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REPORT OF SYMPOSIUM

APPLICATIONS OF ADVANCED AND INNOVATIVE COMPUTATIONAL METHODS TO DEFENSE SCIENCE AND ENGINEERING

J. C. Nall, *Project Leader*

November 1994

INSTITUTE FOR DEFENSE ANALYSES
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APPLICATIONS OF ADVANCED AND INNOVATIVE COMPUTATIONAL METHODS TO DEFENSE SCIENCE AND ENGINEERING

J. C. Nall, *Project Leader*

W. J. Hurley
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INSTITUTE FOR DEFENSE ANALYSES
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PREFACE

This symposium was proposed and sponsored by the Institute for Defense Analyses (IDA) to use the talents of the alumni of the Defense Science Study Group (DSSG) to address important issues related to defense. The DSSG is a program of education and study for a select group of outstanding young professors of science and engineering. The purpose of the program is to build a bridge of understanding between these professors and the defense community so that they will be better prepared to conduct defense related research and to serve as advisors, consultants, or members of study groups and panels of the DoD and other components of the U.S. Government.

The symposium was held at IDA from October 31 through November 2, 1994. The theme was *Applications of Advanced and Innovative Computational Methods to Defense Science and Engineering*. The purpose was to use the alumni of the DSSG program and several other key academics as a core group to discuss advanced and innovative ways that computers are used in academic research. To complement the academic briefings, a group of the DoD and DOE scientists presented briefings on their defense related research. Discussions centered around the important work, especially in the area of massively parallel processing, that is being done by the two groups of researchers.

The theme for the symposium was proposed by Dr. Anita K. Jones, the Director, Defense Research and Engineering. Her purpose was to help ensure that the DoD was benefiting to the fullest extent possible from advanced computational methods being used in academic research. Those persons responsible for arranging the symposium are especially indebted to Dr. Jones for encouragement and support, and for setting the tone of the symposium with her keynote address. They are also indebted to Professor Steven E. Koonin who served so effectively as the moderator of the symposium, to Dr. Russell Herndon who helped identify key speakers from the DoD, and to Dr. Maile E. Smith and Dr. Norman R. Howes of IDA who prepared this report.

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TABLE OF CONTENTS

DISCUSSION

APPENDIXES

LIST OF TABLES

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DISCUSSION

A. INTRODUCTION

The technologies involved in parallel computing have made tremendous strides in the last 25 years. During the late 1960s, the first commercial multiple processor computers that were produced incorporated only a few processors. Today, massively parallel machines have been produced incorporating over 1,000 processors, although typical configurations tend to be tens of processors for shared memory machines and as many as a few hundred processors for distributed memory machines. Networks of work stations, with hundreds of nodes, have been used to solve large problems in science and engineering. The history of high-performance computing (HPC) shows that the Department of Defense (DoD) has played an active role in funding the development of many advances in computing. During the last decade, the Advanced Research Projects Agency (ARPA) has provided extensive funding for parallel architecture development, culminating in the U.S. Government's High Performance Computing Initiative.

Currently, parallel computer techniques are used by researchers to solve many problems in science and engineering. The fact that these techniques are widely used is a testament to their successful development. The scientific community has embraced parallel computing to allow researchers to solve problems that only a decade ago appeared intractable. Industry, with a few notable exceptions, has been slow to adopt parallel processing to aid in the manufacturing process because of the unavailability of software and the expense of large parallel machines. The main use of parallel processing in industry today is in the information industry for database servers, where the software is "transparent" to the user. The entertainment industry is becoming a large user of HPC, but the extent to which they are using parallel computing is not clear. What is clear, however, is that the DoD was instrumental in funding the development of parallel computers, but the increase in their use among non-DoD users has resulted in a market where the DoD is not the major customer. Thus, the DoD may find it practical to work even more closely with academia, the information industry, and the entertainment industry to ensure that it continues to be a major player in this important technical area.

The principal topic of discussion during the 3-day symposium was parallel processing, as done on vector machines, massively parallel machines, or networks of work stations. The broader topics of HPC, the Information Superhighway, and development of techniques to manage large databases were only discussed tangentially. Presentations were given by many academic and government researchers, either by those who use parallel computing machines in their work or by those who are working in the field of computer science to develop new technologies and computer architectures.

Many of the presentations were in the area of parallel computing: where it is today, where it is going, and what it can do. Others presented examples of applications of parallel computing to a wide number of problems in science and engineering.

The text of this paper attempts to summarize the presentations and to capture in short form the general and specific highlights of the discussions held during the symposium. Appendix A shows the agenda and Appendix B lists the names and addresses of the attendees. Finally, Appendix C presents copies of all of the briefing aids used by the various speakers.

B. SUMMARY OF THE KEYNOTE ADDRESS AND OVERVIEW PRESENTATIONS

In the Keynote Address delivered by Dr. Anita Jones, the Director, Defense Research and Engineering, she noted that the DoD is currently funding research in many "Computational Technology Areas." These areas, along with the number of DoD-funded researchers involved are shown in Table 1. To support this research, the DoD has established 10 computational centers in the United States, each run by one of the military services. The hardware at each of these centers is impressive, as shown in Table 2. The DoD is also establishing a network to allow access to its machines and is developing software to support remote computing. The real challenge to using these machines, as noted by Dr. Jones, lies in the ability to produce software tools and to create an infrastructure to support the user. She identified five problems that must be overcome before parallel computing becomes a widely accepted tool among DoD users. These are:

- Simplify remote use of computational resources
- Exploit high-speed, reliable communications
- Harness development from outside the DoD
- Build scalable, error free software
- Support users with expert consultation.

Table 1. Computational Technology Areas, Research Groups, and Researchers

Computational Technology Area	No. Research Groups	No. DoD Researchers
Computational Structural Mechanics	67	1,466
Computational Fluid Dynamics	94	2,071
Computational Chemistry and Materials Science	47	723
Computational Electromagnetics and Acoustics	45	828
Climate/Weather/Ocean Modeling	17	450
Signal/Image Processing	37	879
Forces Modeling and Simulation/C4I	28	895
Environmental Quality Modeling and Simulation	10	377
Computational Electronics and Nanoelectronics	9	79

Table 2. Current Computational Capabilities in the DoD

Major Shared Resource Centers

- Army Research (Cray 2 & KSR)
- Air Force Dayton (Paragon)
- Army Vicksburg (C-90 & Y-MP)
- Naval Ocean (C-90 & Y-MP)

Distributed Centers

- Naval R&D Center (Convex SPP & Paragon)
- Naval Research Laboratory (CM-5)
- Air Force Rome Laboratory (TBD)
- Air Force Eglin AFB (Cray T3D)
- Air Force Maui (IBM SP-2)
- Army HPC Research Center (CM-5)

The meeting continued with a presentation on Grand Challenges by Dr. Andrew White of the Los Alamos National Laboratory. The Grand Challenges were identified as problems in science and engineering that are not tractable using current technologies, but may be penetrable with future computing technologies. To augment the Grand Challenges, a list of National Challenges has been created that includes problems whose solutions would improve the quality of life in America. Typical Grand Challenges and National Challenges are shown in Table 3. Dr. White discussed how the view of what constitutes a Grand Challenge has evolved since the inception of the term several years ago. Initially, all of the Grand Challenges were scientific in nature. Now, the emphasis is shifting toward problems that are still scientific in nature, but whose solution would have a marked benefit to society.

Table 3. Grand and National Challenges

Typical Grand Challenges
- Weather, climate, and global change
- Design of drugs
- Enhanced oil and gas recovery
- Semiconductor research
- Superconductivity research
- Transportation

Typical National Challenges
- Crisis and Emergency Management
- Digital Libraries
- Electronic Commerce
- Health Care
- Energy Management

Parallel computing has allowed researchers to make significant progress in many of the Challenge areas, but much remains to be accomplished. Dr. White presented examples of progress in areas such as predicting the topography of the ocean surface, characterization of novel materials using molecular dynamics calculations, and understanding flow in porous media. All three of these examples involve research on larger problems whose solutions would indeed benefit society, those being prediction of global climate change, molecular (i.e., drug) design, and recovery of oil from underground porous rock, respectively.

Professor Geoffrey Fox from Syracuse University presented a talk entitled *Dual-Use Issues for High Performance Computing and Communications (HPCC) Defense Applications*. In his talk, he examined the roles played by government, the manufacturing industry, the information industry, academia, and the entertainment industry in the broader field of HPCC. HPCC includes far more than the use of parallel machines that were the main topic of this meeting. It includes other types of computer architectures as well as the exploding field of information storage, retrieval, and exchange.

Dr. Fox suggested that the future of HPCC will be driven by information storage, retrieval, and exchange, and thus the market for computer architectures that support these functions will flourish. The demand for parallel processing machines that are used to solve scientific problems, such as those problems outlined in Table 1, will only be a small part of the overall market. Thus, he believes that the DoD will become heavily reliant on dual-use technologies and systems to support its research.

Dr. Fox also noted that the manufacturing industry (e.g., airplane and automobile manufacturers) has been slow to adopt parallel processing to aid in the manufacturing process. This is because of the expense involved in purchasing and using these computers. As noted by Dr. Jones, there is little software available to make these machines easy to use, and thus the cost of using them for industry is unacceptably high. Thus, Dr. Fox suggested that the U.S. Government provide support to the manufacturing industries that need HPCC in order to ensure U.S. leadership in the future.

Professor William Dally of the Massachusetts Institute of Technology outlined current capabilities and trends toward future capabilities in processors. His analysis of the state of processing indicates that bandwidth is becoming the most critical resource as opposed to processing capability. He suggested that the ideal computer architecture for HPC would have multiple processors with the illusion of a shared memory. In other words, it would present the user with a virtual machine that has a shared memory architecture, even though the physical architecture might employ distributed memory. However, there was not general consensus among the symposium participants on the suggestion. Some suggested that the ideal architecture must be matched to a particular problem; others suggested that a balanced architecture would evolve and would have some utility for all problems.

At the end of his talk, Professor Dally posed a question that stimulated significant discussion. Given the naturally occurring rapid rate of growth in supercomputing capability (e.g., processor capability is doubling about every 2.8 years), is there a payoff in trying to accelerate this growth rate? In other words, are there problems unsolvable today that are so urgent that we should invest more into developing even faster computers than those projected for the next few years? If so, what are these problems? In the ensuing discussion, very few candidates surfaced. The best related to solving time urgent problems where the user of the data cannot wait very long for a solution. For example, the National Weather Service cannot wait for days for its models to run when it produces its daily weather forecasts.

C. SUMMARY OF THE TECHNICAL SESSIONS

At this point in the meeting, the focus of the talks shifted to looking at certain specific applications of parallel computing. Talks were grouped into six sessions, each on a particular technical area of interest to the DoD. Each session is briefly summarized below.

1. Nuclear Weapons

Two talks were presented during this session, each on very different subjects. One was an overview of the role HPC could play in predicting the performance of the U.S.'s nuclear weapons in the stockpile as well as possible new designs. This role becomes especially critical as the U.S. moves into an era of limiting or prohibiting underground nuclear tests. The second talk presented some very detailed hydrodynamics calculations that were used to model the propagation of a shock wave through rock. This type of calculation was necessary to support the U.S. effort to monitor and verify Soviet underground nuclear tests.

2. Information Technology/Signal Processing

The talks in this session were quite different in nature. The first was a high-level presentation that outlined many ARPA programs in information sciences. Because of the vast amounts of information needed by today's war fighters, ARPA's program offers high payoff for U.S. battlefield efforts in intelligence, targeting, and communications. The second presentation illustrated the use of massively parallel machines to support research in signal processing, for both space-based radars and for ground-based radio astronomy.

3. Simulation Based Design

The talks in this session showed how computing is beginning to be used to facilitate the process of designing and manufacturing large systems. In the past, computing might have been used to design individual parts of a system, such as optimal wing structures, by examining the flow of air around a wing. Now, by creating a design database of the system, it is becoming possible to alter one small part of a large system and observe how the entire system must be adjusted to accommodate that change. An example was shown from the process of ship design in which the designer moved a structural support inside a ship and the new design programs automatically altered the locations of the electrical cabling and ductwork immediately, thus allowing a redesign to occur in seconds.

4. Materials/Processing

In this session, progress in using parallel processing to predict characteristics of atoms and molecules was vividly illustrated. Researchers are now able to examine molecules and their reactions, which only a decade ago were considered too large to study via the standard techniques of quantum chemistry. Examples that are of interest to manufacturing, such as reactions of molecules in plasmas used for surface etching, were shown. Other examples included studies of new superconducting materials.

5. Computational Fluid Dynamics

In this session, the revolution brought about by parallel processing in Computational Fluid Dynamics (CFD) was apparent. Research was presented in which scientists are able to predict properties of flows so accurately that computation has now become an integral part of experiments. Calculations are now so accurate in some areas that they are used to guide researchers in their design of experiments and theoretical models. CFD calculations were shown which aid in designing spacecraft thrusters, thus enhancing the maneuverability of satellites on orbit. Calculations were presented that are allowing scientists to gain fundamental understanding of the characteristics of turbulent flows.

The session ended with an overview of CFD research and massively parallel processing work sponsored by the Naval Research Laboratory. The areas covered were quite broad and of critical importance to the Navy. For example, work is being performed to simulate air wakes from moving ships, wakes from torpedo launches, detonation fronts from explosions, and jet noise from high speed civil transport planes. In all of these areas, massively parallel processing is allowing the Navy to begin solving problems that were intractable only a decade ago.

6. Automatic Target Recognition

Automatic Target Recognition (ATR) has been, and will continue to be, a large area of research for the DoD. Problems range from finding a target in real time on a screen to surveying massive amounts of imagery data for a particular target of interest. An example of an ongoing ARPA target acquisition program, Tier II Plus Unmanned Air Vehicle, was discussed. The session concluded with a presentation on research in ATR using the ARPA-funded programming tool, Khoros.

D. HIGHLIGHTS OF DISCUSSIONS

After hearing the talks, the symposium attendees, led by the moderator, Dr. Steven Koonin, discussed the role and future of parallel computing in DoD science and research. There was general consensus among the group that computing is now crucial to doing scientific research in many areas of importance to the DoD. There was also a general consensus that the United States currently has a lead in the technologies involved in parallel processing, but it is not obvious that the lead will be maintained. The attendees also agreed that the expertise for the development of new technologies to support parallel computing comes from academia and the commercial world, and not from within the DoD. Thus, the group felt that the DoD, with its declining budgets, should continue to reach out to the commercial world and to academia for expertise as to what is really possible with these powerful machines. Many attendees thought that this is an area in which academia could aid the DoD in finding the best ways to implement the use of parallel computing for applications related to scientific and engineering research.

Another issue that was raised regarded the different types of parallel machines being used by researchers. On the one hand, there are the groups of work stations that can be networked together to operate as a parallel machine by using experimental software such as PVM, Linda, ISIS, etc. On the other hand, there are the massively parallel, distributed memory multiprocessor machines, such as Intel's Paragon and Touchstone Sigma, or machines by Thinking Machines or Connection Machines. The recent bankruptcy of Thinking Machines led the group to question the commercial viability of the distributed memory multiprocessor machines, especially in light of the fact that there exists little software to support computing on these machines. These machines are rather user-unfriendly, and therefore the group was concerned that a large commercial market may never develop for such machines and the DoD may be left as the only user. With such a small market, the DoD would then be forced to bear the entire cost of any research and development for more advanced machines.

The group agreed that new techniques of visualizing the results of many of these applications are needed. Because these new computers allow researchers to examine problems in greater dimensions over longer time scales, plodding through a pile of computer output is often inadequate as a way for researchers to understand the data being produced. New techniques for visualization have proven especially useful in computational fluid dynamics and molecular design. During the symposium several speakers showed films of fluid flows over a variety of surfaces, where the flows were calculated using CFD techniques. Only in the last 10 years, with image processing terminals becoming readily available, has the production of such research-enhancing aids become routinely available to academic researchers. The session attendees felt this was an important area and that it should not be neglected relative to other areas of research.

There were a number of topics relating to parallel computing on which the group raised questions, but did not come to any answer or consensus. These could be viewed as issues which, if resolved, might strengthen the role and position played by parallel computing in the DoD and United States as a whole.

The first issue relates to the Grand and National Challenges. The group believed that significant progress might be made earlier in some of them than in others. They also believed that some of the Challenges might benefit more from the next generation of computers, relative to others. In particular, they believed that more powerful computing capability would offer a significant improvement in the area of climate change research. Here, the large general circulation models that are run today are not using small enough grid steps over the surface of the earth and up through the atmosphere that are necessary to produce results with the desired degree of accuracy. The group suggested that the United States might wish to give consideration to determining which of the Grand and/or National Challenges might most benefit from advances in computer development, and initiating a program to demonstrate progress in solving that particular problem.

The participants were also mildly concerned about the recent emergence of the National Challenges. Solving the National Challenges will require innovation in database management, information storage and retrieval, and the maintenance and acquisition of timely data. These problems are of great interest in the burgeoning information industry, which will channel its research into those areas. On the other hand, solving the Grand Challenges will require innovation in the above areas, as well as in developing more powerful massively parallel machines. Thus, there was a modest level of concern that the country will focus on the technologies for solving the National Challenges over those for the Grand Challenges; therefore, the research into scalable, massively parallel machines might decline.

The DoD must also be able to take advantage of the progress made by the information and entertainment industries as they drive HPCC technologies. This is an area that should not be ignored by the DoD. These two industries are huge players in driving new technologies in high performance computing and communications. The DoD should remain abreast of the developments in this field, and leverage them to suit its needs whenever possible. HPCC and all of the information-transfer capability that it entails will be critical for battle management systems of the future. If progress is to be made in real-time operational systems that use parallel computing (i.e., the battle management systems of the future), it might be accomplished in these industries.

Another issue relates to the role played by massively parallel machines in the National Defense. If the commercial market for these machines is going to dwindle over the next several years, the DoD must decide if it needs to support the industry. The group, as a whole, does not have access to much of the DoD work that uses these supercomputers. Given that, the DoD should assess its needs as well as the risks involved if the United States were to lose its lead in the field, and be prepared to take action, if deemed necessary.

Along these lines, the DoD needs to know the cost of developing reasonable software for MPPs. Currently, these machines do not generally have stable operating systems, good debuggers, and utilities that allow programmers to distribute processes automatically to processors. Until the cost (and benefit) of this type of software is understood, it will be difficult to predict the future of this field.

Another issue that arose comes from the fact that DoD-funded research is no longer the only research in parallel computing. Although the DoD was crucial in establishing the field, parallel computing development is now being driven not only by the needs of the DoD, but also by academic and information industry workers. The DoD must decide what role, if any, it will play in the larger U.S. Government effort to set standards and provide the infrastructure for the world of parallel computing and simulation.

The session concluded with a suggestion that the DoD might wish to consider expanding its partnerships with academia in the area of parallel processing. The large cost associated with research in parallel computing makes the manufacturing industry hesitant to undertake new ventures. The DoD, on the other hand, has a long-term view of research in order to receive a payoff. Due to cutbacks in industrial research, academia is now the major institution performing fundamental research in America. Thus, the participants suggested the DoD continue to work closely with academia to maintain U.S. leadership in the field and to ensure that the DoD's future needs will be met.

Appendix A

AGENDA

DEFENSE SCIENCE STUDY GROUP ALUMNI SYMPOSIUM

APPLICATIONS OF ADVANCED AND INNOVATIVE COMPUTATIONAL METHODS TO DEFENSE SCIENCE AND ENGINEERING

OCTOBER 31 - NOVEMBER 2, 1994

IDA BOARD ROOM

AGENDA

Monday, October 31

INTRODUCTION

0830	Refreshments	
0855	Opening Remarks	Julian Nall DSSG Program Director
0900	Welcome	General Larry Welch President, IDA
0910	Keynote Address	Anita Jones Director, Defense Research and Engineering
0945	Remarks by Moderator	Steven Koonin California Institute of Technology

OVERVIEWS

1000	Grand Challenges	Andrew White LANL
1100	Break	
1115	Dual-Use Applications	Geoffrey Fox Syracuse University
1215	Lunch	
1315	Architectures	William Dally MIT

Monday, October 31 (Continued)

SESSIONS

Nuclear Weapons

1415	Advanced Computation for Stewardship of the Stockpile	Victor Reis DOE Andrew White LANL
1515	Application of MMP to the Solution of Environmental Modeling Problems and Nuclear Test Ban Verification (Not Briefed)	James Lewkowicz Phillips Lab AFMC
1600	Break	
1615	Multidimensional Hydrodynamics as a Tool in Nuclear Test Ban Verification	Frederick Lamb Univ. of Illinois
1645	Discussion of Session	
1715	Adjourn	
1745	Reception in IDA Building 2001, Suites 121/122/123	

Tuesday, November 1

0800	Refreshments	

Information Technology/Signal Processing

0830	Technologies for the National Information Infrastructure	Randy Katz ARPA/UC Berkeley
0915	Very High Speed Signal Acquisition and Processing	Thomas Prince California Institute of Technology
0945	Discussion of Session	
1000	Break	

Tuesday, November 1 (Continued)

Simulation Based Design

1015	Defense Needs in Simulation Based Design	Gary Jones ARPA
1100	Advanced Computer Methods for Simulation Based Design	Anthony Patera MIT
1130	Lunch	
1230	Manufacturing Simulation	Kurt Fickie Aberdeen
1315	Discussion of Session	

Materials/Processing

1345	Data for Modeling Materials-Processing Plasmas: The Impact of Parallel Computers	Vincent McKoy California Institute of Technology
1445	Break	
1500	Computer Applications for Crystal Growth Phenomena	Thomas Halsey Exxon Research Laboratory
1530	High Performance Computational Pursuit of Strategic Materials Properties	Warren Pickett NRL
1615	Competitive With Experiments?: The Future of Molecular Modeling	Douglas Dudis Wright-Patterson AFB
1700	Discussion of Session	
1730	Adjourn	

Wednesday, November 2

0800	Refreshments	

Computational Fluid Dynamics

0815	Exploiting Massive Parallelism to Simulate Complex Turbulent Flow	Paul Woodward Univ. of Minnesota
0915	MPP Simulations of Plasma Thrusters on Spacecraft	Daniel Hastings MIT
0945	Large Scale Data Acquisition and Processing in Turbulent Flows	Werner Dahm Univ. of Michigan
1015	Break	
1030	High Performance CFD Simulation for Priority Real-Time Applications	Jay Boris NRL
1115	Discussion of Session	
1145	Lunch	

Automatic Target Recognition

1245	Automatic Target Recognition (ATR) for Wide Area Surveillance	Jonathan Schonfeld ARPA
1330	ATR Algorithm Development Using Khoros	Robert Hummel NYU
1400	Discussion of Session	
1415	Break	

Summary

1430	Discussion and Key Findings	Steven Koonin
1600	Adjourn	

Appendix B

LIST OF ATTENDEES

DEFENSE SCIENCE STUDY GROUP ALUMNI SYMPOSIUM

APPLICATIONS OF ADVANCED AND INNOVATIVE COMPUTATIONAL METHODS TO DEFENSE SCIENCE AND ENGINEERING

AT

INSTITUTE FOR DEFENSE ANALYSES

OCTOBER 31 - NOVEMBER 2, 1994

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Appendix C

BRIEFING AIDS USED DURING THE SYMPOSIUM

INTRODUCTION AND OVERVIEWS

Keynote Address

Dr. Anita K. Jones

Director Research and Engineering, DoD

Applications of Advanced and Innovative Computational Methods to Defense Science and Engineering

Presented by:

Anita Jones
Director, Defense Research and Engineering

October 31, 1994

1

Computational Technology Areas, Research Groups and Researchers

Computational Technology Area	# Research Groups	# DoD Researchers
Computational Structural Mechanics	67	1,466
Computational Fluid Dynamics	94	2,071
Computational Chemistry and Materials Science	47	723
Computational Electromagnetics and Acoustics	45	828
Climate/Weather/Ocean Modeling	17	450
Signal/Image Processing	37	879
Forces Modeling and Simulation/C4I	28	895
Environmental Quality Modeling and Simulation	10	377
Computational Electronics and Nanoelectronics	9	79

Current HPC Capability in the US

- University
  - National Science Foundation Supercomputer Centers
  - Many HPC Capable University Sites
- Government
  - Laboratories: DOE & DoD
  - Others: NSA, NASA, NIST, NOAA, NIH, EPA
- Industry
  - Aeronautics
  - Automotive
  - Pharmaceuticals
  - Petroleum

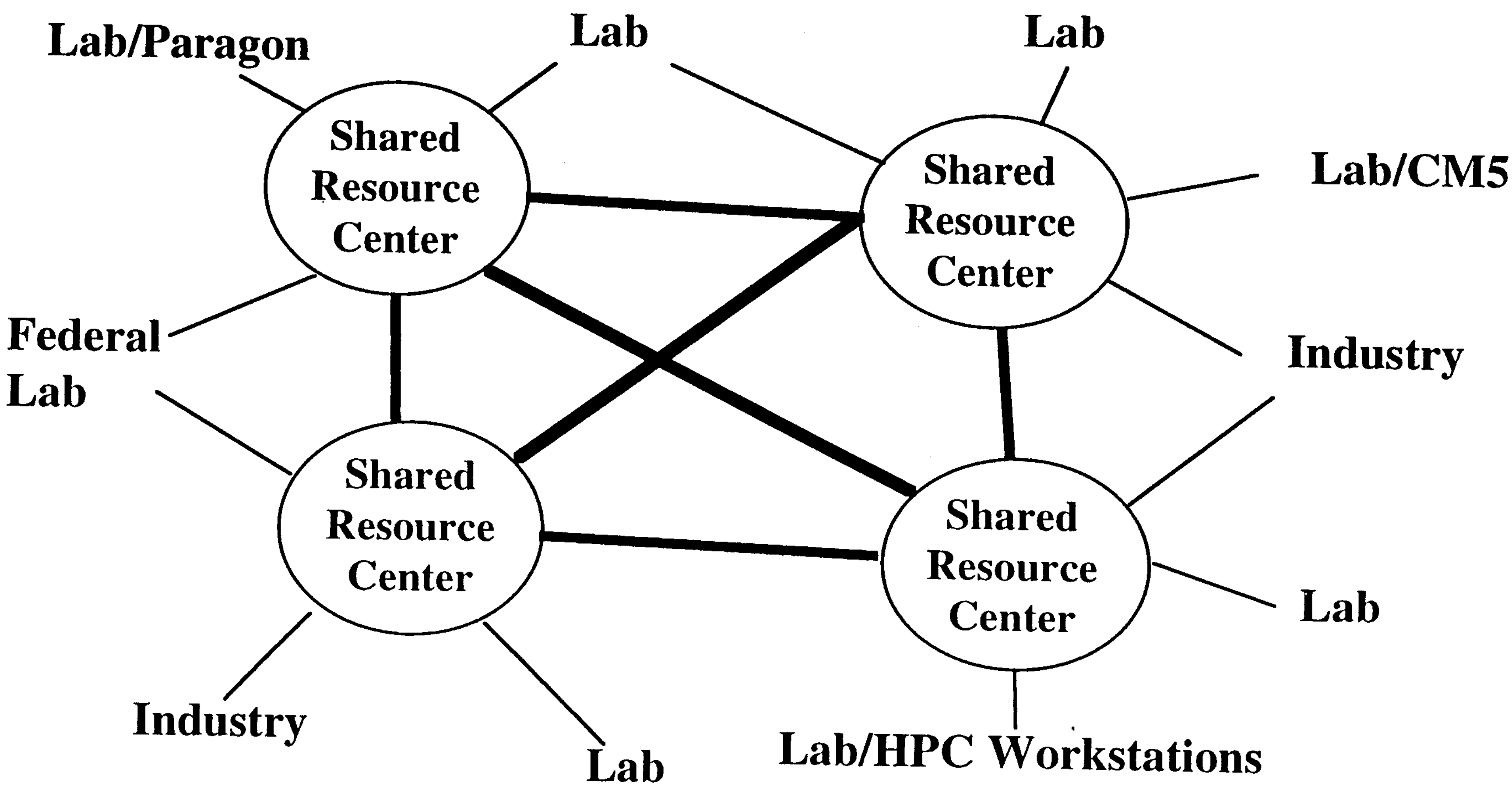
Current Computational Capabilities in DoD

- **Major Shared Resource Centers**
  - Army Research (Cray 2 & KSR)
  - AF Dayton (Paragon)
  - Army Vicksburg (C-90 & Y-MP)
  - Naval Ocean (C-90 & Y-MP)
- **Distributed Centers**
  - Naval R&D Center (Convex, SPP & Paragon)
  - Naval Research Laboratory (CM-5)
  - AF Rome Laboratory (TBD)
  - AF Eglin AFB (T3D)
  - AF Maui (IBM SP-2)
  - Army HPC Research Center (CM5)

Current Computational Capabilities in DoD (Continued)

- Interim Defense Research & Engineering Network
  - T3 Backbone Across Country (45 MBits/sec)
  - Links 50 Laboratories Together
    - » 7 Sites Linked via T3 Line
    - » Rest Linked via T1 Line
  - T3 Gateway to National Research & Engineering Net (NSF)
- Software Tools & Application Development for Scaleable Systems
  - DoD Laboratory Facilities Used for Production Work
  - Service Research Offices Sponsor Scientific Applications

Tomorrow's High Performance DoD Computing Infrastructure



5

Centers Will Specialize in Application Areas

Computational Technology Area	Army Vicksburg	Naval Ocean	Army Research	AF Dayton
Computational Structural Mechanics	X		X	X
Computational Fluid Dynamics	X	X	X	X
Computational Chemistry and Materials Science			X	X
Computational Electromagnetics and Acoustics			X	X
Climate/Weather/Ocean Modeling	X	X		
Signal/Image Processing	X	X	X	
Forces Modeling and Simulation/C4I	X	X	X	
Environmental Quality Modeling and Simulation	X	X		
Computational Electronics and Nanoelectronics			X	X

The Challenge Lies in the Software, Tools & User Support Infrastructure

- Simplify Remote Use of Computation Resources
- Exploit High Speed, Reliable Communications
- Harness Development from Outside DoD
- Build Scaleable, Error Free Software
- Support Users With Expert Consultation

Defense Science & Technology

Dr. Anita K. Jones
Director, Defense Research & Engineering

Post Cold War: New Demands of a New Era

- Today's Competitor is the Global Arms Market
- Must Maintain Military Technological Superiority with Reduced Budget
- Broader Military Demands: Peacekeeping & Counterproliferation
- The U.S. is Challenged Economically

Chart 1

Strategy for a Response to these New Demands

- Focus Technology on Achieving the Joint Warfighting Capabilities
- Use Technology to Reduce the Cost of Systems
- More Rapidly Transition Technology to the Warfighter
- Develop Technology as Base for Both Commercial & Military Products
- Maintain Superiority in Uniquely Military Technologies

Chart 2

Joint Staff Future Joint Warfighting Capabilities

- To Maintain Near Perfect Real-Time Knowledge of the Enemy and Communicate that to all Forces in Near-Real-Time
- To Engage Regional Forces Promptly in Decisive Combat on a Global Basis
- To Employ a Range of Capabilities More Suitable to Actions at the Lower End of the Full Range of Military Operations which allow Achievement of Military Objectives with Minimum Casualties and Collateral Damage
- To Control the Use of Space
- To Counter the Threat of Weapons of Mass Destruction and Future Ballistic and Cruise Missiles to the CONUS and Deployed Forces

Chart 3

Strategy: How to Proceed

New

- Affordability: Reduce Cost of Systems
- Dual Use: Strengthen the Integrated Commercial-Military Industrial Base
- Transition Technology Rapidly to the Warfighter
- Integrated Technology Plan

Emphasize

- Promote Basic Research
- Assure Quality & Superiority of Technology

Chart 7

Reduce Cost

Reduce Weapon and Support System Life Cycle Cost

- Use Best Commercial Products, Practices, and Capabilities
- Invest in Manufacturing S&T and Improve Manufacturing Processes
- Exploit Advanced Distributed Simulation
- Insert Technology into Long Lived Systems

Chart 7a

Commercial-Military Cooperation

Integrated High Performance Turbine Engine Technology

Team
- **Air Force, Navy, Army, NASA, Allied Signal, Allison, General Electric, Pratt & Whitney, Textron Lycoming, Teledyne Ryan, Williams**

Funding
- **1994 DoD: $132M NASA: 17M Industry: $94M**

Objectives
- **Turbofan/Turbojet Thrust/Weight Ratio:**
  - +30% by 1991, +60% by 1997, and +100% by 2003; -25% Cost by 1997
- **Turboshaft/Turboprop Specific Fuel Consumption:**
  - -20% by 1991, -30% by 1997, and -40% by 2003

Chart 7b

Commercial-Military Cooperation

Integrated High Payoff Rocket Propulsion Technology

Team
- **Army, Navy, Air Force, NASA, Aerojet, Atlantic Research, Hercules, Kaiser Marquardt, Rocketdyne, Rocket Research, Thiokol, TRW, United Technologies**

Funding
- **1995 - DoD: $50M Industry: $30M (est)**

Objectives
- **Boost/Orbit Transfer:**
  - 2000: +5 sec Isp; +30% Thrust/Weight; -25% Failure Rate
  - 2010: +20 sec Isp; +100% Thrust/Weight; -75% Failure Rate

Chart 7c

Commercial-Military Cooperation

Advanced Synthesis and Processing of High Performance Composites

Team
- Naval Air Warfare Center, ARPA, Los Alamos, NASA Lewis, GE Aircraft Engines, Pratt & Whitney, McDonnell-Douglas, Hexcell Corp, Univ of Virginia

Funding
- ARPA: $4.5M Industry: $4.8M (24 Months)

Objectives
- Develop Low Cost Manufacturing Process and Specifications for High Performance (High Strength at High Temperature) Metal & Ceramic Composite Tape Materials for Aerospace Structures.

Chart 7d

Commercial-Military Cooperation

National Rotorcraft Technology Center

Team
- Army, Navy, NASA, FAA, Army Rotocraft Centers of Excellence (Georgia Tech, Maryland, RPI), Bell, Boeing, McDonnell-Douglas, Sikorsky

Funding
- 1996 - 2001: Government: $80M   Industry: $80M

Objectives
- Reduce Civil/Military Design Requirements, Specification, & Standards
- Increase Passenger & Community Acceptance
- Augment U.S. Air Traffic Control Infrastructure; Achieve 24-hour, All-Weather, Civil Rotocraft Operation

Chart 7e

Commercial-Military Cooperation

Sematech

Team	• DoD/ARPA, Advanced Micro Devices, Motorola, National Semiconductor, AT&T, Digital, IBM, NCR, Hewlett Packard, Rockwell International, Intel, Texas Instruments
Funding	• 1994- DoD: $90M Industry: $90M
Objectives	• Solve the Technical Challenges Required to keep the U.S. Number One in the Global Semiconductor Industry

Chart 7f

Grand Challenges

Dr. Andrew White

Los Alamos National Laboratory

Grand Challenges

1997

1994

1991

Andy White
Halloween, 1994

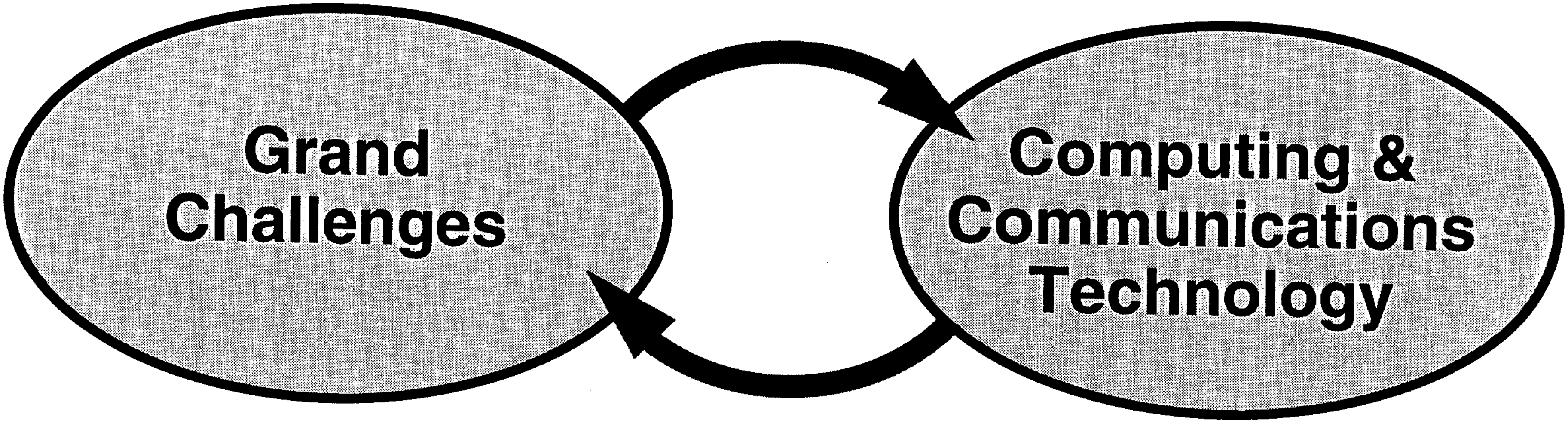
Grand Challenge Characteristics

1991

- Complex
- Massive
- Important
- Risky
- Inaccessible
- Drive the development of a new generation of technology

Grand Challenges 1991

- Weather, climate, & global change
- Materials science
- Semiconductors
- Superconductivity
- Structural biology
- Design of drugs
- Human genome
- Quantum Chromodynamics
- Astronomy
- Transportation
- Vehicle signature
- Turbulence
- Vehicle dynamics
- Nuclear fusion
- Combustion
- Enhanced oil and gas recovery
- Ocean sciences
- Speech
- Vision
- Undersea surveillance for ASW



- Teraflop (1000 x) computing capability
- Gigabit national networks
- Solve a broad range of Grand Challenges
- Involve HPC technology in national education and training programs

Production Accounts
DOE_HPCRC@lanl.gov

Parallel Ocean Program
Isopycnal ocean model
Flow in porous media
Novel materials
Metal forming
Validation of the standard model
Combustion and fluid dynamics
Plasma turbulence
Gyrokinetic transport

SkiHi atmospheric model
Arctic ocean model
Spectral ocean model
Electromagnetic particle code
Galaxy formation
Interacting systems
Multigrid methods
Turbulence model
Transport methods

Applications

- Global climate
- Novel Materials
- Flow through porous media
- Hydrodynamics

|| Apps $||_\infty$ has been better than anticipated

Global Ocean

- POP is a Bryan-Cox-Semtner 3D ocean model
- Streamfunction replaced with surface-pressure formulation
- Rigid lid replaced with free-surface
- 78°S to 78°N, 1280 x 896 x 20 grid
- Resolution is 31 km (0°) to 7 km (78°)

Model uses actual topography and predicts sea surface height

Performance

- Time step: 30 minutes
- Run time (including I/O):
  - 28 hours/year on 256 CM-5 nodes
  - 18 hours/year on 512 CM-5 nodes
- Memory: 4.5 GBytes
- I/O: 50 GBytes/year
- I/O rate: ~ 1 MByte/sec

Model resolves mesoscale eddies
EJIP, NWAG, WAX, SEAMOS collaboration

Novel Materials

- Computational research project
- Molecular dynamics (e.g. L-J)
- Target - 10^9 atoms (μ^3)
- 1993 Gordon Bell finalist @ 59 Gflops
- Visualization >> simulation
- Embedded atom, long-range forces
- Semiconductors, polymers, proteins

Scale-up to macro-systems is key

Hydrodynamics

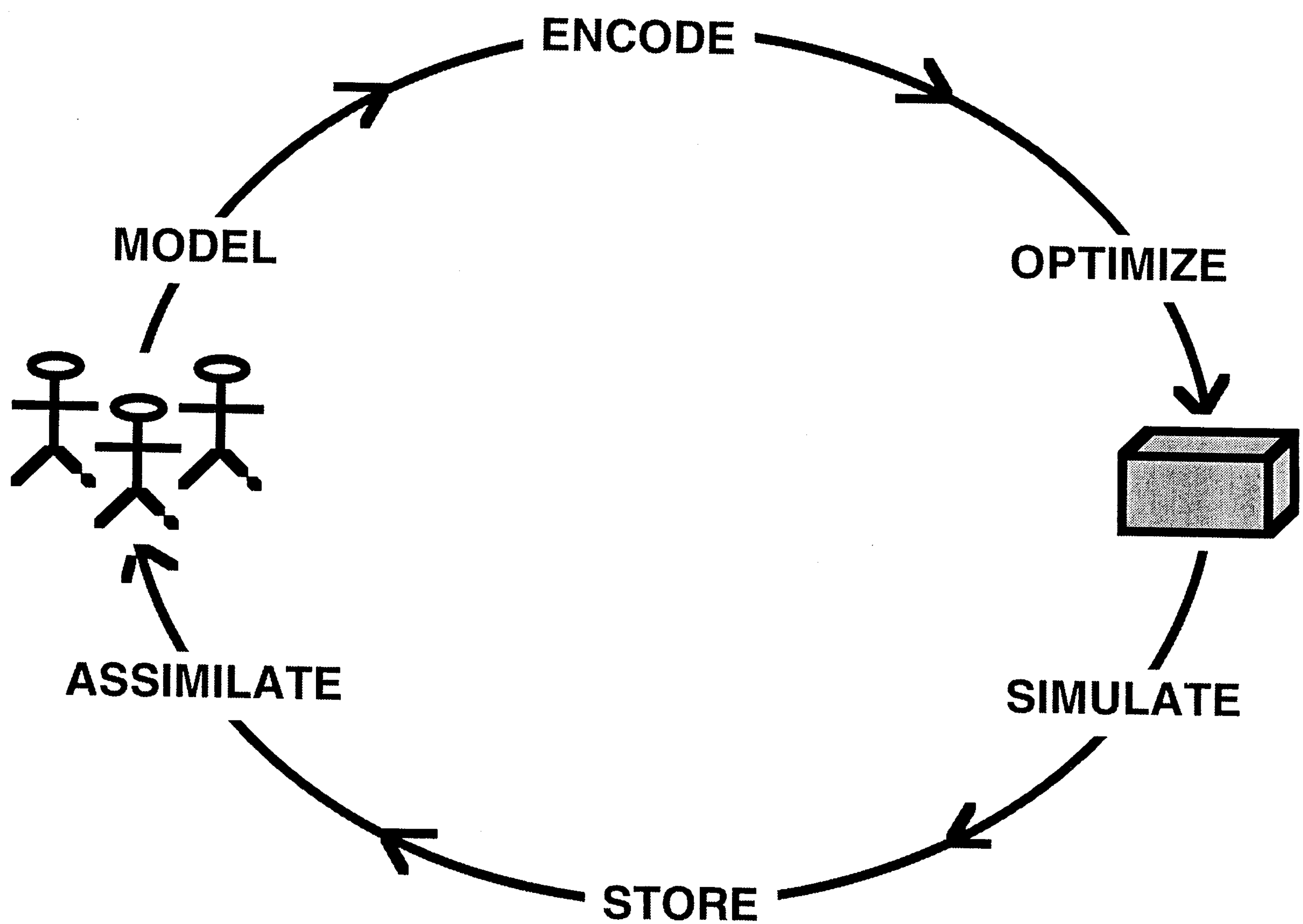
- High speed flows
- PAGOSA: explicit, Eulerian code
- 2 million zones, 10.3 hrs on 512 nodes of CM-5
- Production CM-200s
- Memory > speed
- Direct technology transfer from nuclear weapons program
- Collaboration with industry, DoD

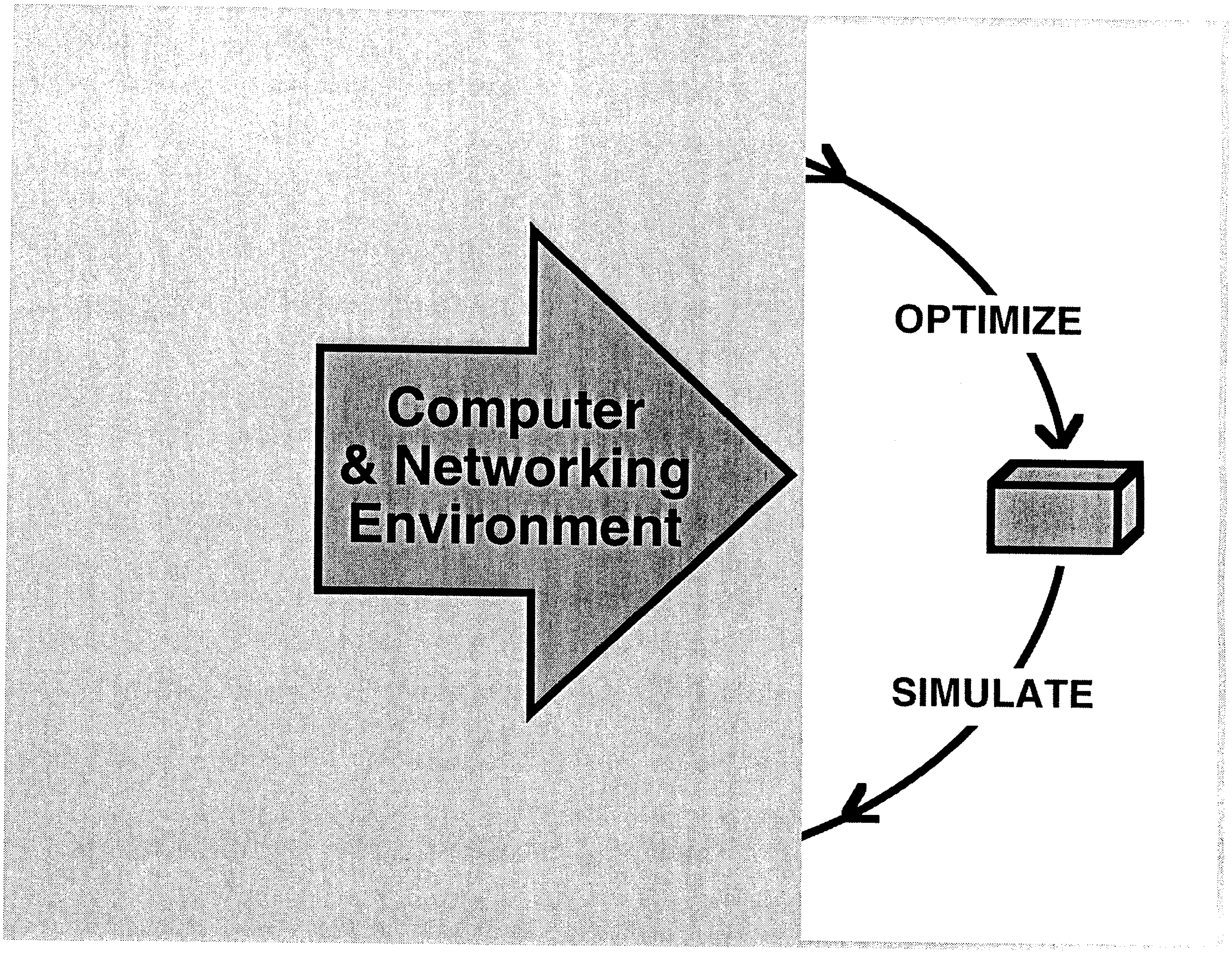
Flow in Porous Media

- Computational research project
- Multiphase Darcy's Law from pore scale simulations
- Replaces Laboratory experiments
- Lattice Boltzmann technique
- Enhanced oil recovery (Mobil), groundwater, remediation

Scale-up to macro-systems is key

Problem-solving Process




Computer
& Networking
Environment
OPTIMIZE
SIMULATE

TeraScale Machine:
(Terabit/sec, Terabyte, Teraflop)

- ≈ 2000 nodes
- ≈ 0.5 Gflop/node
- ≈ 512 Mbytes/node
- ≈ 500 Mbytes/sec/node
- ≈ 1996
- ≈ $100M

Teradactyl or Terasaurus?

CASA Gigabit Testbed

- SDSC - CIT - JPL - LANL
- Fusion of Geophysical data, combustion chemistry, global climate
- 1993: link from SDSC to JPL
- 1994: link from SDSC to LANL
- $\|\text{Performance}\|_\infty$ > 600 Mbits/sec

Nonlinear speed-up possible in heterogeneous systems

OK, but what about the marketplace?

Mainframes are the target for parallel computer vendors

ATM is the answer to all of our prayers

Biographical information is the focus of data storage

Entertainment will provide visualization capabilities

Super¢omputing

"1993"	
Computer Industry	$233.0B
Hardware Industry	$114.0B
Supercomputers	$ 2.0B
High-end systems	$ 0.8B
"1998"	
Supercomputers	$ 4.0B
High-end systems	$ 0.5B

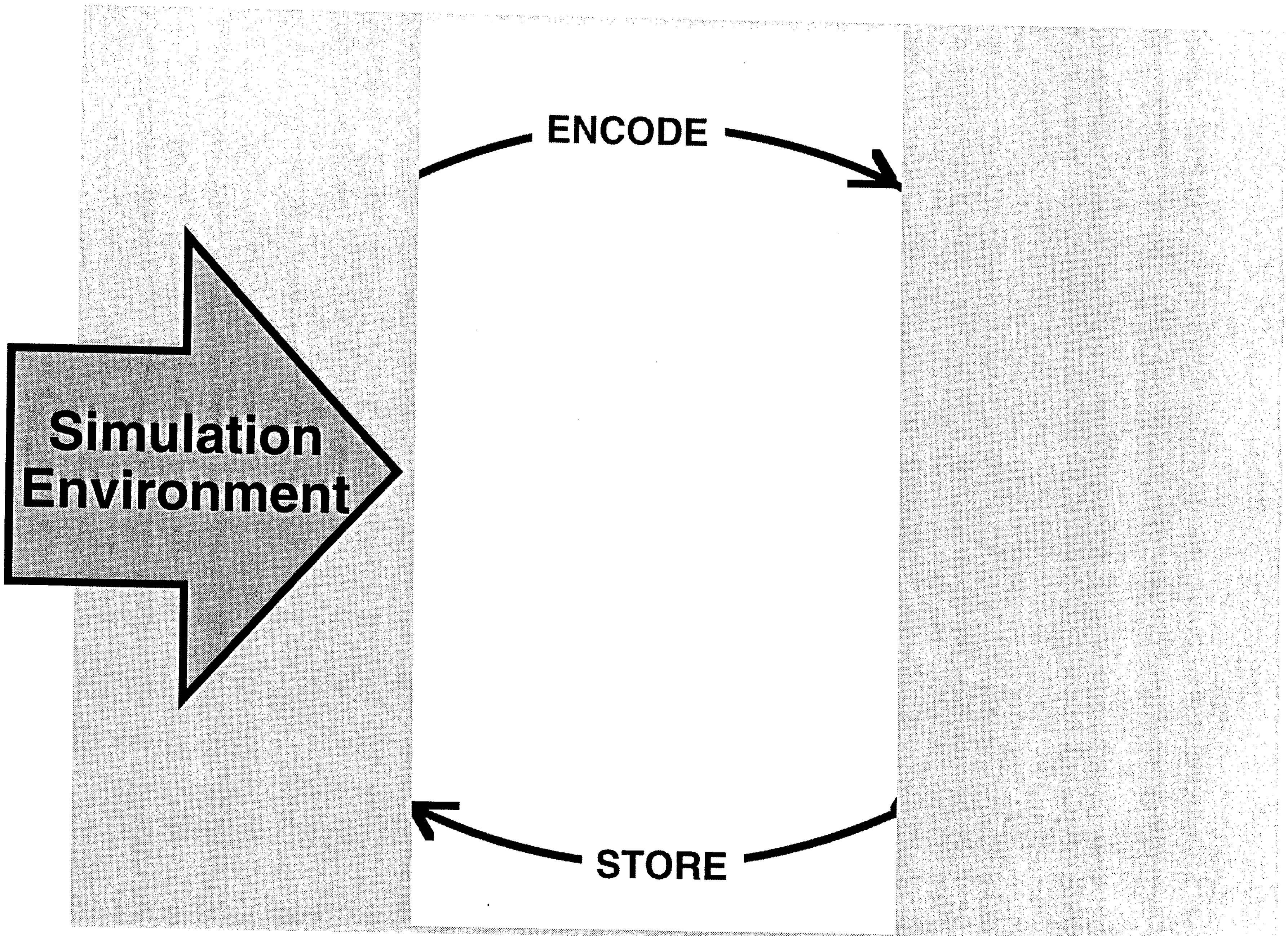
Advanced Computing

- HPC market, Commercial market
- Industry overpopulated & fragile
- No common development target
- Reliability, maturity still lacking
- Workstations inexorably gaining
- Computational science

Little diffusion of software, capability Still critical for success

Application Characteristics

- Complex
- Massive
- Important
- Risky
- Drive the development of a new generation of technology
- Urgent
- Interdisciplinary
- Inaccessible to other techniques
- National in scope
- Societal in effect

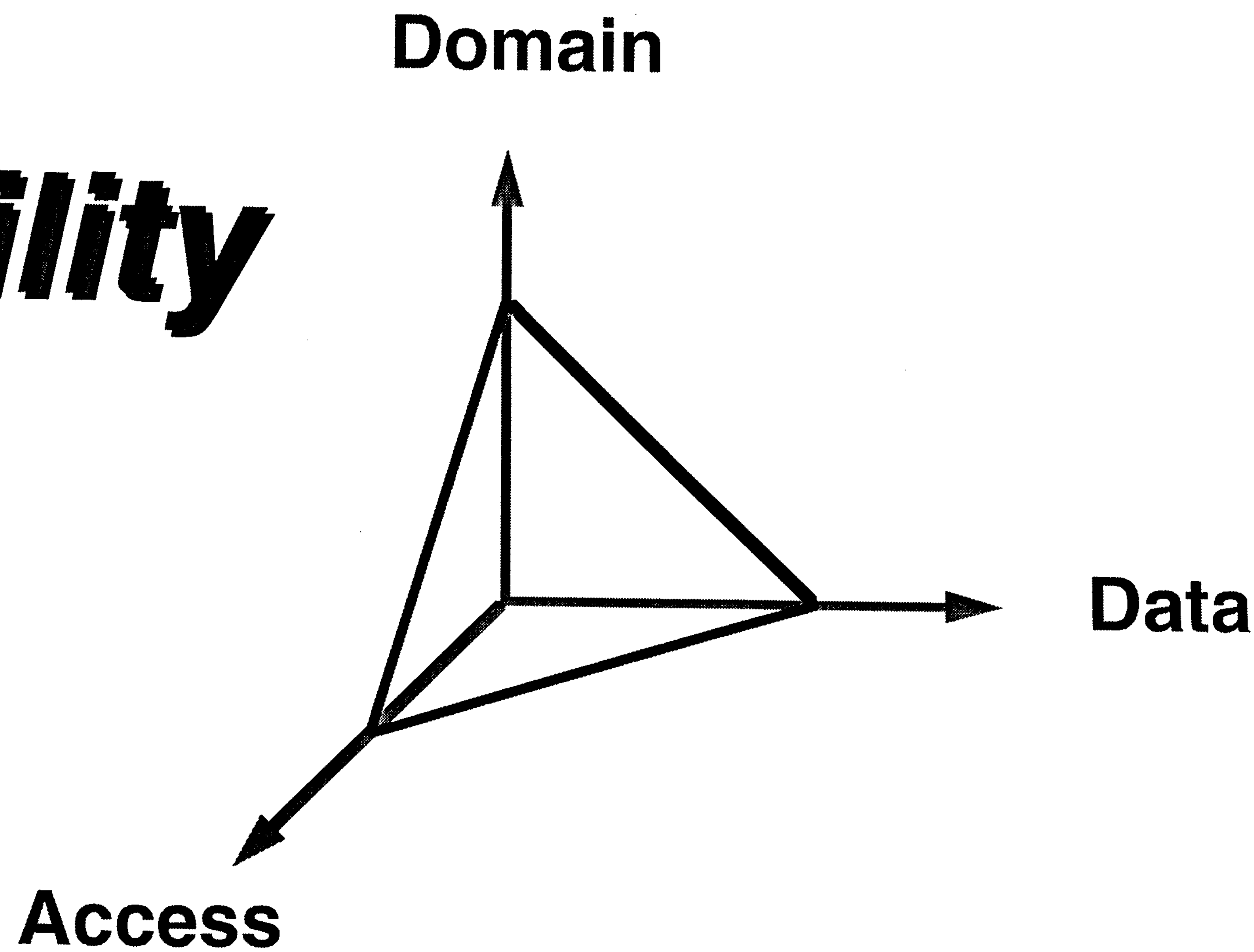

ENCODE
Simulation
Environment
STORE

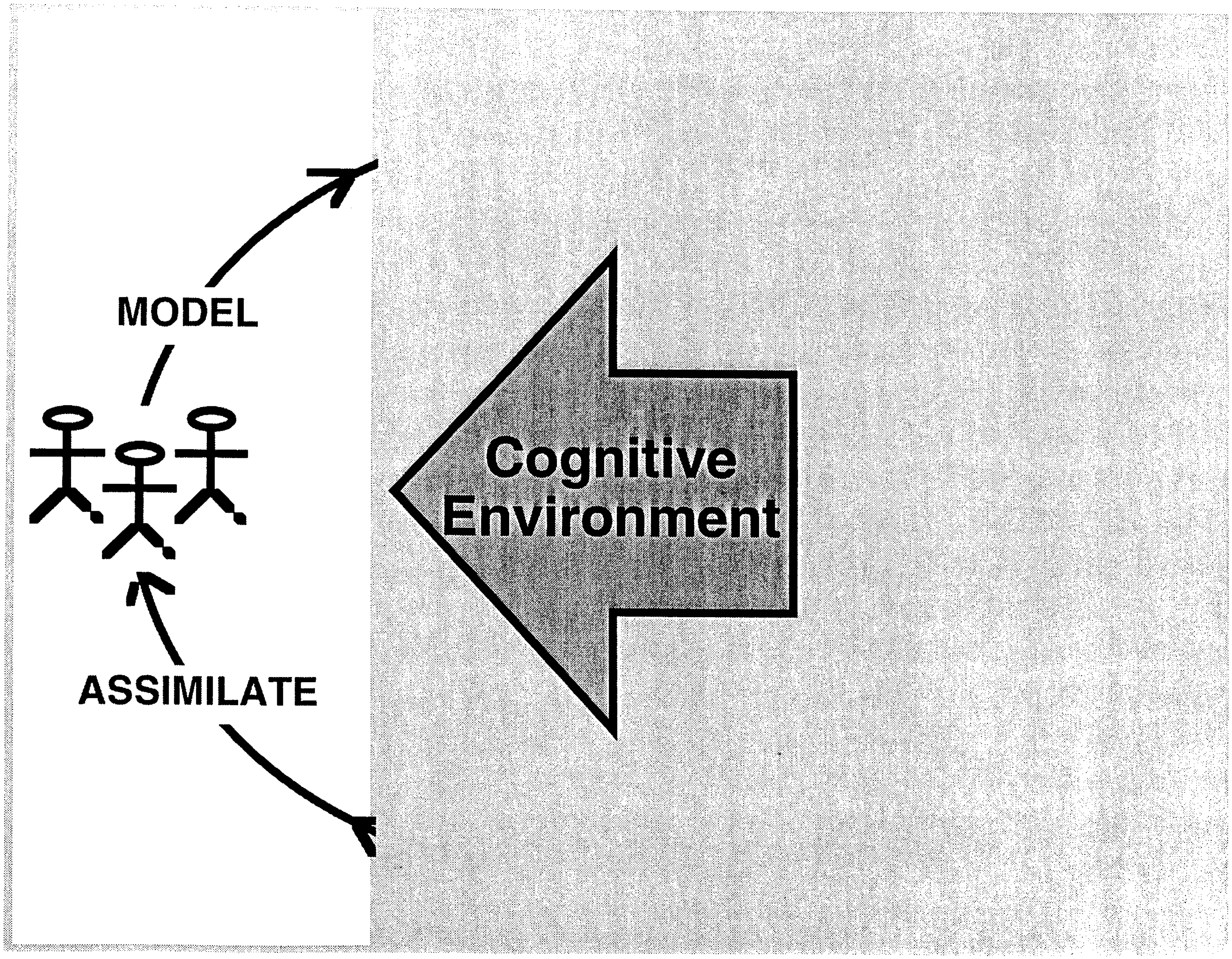
Characteristics of the Simulation Environment

- Capable
- Scalable
- Insensitive to platform (HPF, C++,...)
- Insensitive to distance

Agile
Accessible to customer

Agility

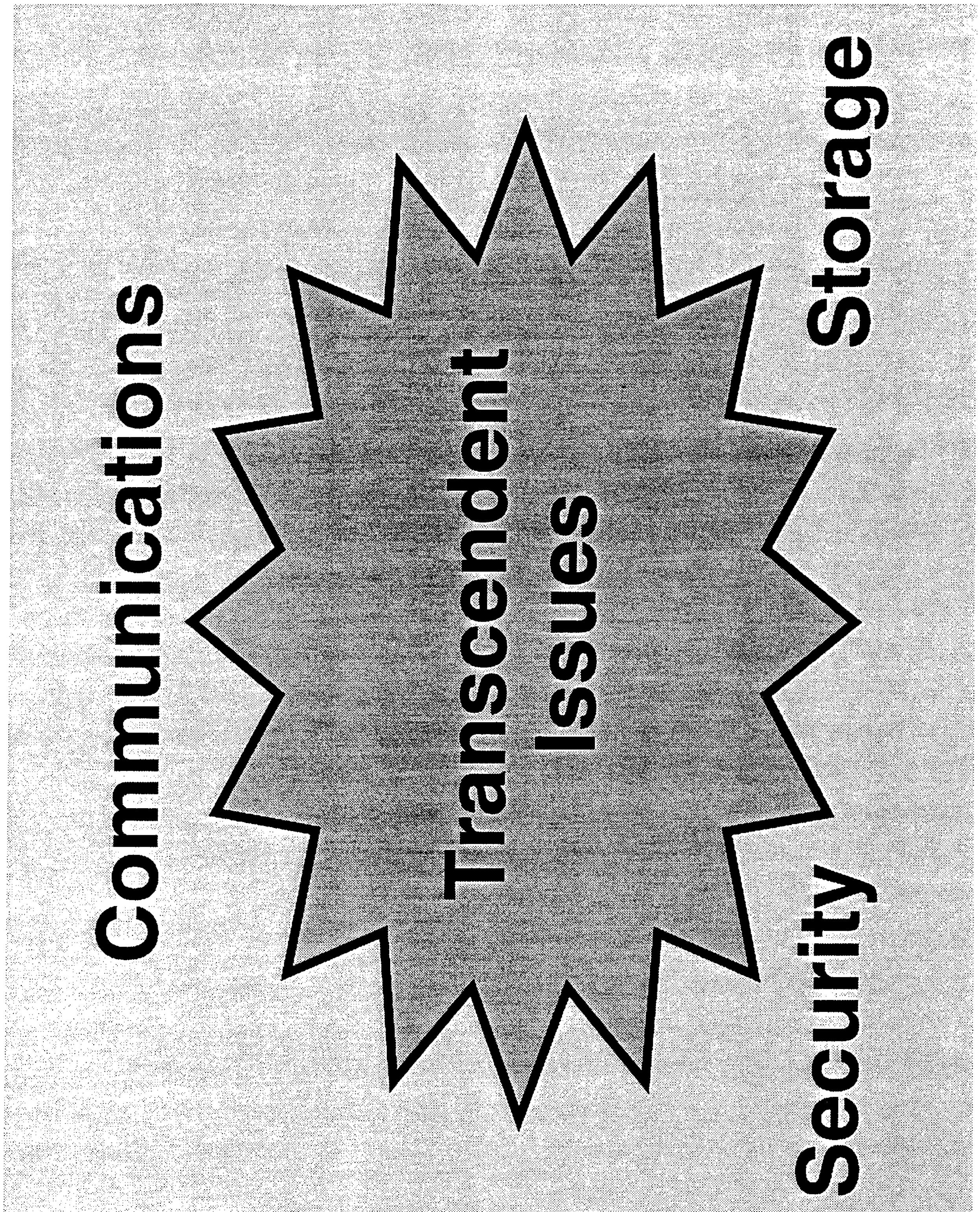


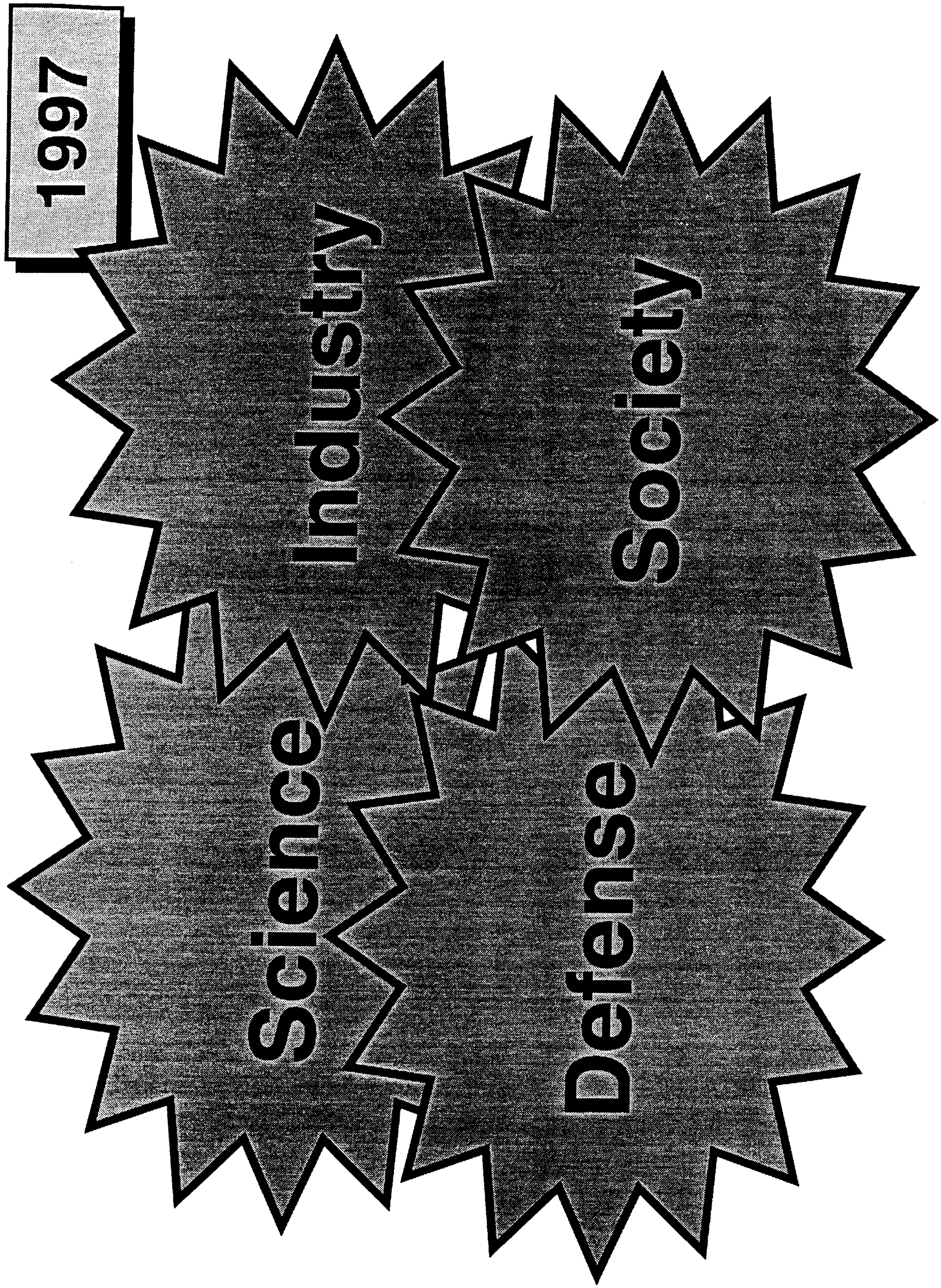

MODEL
Cognitive
Environment
ASSIMILATE

Cognitive Environment

- Ω Multimedia resources for recording/accessing knowledge
- Ω Collaborative tools for allowing virtual teams to interact
- Ω Data analysis, aggregation, and visualization tools
- Ω Syntactic translation of knowledge, information, and data

New cognitive tools can qualitatively transform the way we solve problems.


Communications
Transcendent
Issues
Security
Storage


1997
Industry
Society
Science
Defense

Defense

- *Stockpile stewardship*
- Nonproliferation
- Low-lethality warfare
- Conventional weapons
- EM signatures

Science

- *Material properties*
- *QCD*
- *Tokamak design*
- Electronic structures
- Molecular design
- Desalination

Industry

- *Gas and oil*
- *Information*
- *Virtual design*
- *Financial*
- **Automotive**
- **Medical technology**
- **Steel and metallurgical**
- **Semiconductor**

- *Global climate*
- *Energy demand management*
- *Environmental emergencies*
- *Predictive epidemiology*
- Economic forecasting
- Digital libraries
- Health care
- Global ecology
- Transportation

Society

National Challenges

- **Digital Libraries** (NSF, ARPA, NASA, NOAA, NASA)
- **Crisis and Emergency Management** (ARPA, NOAA, NSF)
- **Education and Lifelong Learning** (NSF)
- **Electronic Commerce** (ARPA, NIST)
- **Energy Management** (DOE)
- **Environmental management and Waste Minimization** (DOE, NASA, NOAA, ARPA)
- **Health Care** (NIH, ARPA, NSF)
- **Manufacturing Processes and Products** (ARPA, NASA, NIST, NSF)
- **Public Access to Government Information** (ARPA, NSF, DOE, NASA, NOAA, EPA, NIH)

Continue investment in Grand Challenges

- Critical, urgent applications
- Inaccessible
- National, societal in effect

Focus tactical software goals

- Common, scalable software
- Agile tools and resources
- Begin deployment of cognitive tools

Bottom Line

Dual-Use Applications

Professor Geoffrey Fox

Syracuse University

The Virtual Corporation for
HPCC Software and System Development

Dual-Use Issues for HPCC Defense Applications

Institute for Defense Analysis Meeting

October 31,1994

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Components of Presentation (Available on World Wide Web)

- Specialized Foils on Dual-Use issues for HPCC DoD Applications
- List of 33 Broad HPCC Application Areas coming from InfoMall Survey of New York State Industry
- Set of Anecdotal Comments on various Industries gathered in Survey
- Set of Computer Science Comments on Applications
  - Software and Hardware Architecture Issues
- Set of Application Related Comments and Elaborations
- Link to Federal Programs and Guidelines
  - Official 1994 and 1995 Federal HPCC and NII Documents
  - Technology pages from Federal agencies and laboratories -- examples given from ESC and Rome Laboratoryu
- Links to World Wide Web Pages describing HPCC activities Internationally
  - For instance Home Pages for Grand Challenge Projects
- List of InfoMall members and their relevant Expertise
- Link to National Software Exchange for Detailed HPCC Technology Issues
  - In particular detailed High Performance Fortran Server
  - And to HPCC Glossary and list of Products

The Dual-Use Philosophy

- This approach is built around observation that in today's shrinking defense budgets, military products must share wherever possible hardware software and maintenance components with civilian arena
- Rapidly changing technologies accentuate the importance of this approach
  - A typical military system takes 5 to ten years to build and is out of date, when delivered
  - The dual-use philosophy advocates design as set of dual-use modules which can be replaced by latest (civilian) technology in incremental fashion
- The same philosophy encourages multi-use or modular or component approach to produce reusable technologies and applications for several civilian and military applications
  - For example, multimedia databases can be used in
  - Military Command and Control, Health Care, Business and Government Decision Making, Education and Entertainment

An Example to Illustrate Importance of Dual-Use Philosophy

- A Real Example: Need a data-base system for a military vehicle which will remain nameless
  - In year X, evaluate civilian databases and find them wanting (too slow)
  - Design proprietary hardware and software using technologies of year X
  - Deliver system in year X+5 and find
    - Civilian microprocessors have increased in performance by a factor of 25 but there are no resources to adapt custom hardware and software to use these new civilian technologies
    - The multi-billion dollar civilian database industry has:
      - Increased database functionality adding object-oriented features
      - Ported database to latest microprocessors
      - Parallelized Database
- Thus resultant system cannot be improved, is a factor of 100 slower than best civilian alternative, and DoD must pay contractor to maintain system for next 20 years

Opportunities for HPCC in the Science and Engineering Simulation Arena

- In spite of the large and very succesful national activity, simulation will not be a large "real world" sales opportunity for MPP's
  - Maybe difficulties for Thinking Machines illustrate this
- However some areas of national endeavor will be customers for Mpp's used for simulation
  - Large Scale Academic Calculations
    - Value of Increased Computation demonstrated in many disciplines
    - Codes are sufficiently small that software engineering considerations of adapting 1,000,000 lines not so important
  - Petroleum Industry
    - Resevoir Simulation
    - Siesmic Data Analysis
  - Some Earth and Space Science including
    - Climate and Weather Forecasting

Some Simulation Areas which will be Difficult to exploit in near term

- Some areas which may adopt HPCC for simulation in relatively near future
  - Pharmaceutical Industry
    - Intense and brilliant academic (government research laboratory) effort in biochemical molecular modelling
    - But "Computer Designed Drugs" are not sufficiently promising to clearly justify purchase of large MPP's by drug industry
  - Financial Industry
    - MPP's being used by Prudential but in spite of success, they are not yet being generally adopted
    - Networks of Workstations severe competition as many problems are "embarassingly parallel"
  - Electrical Power Industry
    - Value seems clear for planning and real time control but
    - Industry conservative and faced with growing near term competition

Suprisingly Difficult and Suprisingly Promising Areas for HPCC in Simulation

- The role of HPCC in Manufacturing is quite clear and will be critical to
  - Agile Manufacturing and the year 2010 Manufacturing Industry but for
    - Major fields including
    - Aircraft
    - Cars
  - HPCC will *not* have a major impact for simulation in the next few years
- On the other hand for
  - War Games and Simulations of Complex Scenarios
  - Role of MPP's can be expected to grow especially when couplerd as in (old) SIMNET with high speed geographically distributed networks
  - Note this is different basic software technology
    - Event driven -- not time stepped -- simulation

Why is it hard to use HPCC in Manufacturing-I?

- Return on Investment Unclear:
  - Amdahl's law for use of HPCC in Industrial Simulation
    - If Simulation was only 10% or less of original design and manufacturing cycle, then can only gain this 10% by speeding up simulation
    - And this speedup comes at huge software engineering cost ...
      - Codes are long and expertise to convert to parallelism may no longer exist in new "slim" companies after layoffs , buyouts and freeze on hiring new employees with knowledge of new technologies such as HPCC
      - New codes must be validated by extensive tests before use
        - Remember we can't solve full Navier-Stokes Equations yet and so some approximations necessary
- The Industry is in a very competitive situation and focussed on short term needs

Why is it hard to use HPCC in Manufacturing-II?

- In March 1994 Arpa Meeting in Washington, Boeing(Neves) endorsed parallel databases and not parallel simulation
  - Similar comment made to me by Major Brokerage
    - "Financial Modelling (on MPP) gets the headlines but information services are the critical problem"
- Aerospace Engineers are just like University Faculty
  - They prefer to use their own workstations and not central Supercomputers
- There is perhaps some general decline of Supercomputer Industry
  - As performance of technology increases
  - Users don't take full advantage of this performance Increase
    - Rather buy somewhat more powerful computers at somewhat lower cost

Multidisciplinary Analysis and Design as a Critical use of HPCC in Manufacturing?

- MAD (Multidisciplinary Analysis and Design) links:
  - Structural, Fluid flow, electromagnetic signature, manufacturing process computations
  - Design, Manufufacturing, Sales and Support Functions
- (Includes MDO -- Multidisciplinary Optimization)
- Link Simulation and CAD Processes
  - Technically link CAD databases (using parallel database technology) to MPP simulations
- This is really important application of HPCC as addresses "Amdahl's Law" as we use HPCC to support full manufacturing cycle -- not just one part! Thus large improvements in manufacturers time to market and product quality possible.
- BUT must change and even harder integrate:
  - ALL software used in Manufacturing and this now comes from different vendors
  - The way of doing business in company
    - New job skills and cultures -- the hardest problem

Role of Government and DoD in HPCC Simulation Applications

- The limited nearterm industrial use of HPCC implies that it is critical for Government and DoD to support and promote
- DoD Simulation: Dual-Use Philosophy implies
  - Can use Commercial MPP hardware and basic systems software
  - Cannot rely on commercial market for application and sophisticated systems software and indeed hardware targeted at engineering and science simulation
- Manufacturing Support can lead to future US Industry leadership in advanced HPCC based manufacturing environments 10-20 years from now
  - Industry cannot afford and even consider long term investment needed to integrate HPCC into manufacturing
  - Government should support long-term not short-term needs
  - Government must involve manufacturing Industry in its plans
  - Currently federal Initiatives are correctly involving Industry in more major fashion than before but focussing on short term needs

The HPCC Software Industry is not Viable in Simulation Area

- An HPCC Software Industry is essential if HPCC field is to become commercially succesful
- The HPCC Simulation market is small
- This market is not used to paying true cost for software
  - As cost traditionally bundled with hardware and one can get
  - Federal Grants to develop software yourself ....
- There is a lot of excellent available public domain software (funded by federal government)
- Small Businesses are natural implementation of HPCC Software Industry
  - Plenty of talented Entrepreneurs
- Two InfoMall Success Stories
  - Portland Group: Commercializing High Performance Fortran Compiler developed at NPAC. We are not competing with them but adding value
  - Applied Parallel Technologies:Developing with NIST ATP and Venture Capital portable database exploitation tools
    - NPAC provides HPCC facilities, expertise and contact with best of class international software activities

Anecdotes from HPCC Software Industry Arena

- Anecdotes from Thinking Machines (TMC) April 94 before the fall
  - "They would like to be a software company but you can only sell software if bundled with hardware"
  - Customers did not buy TMC hardware because TMC's software was too good and so one couldn't then get the federal grants to improve parallel systems software
- Anecdote from Digital September 94:
  - Digital cannot make money on their scientific software package for alpha workstations
  - If Digital charged true cost of development and maintenance, users would make do with good (but not optimized or as complete) public domain software
  - So if workstation market not viable for simulation software, how can much smaller MPP market lead to viable business plans?

National Challenges will drive the adoption of HPCC in the "Real World"

- These can be defined simply as those HPCC applications which have sufficient market to sustain a true balanced HPCC computing Industry with viable hardware and software companies
  - With this definition, some "Grand Challenges" such as Oil Exploration are National challenges
- Alternatively one can define National Challenges by the HPCC technologies exploited
  - High speed geographically distributed (ATM) networks i.e.
  - The National Information Infrastructure (NII) with several hundred million clients and perhaps some 10,000 MPP based high performance multi-media servers
  - Large scale text, Image and Video databases fed by Satellites, Information produced by National Enterprise such as credit card slips etc.

The National Challenges Identified by the Federal HPCC Initiative

- Crisis and Emergency Management
  - Civilian words for scaled down Military Command and Control
- Design and Manufacturing
- Education and Lifelong Learning
- Electronic Commerce
- Energy Management
- Environmental Monitoring
- Health Care

Why is Dual-Use Critical for National Challenges?

- The National Challengies have been correctly identified as the the major HPCC opportunity and there is a
- Reasonable list of targeted Government areas BUT
- The Entertainment and Consumer Information Industry will set the standards and drive the technology
- One must set up collaborations with:
  - Companies such as Time-Warner, Disney, Nintendo and Microsoft
  - Fields such as Journalism and the Video Game Software Community
- Health Care and Electronic Commerce may be large enough areas to sustain their own enterprise but some such as
- Military Command and Control and Education are not
- However the GII (Global Information Infrastructure) will force common standards and one canNOT go it alone in any area!
- So Dual-use or Multi-use development of modular HPCC technologies, services and applications essential

Dual-Use Command and Control HPCC Applications and Why is Global Grid Concept Essential

- Command and Control (C^2 , C^4I, BMC^3IS) is largest HPCC Opportunity in DoD
- It is Dual-Use to the NII and Large Scale Database Decision Support Applications which will dominate the civilian use of HPCC
- This Dual-Use approach to Command and Control demands the Global Grid Concept at the low (hardware) level
- There will not be a separate DII (Defense Information Infrastructure) just as there is not a separate Interstate Highway System for DoD Vehicles
- Even if you built the DII, the commercial GII will always have much higher bandwidth and so one would want to use it

Naive Definition and Discussion of Global Grid

- The Communications System used in International Wartime Command and Control will be the commercial Global Information Infrastructure(GII) augmented by
  - Location(Theater) and DoD specific physical network extensions to take GII from commercial drop-off point to battlefields.
  - Necessary Security and Priority services on the commercial networks to ensure appropriate "quality of service" for use by DoD in battle-critical situations
- Clearly Global Grid is essential and Critical Underlying Concept for Dual-Use Command and Control which needs major attention by DoD
- An Anecdote: Similar cost arguments says that communities should not develop the NII separately for Public(Government) Information, Health Care and Education
  - We only want one NII with Multi-Use applications and technologies

Dual-Use Applications of InfoVision to Command and Control: Video Information on Demand

- Basic InfoVision Service is Tens of thousands of hours of Digital Video with Index (Video Browsing) formed from
  - Text Database to resolution of a few seconds of clips
  - Later Speech Recognition including Language Translation
    - CMU InfoMedia Project with Public TV
  - Maybe Image Processing
- Educational application uses Reuters and CNN News services as an online resource to support social studies, science and foriegn language classes
- Medical Application stores Echo Cardiograms and other video material digitally as Online support for telemedicine
  - One Syracuse Doctor has several thousand such video tapes
- Government Application uses multimedia data from world news services to support political decisions.
  - Pioneered by Maxwell School at Syracuse University
- Defense applications stores combat videos to allow commanders to access and plan missions

Dual-Use Applications of InfoVision to Command and Control: Image Information on Demand

- Basic InfoVision Service is a set of Images stored in Multiresolution (Kodak Photo-CD) format indexed by:
  - Text database as in current Kodak Picture Exchange service with some 100,000 professional photos indexed by hand by criteria of relevance to production houses
  - Image Processing to identify anomalies(medicine) or particular targets(Defense)
- Cutural application stores all the photographs and pictures in museum
  - several examples available on Internet and more will come
- Commercial enterprise has set of Images you can choose and edit for T-shirts on demand
- Medical Application uses Image Processing to screen images to find those which surgeons need look at for potential pathologies
- Defense application identifies targets for missions and in real-time for weopens

Dual-Use Applications of InfoVision to Command and Control: Text Information on Demand

- Basic InfoVision Service is large scale Alphabetic and Numerical database supported by
  - Standard and enhanced SQL from Informix,Oracle, Sybase ....
  - Natural Language front end supporting advanced semantic and full text analysis
  - Set of "Data-Mining" (Statistical) Tools
- Education application is full text analysis of current Dept. of Education ERIC database
- Commercial application is Credit Card company analysing card transactions to discover customer preferences -- market segmentation
- Government application is Patent Office using Semantic Analysis on existing 100 gigabyte database to process new patent claims more accurately
- Defense application has Intelligence officers analysing the World's digitized Newspapers to identify terrorist patterns
- Defense Logistic application analyses operational records to optimize stockpiling of parts and identify unreliable suppliers

Dual-Use Applications of InfoVision to Command and Control: 3D Interactive Terrain Navigation

- Basic Infovison service uses digital map and elevation data (from Satellites and USGS) combined with 3D rendering to allow interactive journeys
  - Including ability to "click" on terrain locations to obtain multimedia information
  - This is natural "Mosaic" interface for spatially labelled data
- Educational application allows teacher to generate historical and cultural multimedia data and allow classes to explore in "virtual field trips"
- Local Government applications allows City Planners to superimpose building CAD data to support wide scale 3D Planning
- Tourist application allows travel agencies to offer virtual trips to potential vacation locations
- Community application offers a full Interactive Yellow Pages
- Defense Application allow Mission planners to navigate potential battlefields to find unexpected hazards and opportunities

Dual-Use Applications of InfoVision to Command and Control: Path Planning for Spatial Reasoning

- Basic InfoVision Service is Two or Three map superimposed with a set of Image Processing and Spatial Reasoning Tools
- Common tool in systems such as ASAS (All Source Analysis System) is Minimum Path Algorithm
- Commercial Application extends current CDROM based route planning systems such as Automap amnd Mapinfo using GPS if necessary (Global Positioning Satellite)
- Can extend Service to multiple vehicle planning for aircraft and vehicle management
- Defense application couples map, terrain data (which tanks can go in what areas in what weather) to plan and analyse both your and their troop movements

Dual-Use Applications of InfoVision to Command and Control: Correlation Analysis for Spatial Reasoning

- Basic InfoVision service is a set of spatially labelled Information combined with appropriate decision support tools
- Typical Defense application is a correlation algorithm which clusters electronic and other information into groups which are supposed to come from a single source. This is followed by an identification algorithm which classifies nature and behavor (moving or static) of source
- Health Care application would use medical records and location of patients to plan optimal location of clinics and needed expertise of doctors
- There are several similar commerce (where you you put bank branchs) and community (optimizing government services) applications
- Using a global database, this type of anaysis of spatial data with geographic browsing can be used to study possible export and marketing strategies to choose best countries as targets for a particular product

Dual-Use Applications of InfoVision to Command and Control: Simulation on Demand

- Basic InfoVision Service is ability to initiate and display simulations running on appropriate NII servers
- Brokerage application allows trader to invoke several different economic simulations to support real-time trading decisions
- Educational Application allows teacher to access library of Grand Challenge Simulations to illustrate Motion of Hurricanes and other Physical Phenomena (Valuable in all areas of education from K-12 to graduate physics education supported by colliding black hole simulation).
- Defense Application supports Commander with "What-If" simulations for possible battle scenarios. This could be:
  - Event driven tactical simulation (war game) or
  - Time stepped weather simulation linked to terrain navigation application

The Virtual Corporation for HPCC Software and System Development

Overview of HPCC Applications in Industry

Background for Institute for Defense Analysis

Meeting October 31,1994

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Categories of Industrial and Government Applications of HPCC (with reference to academic applications)

- Define information generally to include both CNN headline news and the insights on QCD gotten from lattice gauge theories
- Information Production
  - e.g. Simulation
  - Major concentration of MPP and HPCC at present
- Information Analysis
  - e.g. Extraction of location of oil from seismic data,
    extraction of customer preferences from purchase data
  - Growing area of importance and Short term major MPP opportunity in decision support combined with parallel databases
- Information Access and Dissemination - InfoVision
  - e.g. Transaction Processing, Video-On-Demand
  - enabled by National Information Infrastructure
  - Very promising medium term market for MPP but need the NII to be reasonably pervasive before area "takes off"
- Information Integration
  - Decision support in business
  - Command and Control for Military
  - Concurrent Engineering and Agile Manufacturing
  - Integrates Information Production, Analysis, Access
  - Largest long term market for MPP

Tables of Industrial HPCC Applications 1 to 4:SIMULATION

Item	Application Area and Examples	Problem Comments	Machine and Software
1	**Computational Fluid Dynamics**	PDE, FEM Turbulence Mesh Generation	SIMD MIMD for irregular, adaptive **HPF(+)** Unclear for adaptive irregular mesh
2	**Structural Dynamics**	PDE, FEM Dominated by Vendor Codes (e.g. NASTRAN)	MIMD as Complex geometry **HPF(+)**
3	• **Electromagnetic Simulation** • Antenna Design • Stealth Vehicles • Noise in high frequency circuits • Mobile Phones	PDE Moment method (matrix inversion dominates) ——— Later FEM, FD? Fast Multipole	SIMD **HPF** ——— SIMD, MIMD, **HPF(+)**
4	**Scheduling** • Manufacturing • Transportation (Dairy delivery to military deployment) • University Classes • Airline Scheduling of crew, planes in static or dynamic (Midwest snowstorm) cases	Expert systems and/or ——— Neural Networks, Simulated Annealing ——— Linear Programming (hard sparse matrix)	MIMD (unclear speedup) Asyncsoft ——— SIMD **HPF** ——— MIMD **HPF+ ?**

PDE	Partial Differential Equation	**VR**	Virtual Reality
FEM	Finite Element Method	**HPF**	High Performance Fortran [HPFF92a]
FD	Finite Difference	**HPF+**	Natural Extensions of HPF [SCCS-255]
ED	Event Driven Simulation	**MPF**	Fortran plus message passing for loosely synchronous software
TS	Time Stepped Simulation		
CFD	Computational Fluid Dynamics	**Asyncsoft**	Parallel Software System for (particular) class of asynchronous problems

Note on Language: HPF, MPF are illustrative for Fortran
one can use parallel C, C++ or any similar extensions of data parallel or message passing languages

Tables of Industrial HPCC Applications 5 to 8: SIMULATION

Item	Application Area and Examples	Problem Comments	Machine and Software
5	**Environmental Modeling** - Earth/Ocean/ Atmospheric Simulation	PDE, FD, FEM Sensitivity to data	SIMD MIMD for irregular, adaptive mesh **HPF(+)** Unclear for adaptive irregular mesh
6	**Environmental Phenomenology** - Complex systems e.g. lead concentration in blood	Empirical models Monte Carlo and Histograms	Some SIMD MIMD more natural **HPF**
7	**Basic Chemistry** • Chemical Potentials • Elemental Reaction Dynamics	Calculate Matrix elements Matrix Eigenvalue Multiplication, Inversion	MIMD (maybe SIMD) **HPF**
8	**Molecular Dynamics** • Biochemistry • Discrete Simulation Monte Carlo in CFD (DSMC) • Particle in the cell (PIC)	Particle Dynamics with irregular cutoff forces Fast Multipole methods Mix of PDE and Particles in PIC or DSMC	**HPF(+)** or MPF for fast multipole

PDE	Partial Differential Equation	**VR**	Virtual Reality
FEM	Finite Element Method	**HPF**	High Performance Fortran [HPFF92a]
FD	Finite Difference	**HPF+**	Natural Extensions of HPF [SCCS-255]
ED	Event Driven Simulation	**MPF**	Fortran plus message passing for loosely synchronous software
TS	Time Stepped Simulation		
CFD	Computational Fluid Dynamics	**Asyncsoft**	Parallel Software System for (particular) class of asynchronous problems

Note on Language: HPF, MPF are illustrative for Fortran
one can use parallel C, C++ or any similar extensions of data parallel or message passing languages

Tables of Industrial HPCC Applications 9 to 13: SIMULATION

Item	Application Area and Examples	Problem Comments	Machine and Software
9	**Economic Modeling** ● Real Time Optimization ● Mortgage backed securities ● Option Pricing	Individual (Monte Carlo) Full simulations of portfolios	SIMD,**HPF** MIMD, SIMD Integration software
10	**Network Simulations** ● Electrical Circuit ● Microwave and VLSI Chip ● Biological (neural) Circuit	Sparse matrices; Zero structure defined by network connectivity	MIMD **HPF** for matrix elements MPF/library matrix solve
11	**Particle Transport Problems**	Monte Carlo methods as in neutron transport for explosion Simulations	MIMD **HPF**
12	**Graphics** (rendering) Hollywood Virtual Reality	Several operational Parallel Ray Tracers Distributed model hard	MIMD Asyncsoft for distributed database **HPF** for simple ray tracing MPF for best algorithms
13	**Integrated Complex Systems Simulations** ● Defense (SIMNET, Flight Simulators) ● Education (SIMCITY) ● Multimedia/VR in Entertainment ● Multiuser virtual worlds ● Chemical & Nuclear Plants	Event driven (ED) and Time Stepped (TS) Simulations. Virtual Reality Interfaces. Database backends. Interactive	Timewarp or other Event Driven (ED) Simulation needs Appropriate Asyncsoft Integration Software Database **HPF+** for TS simulation

PDE	Partial Differential Equation	**VR**	Virtual Reality
FEM	Finite Element Method	**HPF**	High Performance Fortran [HPFF92a]
FD	Finite Difference	**HPF+**	Natural Extensions of HPF [SCCS-255]
ED	Event Driven Simulation	**MPF**	Fortran plus message passing for loosely synchronous software
TS	Time Stepped Simulation		
CFD	Computational Fluid Dynamics	**Asyncsoft**	Parallel Software System for (particular) class of asynchronous problems

Note on Language: HPF, MPF are illustrative for Fortran
one can use parallel C, C++ or any similar extensions of data parallel or message passing languages

Tables of Industrial HPCC Applications 14 to 18
Information Analysis - "Data Mining"

Item	Application Area and Examples	Problem Comments	Machine and Software
14	**Seismic and Environmental** data analysis	No oil in NY State. Parallel Computer already important	SIMD, maybe MIMD needed **HPF**
15	**Image Processing** • Medical Instruments • EOS (Mission to Planet Earth) • Defense Surveillance • Computer Vision	Commercial Applications of Defense Technology. Component of many Information Integration Applications e.g. Computer Vision in Robotics	Metacomputer Low Level SIMD, **HPF** Medium/High level MIMD **HPF(+)** Software Integration Asyncsoft Database
16	**Statistical Analysis** Packages (libraries)	Optimization Histograms (see category 4)	**HPF+** adequate for many libraries
17	**Healthcare Fraud** Inefficiency Securities Fraud Credit Card Fraud	Linkage Analysis of database records for correlations	SIMD or MIMD Parallel Relational Database Access Plus category 16)
18	**Market Segmentation**	Sort and Classify records to determine customer preference by region (city --> house)	Some cases are SIMD Parallel Database Plus category 16

Table of Industrial Applications 19 to 24 for Information Access InfoVision - Information, Video, Imagery and Simulation on Demand

19	Transaction Processing • ATM (automatic teller machine)	Database-most transactions short. As add "value" this becomes Information Integration	Embarrassingly Parallel	MIMD Database
20	Collaboration • Telemedicine • Collaboratory for Research • Education • Business	Research Center or doctor(s) - patient interaction without regard to physical location	Asynchronous	High Speed Network
21	Text on Demand • Digital (existing) libraries • ERIC Education database, • United Nations - Worldwide newspapers	Multimedia database Full text search	Embarrassingly Parallel	MIMD Database
22	Video on Demand • Movies, News (CNN Newsource & Newsroom), • Current cable, • United Nations - Policy Support	Multimedia Database Interactive VCR , Video Browsing, Link of video and text database	Embarrassingly Parallel for multiple Users Interesting parallel compression	MIMD Database Video Editing Software SIMD Compression
23	Imagery on Demand Kodak GIODE • "clip art" on demand • Medical images • Satellite images	Multimedia database Image Understanding for Content searching and (terrain) medical feature identification	Metaproblem Embarrassingly Parallel plus Loosely Synchronous Image Understanding	MIMD but much SIMD image analysis
24	Simulation on Demand • Education, Tourism, City planning, • Defense mission planning	Multimedia map database Generalized flight simulator Geographical Information System	Synchronous terrain rendering with Asynchronous Hypermedia	SIMD terrain engine (parallel rendering) MIMD database **Integration** software

First Four Table Entries for Applications 25 to 33: Information Integration

- These involve combinations of Information Production, Analysis, Access and Dissemination and thus need the Integration of the various Software and Machines Architecture Issues discussed there
- Sometimes Called System of Systems
- 25: Military and Civilian Command and Control (C^2, C^3, C^4I ....)
  - Battle Management, Command,Control,Communication,Intelligence and Surveillance (BMC^3IS)
  - Military Decision Support
  - Crisis Management -- Police and other Government Operations
  - SIMNET simulates this and with people and computers in the loop has many of same issues
- 26 to 28: Applications of InfoVision Services
  - Generalize Compuserve,Prodigy, America Online, Dialog and Other Information Servives
  - 26: Decision Support for Society
    - Community Information Systems
    - Travel and Generalized Yellow Page Services
  - 27: Business Decision Support -- One example is:
    - Health Care with Image and Video databases supporting telemedicine
  - 28: Public Administration and Political Decision Support
    - Government Information Systems
    - Maxwell School at Syracuse University teachs use of realtime video to aid world wide decisions (United Nations)

Second Five Table Entries for Applications 25 to 33: Information Integration

- 29: Real-Time Control Systems
  - Robotics uses Imagery to make decisions(control vehicles)
  - Energy Management controls power use and generation
- 30: Electronic Banking
  - Requires Security, Privacy, Electronic Cash etc.
- 31: Electronic Shopping
- 32: Agile Manufacturing -- Multidiscplinary Design and Concurrent Engineering
  - Combines CAD with Applications 1 to 3
  - Requires major changes to Manufacturing Infrastructure and Approach
- 33: Education
  - InfoMall Living Textbook -- 6 Schools on ATM network linked to HPCC InfoVision Servers at NPAC

Abbreviations used in tables of Industrial Applications of HPCC

PDE	Partial Differential Equation
FEM	Finite Element Method
FD	Finite Difference
ED	Event Driven Simulation
TS	Time Stepped Simulation
CFD	Computational Fluid Dynamics
VR	Virtual Reality
HPF	High Performance Fortran
Adaptive	Software for Irregular Loosely Synchronous Problems handled by pC++, HPF extensions, Message Passing
Asynchronous (AsyncSoft)	Software for asynchronous problems
Integration Software	Software to integrate components of metaproblems

Core Enabling HPCC Software Technologies for Information Production (Simulation)

- PVM, Express, Linda, MPI
- ISIS (Cornell)

- High Performance Fortran (HPF) Compiler
- High Performance C, C++ Compiler

- HPF Extensions - PARTI
- Parallel / Distributed Computing Runtime Tools
- ADIFOR (Differentiate Fortran Code)
- AVS and Extensions
- High Performance Fortran Interpreter
- Image Processing
- Parallel Debugger
- Parallel Performance Visualization
- Parallel Operating Systems
  - I/O
  - Scheduling
- Virtual Reality
- Event Driven Simulator

Core Enabling HPCC Algorithms and Components for Information Production (Simulation)

- Mesh Generation
- SCALAPACK
- Sparse Matrix Solvers - Templates and libraries (Direct and Iterative)
- Particle Dynamics Kernels - Templates and Libraries ($O(N^2)$ to fast multipole)
- Optimization Methodology and Templates
  - Linear programming
  - Non-linear programming
- Scheduling (neural-net, parallel) Templates

Core Enabling HPCC Technologies
Information Analysis, Access, Integration

- Parallel (Relational) Database e.g. Oracle 7.0
- Object database
- High Speed Networks
- Multilevel Mass Storage
- Integration Software ("glue")
- Integration of Parallel and Distributed Computing
- Multimedia Support
  - Video Browsing
  - Image Content
  - Full Text Search
  - Real time I/O (disk ---> network)
- ATM Network Protocols and Management
- Compression
- Parallel Rendering
- Linkage Analysis (between records of database)
- Sorting (large databases)

Core Enabling HPCC Technologies Information Analysis, Access, Integration *continued*

- Collaboration Services
  - Multi user video conferencing
  - Electronic whiteboards, etc.
- Security and Privacy
- Usage and Charging Algorithms
- Televirtuality
  - The world as a metacomputer
  - Naming
  - World Wide Web
- Human-Computer Interfaces
  - Mosaic Client
- Information Organization
  - Mosaic Server
- Image Processing
  - Terrain Rendering
  - Kodak Photo-CD
- Geographical Information Systems
  - Spatial databases

Some Anecdotes from New York State InfoMall Survey of Industrial HPCC Applications

- Carrier (Syracuse) competing with Japanese who build quiet air conditioners. Need 3-D CFD simulations including acoustics.
- Major aerospace company - engineers are using a network of RS6000's for large CFD simulations.
  - Excellent speedup but troubled by poor O/S support for such distributed computing
  - Viewed parallel computing as uninteresting
    - Because for their problem, i860 node on Intel Touchstone had poor cost-performance compared to RS6000
- Teraflop machine in a submarine will allow adaptive 3-D beamforming.
  - (SIMD) Signal processing (matrix algebra) combined with irregular partial differential equation solution for acoustic propagation in ocean.
  - but submarine not so critical to nation these days .... (seawolf)
- Global competition and DoD cutbacks ---->
  Aerospace and other manufacturing companies are typically cutting back in personnel and research ---->
  Hard to integrate new technologies .....

HPCC Industrial Applications in Environmental Modeling

- Several diverse applications

    Global warming
    Pollution
    Oil reservoir
    Acoustic signals in a real ocean to detect (hide) submarines

- Share partial differential equation algorithms between disciplines and with CFD, structures

    Direct solvers
    Conjugate gradient
    Domain decomposition
    Multigrid
    Adaptive meshes

- Major federal activities in
  - DOE CHAMMP
  - NOAA
  - NASA (Goddard)

Particle Calculations
Chemical Potentials and Scattering

- Caltech (Kuppermann, McKoy) showed successful hypercube implementations of reactions such as $e^- Si$, $H_2 + H$ scattering
  ----> such problems important for catalysts
- These and MOPAC Gaussian90 (find potentials) dominated by matrix algorithms - multiplication, inversion and eigenvalues
  - use AVS to separate into components
- Computational Electromagnetics has similar computational structure

Physics and Chemistry Molecular and other Particle Dynamics

- CHARMM used extensively in industry
  100,000 lines - hard to parallelize
  - No good SIMD version
  - Adhoc MIMD version
- Academic astrophysics code with new algorithm (fast multipole) running with > 10^6 particles on Delta at Caltech

Electrical Power and Other Network Simulations

- Niagara Mohawk's transmission system described by 4000 X 4000 sparse matrix (~12 nonzero elements in each row)
- Use to plan and control electrical distribution and to recover from circuit damage
- NiMo could use small parallel MIMD machine - problem not very big
- Large teraflop machine could control nation's power?

Related Network Simulations - Chip, Phone, Gas, Cortex

- NYNEX currently does not use sophisticated simulations in planning new installations. Has large databases of information to guide simulation
- All are physical networks with mainly local connections

Dual-Use Image Processing and Related Technologies

- Defense (SDI ...) Technology
  - Sensors and Image Processing
  - Command and Control (decision aids)
  - Tracking
- Has interesting applications to the next war (i.e. to global economy)
  - Entertainment
  - Sports
  - Medicine
  - Robotics
  - Manufacturing
  - General information systems ....

OLTP - Online Transaction Processing

- This is dominant use of computers in business and ~80% of business use involves transactions which are short, taking < 1 second ----> can parallelize simply by processing several users simultaneously
  - Oracle 7.0 on shared (KSR,Teradata,Sequent) and distributed memory (Meiko, nCUBE)
- OLTP unlikely to need a "teraflop" machine unless we add sophisticated processing to database access
- Teradata (--> NCR --> AT and T) is largest parallel computer vendor whose systems are used to summarize inventories (etc.) and parallelized similarly over several small records.

Anecdotes from Insurance Industry

- Empire Blue Cross / Blue Shield in Syracuse processes
  - 6.5 million transactions per day using an IBM3090-400 with a data center of 200 people
  - Expects IBM ES9000 to allow system to expand gracefully for future growth
  - Already all documents are scanned in and store in archives
  - Interested in fault tolerance
  - Does not need high performance unless goals change ....
  - Consumer Reports estimates that 20% of health care costs ($200B) is waste ....

Anecdotes from Running Stock Exchanges

- SIAC runs the New York and American stock exchanges
- Already uses parallel computing implemented appropriately on distributed networks ("embarrassingly parallel")
- 2 acres (~300) Tandem computers interfacing network of PC/workstations to calls from brokers
- 2000 stocks in NYSE decomposed in load balanced fashion over traders and associated PC's (~500)
- Fault tolerance and network management are key issues
- A few minutes downtime per year are allowed

....

More Anecdotes from the Insurance Industry

(Health Insurance example)

- Large NY State Insurance Company spends \$70M a year in Syracuse on data processing.
- Hardware and operation costs "negligible" (<10%) for modest IBM3090
- Cost is application programmers developing new software or maintaining old code - your grandfather's policy is an important dusty COBOL deck.
  - ~15 million lines of COBOL
  - ~3 year backlog for new application codes
- Where should they use high performance computing?
- Innovative insurance companies scan documents but don't need HPC
- Clearly need a more productive software model

The Case for Parallel COBOL?

- Parallel computing is clearly applicable for the myriad of small transactions
  - We can in parallel each get money from our ATM for our trip
- But there are important "batch jobs" typically written in COBOL
  - e.g. Summarize corporate inventories
- This is the dusty COBOL deck problem.
  Both
  - Parallel processing
  - 24 hour a day operation implied by global economy - large programs used to run overnight, but our night is day somewhere in the world!
  Causes difficulties
- Need "High Performance COBOL" compilers?

Anecdotes from Information Industry

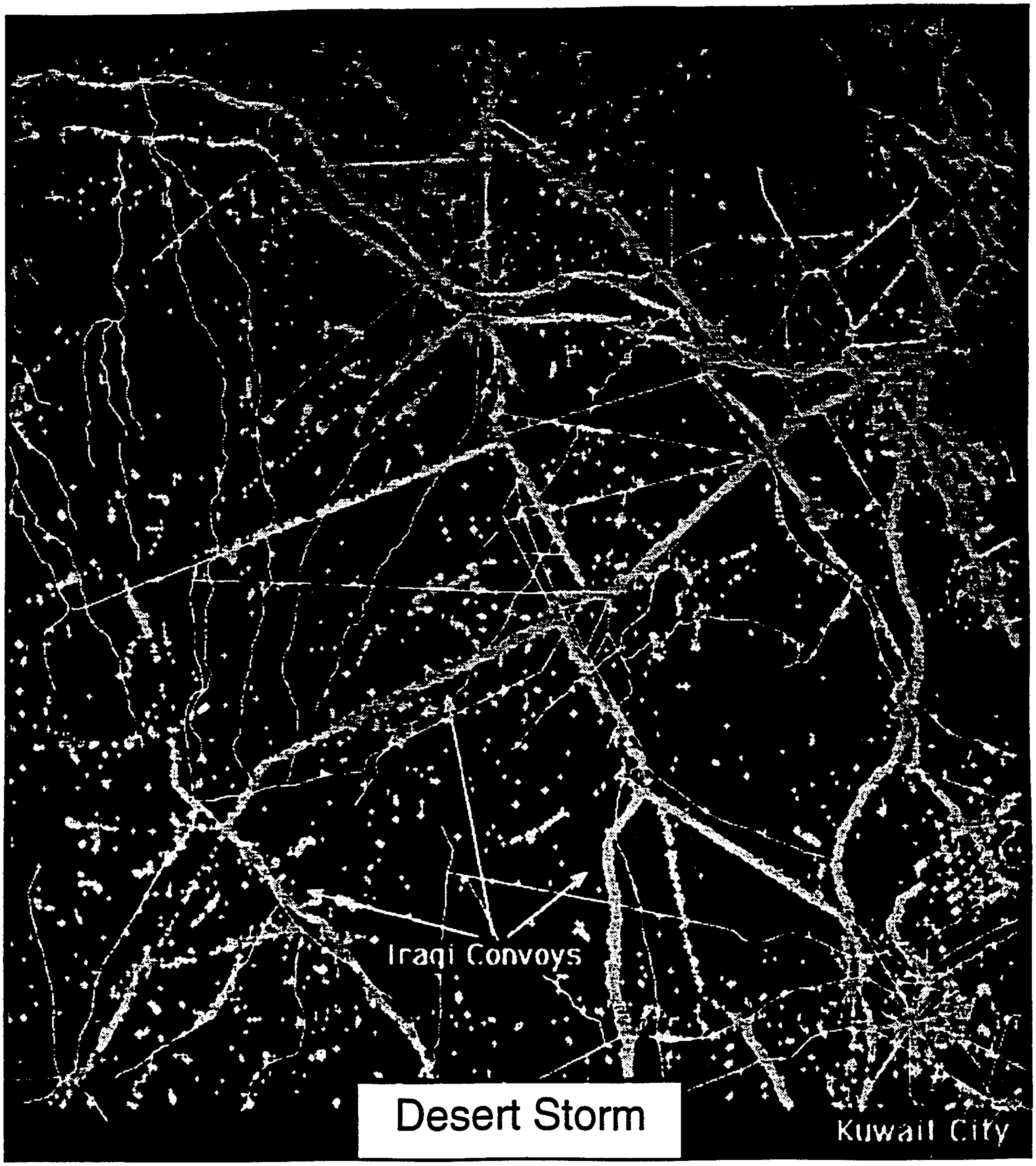
- Dowquest already uses two CM-2's to extract information from an online database of financial articles.
  - Generalized in WAIS system by Thinking Machines
- A small Rochester company making CD-ROM's would like to complete task more quickly as need to run several times to get error free CD-ROM.
- Low end (PC) multimedia systems will revolutionize information presentation (DVI specialized hardware for realtime CDROM animation)
  - But will need parallel supercomputer for intelligent dynamic searches
- SIAC uses 3090's after hours to find unusual correlations which could signify fraudulent trading
- Otis has ~1 million elevators and is considering a central database to accumulate operating history. One could then analyze with neural networks or an expert system to find "signatures" that allow one to schedule preventive maintenance and avoid "callbacks" - customer induced repair calls
  - Japanese elevators have a very good reputation for reliability (>10 times better than United States ?)

Command and Control and Avionics

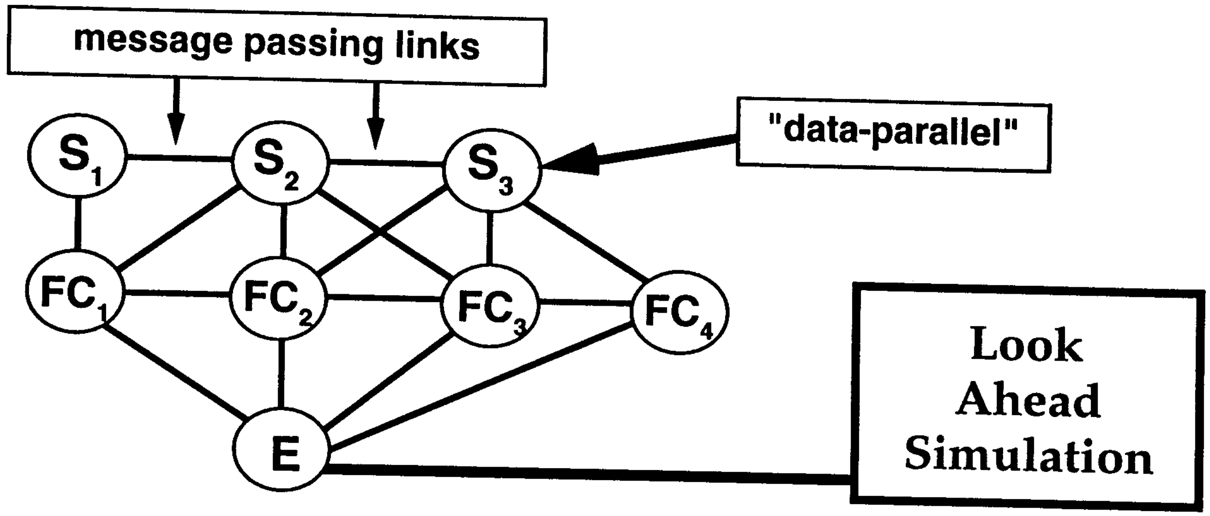
- DOD maybe only will sponsor about two new airframes in the next ten years doe to peace dividend ----> maybe no more aircraft for given company
- But we can consider replacing all existing computers in:
  - aircraft
  - ships
  - local and global commands in all branches of DOD
- What will factor of 1000 increase in performance allow us to do in:
  - Avionics: claim no more Mips needed, but can at least waste Mips and use standard distributed software
  - Mission Control: signal processing and planning will surely be able to use any available Mips - "Pilot's Associate", but many new algorithms still to be discovered.

Image From Joint Stars (Grumman, PAR Technology)

"The Mother of All Retreats"
(Secretary Cheney)



Heterogeneous Metaproblem Structure for Command and Control



- S_i: Satellite with: Image processing, Kalman filter, Stereo match — Synchronous or loosely synchronous
- FC_i: Fire Control platform with loosely synchronous target-weapon pairing algorithm
- E: Overall Asynchronous expert system

Rome Laboratory Parallel Software Engineering Cooperative

- CRDA - Government-Industry Research and Development Agreement - allows government (laboratory staff and in principle subcontracts) and industry to work together
  - Important mechanism for government to interact with and focus funds on introducing high technology into industry
- Current(1993) Membership:

Large Organizations:

Aerospace
Grumman (Data Systems)
ITT
MITRE
Motorola (Federal Systems)
Raytheon

Small organizations:

Symbiotics
Ultra

Rome Laboratory Parallel Software Engineering Cooperative

- Cooperative is focussed on software
  Operating systems, Languages, tools and system integration for
  - BMC^3IS =
    Battle Management, Command-Control-Communication, Intelligence and Surveillance
  - Military version of large scale information processing
    - Heterogeneous distributed sensors and processors
    - Real time embedded systems
- Even if little new military equipment is funded by DOD, could and should upgrade control systems in existing ships, tanks, aircraft, control centers ....

Some HPCC Software Questions for BMC^3IS

- What is the appropriate virtual machine(s)
  i.e. (industry standard) computing model for BMC^3IS ?
- How important is ADA ?
  - Next upgrade (ADA9X) of ADA will not address deficiencies in area of (data) parallel computing
  - ADA mandated by DOD but not used in analogous commercial applications (C++ dominant ?)
  - DOD wants to use civilian facilities for "agile manufacturing"
    - Can it afford different software standards ?
  - DOD mandates ADA but it does NOT mandate parallel computing be used in , say, simulation of AX (next Navy plane)
- Does parallel software engineering mean anything to a wide community?

Anecdotes from Use of Computers in Large Organizations

- New York Health Department Syracuse office only has home PC's and old (? 6 years) UNIX systems rescued from bankrupt hospitals
  - They take several weeks to access central databases in Albany and produce charts of medical statistics for the Central New York region
- Large utility is interested in expert system/neural networks which can be used to analyze bill payment data and predict when payments expected
- Large credit card company rumored to be interested in analyzing credit card receipts to discover more than you know about your family's buying habits

Issues for Financial Modeling

- Wall Street already has some parallel machines installed and likely to increase use of parallel computers
- Rapid prototyping critical as financial instrument, mix of investments in portfolio and models change rapidly
- Mortgage backed securities (Zenios) at Wharton School and option pricing well studied. New optimization methods very promising

Anecdotes for Use of Computing in Financial Community

- One Wall Street company makes major use of C and C++ - 200,000 lines of code in just one application.
- Another company says modeling is very appealing but information processing is the real problem for corporation
- New Optimization Methods and Monte Carlo Simulations of growing Interest

HPCC Issues for Virtual Reality(VR)

- Is " by definition " the highest bandwidth and richest human-computer interface
- Thus natural HPC user interface
- Need HPCC to create virtual worlds
- VR is high end multimedia - multimedia is rapidly evolving "low end" technology
- VR is used by customer to "experience" new car which will be built by "Agile Motors Inc."(Car company employing Agile Manufacturing)
- VR is used in medical rehabilitation and diagnosis. Patient can be stimulated and motivated as virtual world fills in for impaired patient capabilities
- VR is used in new sports delivery systems to experience "world according to favorite player" as detected by sensors and HPC image processing

History and Key Issues for MADIC -- The Multidisciplinary Analysis and Design Industrial Consortium

Multidisciplinary Analysis and Design Industrial Consortium

- Industry imitations provide strong incentive for collaboration between firms and with universities and government
- MADIC organized through NPAC in March 1992
- Initial organization supported by NASA, New York State (NPAC INFOMALL program)
- Member firms pay annual fee for administrative expenses
- NASA regards MADIC as its "CAS (Computational Aerosciences) Consortium"
- MADIC members form teams to address specific projects

Objectives of MADIC Multidisciplinary Analysis and Design Industrial Consortium

- Define systems architecture and software requirements for an automated multidisciplinary analysis and design system implemented in a heterogeneous computer environment
- Identify gaps in existing technology base
- Facilitate joint ventures
  - Between member companies
  - Between member companies and government agencies
- Influence Federal HPCC program
  - Software research and development
  - Machine access and training
- Provide a mechanism for technology transfer

MADIC Industrial Consortium Members as of 1993

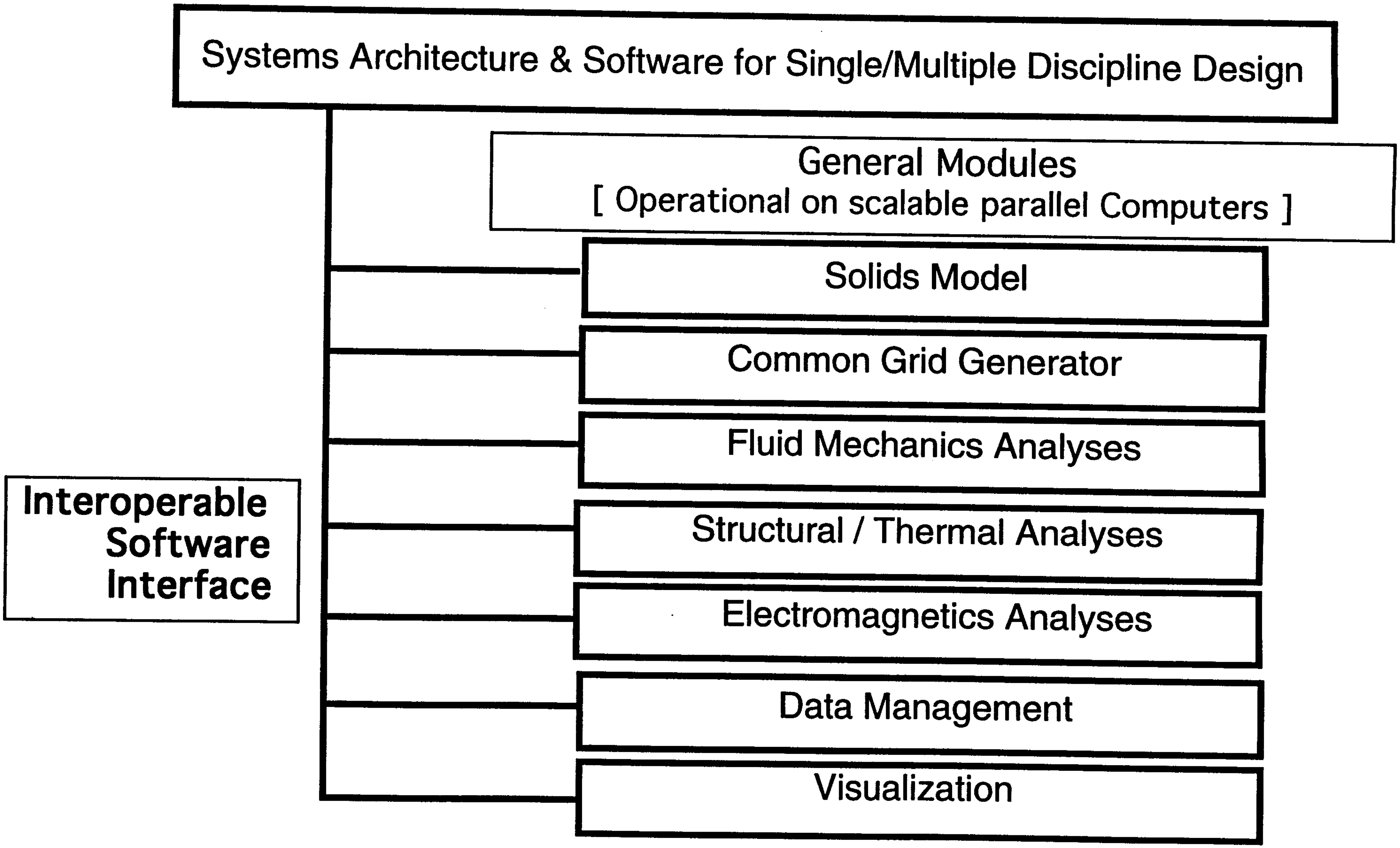
- Allison Gas Turbines
- Boeing
- Ford Motors
- General Electric (Corporate R&D, aircraft engines)
- General Motors
- Grumman
- Lockheed
- McDonnell Douglas Aircraft
- Northrup
- Rockwell
- United Technologies Research Center representing (Otis, Pratt & Whitney, Sikorsky)
- Vought Aircraft

The USMADE Project of MADIC Industrial Consortium

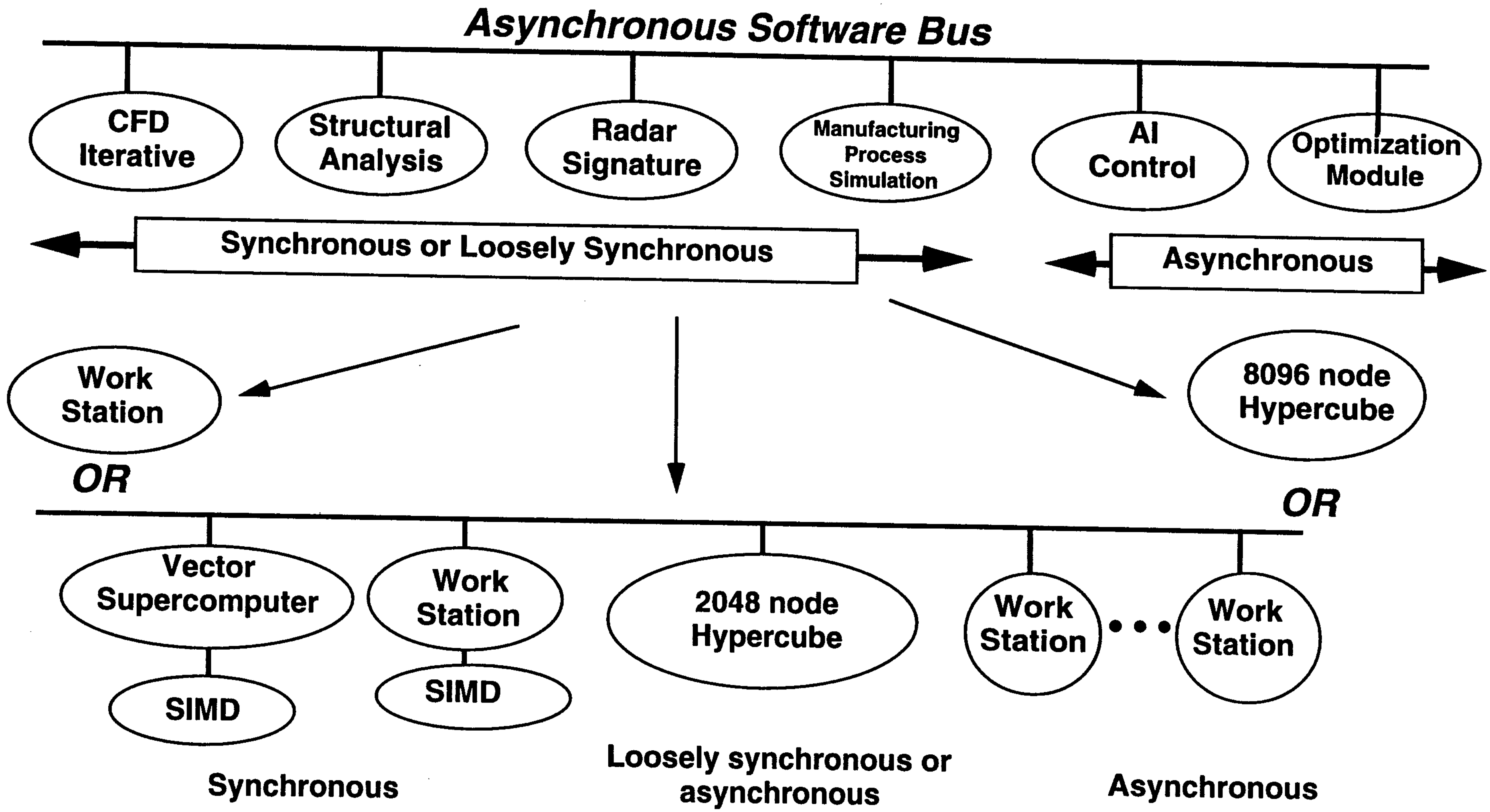
United States Multidisciplinary Analysis and Design Environmei

- Integrated Environment
- Multiple discipline
  - Fluid Dynamics
  - Structural mechanics, dynamics
  - Electromagnetics
  - Heat transfer
  - Controls
  - Manufacturing
  - ...
- Engineering analysis
- Design optimization

Software Bus Structure of USMADE



The Mapping of Heterogeneous Metaproblems onto Heterogeneous Metacomputer Systems



INFOMALL and the National Information Infrastructure

Media
Entertainment
Telephone
Cable (communications)
Computing
Video game

Industries will partner to provide

Digital Information Services

Initially provide

Entertainment (Video on Demand)
News
Interactive TV - Shopping etc.

These will justify capital investment to create

National Information Infrastructure (NII)

How can these be exploited for defense, business use, academic research, education, creation of HPCC Software Industry?

NII Compute & Communications Capability in Year 2000 --> 2005

100 Supercomputers at a teraflop	10^{14} flops/sec (100% duty cycle)
100 Million NII Connections	10^{14} bits/sec --> words/sec (x~0.1 duty cycle?)
100 Million home PC's, Videogames, Settop boxes at 100 --> 1000 megaflops	10^{16} --> 10^{17} flops/sec (x~0.1 duty cycle?)
1000 --> 10000 High Performance Multimedia Servers	10^{15} --> 10^{16} ops/sec (100% duty cycle)

Each has capital value of order $100 Billion

Ultimate Vision and Implementation of NII and InfoVision

- InfoVision is ultimate client server application
  - 10^8 clients - each of which could be (small) servers
  - 10^4 large (~$10M) parallel servers

- Democracy on the NII (Gore)
  - Everybody can access information on the NII
  - Everybody has equal opportunity to put information on the NII

What will National Information Infrastructure give us?

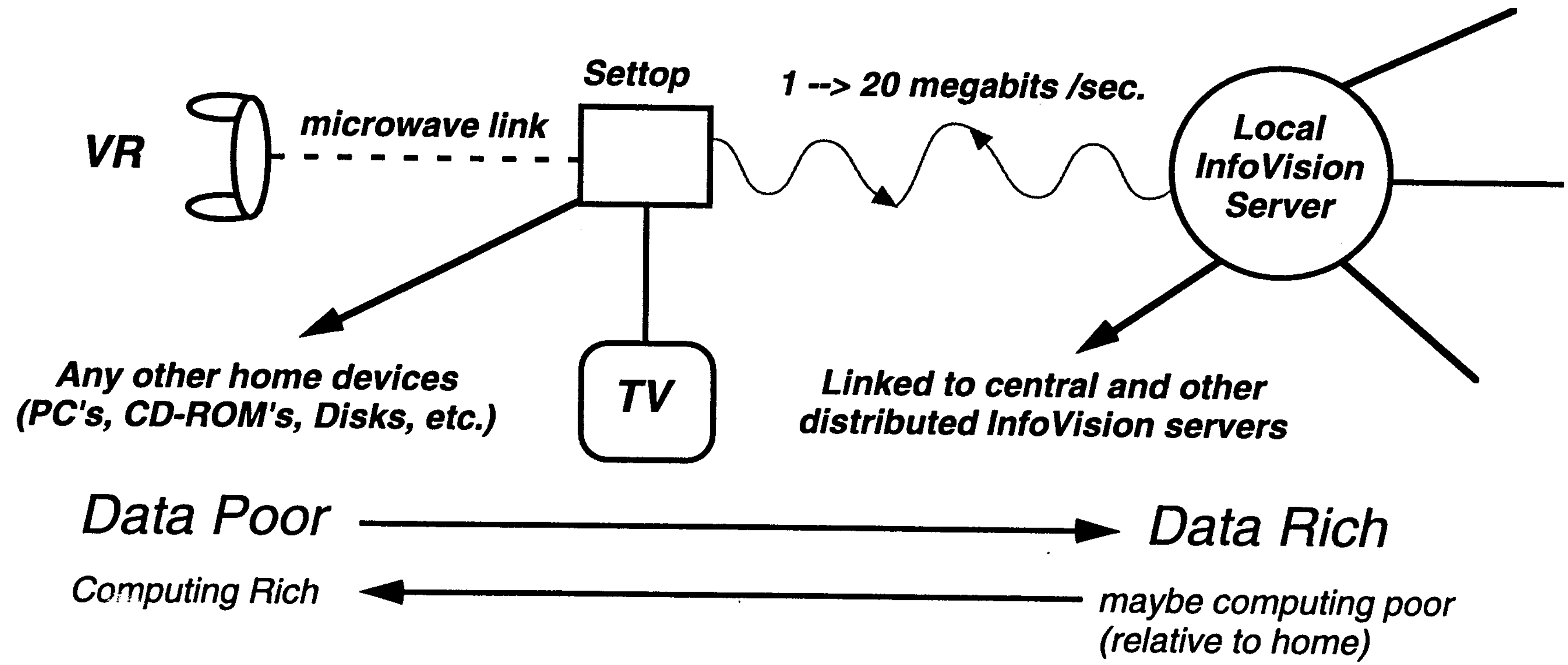
- Every Military "Unit", "Every" Business Office, Every school "desk", "Every" home (approximately any place on cable or accessible by wireless ot other communication device) will have a two-way high speed link to the NII
  - about 10 Megabits/second compared to
  - modem - 10 Kilobits/second
- "Resolution" of Military Unit and School Desk Unclear

- What does this factor of 1000 increase in performance do for the home?
  - TV + Settop Unit becomes Computer
    (analog) (interactive digital)
  - Modem & home PC supporting text interfaces becomes interactive full (VHS → HDTV resolution) video receiving unit
  - Interactive implies that you can choose what you want when you want it.

- These consumer developments will drive MPP use
  - consumer products drives better high end business and research user level products e.g., cheap Virtual Reality Interfaces
  - MPP's are information servers for consumers, business, research

InfoVision is a Set of HPCC Applications on the NII/GII

Information Video Imagery and Simulation on Demand



- ❑ **Defense (Dual-Use), Business and Research environments will be set up in a similar way to leverage mass market and common NII. Obviously different services in detail and different functionality trade offs.**

Architectures

Professor William J. Dally

Massachusetts Institute of Technology

What can Parallel Computing do for Defense Science and Engineering?

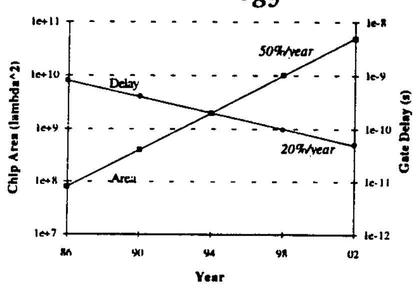
William J. Dally
Massachusetts Institute of Technology

October 31, 1994

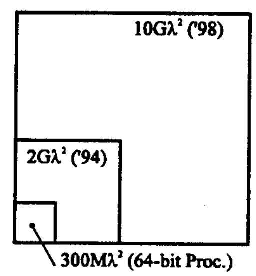
Outline

- *Technology Trends*
  - *Why parallel computing?*
- *Parallel Computer Architecture*
- *Leveraging Commodity Technology*
- *Case Study*
- *Futures*

Trends in Integrated Circuit Technology

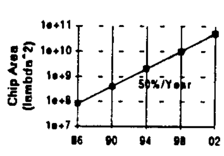


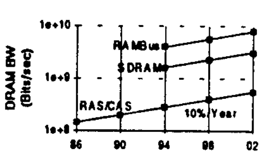
Scaling of Circuit Technology



Bandwidth vs. Capacity of DRAMs

- *Capacity increases 50% per year vs 10% for BW*
- *Time constant growing at 40% per year*
- *Move to high bandwidth parts resets clock 5 years*





Scaling of Arithmetic, Memory, and Bandwidth

- *Arithmetic performance improves with area and speed (70% per year)*
- *Memory capacity improves with area (50% per year)*
- *Bandwidth improves with speed (10% - 20% per year)*
  - *Bandwidth is becoming the most critical resource*
  - *Arithmetic (processing) is becoming the least critical*

Cost of Bandwidth vs. Distance

Cost of 1GB/s vs distance

Packaging Level	Dist	Cost. ($)	
Local on chip	2mm	0.06	wire
Global on chip	15mm	0.50	wire
Between chips	10cm	12.00	chip pins
Between boards	30cm	50.00	connectors
Between cabinets	10m	200.00	cables+conn
Between buildings	200m	2000.00	fiber+xcvrs

Technology in 2010

- CMOS Integrated Circuits
  - 0.05μm CMOS, 3.5cm x 3.5cm. (2Tλ^2)
  - 2GHz clocks
- Processors
  - 4K per chip (@ 500Mλ^2/proc)
  - 8TFLOPS/chip (@ 2GHz)
- Memory
  - 20G bits/chip (@ 100λ^2/b)
- 5K pins/chip
  - 500μm area grid

Then and Now

	1994	2010		Δ
Area	2G	2T	λ^2	1K
Frequency	200M	2G	Hz	10
Processors	4	4K		1K
FLOPS	800M	8T		10K
Pins	500	5K		10
Global wires	100K	1M	b/m²	10
Pin BW	100G	10T	b/s	100
Memory	16M	16G	b	1K
Memory/PBW	160μ	1.6m	s	10
FLOPS/PBW	8m	800m	OP/b	100

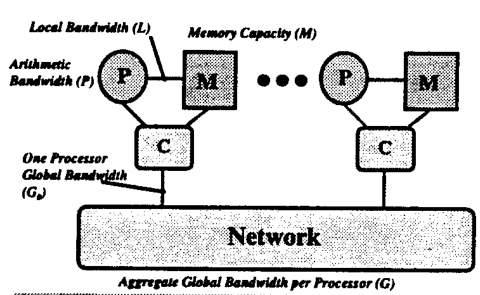
Implications of Technology Trends

- Processors are cheap relative to memory
  - Many processors in a system
  - Increase P:M ratio - cost balanced design
- Bandwidth is expensive and gets more so with distance
  - Optimize use of bandwidth, not processing
  - Exploit locality - use bandwidth where it's cheap
  - Non-uniform memory access

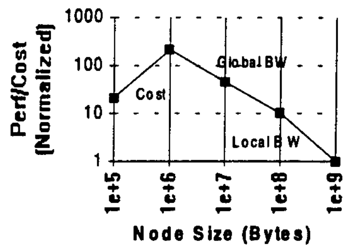
Outline

- Technology Trends
- Parallel Computer Architecture
  - Grain Size
  - Bandwidth ratios
  - Mechanisms
- Leveraging Commodity Technology
- Case Study
- Futures

A Generic Parallel Computer



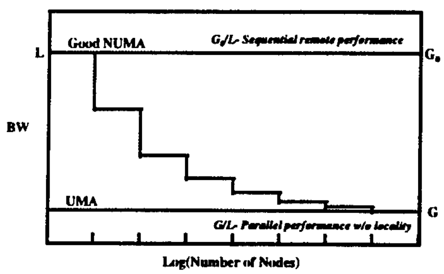
Granularity



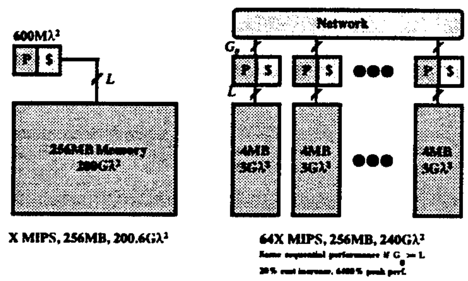
Cost-Balanced Architecture

- *Traditionally balance processor performance to memory capacity*
  - *1MB of memory per MIPS of processor*
  - *This leads to machines that are all memory*
- *More efficient to balance costs of communication, memory, processing*

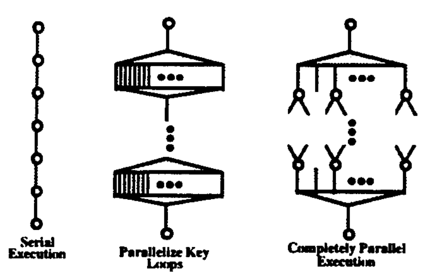
Bandwidth Ratios



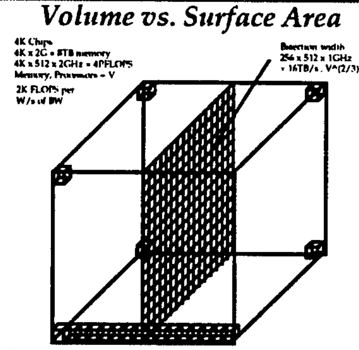
A Parallel Computer should be a Good Sequential Computer



Incremental Migration of Software

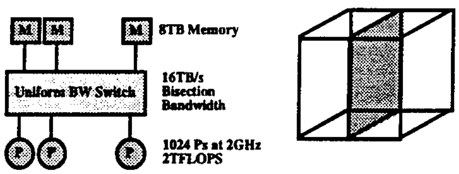


Volume vs. Surface Area



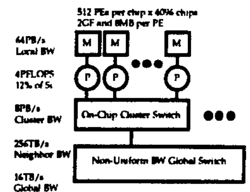
Uniform BW Architecture Does not Scale

- *Global bandwidth scales as V^(2/3)*
- *.006% of silicon provides processing to match BW*



Clustered Architecture Exploits Locality

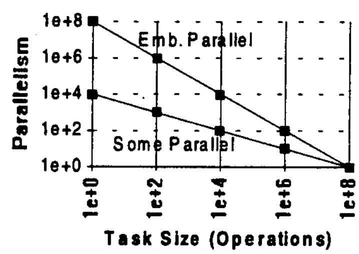
- *12% of silicon provides 4PF processing*
- *Can emulate similar cost uniform BW architecture*
- *2000x more cost effective for local computations*



Mechanisms

- *Applications should see latency and bandwidth set by physical limits on short messages.*
  - *e.g., 300ns and 300MB/s vs. 50μs and 2MB/s*
- *Sequential programs should run well and be incrementally parallelized*
- *Requires*
  - *Shared address space*
  - *User-level communication*
  - *Cache coherence - to automatically exploit locality*
  - *Fast synchronization - local and global*
  - *Latency tolerance*

Agility Enables Parallelism



The Impact of Architecture

- *A good architecture reduces the parallel software problem to fundamentals*
  - *Identify parallelism*
  - *Exploit locality*
- *A bad architecture burdens the programmer with incidentals*
  - *Manage multiple address spaces*
  - *Coalese messages and tasks to avoid startup overhead*

Outline

- *Technology Trends*
- *Parallel Computer Architecture*
- ***Leveraging Commodity Technology***
- *Case Study*
- *Futures*

Technologies - Commodity and Custom

Technology	NR	R	Q
Integrated Circuit Fabrication	$500M	$100	5M
Processor Design	$20M	$100	200K
Parallel Computer System	$50M	$1M	50
System Software	$100M		
Application Suite (100 codes)	$500M	$100K	5K

Exploiting Locality

- Inter-Processor Networks
  - Provide high "Neighbor" BW
  - Latency and BW should approach physical limits
- Data placement
  - Partition data so majority of accesses are local.
  - Need 3200:160:16:1 (Local, Cluster, Neighbor, Global)
- Caching
  - Automatic, coherent management of entire memory can automatically place and migrate data to exploit locality.
- Limited by communication requirements of algorithms
  - e.g., FFT needs O(N) communication for O(NlgN) ops.

Tolerating Latency

- Keep local resources busy while waiting for global requests
- Multithreading
  - Multiplex several "virtual processors" on hardware
  - Zero-cost context switch when waiting
  - Requires excess parallelism to cover latency
    Pex = Max(1, T x g)
- Pipelined memory system
  - Memory system must support many outstanding requests
  - Flow-control required to avoid deadlock/livelock

Parallel Software

- Most problems have lots of parallelism
  - FFT O(N), LUD O(N), Eval Model O(N)
  - Almost no "serial" problems (or real "serial fraction")
    - this is just code that hasn't been converted
- Parallel software hard today because
  - Machines have poor communication and synchronization
    - Need fast networks, low overhead interfaces, synchronizing memory
  - Management of locality and bandwidth is not well understood
    - Need global coherent memory, bandwidth optimized applications

Parallel Software (cont.)

- <u>Little economic incentive to develop parallel software today</u>
  - 300M$ parallel market vs. 100GS serial market
  - Tools are primitive

Invest in what the market ignores: Scalability

- Desktop/Settop systems drive technology
  - process technology
  - processor designs
  - memory designs
  - small-scale software
- Ignores scalability
  - global packaging technology
  - latency hiding mechanisms
  - exploitation of locality
  - scalable software

Outline

- *Technology Trends*
- *Parallel Computer Architecture*
- *Leveraging Commodity Technology*
- *Case Study*
  - *MIT J-Machine*
  - *Cray T3D*
- *Futures*

Outline

- *Technology Trends*
- *Parallel Computer Architecture*
- *Leveraging Commodity Technology*
- *Case Study*
- *Futures*
  - *Parallelism from the desktop up*
  - *Obstacles and opportunities*

Parallelism on the Desktop

- *Year 2000 - 25Gλ^2 chips - 4P+M*
  - *4 processors with 8MB each (2%P)*
    - *PCs with single chip (4P)*
    - *Servers/worstations with 10s of chips (~100P)*
    - *Supercomputers with 10^3 to 10^4 chips (~10^4P)*
- *Systems share*
  - *IC fabrication technology*
  - *Core processor and memory design*
  - *Modestly parallel software modules*
- *High end systems also need*
  - *Latency hiding and locality features in processor*
  - *Massively parallel software modules*
  - *High bandwidth global networks*

Parallel Computer Companies are Struggling

- *Their products are networked workstations*
  - *e.g., CM5, Paragon*
  - *Its cheaper to buy the workstations and network them*
- *Converting sequential software is hard*
  - *w/o mechanisms*
    - *shared memory, latency hiding, and cache coherence.*
  - *w/o fast access to global memory (G_c<<L)*
- *There are few 3rd party applications*
- *They focus only on the vanishing high-end market*

Opportunities

- *>10x performance/price gain by increasing P:M*
- *Incremental migration of programs*
  - *Mechanisms for locality, latency, shared address space*
  - *Bandwidth balance (L~G_c)*
- *Parallelism is moving downward in the market*
  - *SMP servers with up to 64 processors today*
  - *parallel desktop machines in a few years*

Conclusions

- *Technology trends motivate parallelism*
  - *70% per year increase in area x speed*
  - *Non-uniform scaling of processor, memory, and communication*
- *Parallel architecture enables software*
  - *Cost-balanced granularity*
  - *Bandwidth hierarchy (L=G_0>>G)*
  - *Mechanisms*
- *Invest in what the market ignores*
  - *Use IC technology, sequential software*
  - *Develop mechanisms, parallel software*
- *Supercomputers are time machines*
  - *Is this still valuable?*

NUCLEAR WEAPONS

Advanced Computation for Stewardship of the Stockpile

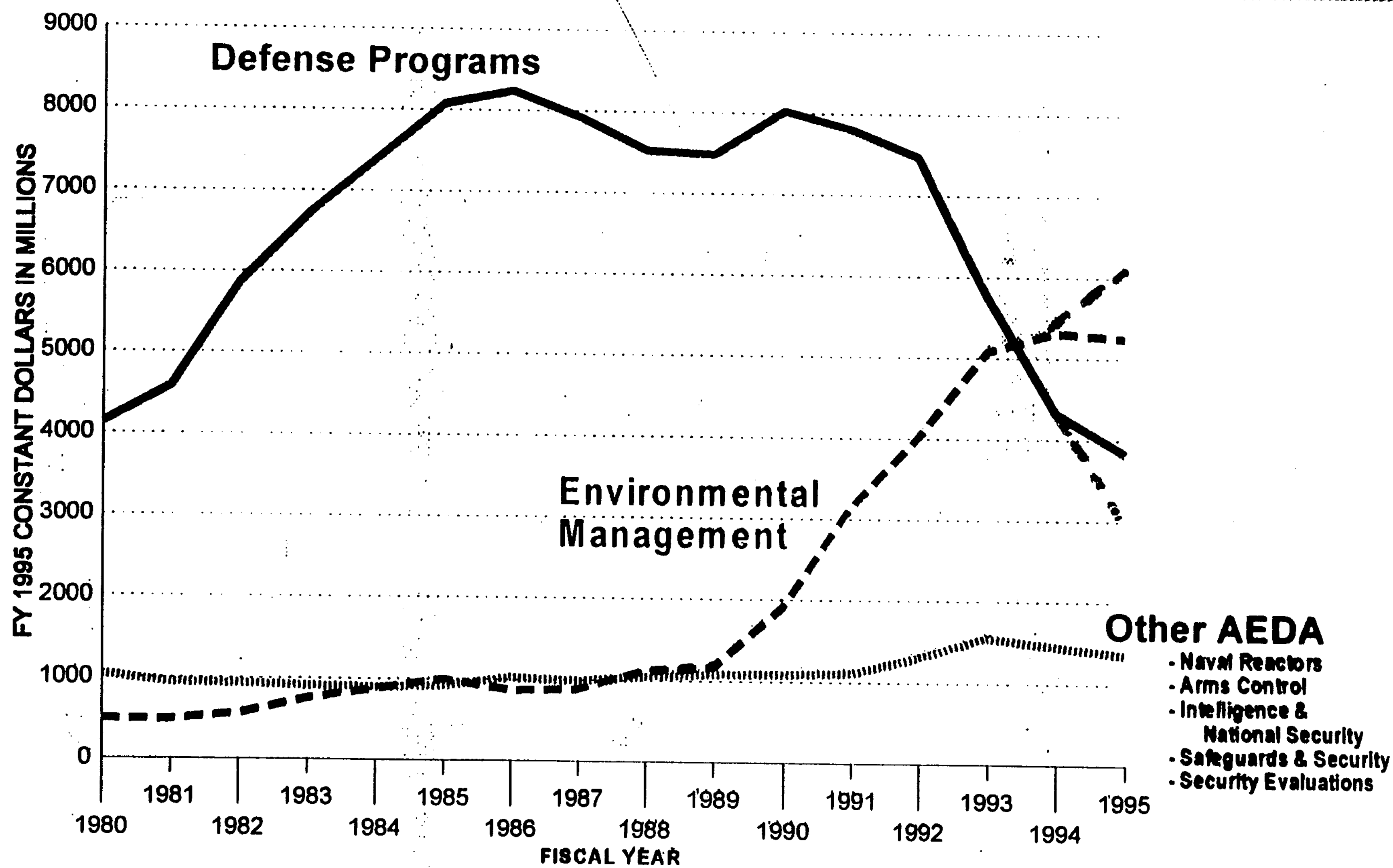
Dr. Victor Reis

Department of Energy, DOE

Dr. Andrew White

Los Alamos National Laboratory

HISTORY OF ATOMIC ENERGY DEFENSE ACTIVITIES FUNDING

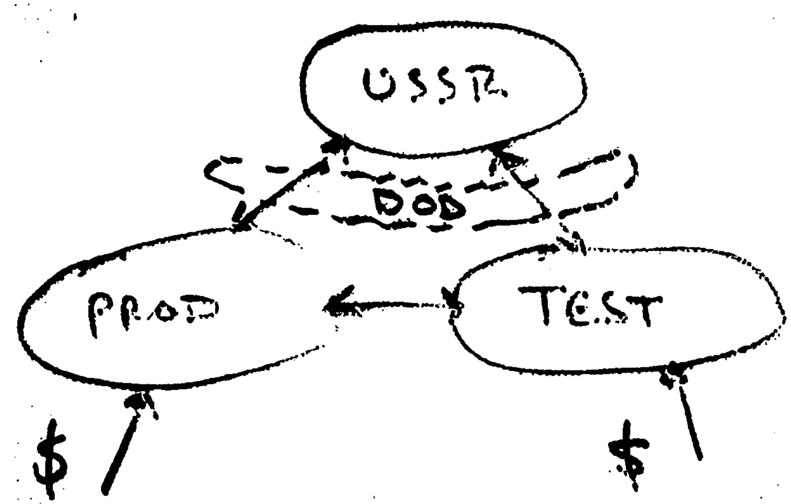


COLD WAR MODEL

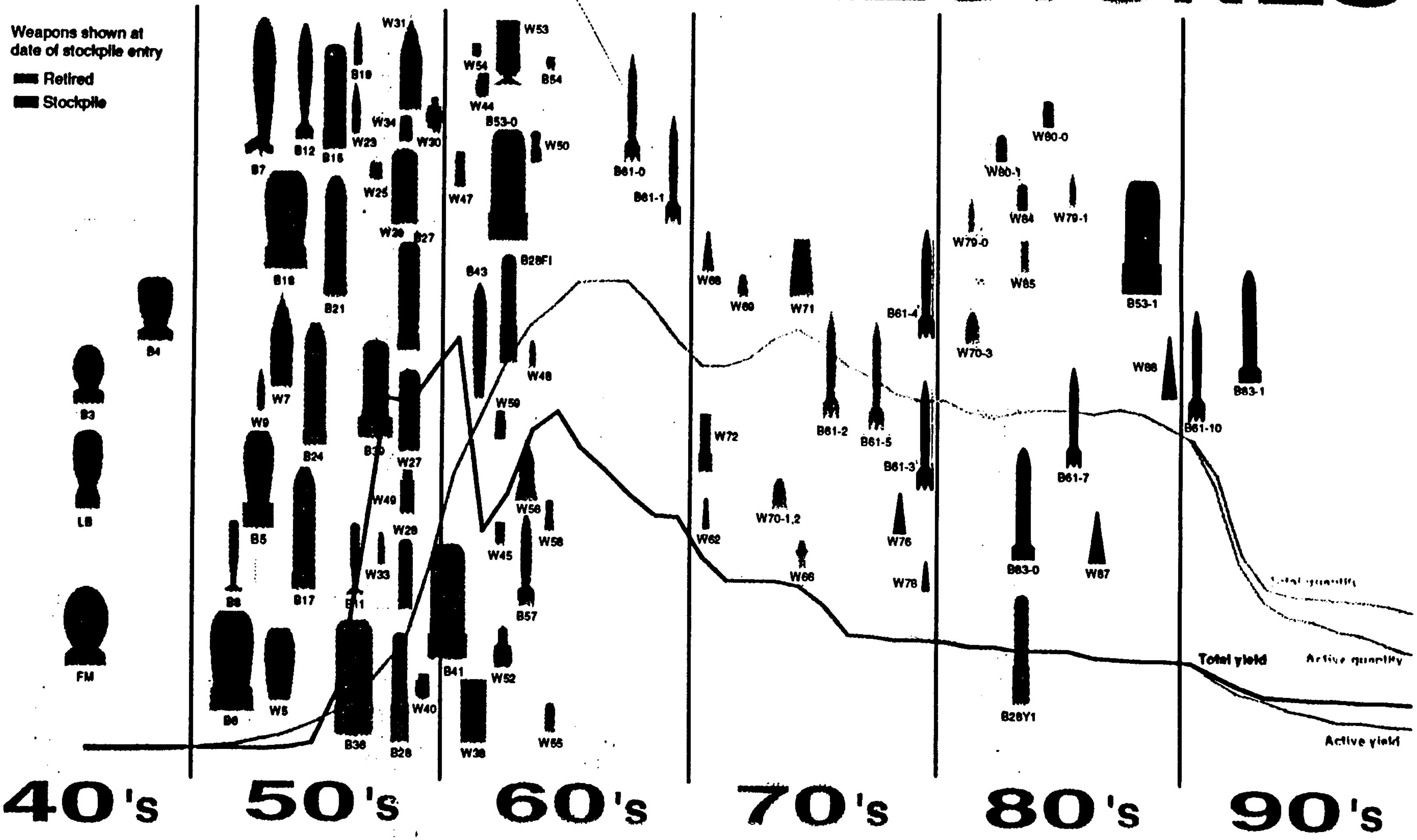
MISSION: DETER WAR WITH U.S.S.R.

PRODUCT: NUCLEAR WEAPONS (LOTS)

S&T CHALLENGE:
- YIELD/WEIGHT
- SURETY
- TYPES



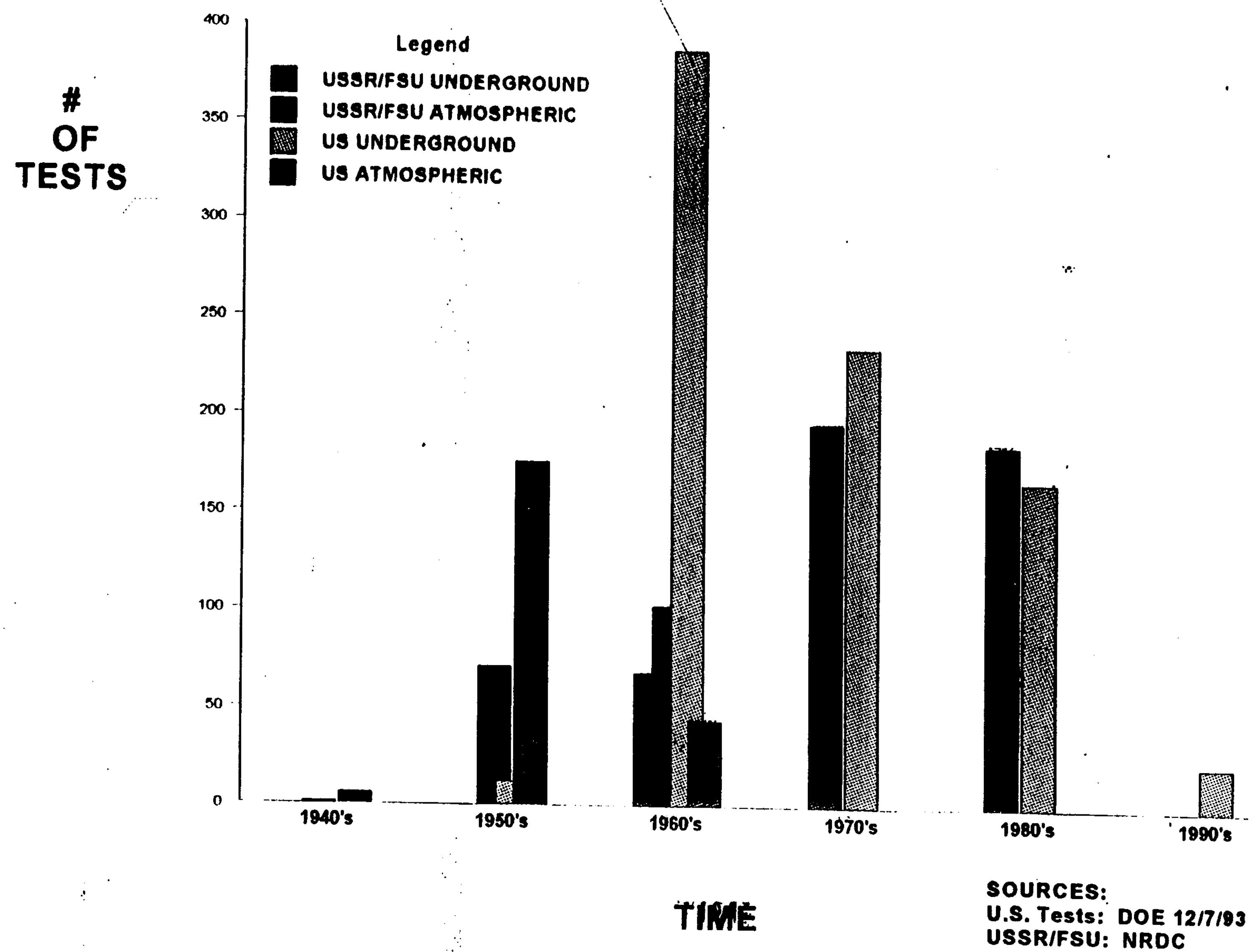
STOCKPILE MILESTONES



Sandia National Laboratories

12610:JB-QX-5/94

WORLDWIDE NUCLEAR WEAPON TESTING
(1945 - 1993)



NEW [illegible]

MISSION: REDUCE NUCLEAR DANGER

- DETER WAR
- SUPPORT ARMS CONTROL & NON-PROLIFERATION
- CLEAN UP & MATERIALS CONTROL

PRODUCT: (DEF. PROG.)

- SAFE, SECURE, RELIABLE WEAPONS
  - W/O TESTING
- RECONFIGURED (LOWER COST) COMPLEX
- DISMANTLED WEAPONS

RESUME TEST, PRODUCTION ⇓ SPRINGBACK

S&T CHALLENGE: NO TESTING

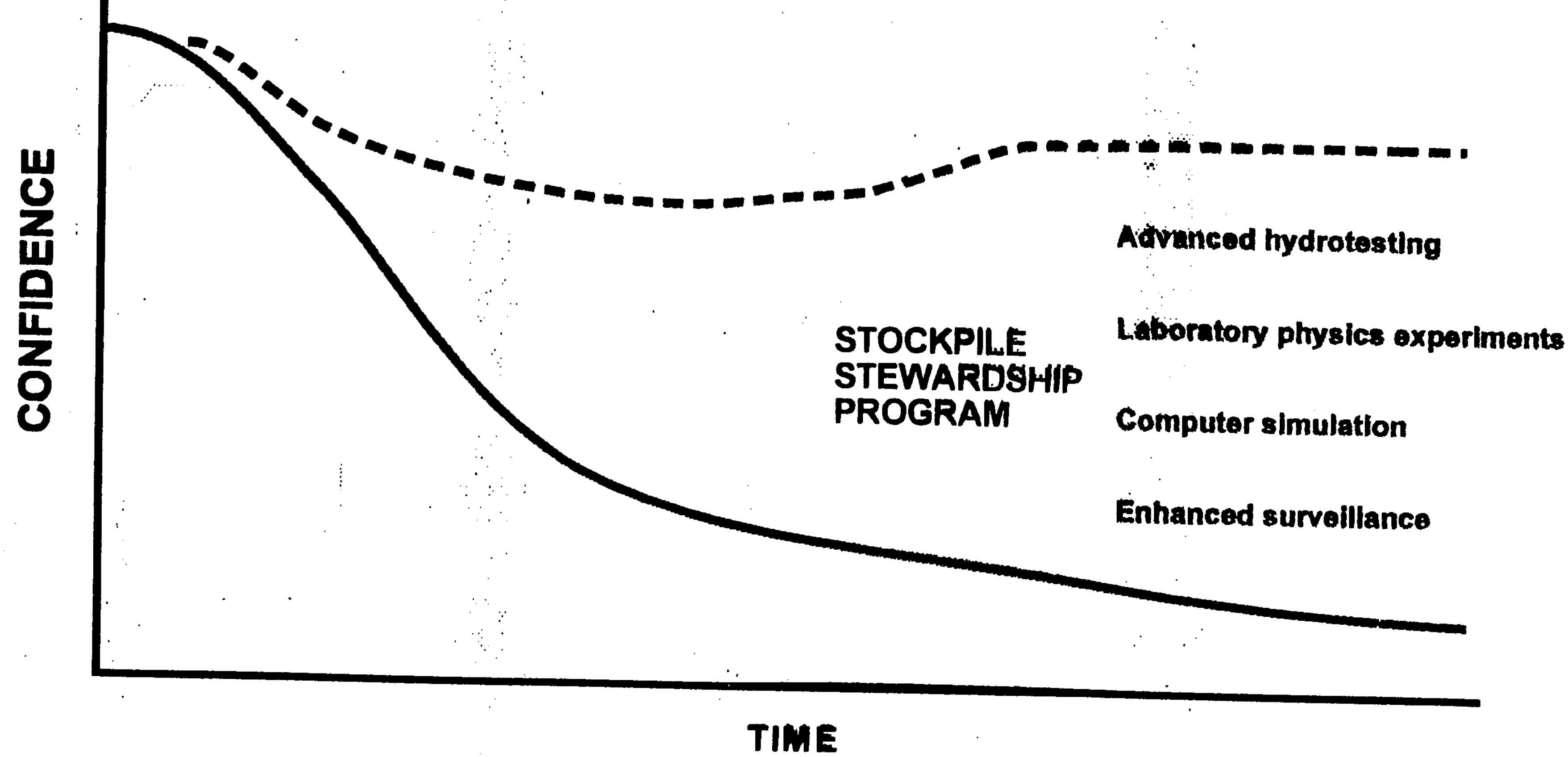
"NO" NEW DESIGN/PRODUCTION

⇒ SCIENCE BASED STOCKPILE STEWARDSHIP

⇒ ACCELERATOR PRODUCED TRITIUM

STOCKPILE STEWARDSHIP PROGRAM

The objective of the Plan for Stockpile Stewardship is to maintain a high level of confidence in the safety, reliability and performance of the U.S. nuclear weapons stockpile in the absence of nuclear testing.   President Clinton -- November 3, 1993



EFFECTIVELY IMPLEMENTED, A STOCKPILE STEWARDSHIP PROGRAM WILL MITIGATE THE LOSS OF CONFIDENCE

ACCELERATED STRATEGIC COMPUTING INITIATIVE

Andy White

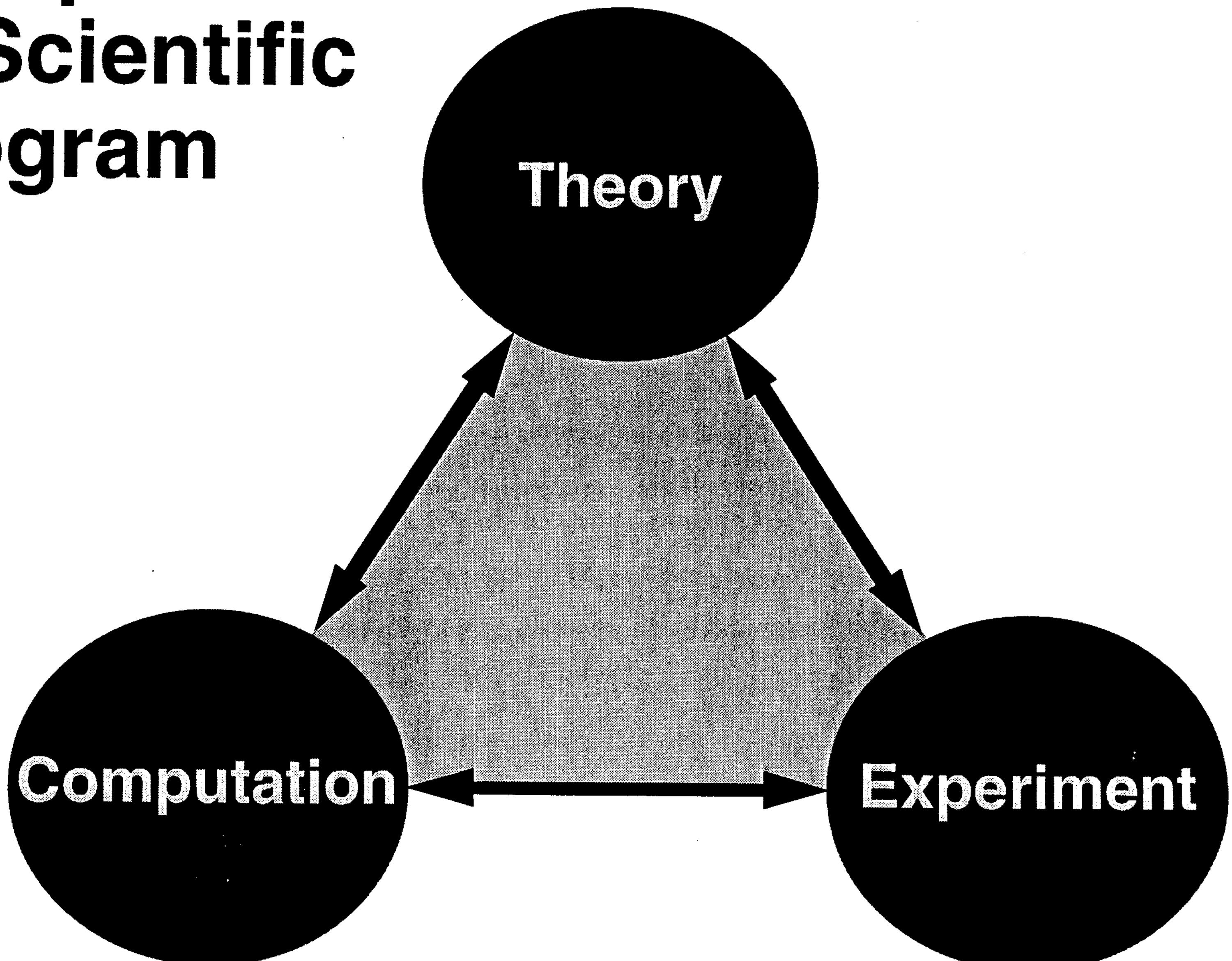
31 OCTOBER 1994

Accelerated Strategic Computing Initiative

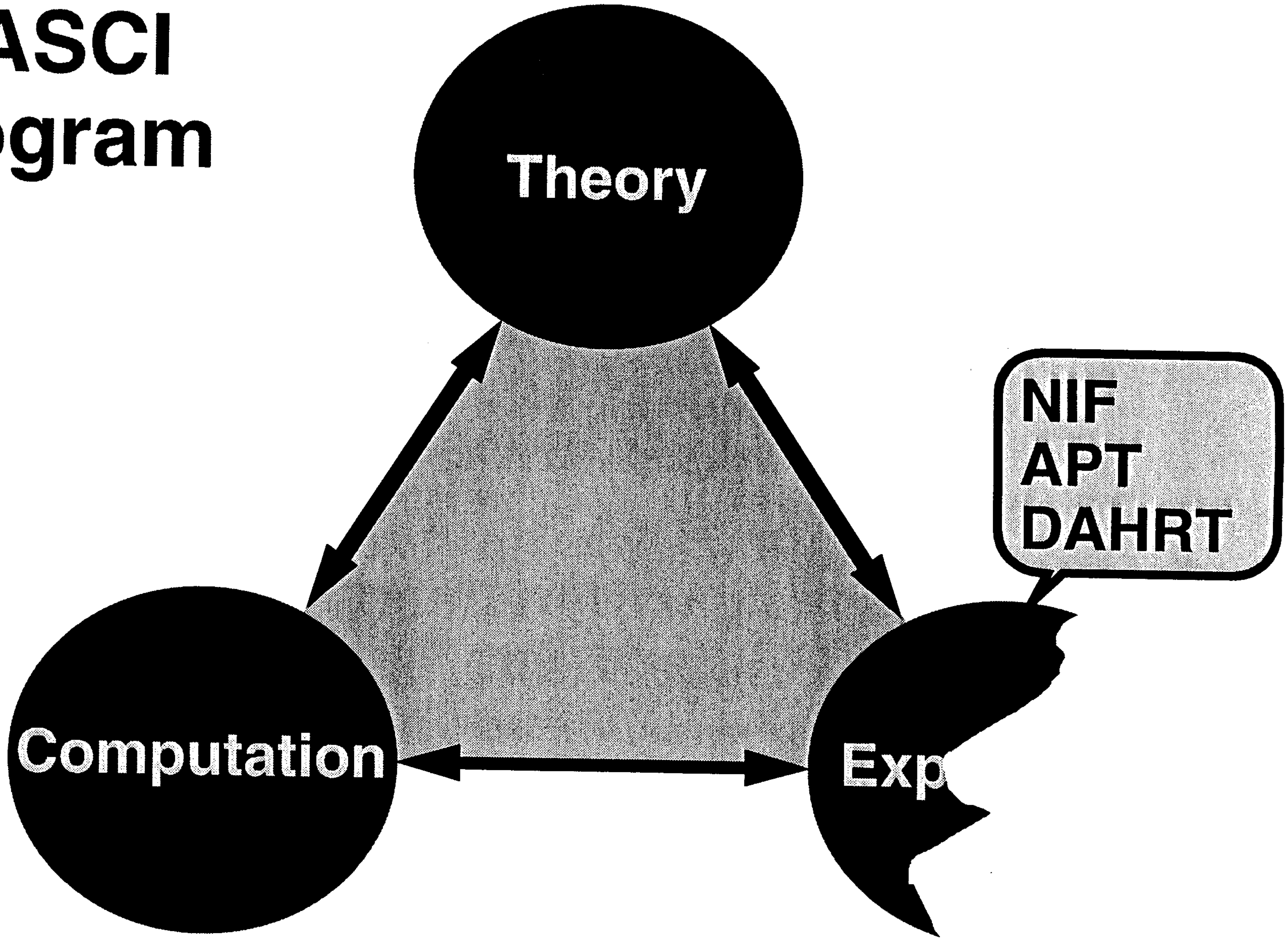
Grand Challenge: *Prediction of nuclear weapons performance* in a broad, unpredictable range of circumstances

Enabling technology: *High performance computing* is essential to the success of Science-based Stockpile Stewardship, particularly without weapons testing

Components of Scientific Program



Components of ASCI Program



1976

- DP is a primary driver for Computational Science and High Performance Computing
- Problems are critical to national security
- Integrated weapons tests provide validation for modeling and simulation
- DP has a major effect on the industry

1994

- DP is *not* a principal player in High Performance Computing program
- Problems are critical to national security, *but*
- *No* integrated weapons tests to provide validation for modeling and simulation
- DP can have a major effect on industry, *if*

Possible Problems are ...

Aging

- Cracks, corrosion, debonding
- Material degradation
- Critical system modifications
- Remanufacture of non-nuclear components

Safety

- Consequences of physical insults
- Abnormal environments
- Dismantlement
- Stolen weapons or terrorist scenarios

Physical Phenomena

- Three dimensional
- Multiple length scales
- Multiple time scales
- Structural deformation, heat transfer
- Chemical reactions, explosives
- Dynamic material response, hydrodynamics
- Shocks
- Radiation transport

But are these ...

Grand Challenges?

<u>Full-scale, 3d accident simulation</u>

- Space: 1 m^3
- Resolution: grain size
  (10^{12} grid points, 10 variables/grid point)
- Time: 1 sec @ $\Delta t = 10^{-5}$ sec

Raw requirements: no AMR, no ν physics, ...

- Memory: 160 terabytes
- Compute time @ petaflop: 28 hours
- Storage: 80 petabytes
- Data rate: 800 Gigabytes/sec

Grand Challenges?

Full-scale, 3d reliability simulation

- Space: 1000 cm^3
- Resolution: moving fronts
  (8×10^{12} grid points, 20 variables/grid point)
- Time: 10^{-4} sec @ $\Delta t = 10^{-9}$ sec

Raw requirements: no AMR, no ν physics, ...

- Memory: 2.5 petabytes
- Compute time @ petaflop: 44 hours
- Storage: 256 petabytes
- Data rate: 1.6 Terabytes/sec

Grand Challenges?

<u>Full-scale, 3d virtual prototype</u>

- Space:
- Resolution:

  ()

- Time:

Raw requirements: no AMR, no ν physics, ...

- Memory: 160 terabytes
- Compute time @ petaflop: 30 hours
- Storage: 160 petabytes
- Data rate: 800 Gigabytes/sec

Simulation Requirements

- Adaptive mesh refinement
- Domain decomposition
- Stable language, programming paradigm
- Scalable from workstations to MPPs
- More sophisticated materials models
- CAD-like setup capabilities
- Portability
- Flexible data structures
- 1d, 2d, 3d

Environmental Requirements

- CASE tools, GUI, CQA
- Data management, mining, and navigation
- Debugging
- Visualization and analysis
- Rapid, large-scale storage

- Collaborative environments
- Multi-media data capability

OK, but what about the marketplace?

Mainframes are the target for parallel computer vendors

ATM is the answer to all of our prayers

Biographical information is the focus of the data storage

Entertainment will provide visualization capabilities

Super¢omputing

"1993"	
Computer Industry	$233.0B
Hardware Industry	$114.0B
Supercomputers	$ 2.0B
High-end systems	$ 0.8B

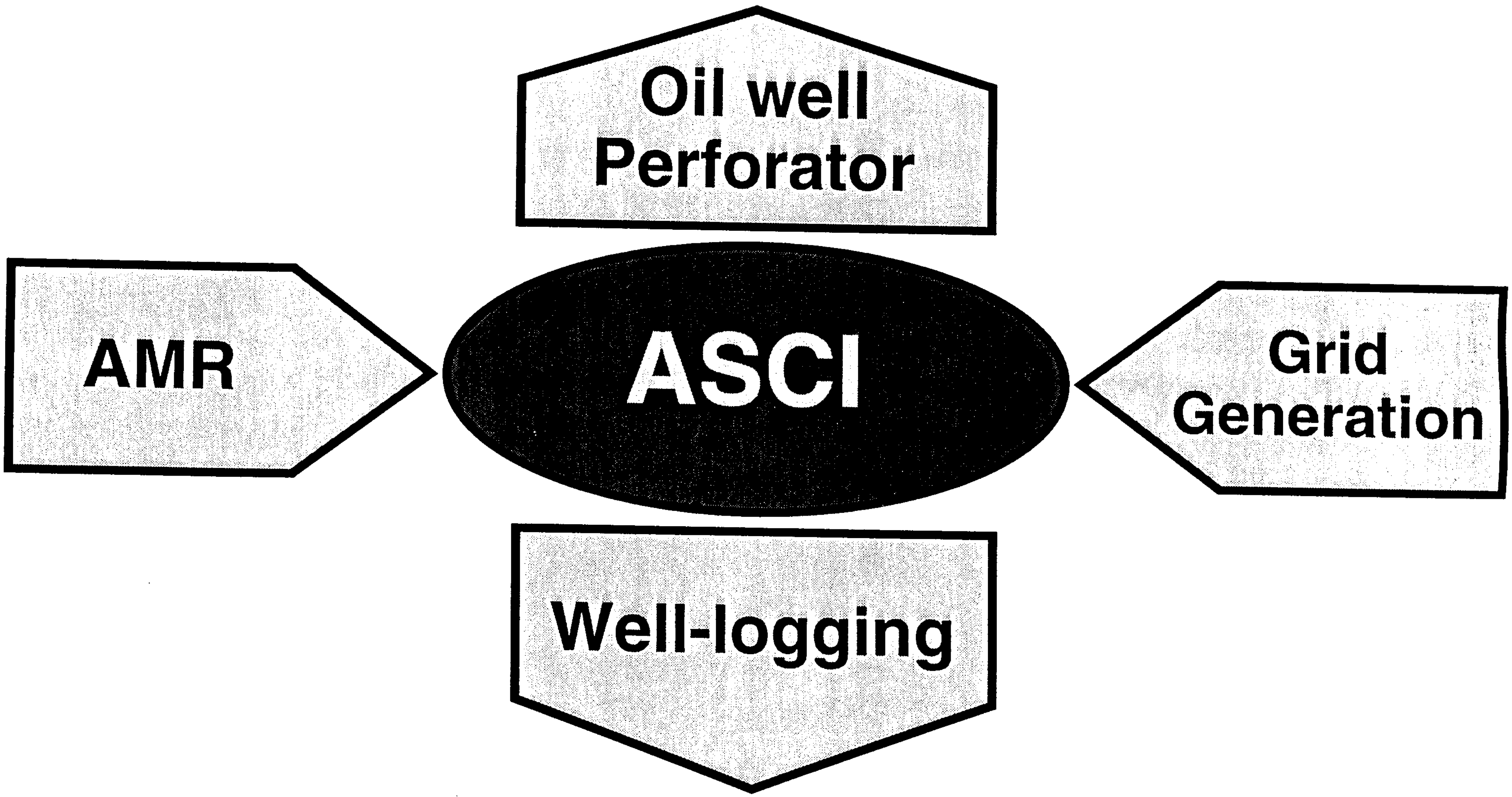
"1998"	
Supercomputers	$ 4.0B
High-end systems	$ 0.5B

TeraScale Machine*

- $\approx$ 2000 nodes
- $\approx$ 0.5 Gflop/node
- $\approx$ 512 Mbytes/node
- $\approx$ 500 Mbytes/sec/node
- $\approx$ 1996
- $\approx$ \$100M

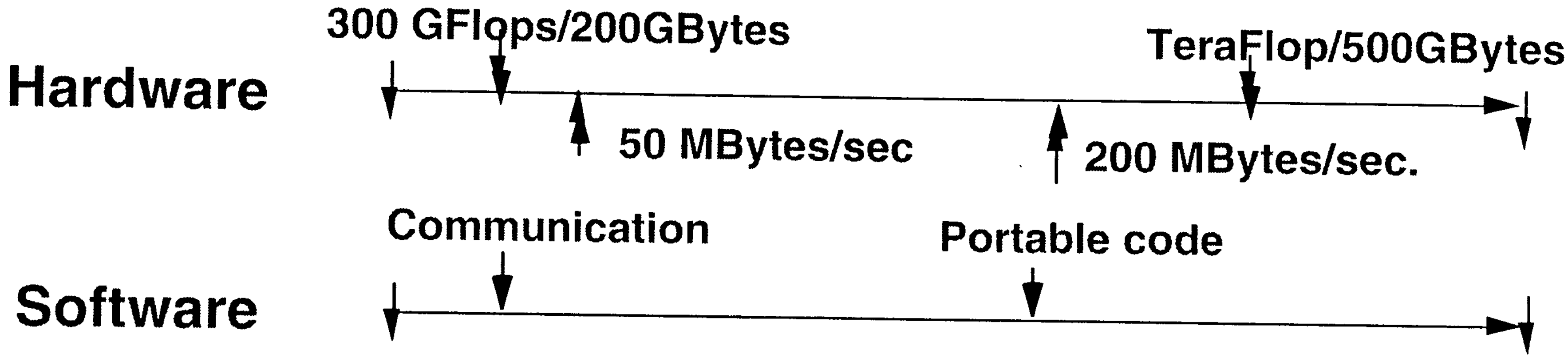
What we need is a ...

Community Effort



ASCI PROGRAM

- Investment in technology and industries



- 5 year strategic partnerships
- Hard technology delivery milestones for all partners (computers, storage, languages, operating systems, algorithms)
- All partnerships linked
- Several partners, selection criteria

1996 Program Outline

<u>Platforms: $24M-$27M</u>

- Multivendor collaborations-at least one large system
- $1.0M-$1.25M/month for each technology investment collaboration

<u>Applications: $15M-$12M</u>

- Three application areas
- $12M for prediction and weapons safety
- $1M-$3M for modeling the production complex

<u>Infrastructure: $6M</u>

- Network, and storage: $5M
- Security: $1M

Issues

- Can ASCI, spending $45M/year, significantly effect the industry?
- How much can one trust the unvalidated results of these simulations?
- How can ASCI take advantage of the community?
- How can ASCI accelerate the production of a petaflop machine by 2010?

Application of MPP to the Solution of Environmental Modeling Problems and Nuclear Test Ban Verification

James F. Lewkowicz

Phillips Laboratory, Hanscom AFB

Application of MPP to the Solution of Environmental Modeling Problems and Nuclear Test Ban Verification

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Geophysics Directorate
29 Randolph Road
Hanscom AFB Massachusetts 01731-3010

Our lack of understanding regarding a variety of important defense related problems in many cases stems from the inability to realistically model complicated geophysical processes that govern the problems. Two examples of such problems are understanding seismic wave radiation from underground nuclear explosions and modeling processes that control subsurface hazardous waste plumes. These areas address DoD high priority requirements in counter/nonproliferation (e.g., Comprehensive Test Ban Treaty monitoring) and the environmental remediation of hazardous waste sites at DoD installations, respectively. Research in environmental remediation also supports DoD counterproliferation efforts to identify and characterize underground structures. Additionally, these areas also have strong *dual use* applications in the oil exploration and engineering industries.

The application of supercomputers known as Massively Parallel Processors (MPP) to the solution of these important DoD problems will be crucial. In fact, the introduction of MPP technology has already made impacts in the solution of complex problems in geophysics, specifically in the solution of seismic wave propagation in complicated Earth models and the processing of ground-penetrating radar for the detection of hazardous wastes. Some of the details about the progress of these advances are discussed in this paper in addition to outlining the challenges that lie ahead.

1. INTRODUCTION

The use of computers has revolutionized the way scientific enquiries are made, and now calculations which were once considered untenable are simple exercises. The evolution of computer technology over the past 35 years has allowed a great expansion of the types of problems that can be solved, and computational turnaround routinely decreases by multiple factors each time a new generation of computers is produced. Computer microelectronics has progressed from the production of the first integrated circuit in 1959 to the manufacture of single, printed circuit computers which can carry out more than ten million instructions per second. This improvement in chip technology has reduced signaling time between components, since the distance between chips has decreased. It has also decreased the net cost per component, and this has led to the idea of putting multiple sequential computers together to greatly enhance net performance. In fact, there is now general agreement that the only way to achieve significant improvement in performance is through concurrent computation, whereby many computers/processors are used in tandem to solve the same problem. Massively Parallel Processor (MPP) technology is an example of this concept. MPP machines combine large numbers of processors (known as nodes) to carry out simultaneous actions on data sets. There are two types of MPP machines; SIMD (Single Instruction Multiple Data) machines simultaneously carry out the same program instructions on multiple nodes, each of which has only a small amount of resident memory. An example of this type of computer is the Connection Machine manufactured by Thinking Machines, Inc. In contrast, MIMD (Multiple Instruction Multiple Data) machines have larger memory storage per node, and thus each node can carry out a separate set of program instructions. Examples of this type of computer include the nCUBE and Cray T3D computers. From the programmer's viewpoint, making an algorithm work on a MIMD machine involves devising a way to decompose the problem into small segments to which an individual node can be assigned, with the results being collated at the end of each individual set of calculations.

2. APPLICATION OF MPP TO DEFENSE-RELATED RESEARCH

Nuclear Test Ban Treaty Verification

Much of our inability to understand the complicated behavior of geophysical phenomena is due to incomplete modeling of the underlying physical processes. Historically, important treaty verification research problems were focused on estimating the yield of relatively large explosions (~150 kilotons) in support of Threshold Test Ban Treaty (TTBT) monitoring. This work was primarily focused on test sites in the Former Soviet Union (FSU). However, with the decline of the FSU and the current negotiations in Geneva to negotiate a Comprehensive Test Ban Treaty (CTBT) an important research goal is to correctly model seismic wave propagation between relatively small nuclear weapons tests and receivers (seismometers) separated by regional distances (500-2000 km). Contrasted to the TTBT monitoring situation, where the US was primarily concerned with monitoring well known test sites, the CTBT monitoring situation is one in which a number of countries have become potential nuclear proliferators. This means that we must be able to understand seismic wave propagation in a variety of geologically diverse areas. Figure 1 depicts a simple picture of the monitoring problem. On the left are shown various seismic sources ranging from mine blasts to earthquakes that must be discriminated from nuclear weapons tests. The various seismic rays emanating from each of the sources are recorded by a seismometer at the Earth's surface. Also shown are simplified seismograms from each of the sources. The problem is to detect and subsequently identify correctly the seismic source associated with each seismogram.

To do this properly many factors must be taken into account, such as strong scattering effects in the shallow crust, source behavior, surface topography and velocity heterogeneities. One of the most widely applied numerical techniques used to solve the seismic wave propagation problem is the finite difference technique, which involves the solution of differential equations with specific boundary conditions over a spatial grid describing a portion of the Earth. This is a numerically intensive process, because to maintain accuracy in computing a time-dependent wavefield, small grid spacing and time steps must be taken. The use of MPP allows efficient solutions of finite difference problems through grid decomposition. The decomposition is done by dividing the spatial grid into segments, each of which are placed on individual nodes. The wavefield is then propagated on each segment of the grid for a single time step, and the results are communicated across nodes before moving on to the next time step. Using this type of parallelization, seismic wave propagation using finite difference techniques becomes feasible for large problems. For example, Figure 2 shows the superposition of a 2-D wavefield calculated using the finite difference method over a heterogeneous structure known as the Marmousi model. The expanding ring on the upper left hand corner of the model represents the spreading seismic wavefront propagating through the medium. The grid dimensions in this problem are 751x2501, and the complete wavefield was generated on 32 nCUBE nodes in approximately 13 minutes using 3000 time steps.

While 2-D techniques have been used in the past to provide significant insight into the physics governing seismic events, it is now possible to solve very large scale 3-D propagation problems. A 3-D wavefield propagation example is shown in Figure 3. The model is a two-layer graben, and the calculation was done on a 400x100x100 element grid. The run time on 64 nCUBE 2 processors was about 40 minutes for 2000 time steps. This type of 3-D modelling can be used in a variety of applications, including nuclear test ban verification, assessment of earthquake hazards, and the dual use technologies of petroleum exploration and civil and hydrological engineering. The ability to use the more realistic 3-D techniques in answering some of the important questions in these fields will add greatly to our understanding of the underlying physics.

Petroleum Exploration and Recovery

Some of the most computationally expensive problems in seismology occur in the petroleum exploration and recovery industries. Along with modelling the complex wavefields which are seen at sensors on the surface and in boreholes, the exploration seismologist is interested in using imaging and inversion techniques to determine the location and properties of subsurface reservoirs. Previously the imaging and inversion techniques were limited to small subsets of data over smaller regions of the Earth, but with the increasing use of MPPs in imaging, more power is available to produce realistic images of subsurface reservoirs. One of the most frequently used imaging techniques in exploration seismology is known as migration. It is primarily done to refocus events reflecting from subsurface horizons to their proper location in time and depth. There are many variations in migration algorithms, each of which has different mathematical approximations to make the calculations more manageable. For example, a 2-D pre-stack Kirchhoff migration code has been used to image the synthetic seismograms produced from the Marmousi model discussed in the previous section. This software can image the entire Marmousi data set (240 seismic sources and 96 receiver sensors) in four minutes. The results from this Kirchhoff imaging procedure are shown in Figure 4, which depicts the Marmousi model at the top of the figure and the imaging results at the bottom. This type of turnaround in computing the migrated image makes iterative imaging (where the velocity model is adjusted slightly and the imaging step is done to check the results) a viable prospect. This is an exciting application of MPP technology to the detection and recovery of petroleum reserves which previously was thought to be in the distant future. The speed and versatility of the MIMD architecture will allow even more powerful 2-D imaging and inversion techniques to be tested on observables, and even the use of 3-D algorithms in the foreseeable future.

Environmental Modeling

It is recognized that the DoD is facing an enormous expense to environmentally restore many, if not all, of its military installations. Estimates of this expense have been projected to be in the billion dollar(s) range. Geophysical modeling and simulation has the potential to save the DoD tremendous expense and there are several environmental problems which are of critical importance to the DoD that can be solved effectively using MPPs. For example, the subsurface migration of hazardous waste materials can lead to potential water table contamination. Ground-penetrating radar (GPR) is a technique used to image the shallow subsurface using high-frequency electromagnetic waves that reflect from subsurface contrasts in dielectric constant. By relating radar propagation velocities to subsurface water content through empirical relations, a potentially important indicator of contamination can be derived. Before a reasonable picture of the subsurface can be obtained, however, several data processing steps must be taken. These include a complicated stacking and enhancement of the GPR data to accurately resolve the positions of reflective contrasts in the subsurface. These steps are computationally intensive, and can be accomplished efficiently by processing algorithms resident on an MPP. As an example, Figure 5 shows a grayscale picture of GPR data acquired in the Chalk River test area in Canada prior to the data processing and imaging steps. There are very few coherent reflectors apparent in the subsurface beside the strong one dipping to the right between Common Midpoints (CMPs) 202 and 902. Figure 6 shows the effects of the processing. The region on the right changes dramatically, with many reflectors emerging from the stack, and the continuity of the reflections on the left is improved. Using the results from the radar propagation velocity processing, the subsurface water content can be estimated for the Chalk River area, as shown in Figure 7. The results show a zone of increasingly shallow high water content from left to right across the profile, which can be interpreted as an indication of a rising water table. Since this region of high water content cuts across the detailed reflection structure, it implies that water-filled porosity and permeability pathways are not constrained to apparent stratigraphic structure.

Another potential environmental application of MPP technology still at a basic research level is the simulation of seismoelectric wave propagation. When seismic waves propagate through a fluid-saturated sedimentary material, electrical current systems are set up in the material, which induce non-radiating fields. When the seismic waves impinge on a contrast in electrical and or mechanical properties, the current systems on both sides form a complex dynamic current system which generates electromagnetic waves. These waves are detectable at the surface of the Earth using dipole antennas. A schematic of this phenomenon is shown in Figure 8. It is possible by performing joint electromagnetic and seismic surveys over shallow crustal areas, a more useful estimate of subsurface properties may be determined. This might lead to powerful indicators of environmental contamination, since the experiment would provide estimates of both the mechanical, fluid and electromagnetic properties underneath the survey area. Examples of the fields generated from an electroseismic survey are shown in Figures 9 and 10. The model in Figure 10 is that of a typical road fill material superposed on top of a glacial sedimentary sequence. The electromagnetic and seismic wavefields are calculated using an MPP to solve the complicated coupled set of equations which describes the seismoelectric phenomena. Figure 10 shows the modeled electrical and seismic wavefields, as well as the difference in electromagnetic signal as a function of the depth of road fill. Without the use of an MPP to calculate the wavefields, the computational expense of testing this potentially powerful technique would be exhorbitant.

Characterization of Underground Structures

The same geophysical modeling techniques that are described above in the section on environmental modeling are directly applicable to the problem of detecting and characterizing underground structures. The importance of this work was highlighted in the the Iraq conflict. For pre-strike targeting purposes, pilots need to know the exact location of underground targets, in addition to characterizing the physical properties of the structure and geology in which the structure has been embedded. In a post-strike mode, additional information, based on geophysical observations and modeling can be useful to discern the level of damage assessment.

3. MPP LIMITATIONS

There are two current limitations on the use of MPP in defense-related geophysical research are in both the hardware and software areas. The hardware limitations include CPU limits on modeling, imaging and inversion algorithms, memory bounds on large modeling problems, and input/output bounds on out-of-core imaging efforts. The software limitations involve input/output functionality (e.g., asynchronous I/O), code portability, code sharing by programmers over communication networks such as the Internet, and programmer training to increase the number of MPP-literate computational scientists.

While software advances have been steady, they have been eclipsed by advances in hardware. What is needed at this time, are efforts to support software development and the training of scientists to utilize MPP in order to exploit fully their potential to solve both DoD and civilian problems.

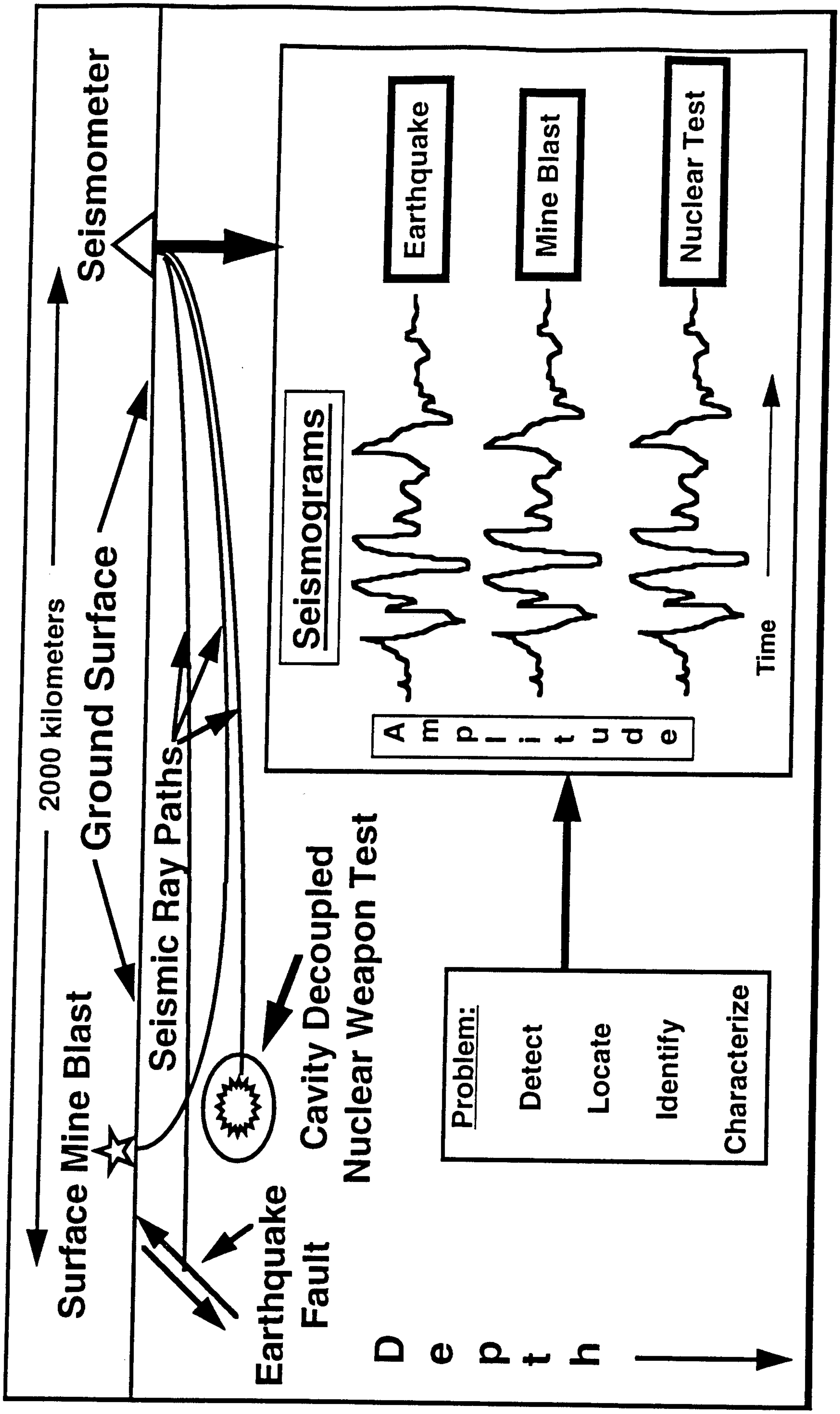
4. CONCLUSIONS AND SUGGESTIONS

As a DoD program manager, with responsibility for contract research programs in both CTBT monitoring and environmental areas, I am most interested in the *application of MPP to the solution of relevant DoD problems*. MPP have the extraordinary potential to provide DoD with the insight and knowledge necessary to solve our most longstanding and difficult problems. However, I am very concerned with the apparent lack of availability of MPP for the general scientific community and specifically the university community. I believe the foundation for advancements in the application of MPP to important DoD and civilian problems will come, in large part, from the young scientists currently being trained in our universities. Therefore, I believe the DoD community should make strenuous efforts to ensure MPP are readily available and the software limitations mentioned above will, through the midnight oil of PhD dissertations, in large part disappear.

One efficient and cost effective way to achieve this goal is for DoD to foster and support partnerships between industry and academia. While there may be many ongoing partnerships, one that I am aware of is between the Massachusetts Institute of Technology (MIT) and nCUBE. nCUBE has placed an MPP at MIT's Earth Resources Laboratory (ERL) and is cost sharing the operation of this computer with ERL. ERL in turn has made this MPP available to a wide audience of students and other users, including providing much needed training on how to utilize the potential of MPP. Everyone, including the DoD, benefits by such partnerships.

5. ACKNOWLEDGEMENTS

All of the calculations discussed in this paper were performed on an nCUBE 2 MPP located at the Massachusetts Institute of Technology's Earth, Atmospheric and Planetary Sciences' Earth Resource Laboratory (ERL). I am indebted to Professor M. Nafi Toksöz, Director of ERL, and his staff, particularly Drs. Delaine Reiter and Joseph Matarese, for many helpful discussions regarding MPP and providing the results of their calculations for inclusion in this paper.



Surface Mine Blast
2000 kilometers
Seismometer
Ground Surface
Seismic Ray Paths
Earthquake Fault
Cavity Decoupled Nuclear Weapon Test
Depth
Problem:
Detect
Locate
Identify
Characterize
Seismograms
Amplitude
Time
Earthquake
Mine Blast
Nuclear Test

Figure 1

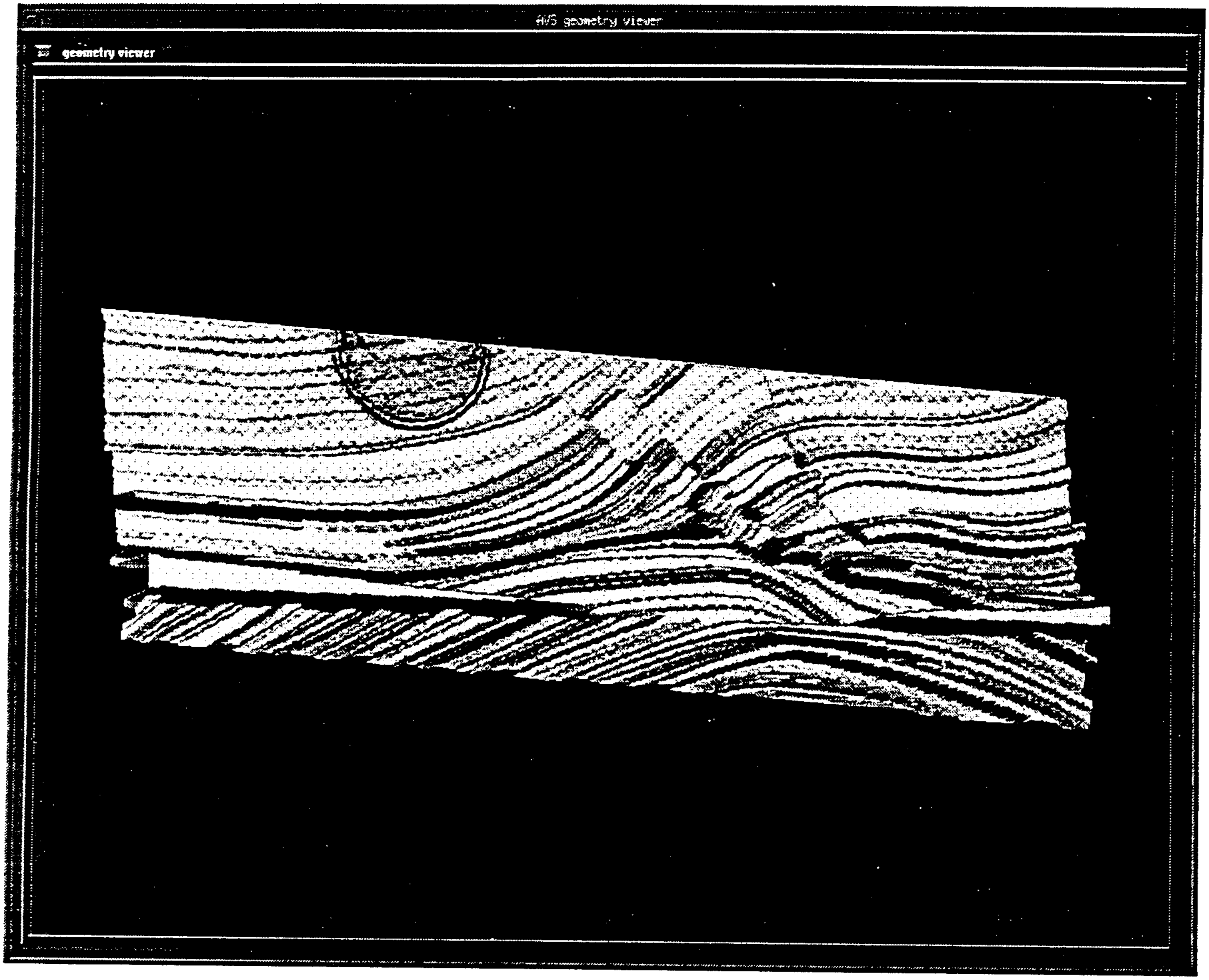


Figure 2

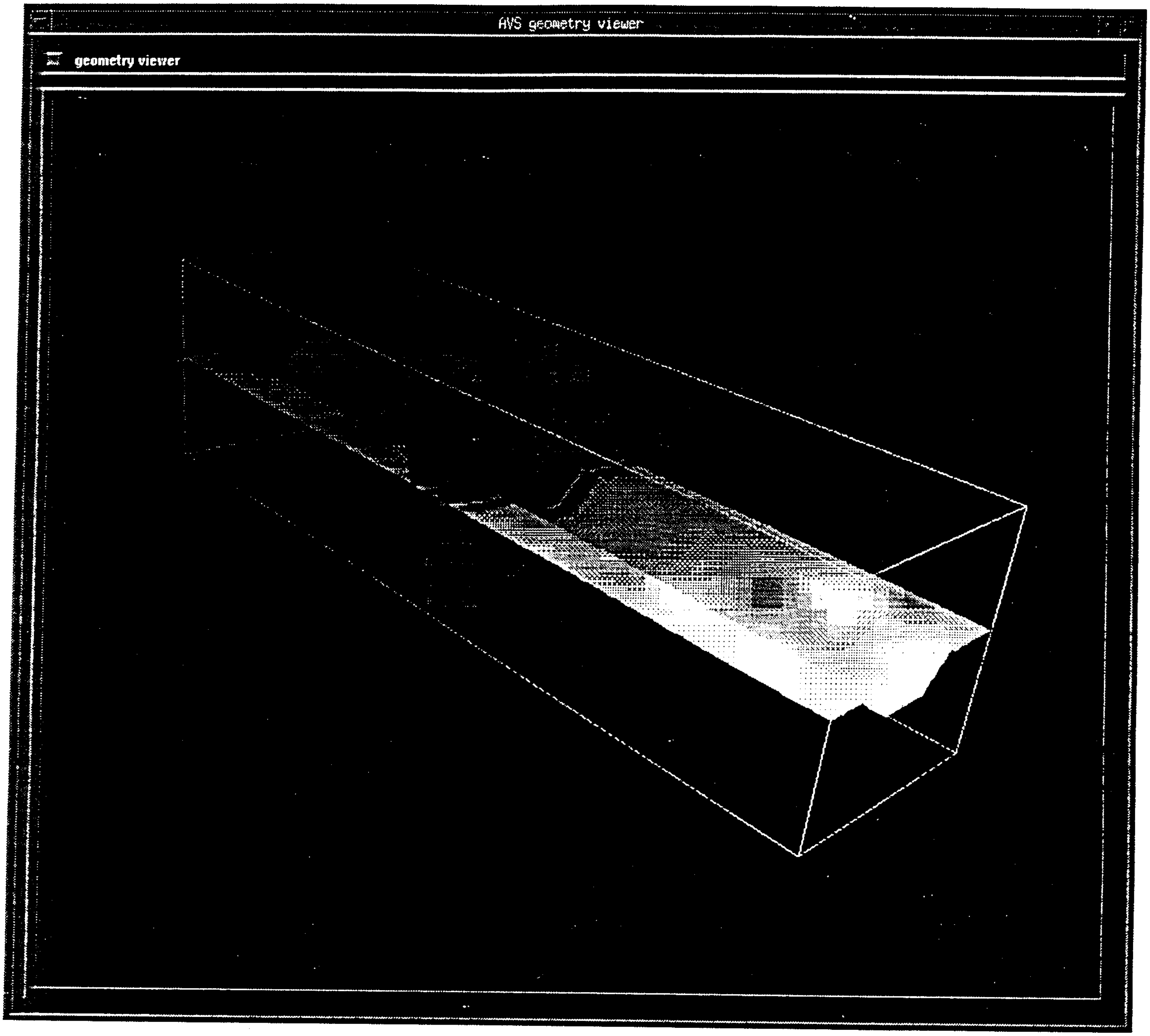


Figure 3

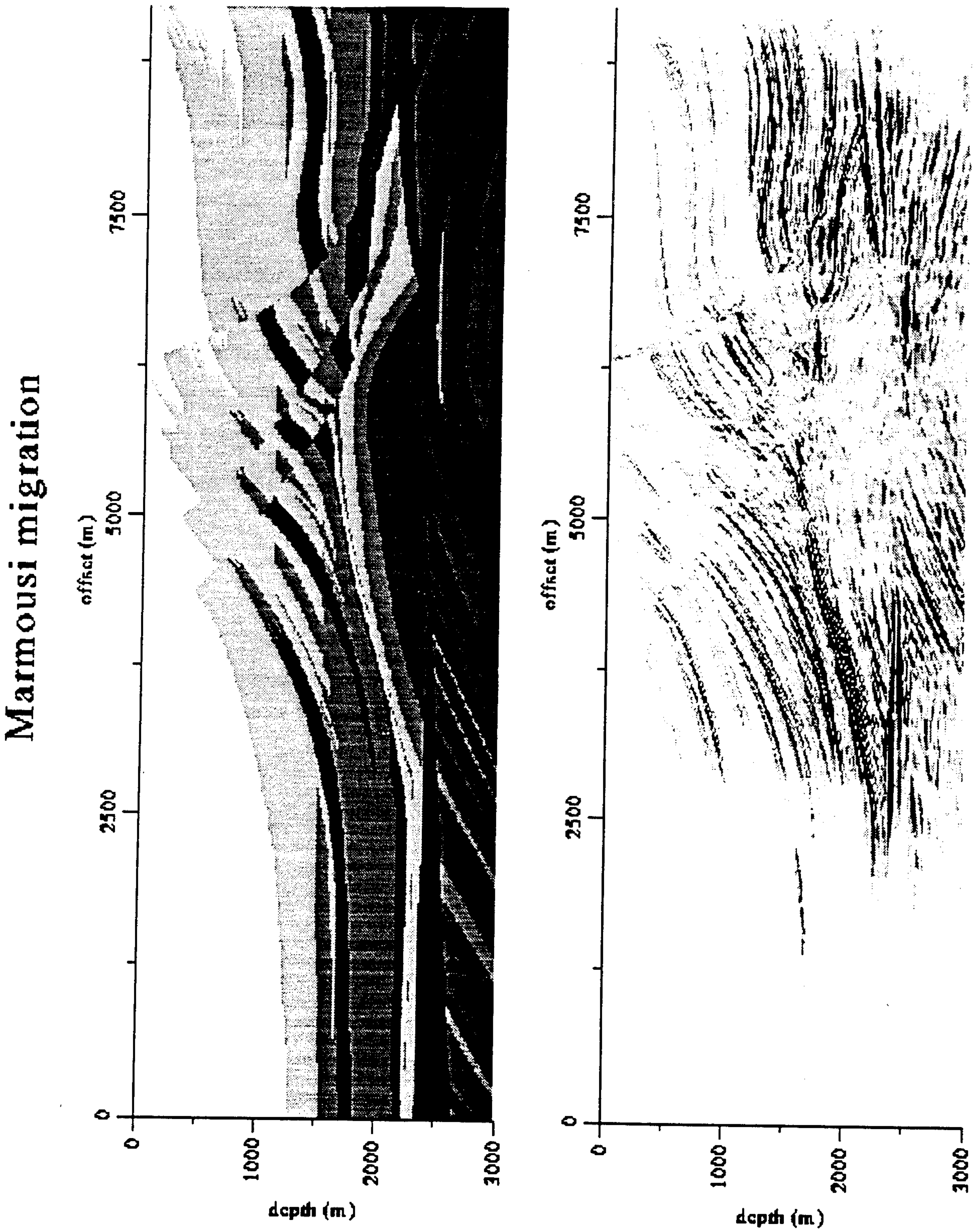

Marmousi migration
offset (m)
depth (m)
0
2500
5000
7500
0
1000
2000
3000
offset (m)
depth (m)
0
2500
5000
7500
0
1000
2000
3000

Figure 4

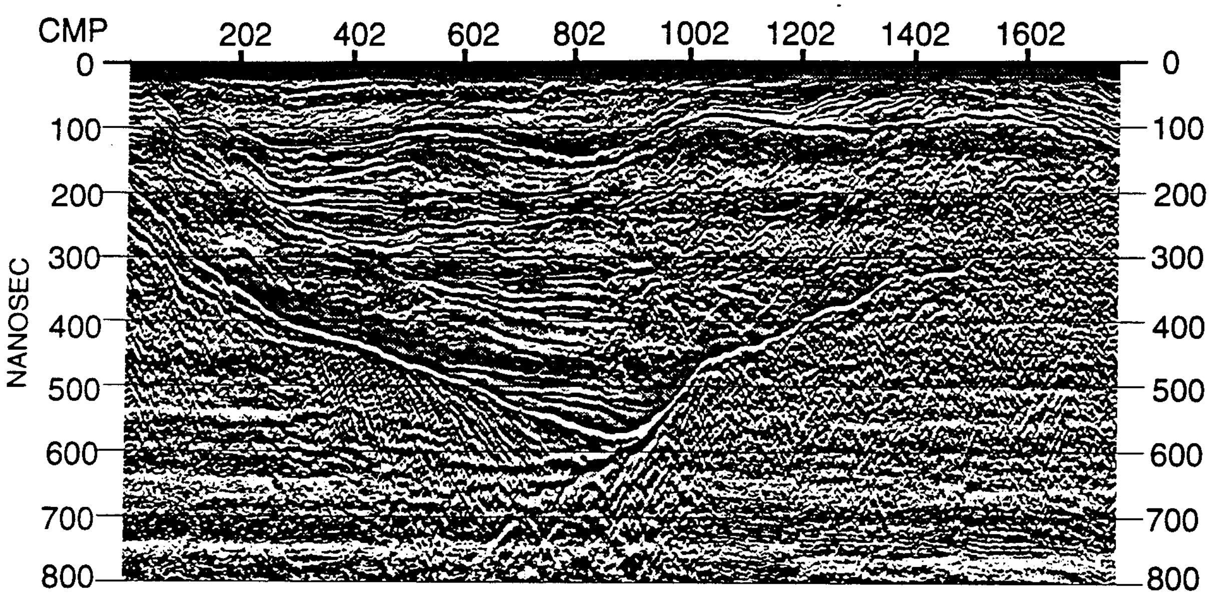
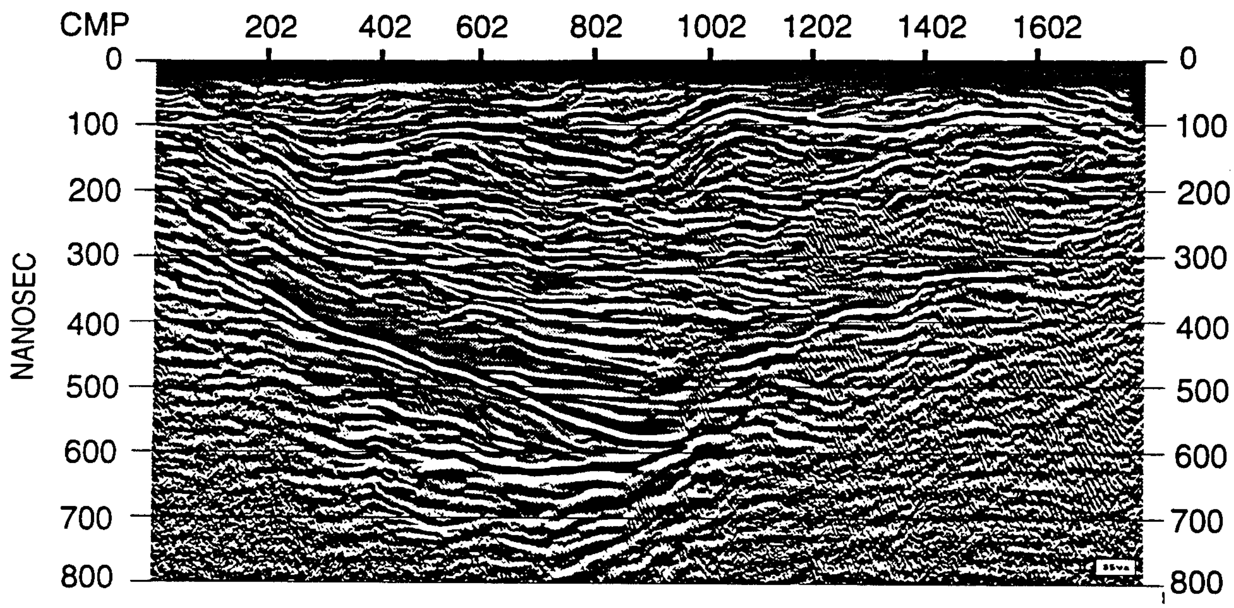
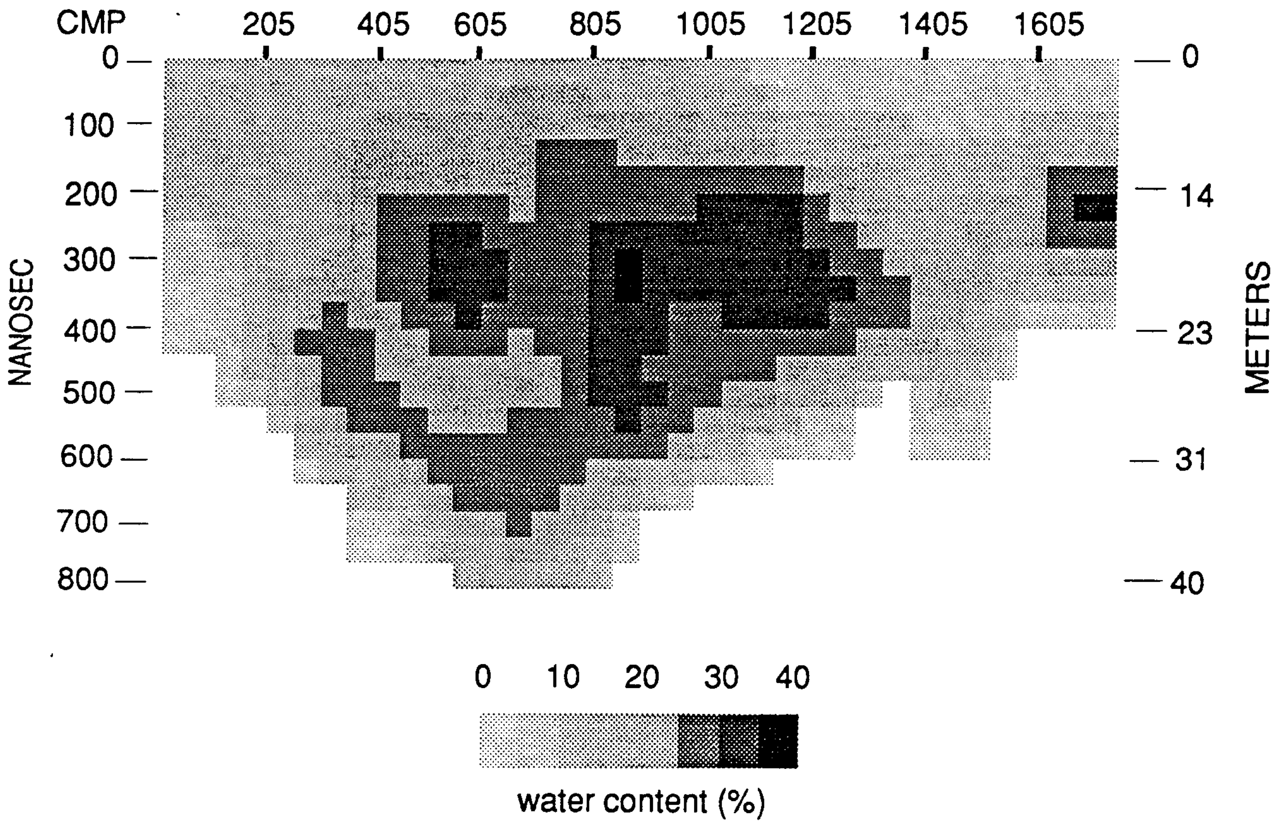

CMP
202
402
602
802
1002
1202
1402
1602
NANOSEC
0
100
200
300
400
500
600
700
800

Figure 5



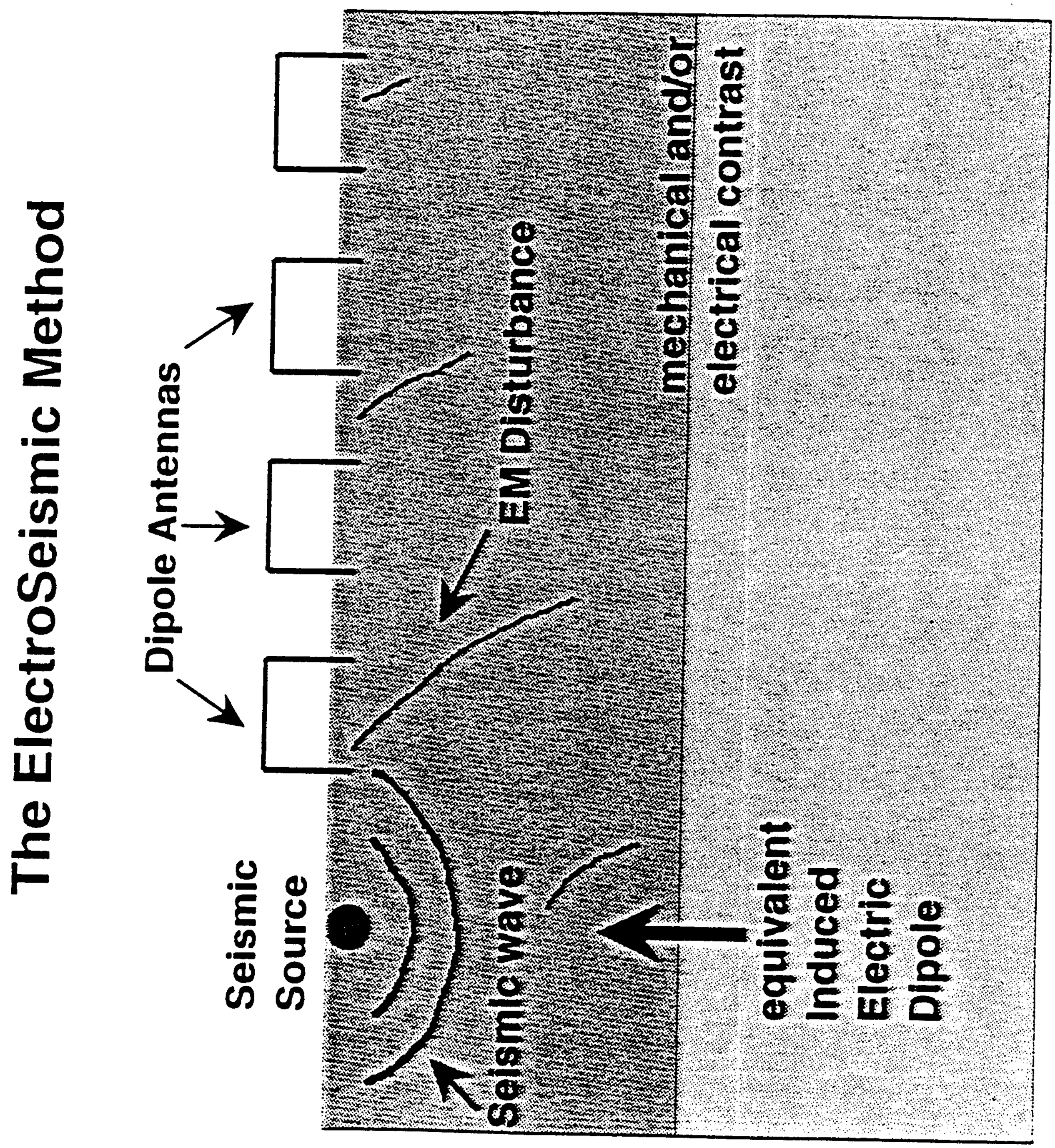
CMP
202
402
602
802
1002
1202
1402
1602
NANOSEC
0
100
200
300
400
500
600
700
800

Figure 6



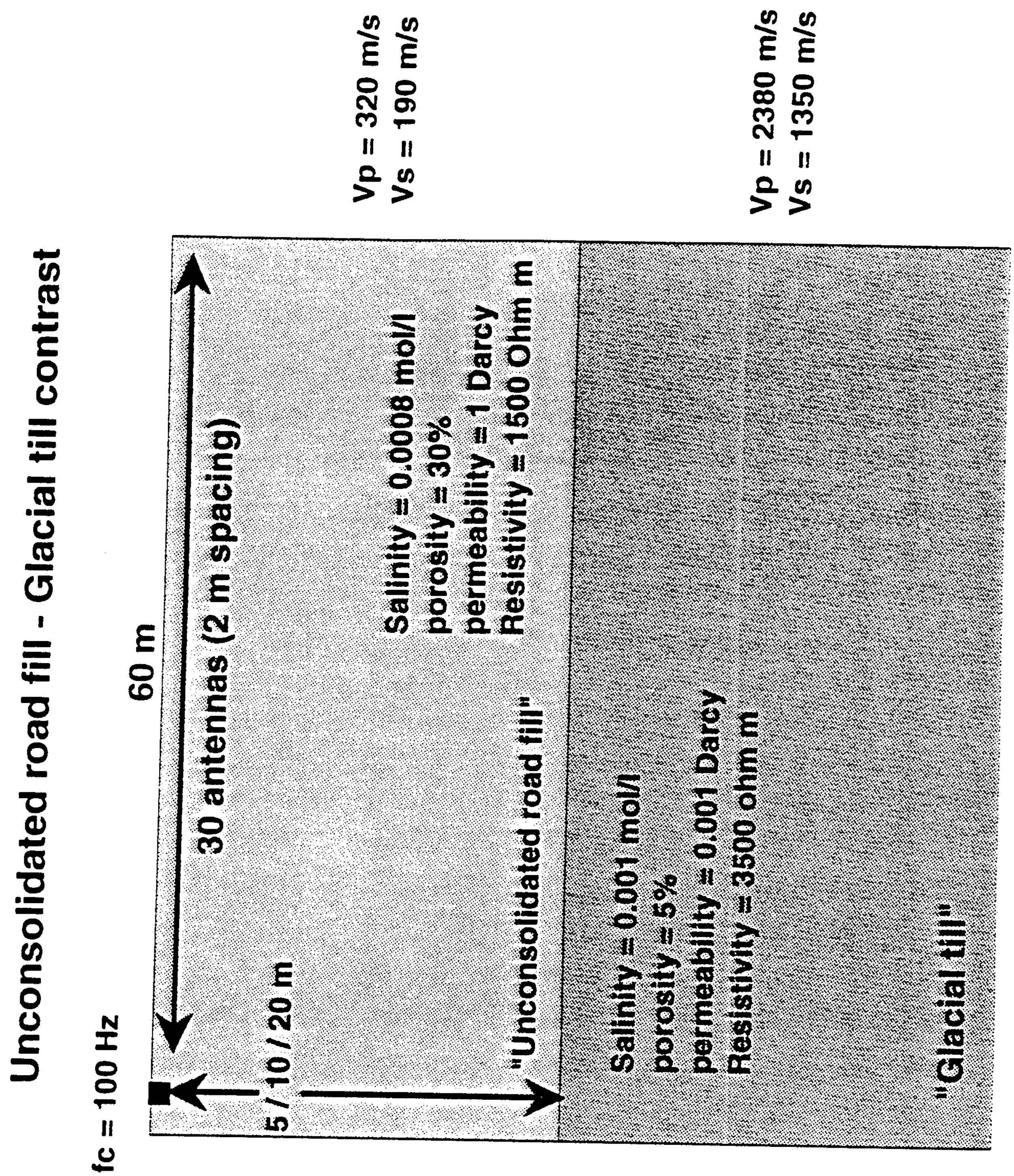
CMP
205
405
605
805
1005
1205
1405
1605
0
100
200
300
400
500
600
700
800
NANOSEC
0
14
23
31
40
METERS
0
10
20
30
40
water content (%)

Figure 7



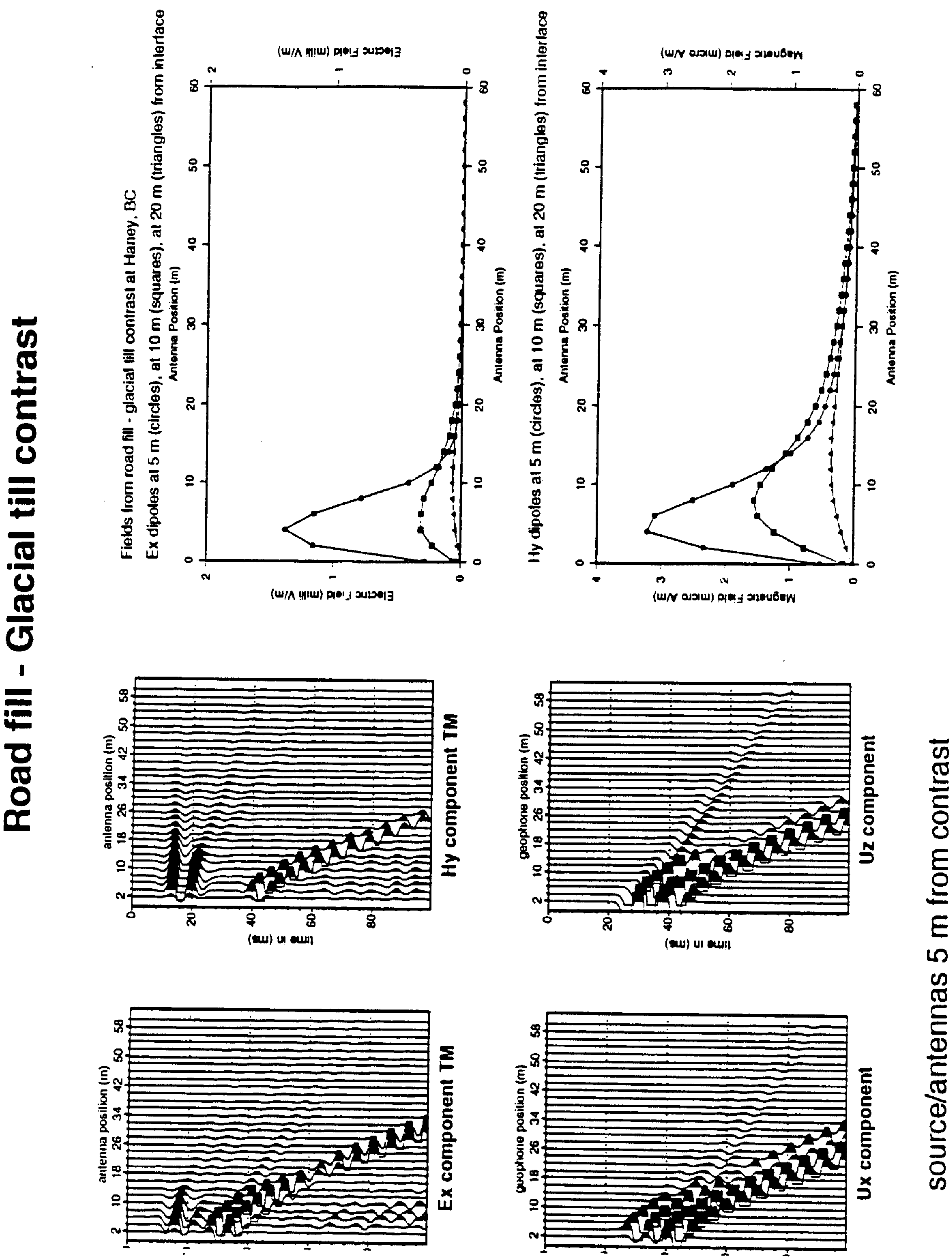
The ElectroSeismic Method
Dipole Antennas
Seismic Source
EM Disturbance
mechanical and/or electrical contrast
Seismic wave
equivalent Induced Electric Dipole

Figure 8



Unconsolidated road fill - Glacial till contrast
fc = 100 Hz
60 m
30 antennas (2 m spacing)
5 / 10 / 20 m
Vp = 320 m/s
Vs = 190 m/s
Salinity = 0.0008 mol/l
porosity = 30%
permeability = 1 Darcy
Resistivity = 1500 Ohm m
"Unconsolidated road fill"
Vp = 2380 m/s
Vs = 1350 m/s
Salinity = 0.001 mol/l
porosity = 5%
permeability = 0.001 Darcy
Resistivity = 3500 ohm m
"Glacial till"

Figure 9



Road fill - Glacial till contrast
Fields from road fill - glacial till contrast at Haney, BC
Ex dipoles at 5 m (circles), at 10 m (squares), at 20 m (triangles) from interface
Hy dipoles at 5 m (circles), at 10 m (squares), at 20 m (triangles) from interface
Antenna Position (m)
Electric Field (milli V/m)
Magnetic Field (micro A/m)
antenna position (m)
geophone position (m)
time in (ms)
Ex component TM
Hy component TM
Ux component
Uz component
source/antennas 5 m from contrast

Figure 10

Multidimensional Hydrodynamics as a Tool in Nuclear Test Ban Verification

Professor Frederick K. Lamb

University of Illinois at Urbana-Champaign

MULTIDIMENSIONAL HYDRODYNAMICS

—UIUC

As a Tool in Nuclear Test Ban Verification

Frederick K. Lamb

Departments of Physics and Astronomy
Program in Arms Control, Disarmament, and International Security

University of Illinois at Urbana-Champaign

DSSG Alumni Symposium

Institute for Defense Analyses
October–November 1994

Research supported in part by ARPA

FKL 10/94

MULTIDIMENSIONAL HYDRODYNAMICS

— *UIUC*

As a Tool in Nuclear Test Ban Verification

- ❑ Background
- ❑ Shock wave methods
- ❑ Simulated explosions
- ❑ Yield estimates
- ❑ Concluding remarks

FKL 10/94

TEST BAN VERIFICATION

UIUC

Background

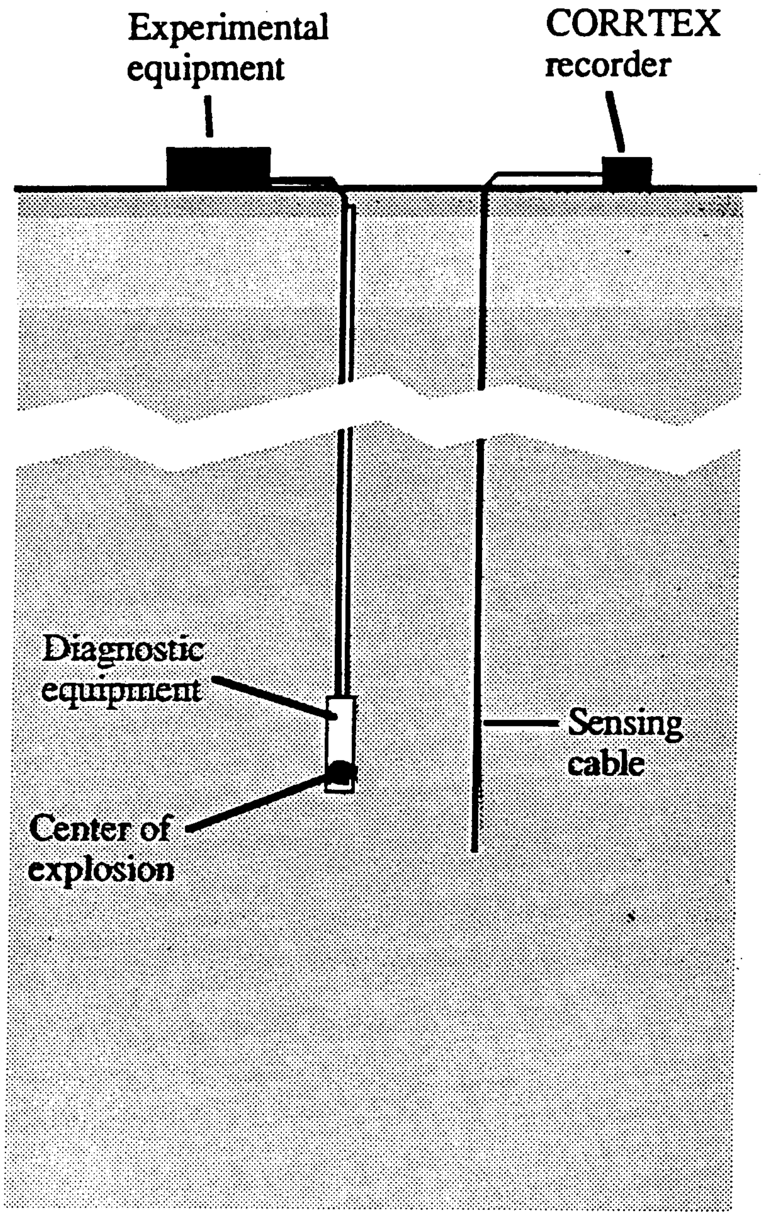
- Hydrodynamic yield estimation methods originally developed for testing program
- When PNET was negotiated in 1974, HYE was incorporated as a verification tool
- In mid-80's, Reagan administration insisted on HYE & CORRTEX sensors for TTBT
  - Unhappy with seismic methods
  - Wanted to signal a higher verification std
  - Wanted to focus attention on past treaties to forestall movement toward a CTBT
- Use of HYE for verification is very different from use in a weapon testing program
- HYE sensors & methods are highly classified
- In 1986, strengths & weaknesses of HYE as a verification tool were poorly known
- I became involved in 1986 due to a request from DARPA's NMRO to the DSSG

FKL 10/94

SHOCK WAVE METHODS

-UIUC

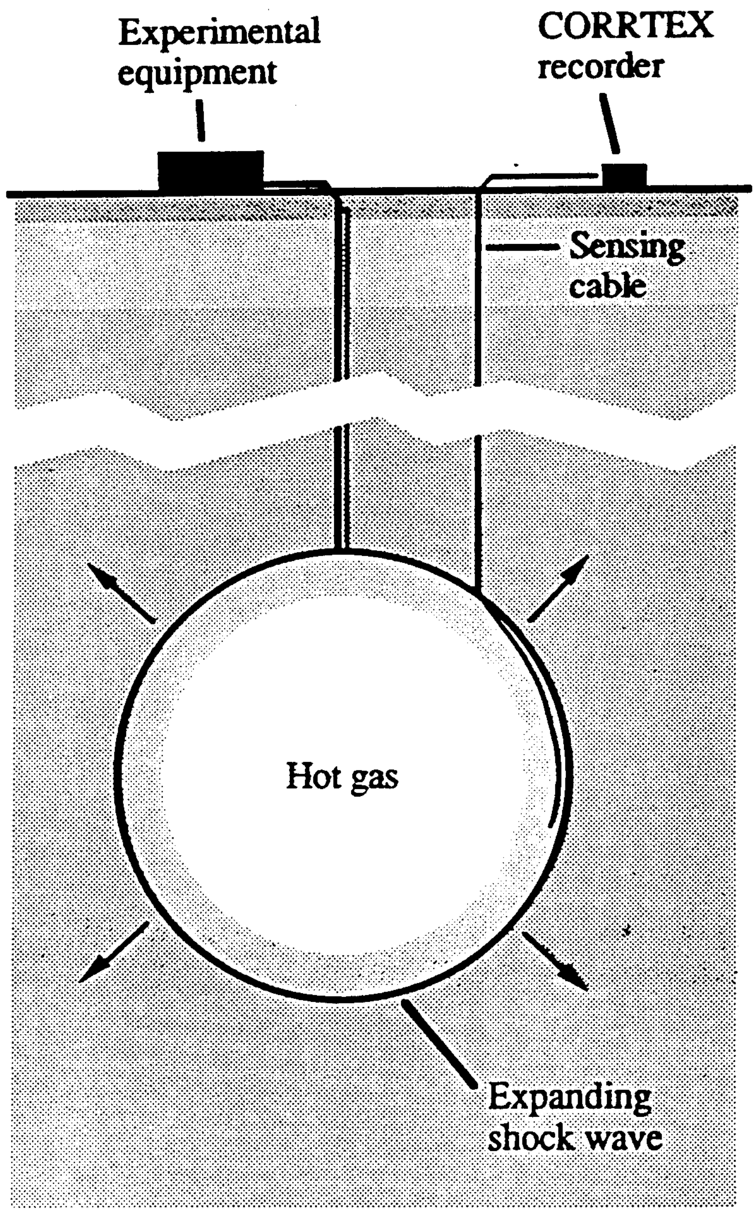
Before Explosion



SHOCK WAVE METHODS

– UIUC

After Explosion



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SHOCK WAVE METHODS

UIUC

Yield Estimation Algorithms

Components

- Model of the motion of the shock front that depends on the yield
- A procedure for fitting the shock-front position predicted by the model to the data

Examples

- ° Power-law model*
- ° Analytical model*
- Similar explosion scaling*
- Simulated explosion scaling*
- Suite of numerical simulations

*Assumes cube-root scaling

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SHOCK WAVE METHODS

UIUC

Cube-Root Scaling

Requirements

- Explosions are spherically symmetric
- Explosion sources all have same e.o.s.
- M, R, P of the sources scale with W
- Ambient media are identical and uniform, can be treated as fluids
- Heat transpot and viscous enegy dissipation behind the shock front are negligible

Scaling

$$R(t;W) = [W/W_{ref}]^{1/3}\ g(t\ [W_{ref}/W]^{1/3})$$

where g(x) describes the evolution in time of an explosion with yield W_{ref}

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SHOCK WAVE EVOLUTION

UIUC

Potential Complications

Complications caused by the source

- Canisters are meters in diameter
- Source shape is aspherical
- Hence shock R vs. t depends on the source

Complications in a uniform medium

- Motion is affected by phase transitions
- Motion is affected by rock strength
- Shock splits into two-wave structure

Complications due to inhomogeneities

- Complex energy flows in pipes/tunnels
- Distortion of shock wave by layers
- Distortion of shock wave by voids

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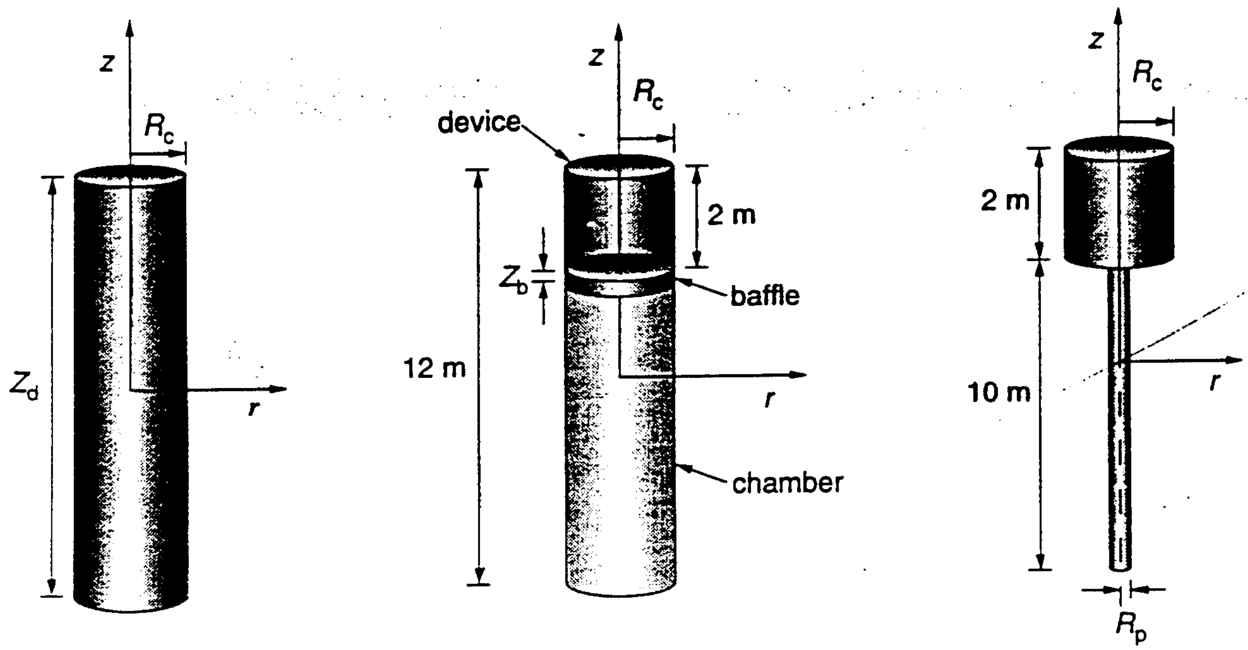
NUMERICAL SIMULATIONS

— UIUC

Explosion Parameters

Source Geometries



Other Parameters

- All explosion have yields of 125 kt
- All explosions are in Westerly granite

FKL

NUMERICAL SIMULATIONS

– UIUC

ZEUS-2D Hydrodynamics Code

- Uses finite-difference equations and a second-order-accurate, operator-split, multi-step, explicit-time integration scheme
- Von Neumann artificial viscosity spreads shock waves over several mesh cells
- Advection is treated using van Leer's monotonicity-preserving algorithm
- Uses the first-order method of LeBlanc to treat material interfaces
- Results presented here use ~10^4 cells
- Code was tested by solving a large suite of test problems
- Simulated explosions were compared with exact analytical solutions for ideal gases and ZEUS-1D simulations for granite

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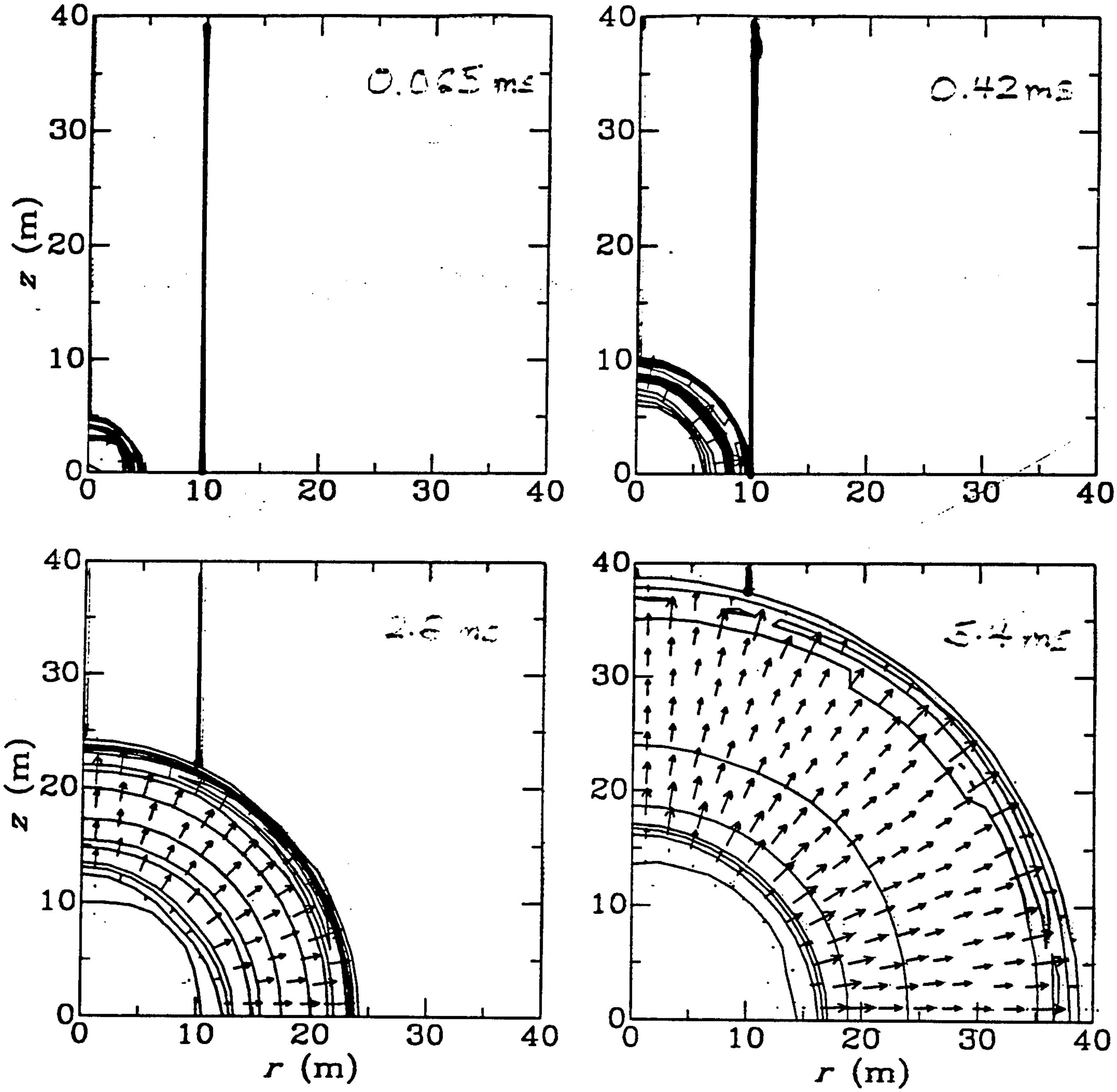
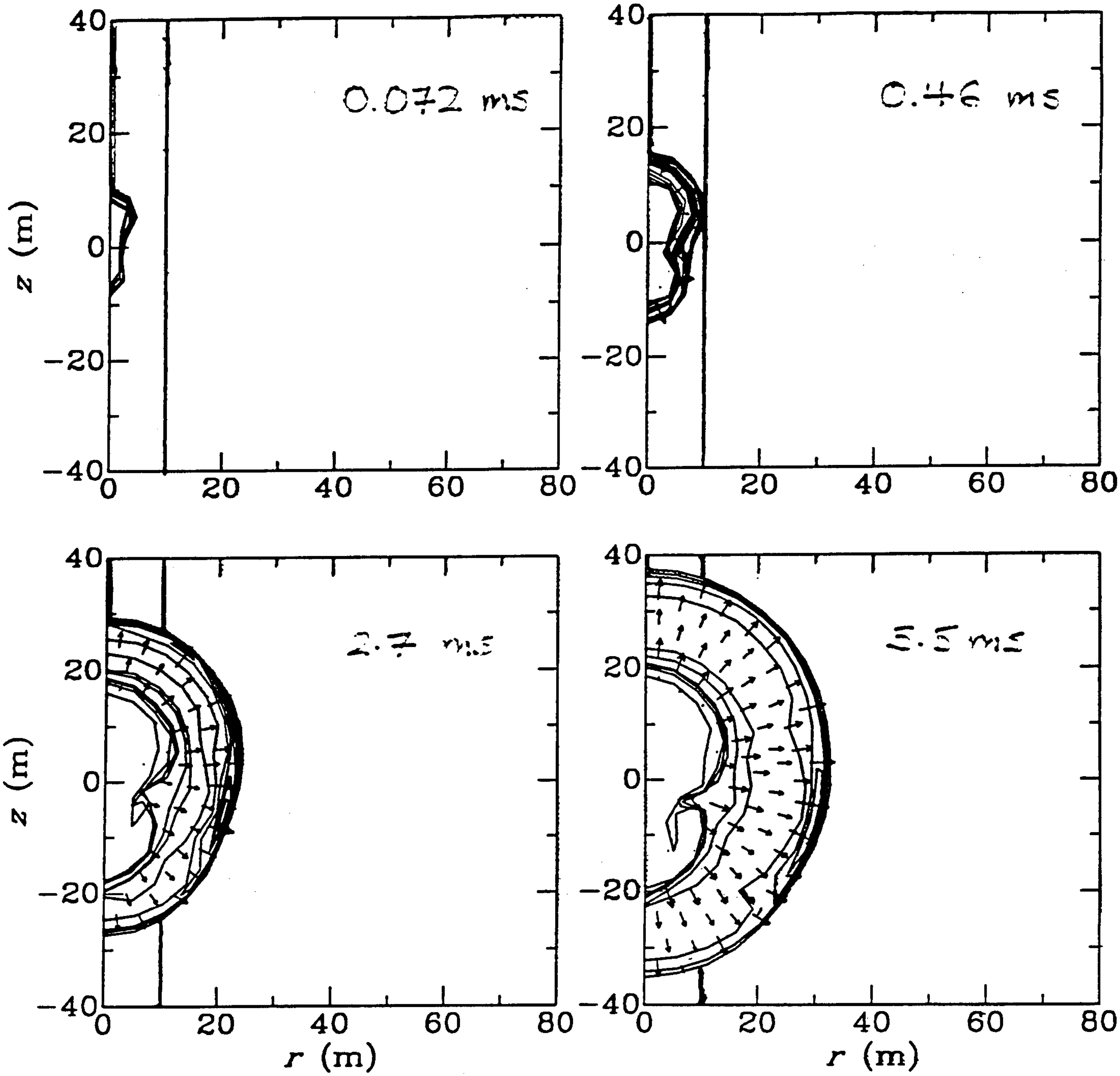
2m × 2m SIMPLE CYLINDRICAL CANISTER



2m × 12m CYLINDRICAL CANISTER W. INTERNAL BAFFLE



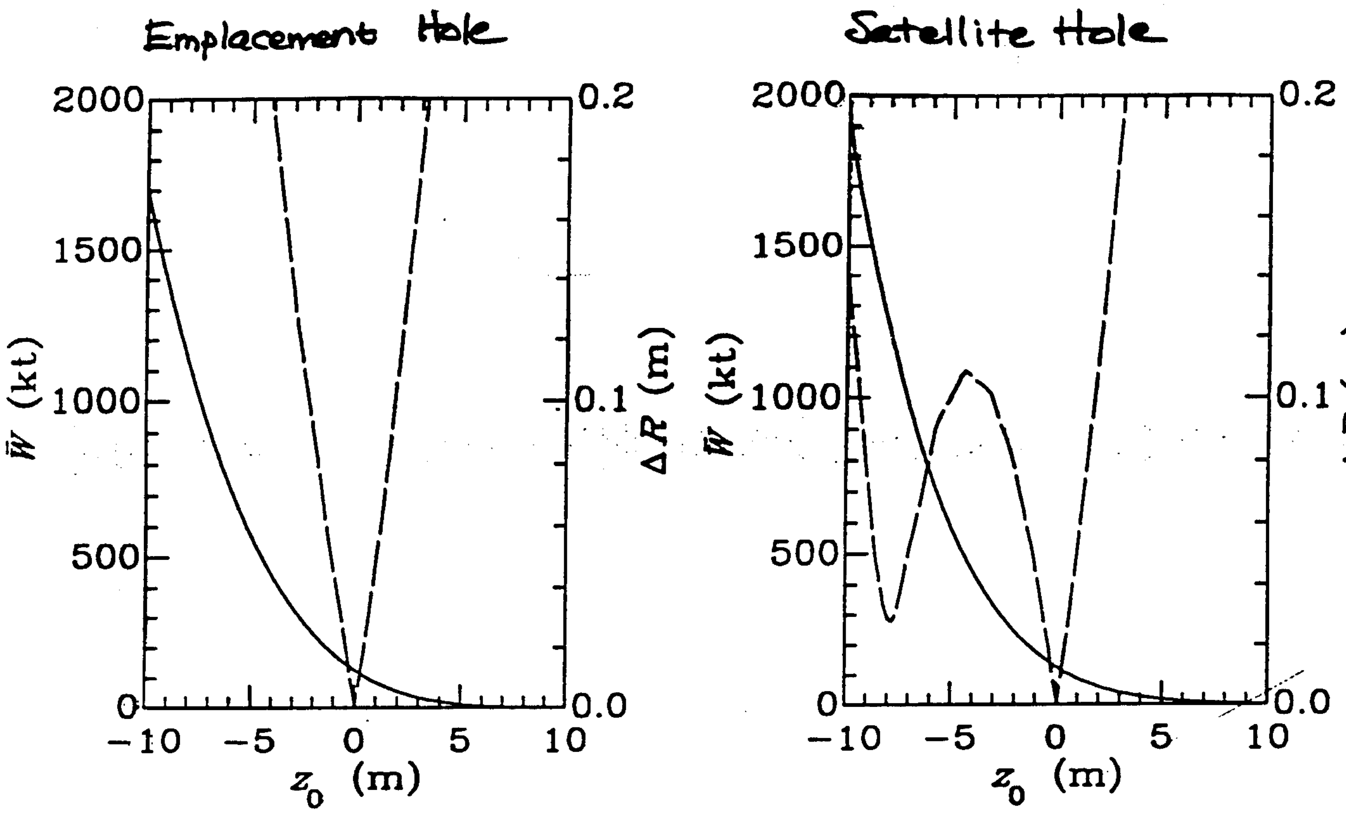
YIELD ESTIMATES

UIUC

Assumptions

- No uncertainties in shock front positions or times
- All exlposions are in Westerly granite
- All explosions are axially symmetric
- Axis of symmetry is known exactly, only the vertical position z_0 is unknown
- 'Unknown' and 'reference' explosions all have same yield (125 kt)
- Data analysis interval is 1.0–2.5 ms

SPHERICAL EXPLOSION
FIT BY SPHERICAL MODEL



Emplacement hole —

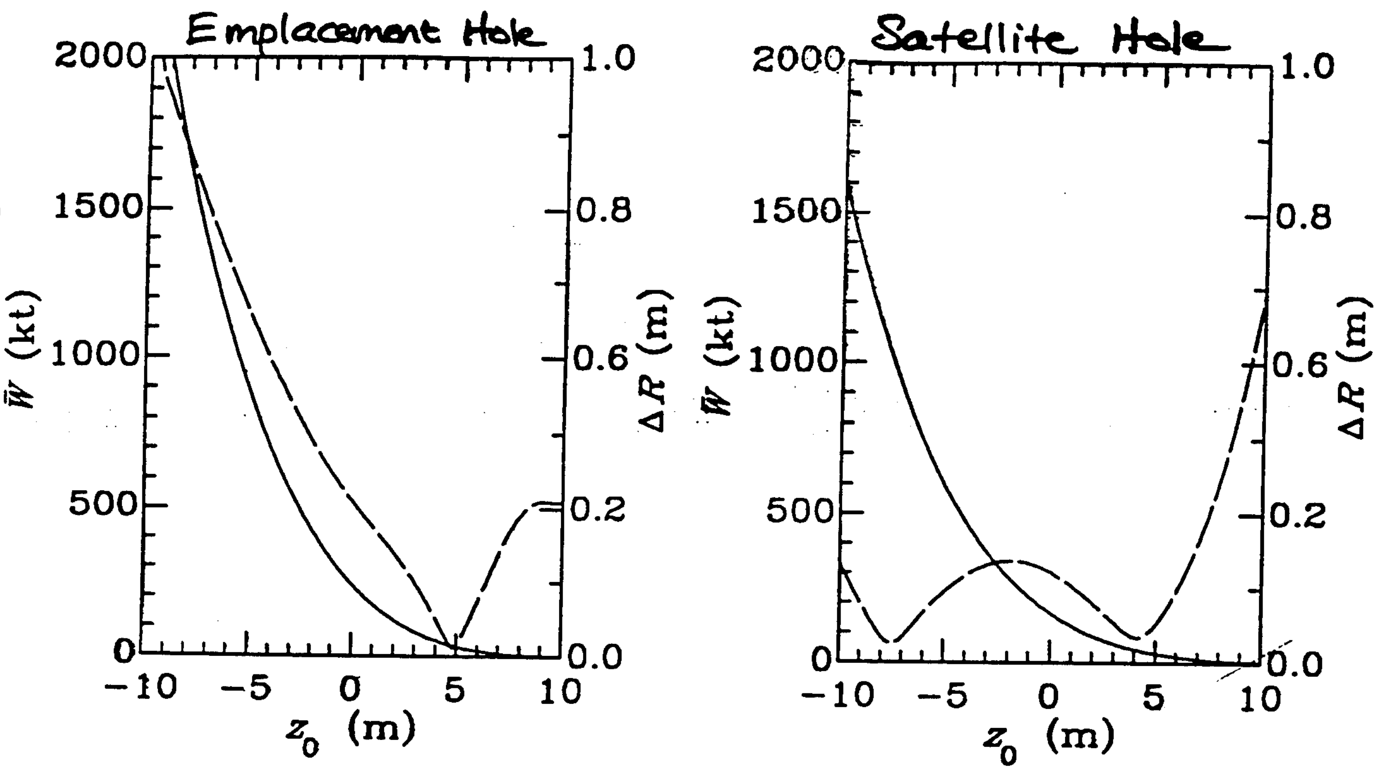
Best solution: $z_0 = 0$, $W = 125$ kt, $\Delta R = 0$

Satellite hole —

Best solution: $z_0 = 0$, $W = 125$ kt, $\Delta R = 0$
2nd solution: $z_0 \simeq -8$ m, $W \approx 1350$ kt, $\Delta R \approx 3$ cm

2m × 10m CYLINDRICAL EXPLOSION

FIT BY SPHERICAL MODEL



Emplacement hole data—

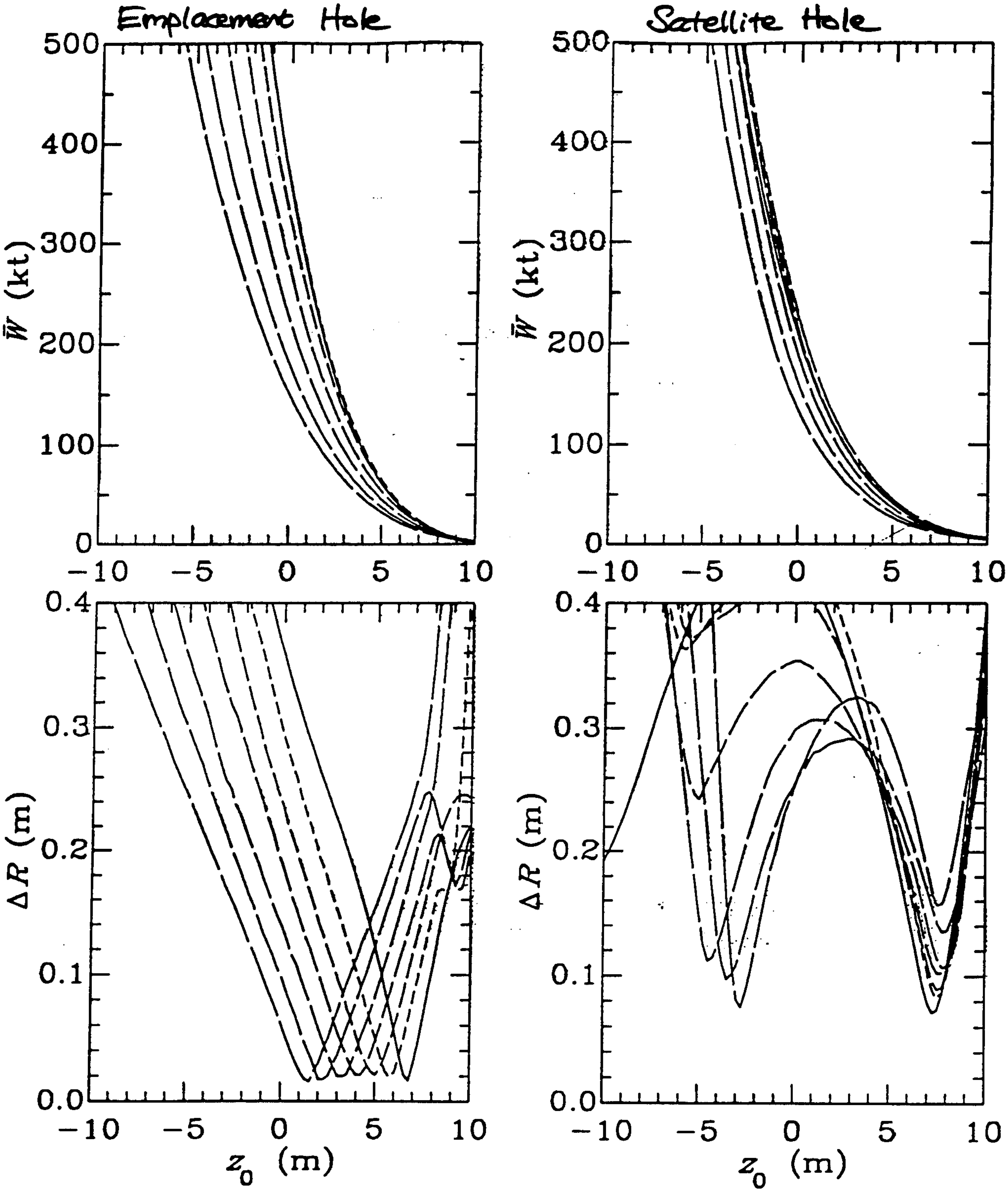
Best solution: $z_0 = 4.8$ m, $W = 35$ kt, $\Delta R = 1.3$ cm

Satellite hole data—

Best solution: $z_0 = -7.6$ m, $W = 10.3$ kt, $\Delta R = 3$ cm

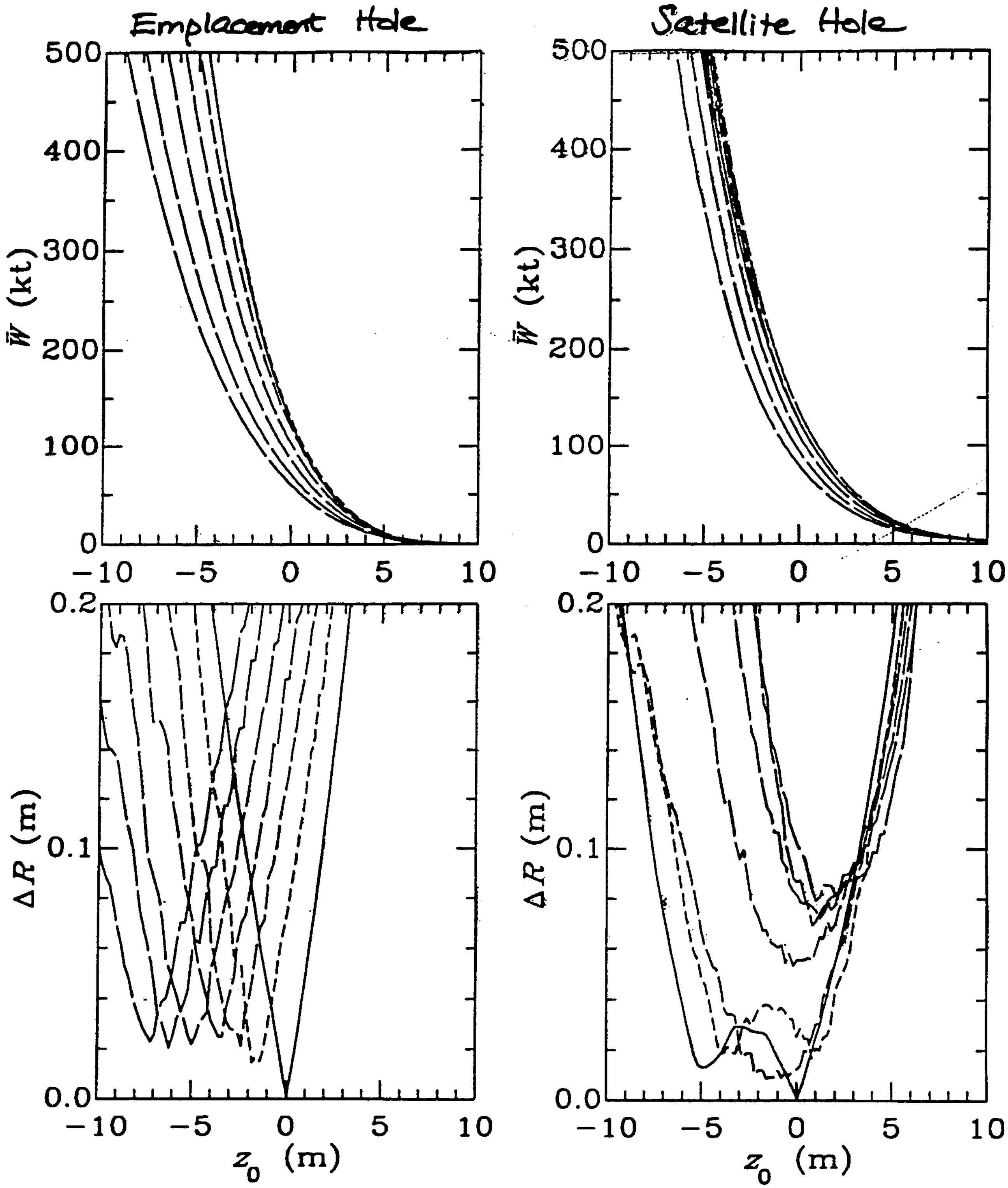
2nd solution: $z_0 = 4.1$ m, $W = 44$ kt, $\Delta R = 4$ cm

2m × 12m CYLINDER W. INTERNAL BAFFLE (INVERTED)
FIT BY SPHERICAL & CYLINDRICAL MODELS



SPHERICAL EXPLOSION

FIT BY SPHERICAL & CYLINDRICAL MODELS



MULTIDIMENSIONAL HYDRODYNAMICS

– UIUC

Concluding Remarks

- HYE problem still unsolved (but less urgent)
- The main difficulty is lack of data: one set of sensing cables does not give enough
- These limitations must be recognized, esp. if HYE is ever used for PNET/TTBT verification
- Inadequate understanding due in part to
  - secrecy
  - lack of will
  - limited access to computers and codes

  plus desire to preserve 3rd generation weapons programs (esp. X-ray laser) led to weak verification protocols

This does not mean that the U.S. should devote more resources to HYE or that the protocols should be renegotiated. Can accept current seismic capabilities or improve them.

FKL 10/94

INFORMATION TECHNOLOGY/SIGNAL PROCESSING

Technologies for the National Information Infrastructure

Professor Randy H. Katz

Advanced Research Projects Agency
and
University of California, Berkeley

The ARPA Research Program in National-Scale Information Enterprises

Randy H. Katz

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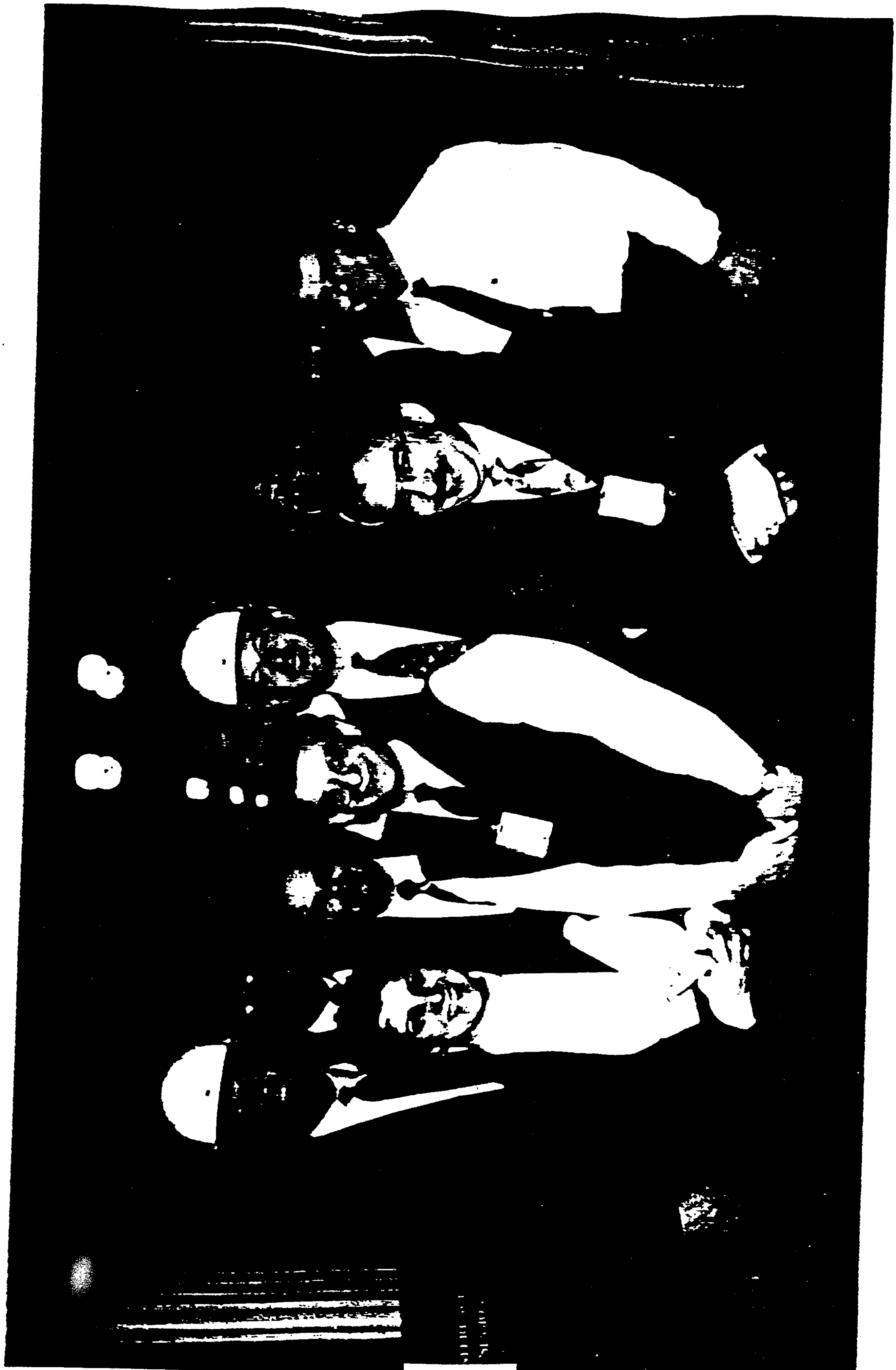

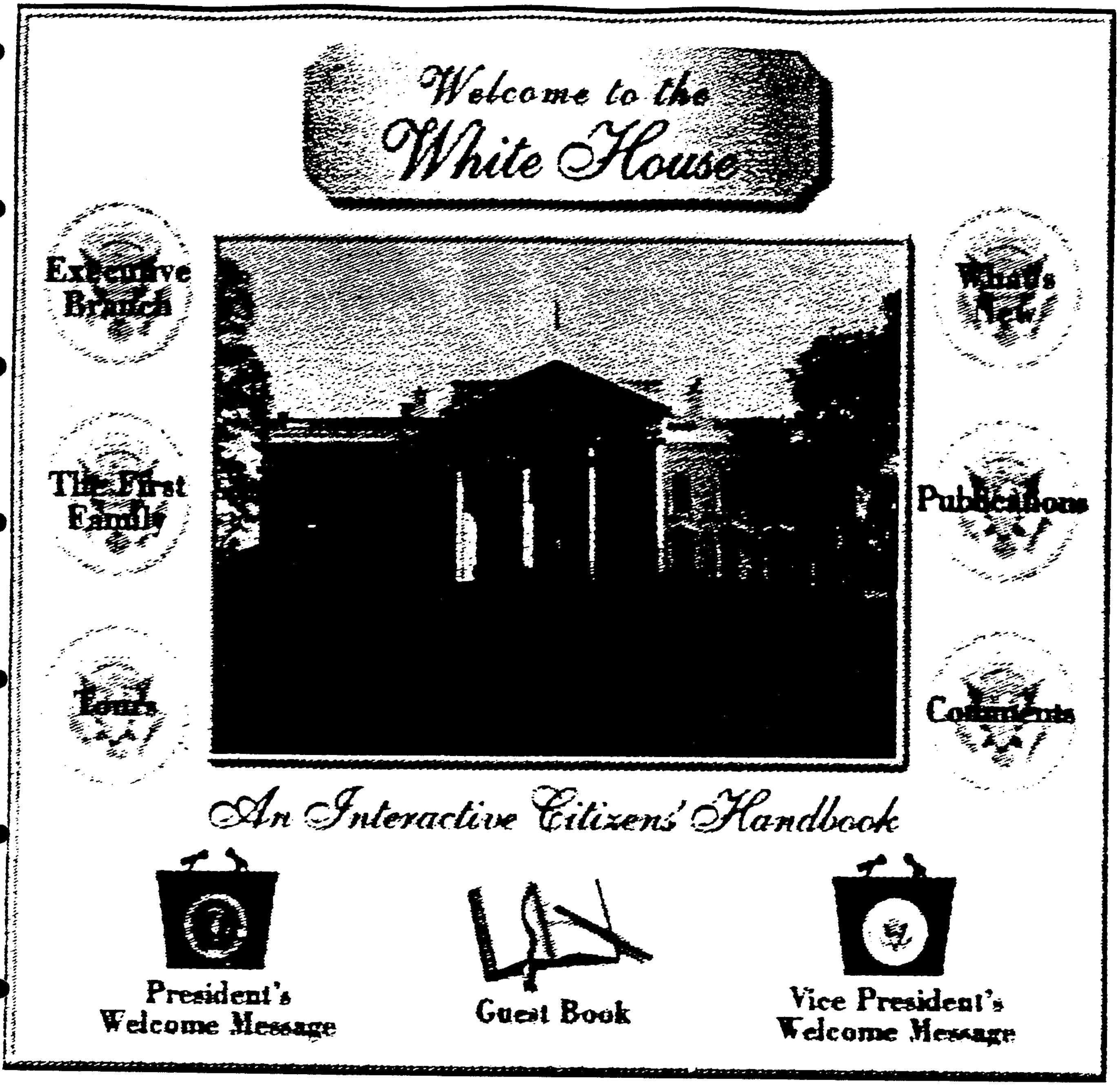

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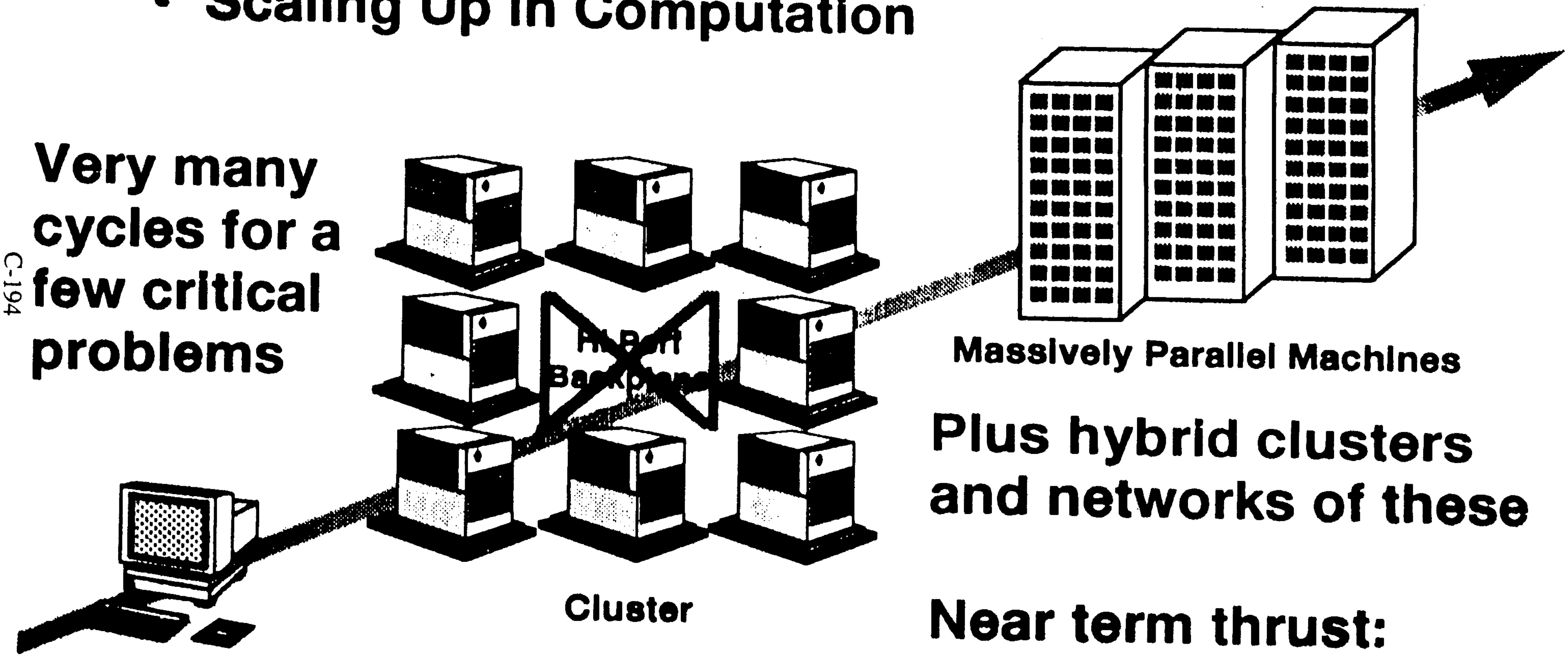
HPCC Scaling

- Scaling Up in Computation

Very many cycles for a few critical problems

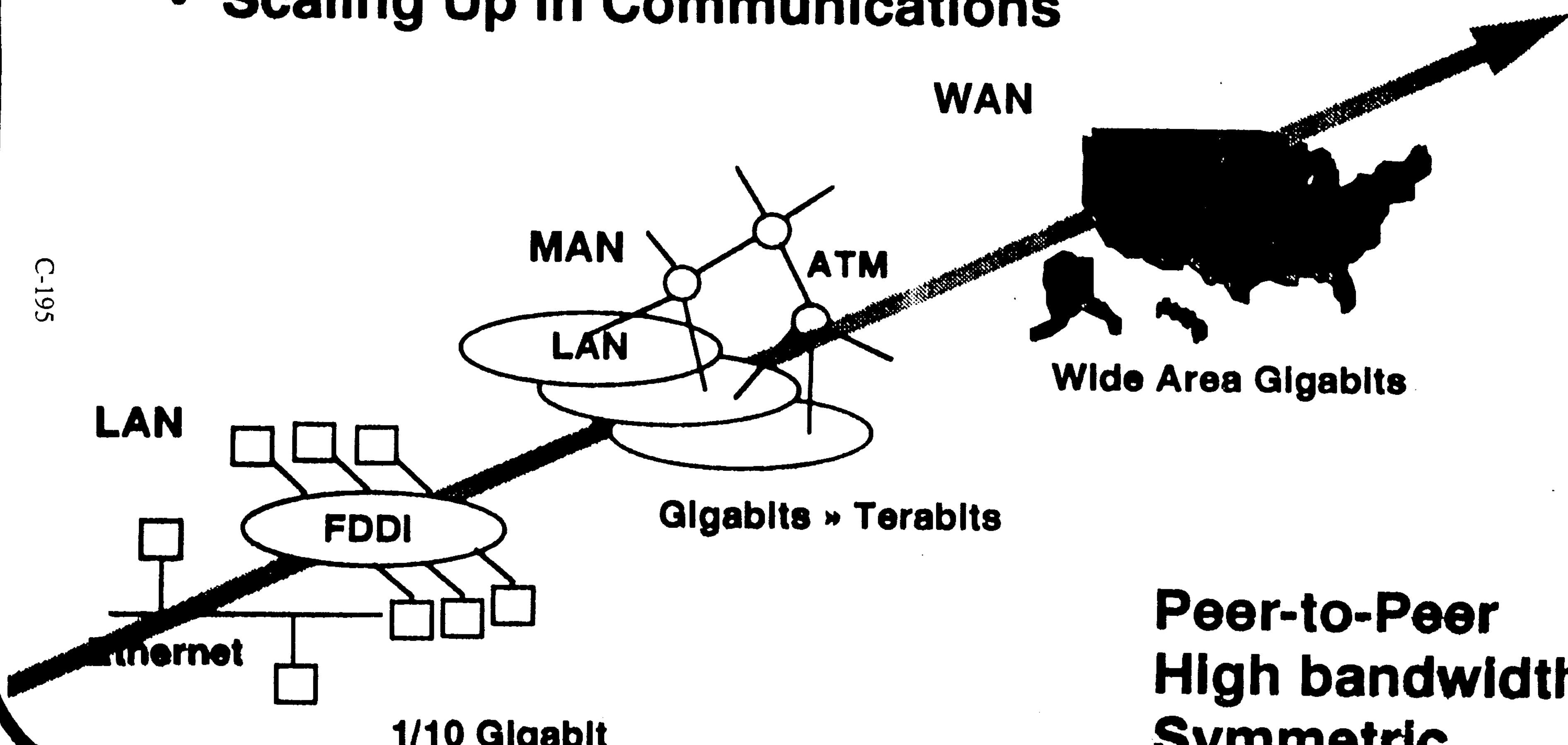


Plus hybrid clusters and networks of these

Near term thrust: unified models of computation

HPCC Scaling

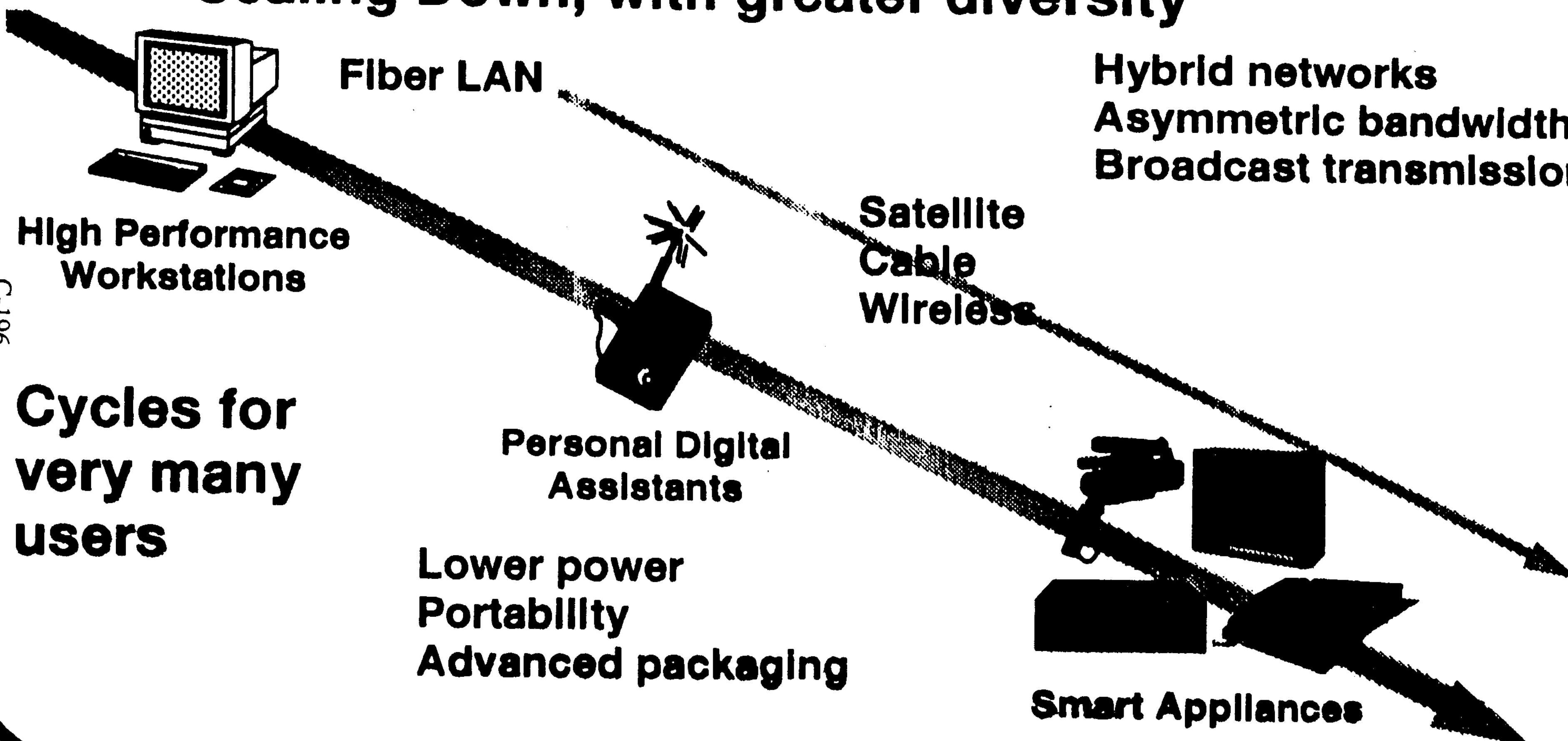
- Scaling Up in Communications



Peer-to-Peer
High bandwidth
Symmetric

HPCC Scaling

- Scaling Down, with greater diversity



Cycles for very many users

Lower power
Portability
Advanced packaging

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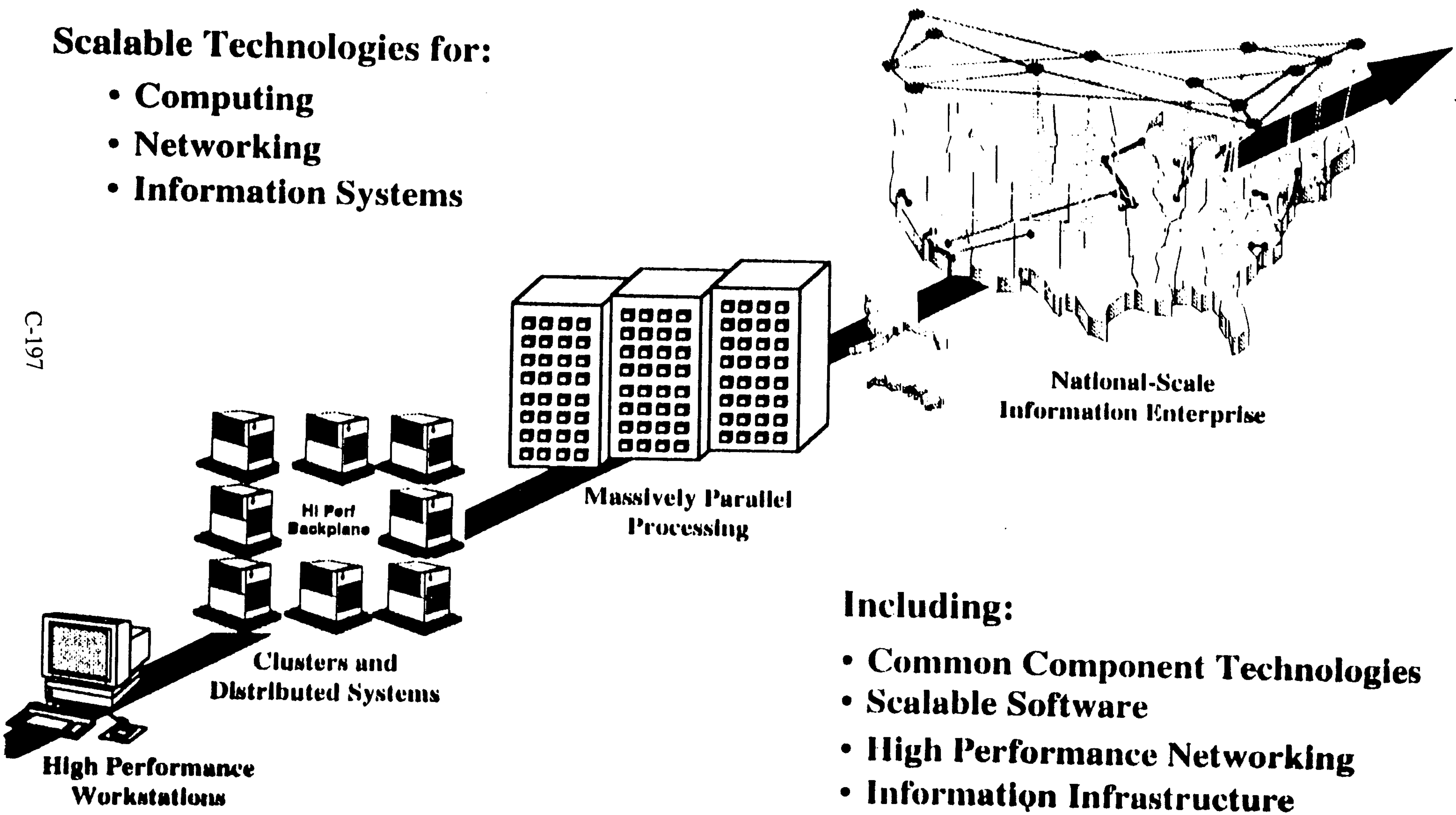
Computing Systems Scaling

Scalable Technologies for:

- Computing
- Networking
- Information Systems



Including:

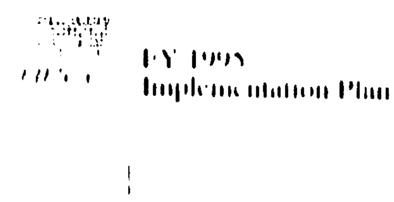
- Common Component Technologies
- Scalable Software
- High Performance Networking
- Information Infrastructure

ARPA

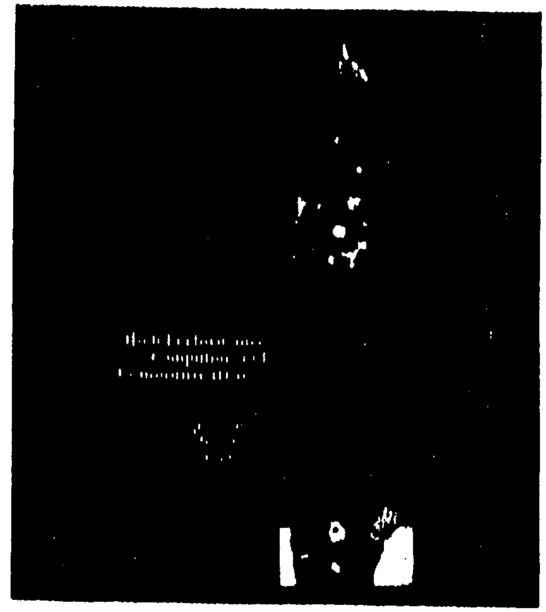
Computing Systems Technology Office

HPC

Federal HPCC Program

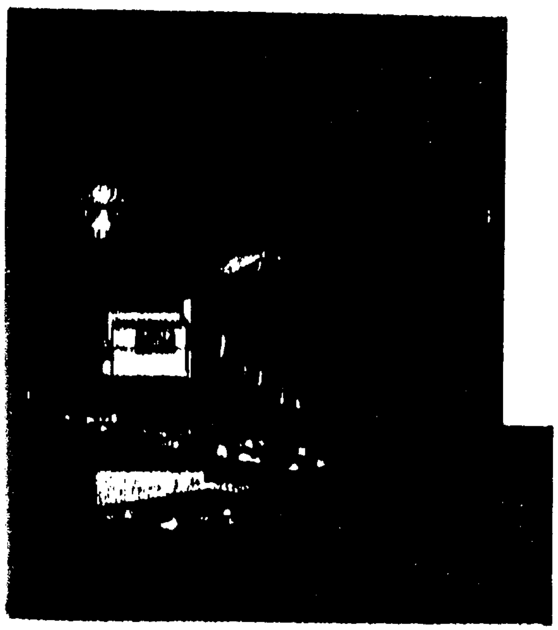


FY 1995
Implementation Plan



FY95
HPCC:
Technology
for the
National
Information
Infrastructure

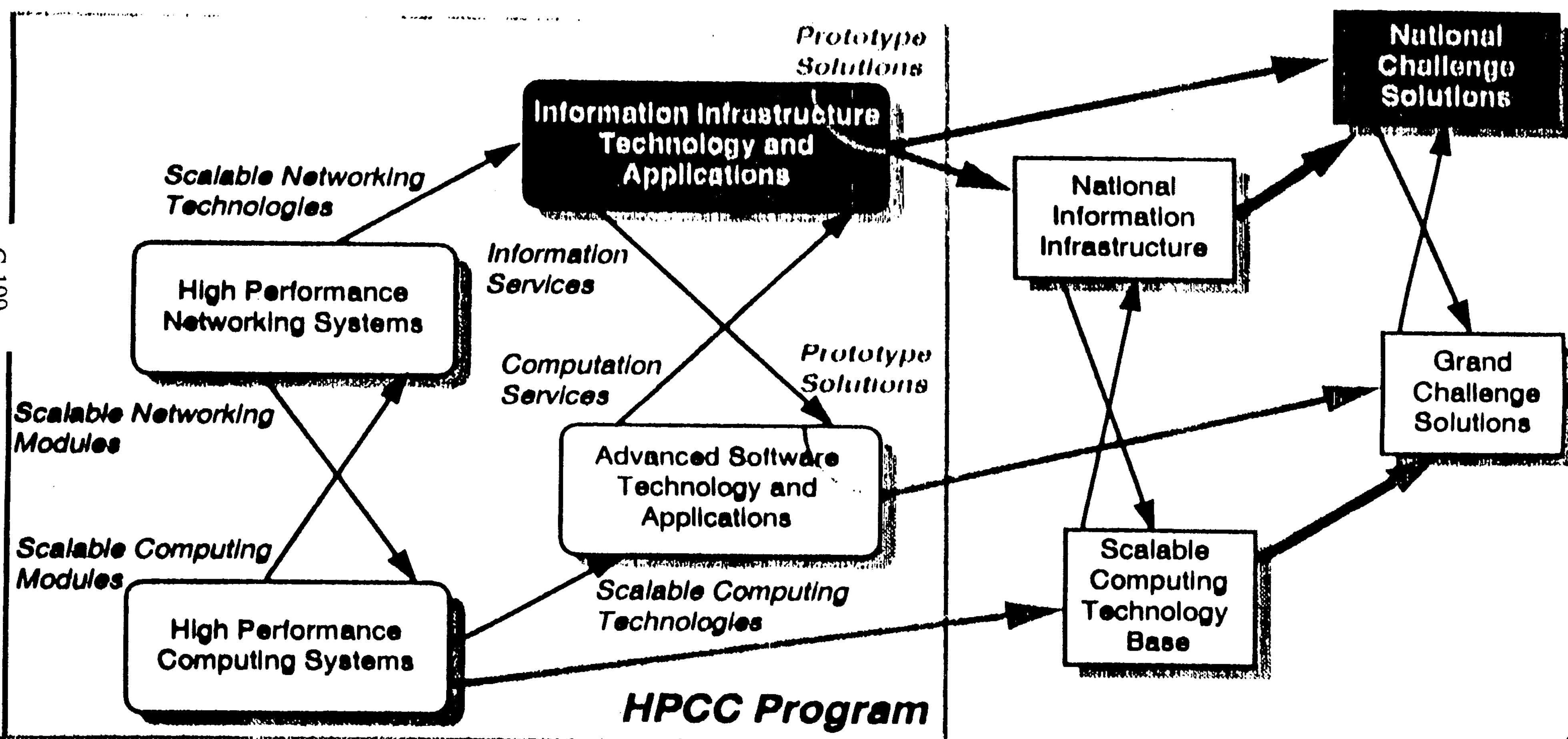
FY95
Implementation
Plan



FY94
HPCC: Toward a National
Information Infrastructure

National Coordinating Office - (301) 402 -4100 or carson@hpcc.gov

HPCC Towards NII: Top Level Relationships



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5

Three Layer Architecture

National Challenges (NCs):
Achieve major new economies of scale

NII supports all kinds of applications, not just NCs

Many services support Grand Challenges as well

National Information Infrastructure (NII):
Provide ubiquitous interconnected computing and communications

Applications

[redacted]

Information

Services

[redacted]

Communications

Bitways

Examples

[redacted]

[redacted]

[redacted]

C-200

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Presentation Outline

- Information Infrastructure Services
- The ARPA/CSTO R & D Program
  - Applications Support Technology
  - Electronic Commerce Technology
  - Digital Libraries Technology
- Information Infrastructure Technology and Applications Inventory
- Testbed Opportunities

Presentation Outline

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Service Definition

- **Distributed system capabilities for access, resource discovery, linkage, dissemination, distribution and security**
- **Services for the applications developer *as well as* end user services**
- **Evolution of the services layer**
  - Today's end-user services become tomorrow's applications building blocks
  - Support for broader classes of users, kinds of usages
  - Greater situation-awareness, context-sensitivities

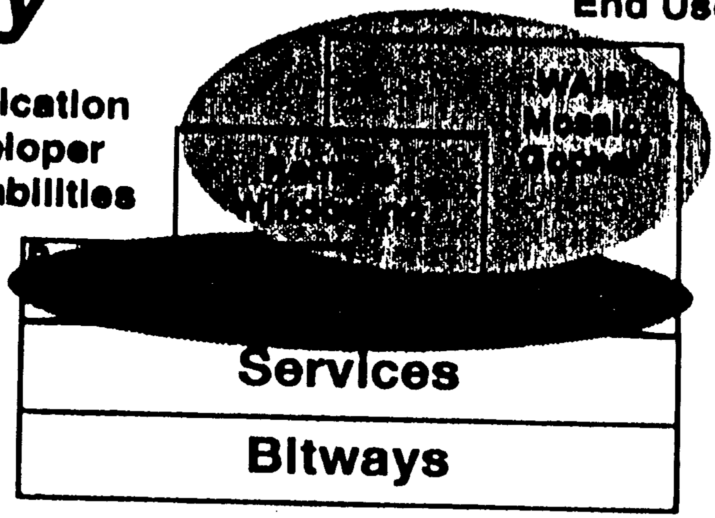
Evolution of Services

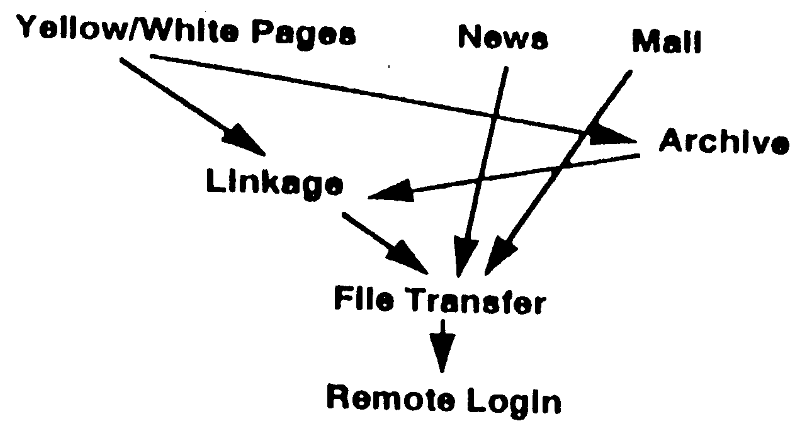
NIE

Today

Application
Developer
Capabilities

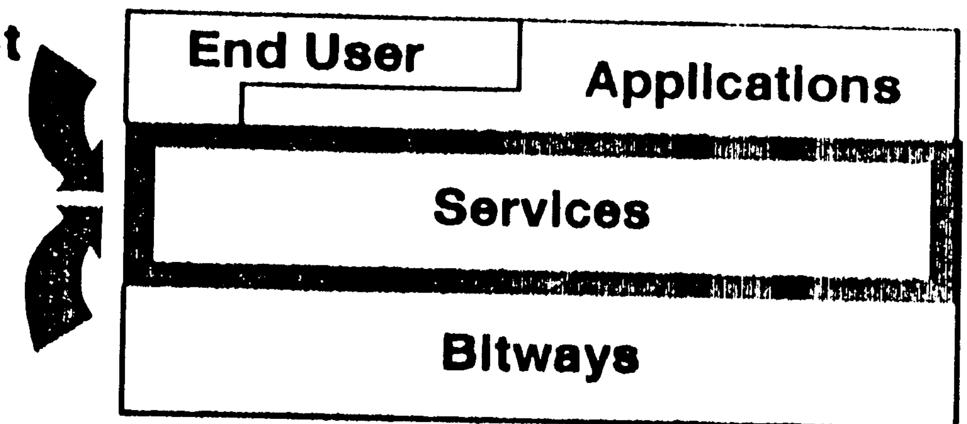
End User Capabilities





Intelligent
Systems

Networks



New Capabilities
Wider Availability
Greater Adaptability
Improved Ease of Use
Scale Up
Better Reliability

Future

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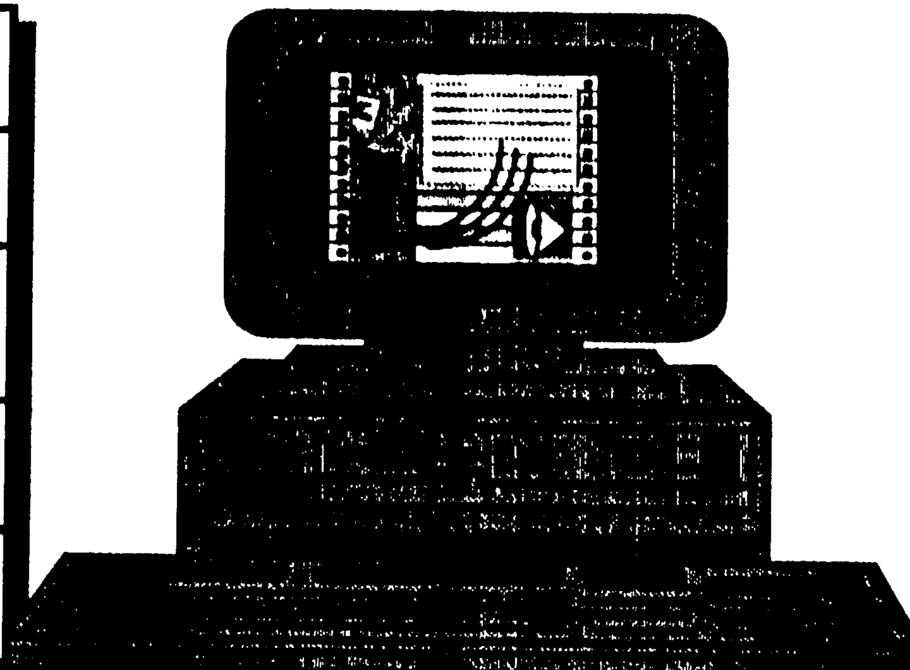
Evolution of Services: e.g., MOSAIC

Today → **Future**

Today
Fixed User Interface
HTML / GIF / Audio
Understands specific formats and data types (but can be extended)
Need explicit knowledge of document location
Fixed comm protocols (WWW, gopher)



Future
Adapts to User Preference
Adapts to display/sound configuration
Platform-Independent Self-describing Digital Objects (no need for a priori translators)
Becomes aware of new documents of interest; Metering/Fee for Access
Adapts to available protocols/network b/w

Multimedia Interface to Network-based Hyperlinked Documents

Viewer- and Network-aware Hyperlinked Objects

ARPA

A Research Program in Service Technology

NIIE

- **Objective**
  - In conjunction with industry and academia, develop an open, robust, highly leveraged service architecture for the National Information Infrastructure; focus on applications developers
- **Approach**
  - Pursue R&D program in new information services; Focus on e-commerce and digital libraries technologies
  - Collaborate on regional and national testbeds to test emerging service technologies and architectures
- **Applications and Benefits**
  - Demonstration of a National Information Marketplace
  - Widespread, spontaneous NII-based commercial transactions
- **Schedule**
  - 1994-6: Regional testbeds; 1997-9: National testbeds

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Presentation Outline

- Information Infrastructure Services
- **The ARPA/CSTO R & D Program**
  - **Applications Support Technology**
  - **Electronic Commerce Technology**
  - **Digital Libraries Technology**
- Testbed Opportunities

Strategic Thrusts

- **Applications Support Technology**
  - Application partitioning and synthesis
  - Adaptation to changing infrastructure capabilities
  - Initial context provided by wireless, adaptive, mobile information systems
- **Fundamental Enabling Technologies**
  - Electronic Commerce Technologies
  - Digital Library Technologies
- **Demonstration projects to drive system architecture development**
  - Cross-cut from applications to services to bitways
  - Leverage and extend existing service and communications capabilities

Program Relationships

Other National Challenge Applications

E-Commerce Technology

Usage Metering/Charging

Application
Support Technology

Adaptation to New Servers, Publishers, Repositories, Institutions, Display Characteristics, Bandwidth Characteristics

Presentation Outline

- Information Infrastructure Services
- **The ARPA/CSTO R & D Program**
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The Vision

"People and their machine should be able to access information and communicate with each other easily and securely, in any medium or combination of media—voice, data, image, video, or multimedia—*any time*, *anywhere*, in a timely, cost-effective way"

Dr. George H. Heilmeier
IEEE Communication Mag.
October 1992

The Vision

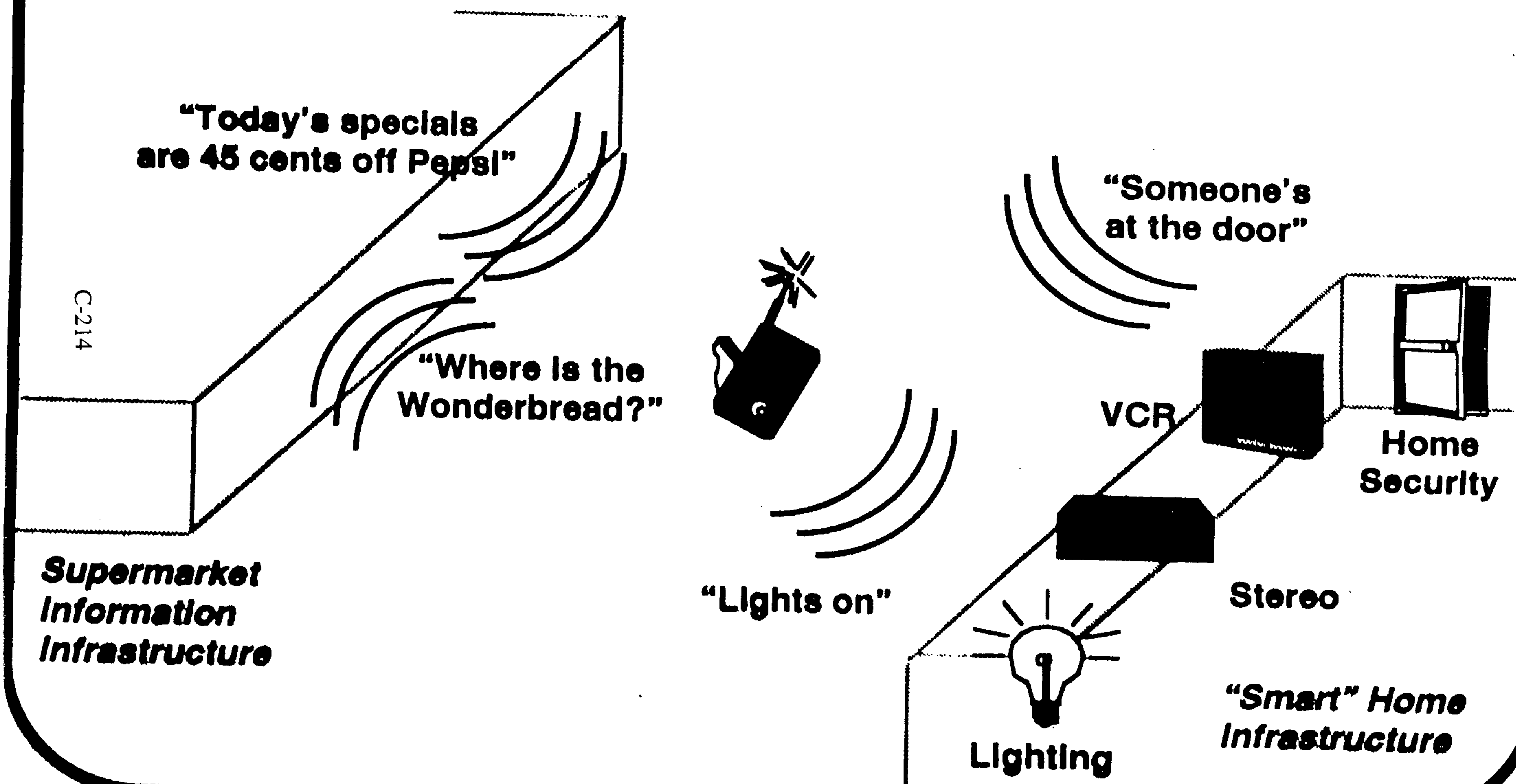
"Going to war with a rifle in one hand and a laptop computer in the other would have been shocking only a few years ago. [Yet] tomorrow's war-fighter will require global access to information and transparent multilevel security in a laptop system. ... Give the battlefield commander access to all of the information needed to win the war ... *when he wants it, where he wants it*, how he wants it."

Gen. Colin L. Powell
Byte Magazine
July 1992

Application Support Technology

- **Generalized approach for discovery and interaction with nearby devices and services**
  - Make possible a kind of "Universal Interactor"
  - Mechanisms to adapt to different kinds of never before encountered services
- **Support for partitioning/function shipping**
  - Partition application between host and infrastructure
  - Move application to service provider
  - Move service "enabler" to application
  - Depends on location of service providers, available bandwidth, preferred network routing, generalized quality of service, energy considerations, usage characteristics

Example: Universal Interactor



Challenges

- Come as you are communications and infrastructures
- No single set of naming and interaction protocols, no global services like Internet naming and directories
- Issues are the same in a very large, evolving wired network as in the wireless network examples as shown

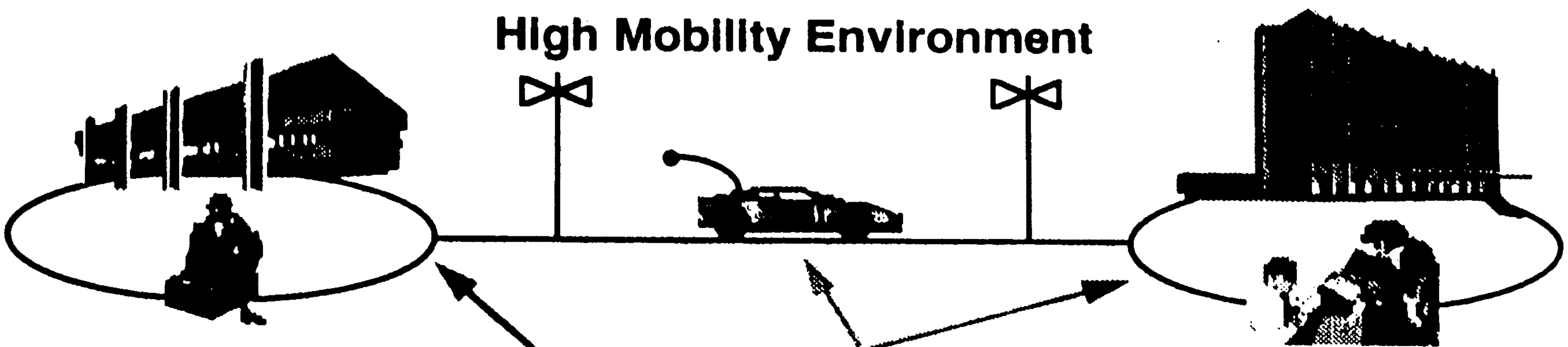
Specific Needed Developments

- Models of services and service interactions
- Explicit service interface descriptions; standard methods for applications to be informed of resource changes
- Algorithms that migrate services near to the application and vice versa
- Models of user behavior, algorithms that surmise user's work patterns and predict future service references
- Benchmarks: extent of "graceful" adaptation to change in resources (e.g., new services, bandwidths, routes to servers, etc.)

Mobile & Wireless Systems Adaptability

To enable users to take their "InfoEnvironment" with them ...

High Mobility Environment



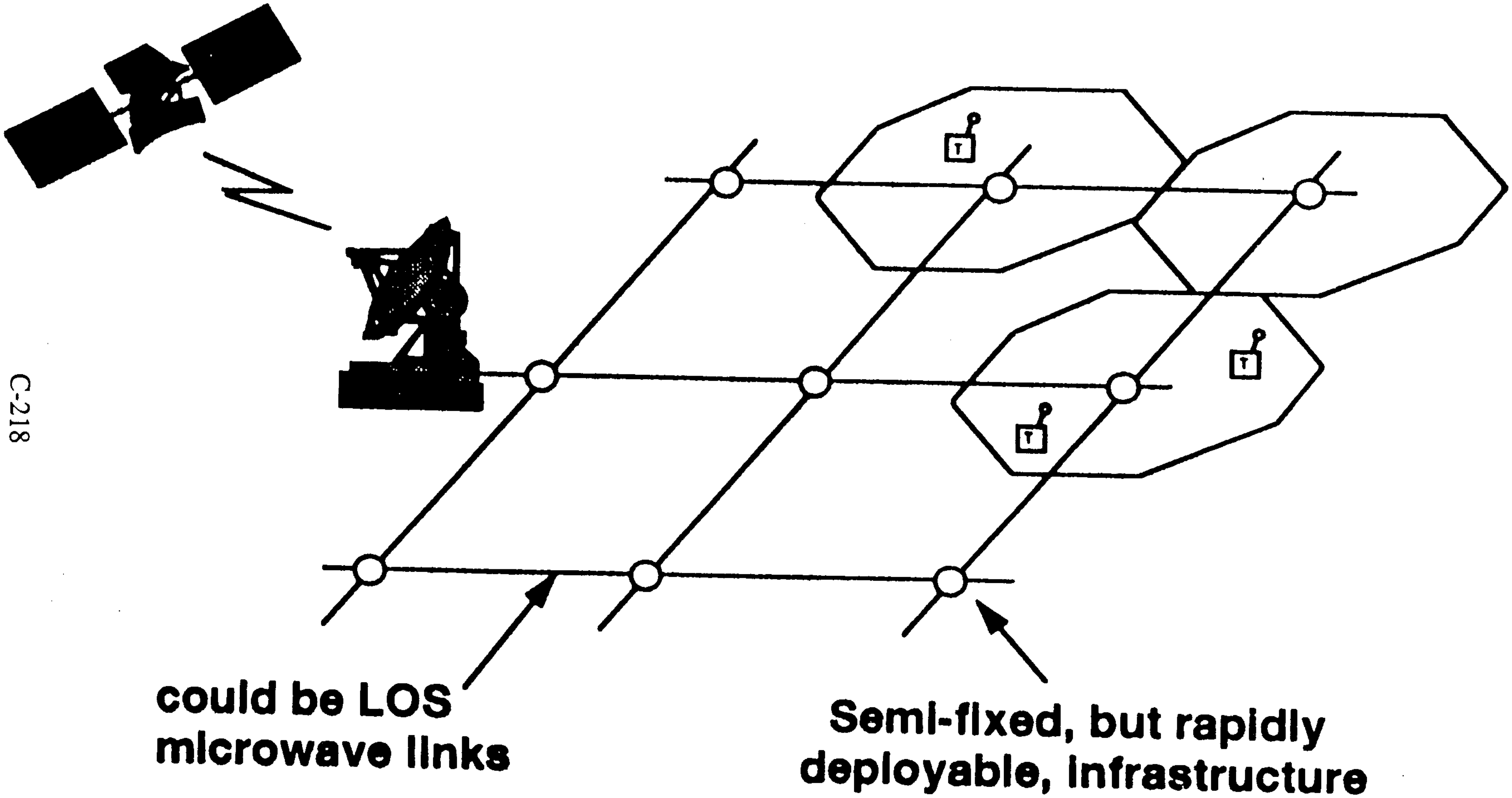
Low Mobility Environment

- **High bandwidth in-building infrastructures**
- **Complex security/privacy issues**
- **Guest users of infrastructure**
- **Protecting privacy of users**

Low Mobility Environment

- **Lower bandwidth outside infrastructures + asymmetric (low b/w uplink, high b/w downlink)**
- **Leverage existing cellular infrastructure where possible; Establish "instant infrastructure" when necessary**

Adaptive Backbone Infrastructure



Program Relationships

Wireless, Adaptive, Mobile Information Systems (WAMIS)

Collaborative Applications within the National Challenges
Location-aware, Bandwidth Sensitive Applications
Digital Libraries, Electronic Commerce

Microsystems: Desig
and prototypes of
tetherless, mu

Decoupled
and Privacy

Support for Application Partitioning/Synthesis
Service Discovery
Adaptation to Changing Environment

Wired Bitways Infrastructure
Internet technology
Security in networks
High performance computing components

Presentation Outline

- Information Infrastructure Services
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- Testbed Opportunities

ARPA

Requirements for Electronic Commerce

NIE

- **Marketplace for Information and Services**
  - Directories (White Pages, Yellow Pages, Catalogs, Ads)
  - Value-added Services (Brokers, Gateways, Active Forms)
  - Electronic Transactions thru security, billing, and payment
  - Open Access: Any provider can add information or services at any time
- **Financial Transactions**
  - Commercial transactions, including bidding, purchase orders, money, letters of credit, and other electronic analogs of current financial instruments
- **Intellectual Property**
  - Control of the use and disposition of intellectual property in electronic form

Core Services for Electronic Commerce

- Discovery/Searching
  - Information clearinghouses
  - Critical for finding service providers,
- Data Interchange and Format Conversion
  - Conversion services for interoperation
  - Critical for EDI and electronic forms
- Authentication and Security
  - Authentication, authorization, confidentiality, privacy, integrity, protection against misuse
- Electronic Payments
  - Digital money, payment orders, escrow, letters of credit, bartering systems, financial instruments, value exchange

Electronic Commerce Infrastructure

Network Management

Fee for Access Documents

Fee for Service (e.g., FAST)

Accounting/ Banking Services

Authorization Services

Authentication Services

Privacy Enhanced Mail

Public Key Crypto Digital Signatures

Needed: a security infrastructure for distributed computing and open networks

Proxies: ability to grant credentials to performed restricted operations under limited conditions

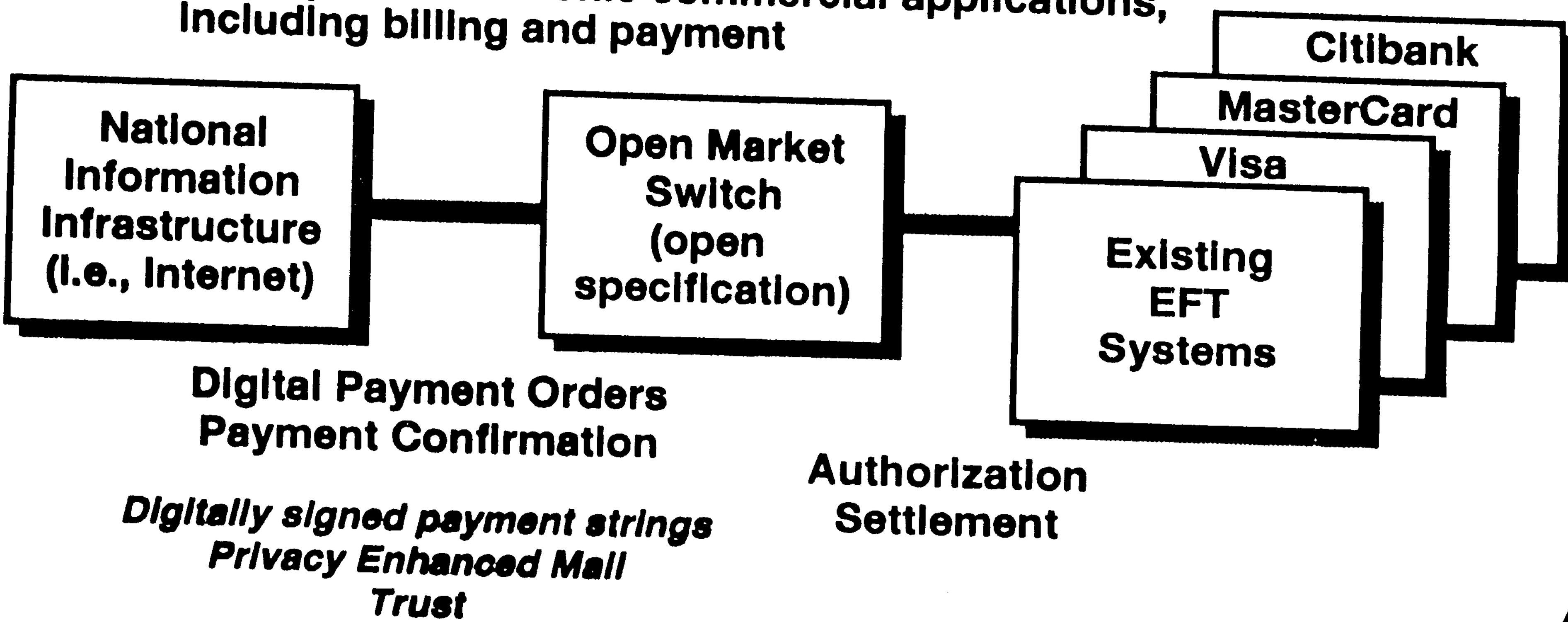
Proxies created by trusted server
carries own restrictions
can't be tempered with

Kerberos: commonly used authentication service based on conventional crypto

A proxy grants the right to withdraw funds (or other quota resources)

Electronic Commerce Infrastructure

- **Open Market System**
  - Basis for National Information Marketplace
  - Widespread electronic commercial applications, including billing and payment



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Presentation Outline

- Information Infrastructure Services
- **The ARPA/CSTO R & D Program**
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  - **Digital Libraries Technology**
- Testbed Opportunities

Requirements for Digital Libraries

- **Object Management**
  - Control the process of storage, retrieval, communication, presentation, and replication of information objects
  - Rich set of composable data types that interact across platforms
- **Intellectual Property Management**
  - Control the use and disposition of intellectual property in electronic form
- **Agents and Brokers**
  - Humans and computer processes that can be tasked to find, filter, and process information on behalf of users or processes

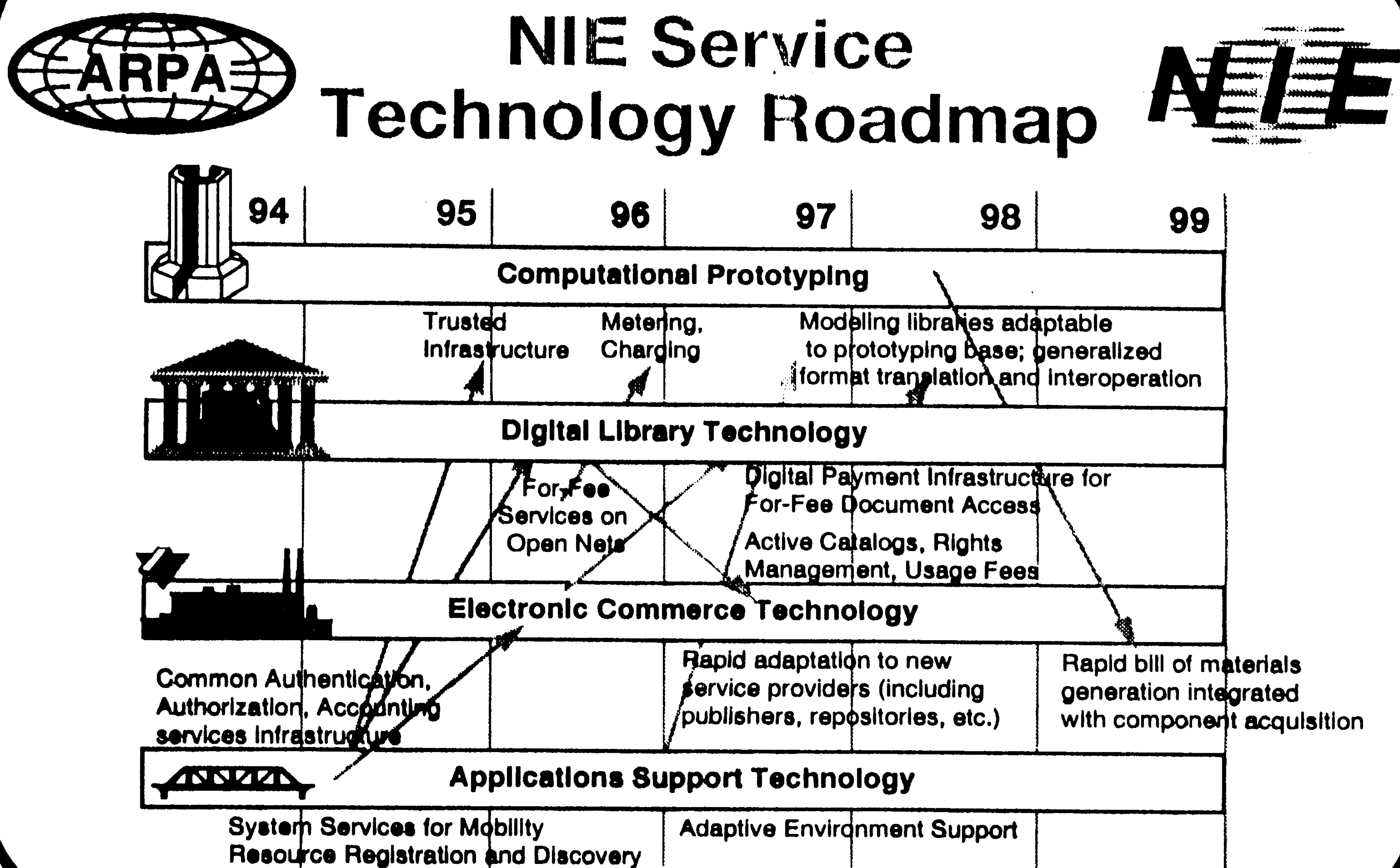
Core Services for Digital Libraries

- **Discovery/Searching**
  - Finding information within the library
  - Strategies for indexing terms
- **Linkage**
  - Pointers that link information, solving problems of long term validity, granularity, versions
- **Data Interchange and Format Conversion**
  - Conversion services between different documents or data formats
- **Repository**
  - Long lived, archival storage services
- **Registration and Publishing**
  - Creation and dissemination of pointers across the net

Computing Systems
Digital Libraries Issues

- Locating documents in the information web
- Shared, distributed, long-lived repositories of documents
- Document translation and interchange
- Scalable registration/recordation system for digital objects
- Rights management system (attribution, fee for use)

NIE Service Technology Roadmap



NIE Service Technology Trends

Key Areas	Today	+2 Years	+4 Years	Impacts
Applications Support Technology - Discovery - Registration - Partitioning - Shipping	• Some software for disconnected ops • Static, non-reactive applications • Little system support for partitioning/shipping	• Demonstration of graceful degradation • Bandwidth sensitive applications • Prototype support for partitioning/shipping	• Pervasive use of general capabilities for dynamically adapting applications to discovered available resources	• Enabling technology base for situation-sensitive applications
Electronic Commerce Technology - Usage Metering - Accounting - Payment - Trust - Brokering	• No trusted network infrastructure • No general purpose building blocks for ecommerce • Limited resource discovery mechanisms	• Common infrastructure for trust, security, & privacy-enhanced operation • General for-fee services on the Internet	• Open architecture building blocks for usage metering, accounting, payment • Advanced brokering services coupled to active catalogs	• Enabling technology for usage metering, accounting, and payment for general applications
Digital Library Technology - Location - Translation - Recordation - Rights Mgmt	• Network hypermedia browsers (Mosaic) • Indexes on-line • Limited on-line technical documents	• Prototype Copyright Management System • For-Fee document access on the Internet • Search/retrieval services	• Operational Rights Management Systems for digital object usage • Integration of library technology with brokers	• Common infrastructure for storing, locating, displaying, metering, accounting, paying for use of digital objects

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Presentation Outline

- Information Infrastructure Services
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  - Digital Libraries Technology
- **Testbed Opportunities**

The Need for Driver Projects

- "The NII -- Just Do It!"
  - John Young, retired CEO Hewlett-Packard Corp.
- Don't do technology in isolation
- Demonstrate the potential for real value to the public; measure and evaluate it
- But avoid application-specific "stovepipes"
- Government's role as neutral third party in developing reference architectures, interfaces, and methods of interoperation

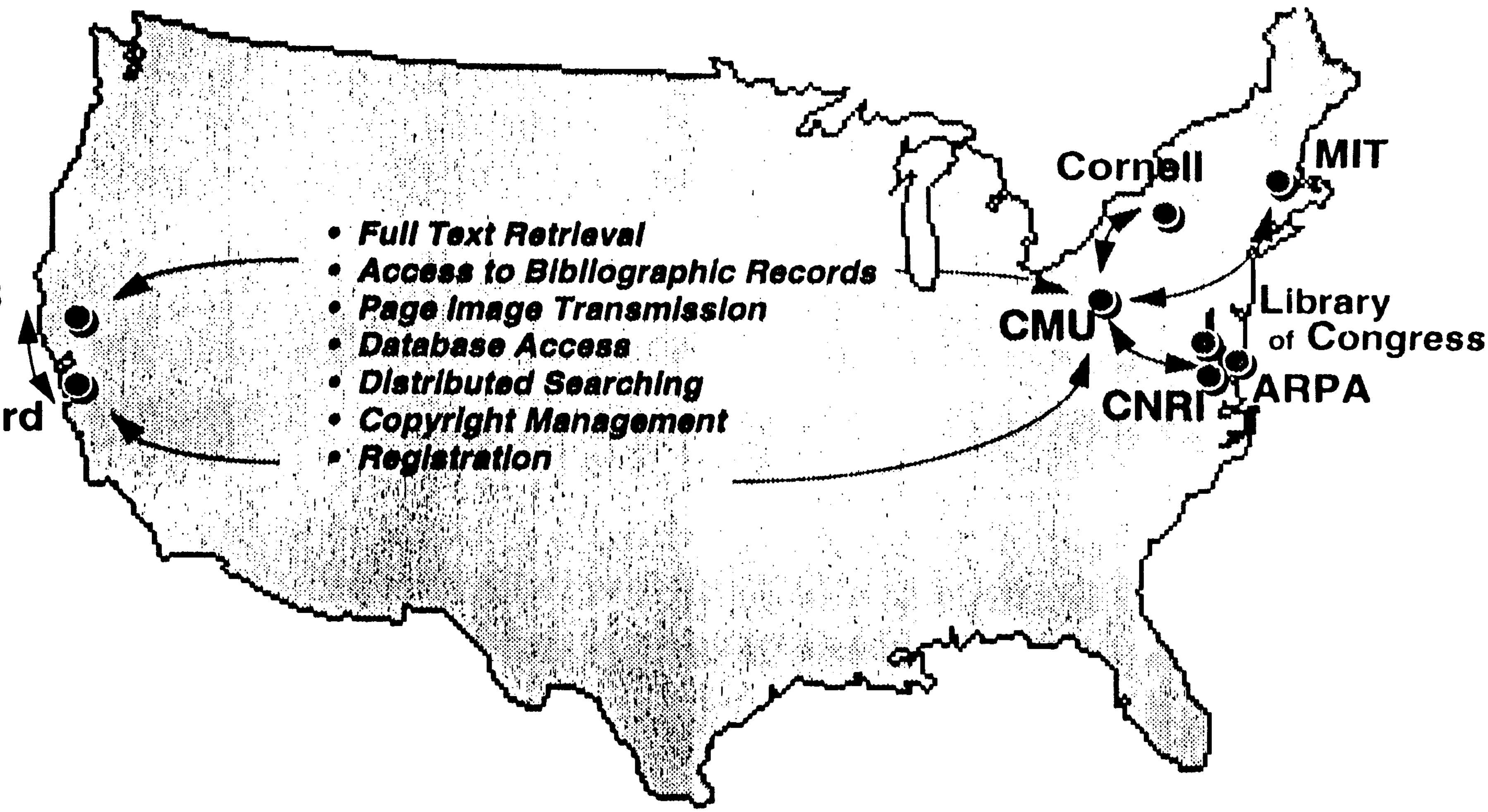
Successful Model: Gigabit Testbeds

	Universities	Partners	Applications
AURORA	Pennsylvania, MIT	Bell Atlantic, Bellcore, IBM, MCI, Nynex	Visual Laboratory Advanced teleconf
BLANCA	Berkeley, Illinois, Wisconsin, LBL	AT&T, Ameritech, Astronics, Bell Atlantic, Cray Research, NCSA, Norlight, Pacific Telesis	Atmospheric storm modeling, radio astronomy imaging, multimedia digital libr
CASA	CalTech, SDSC	JPL, LANL, MCI Pacific Telesis, US West	Geophysical, global climate, chemical reaction
MAGIC	Minnesota, Kansas	LBL, SRI, EROSDC, MSCI, BCBL, DEC, Southwestern Bell, Splitrock Telecom, Sprint	Terrain vis, imagery transport, real time data fusion
NECTAR	CMU, U Pitt	Bell Atlantic, Bellcore	Traveling salesman prob chem flowsheet model
VISTAnet	North Carolina	Bell South, GTE, MCNC	Real time radiation treatment planning

Some ARPA Digital Library Activities

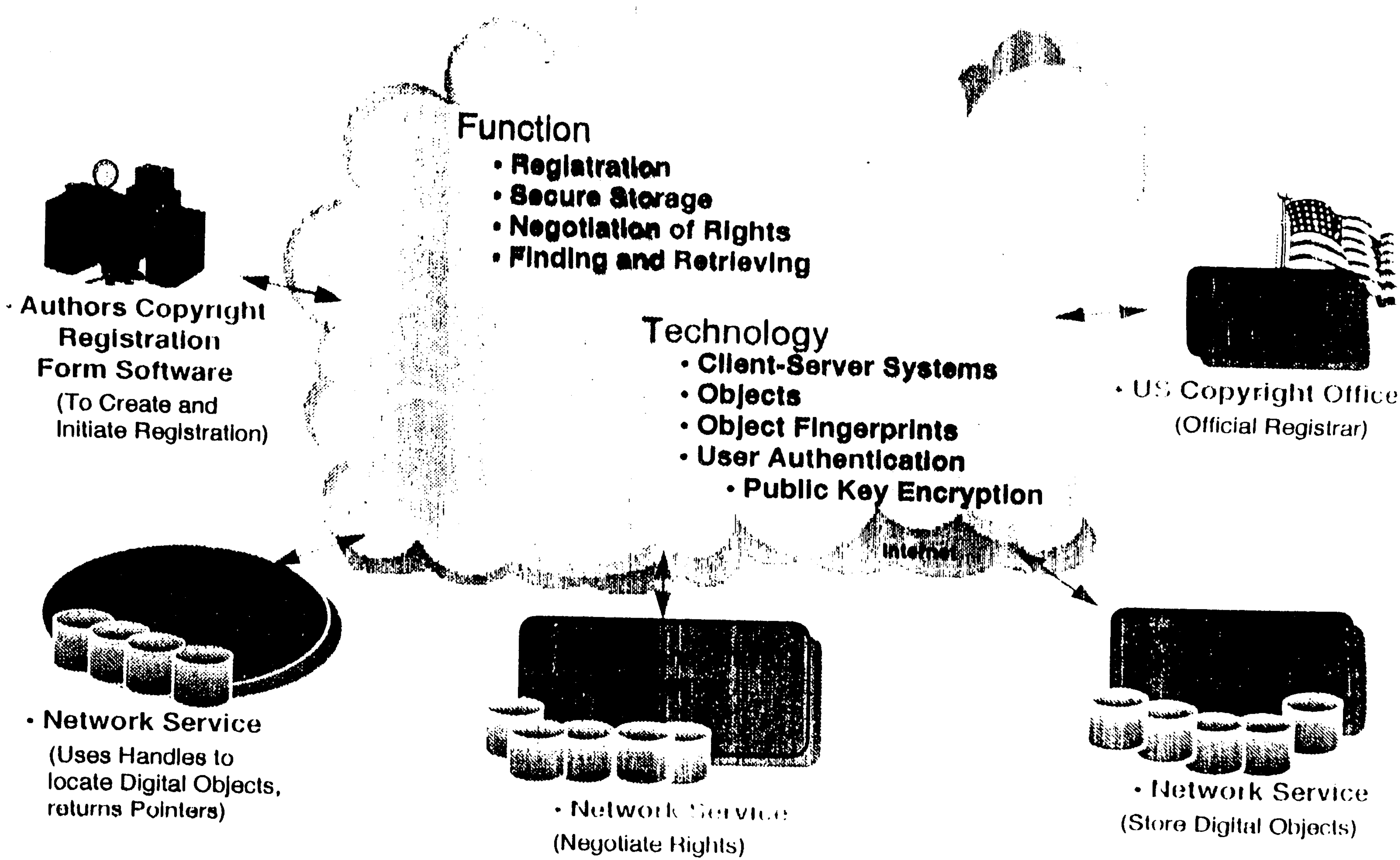
- CS-TR Project (putting Technical Reports online)
- Joint NSF/ARPA/NASA Digital Library Initiative
- NIE proposals (e.g. enhancements/extensions to the Information Web)
- Information brokers, management, etc. (SISTO)
- Applications to health care, education/training
- IITA Activities
  - WWW Coordination
  - Digital Library Conference and Workshop (Spring '95)

Linking Electronic Libraries

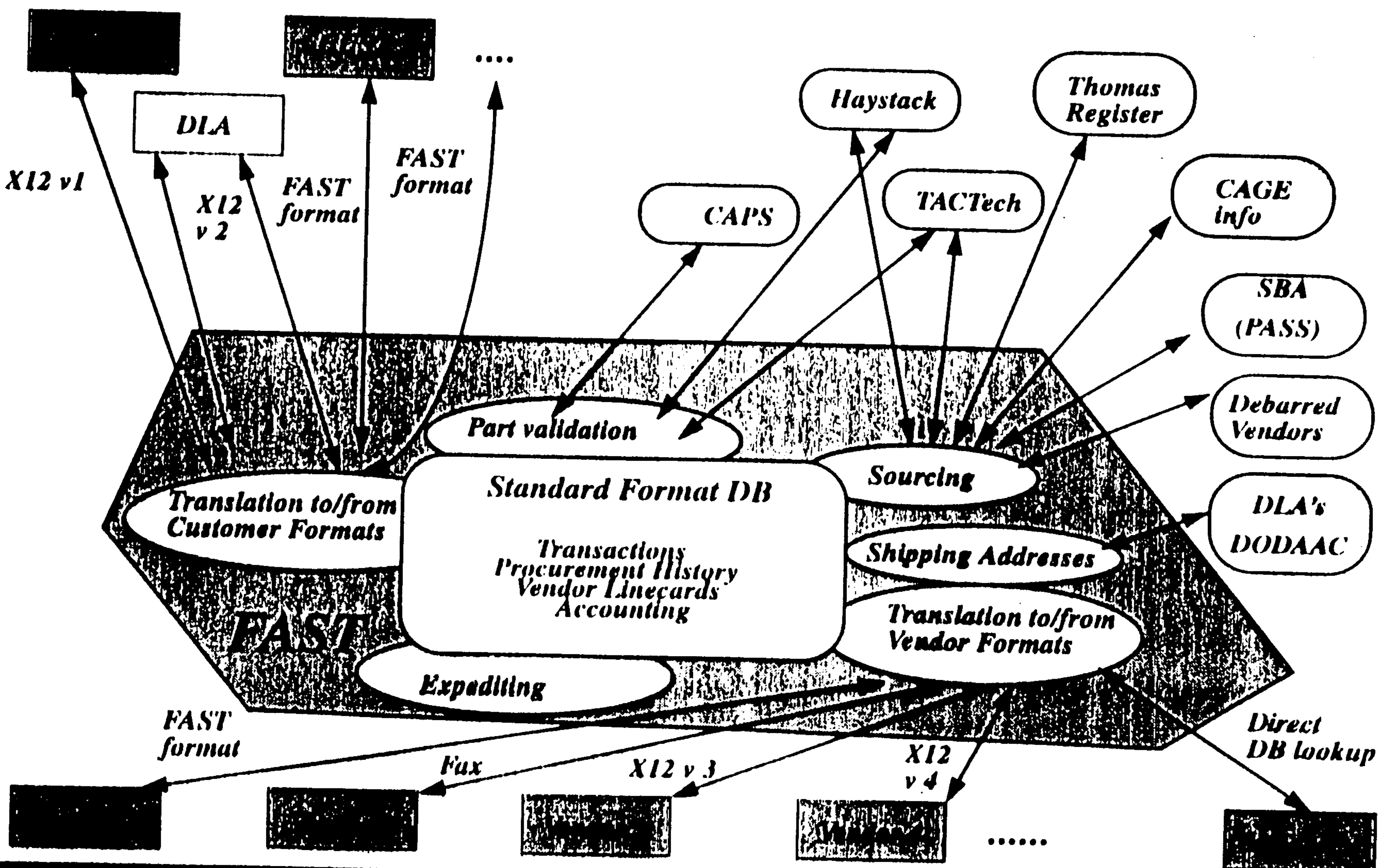


CNRI 1994

Electronic Copyright Management System



DLA Testing FAST's Modular Procurement Service

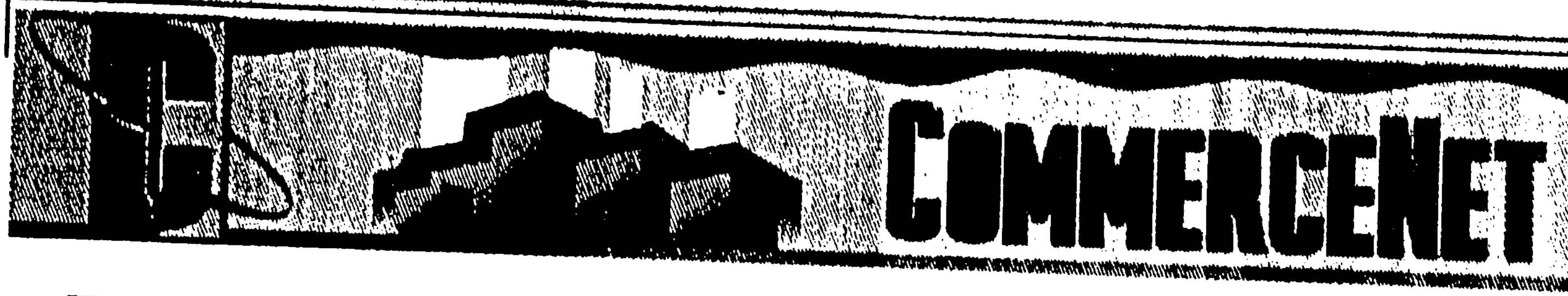


Options Navigate Annotate Hotlist

Fri 8/5/94

CommerceNet Home

CommerceNet Home | Search | Keyword



Welcome to CommerceNet, *an open, Internet-based infrastructure for electronic commerce, created by a coalition of Silicon Valley organizations! A text-only view of CommerceNet is available. Please try out our survey!*

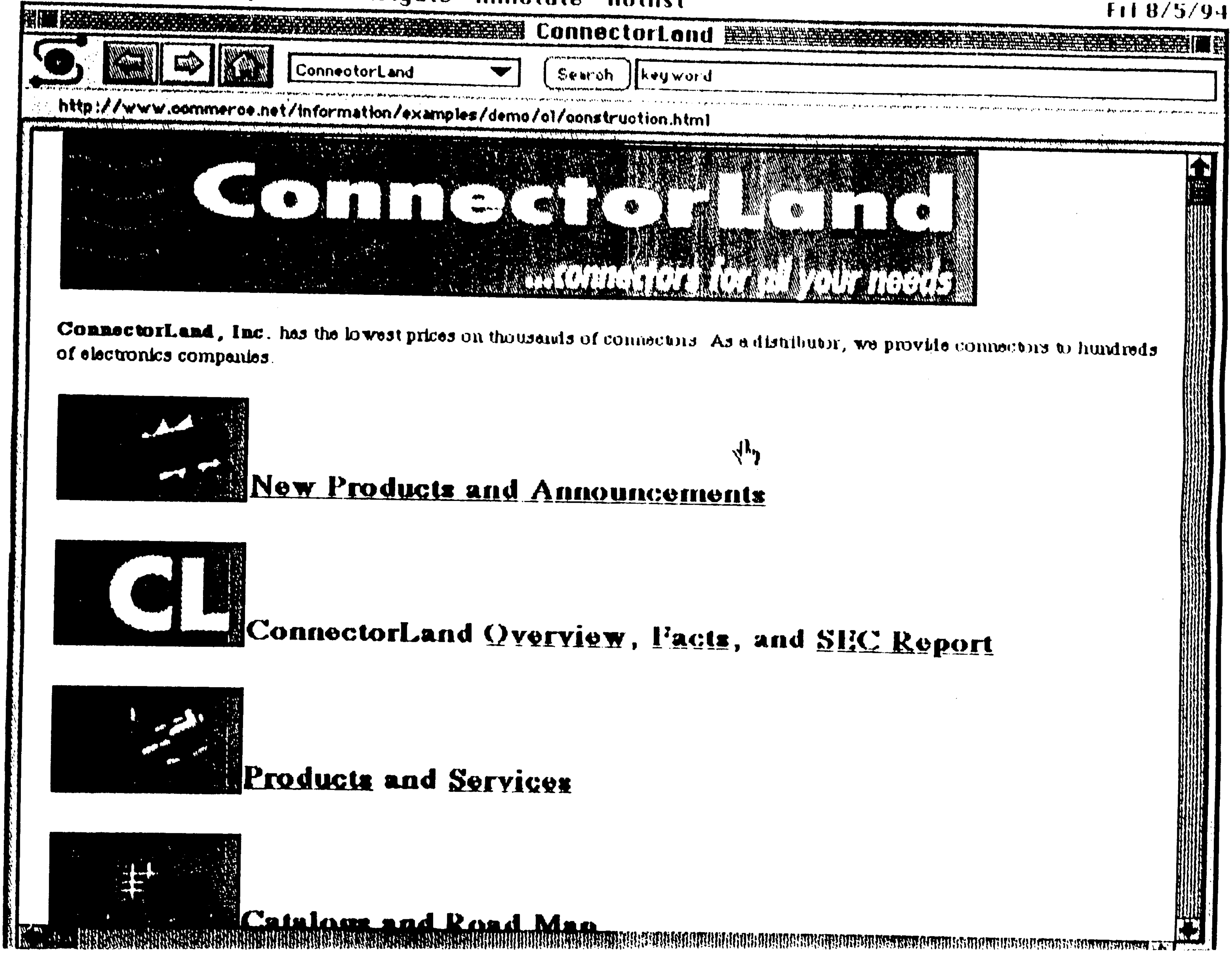
What's New on CommerceNet

CommerceNet Information

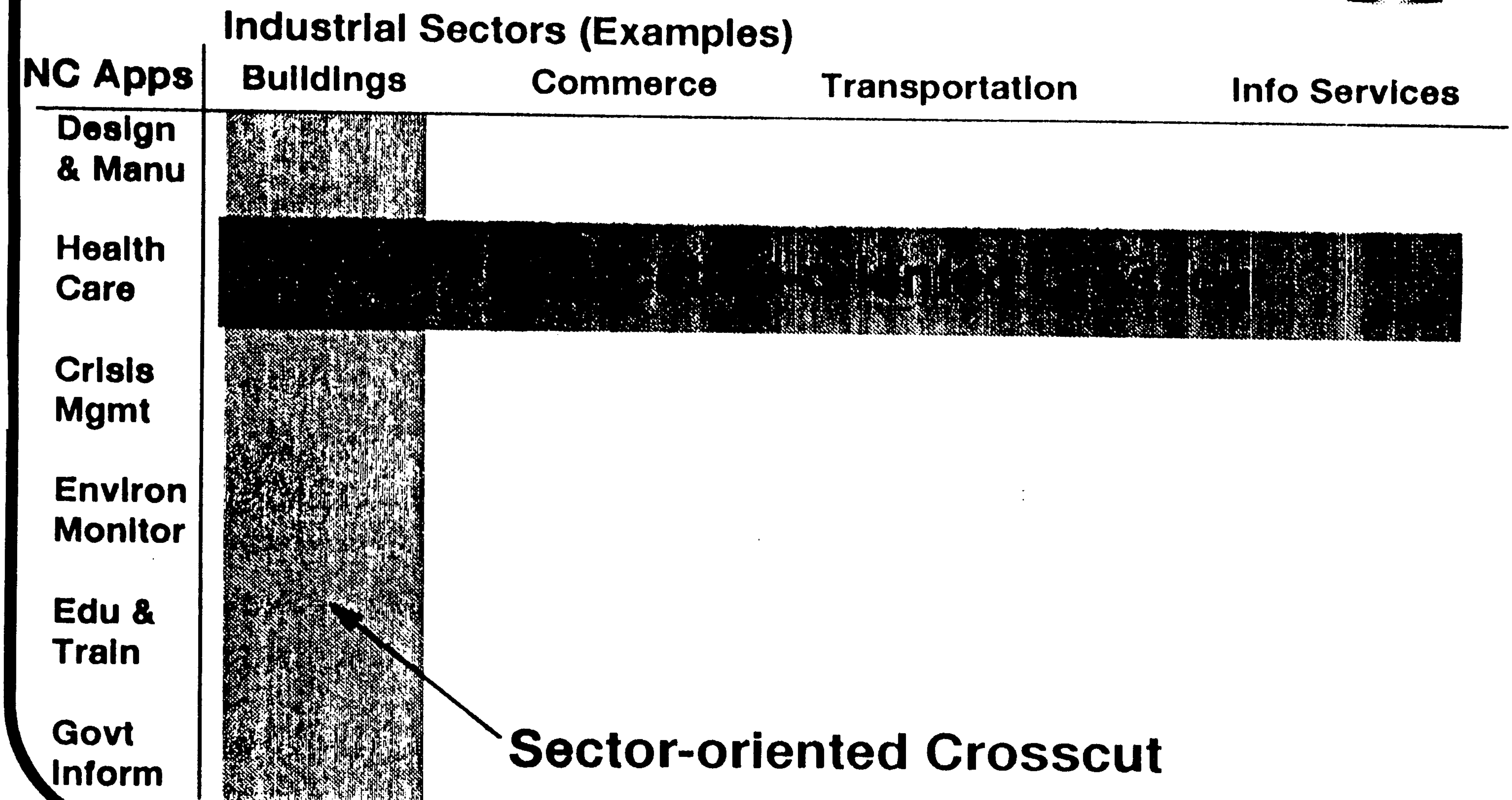
CommerceNet Directories

INFORMATION DIRECTORIES FIND HELP

Questions and comments go to feedback@commerce.net. A text-only index and view are available.


File Edit Options Navigate Annotate Hotlist
Fri 8/5/94
ConnectorLand
ConnectorLand
Search
keyword
http://www.commerce.net/information/examples/demo/cl/construction.html
ConnectorLand
...connectors for all your needs
ConnectorLand, Inc. has the lowest prices on thousands of connectors. As a distributor, we provide connectors to hundreds of electronics companies.
New Products and Announcements
CL
ConnectorLand Overview, Facts, and SEC Report
Products and Services
Catalogs and Road Map

Testbed Strategy



ARPA

Testbed Strategy

NIE

Industrial Sectors (Examples)

NC Apps	Buildings	Commerce	Transportation	Info Services
Design & Manu	Smart Factory	Supply Chain	Material Tracking	Design Expertise
Health Care	Smart Hospitals	Claims Processing	EMS Dispatch	Self Medical Diagnosis
Crisis Mgmt	C & C Center	Crisis Managers for Hire	Logistical Planning	Historic Retrospectives
Environ Monitor	In-building Sensors	Monitoring for Payment	Air Quality Monitoring	Land Use Information
Edu & Train	Electronic Classroom	Courseware Rental	Training Simulators	Multimedia Digital Libraries
Govt Inform	Info Kiosk	Electronic Procurement	Carpool Formation	Government EForms

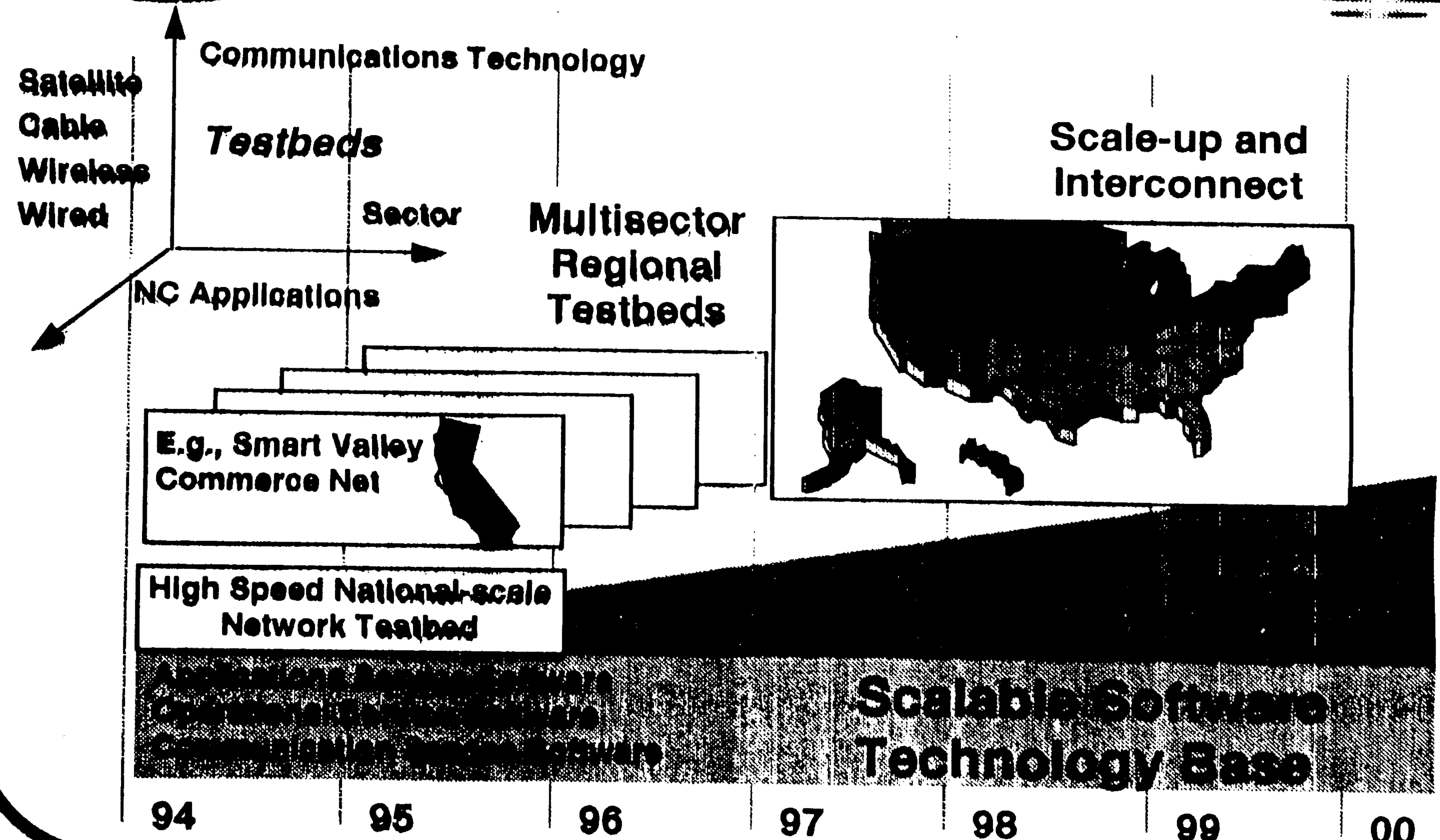
Testbed Strategy

NIE

Industrial Sectors (Incomplete!)

NC Apps	Buildings	Commerce	Transportation	Info Services
Design & Manu		CommerceNet, EINet		CommerceNet, EINet
Health Care				
Crisis Mgmt			IVHS (DoT)	Integrated Public Safety Nets (NPR)
Environ Monitor				NEI, Natl Env Data Index (NPR)
Edu & Train				NSF Eng. Edu. [illegible]
Govt Inform		[illegible] Data Index (NPR)		State of Iowa, North Carolina, USDA (ACE Pro)

Testbed Strategy



For Official Use Only

Very High Speed Signal Acquisition and Processing

Professor Thomas A. Prince

California Institute of Technology

High Speed Signal Acquisition and Processing

Thomas A. Prince
California Institute of Technology

DSSG Symposium
November 1, 1994

SOME DISTURBING QUESTIONS:

WHY IS AN EXPERIMENTAL ASTROPHYSICIST GIVING A TALK AT A COMPUTING SYMPOSIUM?

(ANSWER: BECAUSE IT'S ALMOST HALLOWEEN?)

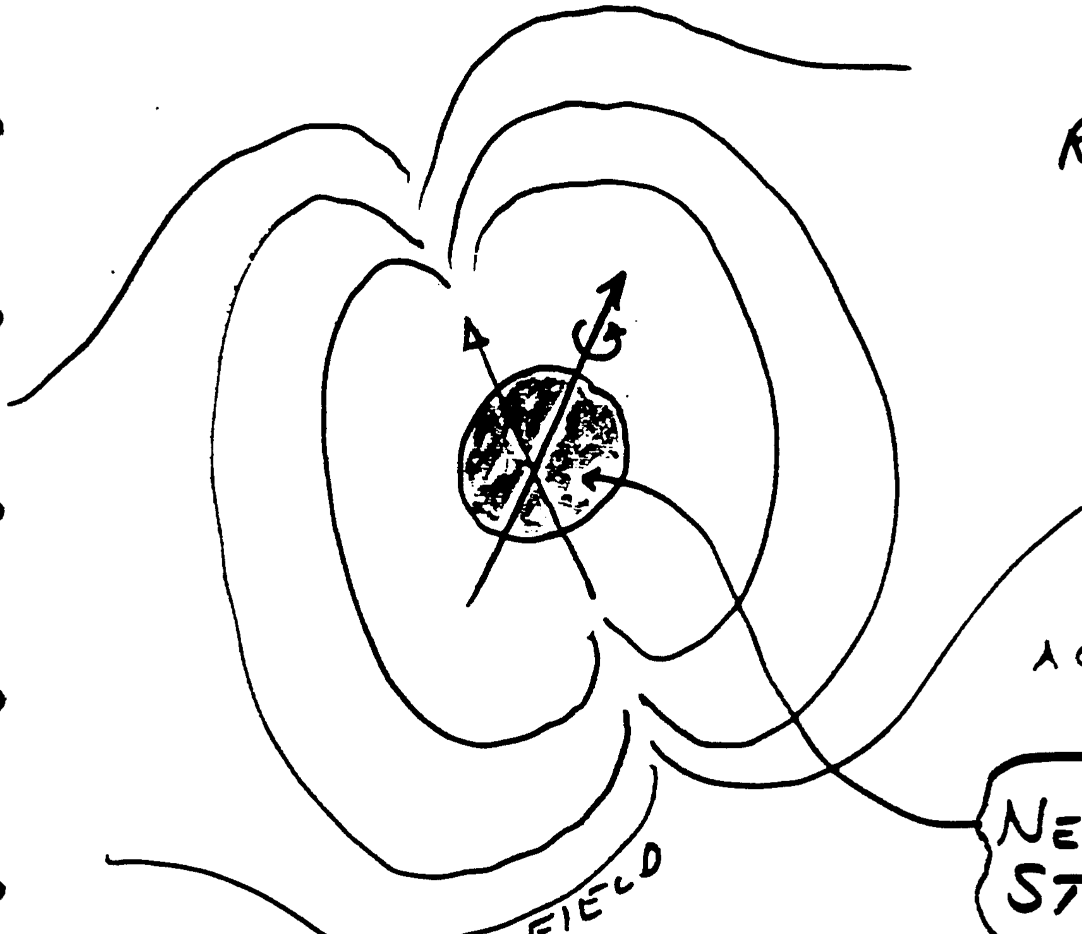
WHO COULD POSSIBLY GET EXCITED ABOUT A TAPE RECORDER?

(ANSWER: AN EXPERIMENTAL ASTROPHYSICIST)

HOW DOES AN EXPERIMENTALIST VIEW A SUPERCOMPUTER?

(ANSWER: IT'S A FANCY OSCILLOSCOPE)

PULSARS



ROTATION:
0.2 → 1000 Hz

MOST EXOTIC
STABLE MATTER
ACCESSIBLE TO DIRECT
OBSERVATION

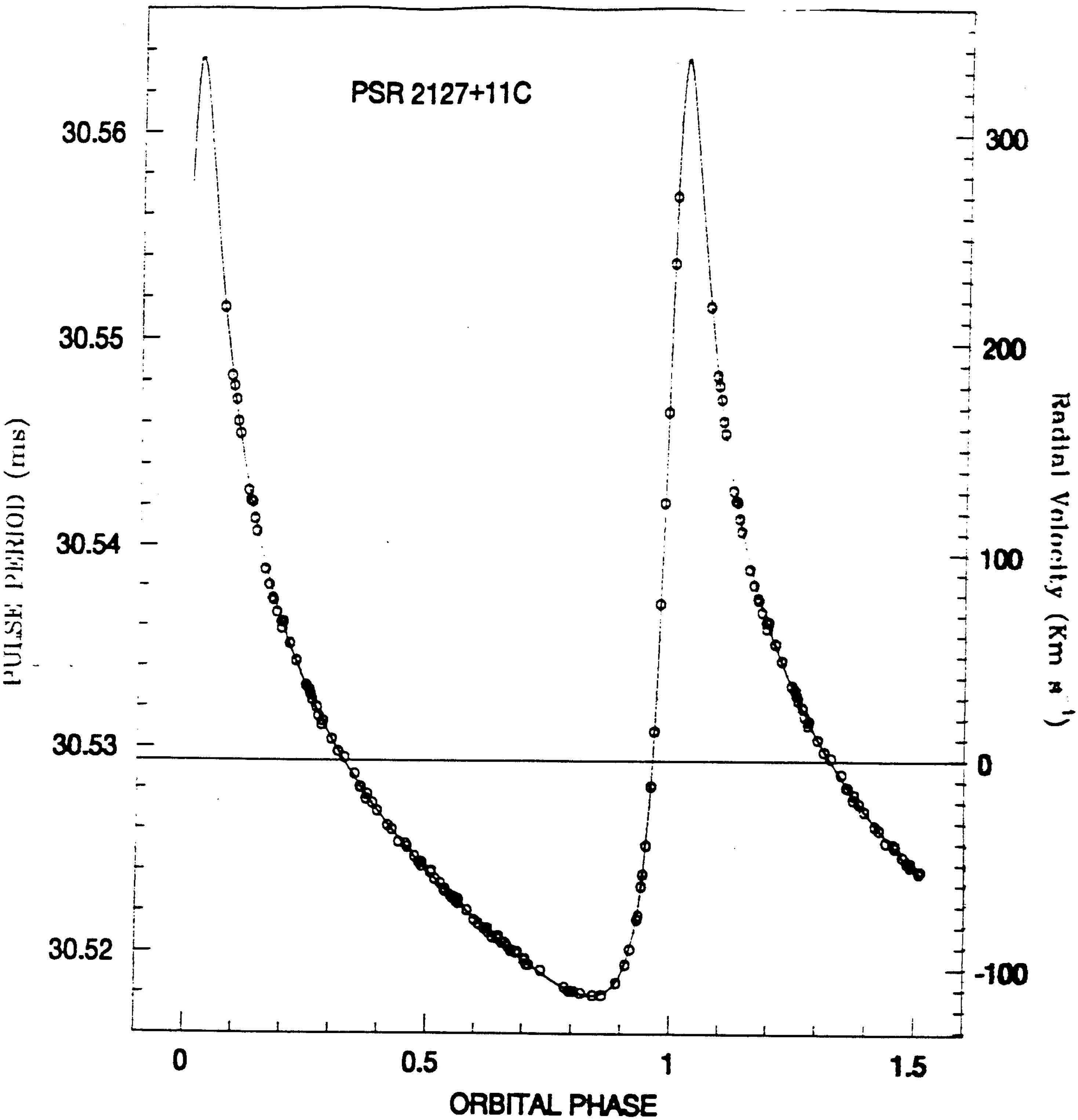
NEUTRON
STAR

MAGNETIC FIELD

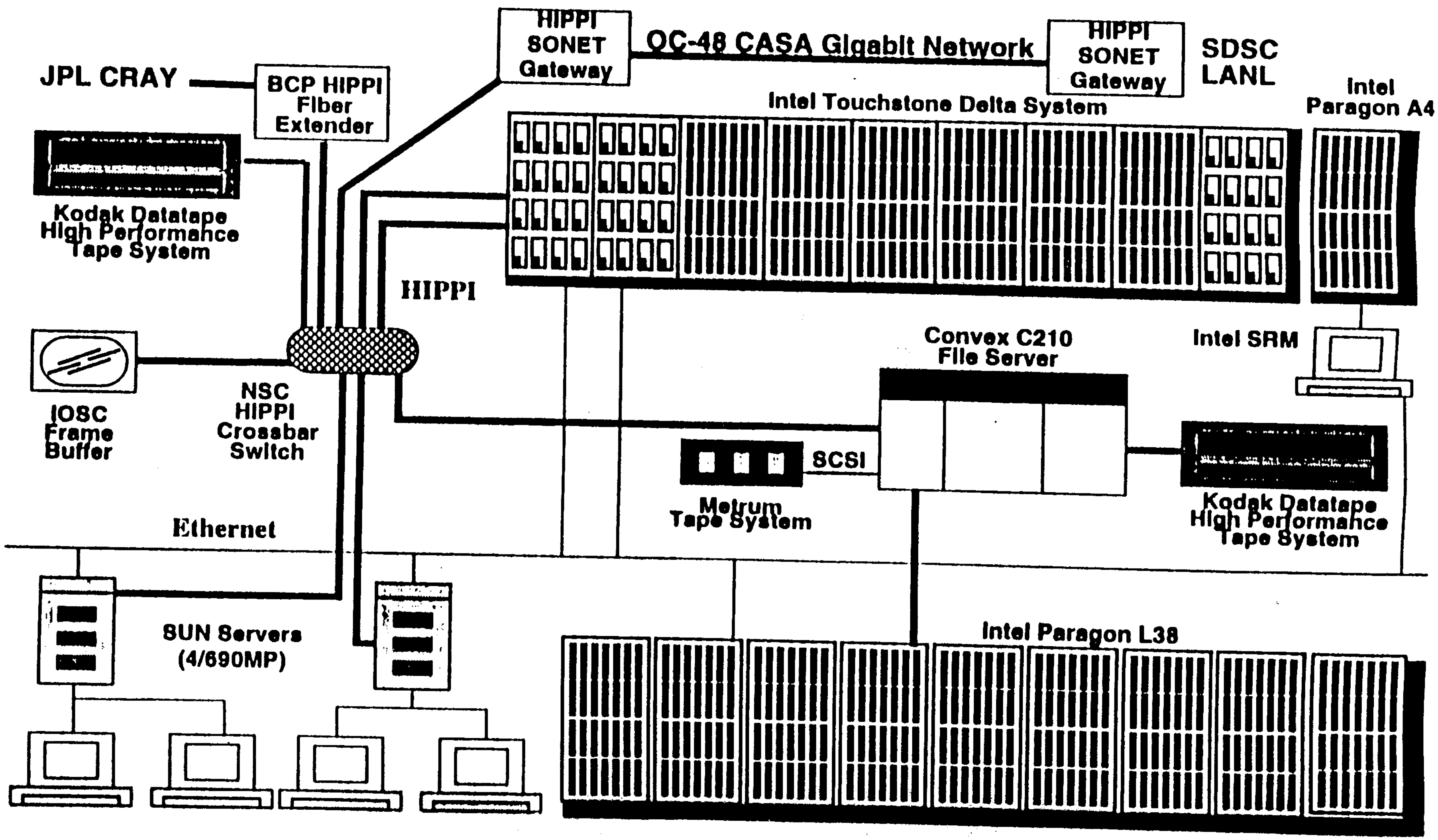
MAG FIELD:
UP TO 1 TRILLION
X EARTH
($10^8 - 10^{13}$ GAUSS)

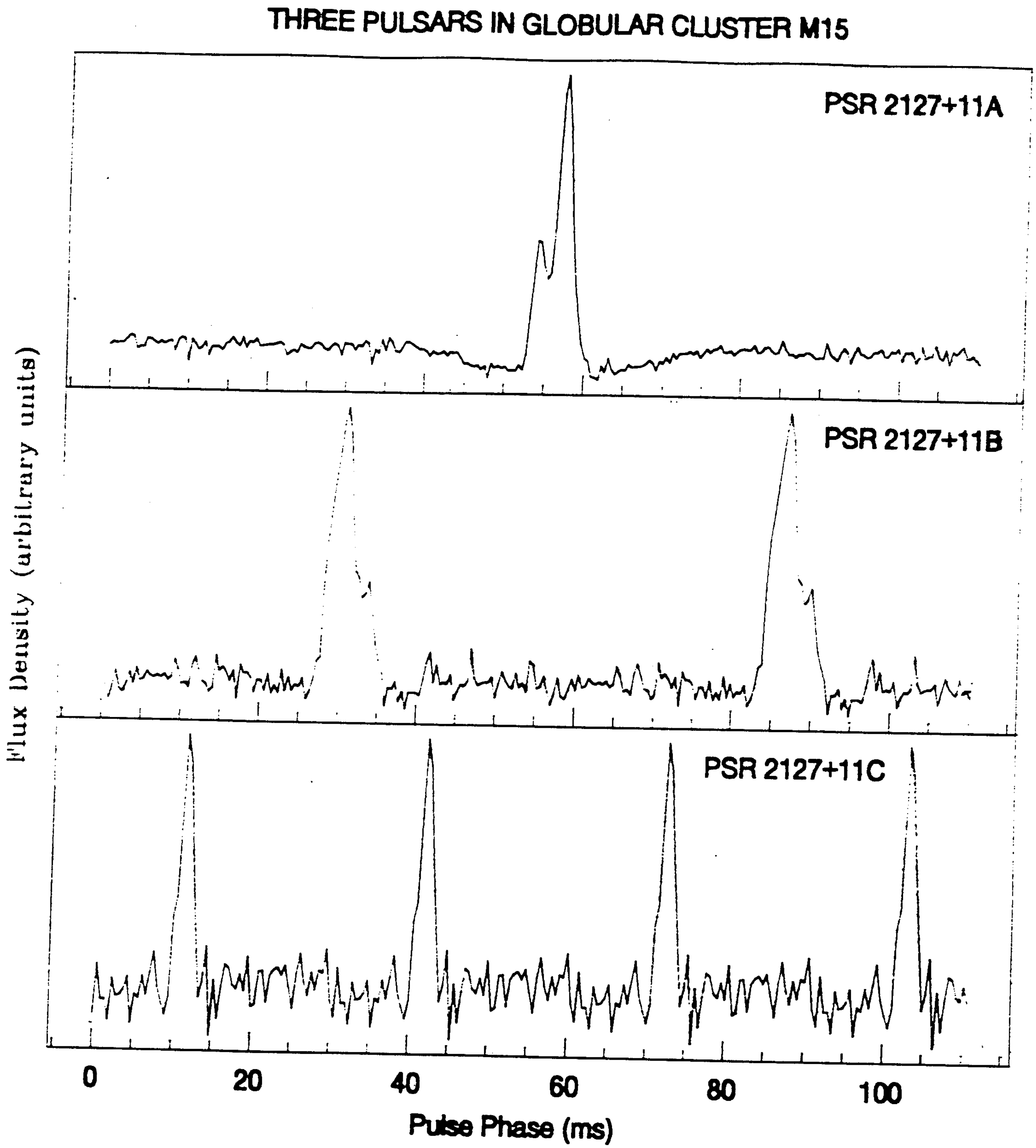
MASS ~ 1.4 SOLAR
MASS

DENSITY ~ 1 BILLION TONS
PER TBS
(10^{15} g/cc)


PSR 2127+11C
30.56
30.55
30.54
30.53
30.52
PULSE PERIOD (ms)
300
200
100
0
-100
Radial Velocity (Km s-1)
0
0.5
1
1.5
ORBITAL PHASE

CSCC COMPUTER ENVIRONMENT

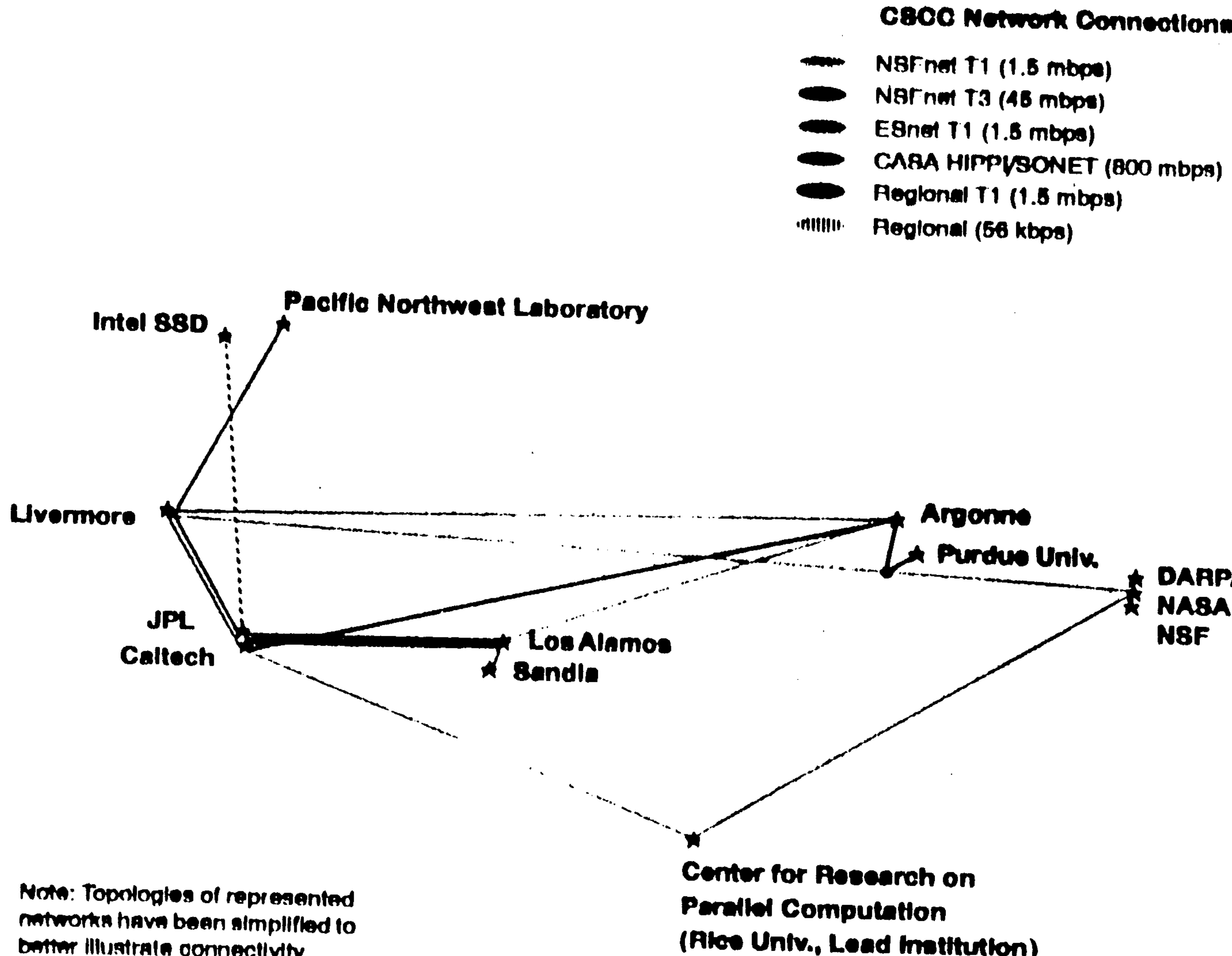




THREE PULSARS IN GLOBULAR CLUSTER M15
PSR 2127+11A
PSR 2127+11B
PSR 2127+11C
Flux Density (arbitrary units)
0
20
40
60
80
100
Pulse Phase (ms)

MPP HARDWARE

FEATURE	DELTA	TREX	RAPTOR	JPL CRAY
MODEL	DELTA	XPS L38	XPS A4	T3D
GFLOPS	30.7	38.4	4.3	38.4
NODES, PE's PER NODE	513, 1 PE	512, 1 PE & 1 Comms Procsr.	52, 1 PE & 1 Comms Procsr.	128, 2PE's
CPU	i860 XR	i860 XP	i860 XP	DEC 21064
SPEED	40 MHZ	50 MHZ	50 MHZ	150 MHZ
INTERNODE	25 MBYTES	200 MBYTES	200MBYTES	300 MBYTE/2
MFLOPS/CPU	60	75	75	150
MB/NODE	16/PE	32	32	64
TOTAL GB	8.2	16.4	1.8	16.4
DISKS IN GB's	93 (RAID0)	67.2 (RAID3)	14.4 (RAID3)	103
TOPOLOGY	2D (16X36)	2D (16X36)	2D (16X4)	3D TORUS



Note: Topologies of represented networks have been simplified to better illustrate connectivity between CSCC sites

Concurrent Supercomputing Consortium (CSCC)

- A consortium of research institutions and federal agencies
- Goal: exploit massively parallel computers for science and engineering calculations
- Caltech is lead institution
- Major initiatives:
  - –Intel Touchstone Delta (1991)
  - –Scalable I/O Initiative (1994)

Concurrent Supercomputing Consortium (CSCC) Membership

- Additional members of the consortium are:
  - Lawrence Livermore National Laboratory
  - Los Alamos National Laboratory
  - Purdue University
  - Sandia National Laboratories

Concurrent Supercomputing Consortium (CSCC) Membership

- The consortium's partners are:
  - Argonne National Laboratory
  - California Institute of Technology
  - Caltech's Jet Propulsion Laboratory
  - The Center for Research in Parallel Computation
    - (a National Science Foundation Science and Technology Center: Rice, Caltech, Argonne, Los Alamos, Syracuse, Tennessee/Oak Ridge)
  - Defense Advanced Research Projects Agency
  - Intel Corporation's Supercomputer Systems Division
  - National Aeronautics and Space Administration (NASA)
  - National Science Foundation programs in computational science and engineering
  - Pacific Northwest Laboratory

What is a High-Performance Computing Environment?

Entire Environment is Important

SCALABLE?

- Ops as well as Flops
- Memory size
- Mass storage
- I/O speed
- Networks
- File systems
- Archival storage
- Operating system
- Software environment
- Algorithms

Definition:

supercomputer, n.

A computer system that turns a compute-bound problem into an I/O-bound problem.

LIMITING FACTORS:

- –Memory
- –Mass Storage
- –I/O Speed

HIGH-END APPLICATIONS: SPECIFIC EXAMPLES

- **Visualization of Planetary Data**
  - Generation of 3-D perspective views with terrain rendering
  - Real time: 200 MB/frame => 13 GB/s I/O
  - On current generation machines: 1 GB/s I/O required

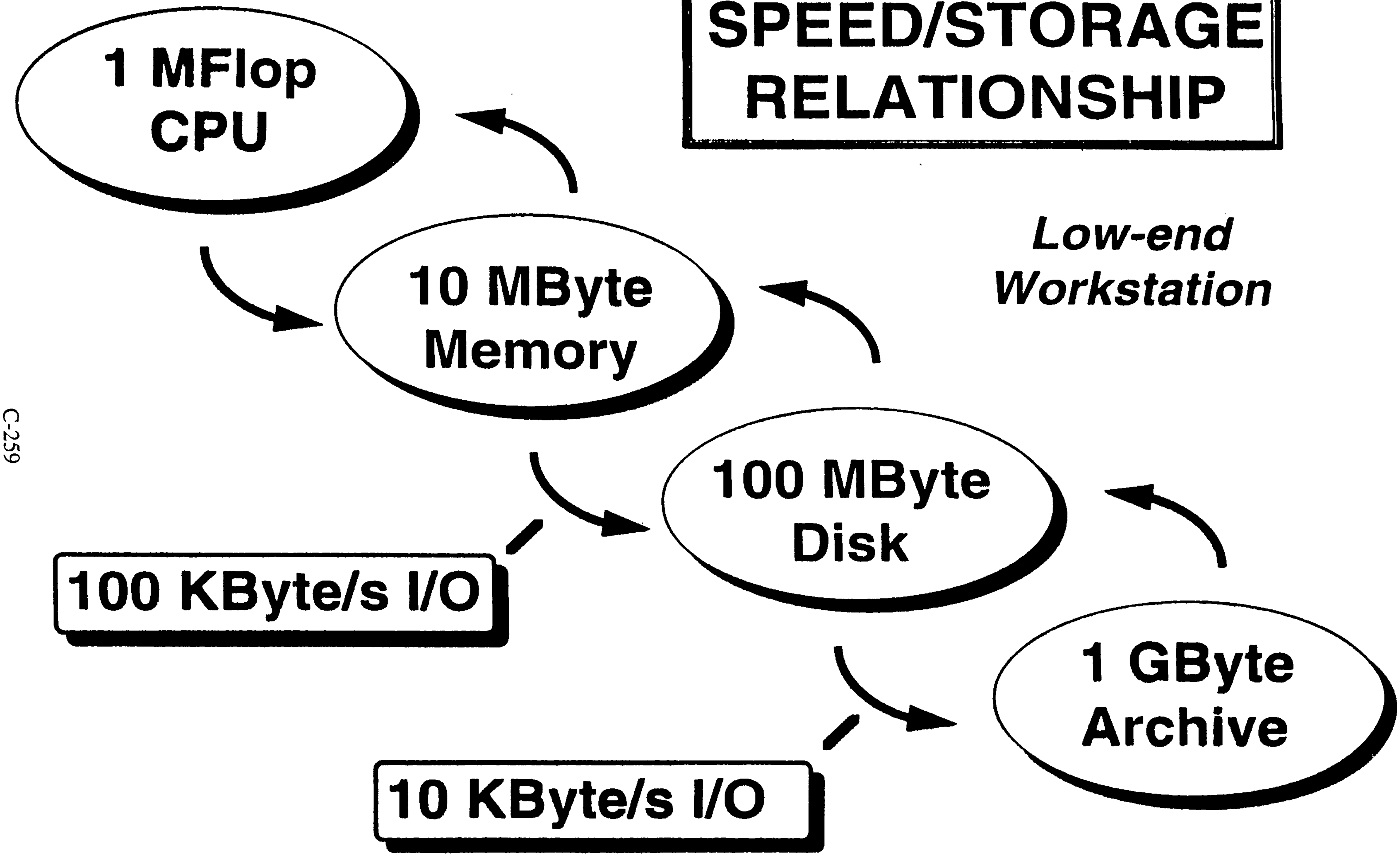
  => *I/O Limited*

- **Electromagnetic Scattering**
  - Topics: Multi-element antennas, airplanes, mm-waves
  - Bi-conjugate gradient finite element computation
  - 3-D surface integrals
  - 200,000 unknowns, 250 GBytes desirable

  => *Memory and I/O Limited*

SPEED/STORAGE RELATIONSHIP

Low-end Workstation



EXAMPLE: FFT (FAST FOURIER TRANSFORM)

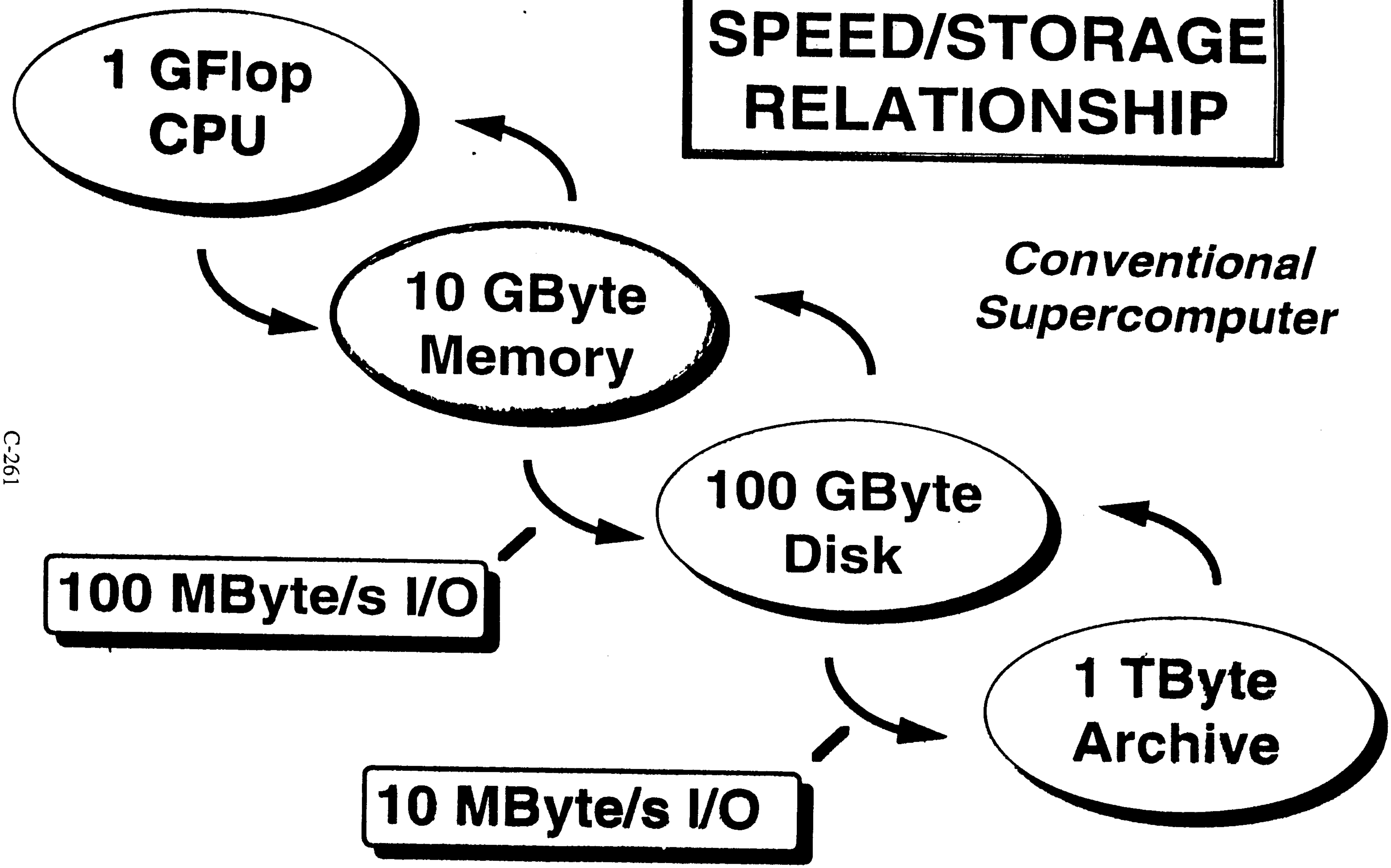
- Basic Assumption: 100 s Calculation
- 10 MBytes ~ 1 MWord (64-bit)
- 1 MFlop in 100s => 100 Flops/Word
- FFT: $\sim 5 \times N \times \log_2 N$
- $N = 10^6$ => 100 Flops/sample

- 100 KByte/s I/O => 10 MByte in 100 s

=> Computation and I/O approximately balanced

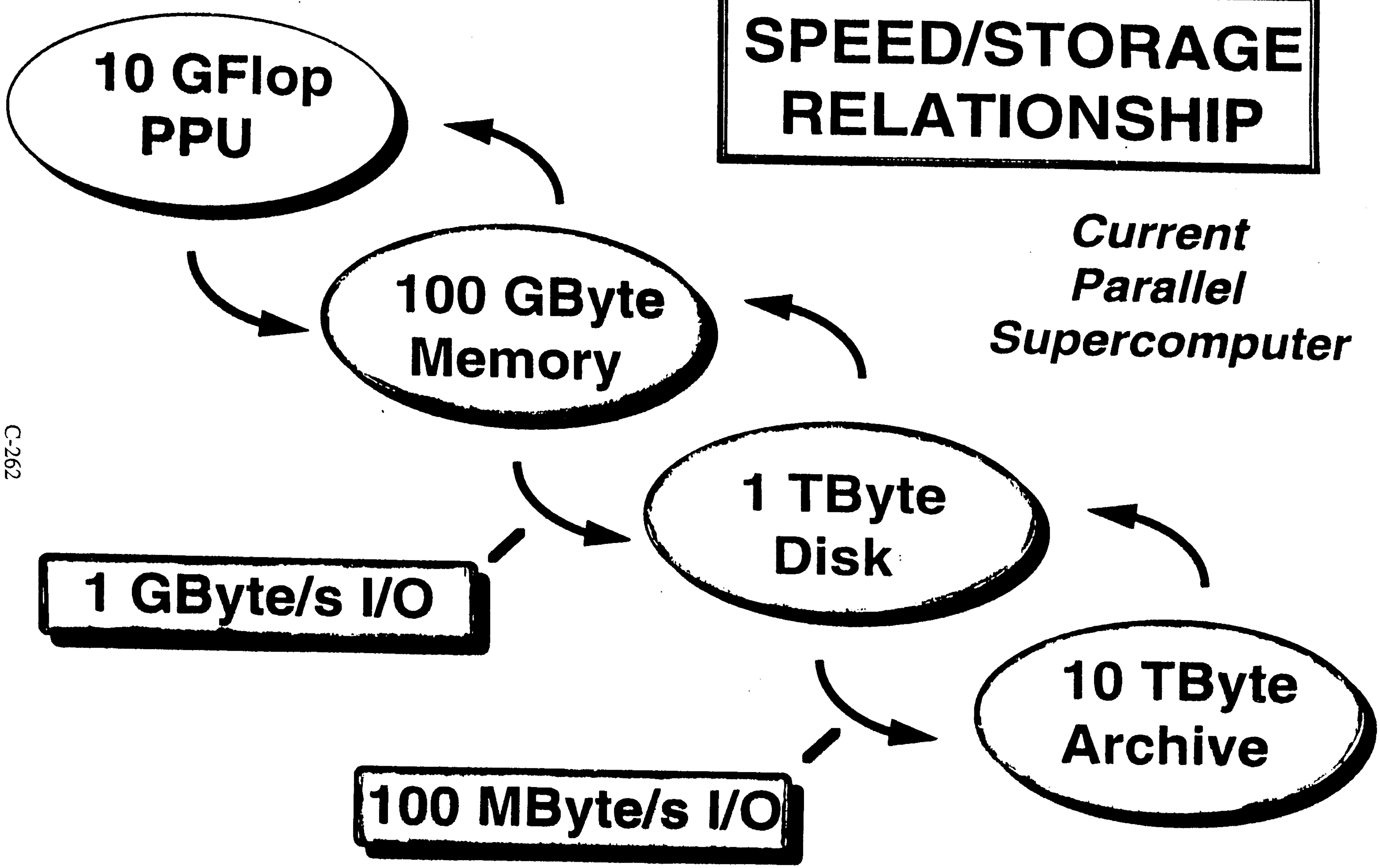
SPEED/STORAGE RELATIONSHIP

Conventional Supercomputer



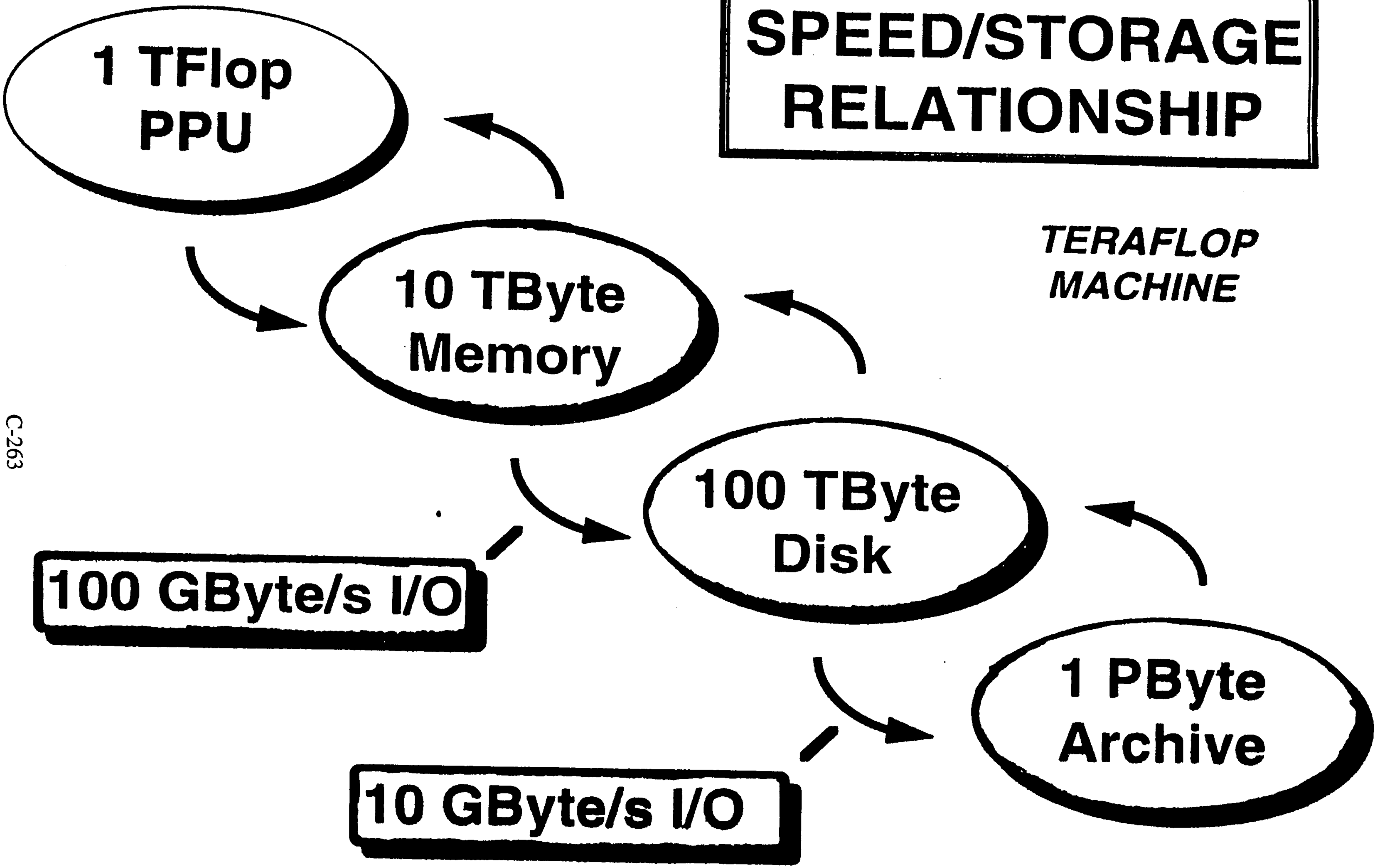
SPEED/STORAGE RELATIONSHIP

Current Parallel Supercomputer



SPEED/STORAGE RELATIONSHIP

TERAFLOP MACHINE



SCALABLE I/O INITIATIVE

- Goal
  - Define and implement *portable* and *scalable* software and hardware techniques for I/O and data management
- Project of the CSCC
- Integrated effort of many research teams
  - System software developers
  - Computer vendors
  - Application teams
- Testbeds:
  - CSCC Intel Paragon at Caltech, IBM SP-2 at ANL, Cray T3D at JPL

SAR Applications

- SIR-C/X-SAR (NASA/JPL)
  - L- and C-band: VV,HH,HV,VH Polarizations
  - 4 Terabytes of data from 10 day shuttle mission
- Analysis on Parallel Supercomputers
  - 512 processor Intel Paragon and 256 processor Cray T3D
  - Goal: Strip-map processing in real time
  - Achieved: Correlation processing faster than real time for individual polarization/frequency channels (10 s processing for 15 s of data collection)
- Evaluation of NASA SAR Free Flyer
  - Require real time processing for 8-12 channels
  - Require large bandwidth and high-volume storage

SAR Applications

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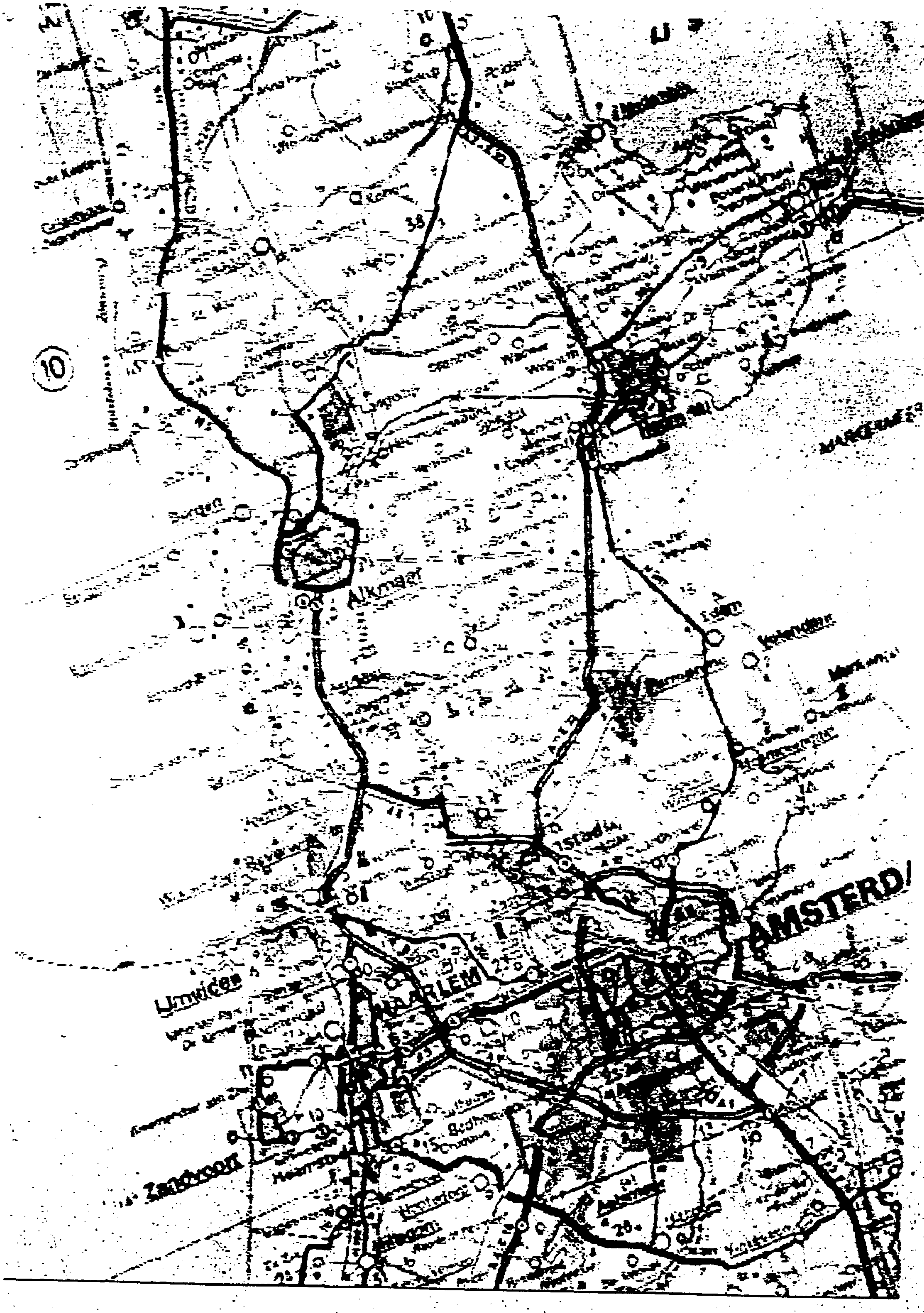
  - Require real time processing for 8-12 channels
  - Require large bandwidth and high-volume storage

$\delta_x =$:

(2653 PIXELS BY 2048 PIXELS)


10
Alkmaar
HAARLEM
AMSTERD
Zandvoort

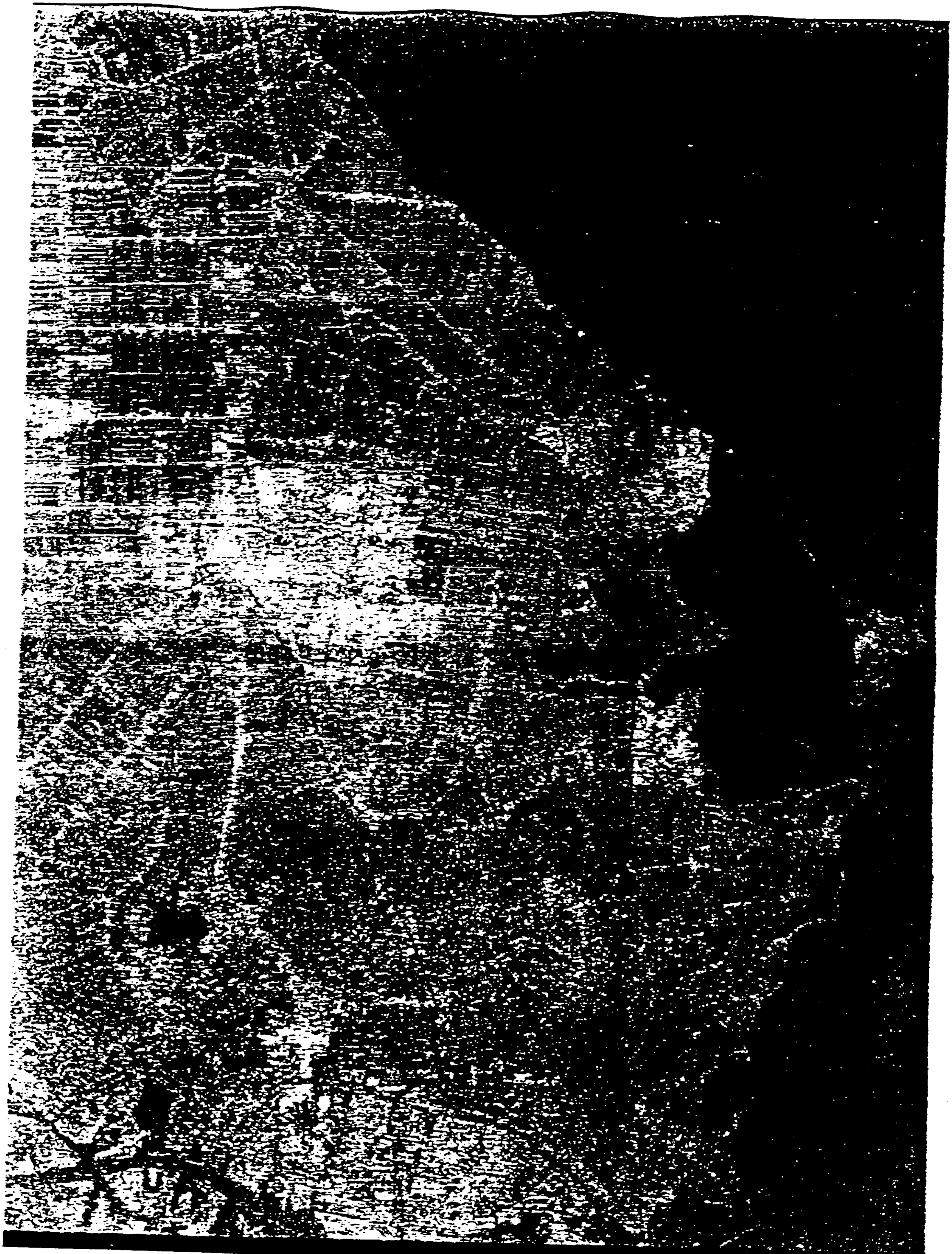


TABLE 1.2 Key Parameters for Free-flying SAR Satellite Systems

Satellite	Seasat	ALMAZ	E-ERS-1	J-ERS-1	Radarsat
Agency/Country	NASA/USA	USSR	ESA	NASDA, Japan	Canada
Launch Date	1978	1991	1991	1992	1995
Altitude (km)	800	280	785	565	792
Frequency Band (GHz)	L(1.3)	S(3.0)	C(5.3)	L(1.2)	C(5.3)
Polarization	HH	HH	VV	HH	HH
Incidence Angle	23°	30–60°	23°	35°	20–50°
Antenna Size (m × m)	10.7 × 2.2	15 × 1.5 (two)	10 × 1.0	12 × 2.2	15 × 1.6
Noise Equiv σ^0 (dB)	−18	-	−18	−20	−21
Swath Width (km)	100	25–50	100	75	50–500
Az Resolution (m)/Looks	23/4	15/2	25/3	30/4	28/4
Range Bandwidth (MHz)	19	Uncoded	13.5	15	11.5, 17.3, 30
Quantization (bps)	Analog	3	5	3	4

TABLE 1.3 Key System Parameters for Selected Airborne SAR Systems

Agency	NASA JPL	NAVY ERIM	CCRS MDA
Aircraft	DC-8	NADC P-3	CV-580
Frequency (GHz)	0.44, 1.25, 5.3	1.25, 5.3, 9.34	5.3, 9.25
Polarization	Quad	Quad	Dual (like, cross)
Az Resolution (m)/Looks	8/4	2.2/1	6/7
Range Bandwidth (MHz)	20, 40	50, 100	100
Swath Width (km)	10–18	6–48	18–65
Look Angle (degrees)	10–65	11–79	0–87
Quantization (bps)	8	6	6
Noise Equiv σ^0 (far range)	−38(P), −40(L), −36(C)	−45(L), −25(C), −31(X)	−41(C)

TABLE 1.4 Key Parameters for the Shuttle Imaging Radar Missions

Mission	SIR-A	SIR-B	SIR-C	X-SAR
Date	1981	1984	1993, 1994	1993, 1994
Altitude (km)	259	225	215	215
Frequency Band (GHz)	L(1.28)	L(1.28)	L(1.28), C(5.3)	X(9.6)
Polarization	HH	HH	HH, HV, VH, VV	VV
Incidence Angle	50°	15–60°	15–60°	15–60°
Antenna Size (m × m)	9.4 × 2.2	10.7 × 2.2	12.1 × 2.8(L) 12.1 × 0.8(C)	12.1 × 0.4
Noise Equiv σ^0 (dB)	−25	−35	−50(L), −40(C)	−26
Swath Width (km)	50	15–50	30–100	10–45
Az/Rng Resolution (m)	4.7/33	5.4/14.4	6.1/8.7	6.1/8.7

$$N_{image} = 4\pi R_{earth}^2 \left(\frac{1}{W^2}\right) f_{earth} \sim 15000 \left(\frac{W}{100km}\right)^{-2} \left(\frac{f_{earth}}{0.3}\right)$$

$$R_{image} = 2\pi R_{earth} \left(\frac{1}{W}\right) \left(\frac{1}{T_{orb}}\right) \sim \left(\frac{1}{13.5s}\right) \left(\frac{W}{100km}\right)^{-1} \left(\frac{T_{orb}}{90min}\right)^{-1}$$

$$R_{data} = 2R_{image} \left[\frac{W^2}{(\delta x)(\delta r)}\right] \sim (3.7MB/s) \left(\frac{T_{orb}}{90min}\right)^{-1} \left(\frac{W}{100km}\right) \left(\frac{\delta x}{20m}\right)^{-1} \left(\frac{\delta r}{20m}\right)^{-1}$$

		SEASAT
Swath Width (km)	W	100 km
Azimuthal Resolution (m)	δx	23 m
Range Resolution (m)	δr	20 m

		Nominal
Fraction of earth surface	f_{earth}	0.3
Radius of earth (km)	R_{earth}	6400
Orbital Period (minutes)	T_{orb}	90

EVALUATION OF A FREE FLYER

$$N_{image} = 4\pi R^2_{earth}\left(\frac{1}{W^2}\right) f_{earth} \sim 15000\left(\frac{W}{100km}\right)^{-2}\left(\frac{f_{earth}}{0.3}\right)$$

$$R_{image} = 2\pi R_{earth}\left(\frac{1}{W}\right)\left(\frac{1}{T_{orb}}\right) \sim \left(\frac{1}{13.5s}\right)\left(\frac{W}{100km}\right)^{-1}\left(\frac{T_{orb}}{90min}\right)^{-1}$$

$$R_{data} = 2R_{image}\left[\frac{W^2}{(\delta x)(\delta r)}\right] \sim (3.7MB/s)\left(\frac{T_{orb}}{90min}\right)^{-1}\left(\frac{W}{100km}\right)\left(\frac{\delta x}{20m}\right)^{-1}\left(\frac{\delta r}{20m}\right)^{-1} \times \underbrace{8}_{\text{SIR-C}}$$

~30MB/s

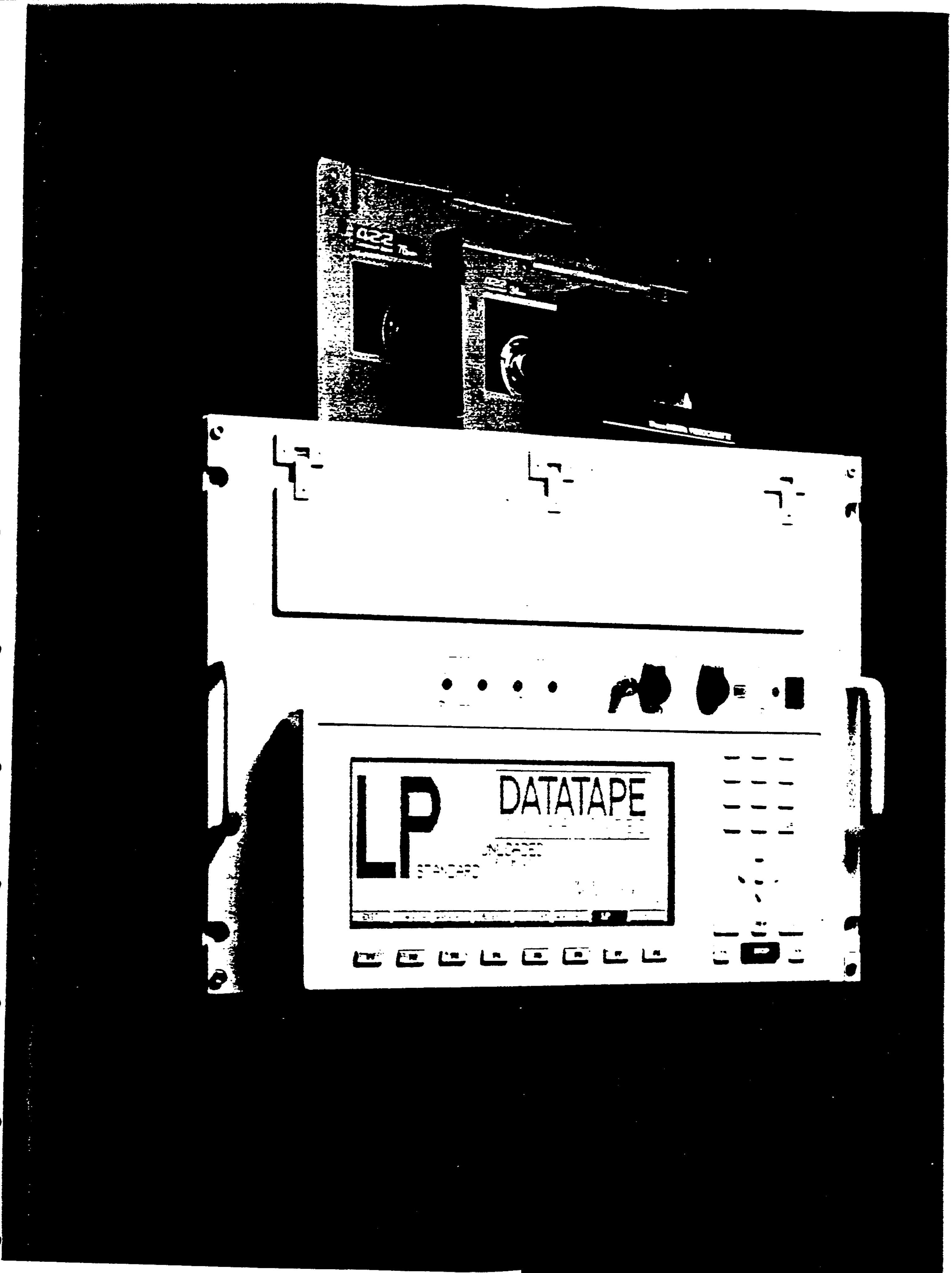
~2.5 TB/d

NEED HIGH BANDWIDTH, LARGE VOLUME ARCHIVAL STORAGE.

ID-1 TAPES?

		SEASAT
Swath Width (km)	W	100 km
Azimuthal Resolution (m)	δx	23 m
Range Resolution (m)	δr	20 m

		Nominal
Fraction of earth surface	f_{earth}	0.3
Radius of earth (km)	R_{earth}	6400
Orbital Period (minutes)	T_{orb}	90


LP
DATATAPE
UNLOADED
STANDARD

Broadband Signal Acquisition

- Digital recording system for signal acquisition
  - 100 MHz bandwidth
  - Based on 400 Mbit/s Datatape LP recorders
  - Custom analog/digital VLSI interface
  - Playback into parallel supercomputre with same recorders
- Application: Radio astronomy
- Advantages over special purpose hardware
  - Flexibility: *post facto* optimization and iteration of detection algorithms
  - Retains full phase information of signal
  - Integrated digital approach to acquisition/reduction/storage

Broadband Signal Acquisition

- Digital recording system for signal acquisition
  - 100 MHz bandwidth
  - Based on 400 Mbit/s Datatape LP recorders (100 GBYTE/CARTRIDGE)
  - Custom analog/digital VLSI interface
  - Playback into parallel supercomputre with same recorders
- Application: Radio astronomy
- Advantages over special purpose hardware
  - Flexibility: *post facto* optimization and iteration of detection algorithms
  - Retains full phase information of signal
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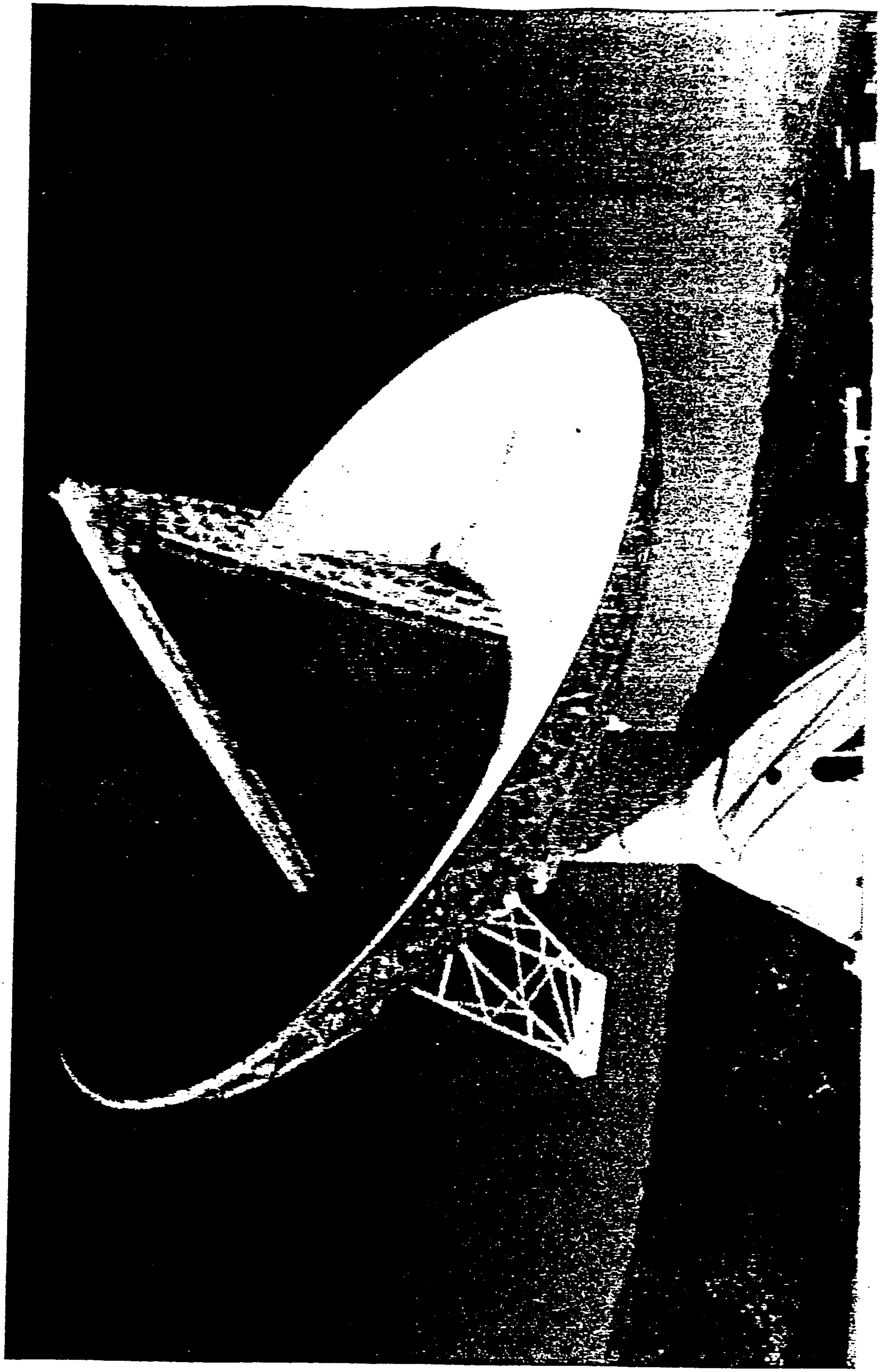
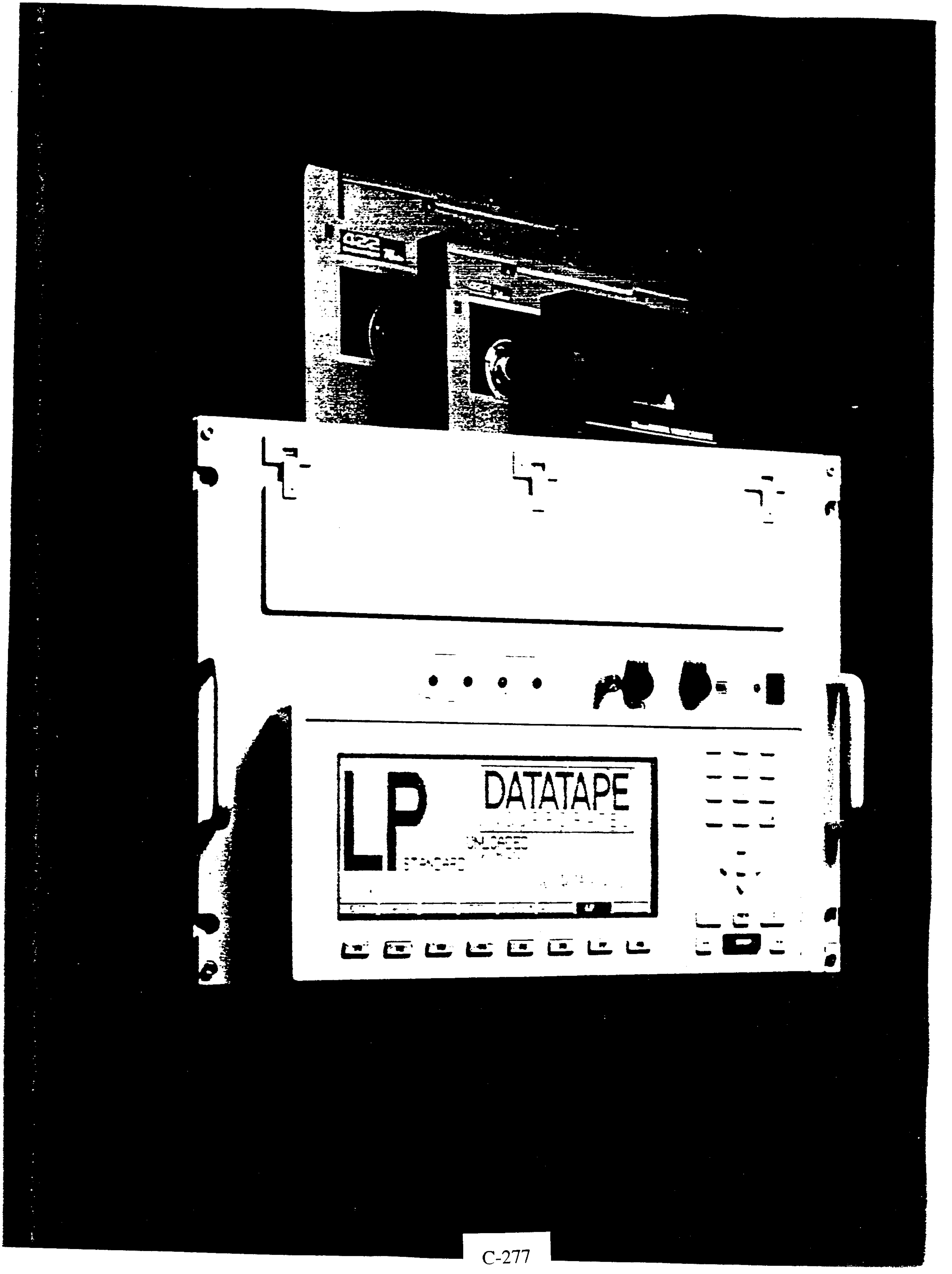
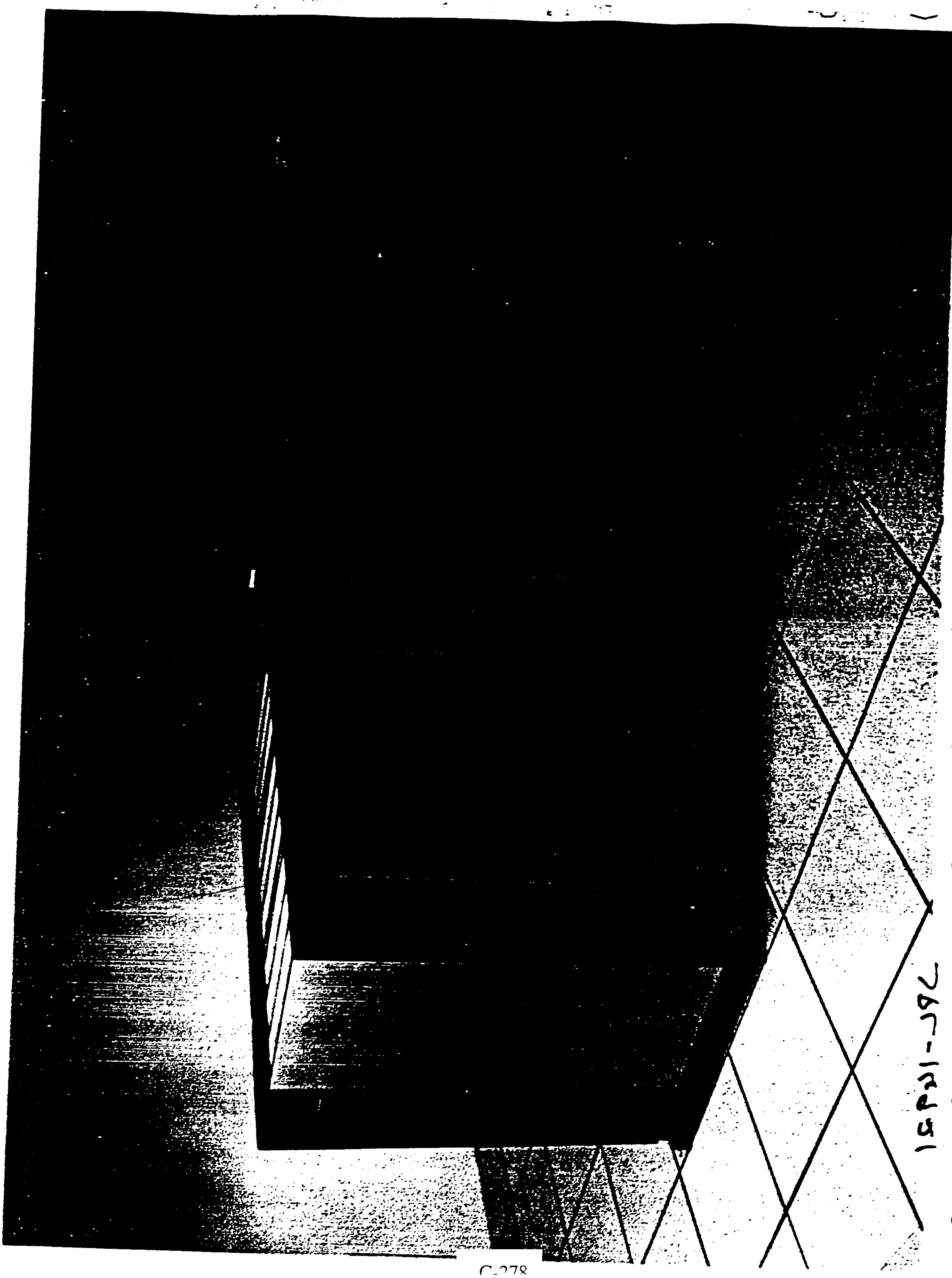
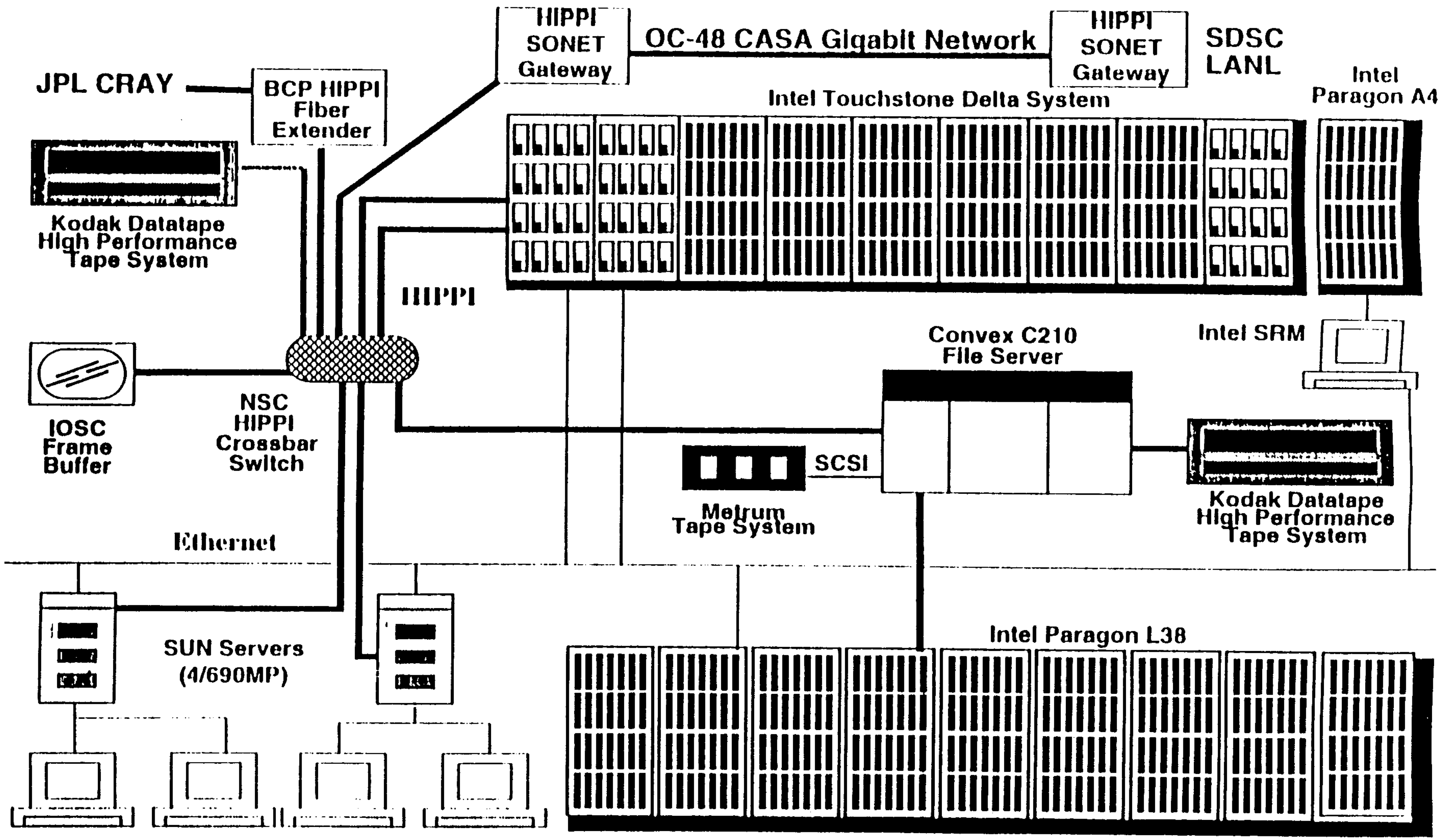



LP
DATATAPE
STANDARD
UNLOADED



1542-1796

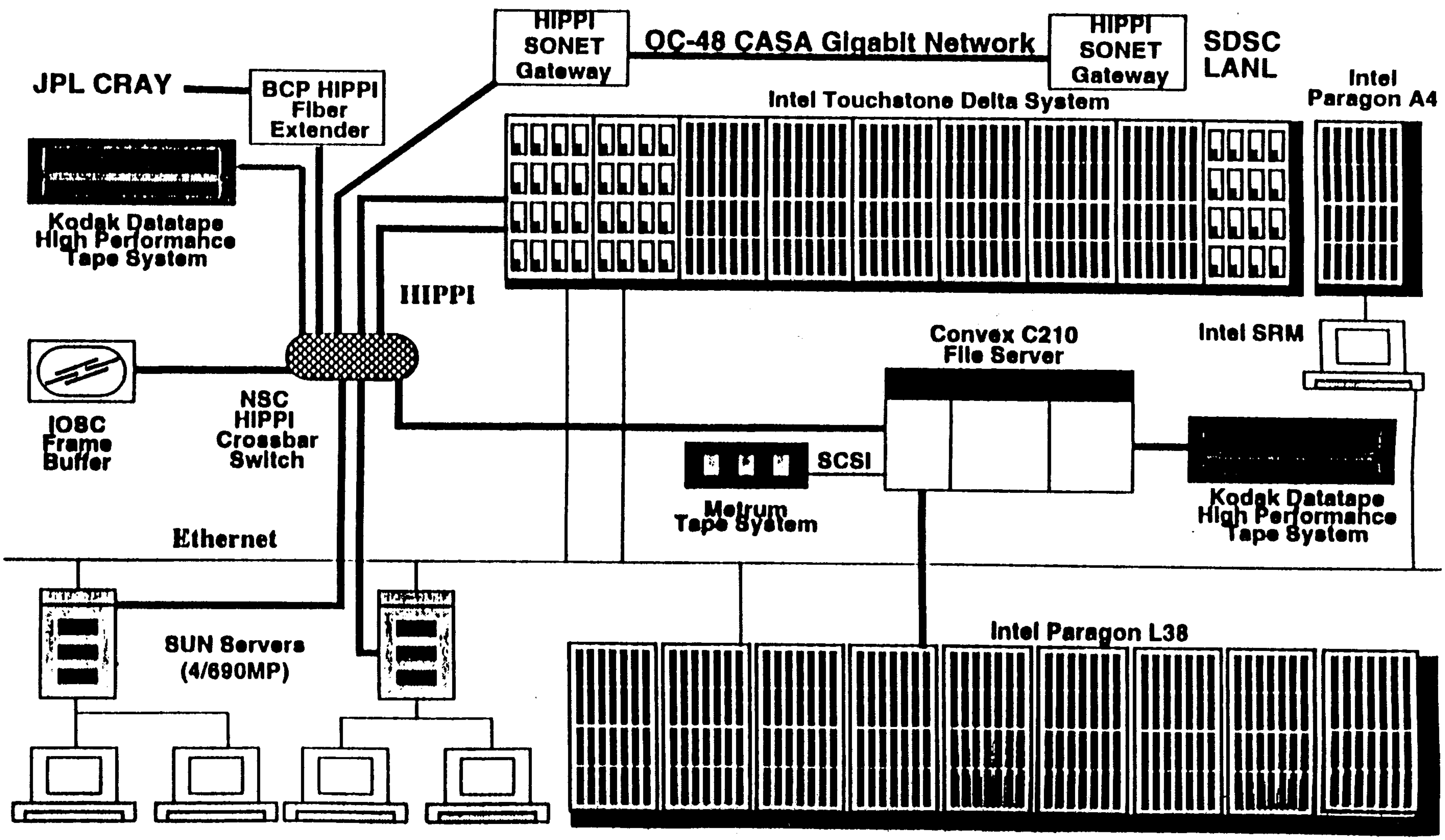
CSCC COMPUTER ENVIRONMENT



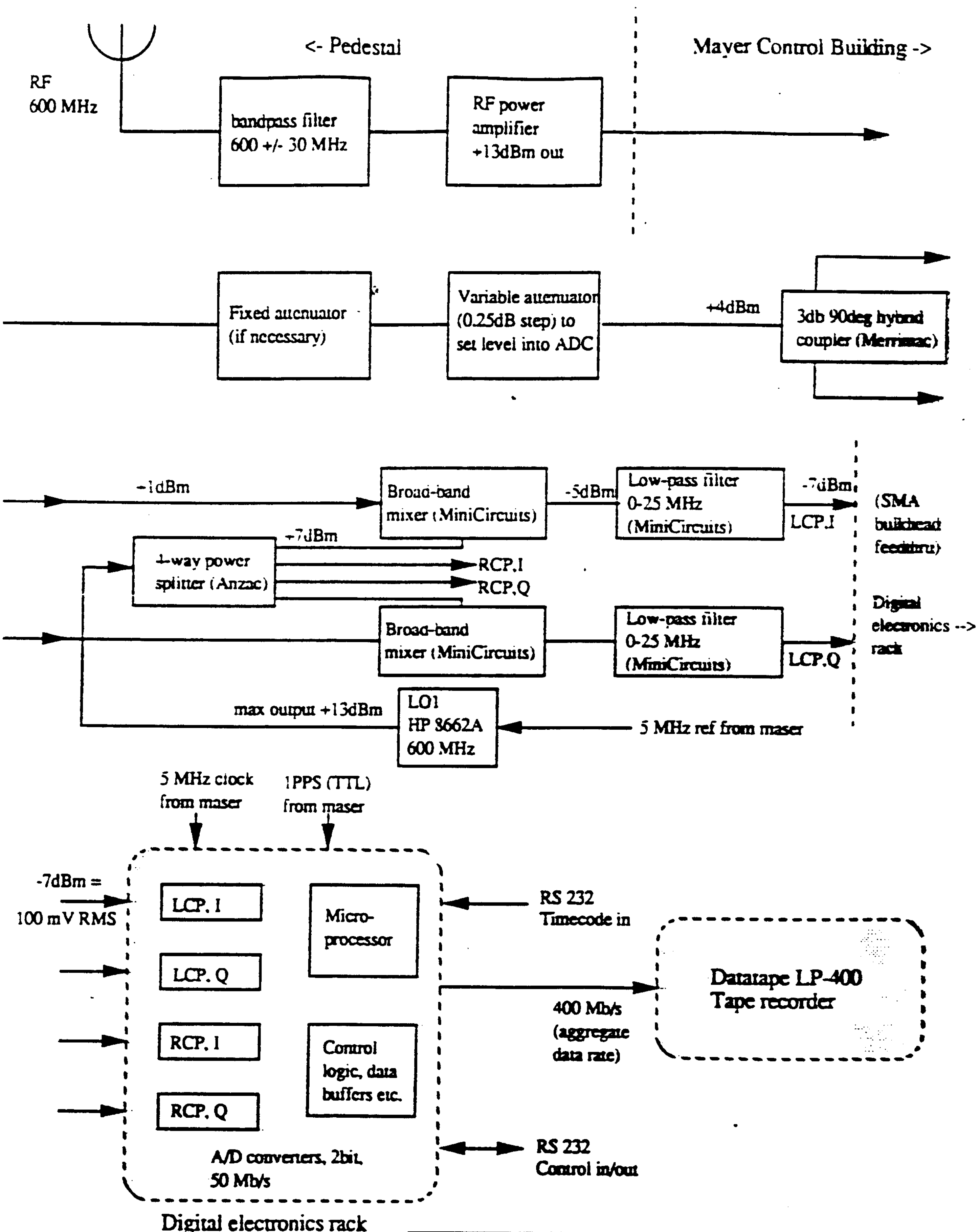
MPP HARDWARE

FEATURE	DELTA	TREX	RAPTOR	JPL CRAY
MODEL	DELTA	XPS L38	XPS A4	T3D
GFLOPS	30.7	38.4	4.3	38.4
NODES, PE's PER NODE	513, 1 PE	512, 1 PE & 1 Comms Procsr.	52, 1 PE & 1 Comms Procsr.	128, 2PE's
CPU	i860 XR	i860 XP	i860 XP	DEC 21064
SPEED	40 MHZ	50 MHZ	50 MHZ	150 MHZ
INTERNODE	25 MBYTES	200 MBYTES	200MBYTES	300 MBYTE/2
MFLOPS/CPU	60	75	75	150
MB/NODE	16/PE	32	32	64
TOTAL GB	8.2	16.4	1.8	16.4
DISKS IN GB's	93 (RAID0)	67.2 (RAID3)	14.4 (RAID3)	103
TOPOLOGY	2D (16X36)	2D (16X36)	2D (16X4)	3D TORUS

CSCC COMPUTER ENVIRONMENT



OVRO 40-m telescope 600-MHz receiver and digital recorder block diagram



Note: Except for LO1 and 4-way splitter, the entire RF-baseband chain must be duplicated for second polarization

Figure 2

SCU 6.3.94

Pulsar Digital Recording System

Overview of digital hardware (single wire-wrap board)

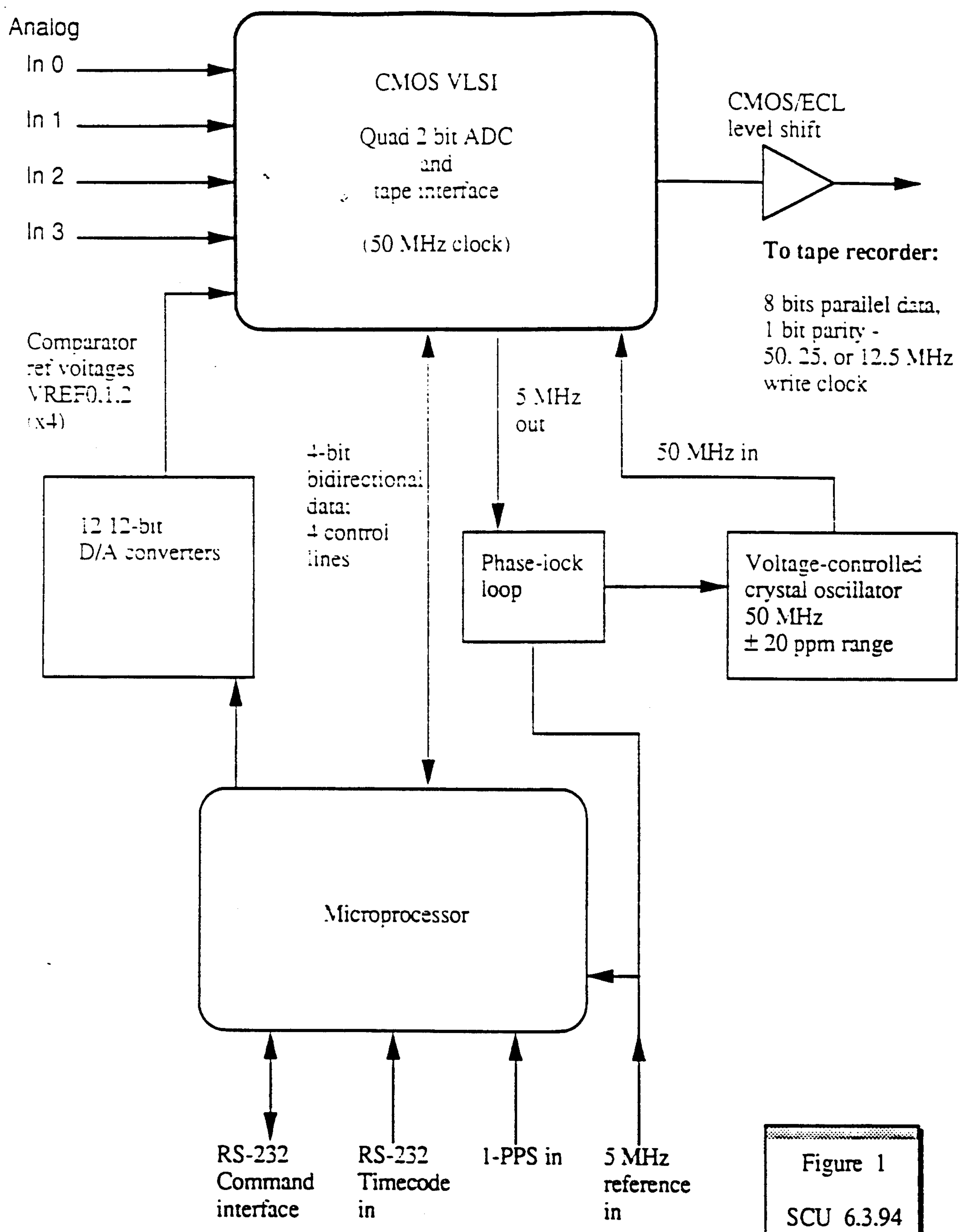
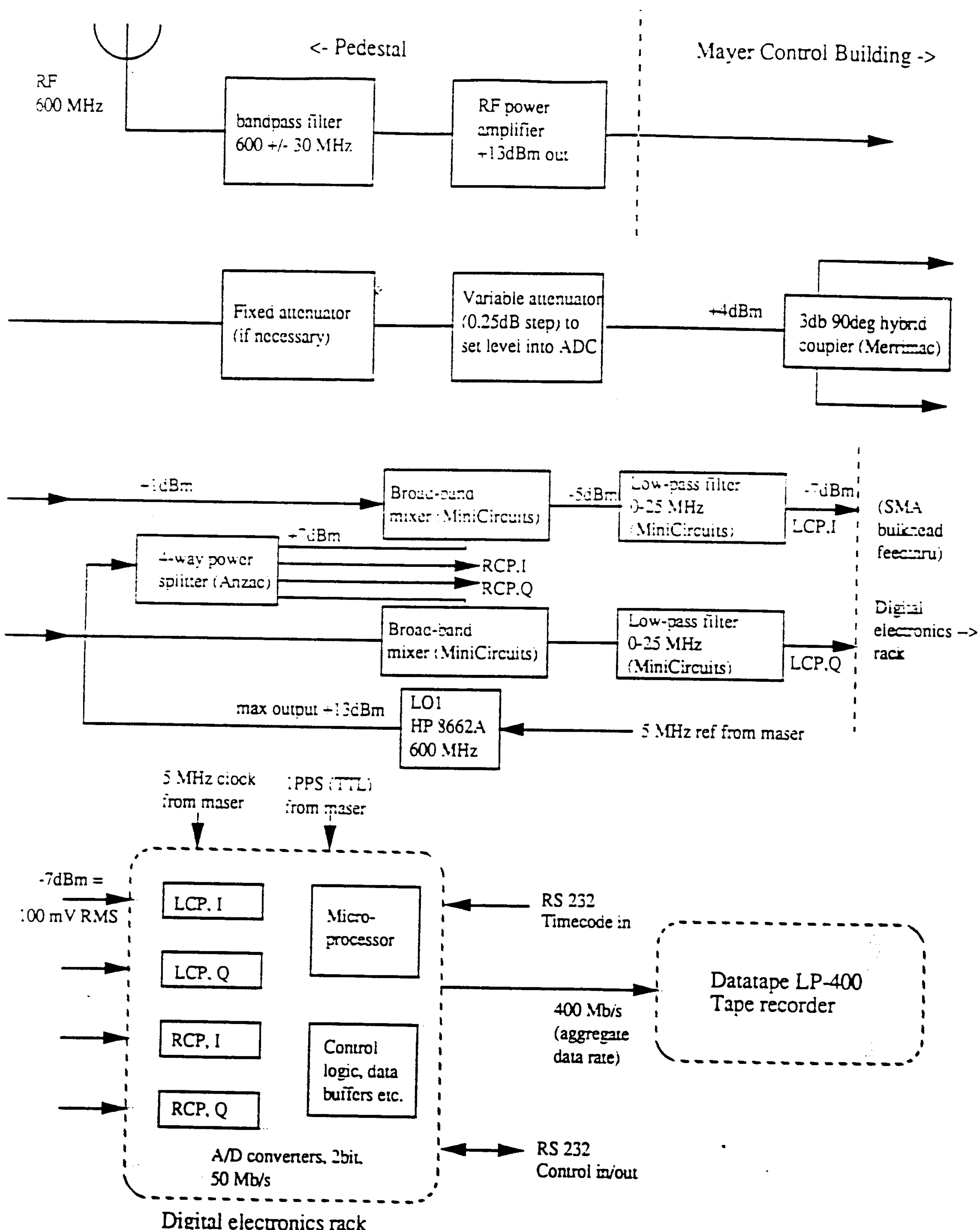


Figure 1

SCU 6.3.94

OVRO 40-m telescope 600-MHz receiver and digital recorder block diagram



Note: Except for LO1 and 4-way splitter, the entire RF-baseband chain must be duplicated for second polarization

Figure 2

SCU 6.3.94

Pulsar Digital Recording System

Overview of digital hardware (single wire-wrap board)

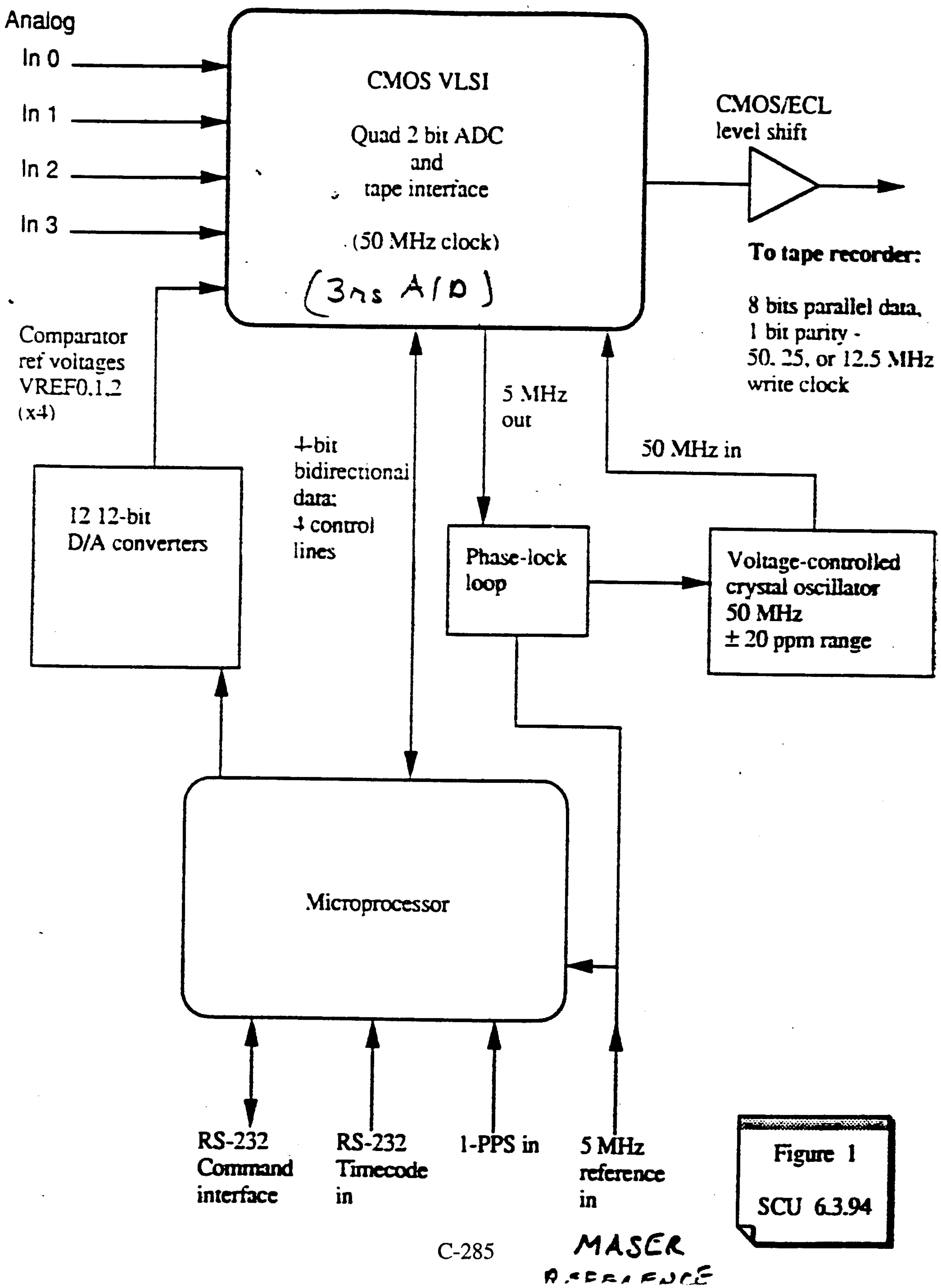
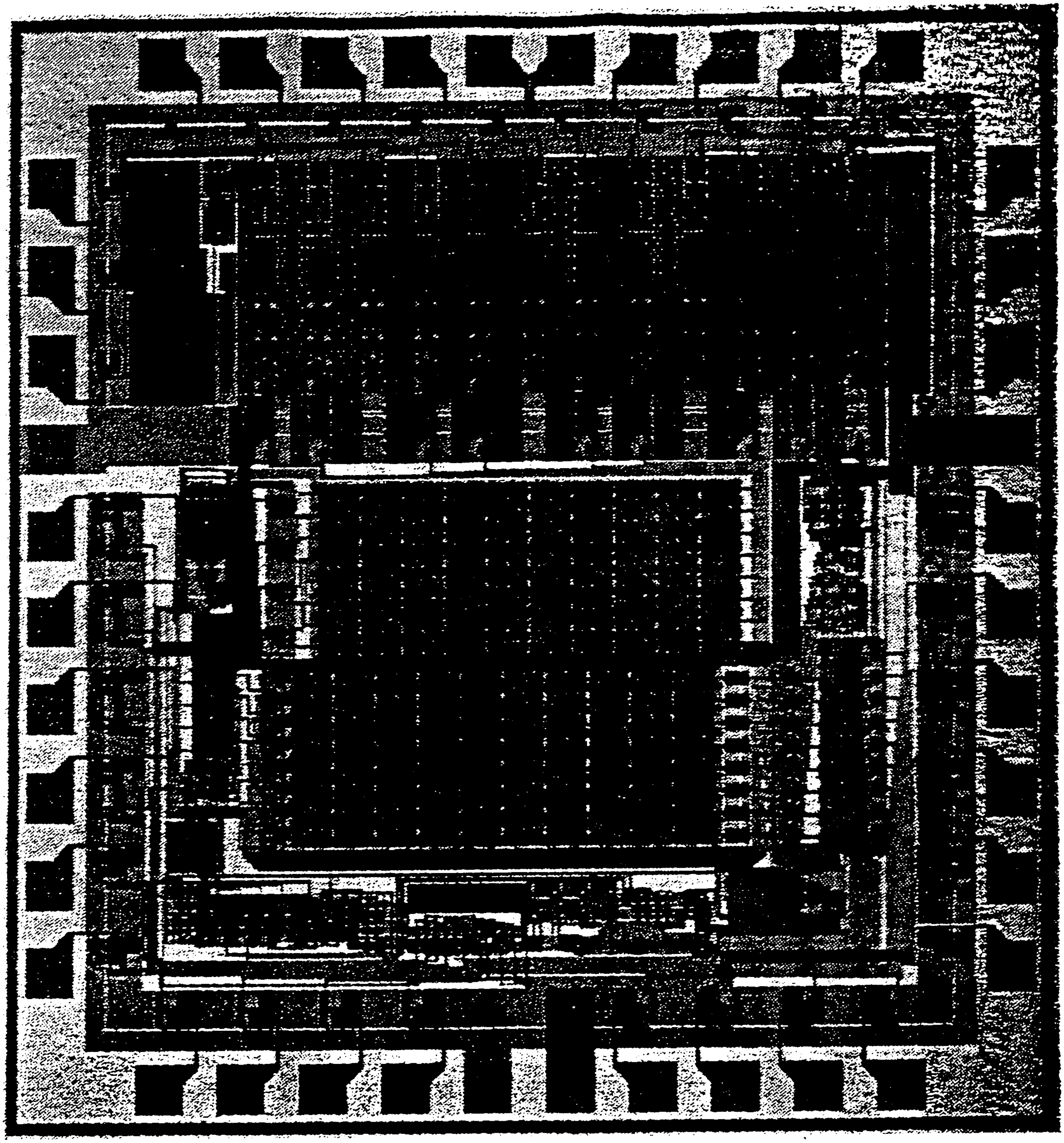
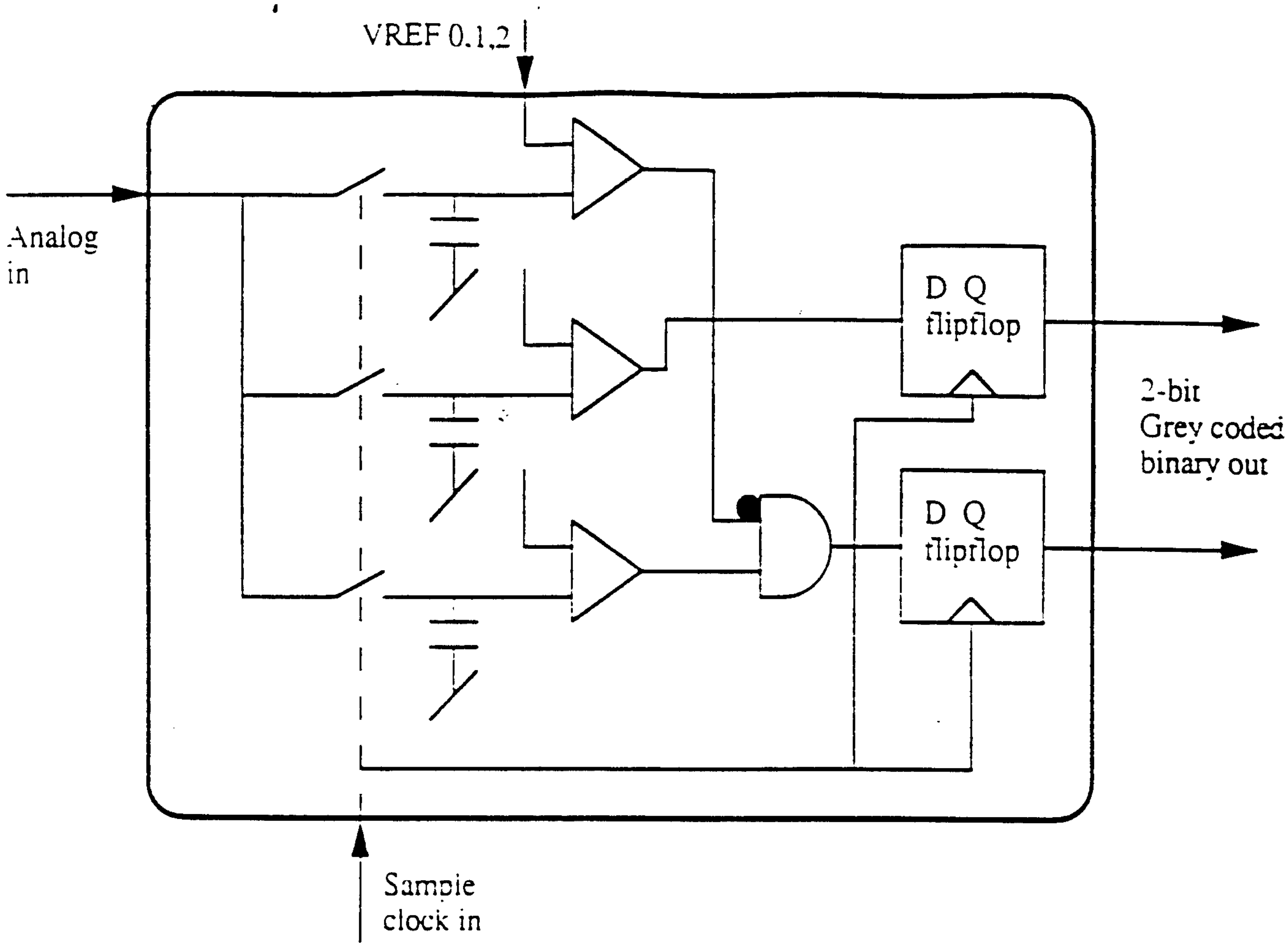


Figure 1

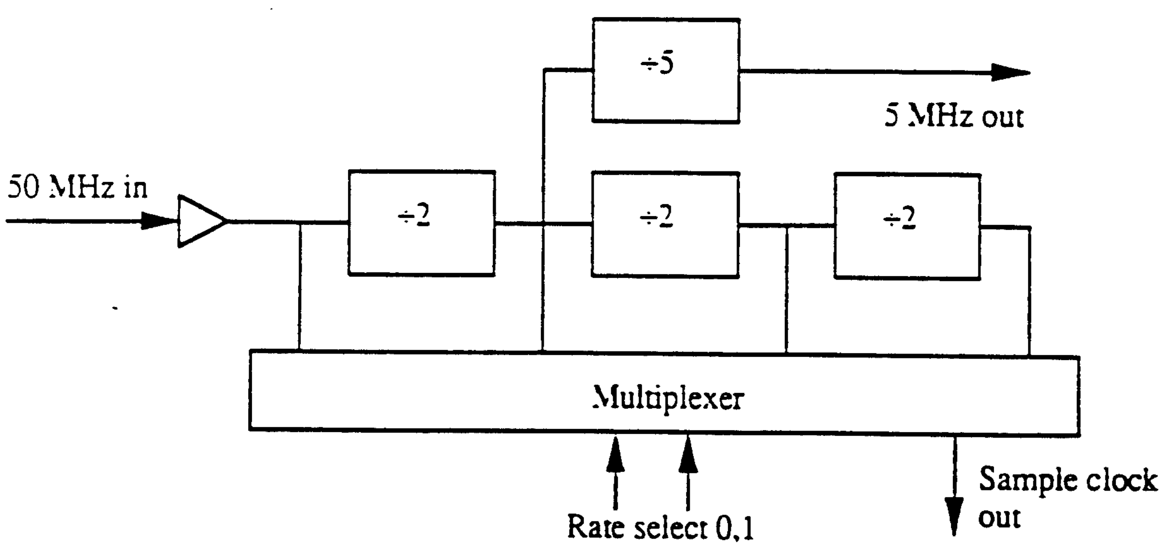
SCU 6.3.94



2-bit flash A/D converter

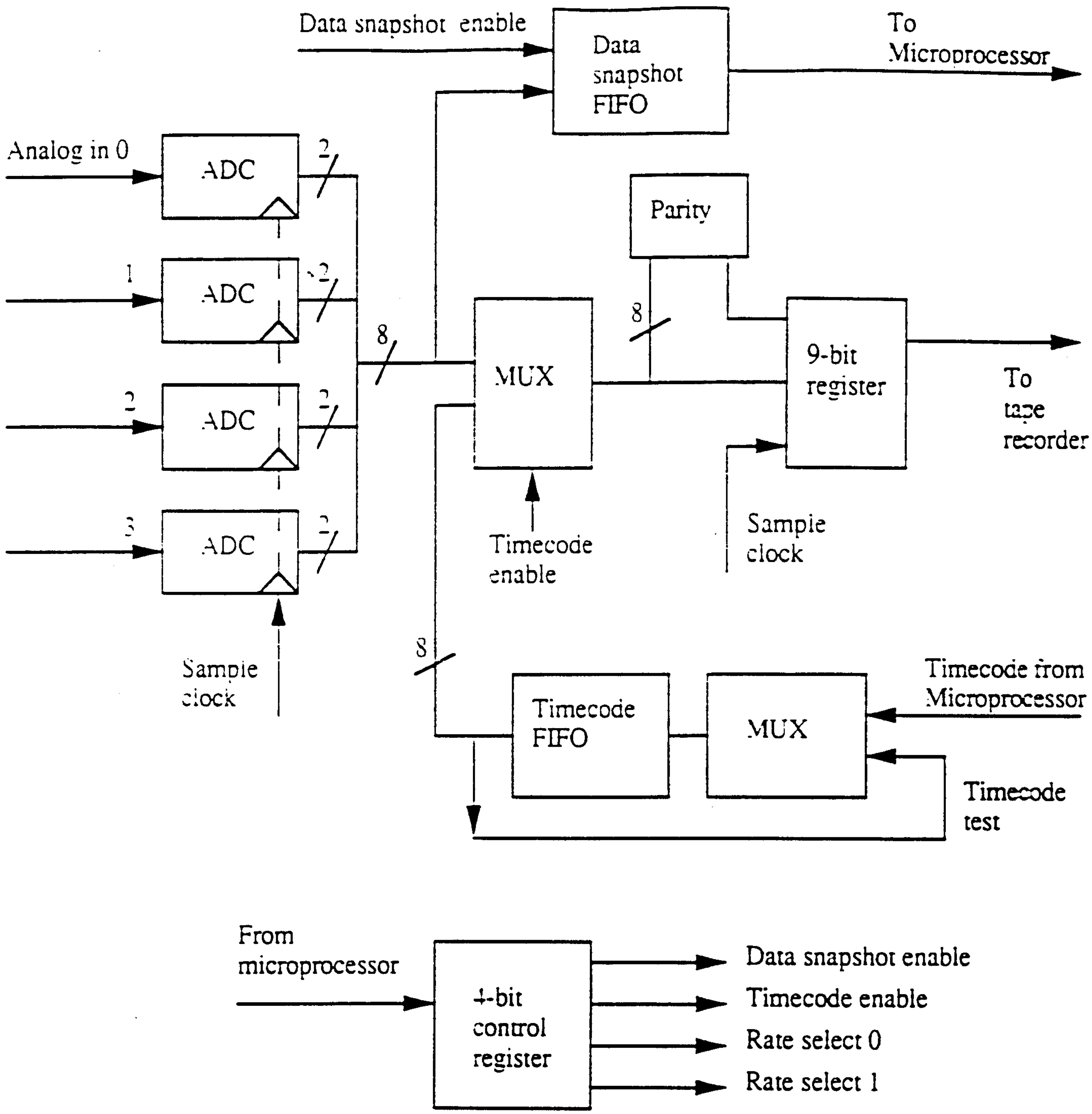


Frequency divider



SCU 6.3.94

VLSI chip - simplified block diagram

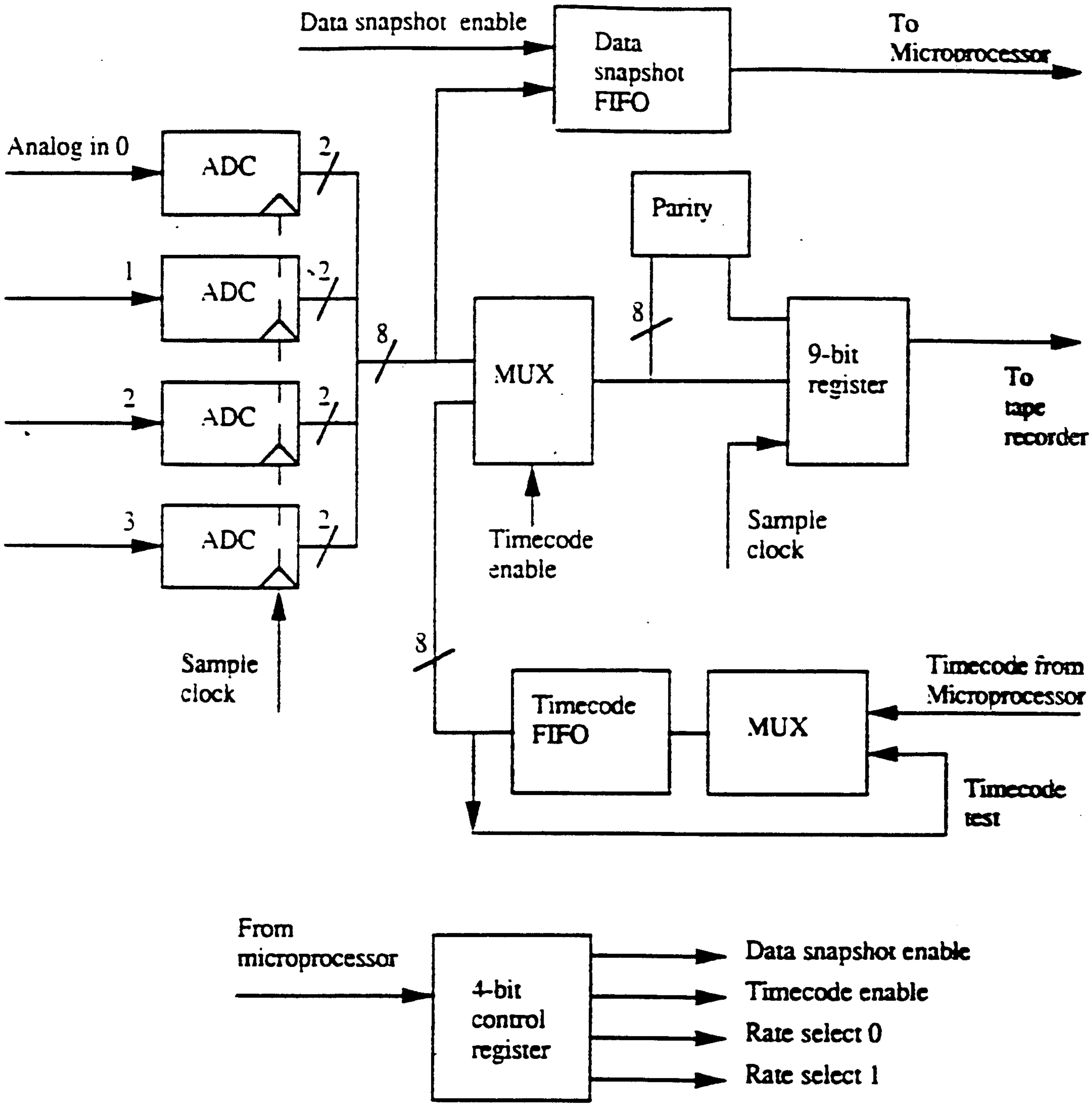


Analog inputs from RF system: (0-25 MHz)

LCP In-phase
LCP Quadrature
RCP In-phase
RCP Quadrature

SCU 6.3.94

VLSI chip - simplified block diagram

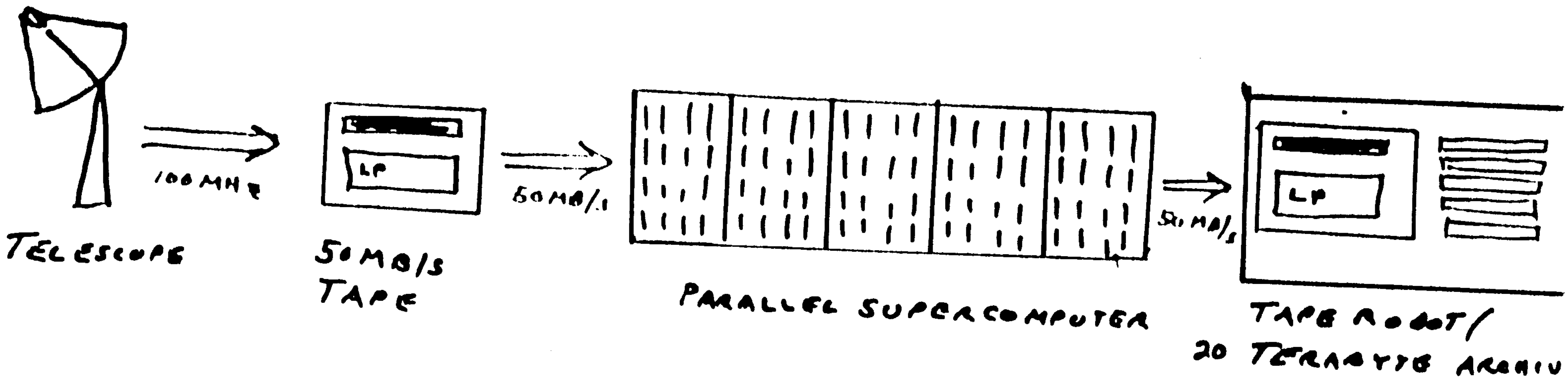


Analog inputs from RF system: (0-25 MHz)

LCP In-phase
LCP Quadrature
RCP In-phase
RCP Quadrature

SCU 6.3.94

Integrated Acquisition/Reduction System



ADVANTAGES

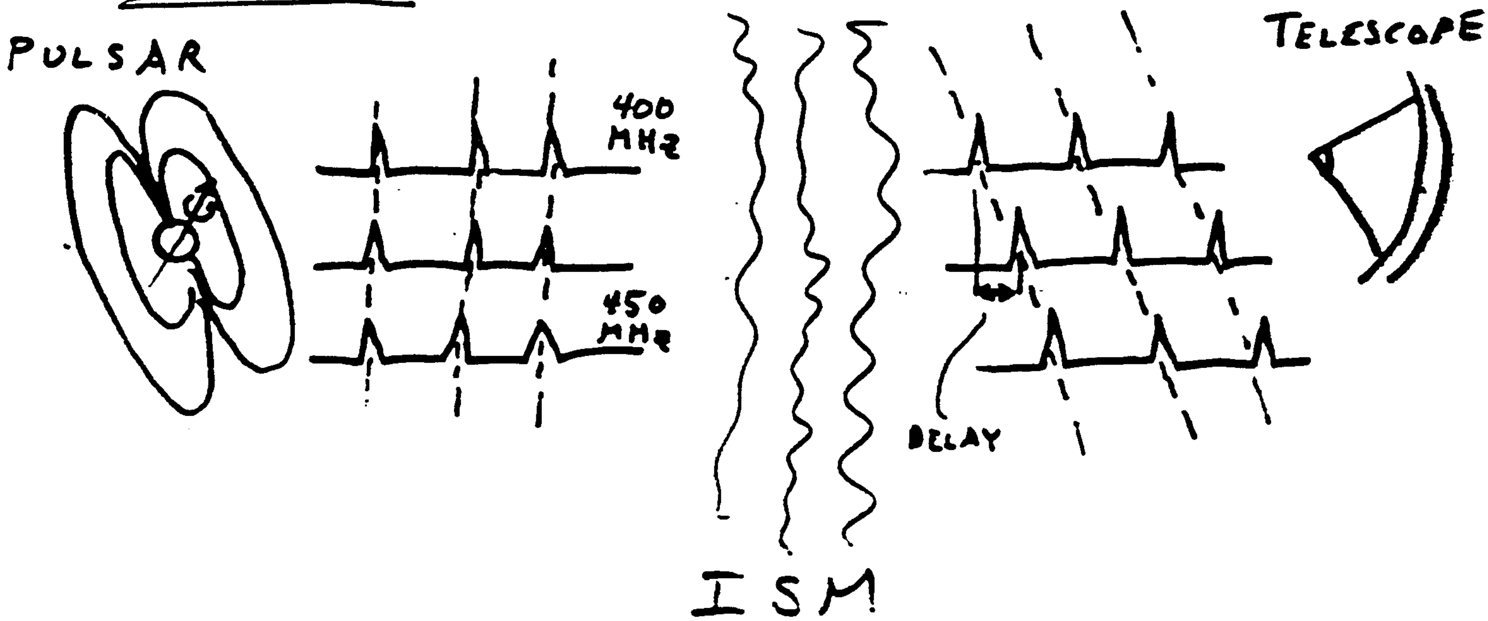
	TYPICAL	BEST	FAST RECORDER
SAMPLING TIME	250 μs	10 μs	10 ns
FREQUENCY CHANNELS	64	1024	ARBITRARY
BANDWIDTH	10-20 MHz	100 MHz	N · 50 MH
		EXPENSIVE COMPLICATED	SIMPLE

\+ POST FACTO OPTIMIZATION AND ITERATION OF SOFTWARE SIGNAL PROCESSING

\+ RETAIN PHASE INFORMATION. ⇒ COHERENT PROCESSING POSSIBLE

THE COMPUTATIONAL PROBLEM (CONT.)

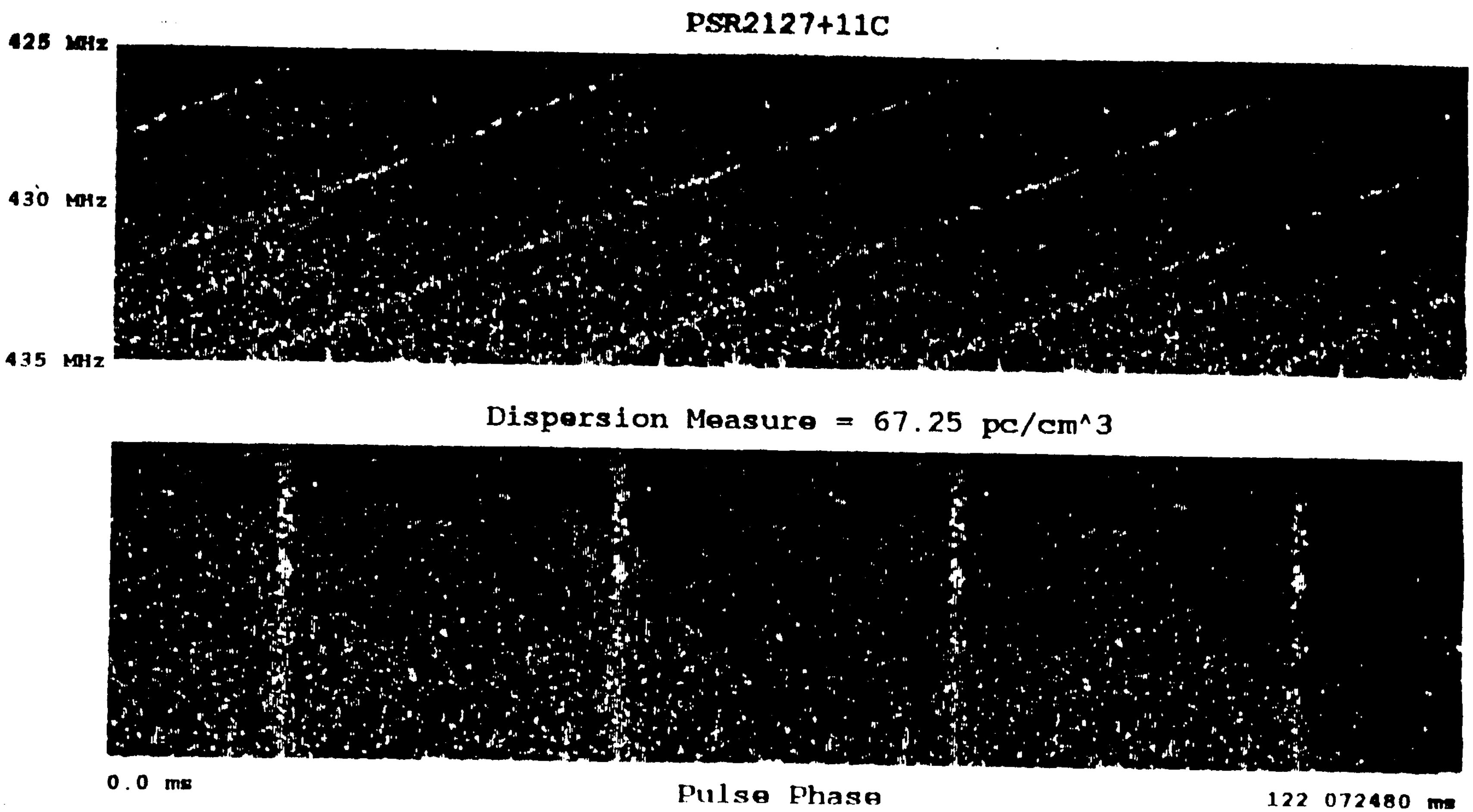
DISPERSION



- DELAY VRS RADIO FREQUENCY IS DUE TO FREE ELECTRONS IN THE INTERSTELLAR MEDIUM.

- MUST "SEARCH" OVER TRIAL DELAYS (OR TRIAL "DISPERSIONS")

⟹ COMPUTING INCREASED BY x 100 - 1000!


PSR2127+11C
425 MHz
430 MHz
435 MHz
Dispersion Measure = 67.25 pc/cm^3
0.0 ms
Pulse Phase
122 072480 ms

FUTURE TRENDS
IN
HIGH SPEED DATA ACQUISITION + REDUCTION

- 10X'S COMPUTE POWER ⟹

  COULD HANDLE 10X'S DATA VOLUME

  * STORAGE TECHNOLOGY IS CRITICAL

- PROGRAM IN BOTH SOFTWARE <u>AND</u> <u>SILICON</u>

  * NEED STANDARDS FOR EASY INTEGRATION OF SPECIAL PURPOSE VLSI

SIMULATION BASED DESIGN

Defense Needs in Simulation Based Design

Mr. Gary W. Jones

Advanced Research Projects Agency

Maritime Systems Technology Office

Simulation-Based Design

1 November 1994

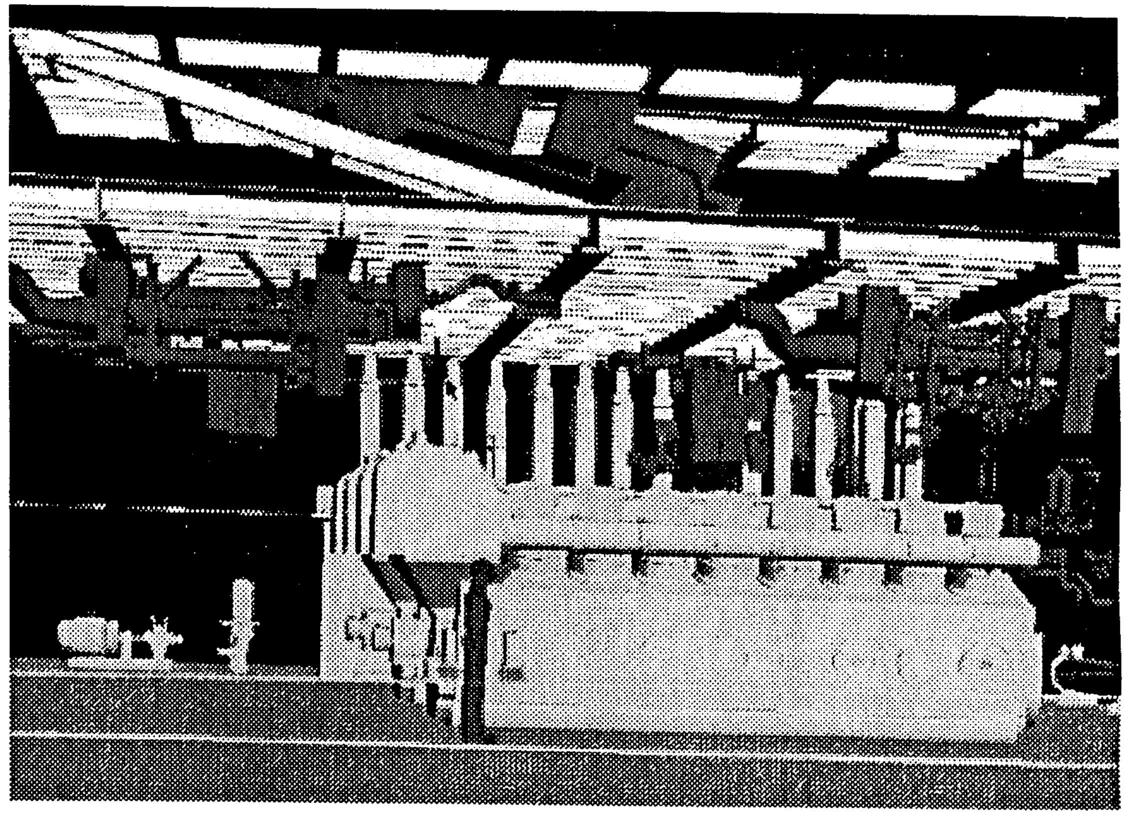
il

(703) 696-2351

Vision

ARPA

A Real Implementation of Technology to Achieve A Revolutionary Improvement in the Acquisition Process for Complex Products.



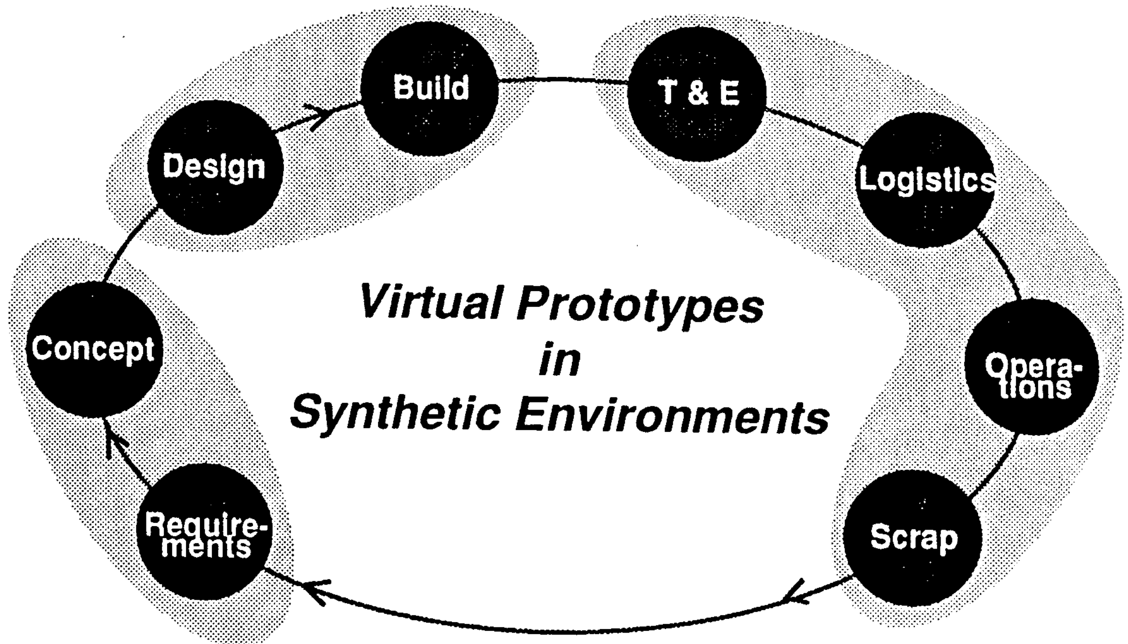
Enable A Revolution

SBD-U-0317-7/22/94

AS OF 7/25/94

Revolutionize the Acquisition Process for Military and Commercial Products

- Distributed, Collaborative Virtual Design Environment
- Virtual Prototyping
  - — Layout
  - — Construction
  - — Operation
  - — Maintenance
  - — Training



Anybody, Anywhere, Anytime, Any System

Transition from Lab to User

ARPA

Personal Computing Analogy

Technology Push

- GUI
- VLSI/Micro-Processor
- Basic
- HPC/Parallel Processing
- TCP/IP & Networking

→ PC / UNIX Operating System →

User Pull

- Word Perfect
- Excel
- DBase
- Turbo Tax
- C++
- X-Windows

Modeling & Simulation

Technology Push

- Widebandwidth Networking
- HPC-Based Workstations
- Distributed Computing
- Visualization Hardware & Software
- Terabyte Databases

→ M&S Deployment to the User →

User Pull

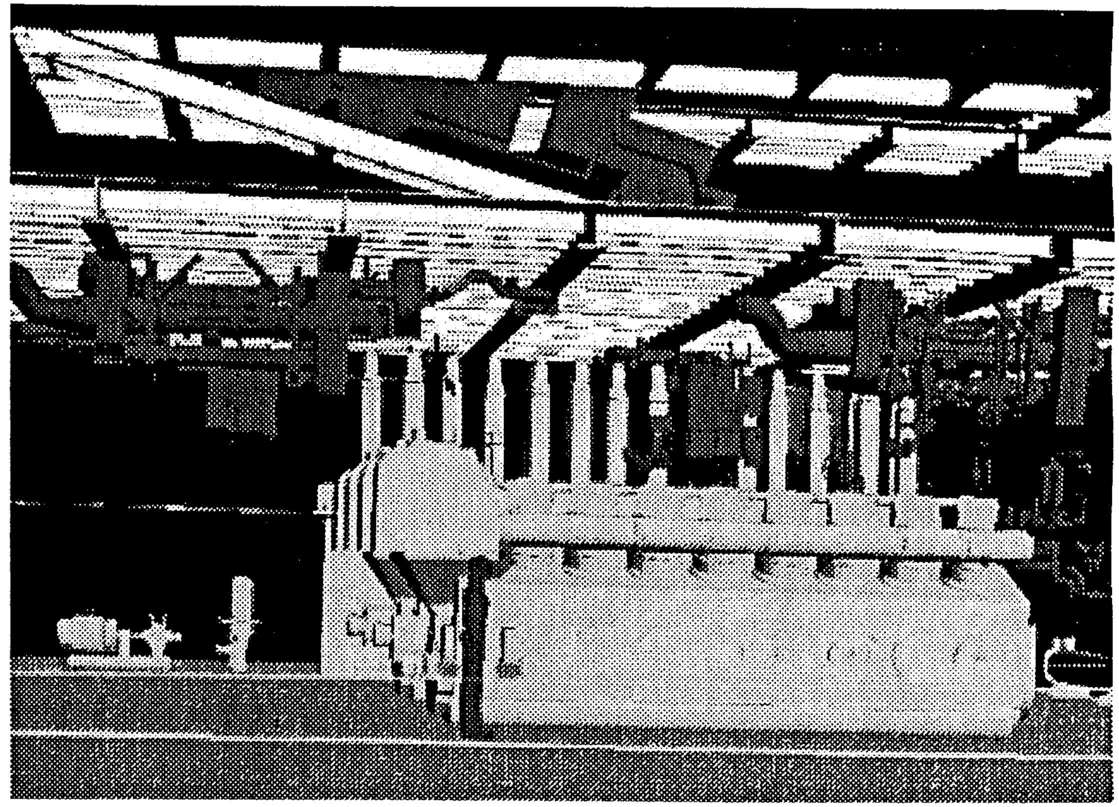
- ?

SBD-U-0243-5/3/94

AS OF 5/3/94

Revolutionary Approach

- Collaborative Synthetic Environment with True Engineering Representations
- Object-Oriented, Distributed Database Supporting Entire Life Cycle
- Enterprise Infrastructure Supporting National Industrial Base

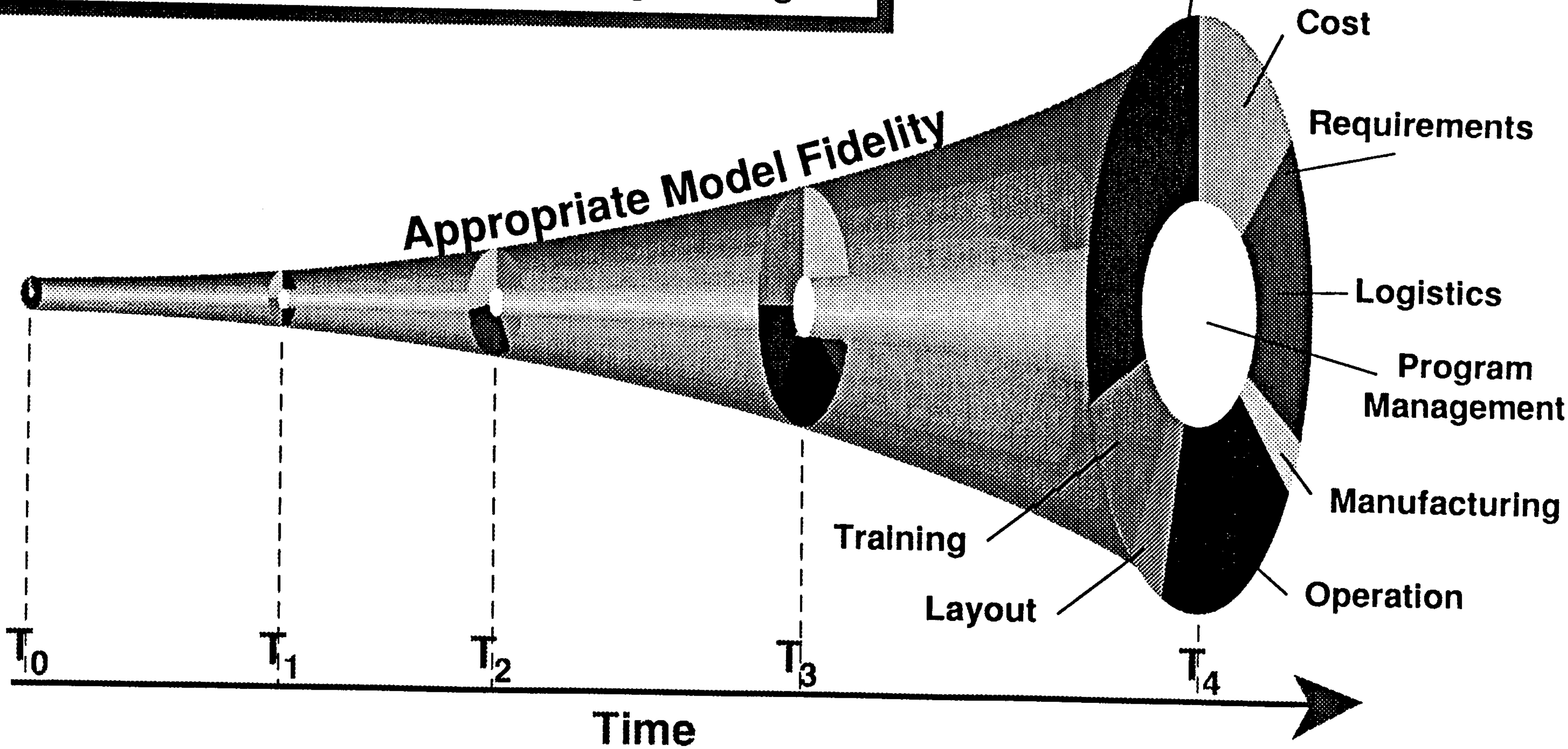


"Electronic" IPPD and Virtual Prototyping

Simulation-Based Design

Our Vision is a Revolutionary Process

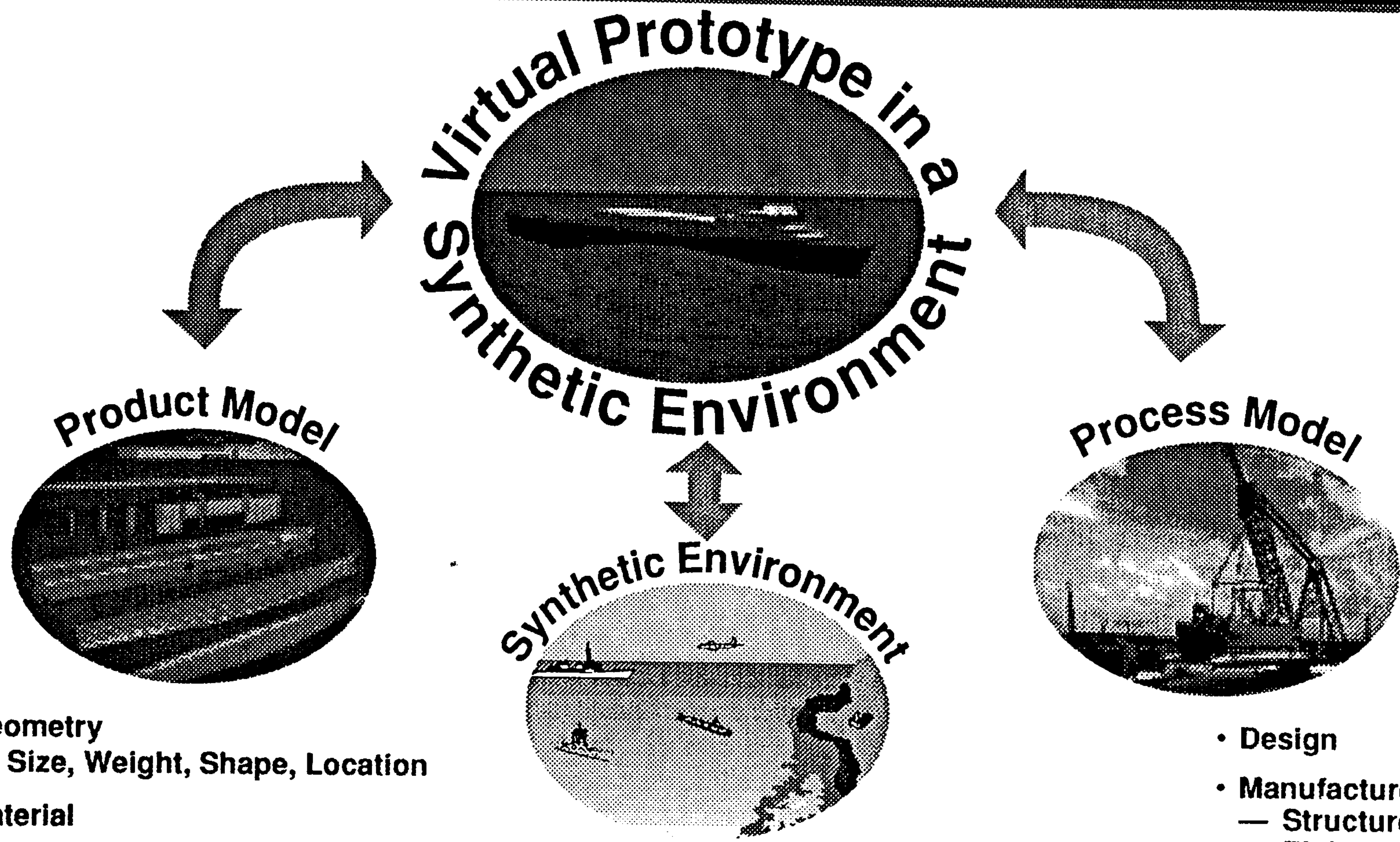
- Integrated Product and Process Models
- Concurrent Engineering to the Limit
- Virtual Prototypes in Synthetic Environments
- Collaborative Distributed Planning & Design



SBD-U-0210-4/5/94

AS OF 5/18/94

Virtual Prototyping



- Geometry
  - — Size, Weight, Shape, Location
- Material
- Performance
  - — Speed, Power, Capacity
- Vendor Info
- Financial

- Ocean Models
  - — Wave/Wind
  - — Salinity
  - — Temperature
  - — Acoustic/Non-Acoustic
- Atmospheric
  - — Wind
  - — Pressure
  - — Temperature
  - — Electro-Magnetic

- Design
- Manufacture
  - — Structure
  - — Piping
  - — Electrical
- Testing
- Training
- Integrated Logistics

SBD-U-0319-7/22/94

AS OF 9/13/94

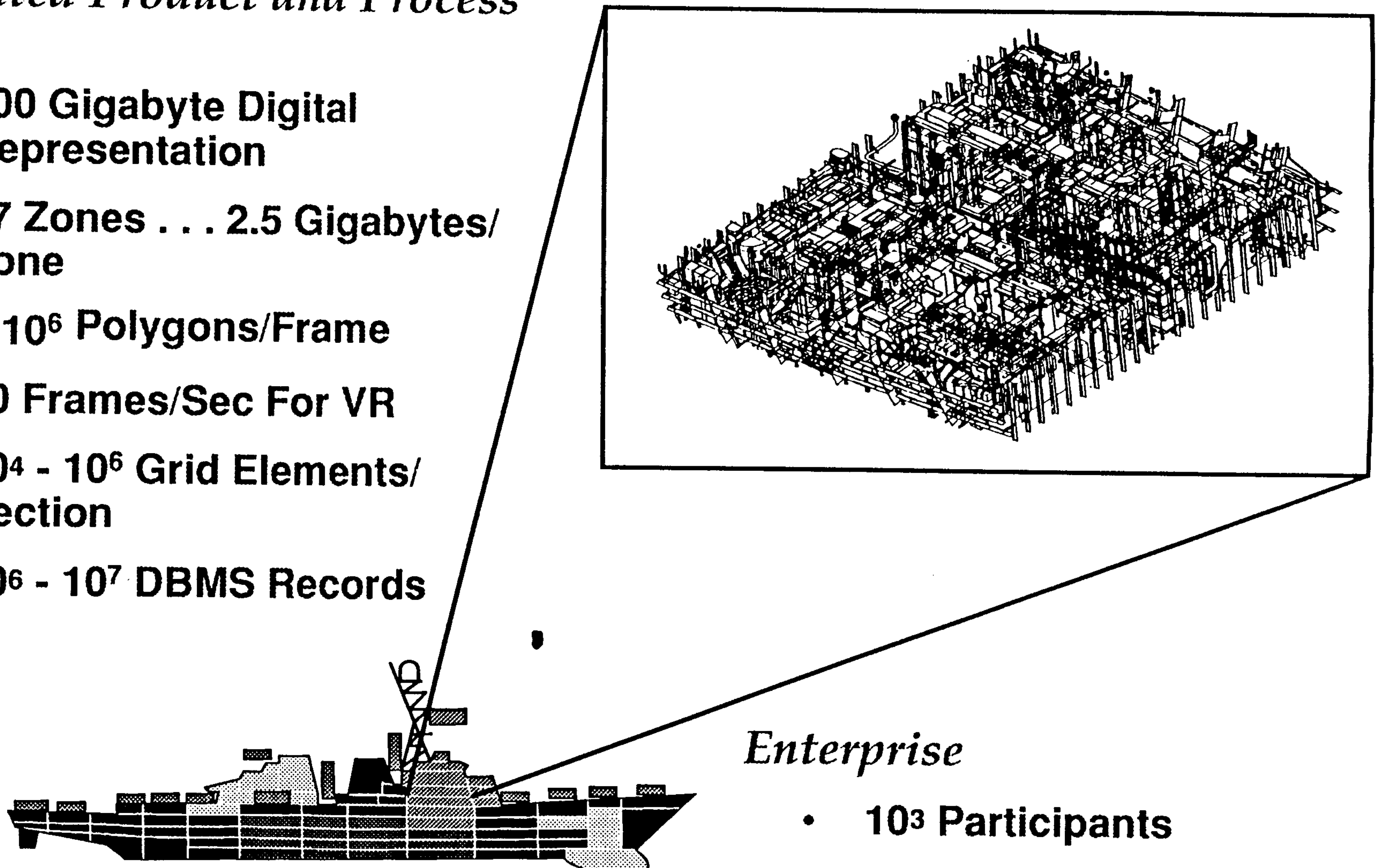
Approach

- Capture and Exploit Technology
- Define an Environment
- Demonstrate Via Challenging Applications
- Leave a Legacy of Extensive Use

Simulation-Based Design
Ship Complexity . . . A Midsized Combatant

Integrated Product and Process Model

- 200 Gigabyte Digital Representation
- 77 Zones . . . 2.5 Gigabytes/ Zone
- ~ 10^6 Polygons/Frame
- 30 Frames/Sec For VR
- 10^4 - 10^6 Grid Elements/ Section
- 10^6 - 10^7 DBMS Records



9,000 Tons

Enterprise

- 10^3 Participants
- 10^2 Transactions/Participant

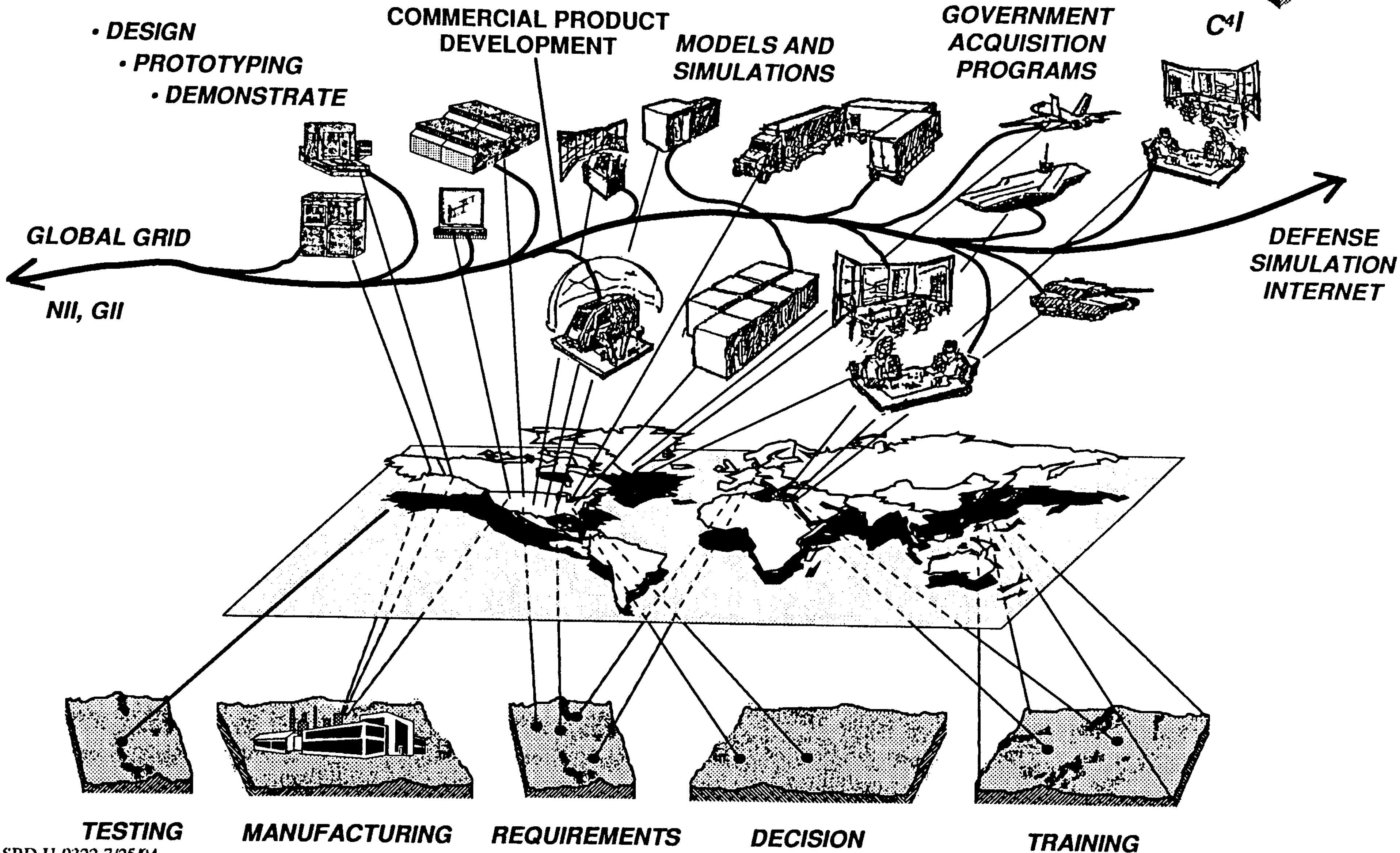
SBD-U-0065-5/19/93

AS OF 11/22/93

Why Change is Necessary

- Current Systems Being Procured Are Increasingly Complex
- Difficult to Affordably Produce What the Mind Can Conceive
- Design and Manufacturing Capabilities Have Not Kept Pace with Technology

Enterprise Infrastructure Network



SBD-U-0322-7/25/94

AS OF 8/30/94

Phase I Demonstration Video

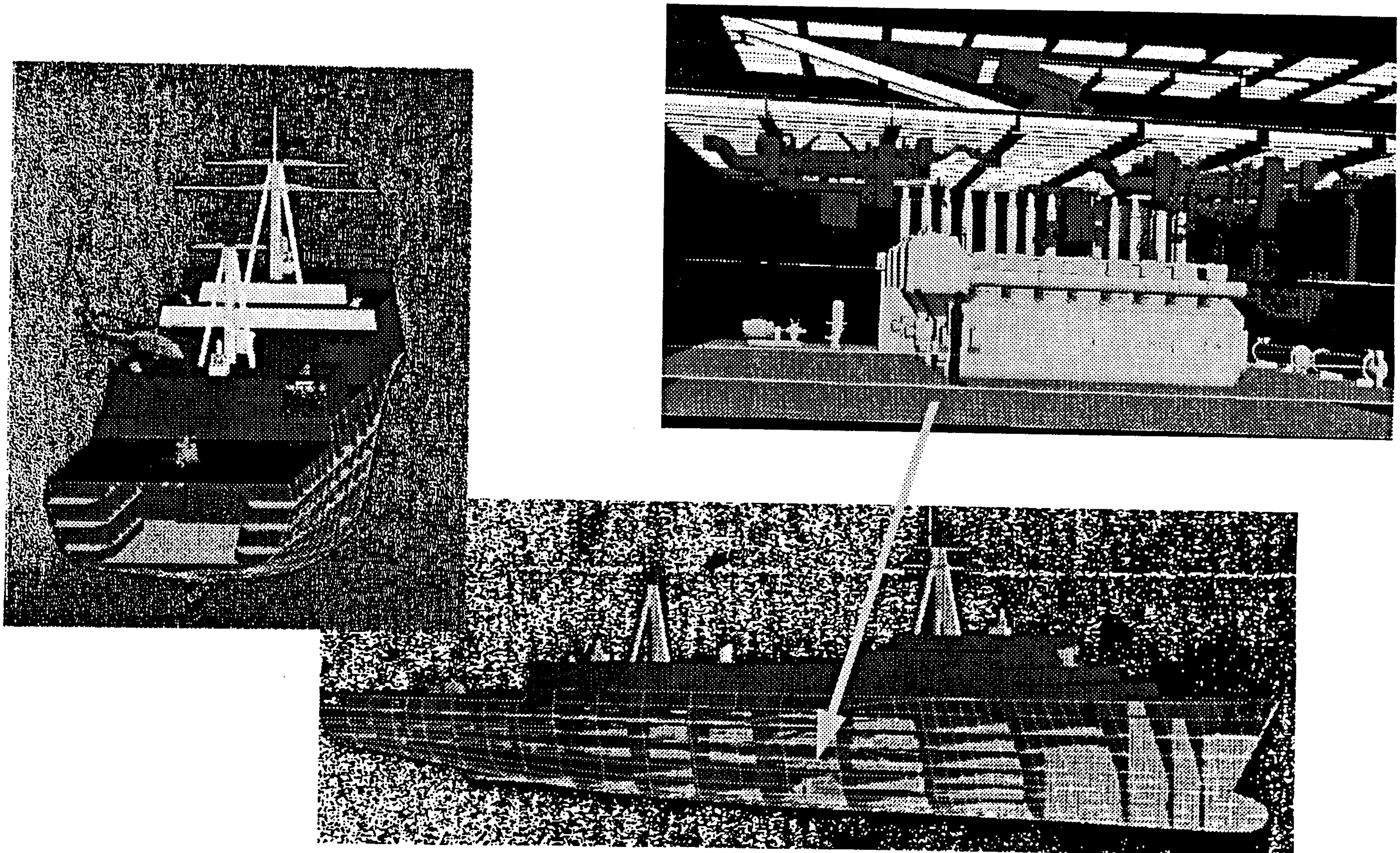
- Video Captured Directly from Computer
- Demonstration Scenario Based on Traditional Acquisition Cycle
- Demonstrates <u>Some</u> of the Technologies
- Documents Accomplishments of Phase I
- Sets the Direction for Phase II

There Were Only Successes

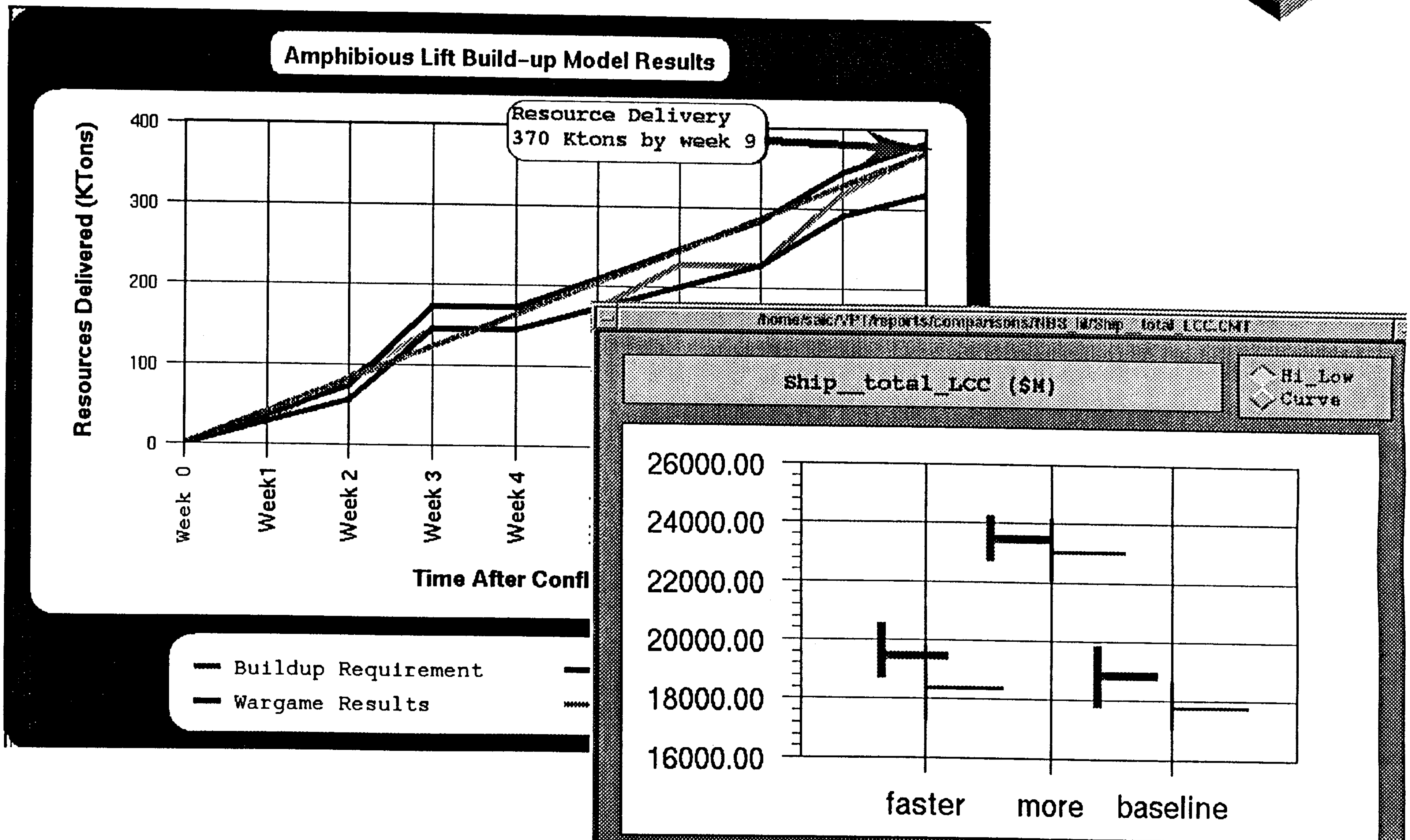
SBD-U-0323-7/25/94

AS OF 7/25/94

Notional Baseline Ship (NBS)



Requirements Results



SBD-U-0335-8/2/94

AS OF 8/2/94

Requirements

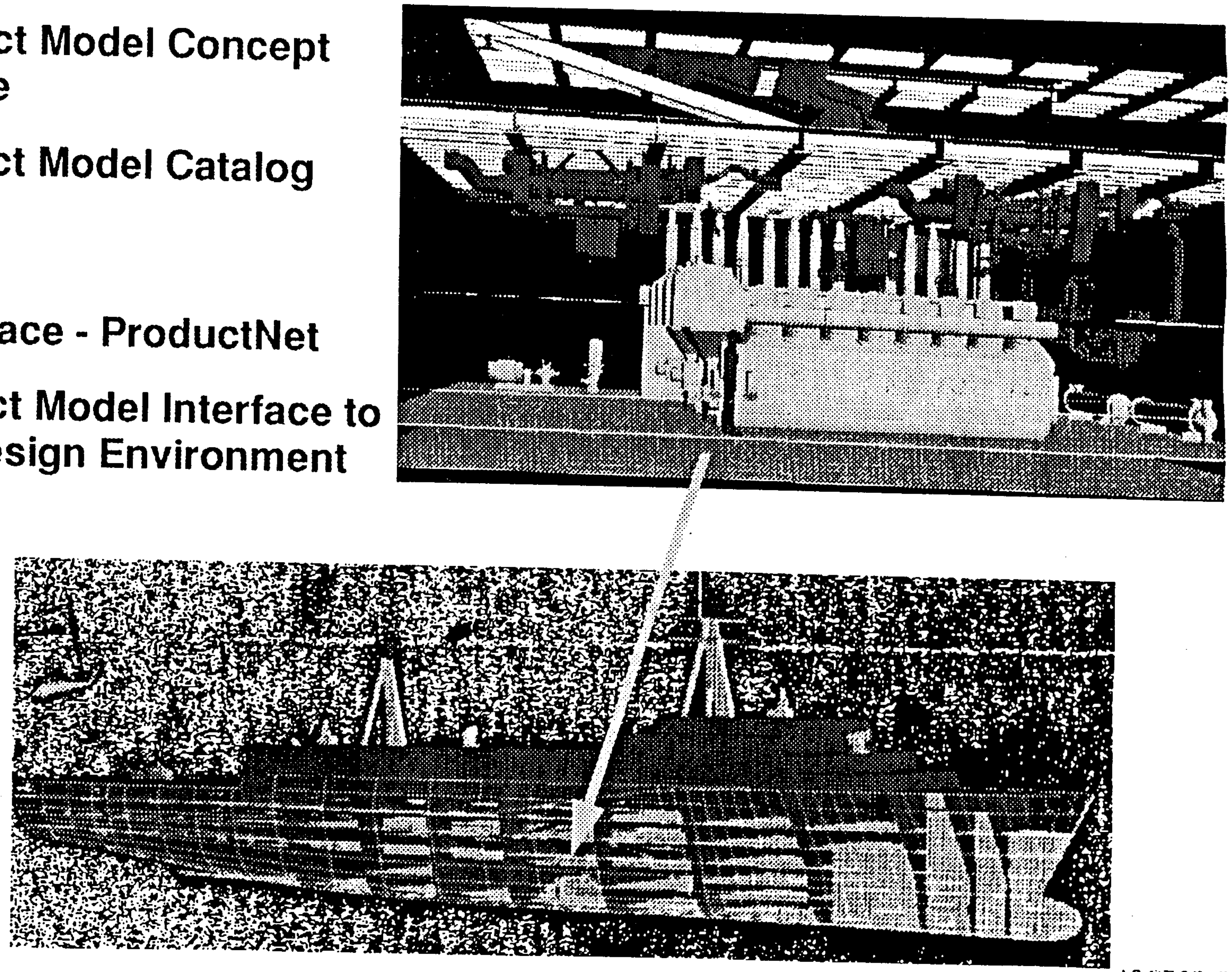
Requirement Development

- Distributed Tools and Data Linked to Multi-Discipline Analysis
- Smart Product Model Integrated with Operational Analysis
- Risk and Uncertainty Analysis Running in the Background
- Allows a Large Number of Tradeoffs to be Made

Concept Formulation

Design and Enterprise/Integration

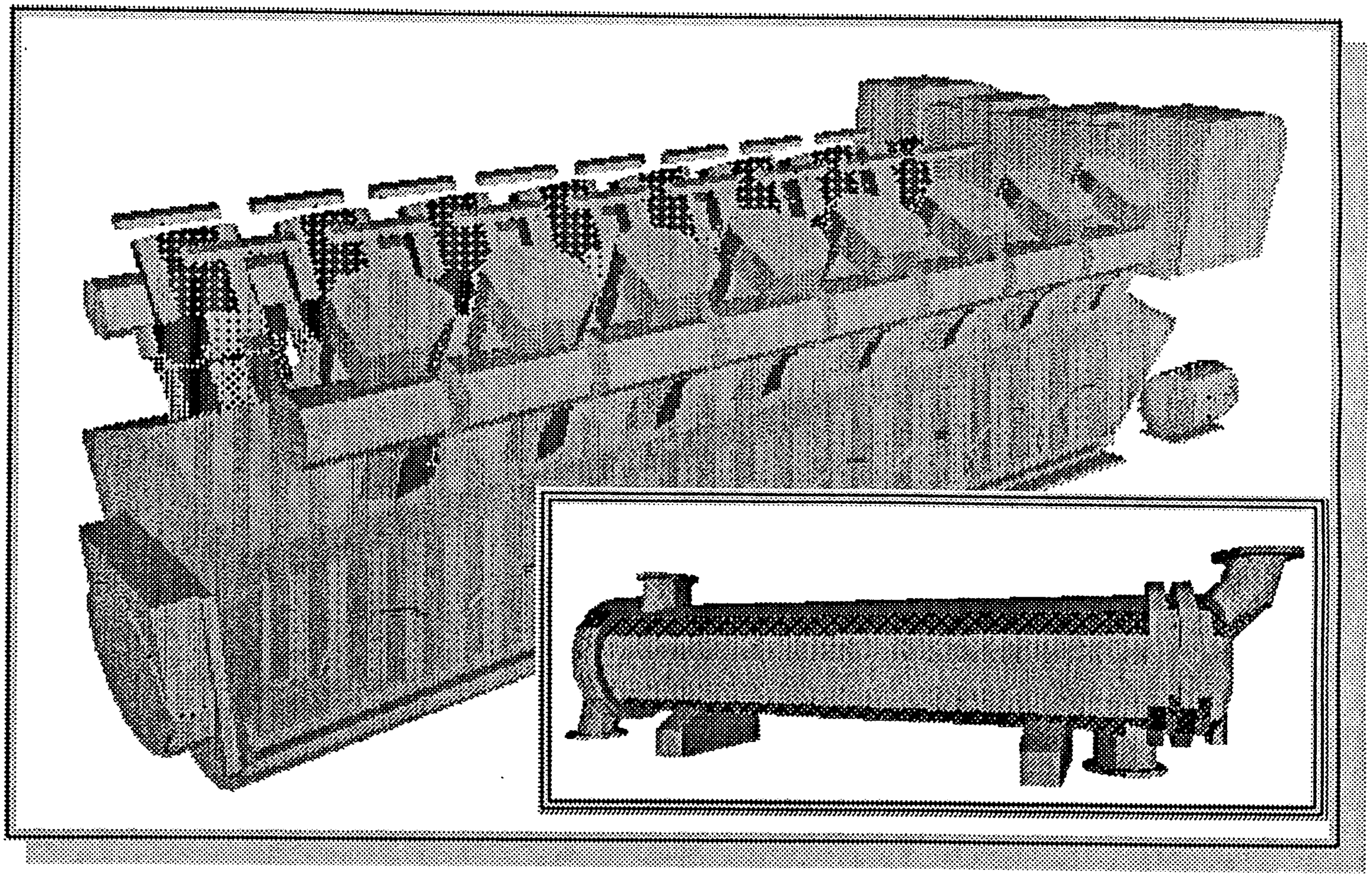
- Smart Product Model Concept and Structure
- Smart Product Model Catalog
  - Text
  - Graphical
- Vendor Interface - ProductNet
- Smart Product Model Interface to the Virtual Design Environment



SBD-U-0307-7/22/94

AS OF 8/31/94

Smart Product Models



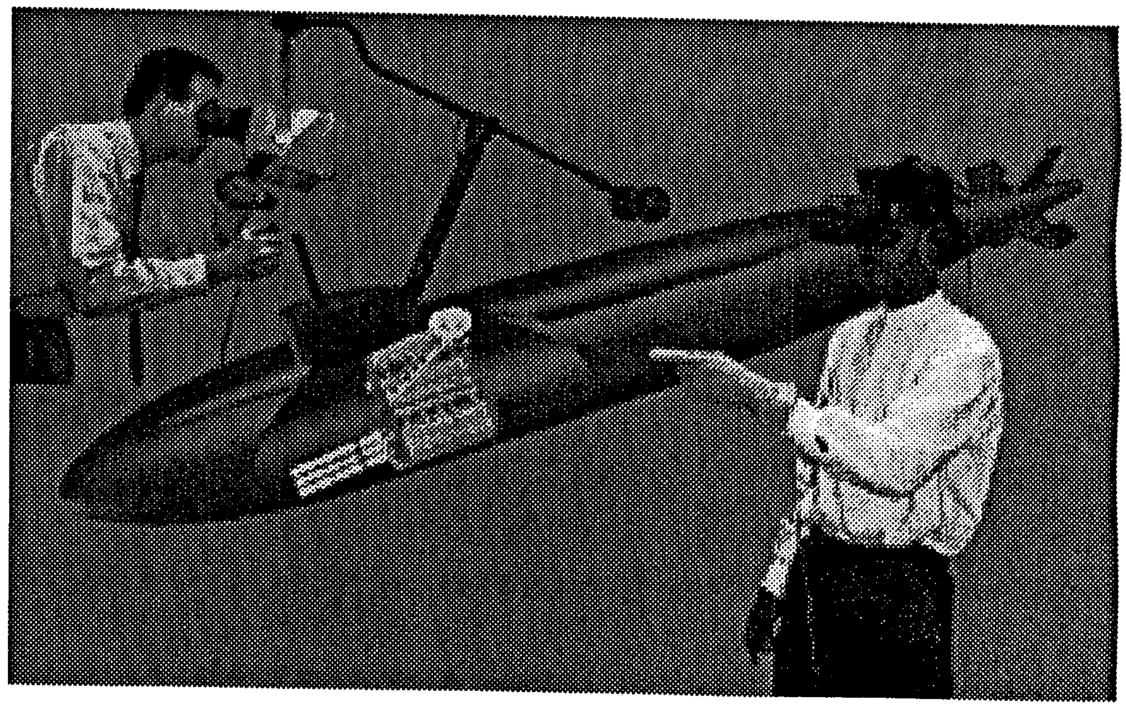
SBD-U-0336-8/2/94

AS OF 8/2/94

Concept Formulation & Design

Human Computer Interfaces

- Multiple Immersion
- Space Mice/Head Mounted Displays/Flat Screens, etc.
- Pointers and Menus in the VDE
- Simultaneous Tasking of Multiple Computers
- Model Generation - data entry and modification
- Augmented Reality
- Smart Objects and Global "Rubber-banding"
- Anthropomorphic as an Input/Output Device



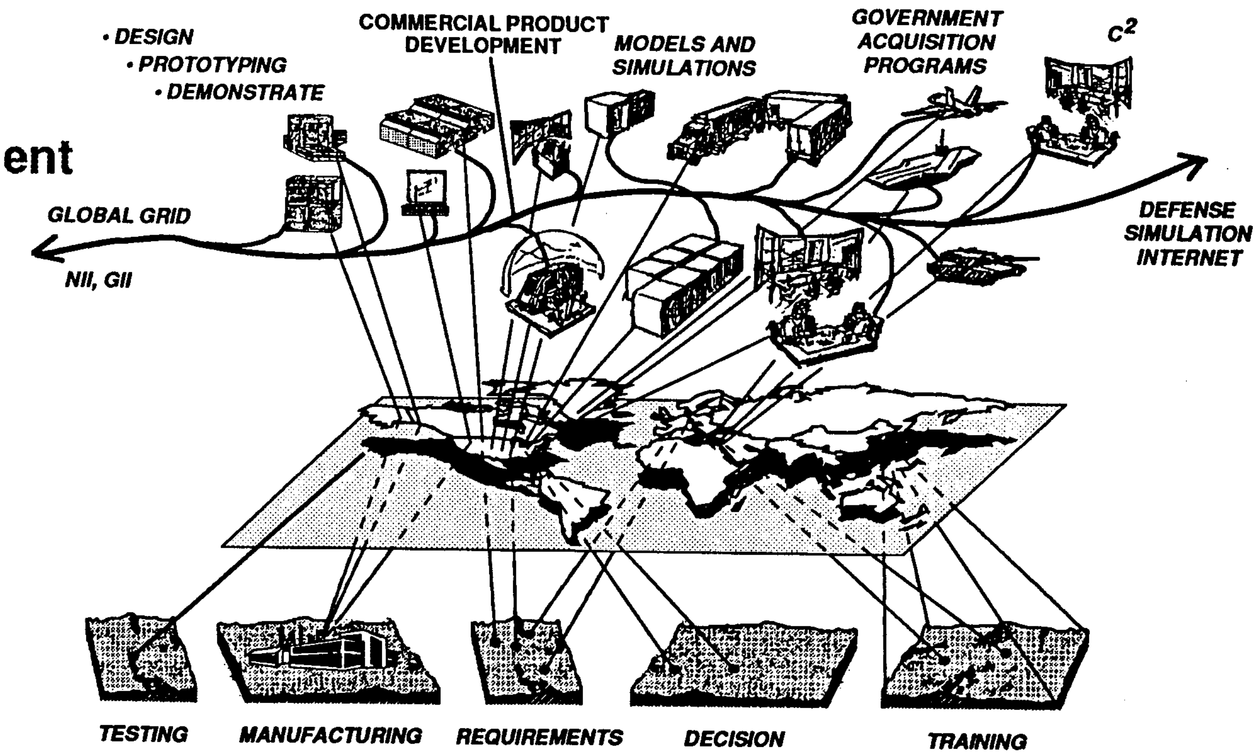
SBD-U-0308-7/22/94

AS OF 9/2/94

Collaborative Design

Network and Communications

- Remote Distributed Immersion
- Area Distribution of the Product Model
- Database Synchronization
- Distributed Interactive Simulation(DIS) in an Engineering Environment
- DIS Linked to a Smart Product Model



SBD-U-0309-7/22/94

AS OF 8/31/94

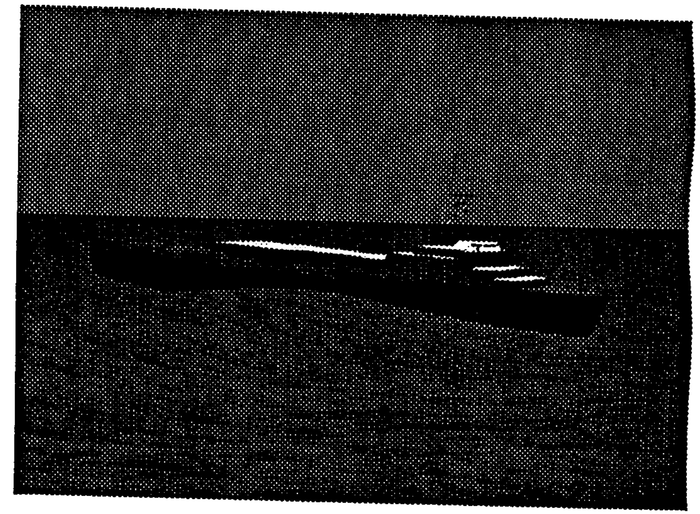
Multi-Disciplinary Analysis

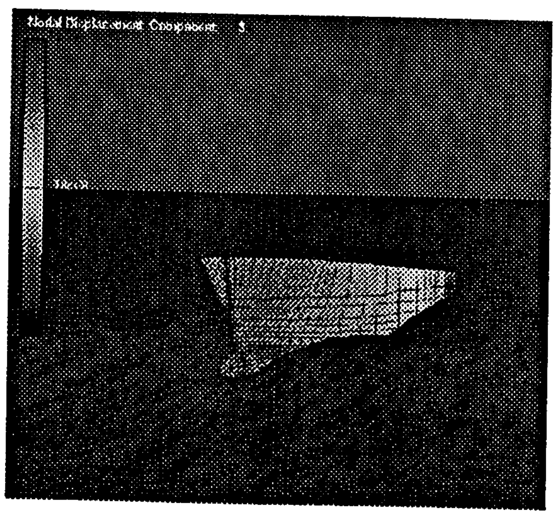
Engineering Analysis

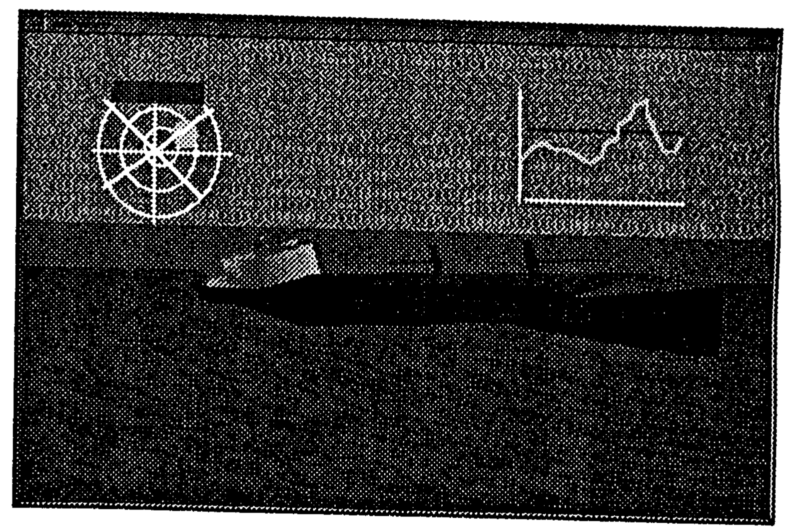
- Coupled Multi-disciplinary Analysis
  — Linear and Non-linear Seakeeping
  — Structures

- Design Optimization
  — Non-intuitive Design Guidance
  — Multi-parameter Optimization

- Distributed High Performance Computing







SBD-U-0310-7/22/94

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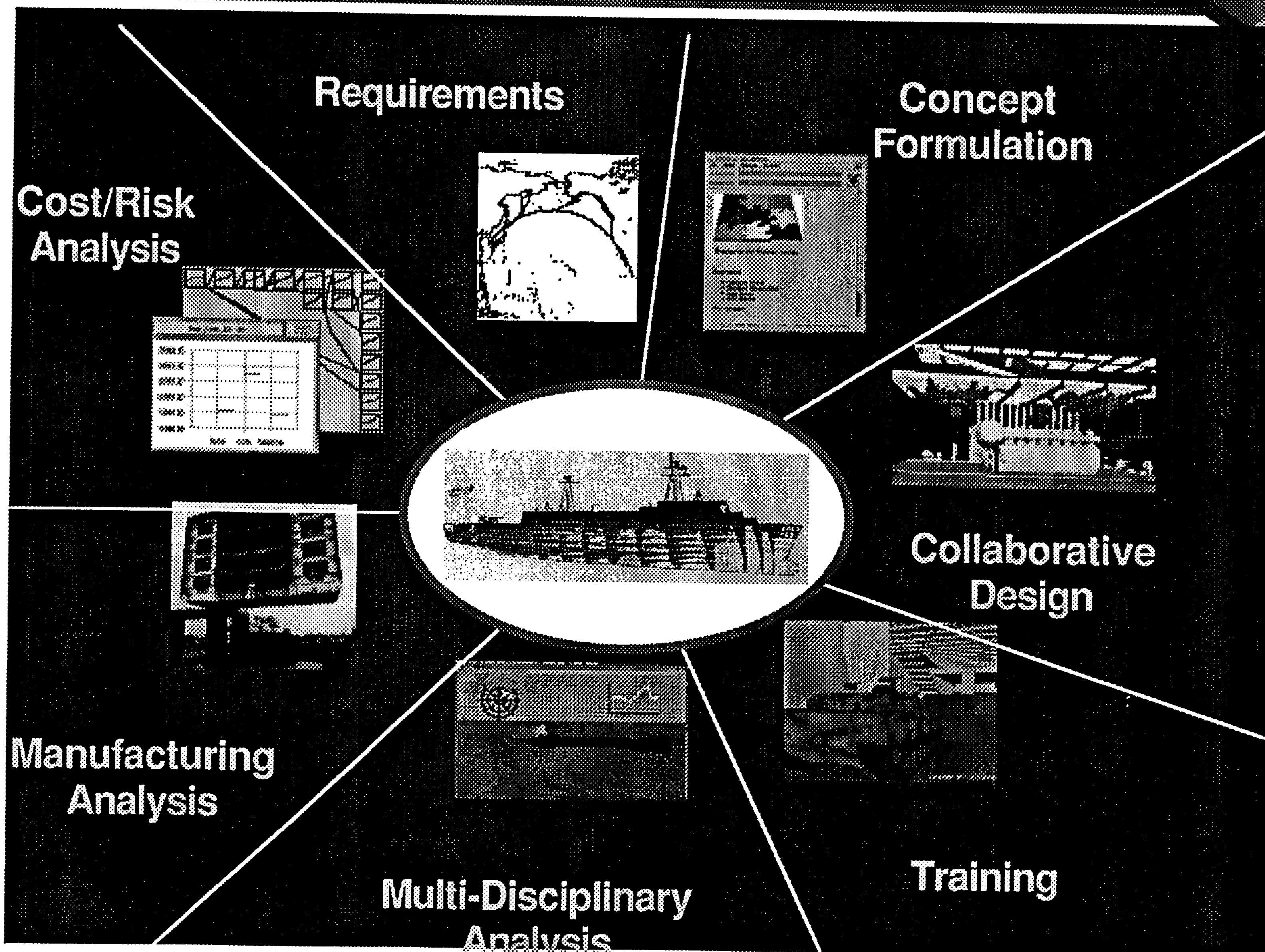
Simulation-Based Design
Phase I Demonstrated (3/93 – 9/94)



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AS OF 9/27/94

Manufacturing

Manufacturing Analysis

- Component Assembly
- Rapid Feedback Impact of Design Changes
  - — Time and Cost
  - — Manufacturing Tradeoffs
  - — Business Decision Aid
- Impact of Alternate Manufacturing Facilities

Training

- Training Link to Early Design
- Smoke and Fire Modeling in VDE
- Multiple Immersion
- Physical Interaction with the VDE
- Sensor Generated Information
  - Characterization of the Environment
  - Update to the Synthetic Environment

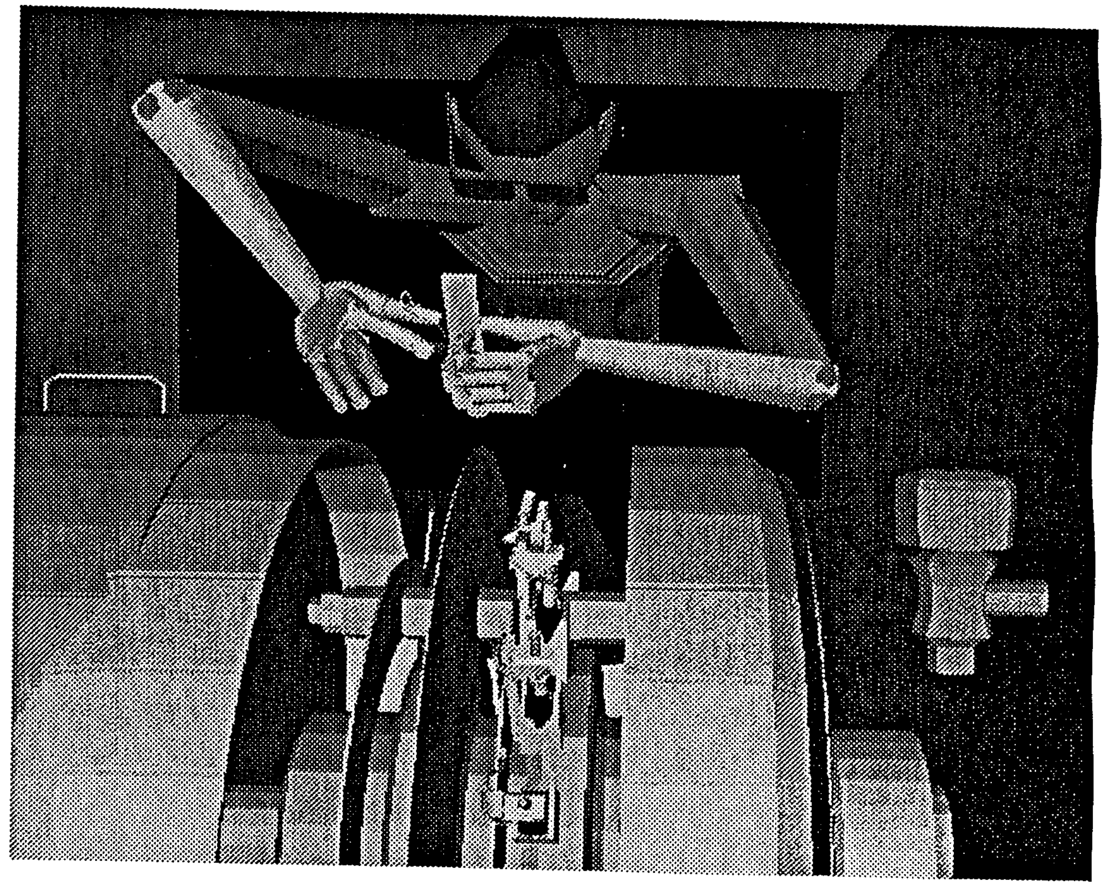
SBD-U-0312-7/22/94

AS OF 9/2/94

Training

Maintenance Analysis

- Use of Anthropomorphics
- Maintenance Accessibility
- Time Motion Studies
- Derivation of Forces and Other Ergonomics Information



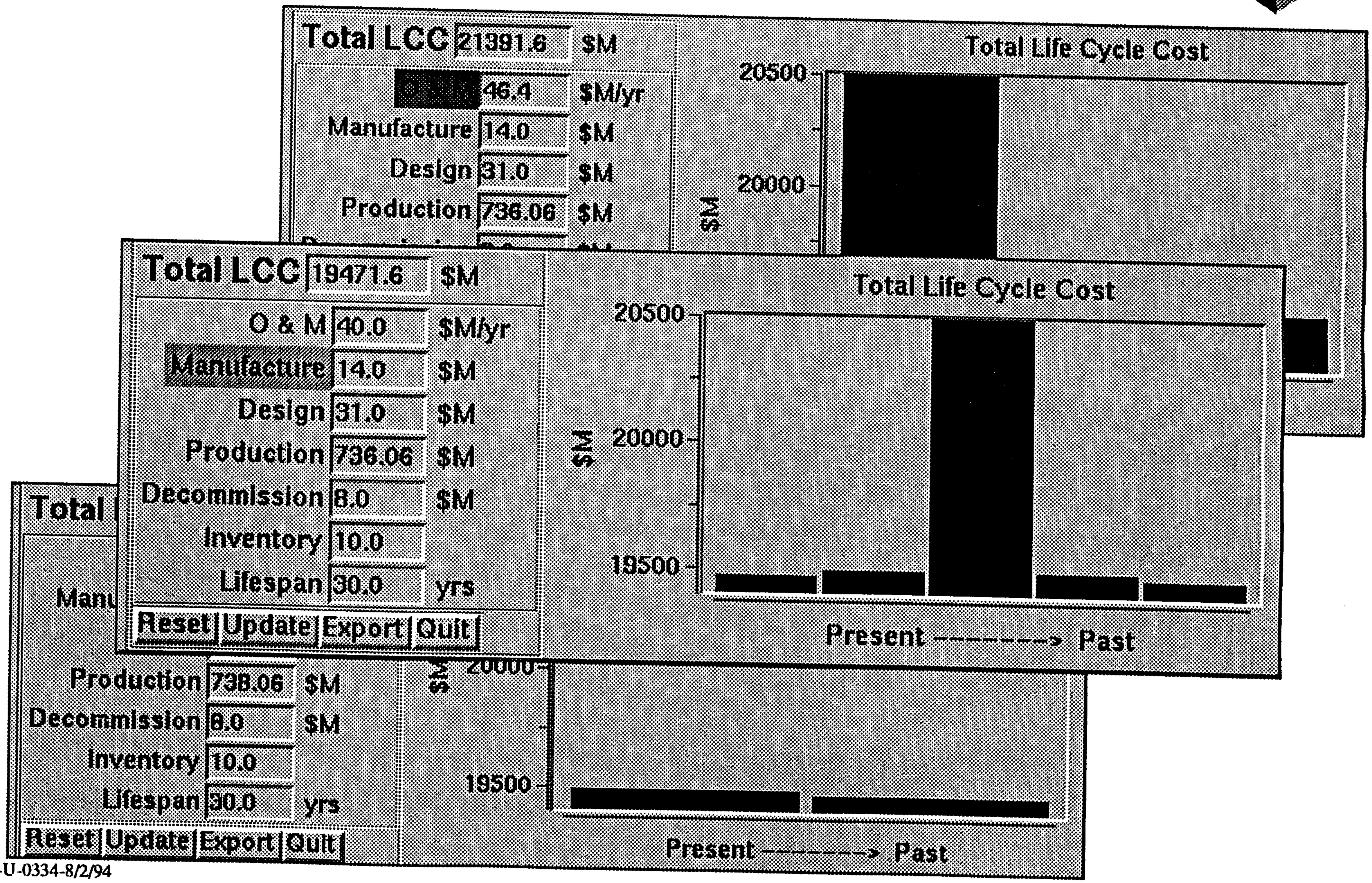
SBD-U-0313-7/22/94

AS OF 8/31/94

Cost Analysis

- **Track, Evaluate, and Manage Uncertainty**
  - — Throughout the Entire Design/Construction Process
  - — Continuously

Dynamic Costing

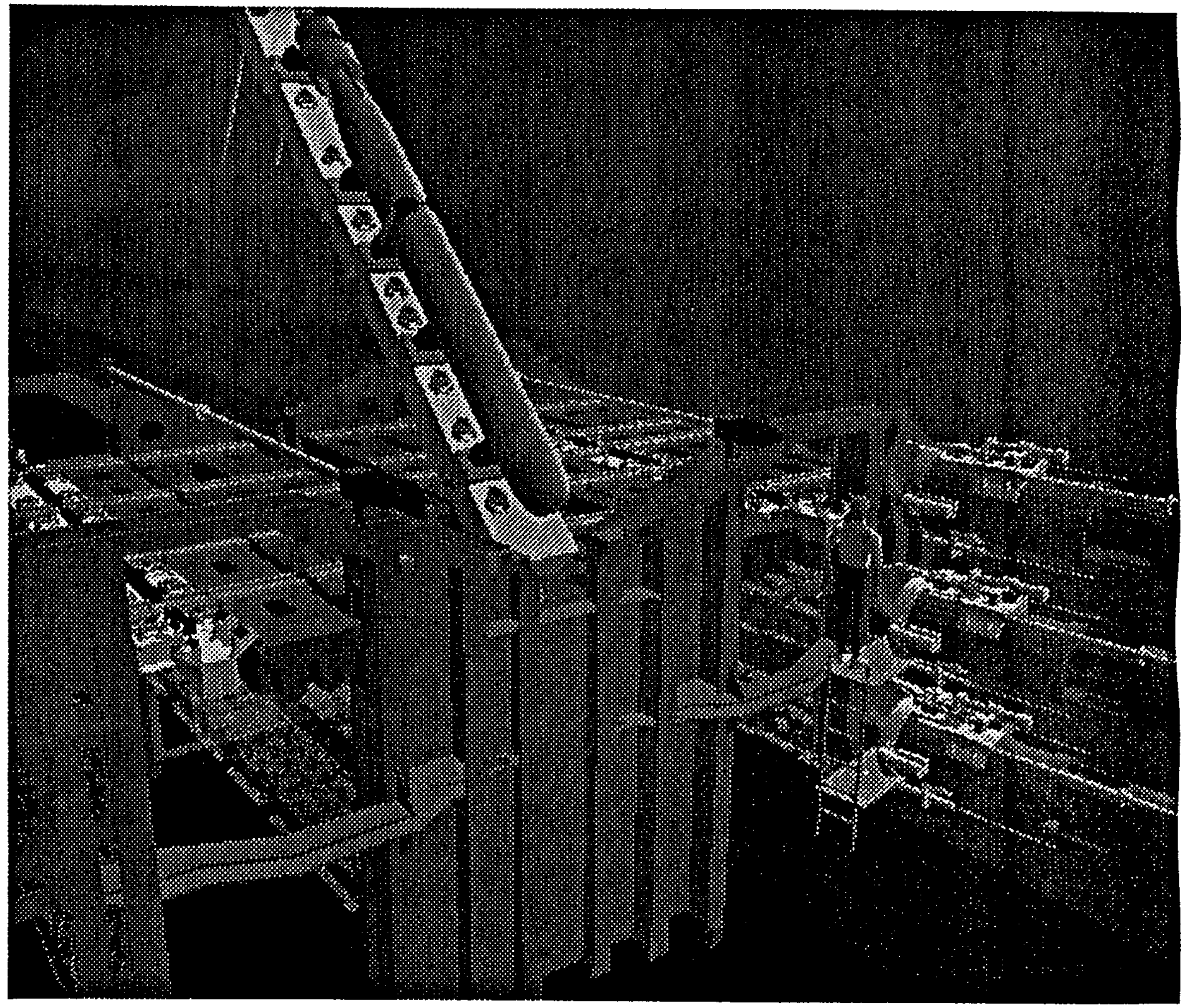


SBD-U-0334-8/2/94

AS OF 8/2/94

Technologies

- Megaprogramming
- Rendering Techniques
  - — Culling
  - — Viewing Frustrum
  - — Resolution



Simulation-Based Design
Technical Challenges

Human Computer Interface	Rendering Technologies Navigation Multiple Immersion	Tracking Portability	Tactile Feedback Voice Recognition
Networking	Bandwidth Distributed Computing Standards and Protocols	Integration of Heterogeneous Systems National Vendor Base	
Modeling	Validation Software Inter-Operability Engineering Analysis Open Architecture - Legacy Codes		
Database	Object Oriented Interface Distributed Data Configuration Control - Multi-Level Security		

SBD-U-0182-10/22/93

AS OF 9/27/94

The Feasibility Demonstrations Were Very Successful

- **ARPA Will Pursue Prototype Development**
- **Need Partnership for Critical Support Applications**

Summary of Demonstrated Utility

ARPA

- Advanced Training During Early Stage Design
- Multi Discipline Engineering Analysis
- Realtime Cost & Risk Assessment
- Early & Continuous Operator Involvement
- Manufacturing Assessment & Tradeoff
- Non Intuitive Guidance for Complex Systems
- Design for Maintainability
- Safe Designs for Hazardous Conditions

Advanced Computer Methods for Simulation Based Design

Professor Anthony T. Patera

Massachusetts Institute of Technology

Bayesian–Validated Computer–Simulation Surrogates for Optimization and Design

Anthony T. Patera
Department of Mechanical Engineering
Massachusetts Institute of Technology

J. Otto, M. Paraschivoiu, S. Yeşilyurt
M. Cruz, C. Ghaddar

DSSG Symposium on
Innovative Computational Methods

IDA, Washington, D.C.
November, 1994

1

OUTLINE

INTRODUCTION

Problem Definition

Direct Insertion *vs* Surrogates

BAYESIAN–VALIDATED SURROGATES

General Framework

Attributes

Contributing "Technologies"

APPLICATIONS

Effective Conductivity of Composite

(Stokes) Drag on Axisymmetric Body

SAMPLE PROOF $(K = L = J = 1)$

$m_\rho(\Upsilon)$ Cumulative Distribution Function

$\mathcal{PAC}$ Statement

$\mathcal{PN}$ and $\mathcal{PC}$ Results

Multiple Studies (*vs* Random Search)

INTRODUCTION

Preliminaries

□ Physical system $\mathcal{M}^{000}$
$\longrightarrow$ mathematical system $\mathcal{M}^{00}$

□ Deterministic mathematical system $\mathcal{M}^{00}$:
$\mathbf{p}$, input vector in $\Omega \subset \mathbb{R}^M$
s, (single) output in $\mathbb{R}^1$ $\quad (\mathbb{R}^K)$
$\mathcal{S}(\mathbf{p}) : \Omega \to \mathbb{R}$, input–output function (L^∞)

□ Global optimization problem (goal):

λ, target output value

$$\mathbf{p}^*(\lambda) = \arg\min_{\mathbf{p}\in\Omega} (\, \Psi(\mathbf{p}, \lambda) = |\mathcal{S}(\mathbf{p}) - \lambda|\,)$$

∘ Extension: $\Psi(\mathbf{p}, \lambda) = \psi(\mathcal{S}(\mathbf{p}), \mathbf{p}, \lambda)$

□ Simulation $\mathcal{M}^0$:

$$\mathbf{p} \in \Omega \xrightarrow{\mathcal{M}^0} R_{\mathbf{p}} = \mathcal{S}(\mathbf{p}) + W_{\mathbf{p}} \text{ (noise)}$$

$$W_{\mathbf{p}} \sim f_{W|\mathbf{P}}(w|\mathbf{p}) = h(\frac{w}{\sigma_W(\mathbf{p})})/\sigma_W(\mathbf{p}) \text{ (sym)}$$

$W^u_{\mathbf{p}}$: unbounded, $h(v) > 0$ for all $v \in \mathbb{R}$
sources: Monte–Carlo variance,...

$W^b_{\mathbf{p}}$: bounded, $h(v) = 0$ for $|v| > c_W$
sources: incomplete iteration,...

□ Complexity conditions:

1. $\mathbf{p} \in \Omega \xrightarrow{\mathcal{M}^0} R_{\mathbf{p}}$ expensive (time, cost)
2. *no* economies of scale for $R_{\mathbf{p}_1}, R_{\mathbf{p}_2}, \ldots$
3. limited regularity (information) for $\mathcal{S}(\mathbf{p})$
4. noise estimable and controllable

Simulation–Based Optimization

□ Exact design problem:

$$\mathbf{p}^*(\lambda) = \arg\min_{\mathbf{p}\in\Omega} |\mathcal{S}(\mathbf{p}) - \lambda|$$

□ Direct Insertion approach:

$$\mathbf{p}^*_R(\lambda) = \arg\min_{\mathbf{p}\in\Omega} |\Re R_{\mathbf{p}} - \lambda|$$

NLP($\mathcal{M}^0$) (simulation as function call)

- robustness ?
- premature termination ?
- mid–process flexibility $(\lambda^{[1]}, \lambda^{[2]}, \ldots)$?
- incorporation of prior information ?
- design interactivity ?

□ Surrogate approach:

1) surrogate construction and validation:

$$\begin{array}{c} \text{prior information} \\ + \\ \mathbf{p} \in \Omega \xrightarrow{\mathcal{M}^0} R_{\mathbf{p}} = \mathcal{S}(\mathbf{p}) + W_{\mathbf{p}} \end{array}$$

$$\textit{construct} \Downarrow \textit{validate}$$

$$\mathcal{M} : \tilde{\mathcal{S}}(\mathbf{p}) \approx \mathcal{S}(\mathbf{p}) \text{ over } \Omega$$

2) surrogate–based optimization:

$$\tilde{\mathbf{p}}^*(\lambda) = \arg\min_{\mathbf{p}\in\Omega} |\tilde{\mathcal{S}}(\mathbf{p}) - \lambda|; \quad \mathrm{NLP}(\mathcal{M})$$

- robust, complete optimization
- significant mid–process flexibility (λ)
- prior information readily integrated
- highly interactive. . . BUT *purposiveness*

How does $\mathcal{S}(\mathbf{p})(\rightarrow R_{\mathbf{p}}) \rightarrow \tilde{\mathcal{S}}(\mathbf{p})$ affect
predictability: $\mathcal{S}(\mathbf{p} \approx \tilde{\mathbf{p}}^*)$? necessary
optimality: $\tilde{\mathbf{p}}^*$ *vs* $\mathbf{p}^*$, $\tilde{\mathcal{S}}(\tilde{\mathbf{p}}^*)$ *vs* $\mathcal{S}(\mathbf{p}^*)$? desirable

6

□ Simple example:

- $\mathcal{M}^{000}$: flow of water past sphere
- $\mathcal{M}^{00}$: incompressible Navier–Stokes

  $\mathbf{p} \equiv \log$ (Reynolds) $\in \Omega \equiv [1,3] \subset \mathbb{R}^{M\equiv 1}$

  $s \equiv$ drag coefficient, c_D; $\mathcal{S}(\mathbf{p}) \equiv C_D(\log Re)$
- optimization problem

  $\lambda \equiv$ target drag coefficient, $\overline{c}_D$

  $(\log Re)^* = \arg\min_{\log Re \in \Omega} |C_D(\log Re) - \overline{c}_D|$
- $\mathcal{M}^0 \equiv$ YOUR CODE HERE

  $R_{\log Re} = C_D(\log Re) + W^b_{\mathbf{p}}(\to 0)$

○ Direct Insertion approach:

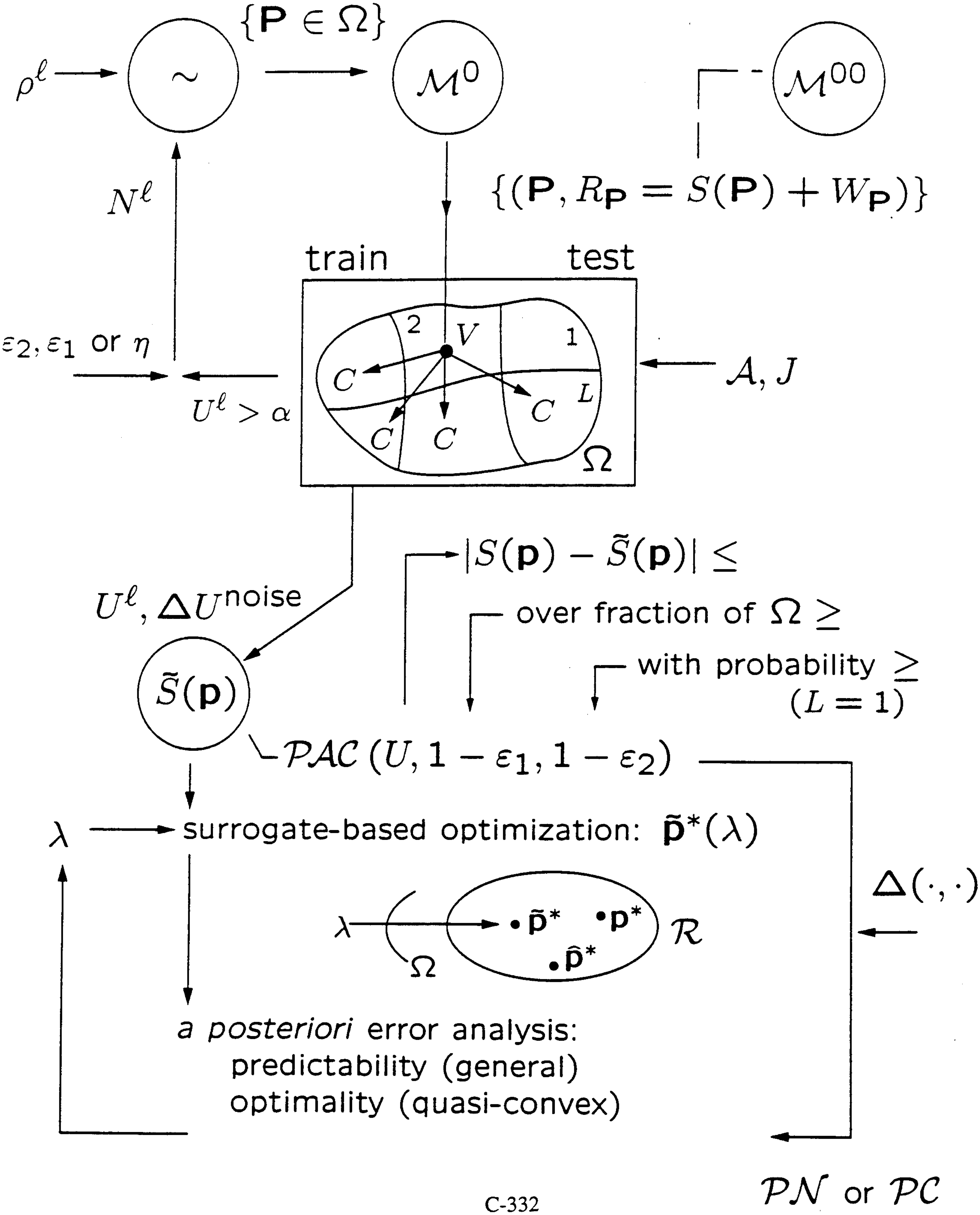
$$(\log Re)^*_R = \arg \min_{\log Re \in \Omega} |R_{\log Re} - \overline{c}_D|$$

- $\mathcal{M}$: $\tilde{\mathcal{S}}(\mathbf{p}) \equiv \tilde{C}_D(\log Re)$

○ Surrogate approach:

$$(\widetilde{\log Re})^* = \arg \min_{\log Re \in \Omega} |\tilde{C}_D(\log Re) - \overline{c}_D|$$

BAYESIAN–VALIDATED SURROGATES



□ Attributes (*vs* alternative schemes):

+ rigorous bounds (*vs* plausible)
+ fixed validation sample size
  (*vs* asymptotic results)
+ verifiable hypotheses on $\mathcal{S}(\mathbf{p})$
  (*vs* convenient assumptions)
+ confidence interval (*vs* expectation)
+ nonparametric framework
  (*vs* $\tilde{\mathbf{p}}^* \sim \rho$ conditional)
+ purposive estimates (*vs* suggestive)
+ elemental, sequential, adaptive
  (*vs* global, batch, open–loop)

± worst–case analysis (*vs* average–case)
± limited resampling (*vs* "1–left–out")

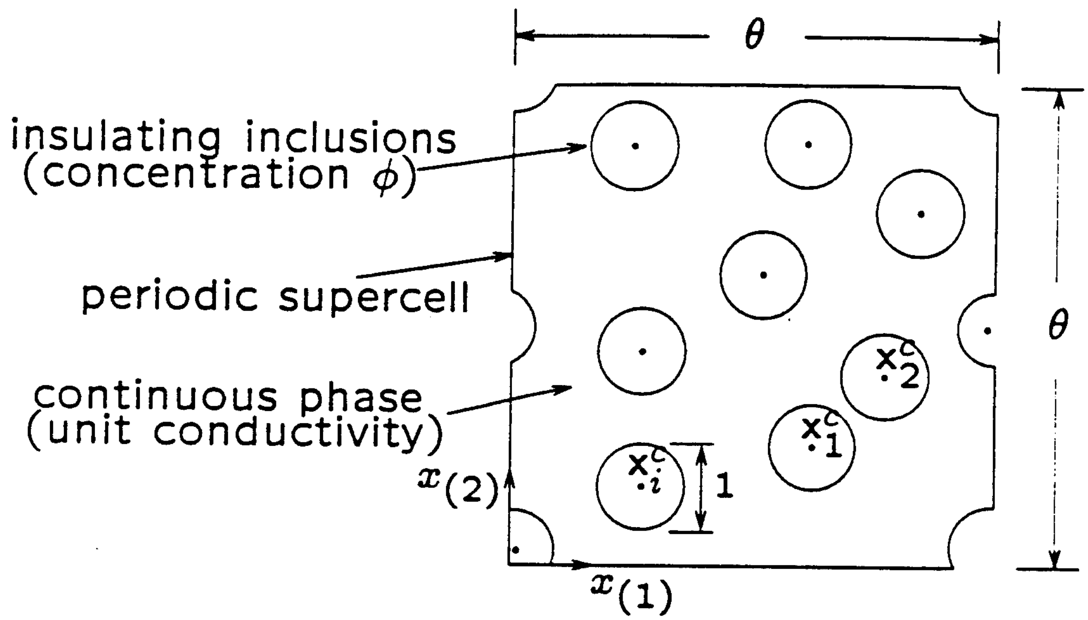
– volumetric ⇒
  poor coordinate localization in $\mathbb{R}^{M\to\infty}$
  unless highly correlated inputs (shape)

□ Contributing "technologies":

- BLUP computer–simulation surrogates [Sacks, Morris, . . .]
- $\mathcal{PAC}$ framework [Valiant, . . .]
- Information–based complexity theory [Traub, Wozniakowski, . . .]
- Discrepancy theory [Niederreitter, . . .]
- Stochastic optimization [Rubinstein, . . .]
- Statistical prediction:
  - experimental response surfaces [Box, . . .]
  - train–test procedures [Weiss & Kulikowski, . . .]
  - tolerance limits, order statistics [David, . . .]
  - nonparametric nonlinear regression [Härdle, . . .]
  - hypothesis–testing [Pratt & Gibbons, . . .]
  - cross–validation techniques [Stone, . . .]
- System identification [Bohlin, . . .]
- Optimization models [Barthelemy, Haftka, . . .]

APPLICATION: Effective Conductivity

□ $\mathcal{M}^{00}$: isotropic, fibrous composite



$\mathcal{K}_r(\phi, \theta, \underline{\mathbf{x}}^c)$:

$$\frac{\text{conduction heat transfer/depth across } x_{(1)} \text{ plane}}{\text{imposed } x_{(1)} \text{ temperature gradient} \times \theta}$$

$$k_e = \mathcal{K}_e(\phi) = \lim_{\theta \to \infty} < K = \mathcal{K}_r(\phi, \theta, \underline{\mathbf{X}}^c) >_{\underline{\mathbf{X}}^c \sim \text{RSA}}$$

$\mathbf{p} \equiv \phi \in \Omega \equiv [0.05, .5] \subset \mathbb{R}^{M \equiv 1}$

$s \equiv k_e$

$\mathcal{S}(\mathbf{p}) \equiv \mathcal{K}_e(\phi)$

□ $\mathcal{M}^0$ (simulation)

◦ Numerical approach

- Monte–Carlo: $< K > \Rightarrow \overline{K}_\phi = \frac{1}{N_r} \sum_{i=1}^{N_r} K_i$
- FEM: $\nabla^2 \chi = \ldots \Rightarrow K_i \equiv \mathcal{K}_r(\phi, \theta_0, \underline{\mathbf{X}}_i^c)$
  variational–bound nip treatment
  automatic *data* parallel partition
  automatic parallel mesh generation (Hecht)
  $\mathbb{P}_2$ isoparametric discretization
  parallel conjugate gradient iteration
  iPSC/860 hypercube implementation

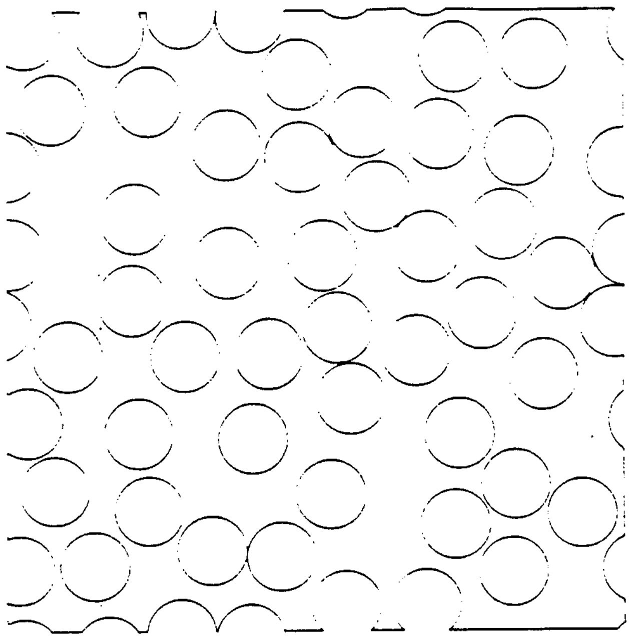
◦ Computational requirements:

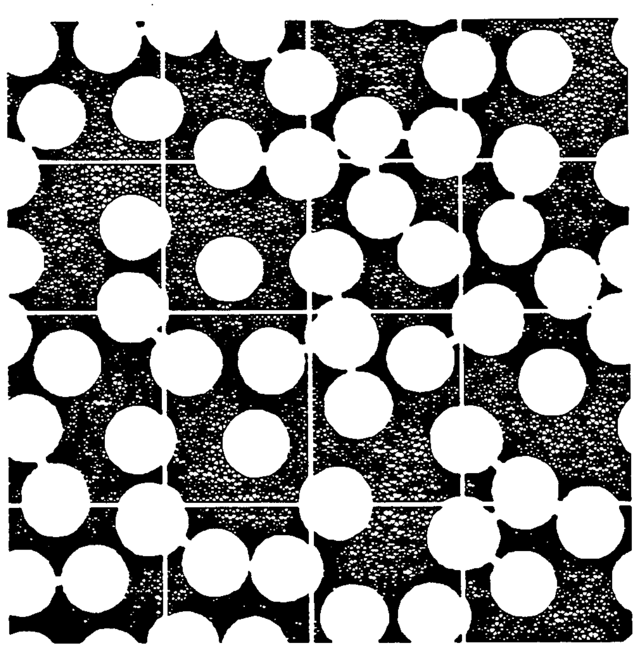
- $\phi = 0.50, N_r = 20 \rightarrow \overline{K}_\phi$
  iPSC/860 (16 nodes): 47 mins, $10
- parallel advantage:

	time	cost
workstation	12×	–
vector super	–	10×

- parallel $\Rightarrow$ time & cost $\downarrow$ OR problem size $\uparrow$

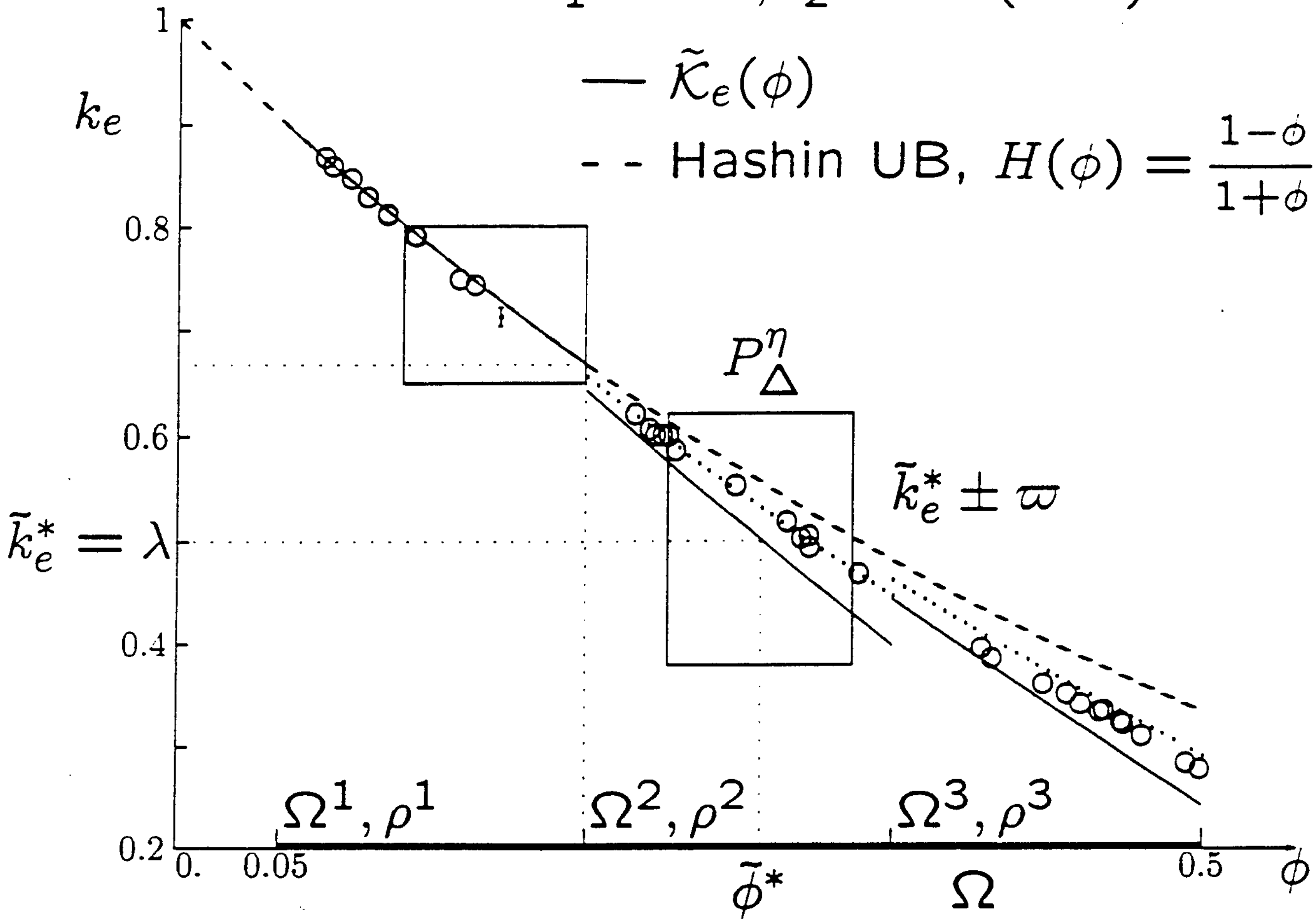
◦ Example: $\mathcal{K}_r(\phi = .5, \theta = 8.86, \underline{\mathbf{x}}^c)$





$$[\mathcal{K}_{r,LB}(\phi, \theta, \underline{\mathbf{x}}^c), \mathcal{K}_{r,UB}(\phi, \theta, \underline{\mathbf{x}}^c)] = [.2839, .2934]$$

□ Train–Test: $\varepsilon_1 = .15, \varepsilon_2 = .15(\to 0)$



○ Simulation (train–test) data:

$[(\phi_j^\ell, \overline{K}_{\phi_j^\ell}), j = 1, \ldots, N^\ell = 12], \ell = 1, 2, L = 3$

$$\overline{K}_{\phi_j^\ell} = \mathcal{K}_e(\phi_j^\ell) + W_{\phi_j^\ell}$$

○ Surrogate (train):

$\ell = 1, \quad \tilde{\mathcal{K}}_e(\phi)|_{\Omega^\ell} = H(\phi)$

$\ell = 2, 3, \quad \tilde{\mathcal{K}}_e(\phi)|_{\Omega^\ell} =$

$$\text{BLUE}_2[(\phi_j^{\ell-1}, \overline{K}_{\phi_j^{\ell-1}}), j = 1, \ldots, N^\ell]$$

∘ Model prediction error estimators (test):

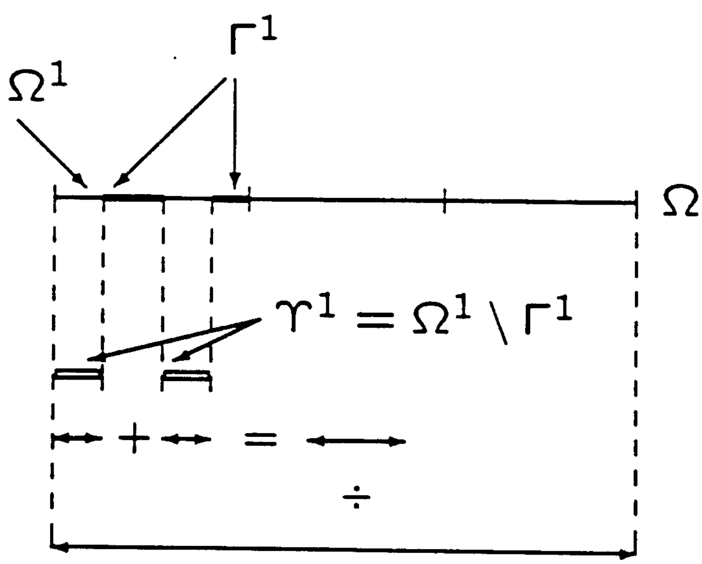
$$U^\ell = \max_{j\in\{1,\ldots,N^\ell\}} |\overline{K}_{\phi_j^\ell} - \tilde{\mathcal{K}}_e(\phi_j^\ell)|,\ \ell = 1,2,3$$
$$= \{.016, .043, .034\} \quad (\cdots\{.016, .006, .019\})$$

∘ *$\mathcal{PAC}$ statement*:

With confidence $\geq 1 - \varepsilon_2 = .85$,
$\forall \ell \in \{1,2,3\}$,
$\exists \Gamma^\ell \subset \Omega^\ell$, with $m_\rho(\Omega^\ell \setminus \Gamma^\ell) \leq \varepsilon_1 = .15$,
such that, $\forall \phi \in \Gamma^\ell$,

$$|\,\mathcal{K}_e(\phi)|_{\Omega^\ell} - \tilde{\mathcal{K}}_e(\phi)|_{\Omega^\ell}\,| \leq U^\ell\,.$$

For $\mathcal{D} \subset \Omega$,
$L > 1, \rho^\ell(\mathbf{p})$ uniform: $m_\rho(\mathcal{D}) = \int_{\mathcal{D}} \mathbf{dp} / \int_\Omega \mathbf{dp}$
$L = 1, \rho(\mathbf{p})$ general: $m_\rho(\mathcal{D}) = \int_{\mathcal{D}} \rho(\mathbf{p})\mathbf{dp}$



$= \quad m_\rho(\Omega^1 \setminus \Gamma^1)$

□ Surrogate–based optimization:

$$\tilde{\phi}^* = \arg \min_{\phi \in \Omega} |\tilde{\mathcal{K}}_e(\phi) - \lambda|$$

$\lambda = .5 \Rightarrow \tilde{\phi}^* = .29;\ \tilde{k}_e^* = \tilde{\mathcal{K}}_e(\tilde{\phi}^*) = \lambda$

□ *A posteriori* error analysis ($\mathcal{PN}$): $\eta = .20$

∘ $\mathcal{P}$rediction $\mathcal{N}$eighborhood $\mathcal{P}_\Delta^\eta = [.24, .33]$

$$\arg \min_{\mathcal{P}' \subset \Omega^{\ell^*} \text{ s.t. } m_\rho(\mathcal{P}') = \eta} \max_{\phi' \in \mathcal{P}'} \Delta(\phi', \tilde{\phi}^*) \text{ (Euclidean)}$$

∘ With confidence $\geq 1 - \varepsilon_2 = .85$,

$$\left.\begin{array}{c} \exists\, \Xi \subset \mathcal{P}_\Delta^\eta, \text{ with } \dfrac{m_\rho(\Xi)}{\eta} \geq 1 - \dfrac{\varepsilon_1}{\eta} = .25, \\ \text{such that}, \forall \phi \in \Xi, \\ |\mathcal{K}_e(\phi) - \lambda| \leq .04(U^2) + .07(\delta) = .12(\varpi)\ . \end{array}\right\} \mathcal{F}$$

∘ *Joint* statement for multiple studies

$q = 1, \ldots, Q,\ \lambda^{[q]} \Rightarrow$

$$\tilde{\phi}^{*[q]}, \tilde{k}_e^{*[q]} (= \lambda^{[q]}), \mathcal{P}_\Delta^{\eta[q]}, \varpi^{[q]}$$

With confidence $\geq 1 - \varepsilon_2 = .85$,

$$\mathcal{F}^{[1]} \text{ and } \mathcal{F}^{[2]} \text{ and} \ldots \mathcal{F}^{[Q]}\ .$$

□ Design scenario(s)

∘ Preliminary design process (potentialities)

$q = 1, \ldots, Q,\ \lambda^{[q]} \Rightarrow$

$\tilde{\phi}^{*[q]}, \tilde{k}_e^{*[q]}, \mathcal{P}_{\Delta}^{\eta[q]}, \varpi^{[q]} \overset{\text{resources}}{\Rightarrow} D^{[q]}[\tilde{\phi}^{*[q]}, \tilde{k}_e^{*[q]}]$

assume: $\forall q \in \{1, \ldots, Q\}, \forall \phi \in \mathcal{P}_{\Delta}^{\eta[q]}$,

$D^{[q]}[\phi, \tilde{k}_e^{*[q]} \pm \varpi^{[q]}]$ acceptable

(*design–performance* "volume")

∘ Final design process (realization)

SELECT $D_f = D^{[r]}[\tilde{\phi}^{*[r]}, \tilde{k}_e^{*[r]}]$

CALCULATE $k_e^A = \mathcal{K}_e(\tilde{\phi}^{*[r]})$ $\qquad (\overline{K}_{\tilde{\phi}^{*[r]}})$

IF $|k_e^A - \lambda^{[r]}| \leq \varpi^{[r]}$, PROCEED

ELSE

FIND $\hat{\phi}^* \in \mathcal{P}_{\Delta}^{\eta[r]}$ such that

$|\mathcal{K}_e(\hat{\phi}^*) - \lambda^{[r]}| \leq \varpi^{[r]}$

SET $D'_f = D^{[r]}[\hat{\phi}^*, \mathcal{K}_e(\hat{\phi}^*)]$, PROCEED

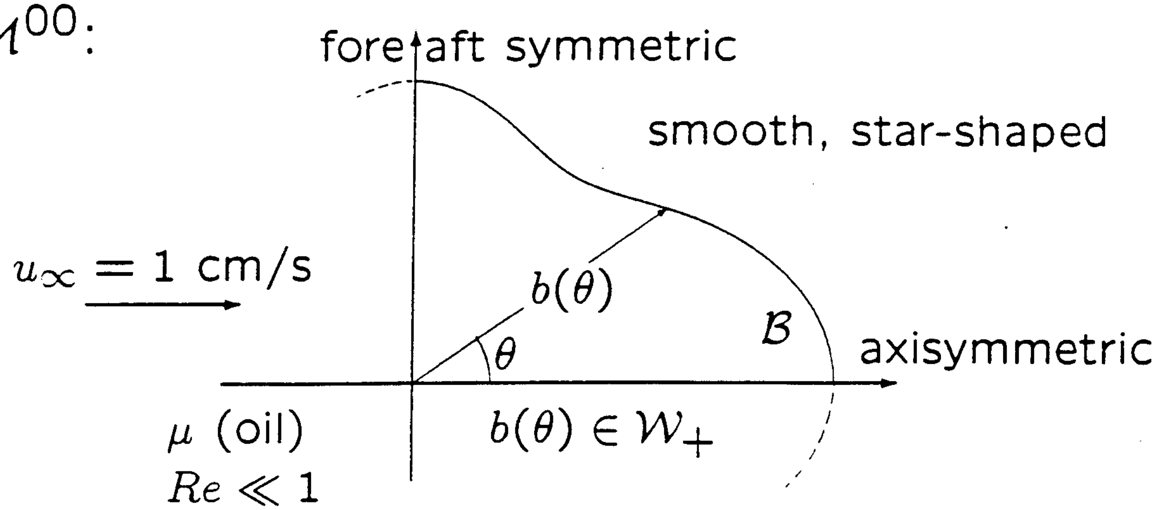
∘ *Un*validated alternative:

preliminary considerations, investments ?

interactive ?

APPLICATION: (Stokes) Drag on Body

□ $\mathcal{M}^{00}$:



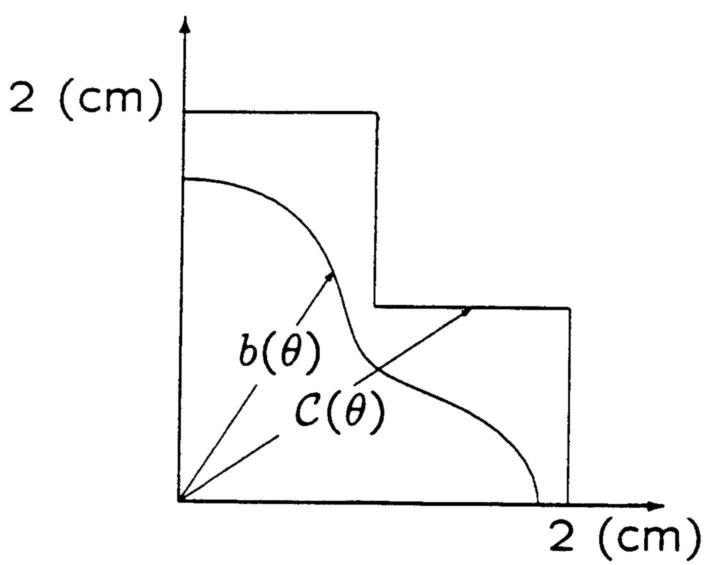
$$b(\theta; \mathbf{a}) = \sum_{i=1}^{M \to \infty} a_i \zeta_i(\theta)$$

$\mathbf{p} \equiv \mathbf{a} \in \Omega \subset \mathbb{R}^{M \to \infty}$; $s \equiv f_D$ (drag force)

$\mathcal{S}(\mathbf{p}) \equiv F_D(b)$; $\tilde{\mathcal{S}}(\mathbf{p}) \equiv \tilde{F}_D(b) = 6\pi\mu u_\infty \bar{r}(b)$

□ Exact design problem: $\lambda = 304$ dynes

$b^*(\theta) = \arg\min_{b(\theta)\in\mathcal{W}_+, b(\theta)\le\mathcal{C}(\theta)} |F_D(b) - \lambda|$



□ $\mathcal{M}^0$ (simulation): negligible noise

- FEM $\mathbb{P}_2-\mathbb{P}_1$ isoparametric discretization
- Uzawa nested conjugate gradient iteration

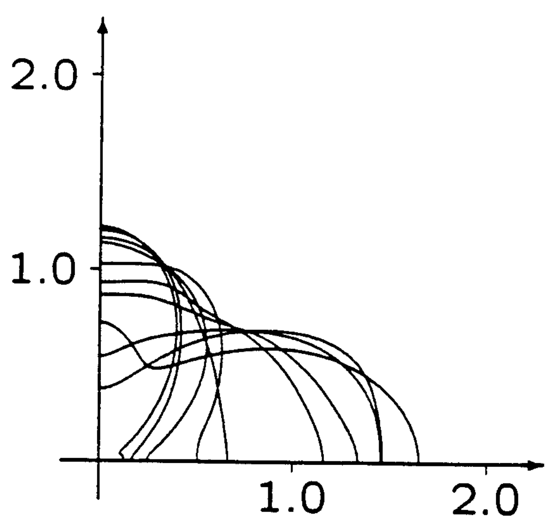
□ Importance function $\rho(\mathbf{A})$:
(*no* $b(\theta) \leq \mathcal{C}(\theta)$ restriction)

○ Random shape process $B(\theta; \mathbf{A})/\overline{r}(B)$
$\Rightarrow$ probability density $\rho(\mathbf{A})$

- radial scale: equivalence relation
- azimuthal scale:

$$E(B(\theta_1; \mathbf{A})B(\theta_2; \mathbf{A}))/\overline{r}^2(B) = g(\theta_1, \theta_2; \xi_B, \sigma_B)$$

○ Test sample: $b(\theta; \mathbf{a}_j)/\overline{r}(b(\theta; \mathbf{a}_j)), j = 1, \ldots$



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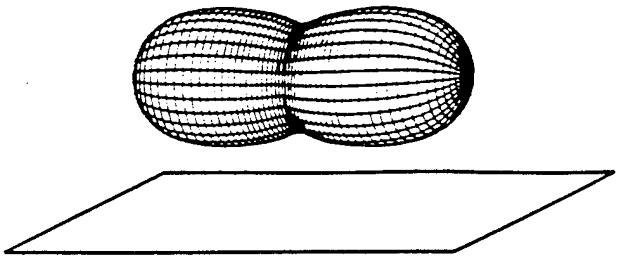
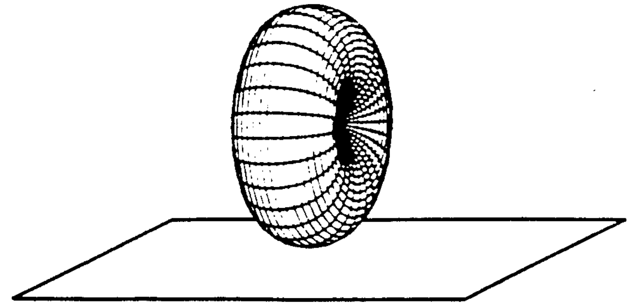
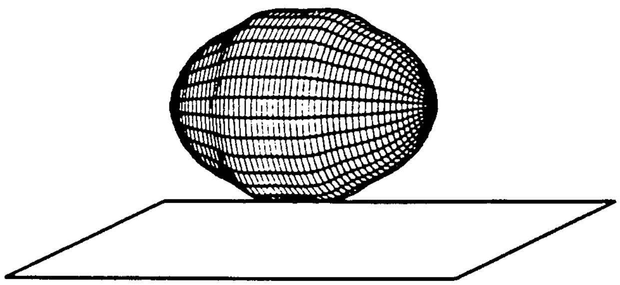
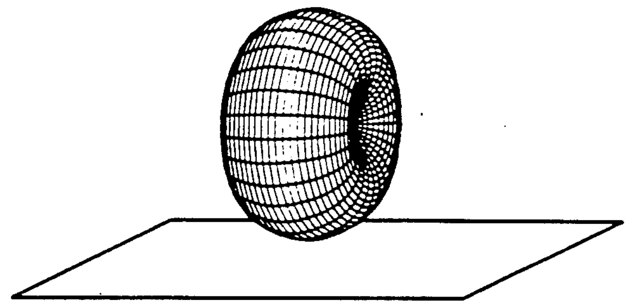
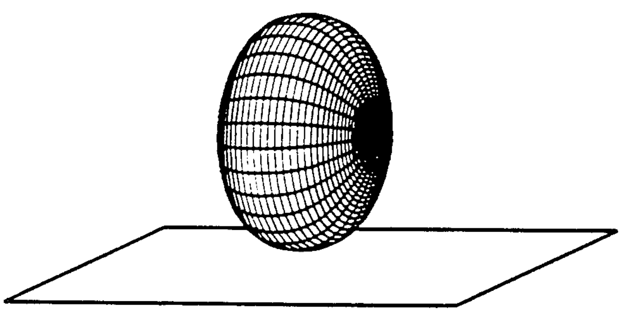
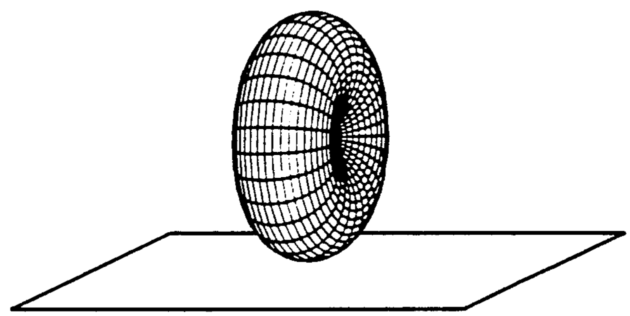


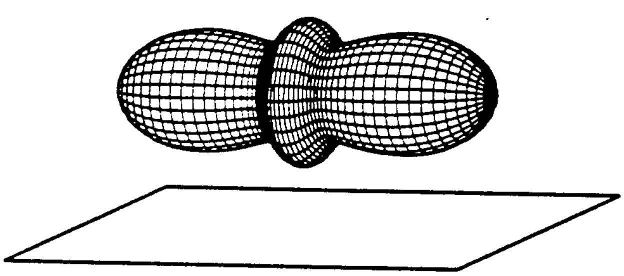


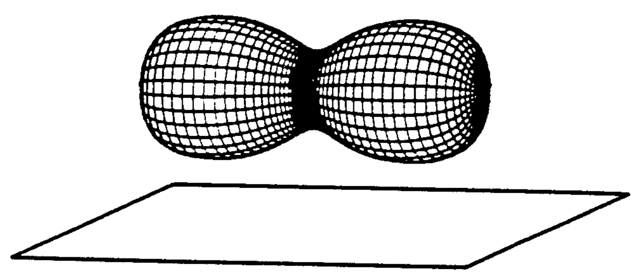


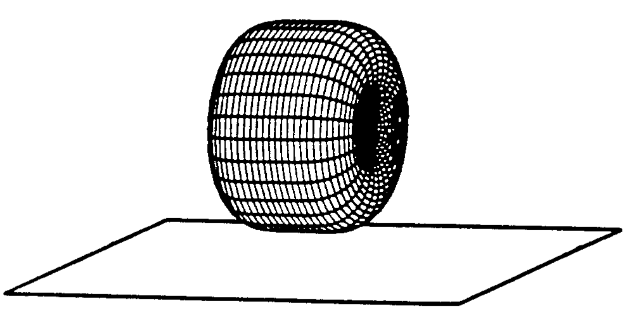


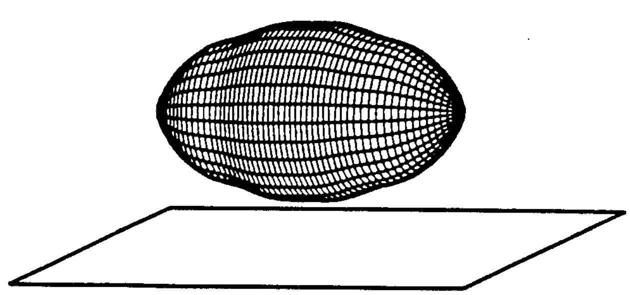












□ Validation: $\eta = .18, \varepsilon_2 = .18$

- model prediction error estimator(e):

$$U = \max_{j \in \{1,\ldots,N=30\}} \frac{\left| \dfrac{F_D(b_j)}{\mu u_\infty \overline{r}(b_j)} - 6\pi \right|}{6\pi} = .17$$

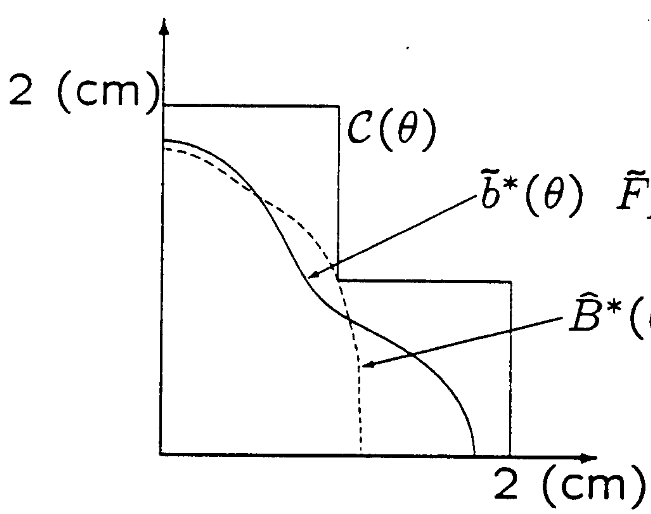
- $\mathcal{PAC}$ *statement*: $(\varepsilon_1 = .06)$

With confidence $\geq 1 - \varepsilon_2 = .82$,

$$m_\rho\{\mathbf{a} \in \Omega \mid \frac{\left| \dfrac{F_D(b)}{\mu u_\infty \overline{r}(b)} - 6\pi \right|}{6\pi} \leq .17\} \geq 1 - \varepsilon_1 = .94 \, .$$

□ Surrogate–based optimization:

$$\tilde{b}^*(\theta) = \ \arg\min_{b(\theta) \in \mathcal{W}_+, b(\theta) \leq \mathcal{C}(\theta)} |\tilde{F}_D(b) - \lambda|$$



□ *A posteriori* error analysis ($\mathcal{PC}$):

∘ Draw ($m = 1$) $\mathcal{P}$roximal $\mathcal{C}$andidate(s)

$$\alpha(b(\theta)) = \arg \min_{\alpha' \text{ s.t. } \alpha' b/\overline{r}(b) \le \mathcal{C}(\theta)} \Delta(\alpha' \frac{b(\theta)}{\overline{r}(b)}, \tilde{b}^*(\theta))$$

$$\mathcal{P}^{\eta}_{\Delta} =$$

$$\arg \min_{\mathcal{P}' \subset \Omega \text{ s.t. } m_{\rho}(\mathcal{P}') = \eta} \max_{\mathbf{a}' \in \mathcal{P}'} \Delta(\frac{\alpha(b) b(\theta; \mathbf{a}')}{\overline{r}(b(\theta; \mathbf{a}'))}, \tilde{b}^*(\theta))$$

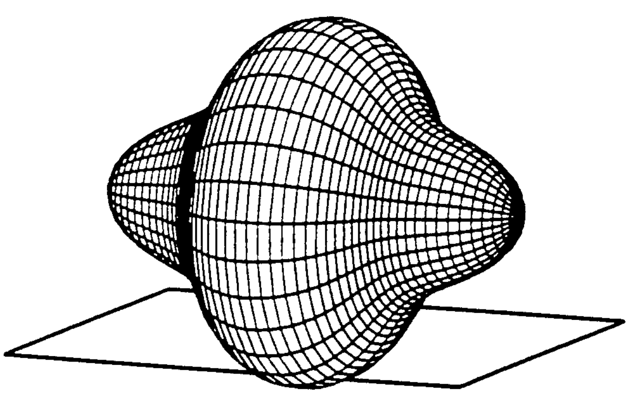
$$\hat{\mathbf{A}}^* (\in \mathcal{P}^{\eta}_{\Delta}) \sim \frac{1}{\eta} \rho(\mathbf{A})|_{\mathcal{P}^{\eta}_{\Delta}}, \ \hat{B}^*(\theta) = \alpha(B) \frac{B(\theta, \hat{\mathbf{A}}^*)}{\overline{r}(B(\theta, \hat{\mathbf{A}}^*))}$$

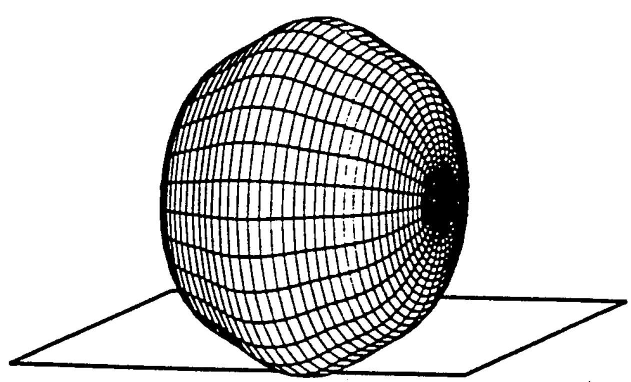
$$\Delta(b_1, b_2) = vol(\text{XOR}(\mathcal{B}_1, \mathcal{B}_2))/vol(\mathcal{B}_2)$$

∘ With confidence $\ge 1 - \varepsilon_2 = .82$,

$$|\, F_D(\hat{B}^*) - \lambda \,| \,/\, \lambda \le U' = .22\,[.06]\ ;$$

joint for different λ, $\mathcal{C}$, $\Delta(\cdot,\cdot)$ (Haussdorf...).



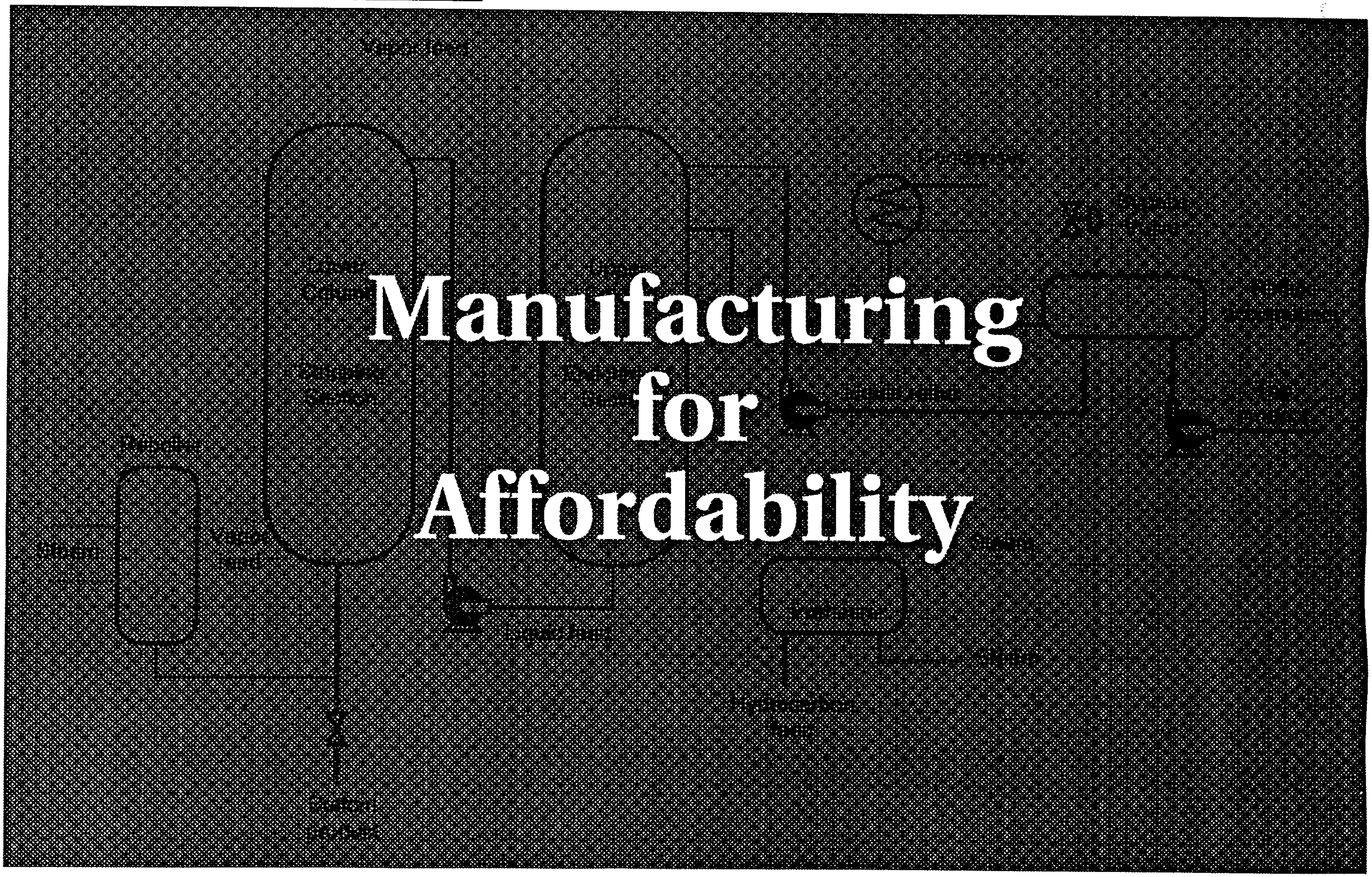


Manufacturing Simulation

Dr. Kurt Fickie

U.S. Army Research Laboratory, Aberdeen Proving Ground

US ARMY RESEARCH LABORATORY



Description

Develop a simulation environment to address materiel processing issues such as flexibility of manufacture, dual-use technologies, military verus commerical specifications, and rapid prototyping. Economic and operational considerations will also be simulated to assist policy makers in "tuning" the warm industrial base based on given defense postures. The immediate focus for the virtual factory will be on process technologies for thick resin composites for land combat vehicles and thin-skin composites for aircraft bodies.

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Rationale

- Some technologies exist primarily due to DoD interest and support.
- They are currently not cost competitive in civilian applications.
- DoD's expenditures will decrease so we must make the technologies affordable or they will die.
- "Dual-use" $\longrightarrow$ make commercially viable.
- Manufacturing simulation is a means to leverage market forces.

Our Analysis

- Virtual reality is 4-6 years off.
- Simulation of 3D, dynamic phenomena is here.

- DoD investment in computing surpasses that of industry.
- CAD/CAM tools are very sophisticated, so virtual prototyping is possible.

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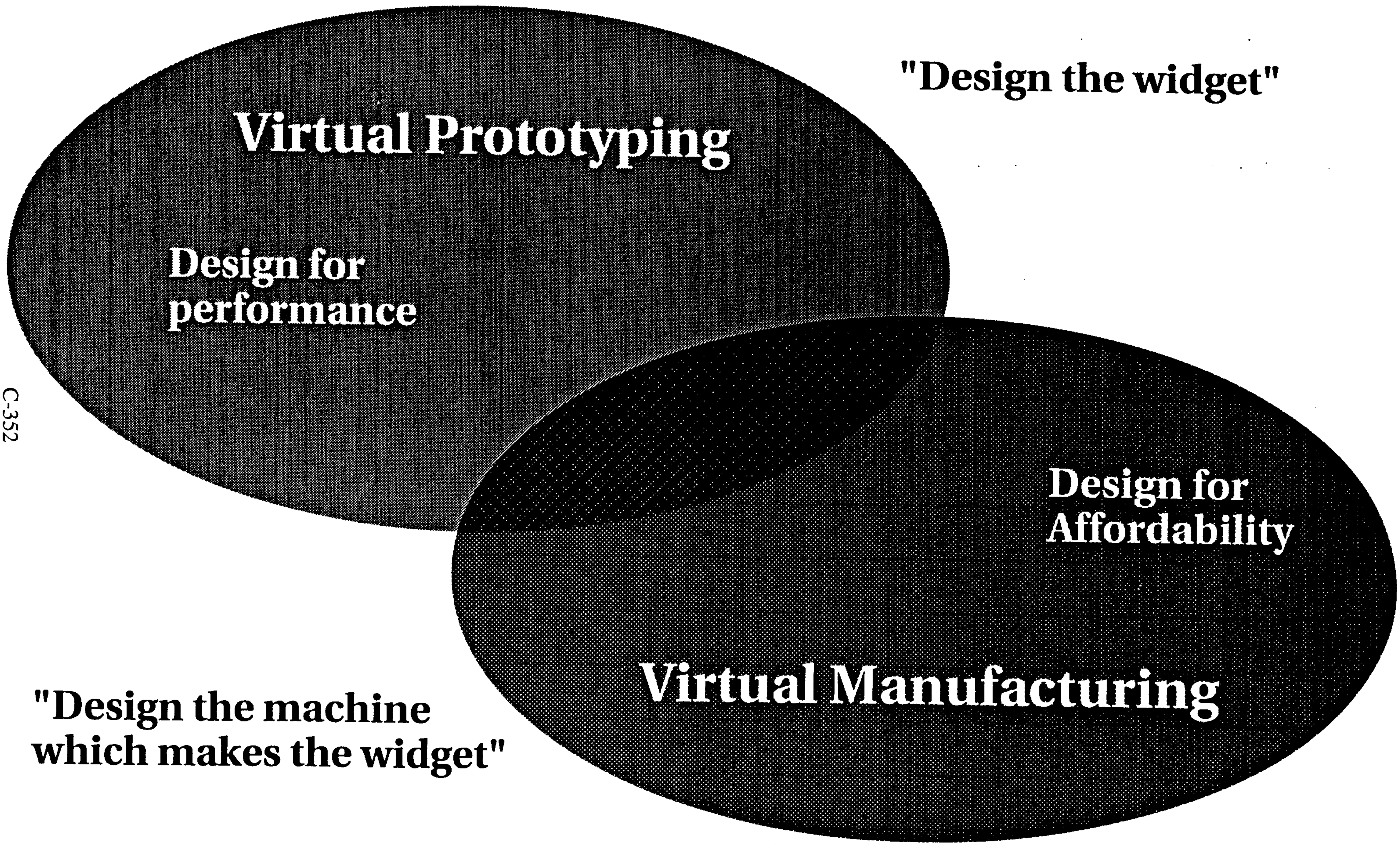
Virtual Factory

"Design the widget"



"Design the machine which makes the widget"

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Why Not Industry/Academia?

- High performance computing assets and modeling expertise are in the DoD or military industries.
- Industry has not yet been convinced large–scale computation turns a profit.
- Integration of indisciplinary research and engineering requires a scope currently beyond existing academic centers and industrial labs.
- Specifications affect cost, so the user must be involved.

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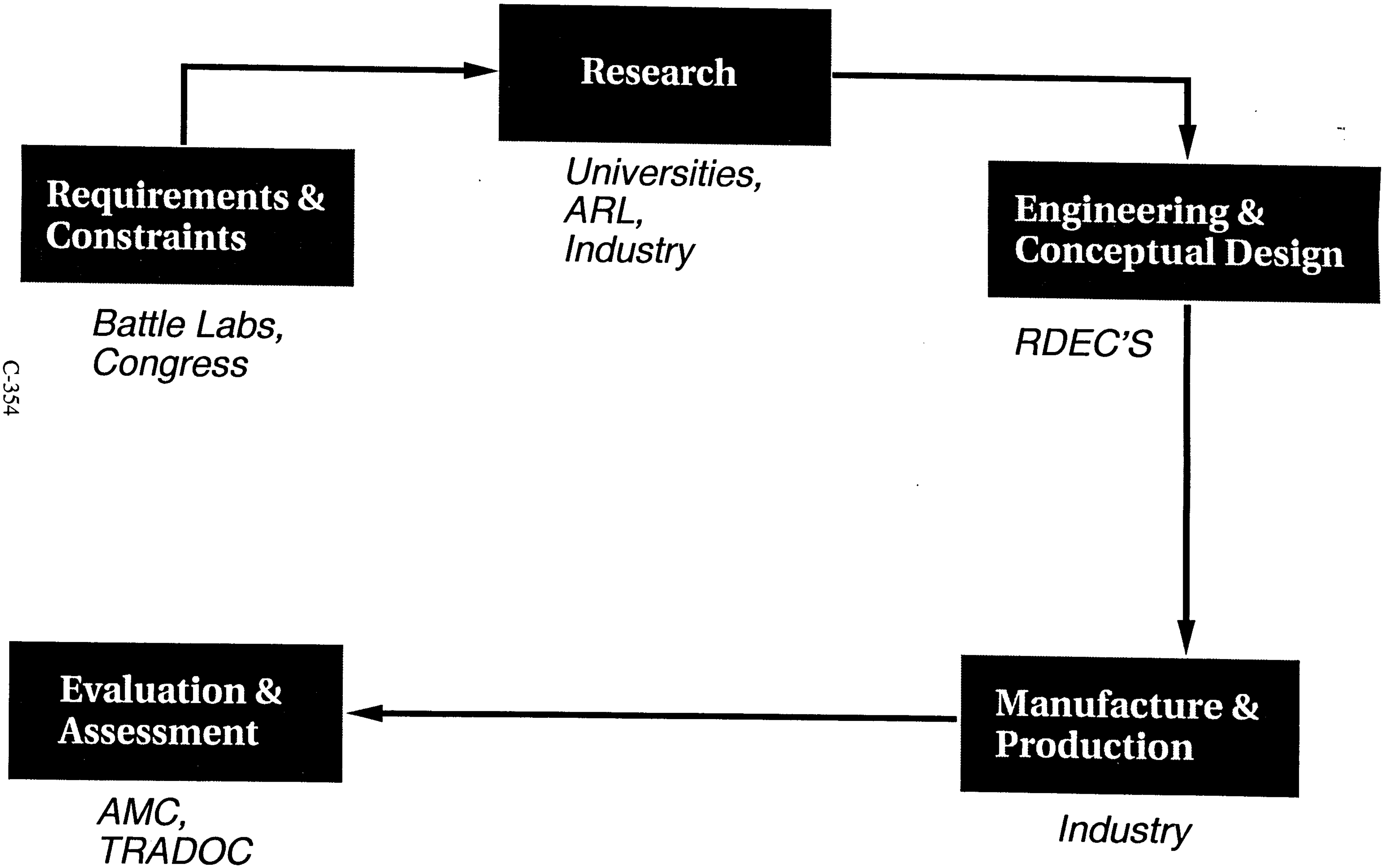
Current Acquisition Cycle



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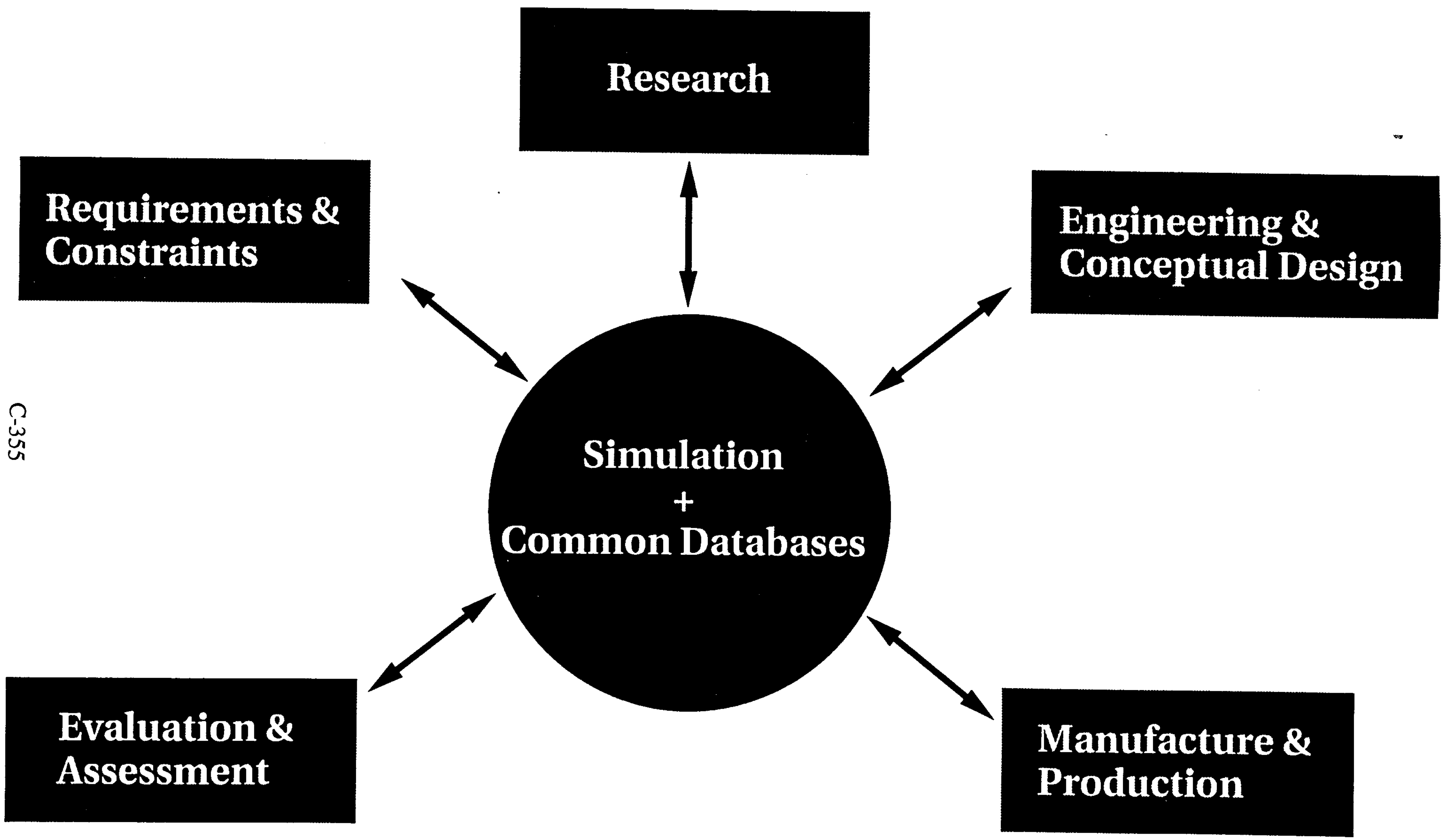
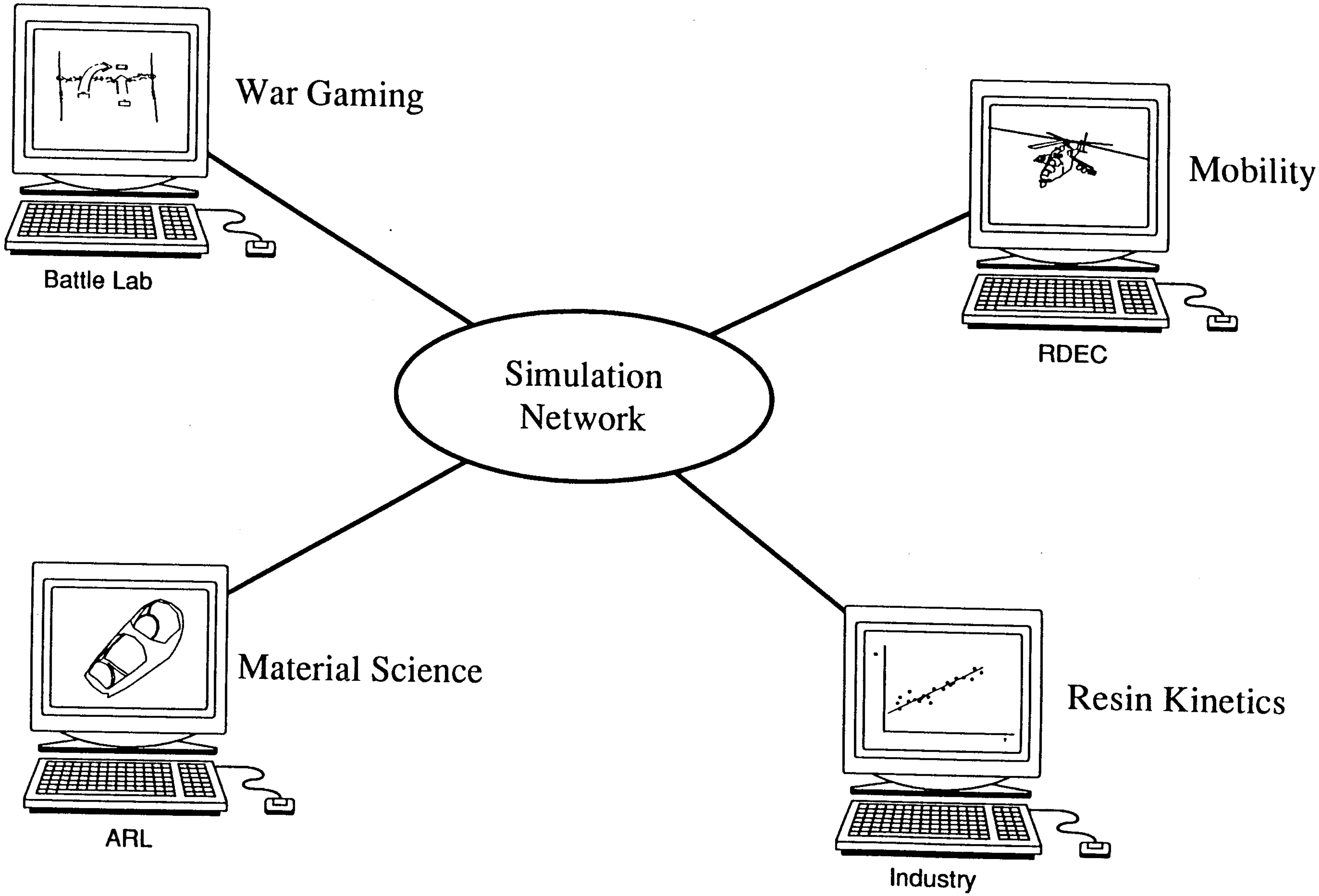
Leveraging Simulation



Interactive Collaborative Environments



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Why Composites?

- Manufacturing issues dominate costs.
- Scaling problems require simulation support.
- Lots of civilian applications, if affordable.
- Lighten the Force: CAV, Comanche.
- Army has long history in low–cost applications.

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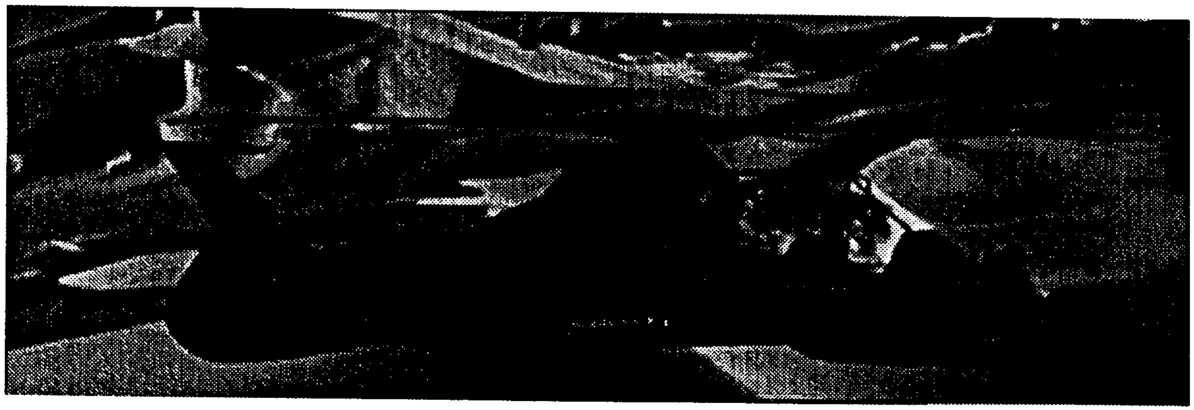
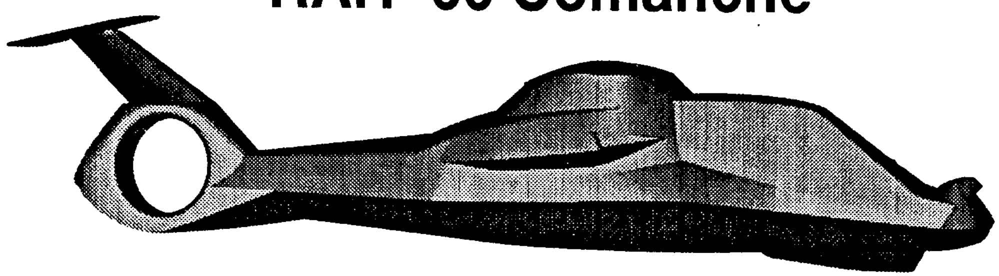
Example Army Applications





RAH–66 Comanche

AH–64D Apache Longbow

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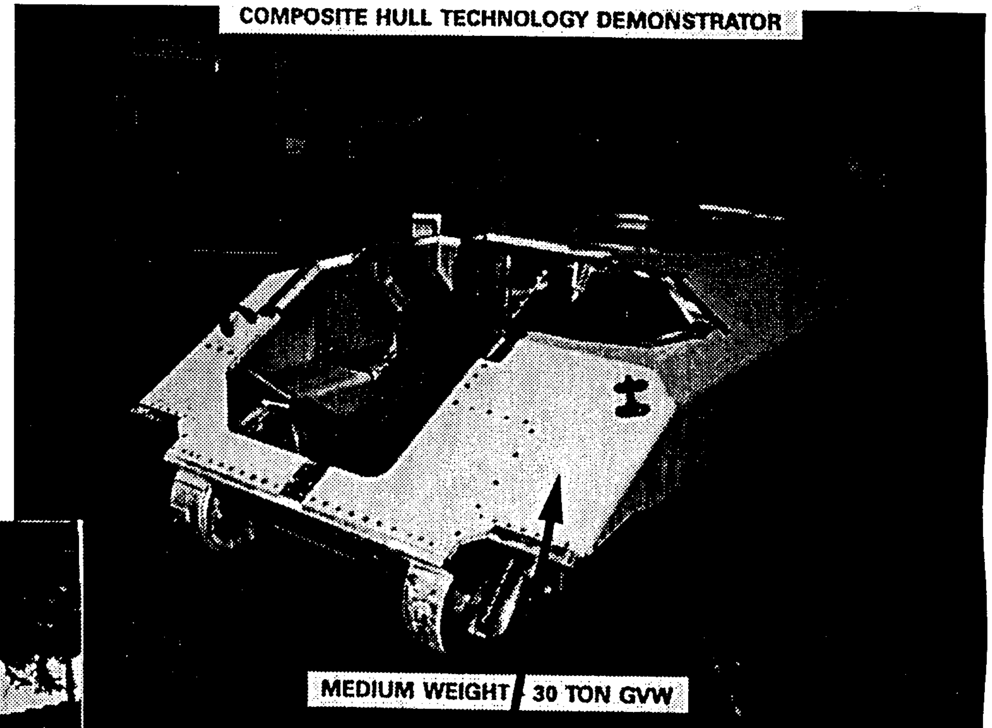
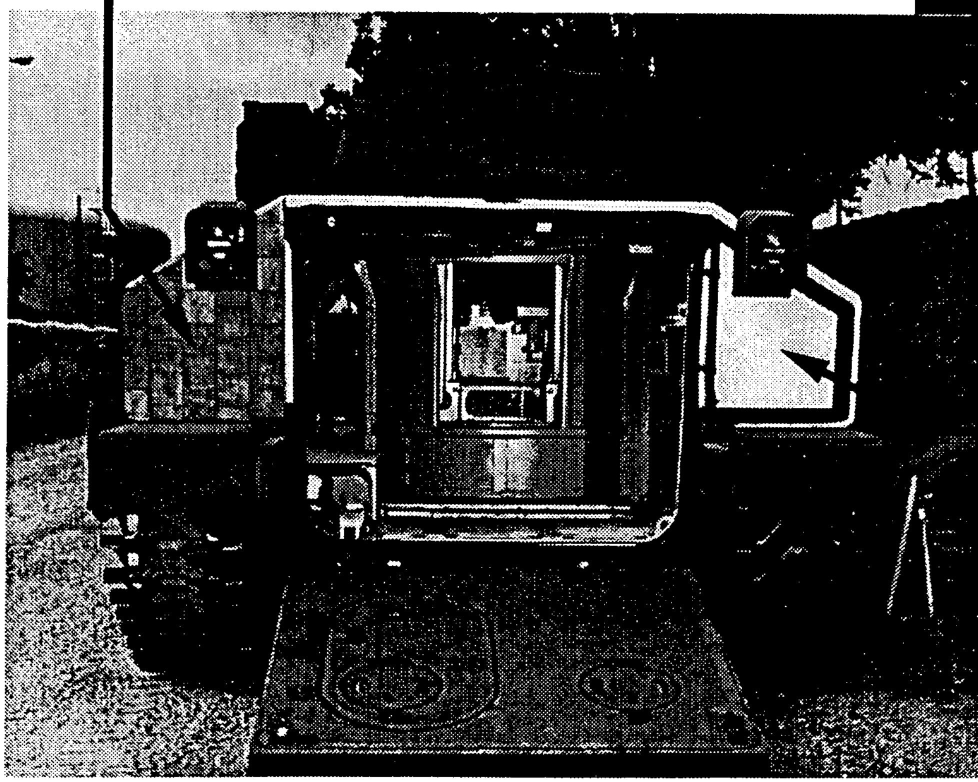
Example Army Applications



Ceramic Plate



Composite Hull

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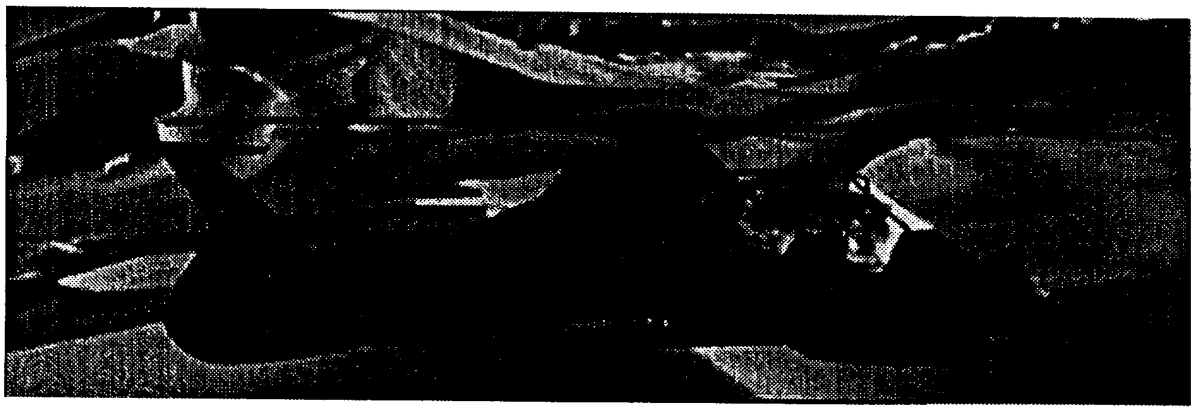
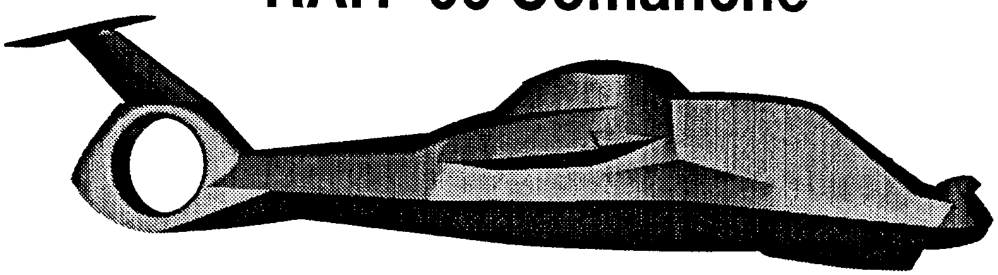
Example Army Applications





RAH–66 Comanche

AH–64D Apache Longbow

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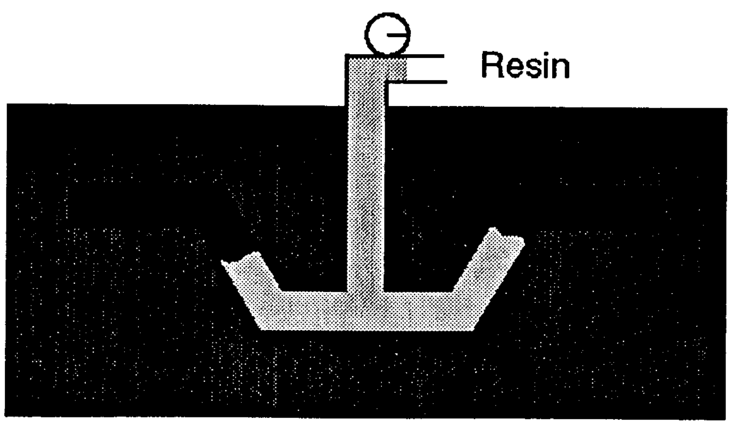
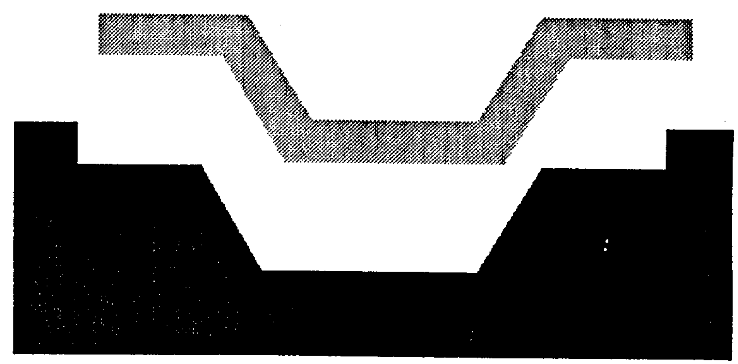
Resin Transfer Molding

Preform Lay-up

Insert preform into mold



Resin injection/Curing



Part removal

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Darcy's Law Flow

$$\boxed{\bar{u} = -\frac{\mathbf{K}}{\eta}\nabla P}$$

+ Heat Transfer

+ Cure Kinetics

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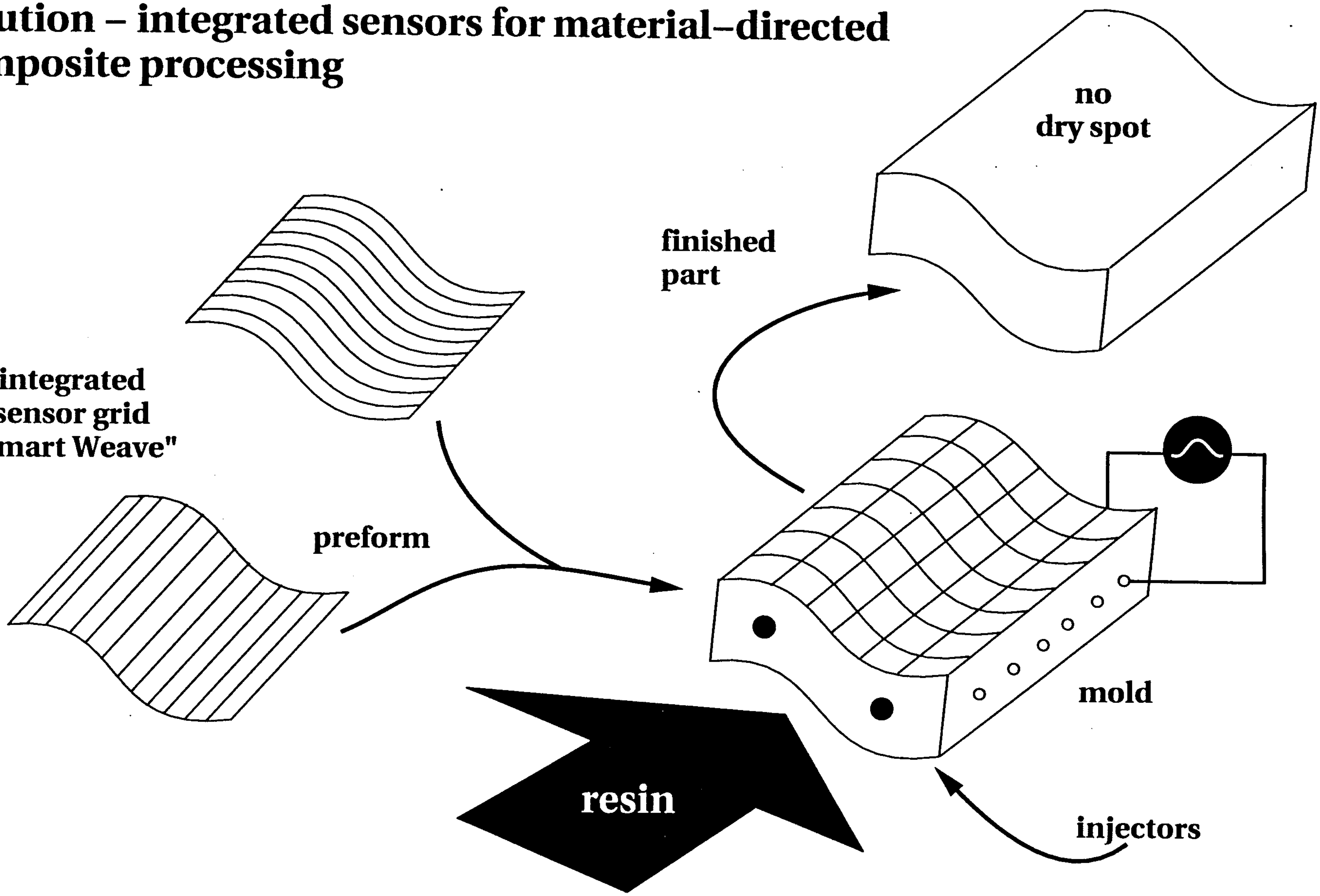
Resin Transfer Molding

Solution – integrated sensors for material–directed composite processing



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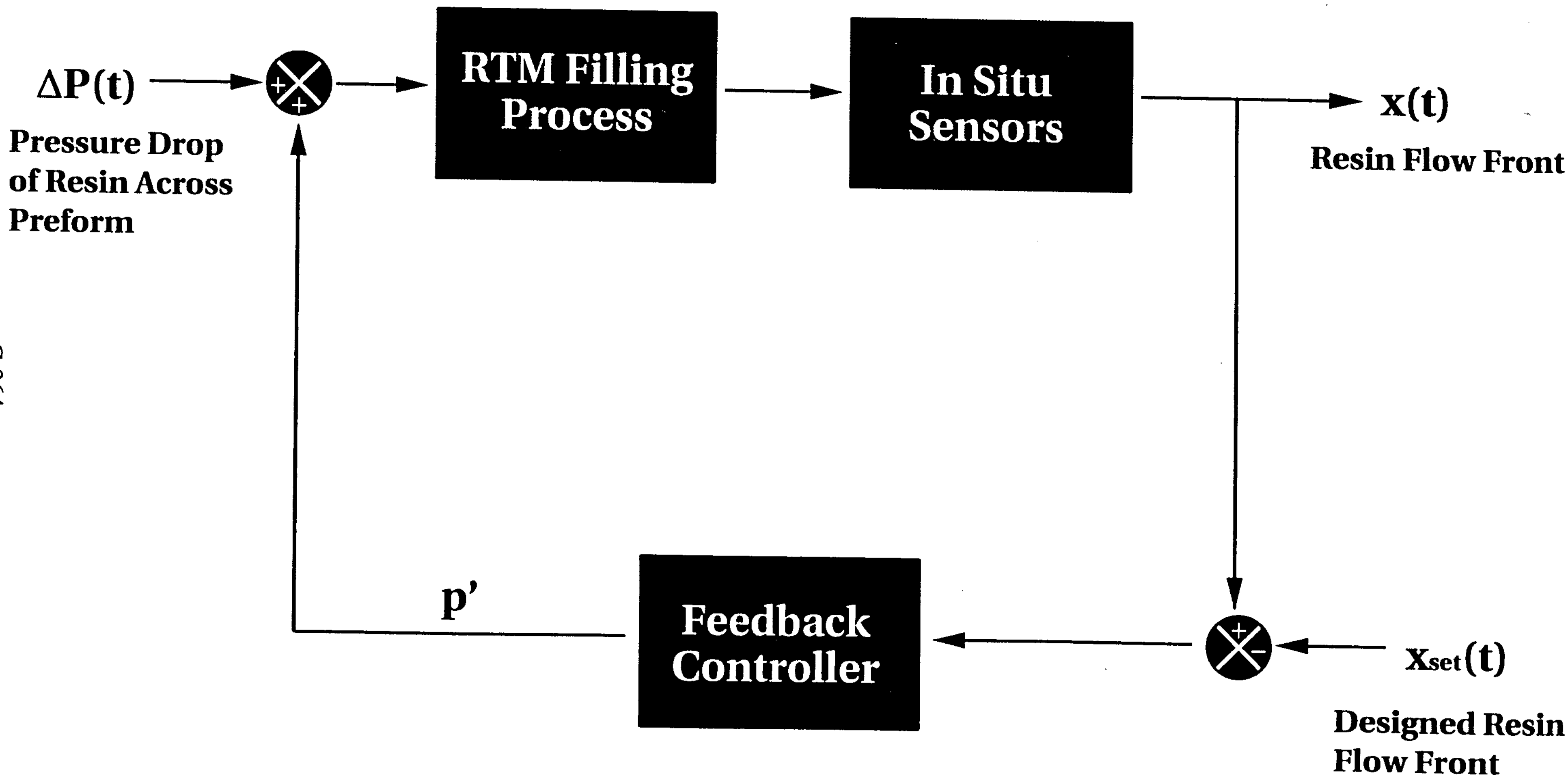
Closed Feedback Control



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In Situ Sensors

Improves reproducibility and quality via feedback control.
Closing the process loop will:

1. Eliminate dry spots

2. Compensate for process variations

Impacts affordability!

Teaming

Sikorsky / ATCOM

Univ. of Delaware

Univ. of Minnesota

Univ. of California, Berkeley

Draper Labs / MIT

FMC / TARDEC

MATERIALS/PROCESSING

Data for Modeling Materials-Processing Plasmas: The Impact of Parallel Computers

Dr. B. Vincent McKoy

California Institute of Technology

Data for Modelling Materials-Processing Plasmas:
The Impact of Parallel Computers

Coworkers: C. Winstead and H. Pritchard

Support: National Science Foundation
Air Force Office of Scientific Research
Sematech, Inc.

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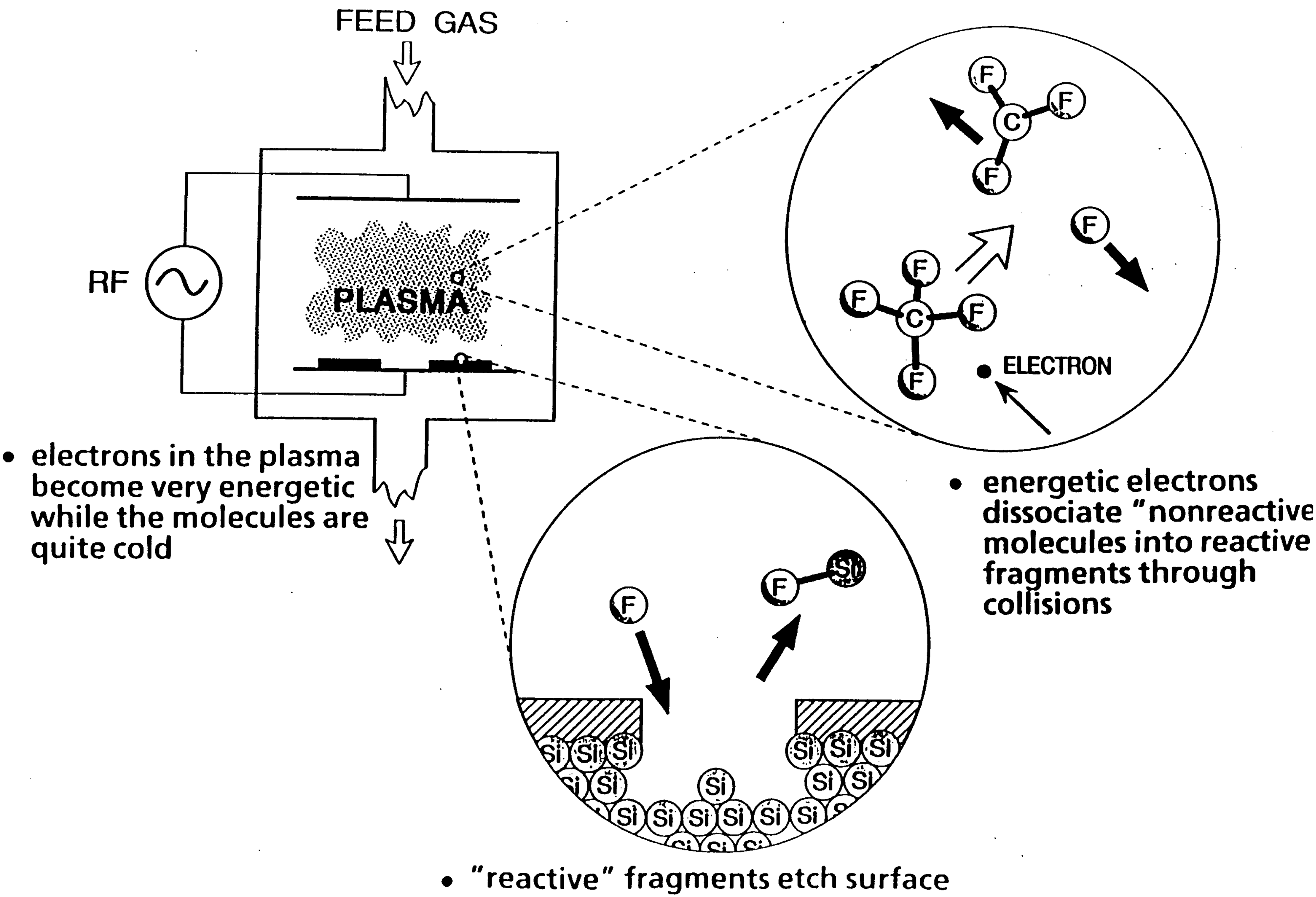
E-mail: BVM@starbase1.caltech.edu

- Schematic illustration of the essential role played by electron impact dissociation in these low-temperature non-equilibrium plasmas:

  - In these plasma reactors, electrons acquire temperatures of hundreds of thousands of degrees Kelvin while the heavy particles have temperatures of hundreds of degrees Kelvin.

  - Electron impact dissociation of feed gases leads to the production of reactive fragments.

  - These reactive fragments are responsible for much of the *chemistry* brought about by these plasmas.


FEED GAS
RF
PLASMA
ELECTRON
F
C
Si
• electrons in the plasma become very energetic while the molecules are quite cold
• energetic electrons dissociate "nonreactive molecules into reactive fragments through collisions
• "reactive" fragments etch surface

- Processing of materials by low-temperature plasmas is one of the most widely applied high-value manufacturing processes in United States industries:

  - Fabrication of semiconductor integrated circuits and other electronic devices.

  - Hardening of tools, dies and industrial metals.

  - Anticorrosion and other coatings deposited on surfaces.

  - Lighting and displays.

  - Hazardous waste remediation.

- Plasma reactors and processes in use today have been developed mainly on the basis of empiricism and statistical optimization. *More rational design procedures are needed to meet future needs.*

- The evolution of simulation tools for plasma processes will depend on progress in plasma modeling techniques and on the *enhancement of the collision cross section data base needed for calculating plasma properties.*

- Because of the fragmentary state of the cross section data base, the hazardous nature of several feed gases, and the difficulty of measurements, particularly for molecular fragments, *computational approaches to the generation of these cross sections have the potential to make a significant contribution.*

- Our objective is to exploit the high-performance and cost-effective computing provided by parallel computers, along with a judicious choice of measurements, to obtain the cross sections for electron-molecule collisions needed for robust modelling of these plasmas.

- A tragic example of the hazardous nature of feed gases of interest in plasma etching. Taken from the recent article by M. A. Dillon et at., J. Phys. B **27**, 1209 (1994).

Elastic scattering and some vibrational excitation cross sections for electron collisions with Si_2H_6

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‡ Department of Physics, Sophia University, Chiyoda-ku, Tokyo 102, Japan
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3.4. Vibrational excitation

During the extension of this work to the realm of vibrationally inelastic scattering, a fatal explosion at Osaka University led to a curtailment of research on silane in Japan. New regulations have made it impossible to conduct research using silanes without very costly laboratory modifications. These circumstances have dictated the premature end of our investigation, but nevertheless we have obtained some results that are relevant to the present discussion and are worth reporting.

- The calculation of cross sections for collisions of low-energy electrons for the gases of interest in these plasmas, e.g., $BC\ell_3$ and $SiC\ell_4$, is computationally intensive.

- In contrast to conventional supercomputers, the high speeds and large memory of parallel computers make a computational approach to generating these cross sections feasible.

- In these studies we use a multichannel extension of the variational principle originally introduced by J. Schwinger. This multichannel variational principle was specifically formulated for applications to electron-molecule collisions.

- Our variational principle can be applied to both elastic and electronically inelastic collisions with general polyatomic molecules. Polarization effects can be included via closed channels.

- As in the original Schwinger method, the trial wave function need not satisfy scattering boundary conditions ; square-integrable functions such as Cartesian Gaussians may be employed.

- Application of this multichannel variational principle leads to a system of linear equations

$$\mathbf{A}\,\mathbf{x} = \mathbf{b}$$

whose solutions yield the scattering amplitudes.

- **A** and **b** are complex matrices with elements

$$A_{ij} = \langle \phi_i | (\frac{1}{N+1} - P)\hat{H} + VP - VG_P^{(+)} V | \phi_j >$$

and

$$b_{im} = < \phi_i | V | \Phi_m (\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N) \exp(i\mathbf{k}_m \cdot r_{N+1}) >.$$

- In a basis of Cartesian Gaussian functions, i.e.,

  $N_\alpha (x-A_x)^\ell (y-A_y)^m (z-A_z)^n \exp(-\alpha |\mathbf{r}-\mathbf{A}|^2)$,

  all integrals needed in the construction of the matrix elements of **A** and **b** can be evaluated analytically, except for those of $VG_P^{(+)}V$.

- The integrals arising in the $<\phi_i|VG_P^{(+)}V|\phi_j>$ term have no known analytic form and must be evaluated by quadrature.

- The high-performance and cost-effective computing provided by parallel computers is the key to our ability to evaluate these $VG_P^{(+)}V$ integrals efficiently and to effectively use this procedure to study electron-molecule collisions.

- To obtain the matrix elements of $VG_P^{(+)}V$ we must evaluate and transform a large number (e.g, 10^9 - 10^{10}) of two-electron integrals of the type

$$\int d^3 r_1 \int d^3 r_2 \alpha(\mathbf{r}_1) \beta(\mathbf{r}_1) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \gamma(\mathbf{r}_2) \exp(i\mathbf{k}\cdot\mathbf{r}_2)$$

where α, β and γ are Cartesian Gaussian functions of the form

$$\mathrm{N}_\alpha (\mathrm{x}-\mathrm{A}_\mathrm{x})^\ell (\mathrm{y}-\mathrm{A}_\mathrm{y})^\mathrm{m} (\mathrm{z}-\mathrm{A}_\mathrm{z})^\mathrm{n} \exp(-\alpha\, |\mathbf{r}-\mathbf{A}|^2).$$

- These integrals, however, can be evaluated analytically with a program containing less than two thousand lines of Fortran.

- To obtain these matrix elements we load the Fortran code for evaluating these integrals on each of the microprocessors of the parallel computer and deal out a subset of integrals to every microprocessor.

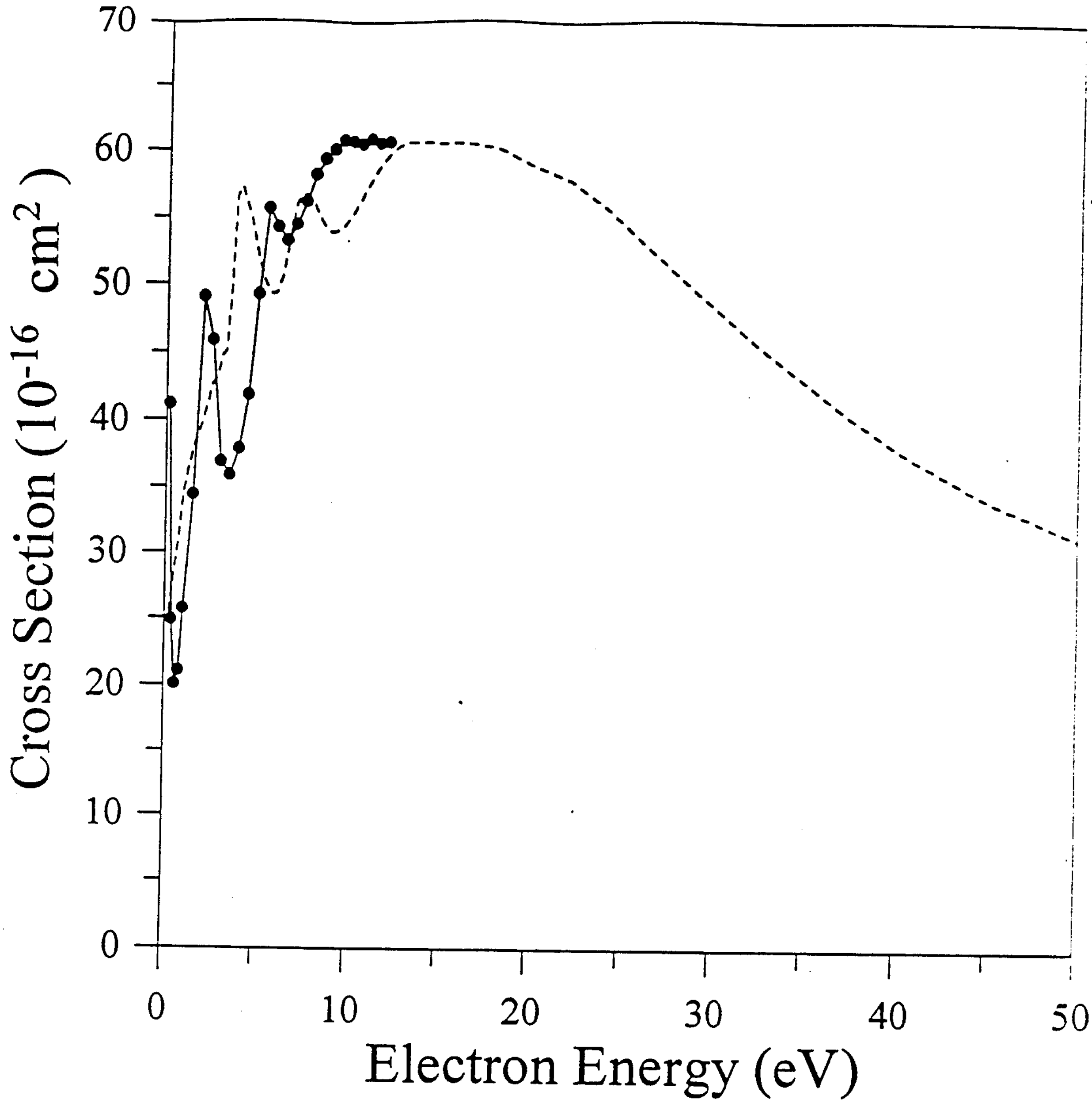
- Transformation of these integrals stored in the microprocessors to generate the final matrix elements is achieved via distributed multiplication of large complex matrices.

- Sustained performance of 5 GFLOP is typical.

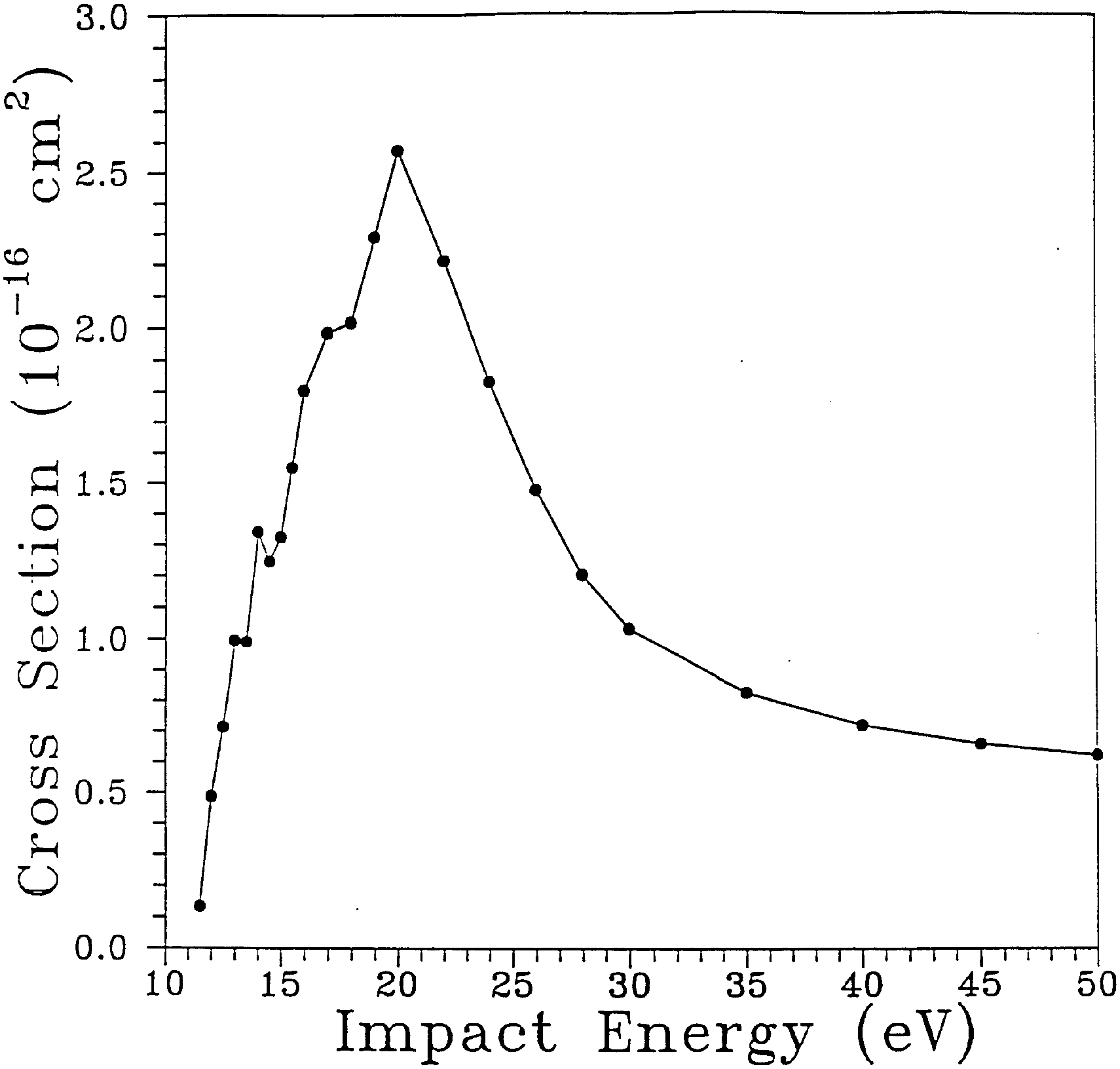
- We have made significant progress in an ambitious project to generate cross section sets for the species $BC\ell_3$, $BC\ell_2$, $BC\ell$, $SiC\ell_4$, $SiC\ell_3$, $SiC\ell_2$, and $SiC\ell$ which occur in boron trichloride ($BC\ell_3$) etching plasmas. This data will enable robust simulations of $BC\ell_3$ etching plasmas.

- Since only limited experimental data are available for $SiC\ell_4$, and none at all to our knowledge, for the remaining molecules, these computations address a clear need.

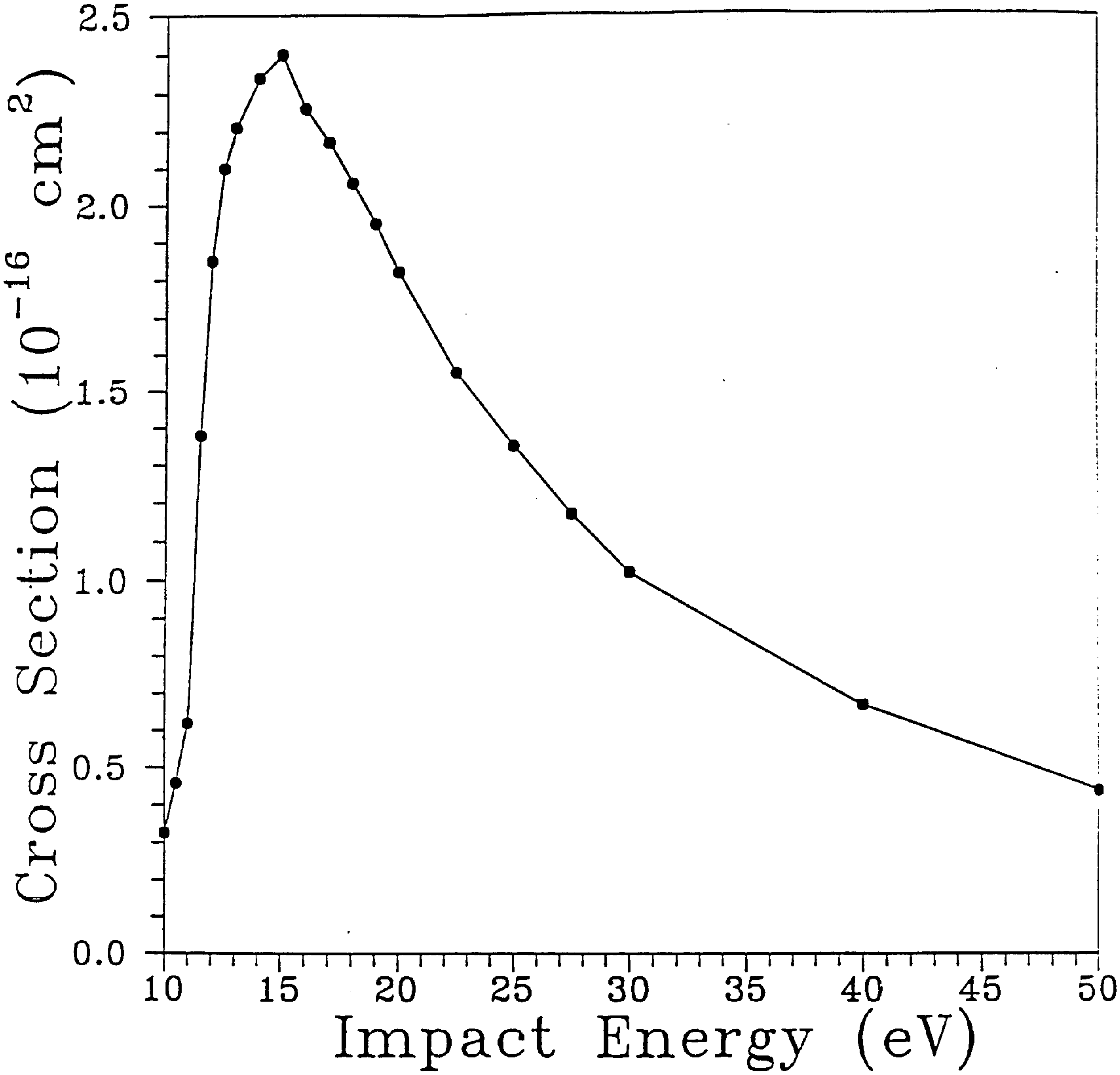
- These studies also provide a challenging opportunity to explore electron collision processes – particularly those involving radicals – about which little is known.



- Cross section for electron scattering by $SiCl_4$: ----, elastic cross section calculated without target polarization; —●—, measured total cross section (H.-X. Wan *et al.*, J. Chem. Phys. **91**, 7340 (1989)).



- Dissociation cross section for BCl_3. This cross section is obtained as the sum of the $6a_1' \rightarrow 3a_2''\,{}^{1,3}A_2''$, the $6e' \rightarrow 3a_2''\,{}^{1,3}E''$, and the $2a_2'' \rightarrow {}^{1,3}A_1'$ electron-impact excitation cross sections.



- Dissociaton cross section for BCl. This cross section includes the $^{1,3}\Sigma^+$, $^{1,3}\Delta$, and $^{1,3}\Sigma^-$ channels arising from $2\pi \rightarrow 3\pi$ electron-impact excitation.

- This work is an early illustration of the significant impact that scalable parallel computers can be expected to have on our ability to model complex physical and chemical systems.

- A proposal to develop high-performance simulation tools for the plasma processes used in microelectronics fabrication is being prepared. The Technology Computer Aided Design (TCAD) group of Intel (Santa Clara) will be a coinvestigator. Parallel computers will play a central role in this effort.

- Such simulation tools can contribute to the development and early evaluation of new equipment for microelectronics fabrication and, hence, to the competitiveness of the industry.

Computer Applications for Crystal Growth Phenomena

Professor Thomas C. Halsey

Exxon Research & Engineering

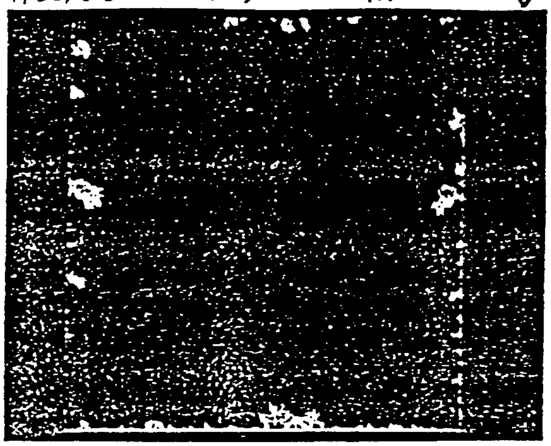
Random Walks and Dendritic Growth

Thomas C. Halsey
Exxon Research

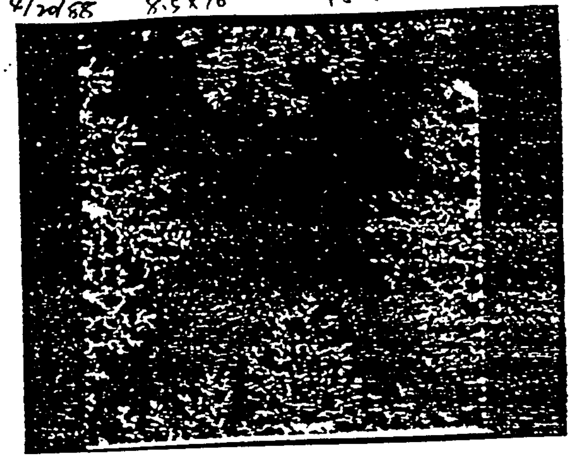
IDA November 1, '94

Levi-Setti, Chabala, + Wang   Ga → GaO

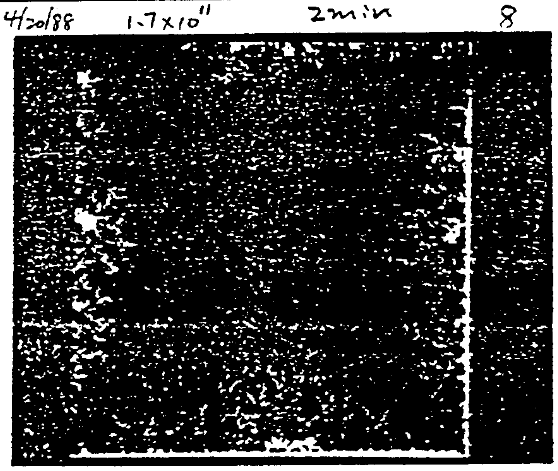
4/20/88   40 μm . Ga^{69} 5



4/20/88 8.5×10^{11} 10 min   10

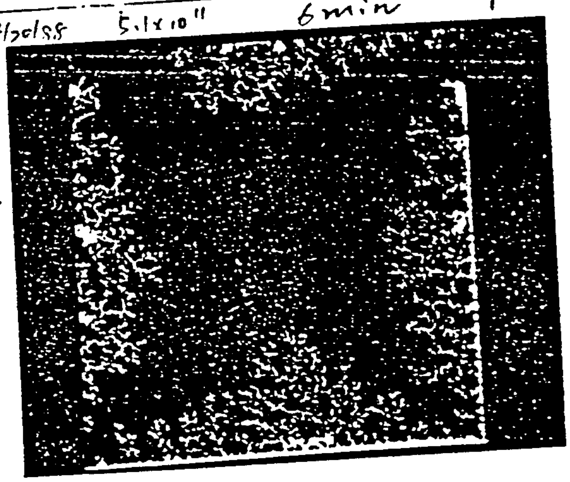


4/20/88 1.7×10^{11} 2 min   8

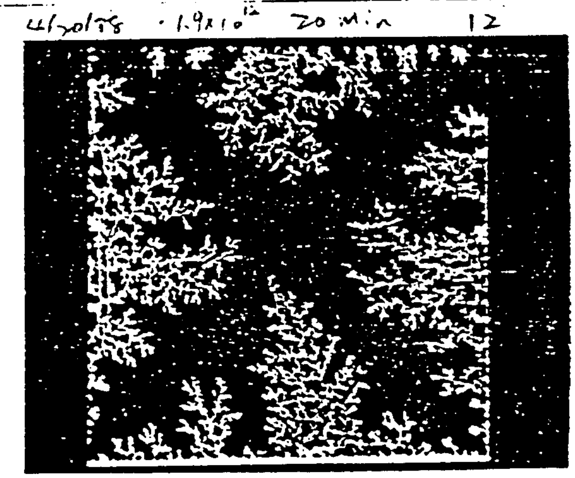


4/20/88 1.2×10^{12} 15 min   11

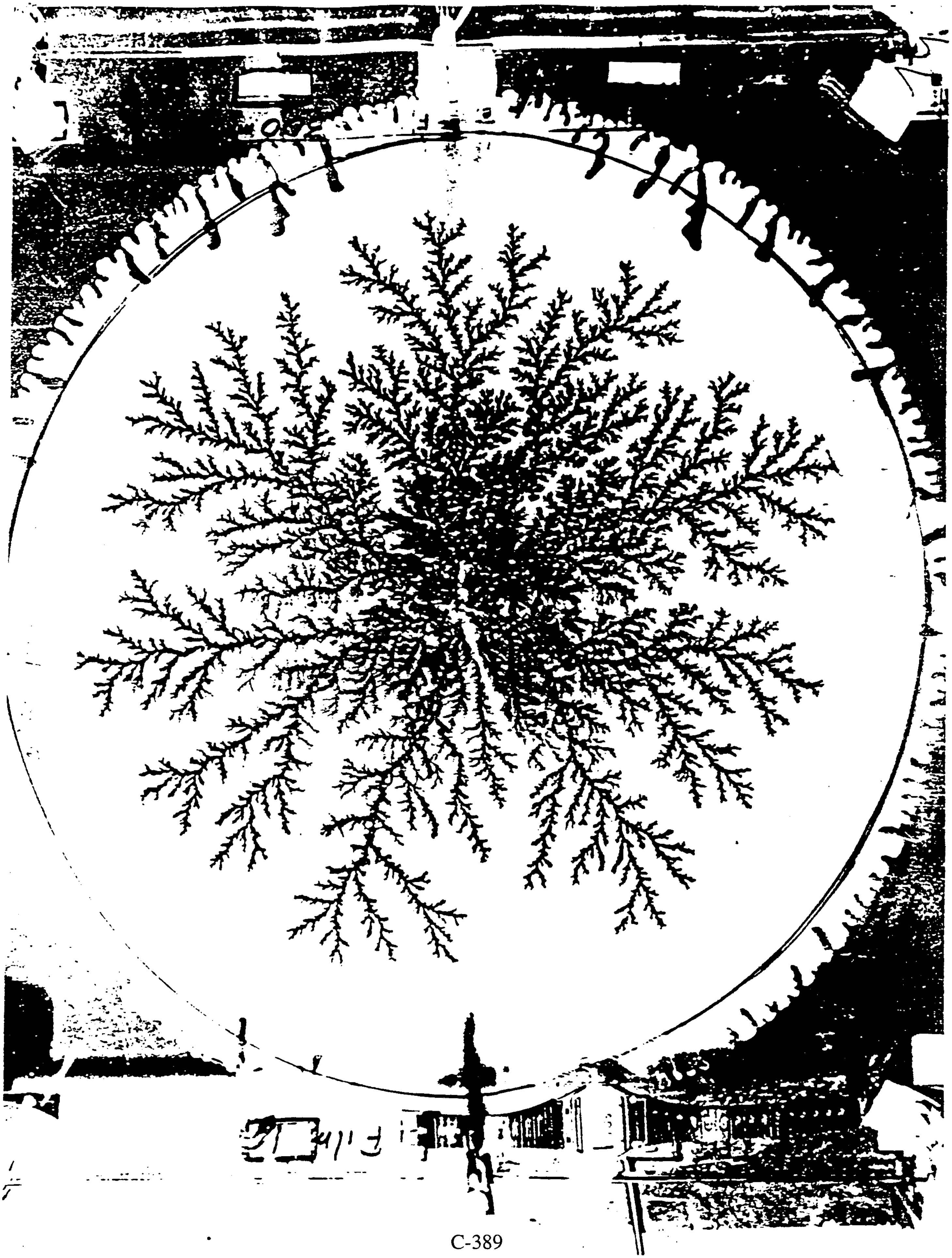
4/20/88 5.1×10^{11} 6 min   9



4/20/88 1.9×10^{12} 20 Min   12

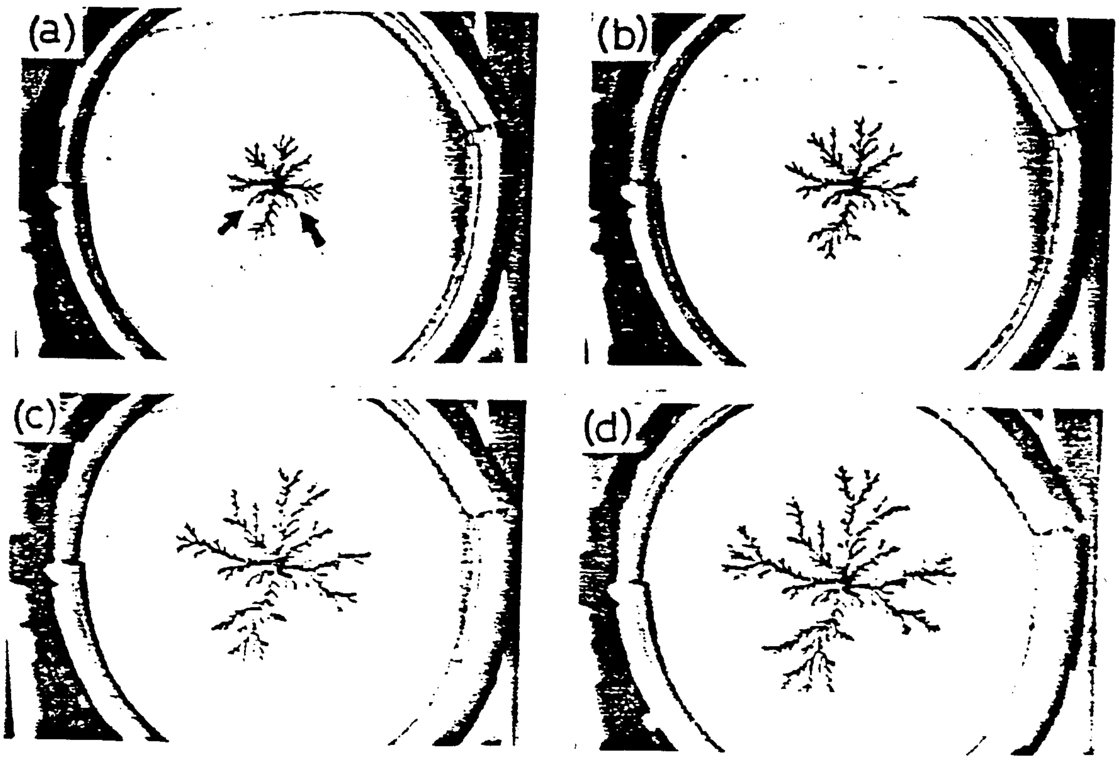


Van Vamm: Water into Mud



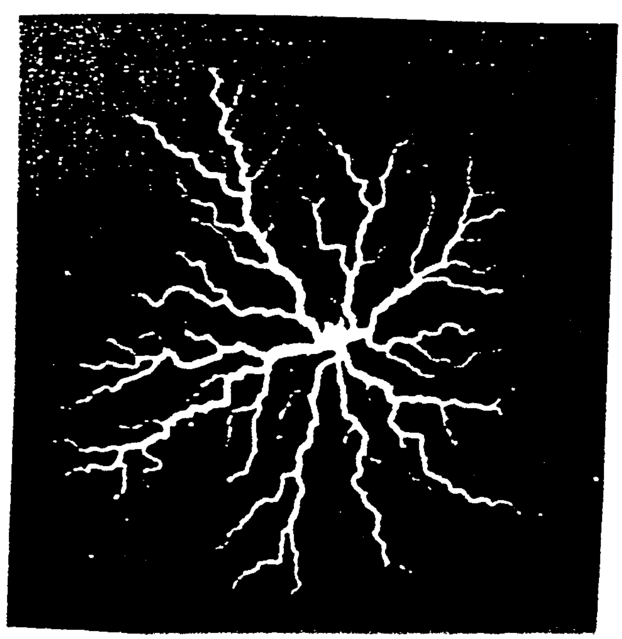
Growing Zn electrodeposit

(Matsushita et al.)

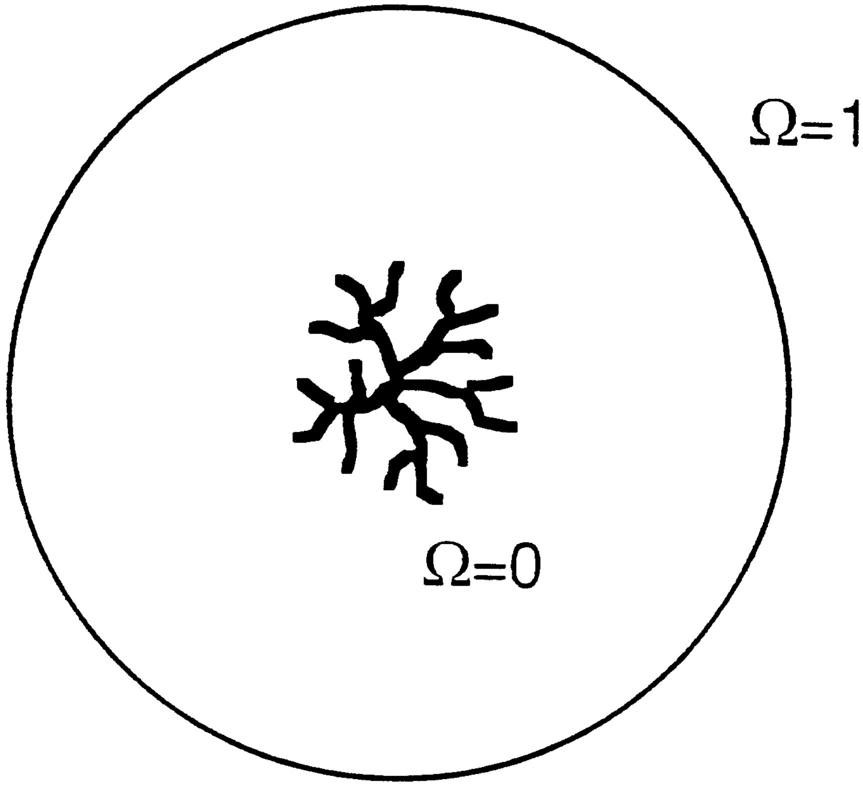


Surface leader discharge

(Niemeyer et al.)



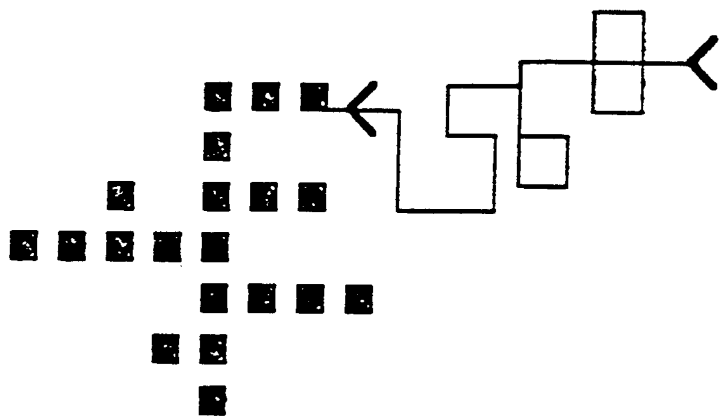
A crude model for electrodeposition:



- 1) Metallic surface is an equipotential of Ω.
- 2) $\Delta \Omega = 0$ in solution, as there is no space charge.
- 3) In solution, current $i(x) = \partial \Omega$.
- 4) At electrodeposit surface, growth rate is proportional to $i(s) = \partial \Omega$.

Diffusion-limited aggregation

- The Witten-Sander algorithm : growth without surface tension.

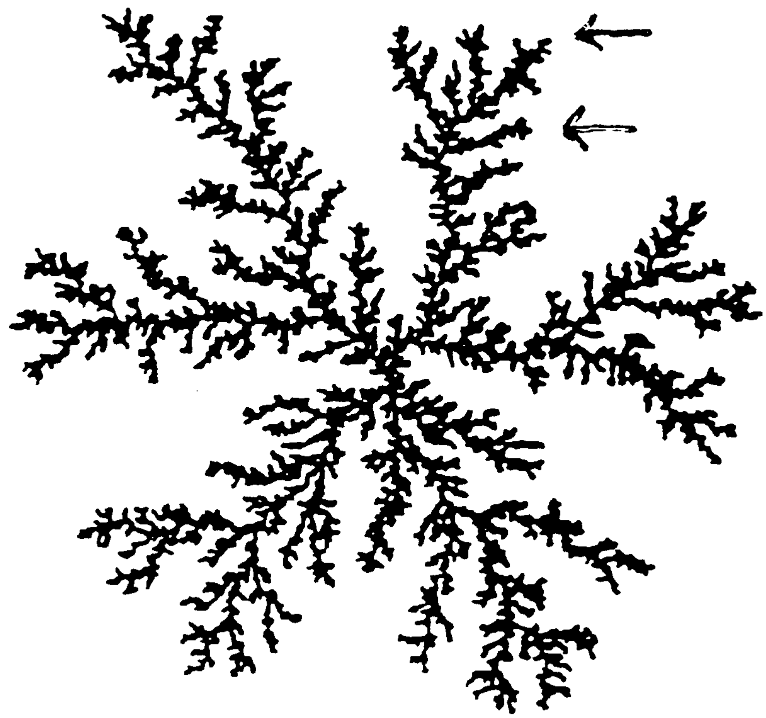


- Particle arrives from infinity. When it strikes seed, it sticks.
- Model for transport-controlled growth in electrodeposition, colloidal aggregation, viscous fingering.
- Structures grown are highly branched, ramified: "fractal"

$$n \sim r^{D}$$

- $D < d$, the dimension of space. Younger aggregates are more dense.

- In $\underline{\underline{d=2}}$, $\underline{\underline{D \cong 1.71}}$
- Example of <u>branched</u> <u>growth</u> with <u>screening</u>



- Diffusive instability
- • Mullins-Sekerka instability
- Analogous to hydrodynamic instabilities
- <u>Unstable</u> <u>growth</u> on all <u>length</u> <u>scales</u>

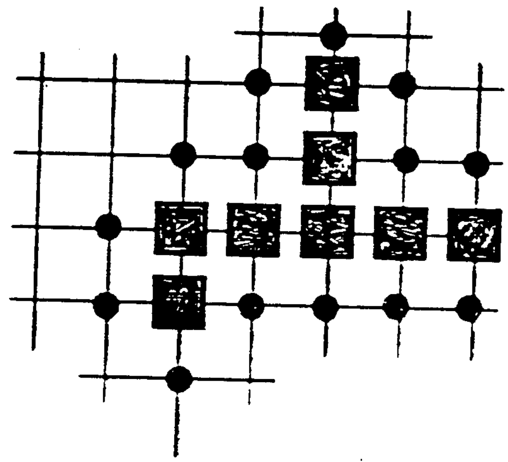
$\Longleftrightarrow$

<u>fractal</u>

Electrostatic analogy

Suppose that the probability density of a particle that has not yet touched the cluster surface is p(x,t); this probability must be zero on the dotted positions.

Elsewhere,



$$\partial_t\, p(x,t) = \Delta\, p(x,t)$$

If we write

$\Omega\,(x) = \int dt\; p(x,t)$

then since $p(x,0) = 0$, and $p(x,\infty) = 0$, we have

$$\Delta\,\Omega(x) = 0$$

And the probability G(s) that the particle first arrives at the surface position s is

$$G(s) = \partial_n \Omega\,(s)$$

electro-deposition model!

Generalization: dielectric breakdown models

- Call the local electric field at the surface in the above problem P(s).
- Then in DLA, the growth probability

$$G(s) = P(s) / \int ds \, P(s)$$

- Niemeyer et al. introduced a set of models for dielectric breakdown in which,

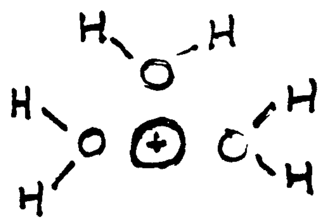
$$G(s) = P^{\eta}(s) / \int ds \, P^{\eta}(s)$$

- In this family of models, the dimension D is observed to be a monotonically decreasing function of η.

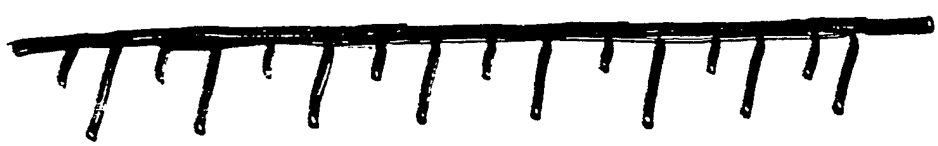
In two dimensions, the lower bound on D is D = 1.

A better model of electrodeposition

Cation is strongly hydrated



Appreciable surface impedance



Current into "double layer" near surface

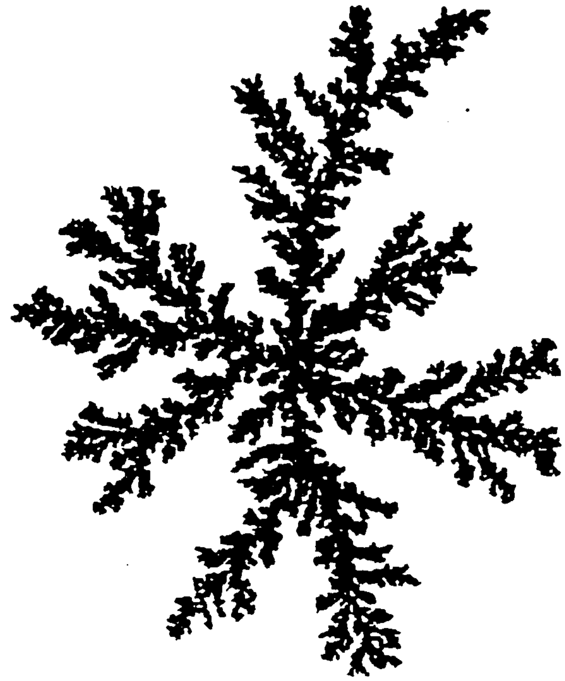
$$i_{sol} \propto \hat{n} \cdot \vec{E} = - \partial_n \Phi_{sol}$$

matches deposition current

$$i_{dep} \propto \underbrace{\Phi_{sol} - \Phi_{metal}}_{\text{double layer potential}}$$

"impedance" boundary condition

Model impedance boundary condition by partially absorbing boundary.

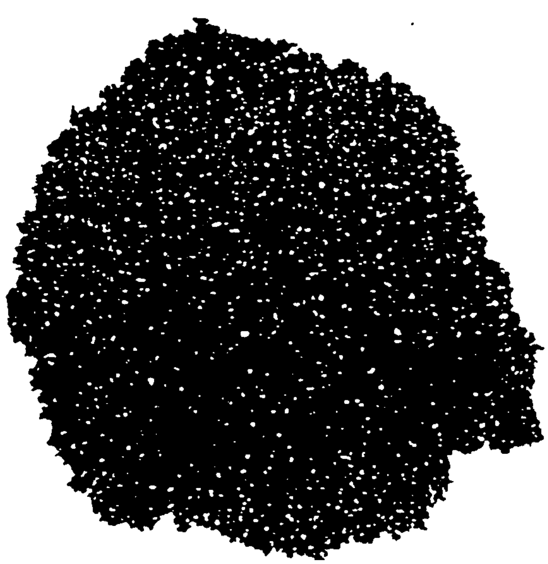


$\lambda = 0.1$

FIG. 5. A 150 000-particle aggregate. This aggregate was grown usin[g a] sticking probability DLA algorithm, with sticking probability $\lambda = 0.1$

Particles stick with probability λ, are reflected with probability $1-\lambda$.

Introduces length scale below which structures are no longer fractal



$\lambda = 0.003$

FIG. 4. A 110 000-particle aggregate. This aggregate was grown using a sticking probability DLA algorithm, with sticking probability $\lambda = 0.003$

Can include

- Surface tension (curvature of surface is source of particle flux)
- Anisotropic surface tension
- Anisotropic kinetic term
- Finite diffusion length

Can't include

- Finite metallic resistivity
- Diffusion + conduction
- Non-linear surface impedance

Monte Carlo simulation of diffusion controlled colloid growth rates in two and three dimensions

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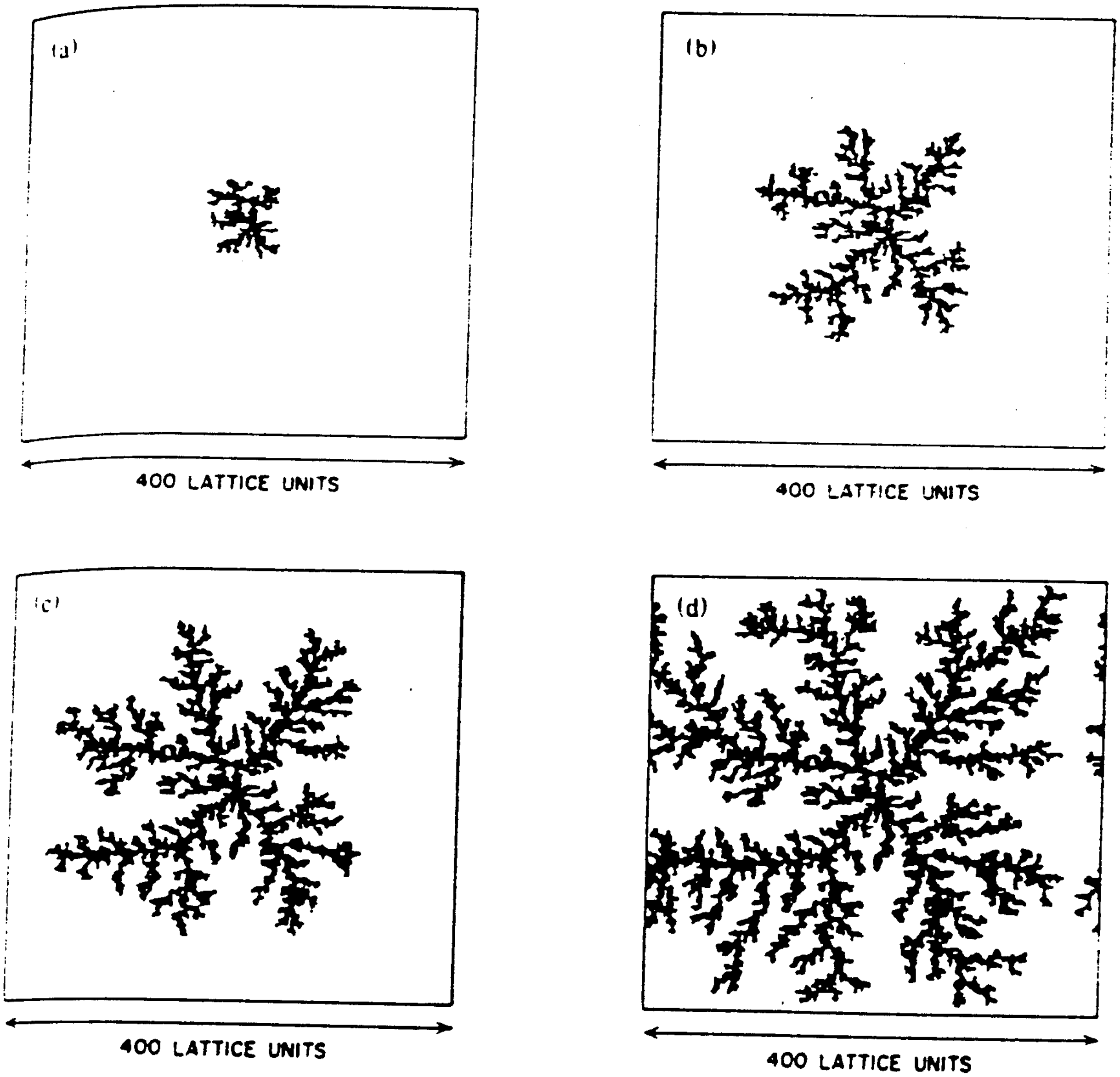
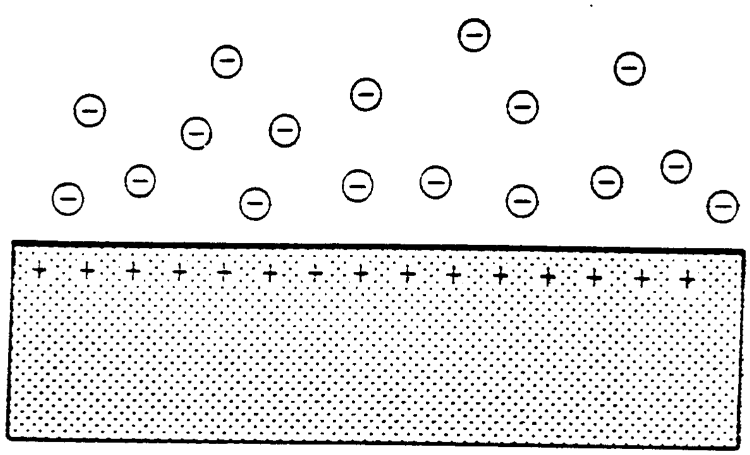


FIG. 1. Growth of a two-dimensional cluster from an initial state containing one seed or growth site and 20 000 mobile sites or particles on a 400 × 400 lattice. (a) At this stage in the simulation 1000 particles have been added to the original seed. This cluster closely resembles a typical cluster of 1000 particles grown using the WS model for diffusion limited aggregation. (b) Five thousand particles have now been added to the cluster which still closely resembles a WS cluster of the same size (number of particles). (c) This figure shows a cluster of 10 000 particles. The cluster still resembles a Witten–Sander cluster but is substantially denser. (d) All 20 000 mobile particles have now been added. The cluster has grown into the periodic lattice images and growth from adjacent lattice images can be seen in this figure.

Frequency dependence of the double layer impedance

If an electric potential is applied between a metallic surface and an electrolyte, a screening layer of charge will come to the surface, forming a *double layer.*



The impedance of this system should be that of a resistor and a capacitor in series.

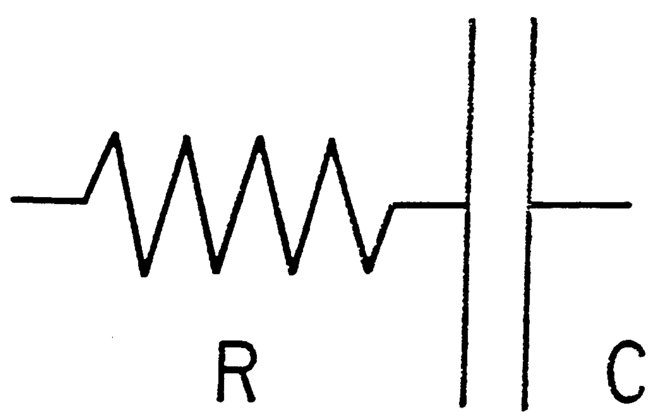
$$Z(\omega) = R + (1/i\omega C)$$

A "Helmholtz" impedance.

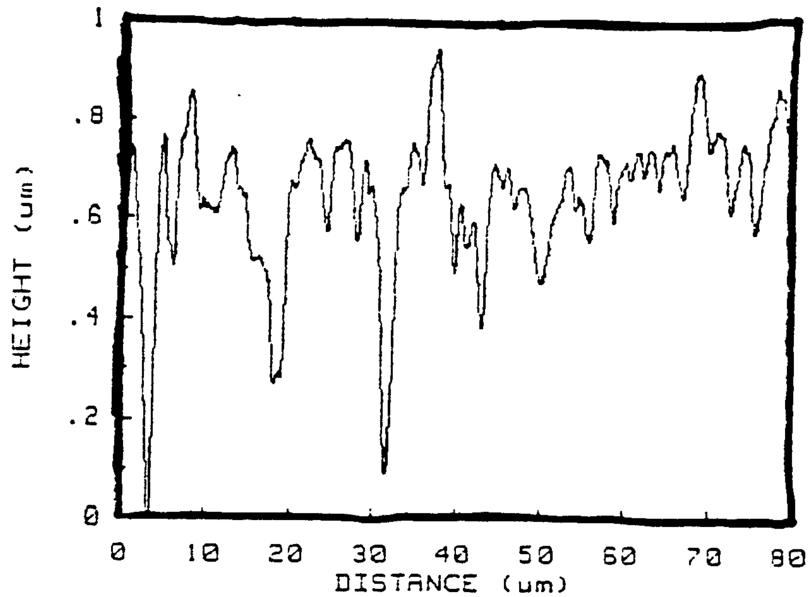
But often one sees instead:

$$Z(\omega) = R + (1/(i\omega)^{\eta} C)$$

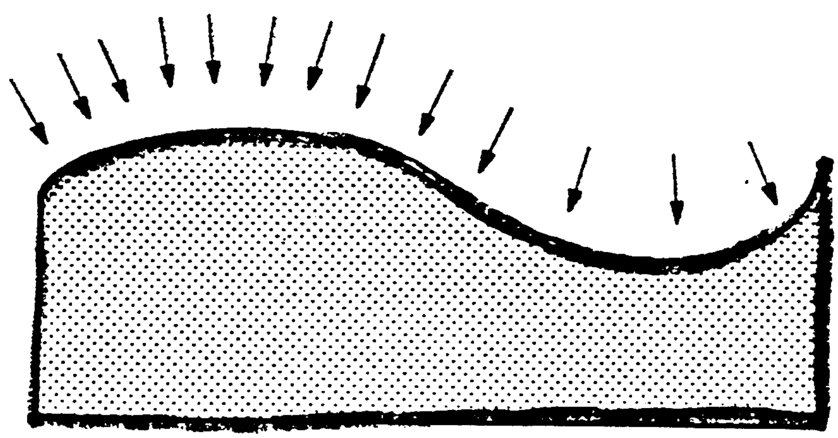
A "constant phase angle" impedance.



Origin of constant phase angle impedance lies in roughness of surfaces:

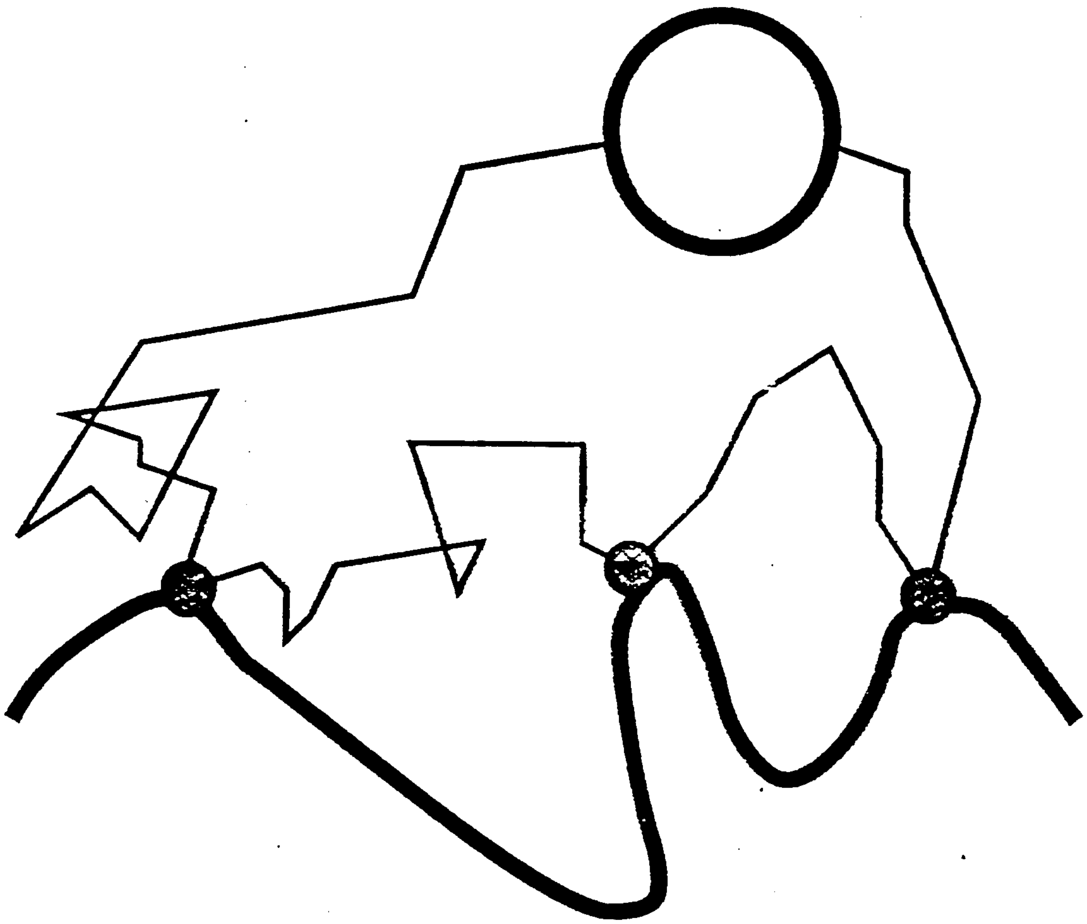


This leads to inhomogeneities in current arriving at surface during charging process.



This process can be analyzed using many of the same methods used in studying diffusive growth models.

Impedance can be expressed in terms of a set of coefficients b(n), which give the probabilities that a random walker starting at one electrode will bounce n times from the other electrode before returning



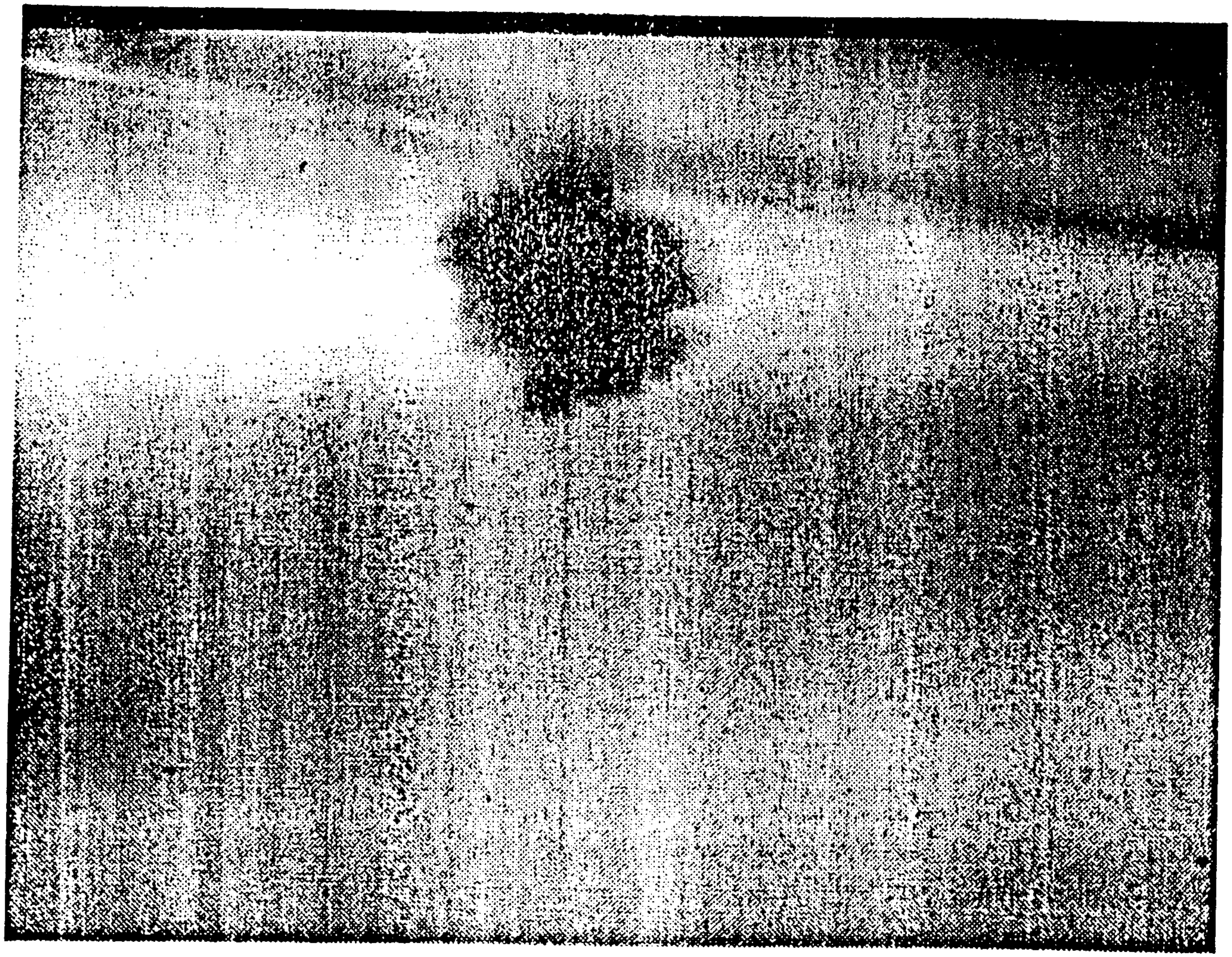
$$Z^{-1}(\omega) = 1 - \sum b(n)\,\lambda^{n}$$

$$\lambda = (1/1+i\omega)$$

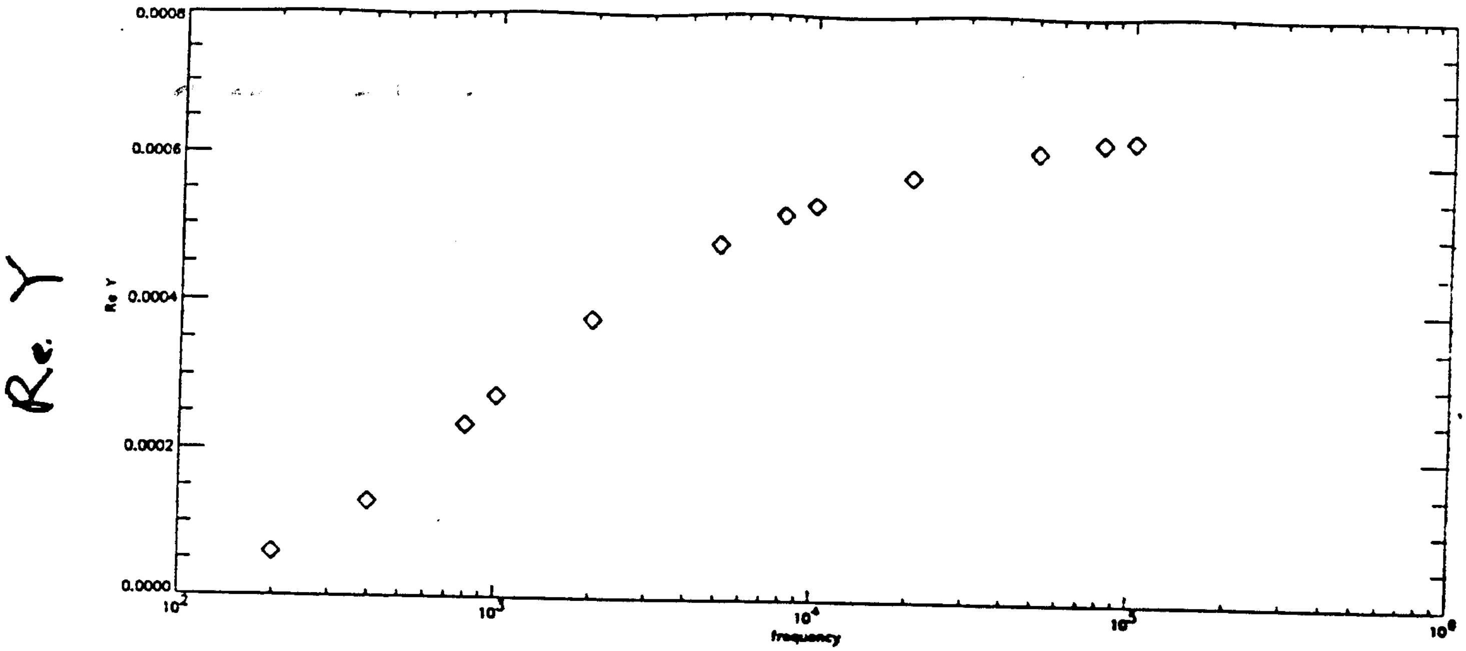
Impedance is a generating function for bounce probabilities

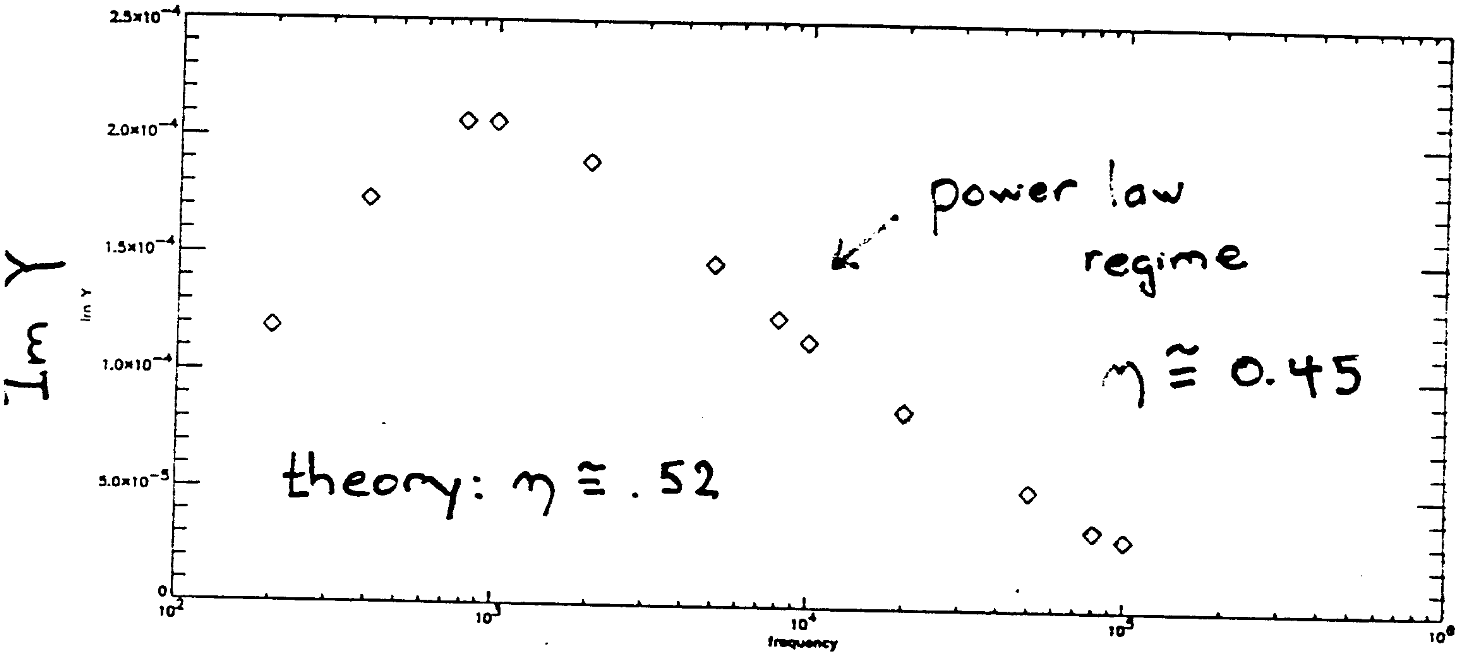
Wilson
+ Grier

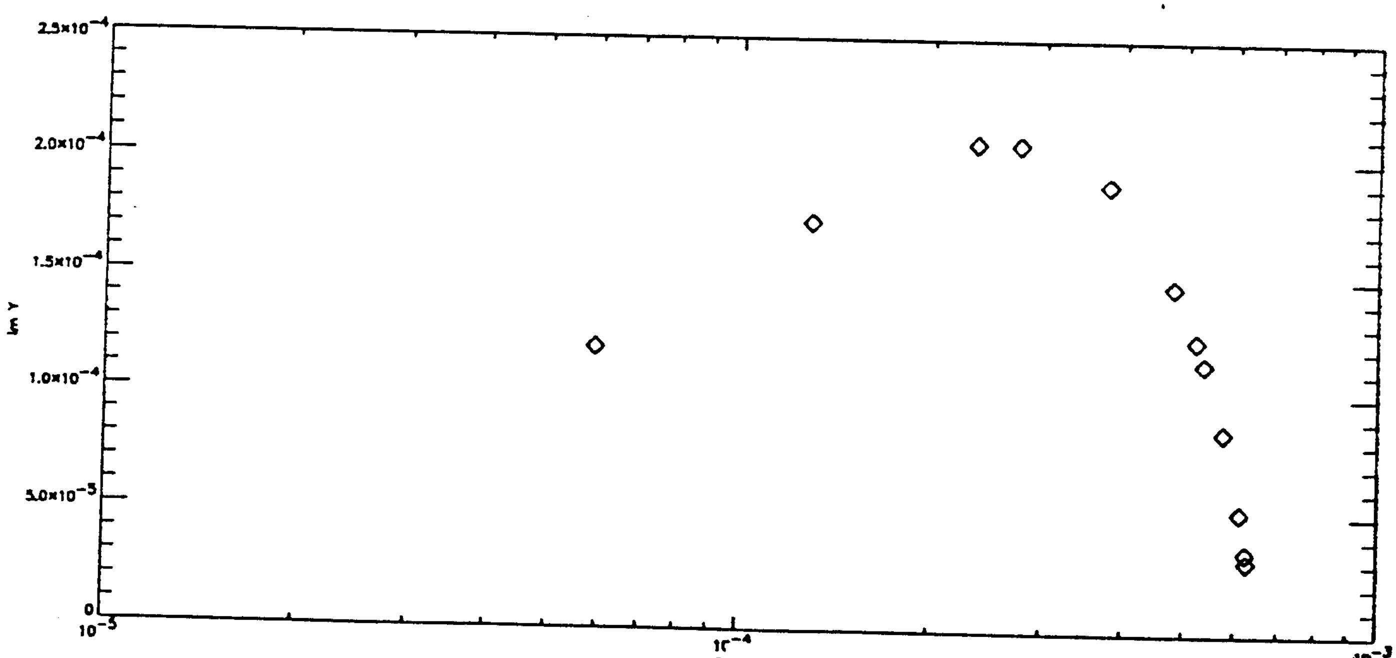
10^{2-3} μm Cu aggregate



.01 M $CuSO_4$
.1 M Na_2SO_4


Re Y
0.0008
0.0006
0.0004
0.0002
0.0000
Re Y
10^2
10^3
10^4
10^5
10^6
frequency


Im Y
2.5×10^{-4}
2.0×10^{-4}
1.5×10^{-4}
1.0×10^{-4}
5.0×10^{-5}
0
Im Y
power law regime
$\eta \cong 0.45$
theory: $\eta \cong .52$
10^2
10^3
10^4
10^5
10^6
frequency


2.5×10^{-4}
2.0×10^{-4}
1.5×10^{-4}
1.0×10^{-4}
5.0×10^{-5}
0
Im Y
10^{-5}
10^{-4}
10^{-3}
R

Remarks

- Direct non-stochastic integration of PDE's making rapid progress (Hele-Shaw flow)
- Random walks - for better or worse, a populist solution
- RW useful for NMR + colloidal studies
- Not useful for hyperbolic problems
- Theory ↔ experiment ↔ numerics
  As our physics improves, numerical needs decline.
- Pattern formation → poor man's Navier-Stokes

High Performance Computational Pursuit of Strategic Materials Properties

Dr. Warren E. Pickett

Naval Research Laboratory

High Performance Computational Pursuit of Strategic Materials Properties

Warren E. Pickett

Naval Research Laboratory

For: Defense Science Study Group Alumni Symposium

"Applications of Advanced and Innovative Computational Methods to Defense Science and Engineering"

Oct 31 - Nov 2, 1994

DoD High Performance Computing Modernization Plan Resources

(in use during FY95)

• Cray Y-MP	8 proc.	128 MW	Navy-NAVO, Stennis SpCntr
• IBM SP2	400 nodes	100 GFLOP	AF-AMOS, Maui
• IBM SP2	64 nodes	20 GFLOP	AF-AMOS, Maui
• Cray C90	16 proc.	512 MW	Army-CEWES, Vicksburg
• Cray Y-MP	8 proc.	128 MW	Army-CEWES, Vicksburg
• CM-5	256 proc.	32 MB	Navy-NRL, Washington DC
• CM-5	896 proc.	28 GB	Army-AHPCRC, Minneapolis
• KSR-1	256 proc.	32 MB/proc	Army-ARL, Aberdeen
• Paragon XP/S	240 proc.	32 MB/proc	AF-Wright Patterson AFB
• Paragon XP/S	336 proc.	16/32 MB/proc	AF-Wright Patterson AFB
• Cray C90		1 GW	Navy-NAVO, Stennis Sp Cntr
• Cray T3D	128 nodes	8GB	AF-Eglin AFB

USAE Waterways Experimental Station (CEWES)

Cray C916/16512 ("C90")

- 512 MWord (1 GB) high speed memory
- 1 GWord (2 GB) solid state device (SSD) memory
- 16 processors
- 16 GFLOP peak performance

Cray Y-MP8/8128 ("Y-MP")

- 128 MWord (256 MB) high speed memory
- 256 MWord (512 MB) SSD memory
- 8 processors
- 2.7 GFLOP peak performance

Maui High Performance Computing Center

Massively parallel IBM SP2 machine architecture

400 node complex:

- 30 frames of SP2 nodes
  - 1 frame = 8 'wide' nodes, or
    16 'thin' nodes.
- 2 switch frames to connect other frames

Node = IBM RS/6000 Model 590 processor

- 66 MHz
- 266 MFLOP

400 Processors ⇒ 100+ GFLOP peak performance

Node configurations available:

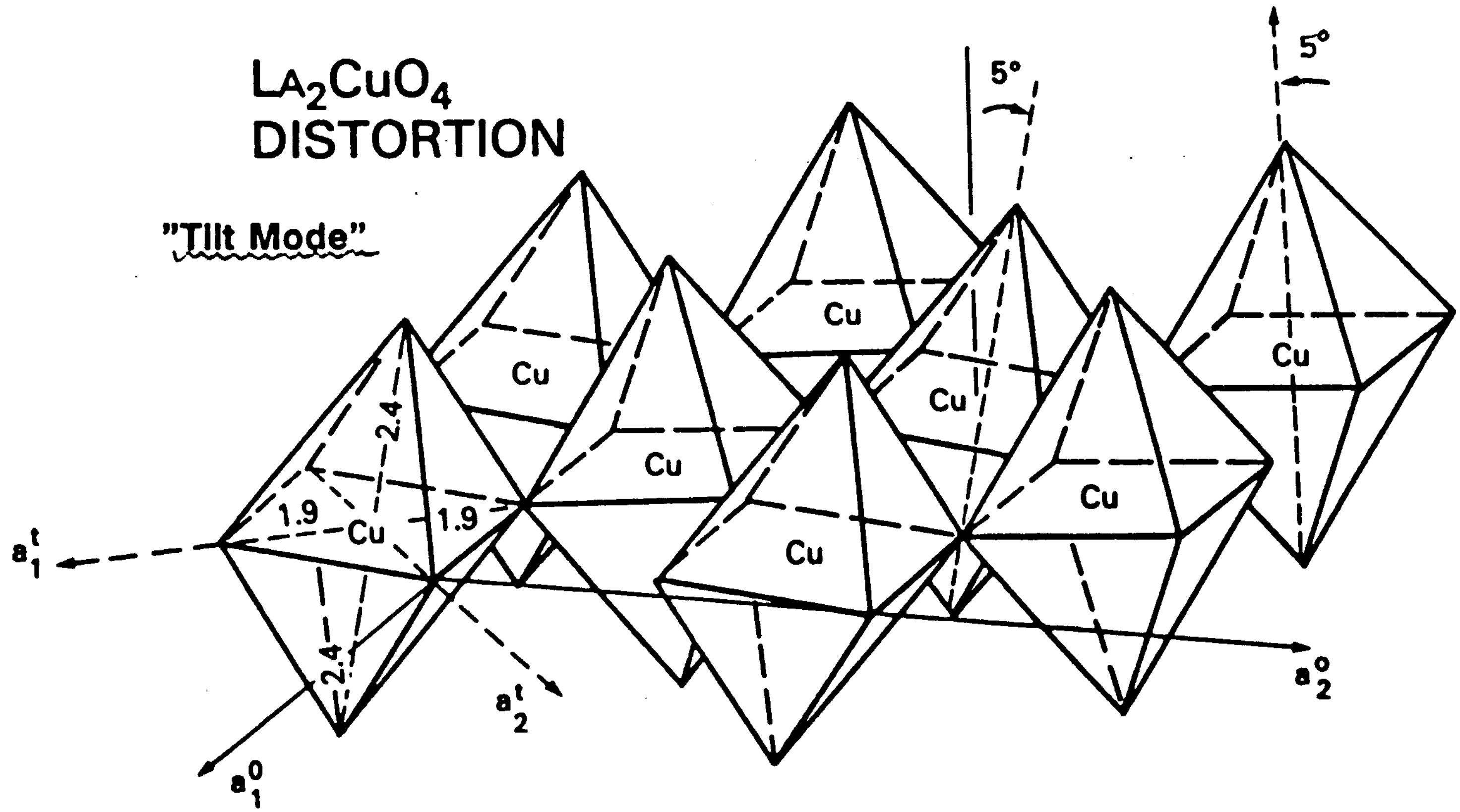
• Thin:	64 MB RAM	1 GB disk	180 MB paging
• Wide:	64 MB RAM	1 GB disk	180 MB paging
• Wide:	128 MB RAM	1 GB disk	244 MB paging
• Wide:	256 MB RAM	1 GB disk	308 MB paging

NRL Code 6690 (Complex Systems Theory Branch) applications:

- first principles electronic structure: more materials/properties
- parametrized tight binding: surfaces/interfaces/defects
- quantum Monte Carlo: one "walker" per node
- clusters & molecules: search configuration space
- molecular dynamics : million-atom systems
- quantum many body theory: under consideration

LA_2CuO_4 DISTORTION

"Tilt Mode"



Lattice Instabilities, Isotope Effect, and High-T_c Superconductivity in $La_{2-x}Ba_xCuO_4$

W. E. Pickett,[1] R. E. Cohen,[2] and H. Krakauer[3]

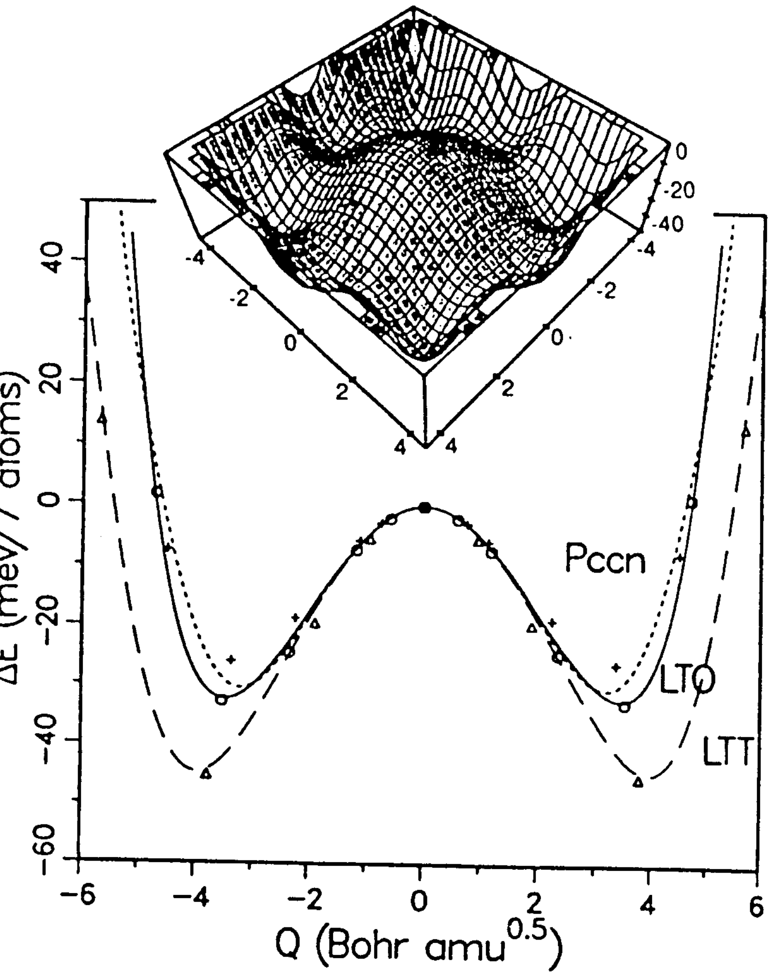


FIG. 1. Energy difference per primitive seven-atom cell of the LTO, LTT, and *Pccn* phases relative to the HTT structure, vs normal-mode magnitude Q. Lines result from a fit of the energy expansion in the text to all calculated energies (symbols). Inset (identical units): A surface plot of the resulting octuple-well energy surface for X-point tilts in the (Q_1,Q_2) plane, with minimum along the diagonal (LTT phase).

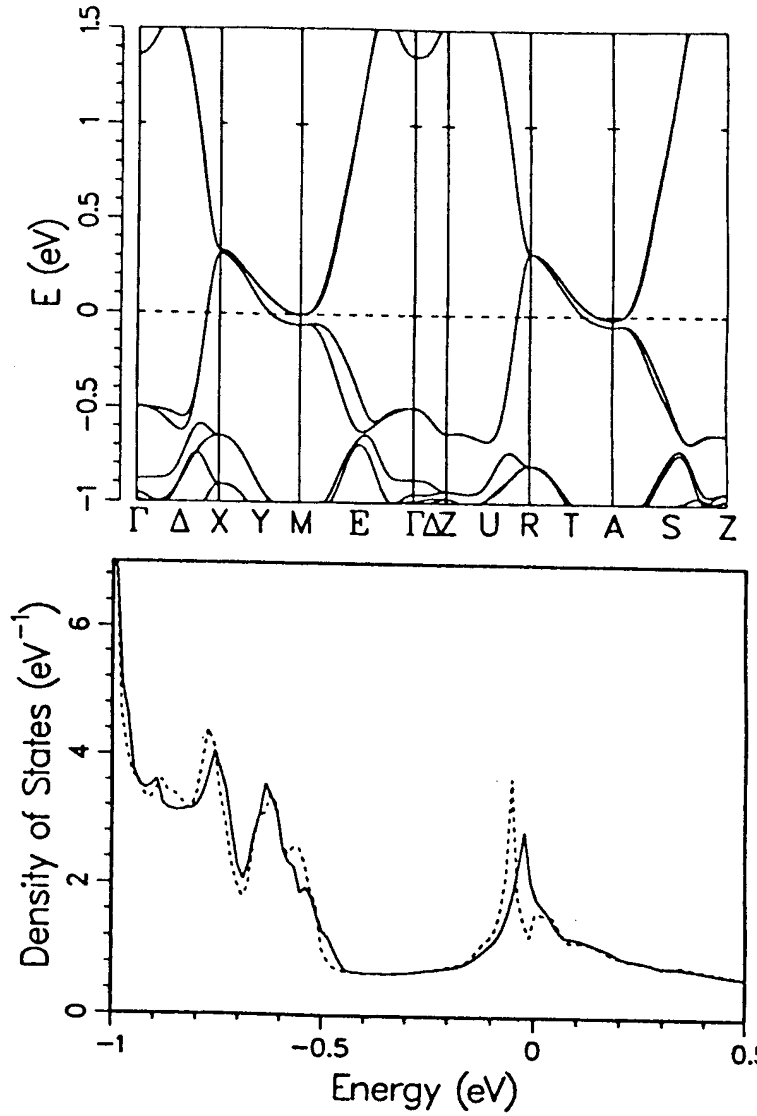


FIG. 2. Top: Energy bands in the LTT structure along high-symmetry directions. Note the gap opening along the M-A zone edge at E_F. Bottom: Density of states near E_F, showing the decrease in $N(E_F)$ by one-half due to the LTT distortion. In both panels the zero of energy is placed at $E_F(x=x_{cr})$.

Novel Superconductors and Semiconductors

David J. Singh and Warren E. Pickett
Complex Systems Theory Branch

- $LuNi_2B_2C$, $LaPt_2B_2C$, YNi_2B_2C etc.
- $IrSb_3$, $CoSb_3$, and related skutterudites and filled skutterudites

References:

W.E. Pickett and D.J. Singh, Phys. Rev. Lett. 72, 3702 (1994).

D.J. Singh, Phys. Rev. B 50, 6486 (1994).

D.J. Singh and W.E. Pickett, Phys. Rev. B 50, 11235 (1994).

M.S. Golden, M. Knupfer, M. Kielwein, M. Buchgeister, J. Fink, D. Teehan, W.E. Pickett and D.J. Singh, Europhysics Lett. (in press).

Question:

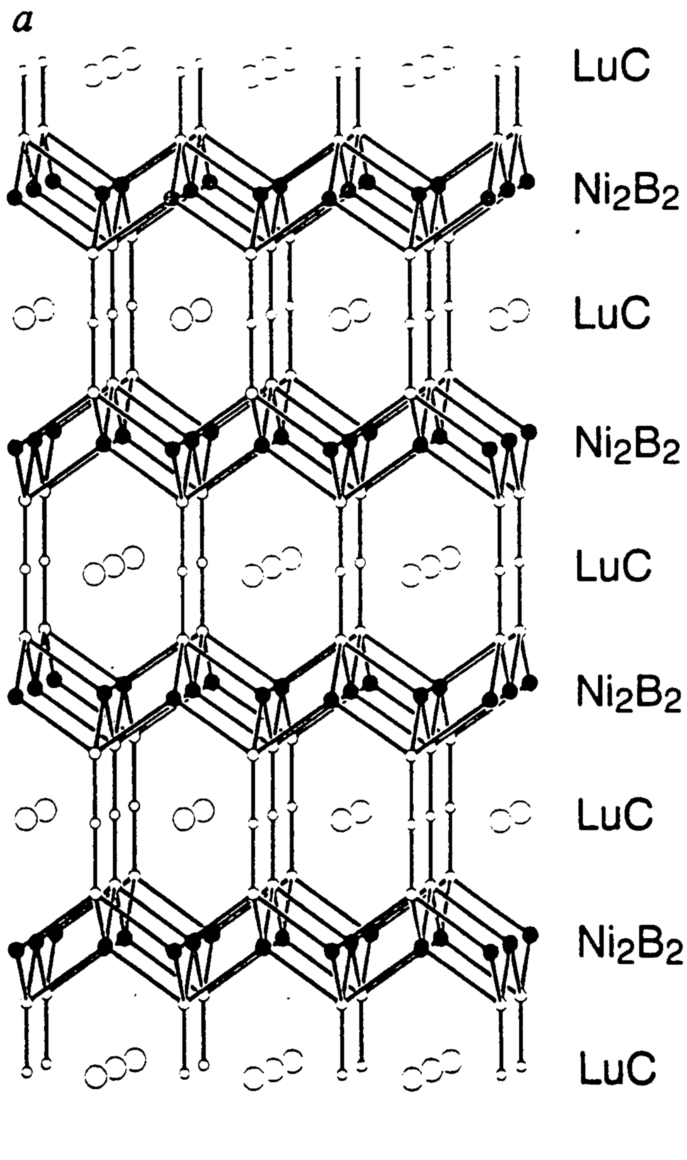
New Physics

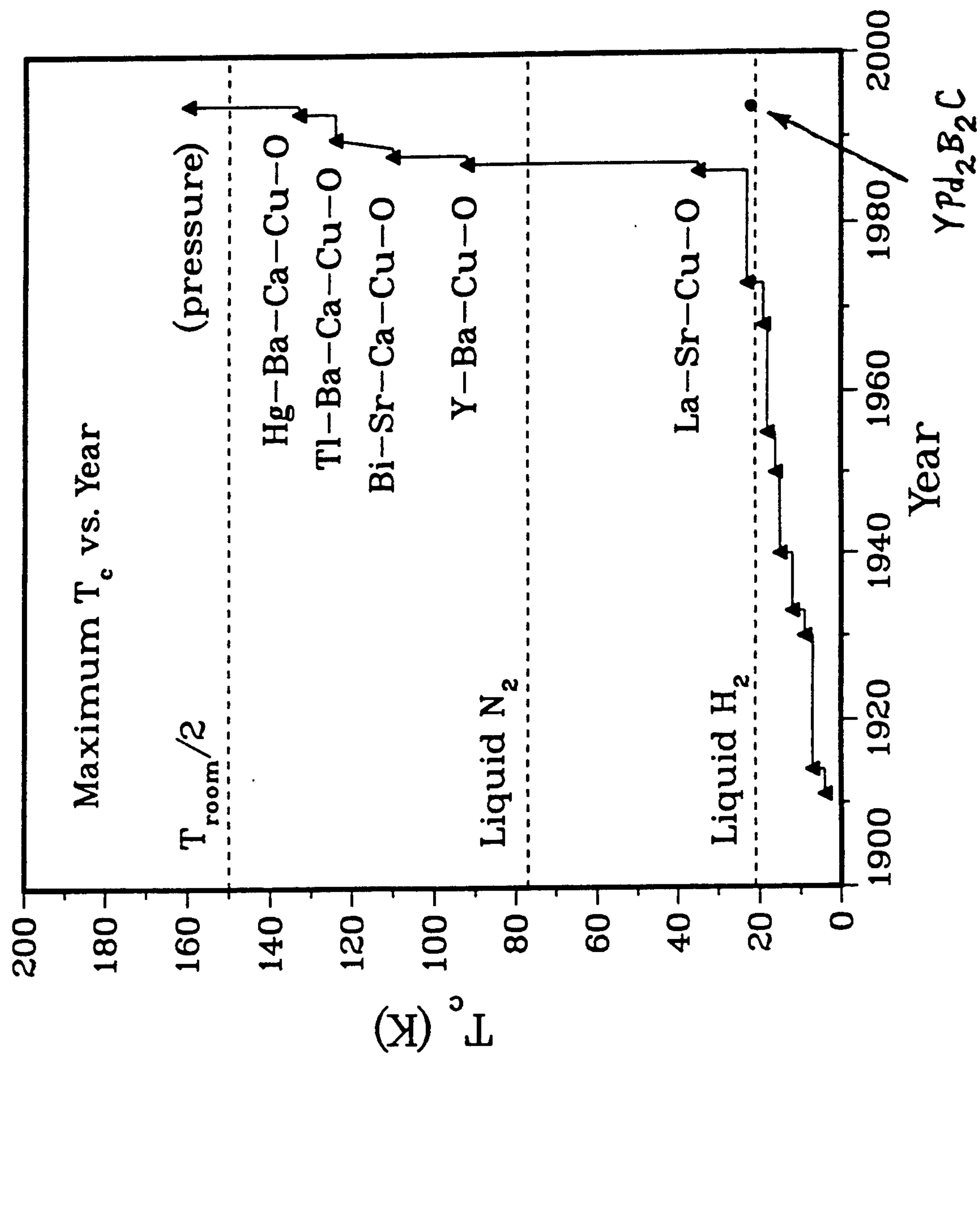
or

New Materials

The crystal structure of superconducting $LuNi_2B_2C$ and the related phase LuNiBC

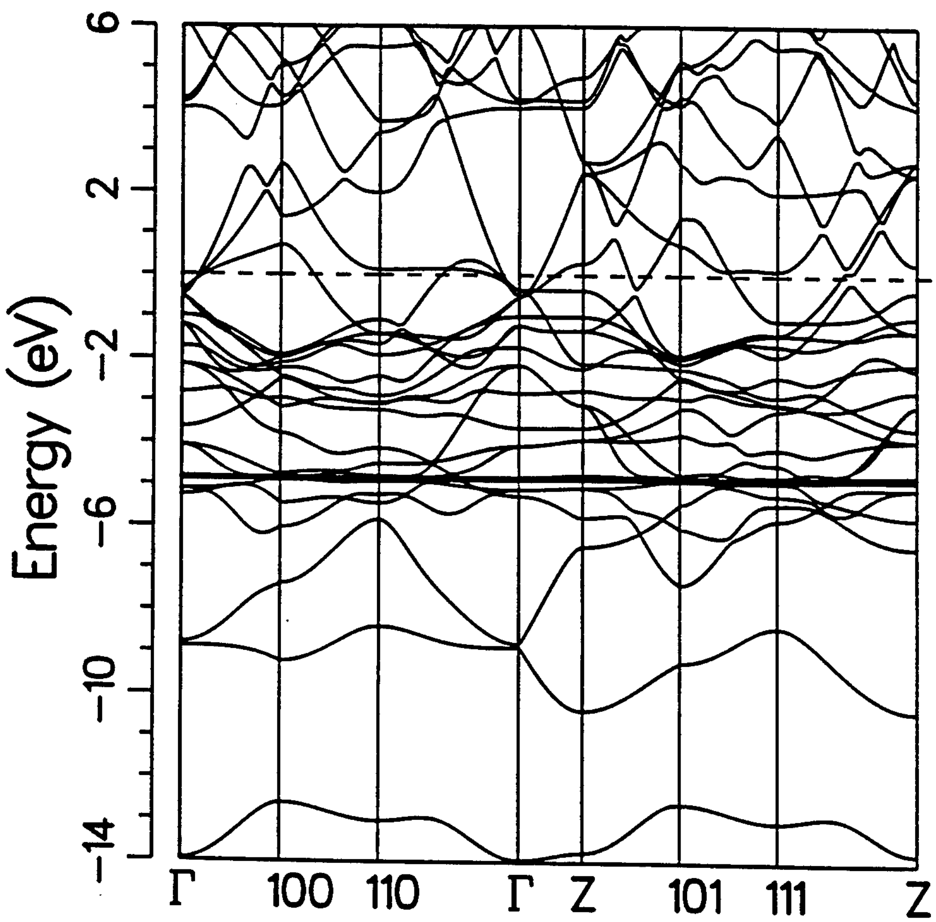
T. Siegrist, H. W. Zandbergen*, R. J. Cava, J. J. Krajewski & W. F. Peck Jr





Maximum T_c vs. Year
$T_{room}/2$
Liquid N_2
Liquid H_2
(pressure)
Hg–Ba–Ca–Cu–O
Tl–Ba–Ca–Cu–O
Bi–Sr–Ca–Cu–O
Y–Ba–Cu–O
La–Sr–Cu–O
YPd_2B_2C
Year
1900
1920
1940
1960
1980
2000
T_c (K)
0
20
40
60
80
100
120
140
160
180
200

$LuNi_2B_2C$ energy bands



$LuNi_2B_2C$ (T_c = 16.6 K)

LDA Calculations:

- Internal Structural Parameter and Raman Frequency Determined Accurately.
- 3D Covalent Bonding. All atoms participate.
- High $N(E_F)$ = 4.8 states/eV.
- Large, complex, 3D Fermi surface.
- Flat band just above E_F: 3D, strongly hybridized Ni, B, C character.
  $\Rightarrow$ Peak in DOS above E_F
- No ferromagnetic instability.

Transport and Superconductivity:

- Fermi velocities: $v_x = v_y = 2.12 \times 10^7$ cm/s; $v_z = 2.09 \times 10^7$ cm/s.
- Drude plasma energies: $\hbar\Omega_p = 5.1$ eV
- $d\rho/dT = (8\pi^2/\hbar\Omega_p^2)k_B\lambda_{tr} \rightarrow \lambda_{tr} \approx 2.6$; (expt. $d\rho/dT \approx 0.4\ \mu\Omega$ cm/K)
- Electron Phonon Interaction: Strong contributions from Ni, B and C.

Implications:

- Conventional, 3D, high DOS, strong coupling superconductor
- Reminiscent of "old" boride, carbide, nitride materials.

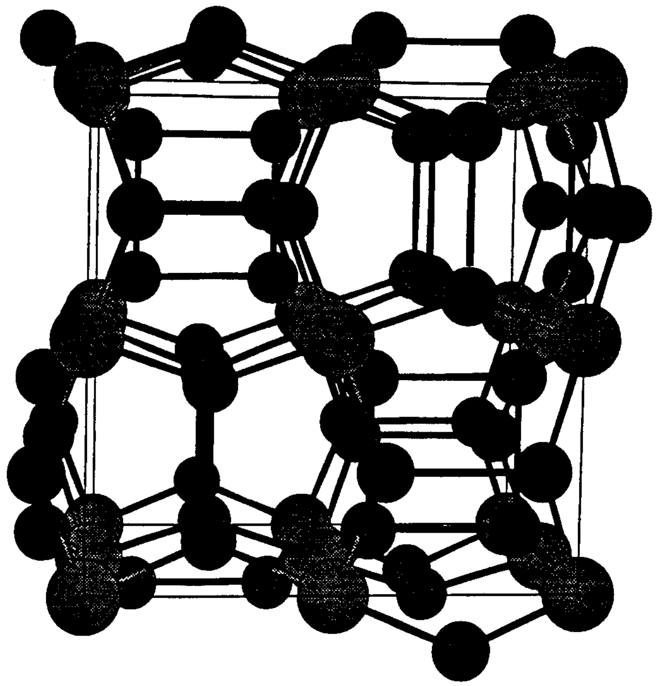
Navy Thermoelectric Technology: Status and Potential

- Clean, Quiet, Reliable Cooling and Power Generation Technology BUT presently very inefficient. → Only niche applications.
- Figure of Merit, $Z = \frac{\sigma S^2}{\kappa}$ is the limiting factor.
  State-of-the-art: $ZT \sim 1$; Goal: Find materials with higher ZT.

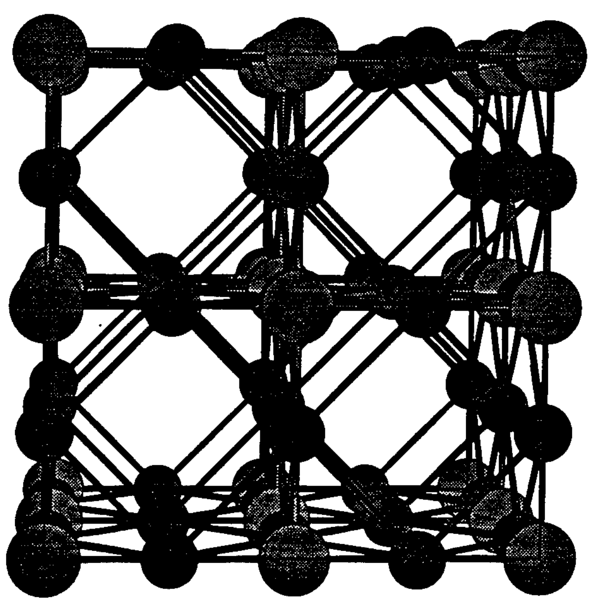
TARGET ($ZT \sim 2$): Refrigeration for Navy Platforms .

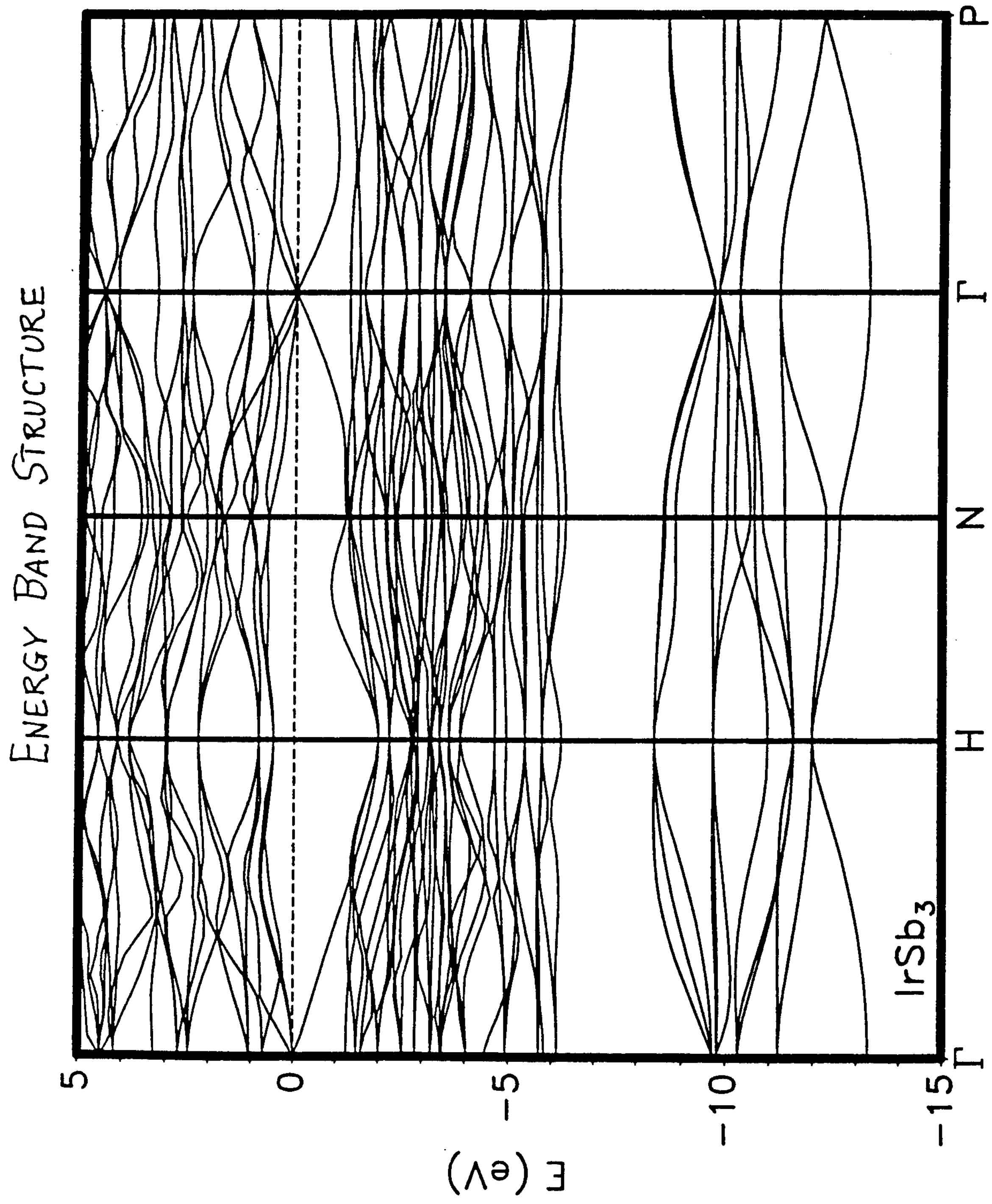
- Decentralized through-the-hull systems
  Benefits: Survivability - decentralized, less ductwork (fire).
  Environmentally Friendly: No CFC's.
  Control: Cooling when and where needed
- Generation: higher ZT ⇒ more power for fixed heat transfer
  Spacecraft: Reduce constraints on electrical power consumption
  Submarines: Possibility for generating power from reactor while operating silently (no moving parts, reduced coolant circulation?)

Skutterudite Structure



(Empty) Perovskite Structure





ENERGY BAND STRUCTURE
IrSb$_3$
E (eV)
5
0
−5
−10
−15
Γ
H
N
Γ
P

Implications of quasi-linear dispersion ($> 3\times10^{16}$ holes/cm^3):

Quasi-Linear	Parabolic
Band Dispersion:	
$\varepsilon(\mathbf{k}) = \alpha k \qquad \mathbf{v}_k = \alpha \mathbf{k}/k = \alpha \hat{\mathbf{k}}$	$\varepsilon(\mathbf{k}) = k^2/2m = \beta k^2 \qquad \mathbf{v}_k = 2\beta \mathbf{k} = \mathbf{k}/m$
DOS:	
$N(\varepsilon) = \dfrac{k^2}{\alpha\pi^2} = \dfrac{\varepsilon^2}{\alpha^3\pi^2} \qquad n(\varepsilon) = \dfrac{\varepsilon^3}{3\alpha^3\pi^2}$	$N(\varepsilon) = \dfrac{\varepsilon^{1/2}}{2\pi^2\beta^{3/2}} \qquad n(\varepsilon) = \dfrac{\varepsilon^{3/2}}{3\pi^2\beta^{3/2}}$
Effective Mass and Hall Number:	
$m_{Tr}^{-1} = 0 \qquad m_C^{-1} = -\alpha/k \qquad R_H = -(nec)^{-1}$	$m_{Tr}^{-1} = 2\beta \qquad m_C^{-1} = 0 \qquad R_H = -(nec)^{-1}$
Conductivity (constant τ):	
$\sigma = \dfrac{e^2\alpha\tau n}{k_F} \qquad \mu = \dfrac{e\tau\alpha}{k_F}$	$\sigma = 2e^2\tau\beta n \qquad \mu = 2e\tau\beta = \dfrac{e\tau}{m}$
Seebeck (constant τ, degenerate):	
$S = \dfrac{\pi^2 K_B^2 T}{3e}\dfrac{\partial \ln\sigma}{\partial\varepsilon} = \dfrac{2\pi K_B^2 T}{3e\alpha}\left(\dfrac{\pi}{3n}\right)^{1/3}$	$S = \dfrac{K_B^2 T}{2e\beta}\left(\dfrac{\pi}{3n}\right)^{2/3}$

Relation to Experiment: $IrSb_3$ (Slack):

Theory: $\alpha = 3.45$ eV Å   Experiment (Hall Number): $n_H = 1.1 \times 10^{19}$ cm^{3}

→ $E_F = -0.24$ eV $k_F = 0.069$ Å^{-1} degenerate and in linear dispersing regime

Calculate Seebeck Coefficient:

i.e. @300K $S = 62\ \mu V/K$ (expt. $72\ \mu V/K$); @600K $S = 123\ \mu V/K$ (expt. $126\ \mu V/K$)

→ Quantitative confirmation

Related Materials:

(1) Skutterudites: $CoAs_3$, $CoSb_3$:

- Zero or near zero gap semiconductors with related single gap crossing band
- $CoAs_3$: parabolic dispersion, $m_h \sim 0.25$; $CoSb_3$: quasi-linear, $\alpha = 3.1$ eV Å
- $CoSb_3$ may be favorable for T.E. (κ may be comparable to $IrSb_3$)

(2) Filled Skutterudites: $(IrSb_3)_4Xe$:

- Insertion of Xe leaves the electronic structure practically unchanged.

→ weak electron phonon interaction for Xe vibrations
negligible changes in electrical transport

May be a good strategy for reducing κ and thereby increasing Z. Can it be made?

- Total energy calculations: Insertion of Xe is endothermic. $\Delta E \sim 10$ Kcal/mole

Some properties of semiconducting $IrSb_3$

Glen A. Slack
GE Research and Development Center, Schenectady, New York 12301
Veneta G. Tsoukala
Oxford University, Oxford, England

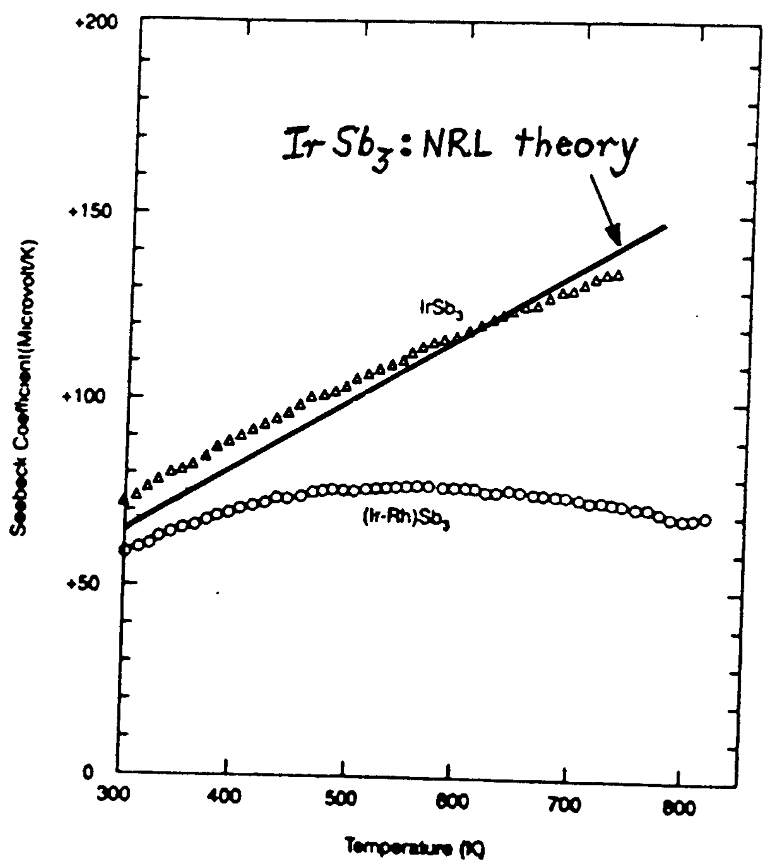


FIG. 7. The Seebeck coefficient vs temperature for $IrSb_3$ and $Ir_{0.5}Rh_{0.5}Sb_3$.

NATURE · VOL 365 · 2 SEPTEMBER 1993

LETTERS TO NATURE

Theoretical determination that electrons act as anions in the electride $Cs^+(15\text{-crown-}5)_2 \cdot e^-$

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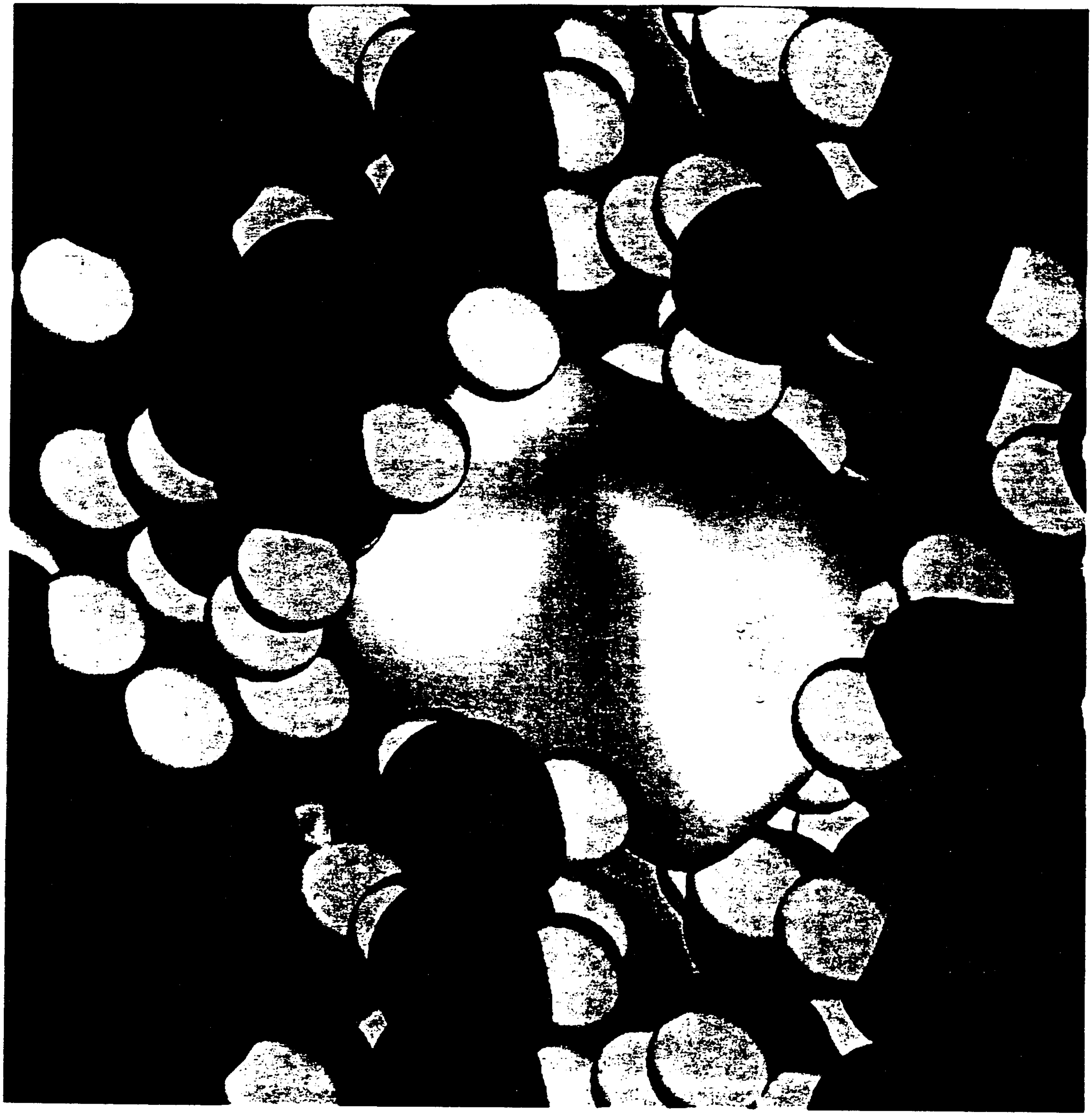
† Department of Physics, College of William and Mary, Williamsburg, Virginia 23187–8795, USA

ELECTRIDES are crystalline salts formed from complexed alkali-metal cations. There has been some dispute as to whether the valence electron from the alkali ion becomes a trapped interstitial anion[1,2] or resides at or near the alkali-metal nucleus[3]. If the former description holds, electrides would represent stoichiometric counterparts of ionic insulators containing 'F-centre' electronic defects. Experiments[1,2] have so far failed to resolve the question. Here we present *ab initio* self-consistent density-functional calculations[4] of the electron distribution in the electride $Cs^+(15\text{-crown-}5)_2 \cdot e^-$. We find that a spatially localized electron is located at the anion site, in accord with the F-centre model. Although the potential is in fact repulsive in this region, the electron is apparently forced to reside here by the need to lower its kinetic energy. We suggest that this picture may hold for other electrides as well.



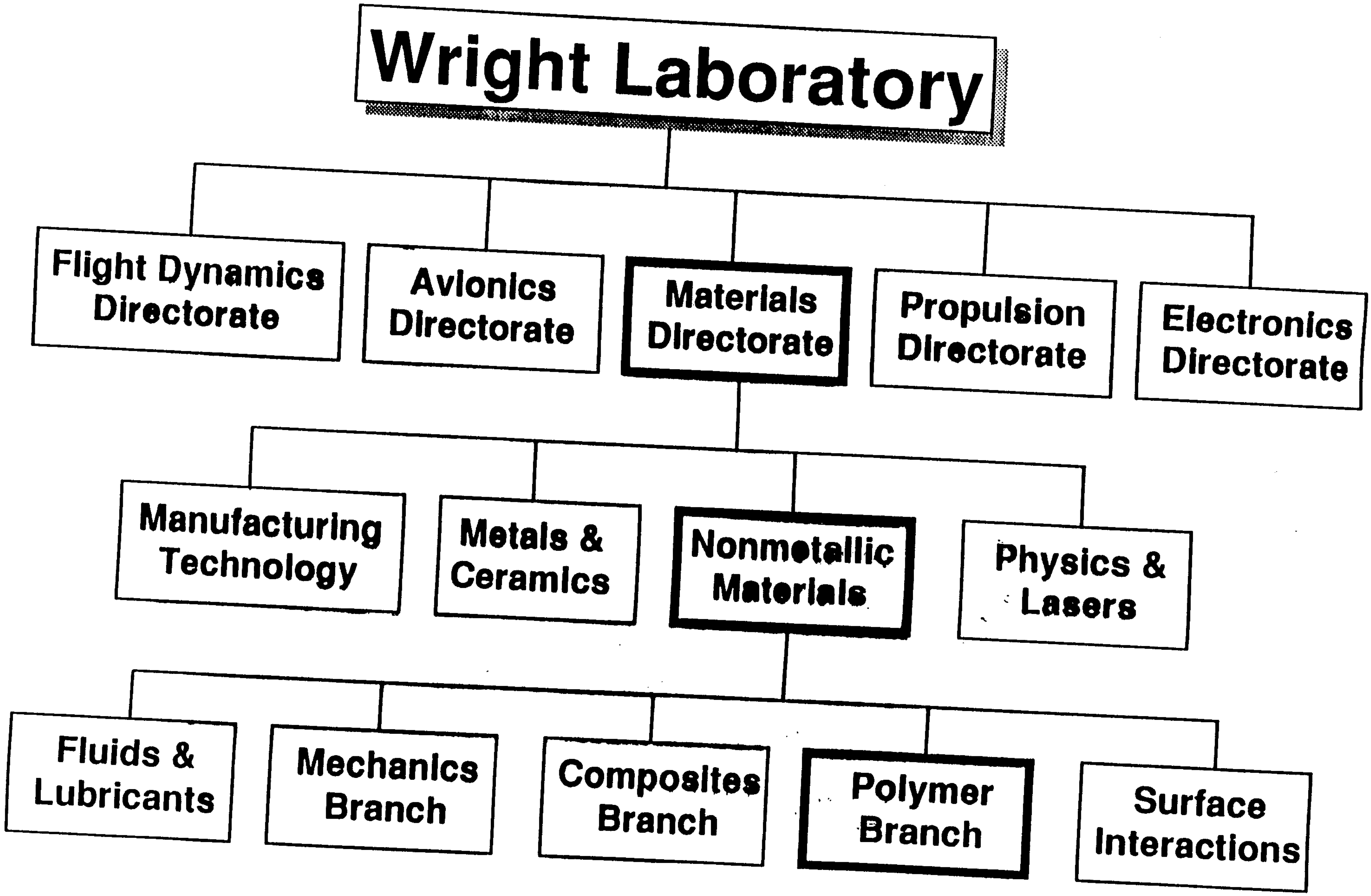
Competitive With Experiment?: The Future of Molecular Modeling

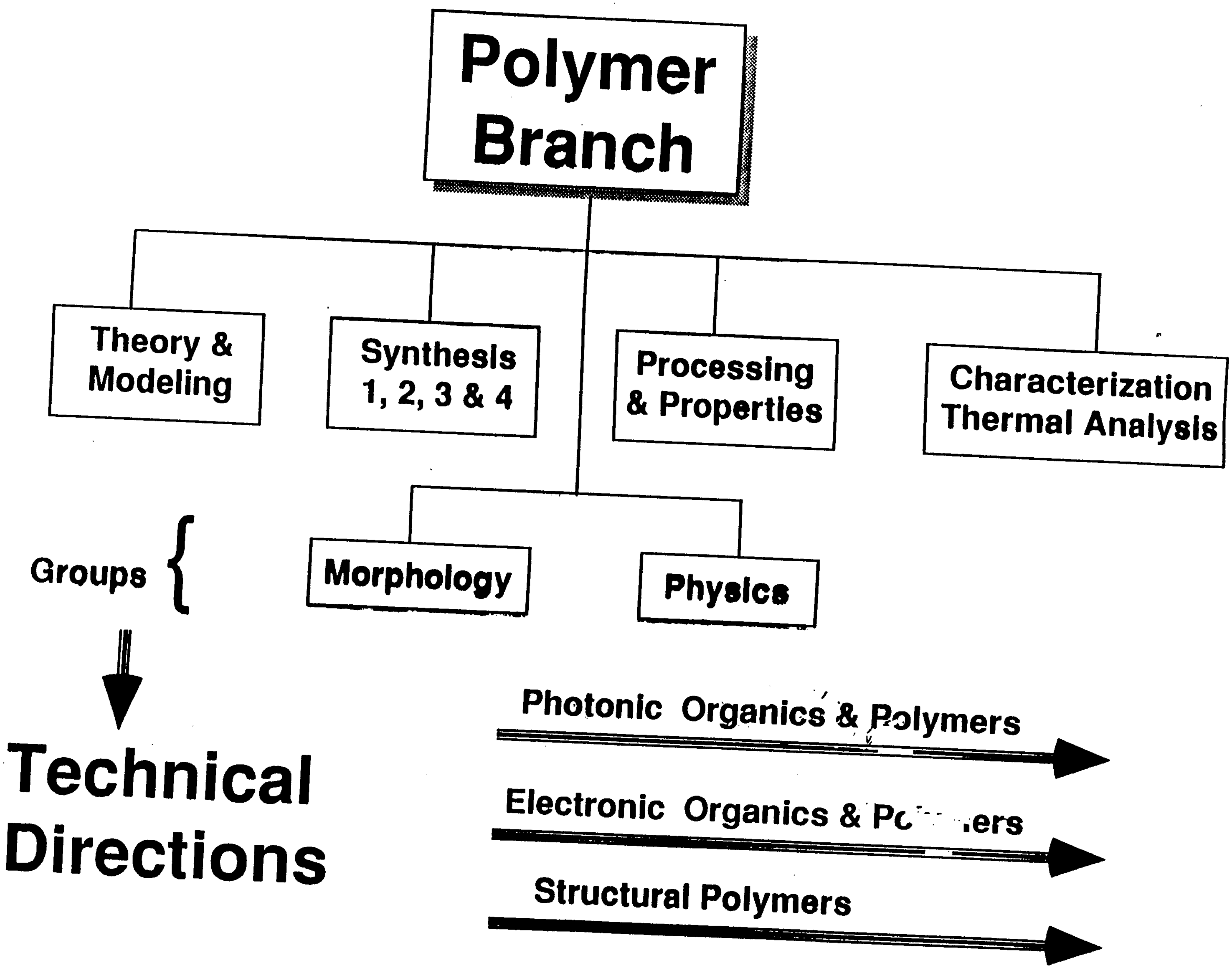
Dr. Douglas Dudis

Wright-Patterson AFB

Competitive With Experiment: The Future of Molecular Modeling ?

Douglas S. Dudis and Alan T. Yeates
Polymer Branch - WL/ MLBP
Materials Directorate - Wright Laboratory
Wright-Patterson AFB, OH 45433


Wright Laboratory
Flight Dynamics Directorate
Avionics Directorate
Materials Directorate
Propulsion Directorate
Electronics Directorate
Manufacturing Technology
Metals & Ceramics
Nonmetallic Materials
Physics & Lasers
Fluids & Lubricants
Mechanics Branch
Composites Branch
Polymer Branch
Surface Interactions


Polymer Branch
Theory & Modeling
Synthesis 1, 2, 3 & 4
Processing & Properties
Characterization Thermal Analysis
Groups
Morphology
Physics
Technical Directions
Photonic Organics & Polymers
Electronic Organics & Po
ers
Structural Polymers

COMPUTATIONAL MATERIALS SCIENCE

WRDC/MLBP

Nonmetallic Materials Division

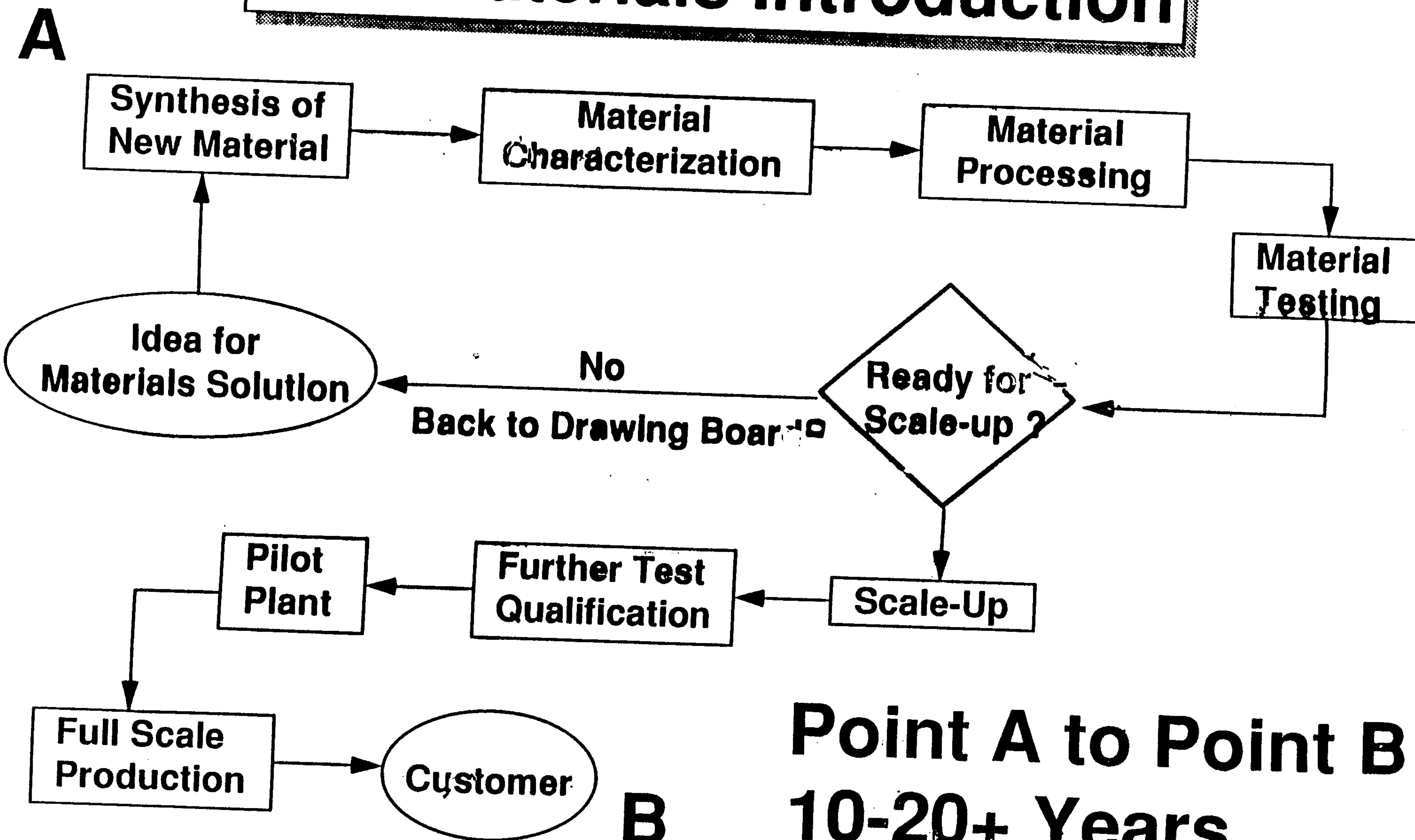
TARGET: ABILITY TO QUANTITATIVELY AND QUALITATIVELY PREDICT MOLECULAR AND BULK PROPERTIES OF MATTER.

- SPECTROSCOPIC
- ELECTRONIC
- MECHANICAL
- THERMODYNAMIC

MOTIVATION: ENHANCE EFFORTS TO DEVELOP ADVANCED MATERIALS

- GREATER EFFICIENCY AND EFFECTIVENESS
- FOCUS AND ASSIST EXPERIMENTAL EFFORTS
- FACILITATE UNDERSTANDING OF ORIGINS OF SPECIFIC PROPERTIES
- ELUCIDATION OF UNDERLYING MECHANISMS
- AVOID EXCESS TESTING OF CANDIDATE MATERIALS
- CIRCUMVENT PREMATURE ELIMINATIONS DUE TO POOR TESTS

Simplified Process for New Materials Introduction



Point A to Point B: 10-20+ Years

When is Modeling Effort "Competitive With Experiment" ?

A Calculation is Competitive with Experiment when we have enough confidence in the methods used that we need not do the experiment or when the theory can challenge an experimental observation.

Example: DuPont

Problem: Important reaction gives two products. One is useful, the other is a waste side product.

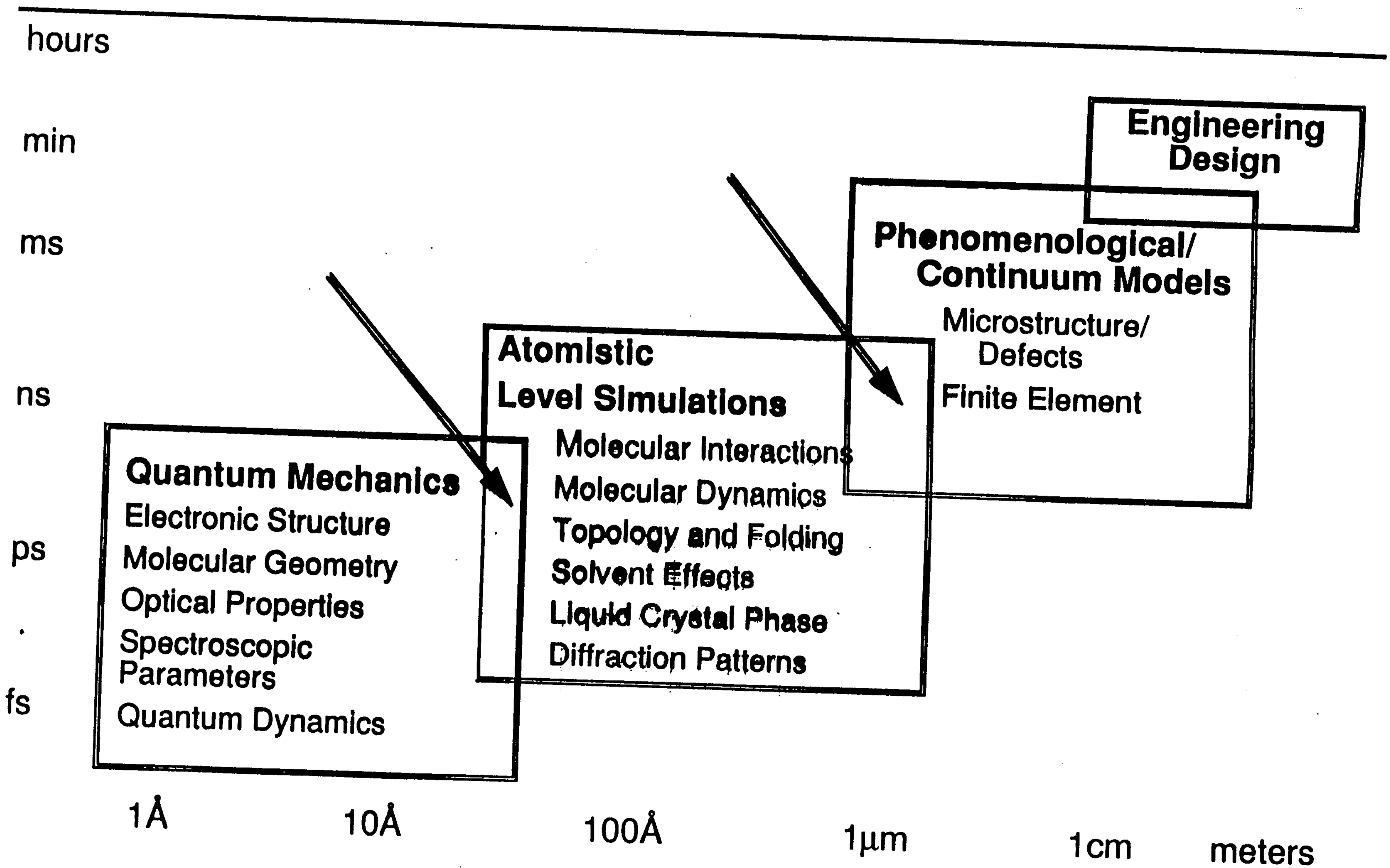
Question: Can a catalytic path be found to convert the undesired side product into the useful product? (Increased yield, decreased waste stream)

Approach: Quantum mechanical methods showed that the undesired product is thermodynamically stable product. Any catalytic scheme would thus convert desired product into the undesired product. That is, any catalyst would be detrimental.

Result: No need for research into this area - it can't work.

Summary: Answer could have been obtained by modeling or by experiment. Modeling was quicker and accurate enough to make multi-million dollar R&D decision = Competitive with Experiment.

MATERIALS DESIGN



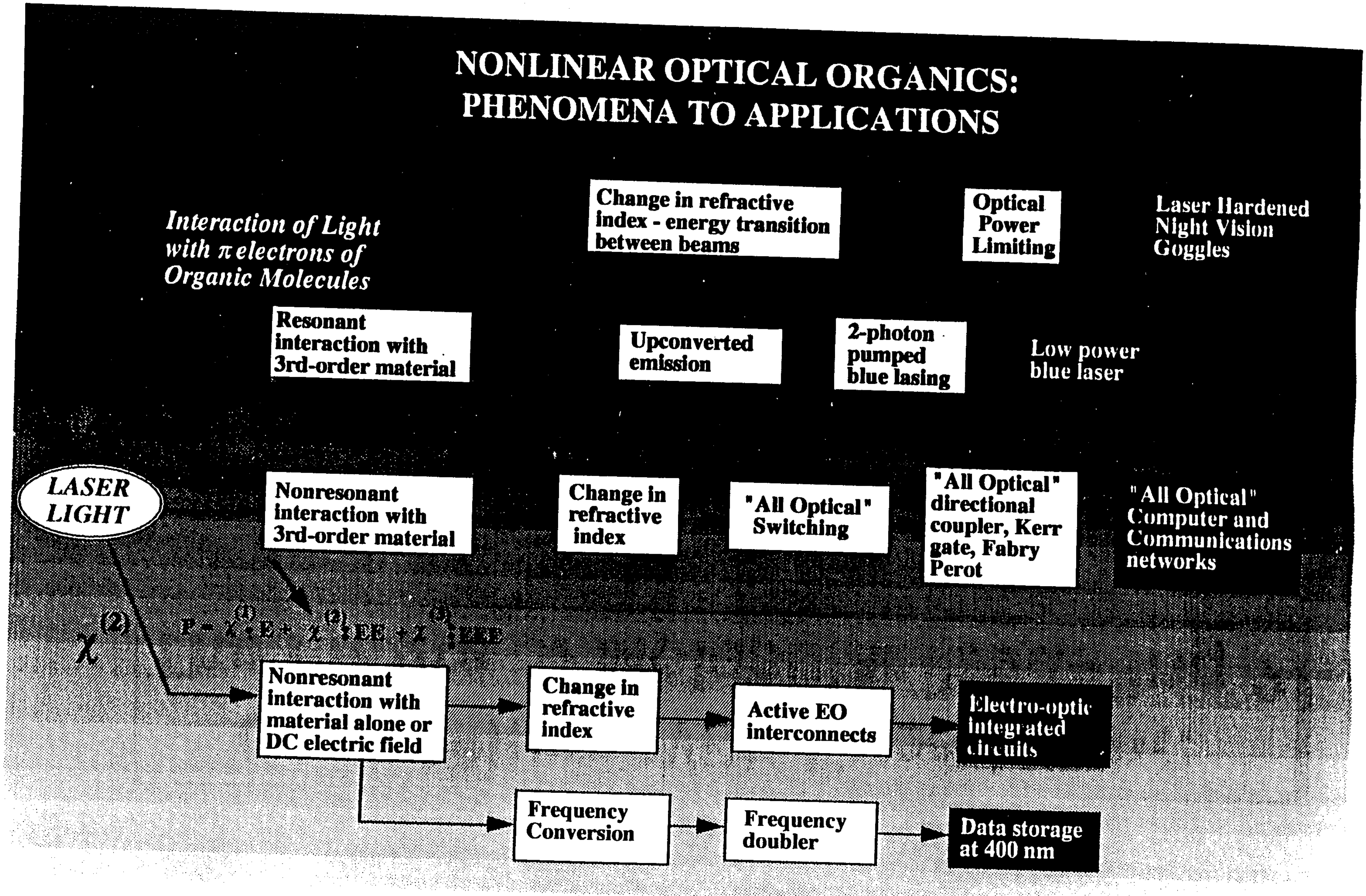
Goddard, Caltech

Atomistic Modeling
~ 1994 Snapshot

No Chemical Reacions

No Dispersion Forces

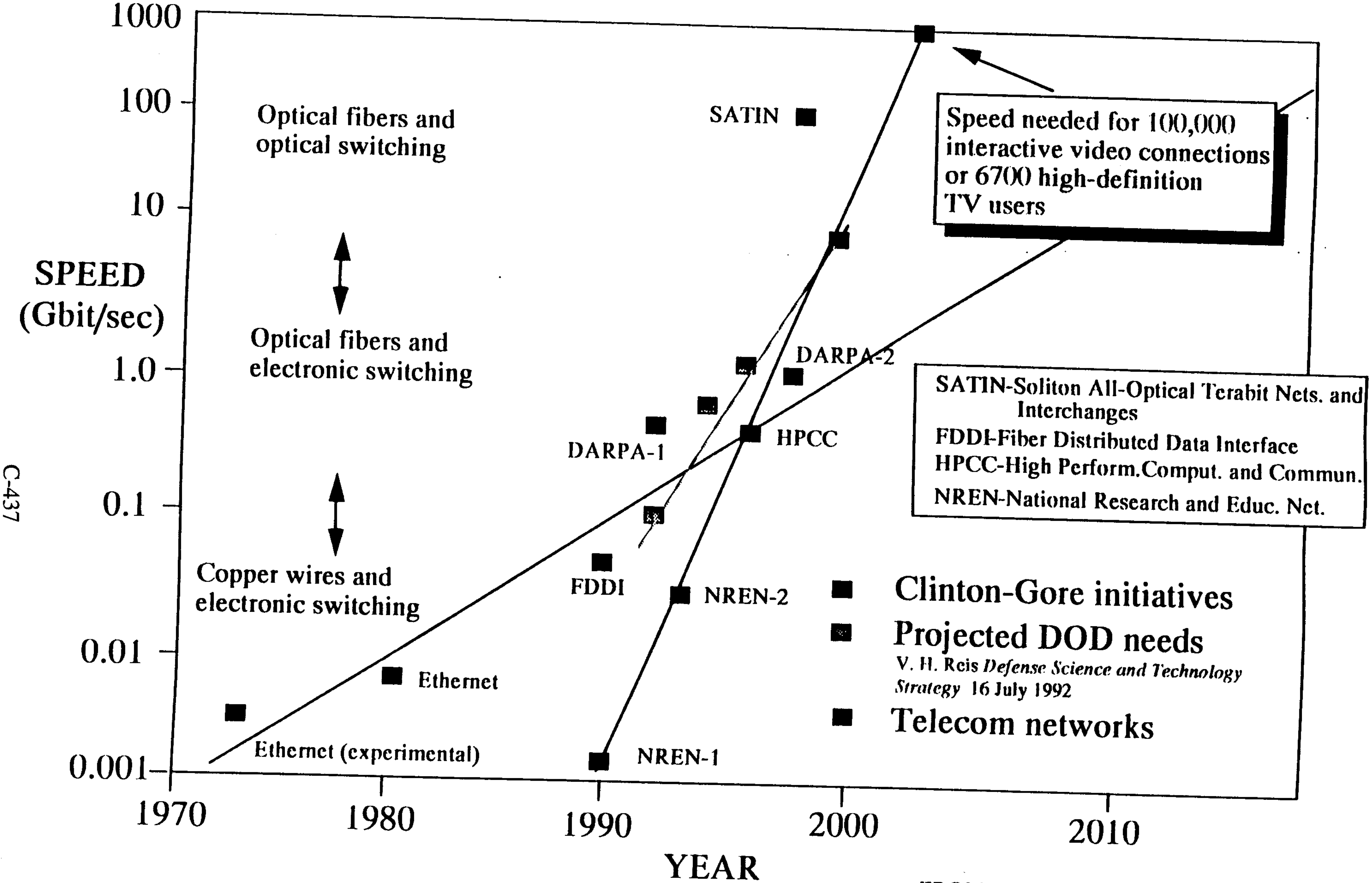
Method	Size	
Molecular Mechanics Molecular Dynamics	~1,000,000 C Atoms	
SemiEmpirical Hartree-Fock	~1000 C Atoms	
Time Independent Hartree-Fock	~40-70 C Atoms	Accurate Structures and Thermodyns (usually)
Time Independent PostSCF Correlated	~14 C Atoms	
Time Dependent Hartree-Fock	~7 C Atoms	
Time Dependent PostSCF Correlated	~2-3 C Atoms	← Truly Competitive with Experiment



NONLINEAR OPTICAL ORGANICS:
PHENOMENA TO APPLICATIONS
Interaction of Light with π electrons of Organic Molecules
Change in refractive index - energy transition between beams
Optical Power Limiting
Laser Hardened Night Vision Goggles
Resonant interaction with 3rd-order material
Upconverted emission
2-photon pumped blue lasing
Low power blue laser
LASER LIGHT
Nonresonant interaction with 3rd-order material
Change in refractive index
"All Optical" Switching
"All Optical" directional coupler, Kerr gate, Fabry Perot
"All Optical" Computer and Communications networks
$\chi^{(2)}$
$P = \chi^{(1)} \cdot E + \chi^{(2)} : EE + \chi^{(3)} \vdots EEE$
Nonresonant interaction with material alone or DC electric field
Change in refractive index
Active EO interconnects
Electro-optic integrated circuits
Frequency Conversion
Frequency doubler
Data storage at 400 nm

BAR 4-94

TRENDS IN NETWORK SPEEDS



FROM: *Physics Today* May 1994

BAR 4-94

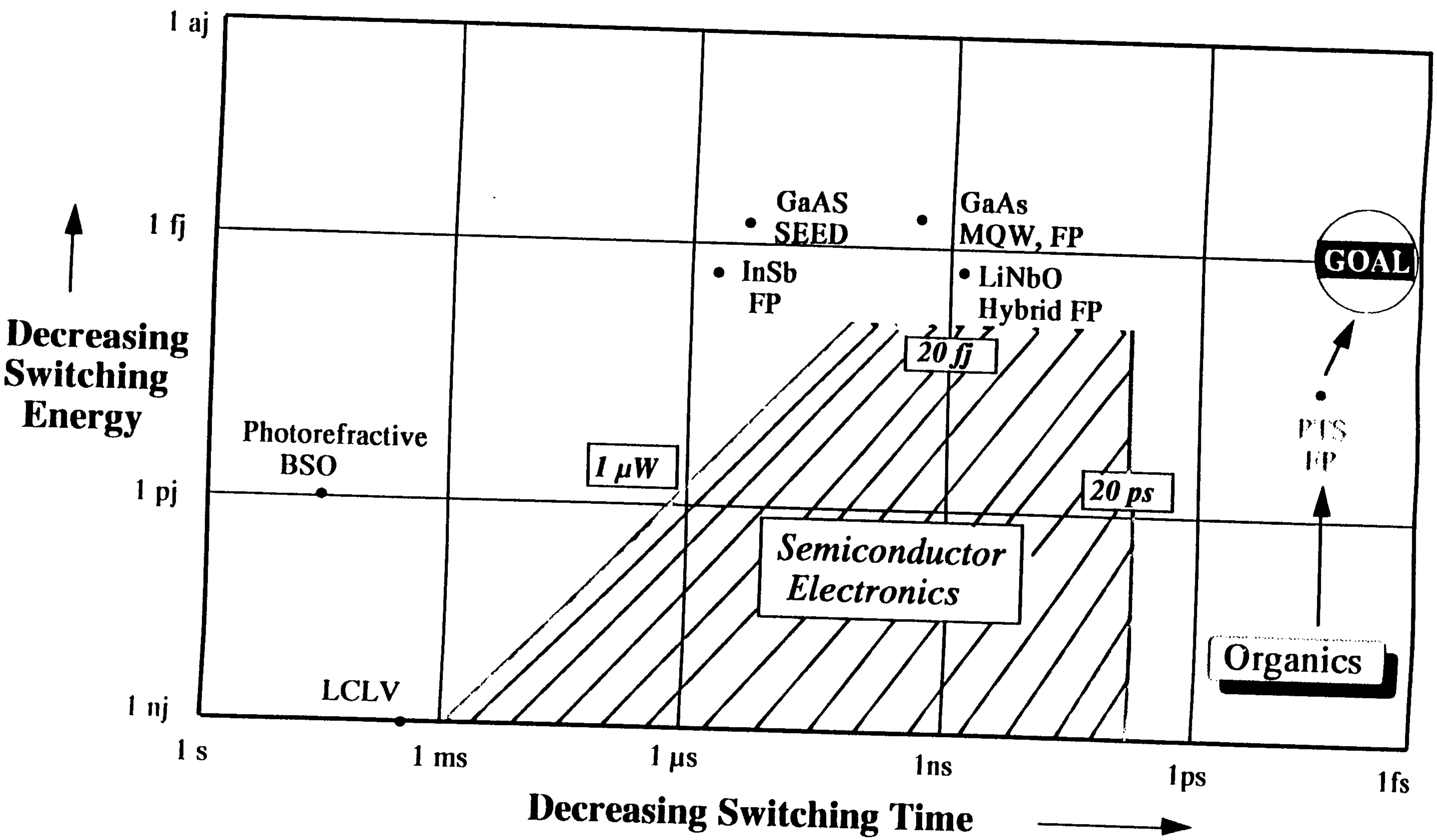
METRICS EO Polymers ($\chi^{(2)}$)

Materials for Electro-Optic Interconnects

Customer Needs	SOA Materials Properties	FA 3 Materials Properties - Current Status
Easily Processed into thin films - spin coatable	yes	yes
Easily electric field poled or self-assembled	yes	poling demonstrated
High EO coefficient (> 30 pm/V) and low optical loss (<0.3 dB/cm at 830 nm	no - high absorption of materials with EO coefficients > than 30 pm/V	10 pm/V - improvement expected
High thermal stability (320°C, 20min) Long term - 95% orig act.- 10 years	320°C stability not demonstrated most chromophores have sensitive groups	experiments in progress high potential for success - use of all aromatic donors and acceptors
Ability to modulate light at high bandwidths (100 GHz) - low dielectric constants	40 GHz Modulation demonstrated but not at 830 nm	Very low dielectric constants due to all aromatic heterocyclic ring structures
Resonable cost, producibility, low toxicity, carcinogenicity	Multiple step synthetic schemes Many are known carcinogens	Enhanced producibility, reduced toxicity/carcinogenicity

BAR 4-94

Switching Energies and Times for a Number of Optical Bistable Switches



BAR 4-94

ENERGY AND DIPOLE EXPANSIONS

IN TERMS OF ELECTRIC FIELDS

$$E(\mathbf{F}) = E^{o} - \sum_{i} \mu_i F_i - 1/2 \sum_{ij} \alpha_{ij} F_i F_j - 1/3 \sum_{ijk} \beta_{ijk} F_i F_j F_k - 1/4 \sum_{ijkl} \gamma_{ijkl} F_i F_j F_k F_l + \ldots$$

$$\mu_i(\mathbf{F}) = \mu_i^{o} + \sum_{j} \alpha_{ij} F_j + \sum_{jk} \beta_{ijk} F_j F_k + \sum_{jkl} \gamma_{ijkl} F_j F_k F_l + \ldots$$

ORIENTATIONALLY AVERAGED POLARIZABILITIES

$$\langle\alpha\rangle = 1/3\,(\alpha_{xx} + \alpha_{yy} + \alpha_{zz})$$

$$\langle\beta\rangle = 3/5\,(\beta_{yyy} + \beta_{yxx} + \beta_{yzz})$$

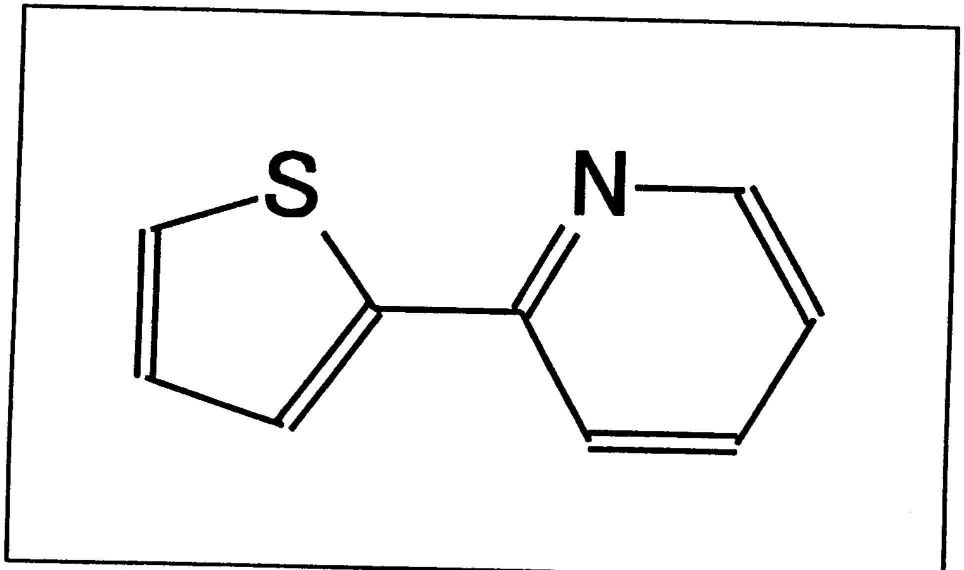
y = major symmetry axis

$$\langle\gamma\rangle = 1/5\,(\gamma_{xxxx} + \gamma_{yyyy} + \gamma_{zzzz} + 2\gamma_{xxyy} + 2\gamma_{xxzz} + 2\gamma_{yyzz})$$

QUANTUM MECHANICAL CALCULATIONS OF POLARIZABILITIES AND HYPERPOLARIZABILITIES

	AB INITIO
FINITE FIELD (FF)	
	SEMI-EMPIRICAL
SUM OVER STATES (SOS)	
	EXTENDED-HUCKEL

Frequency (e.v.)	α's	β's (SHG)	γ's (IDRI)
0.0	103.0565	411.6347	33947.51
0.5	103.8717	454.1714	36577.43
1.0	106.4656	644.6717	46714.13
1.5	111.3836	1852.666	79410.83
2.0	120.0397	1.243633e+13	6.294549e+13
2.5	136.7605	2.727414e+33	1.947792e+34
3.0			



There are Two Kinds of Opportunities for Improvement:

- Those we know about
- Those we don't know about

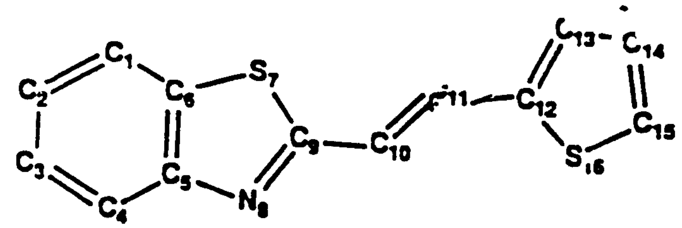


Figure 1: Numbering scheme for 2-([illegible]n thiazolyl)-1-(2-Thienyl)Ethene

Table II: Experimental and Computational Bond Lengths (Å)

Bond	X-ray	AM1	6-31G
C1-C2	1.379(4)	1.392	1.380
C2-C3	1.399(5)	1.402	1.398
C3-C4	1.375(5)	1.389	1.377
C4-C5	1.394(4)	1.406	1.393
C5-C6	1.405(4)	1.433	1.393
C1-C6	1.389(4)	1.390	1.388
C6-S7	1.731(3)	1.681	1.746
C5-N8	1.391(4)	1.408	1.383
N8-C9	1.295(4)	1.324	[illegible].273
S7-C9	1.770(3)	1.73[illegible]	[illegible].767
C9-C10	1.457(4)	[illegible]	[illegible].463
C10-C11	1.321(4)	[illegible]	[illegible].328
C11-C12	1.450(4)	[illegible]	1.459
C12-C13	1.389(4)	[illegible]	1.354
C12-S16	1.721(3)	[illegible]	[illegible]
C13-C14	1.446(4)	1.437	[illegible].432
C14-C15	1.357(6)	[illegible].369	1.345
C15-S16	1.687(4)	1.671	1.725
Δrms		0.021	0.016

Table III: Experimental and Computational Bond Angles (°)

Angle	X-ray	AM1	6-31G*
C1-C2-C3	120.6(3)	120.9	120.9
C2-C3-C4	121.5(3)	121.2	120.9
C3-C4-C5	118.9(3)	118.9	118.8
C4-C5-C6	119.0(3)	119.6	119.8
C1-C6-C5	122.1(3)	120.1	121.5
C2-C1-C6	117.9(3)	119.3	118.1
C5-C6-S7	108.6(3)	109.6	109.0
C6-C5-N8	[illegible]16.3(3)	114.7	115.3
C5-N8-C9	110.3(2)	109.8	111.8
C6-S7-C9	[illegible]9.4(1)	90.9	88.6
S7-C9-N8	[illegible]5.4(2)	115.0	115.4
N8-C9-C10	[illegible]22.2(3)	124.4	121.6
S7-C9-C10	[illegible]22.5(2)	120.6	123.0
C9-C10-C11	[illegible]26.3(3)	122.7	125.2
C10-C11-C12	[illegible]5.4(3)	124.2	126.4
C11-C12-C13	[illegible]24.8(3)	124.5	125.5
C11-C12-S16	[illegible]23.3(2)	124.9	123.9
C12-C13-C14	109.4(3)	111.9	113.4
C13-C14-C15	114.2(3)	111.5	112.3
C14-C15-S16	111.6(3)	112.0	112.1
C12-S16-C15	92.7(2)	94.0	91.6
C13-C12-S16	112.0(2)	110.6	110.6
Δrms		1.6	1.2

What We Should Be Doing: Wayne Gretzky Effect

Don't skate to where the puck is -

Skate to where the puck will be.

COMPUTATIONAL FLUID DYNAMICS

Exploiting Massive Parallelism to Simulate Complex Turbulent Flow

Professor Paul R. Woodward

University of Minnesota

EXPLOITING MASSIVE PARALLELISM TO SIMULATE TURBULENT FLOWS

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Purpose: Exploit massive parallelism in fluid dynamics applications in order to achieve:

1) **Unprecedented flow accuracy,**

2) **Unprecedented flow complexity,**

3) **Generate "experimental" data sets of demonstrated accuracy to guide construction of theoretical models (e.g. turbulence closure),**

4) **Overcome long - standing difficulties:**

   - **Accurate high Reynolds number flows,**
   - **Accurate tracking of multifluid interfaces,**
   - **Flow in or around complex boundaries.**

I. Ways in which massively parallel computing technology is changing the computational fluid dynamics paradigm.

Algorithms which are preferred by MPP's:

1) Explicit or iterative implicit methods which update cells based solely on local data.
2) Regularly structured grids, where each cell is treated in an identical fashion and for which there is no need for indirect addressing.
3) Capturing schemes, where special features of the flow, such as shocks or multifluid interfaces, are automatically captured and handled by the scheme without special tracking techniques which demand a much more elaborate treatment for these special cells.

II. Piecewise - Parabolic Method (PPM):

1) Developed in collaboration with Colella, Fryxell, Edgar, Dai, Porter, and Bailey.
2) Time - dependent, compressible flow with strong shocks, multiple fluids, general equations of state, complex stationary or moving boundaries, magnetic fields. To come: implicit - explicit; improved multifluid treatment; quadralateral grids.
3) Scientific visualization environment.
4) Fortan - P precompiler.
5) PPMLIB project for Cray T3D & ________.

6) Efficient massively parallel implementations.

- 512 - node CM-5: 8 Gflops (2-D),
- 512 - node CM-5: 11 Gflops (3-D),
- 256 - node Cray T3D: 3.75 Gflops (3-D),
- 8 - processor Cray C-90: 3.5 Gflops.
- SGI Challenge Array, 16 machines, 20 processors per machine (100 Mhz), 20 FDDI rings: 4.9 Gflops (32-bit arithmetic).
- SGI Power Challenge Server, 16 processors (MIPS R-8000, 75 Mhz): 1.55 Gflops (32-bit arithmetic).
- Cray C-90 CPU: 450 Mflops.
- MIPS R-8000, 75 Mhz: 98.5 Mflops.
- DEC Alpha workstation: 36 Mflops.
- HP 735 workstation: 30 Mflops.

III. Operations to avoid, in priority order:

1) Data movement from the memory of one processor to that of another.
2) Unbalanced loads & idle processors.
3) Conditional execution of significant code blocks.
4) Interprocessor synchronization events.
5) Indirect addressing.

IV. Tools and tricks we developed for SIMD (CM5):

1) Restrict ourselves to *self-similar* algorithms, for which identical programs can be used to update either the whole grid or any subdomain of the same topology.
2) Pass information between neighboring processors only when update strips of fake cells outside the boundaries of a processor's subdomain of the grid.
3) Developed Fortran-P precompiler to translate our self-similar Fortran-77 codes into efficient CM-Fortran for the Connection Machine.
4) Write code as if memory were infinite, and Fortran-P precompiler automatically equivalences arrays where this is possible.
5) Write vector code for each node, using vector logic (*cvmgm*).

V. Tricks we developed for MIMD (SGI Array):

1) All SIMD tricks listed above.

2) Enhance cache performance via:

   - Reference memory almost exclusively at unit stride.
   - Interleave primary variables in memory and block these arrays to increase locality of memory references in local transpose operations.
   - Overcome memory bandwidth limitations by fitting workspace entirely into cache using private copies of shared data.
   - Equivalence (via Fortran-P precompiler) scratch arrays in workspace so that it fits more easily into cache.

3) Multitasking at a network node via:

   - Explicitly designate very large tasks, generally encompassing many loops or a whole code package.
   - Remove implied barriers at ends of multitasked loops and replace them by conditional barriers (test semaphores).
   - Separate *send* from *receive*.
   - Designate *send* and *receive* as assignments to shared variables.
   - Never multitask disk I/O (already parallel).
   - Save a processor for Unix, I/O, network.

4) Domain decomposition & Load balancing over the Network:

- Domain decomposition generates tasks for network nodes which maximize data reuse and thus best overcomes network latency and bandwidth limitations.
- Domain decomposition balances memory loads.
- Reduce frequency of message passing and increase latency tolerance by introducing explicitly dimensioned buffer of fake zones.
- Separate *send* and *receive*.
- Avoid message copying (*put* and *get*).
- Designate *send* and *receive* by assignments to and from explicitly dimensioned fake boundary arrays. (These can be recognized automatically by the Fortran-P precompiler.)
- Balance loads over network by further decomposition into subdomains and dispatching of subdomains over network. Always send new data back, so that each node requires only one additional subdomain structure and workspace in memory, and message passing topology remains simple.

5) Plugging the numbers in for PPM and for the Silicon Graphics Power Challenge Array:

- 3 - level memory heirarchy:

  4 MB cache, 2 GB shared at node,

  32 GB distributed (assumes 16 nodes).

- 3 - level latency hierarchy:

  60 nsec, 0.8 μsec, 0.5 - 3 msec.

  (assumes switches reset on each event)

- 3 - level bandwidth hierarchy:

  1200 MB/s, 67 - 1200 MB/s, 60 - 180 MB/s.

  (assumes 3 HiPPI interfaces per node)

- 18 CPU's on each of 16 nodes.
- 100 MB/s disk I/O on each of 2 nodes.
- Typical task executed by single CPU (fits into 4 MB cache):

  Pencil of 4x4 strips of 64 zones each:

  4x4x(64+7)x1300 flop = 1.48 Mflop

  ---> 15.0 msec.

  ((4x4 + 4x2x4)x(64+14) + 4x4x64)x5x4 Byte

  = 93.1 KB mem I/O

  ---> 1.32 msec.

- Typical task executed by single node (fits into 2 GB shared mem):

  2 time steps 64x64x64 zone subdomain:

  6x16x16 pencils as above = 2.27 Gflop

  ---> 1.36 sec.

  $2x6x(2x10 + 4x2)x(64+14)^2x5x4$ Byte

  = 39.0 MB message I/O (read+write)

  (27.9 MB time-limiting, 1 net link)

  ---> 32.5 msec. (to shared memory)

  ---> 0.464 sec. (all to network)

  $(64^3 + (64+14)^3)$ x5x4 Byte data to & fro

  = 14.1 MB over 1 net link

  ---> 0.234 sec. (for load balancing)

- Typical task executed by 16-node Array (fits into 32 GB distributed memory):

  <u>5000 time steps on 512x512x1024 grid:</u>

  256x256x256 brick at each node.

  (Memory could accommodate a problem twice this size.)

  Each brick consists of 64 sub-bricks.

  16x6 sub-brick faces sent over network.

  (as if 1/4 of the sub-bricks do netwk I/O.)

  2500x(16x(0.464 + 1.36) + 48x(0.0325 + 1.36))

  = 2500 x 96.3 sec (raw computation)

  = 66.9 hour = 2.79 day

After every 10 time steps, send compressed description of fluid state, with 2 Bytes per word, to the 2 nodes which have attached 100 MB/s disk subsystems.

500 compressed dumps of 2.5 GB each.

1.25 Tbyte data set to be archived.

Requires 500x2500/180 sec = 1.93 hour.

Hence total computation time = 68.8 hour

Total computation = 5807 Tflop.

Overall performance = 2323 Gflop / 99.1 s
= 23.4 Gflops

This estimate does not allow for overlapping message I/O with computation, but it also assumes perfect load balance. Only 17 of the 18 CPU's in each machine are used for computation. The above figures indicate that irregular loads would not result in a significant performance degradation for problems of this size (for the PPM code).

VI. Advantages of this approach for 2-D flow problems:

1) Simulations on grids of 8 million cells are practical.

2) On these fine grids, captured shocks, contact discontinuities, and multifluid interfaces are “razor sharp.”

3) On these fine grids, object boundaries of complex shape can be described accurately without the use of body-fitted grids.

4) The PPM code runs at 8 Gflops on the CM-5 for these problems, and therefore one may, in the supersonic regime, obtain statistically steady flows from direct integration of the governing equations, without having to develop approximate time-averaged fluid equations. Time averages, as in nature, may be taken after rather than before the simulation is performed.

5) Because no body-fitted grids are necessary, objects of complex shape may be moved through the grid according to the dynamic forces acting upon them, which are computed as a natural part of the PPM calculation. Objects may even change shape if this is appropriate.

VII. Examples of 2-D flows computed on the CM-5 at the AHPCRC using the PPM code.

1) The interaction of a Mach 1.3 shock with a wedge. Direct comparison with experiment.

2) Statistically steady Mach 4 flow about a circular cylinder. An exhaustive study of convergence properties of the method.

3) 2-D analog of the sabot discard process. Simulation of a dynamic process with moving boundaries reacting to computed pressure forces generated by the flow. This computation can be seen as a large eddy simulation.

VIII. Additional advantages of this approach in 3-D:

1) On sufficiently fine grids, PPM simulations can be viewed as large eddy simulations -- the largest scales of turbulent motion are resolved, while dissipation of this turbulent energy into heat is accomplished on scales which are unresolved by the grid.

2) PPM calculations on grids of up to a billion cells have been performed on equipment with a list price of under 12 M$ (the Silicon Graphics Challenge Array, Sept., 1993).

3) These fine grids allow us at last to get an accurate look at the Kolmogorov inertial range of homogeneous, compressible turbulence and to compare its behavior to turbulence closure models.

IX. Examples of 3-D PPM simulations.

1) NSF Grand Challenge simulation of turbulent compressible convection in a stratified atmosphere. PPM parallelized on the Cray-C90 at the Univ. of Minnesota and on the Cray-T3D at the Pittsburgh Supercomputing Center. For the first time the interaction of the convection cellular structures with turbulent fluid motions can be studied in a "first principles" calculation without recourse to heuristic turbulence modeling.
2) Billion-Zone Grand Challenge simulation of homogeneous, compressible turbulence using PPM code parallelized on the 320-processor, 16-machine Challenge Array at Silicon Graphics in Mt. View, California. For the first time the detailed structures and behavior of compressible turbulence in the Kolmogorov inertial range may be studied, visualized, and compared in detail with predictions of turbulence closure models.

X. Where does this lead?

1) Simplified new approaches to the simulation of complex, turbulent flows which exploit the fine grids which MPP's and tens of Gflops make possible.

2) Decreased reliance on empirical engineering models and increased use of direct simulation, with the hope of greater confidence in the results when simulating flows in unexplored regimes.

3) Increasingly scalable application codes which operate in a consistent fashion across wide performance and capability ranges starting at the desk top.

4) With the help of new tools like our Fortran-P precompiler and scalable libraries for CFD like PPMLIB, a much reduced barrier to massively parallel computation.

5) With the help of Gigabit networking and powerful flow visualization tools and systems, such as those developed in the AHPCRC's Graphics and Visualization Laboratory, increasingly interactive and natural visual analysis of the extremely large data sets which these simulations produce.

XI. Acknowledgements:

- Moving boundary version of PPM developed in collabration with B. Kevin Edgar.
- Study of shock striking a wedge, of flow about a cylinder, and of 2-D sabot discard performed in collaboration with B. Kevin Edgar and Steven Anderson.
- Study of compressible convection performed in collaboration with David Porter.
- Billion-zone simulation of homogeneous, compressible turbulence carried out in collaboration with David Porter, Steven Anderson, Jim MacDonald, Ken Chin-Purcell, and a team from Silicon Graphics: Richard Hessel, David Perro, Igor Zacharov, Jerold Ryan, Leonard Widra, and Michael Galles.
- Fortran-P precompiler developed in collaboration with Matt O'Keefe, Terence Parr, Steve Anderson, Aaron Sawdey, B. Kevin Edgar, and Hank Dietz.
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- Computer time was provided by the Army High Performance Computing Research Center (AHPCRC) on a 512-node CM-5 Connection Machine, by the Minnesota Supercomputer Institute of the University of Minnesota on an 8-processor Cray-C90, by the Pittsburgh Supercomputer Center on a 256-node partition of a Cray-T3D, and by Silicon Graphics, Inc., on a 16-node, 320-processor Challenge Array.

MPP Simulations of Plasma Thrusters on Spacecraft

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PLASMA SIMULATIONS ON MASSIVELY PARALLEL COMPUTERS FOR ION THRUSTER SPACECRAFT CONTAMINATION

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Overview

- Introduction, Statement of Problem
- Physical Model of Ion Thruster Plume
- Numerical Model and Methods
- Massively Parallel Computing Implementation
- Sample Results
- Conclusions, Future Work

Electric Propulsion

- High *specific impluse* -> **low propellant consumption**
- Typical satellite chemical thruster: Isp = 200-300 s

  ion thruster: Isp = 1000-5000 s
- Higher satellite payload capacity (less fuel required)
- Reduced satellite mass -> reduced launch costs
- Greater propulsive impulse capacity enhances satellite mobility to manuever over to regions of interest around the world

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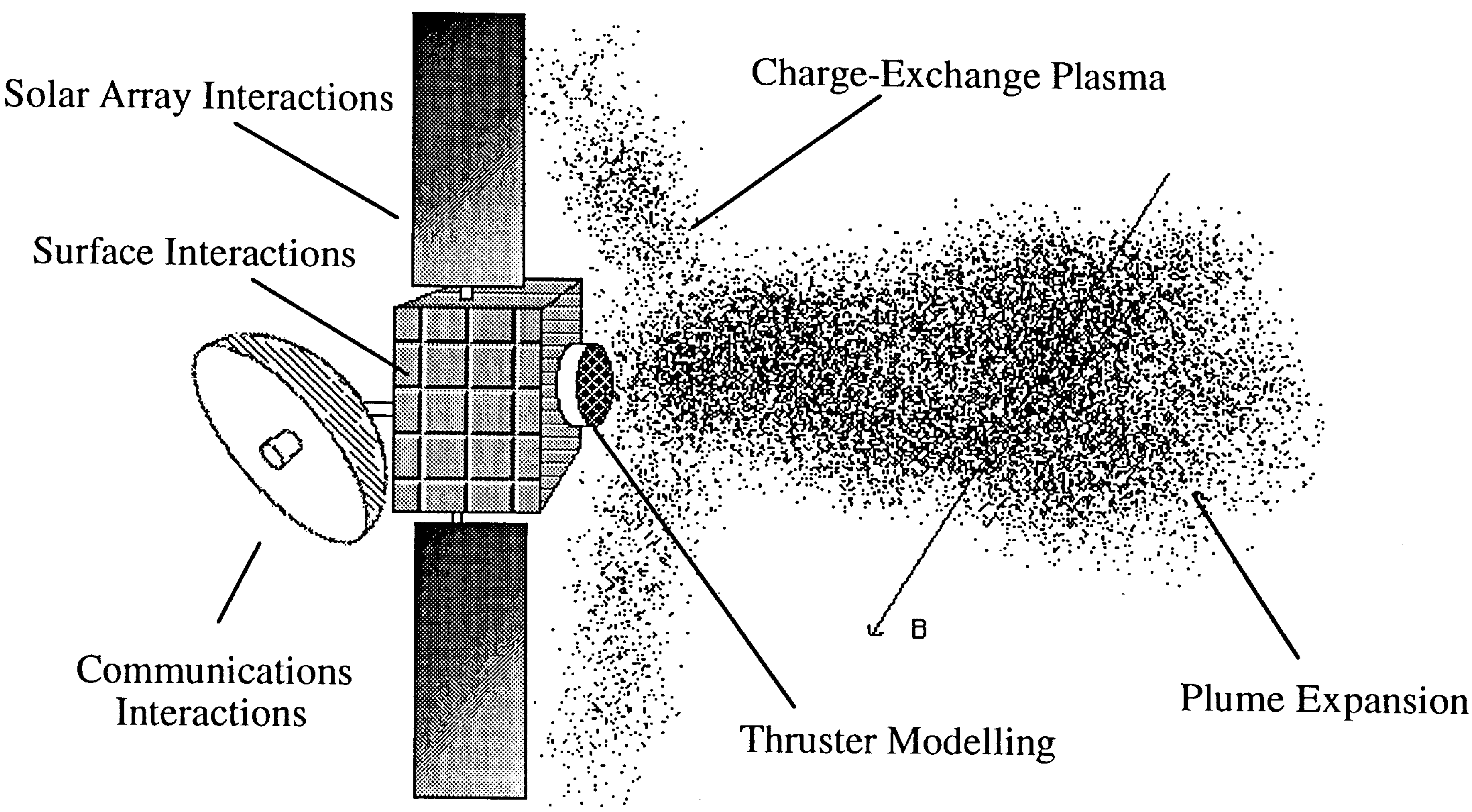
Thruster - Spacecraft Interactions



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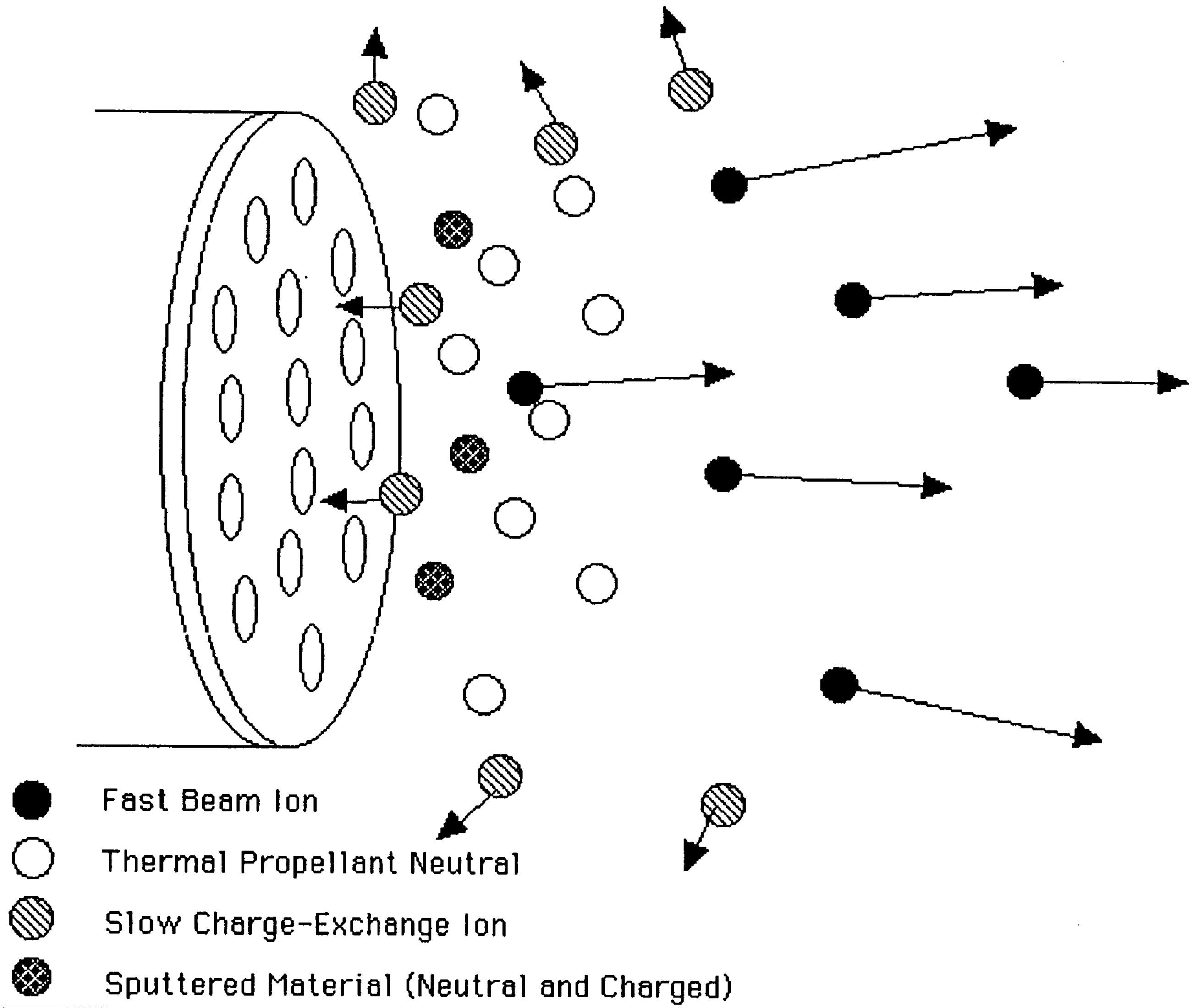
Purpose of Study

- Understand spacecraft contamination by electric propulsion thrusters
- Only simple models are available and ground tests are problematic due to facility effects
- The development of a numerical model with accurate predictive capability will be a major advance in this field where no such model is available
- Apply the model to various mission scenarios and advanced space platforms to aid in thruster-spacecraft integration

Ion Thruster Effluents



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General Computational Approach

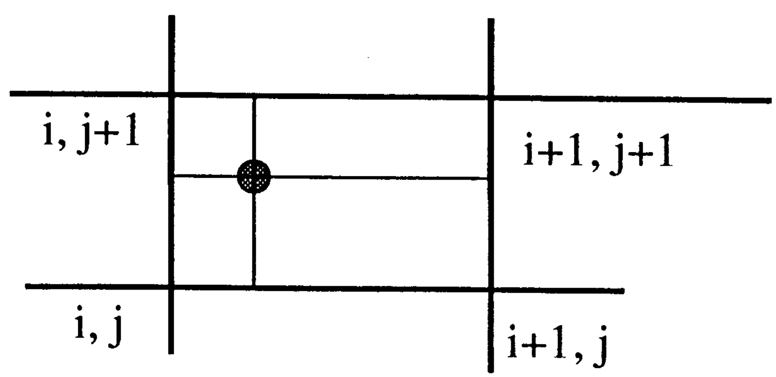
- Model for beam ions
- Model for neutrals
- Volumetric production rate for the charge-exchange (CEX) ions; these ions are treated as particles by the Particle-in-Cell (PIC) method
- Electron fluid model:

  - Isothermal Boltzmann distribution

Particle-in-Cell (PIC) Modelling

<u>Basics of Electrostatic PIC Algorithm:</u>

- Initialize (macro)particles: **x**, **v**
- Weight particles onto a grid to compute density
- Use this density to solve for potential using Poisson's equation, and find **E** field from potential.
- Extrapolate field from grid to particles and move them under this field by integrating the equations of motion.



Hybrid PIC Modelling (cont'd)

Governing Equations:

- Particle Motion: (Lorentz Equation)

$$\frac{d\mathbf{v}_k}{dt} = \left(\frac{q}{m}\right)_k \left[\mathbf{E} + \mathbf{v}_k \times \mathbf{B}\right] \qquad \frac{d\mathbf{x}_k}{dt} = \mathbf{v}_k$$

- Electric Potential: (Poisson's Equation)

$$\nabla^2 \phi = \frac{e\,(\sum_s n_e - \sum_s n_i)}{\varepsilon_o} \qquad \mathbf{E} = -\nabla\phi$$

-> Hybrid Approach: Ions treated as particles, electrons as a fluid. Eliminate restrictive time step conditions.

$$n_e = n_{e\infty} \exp\left(\frac{e\phi}{kT_e}\right)$$

Beam Ion Model

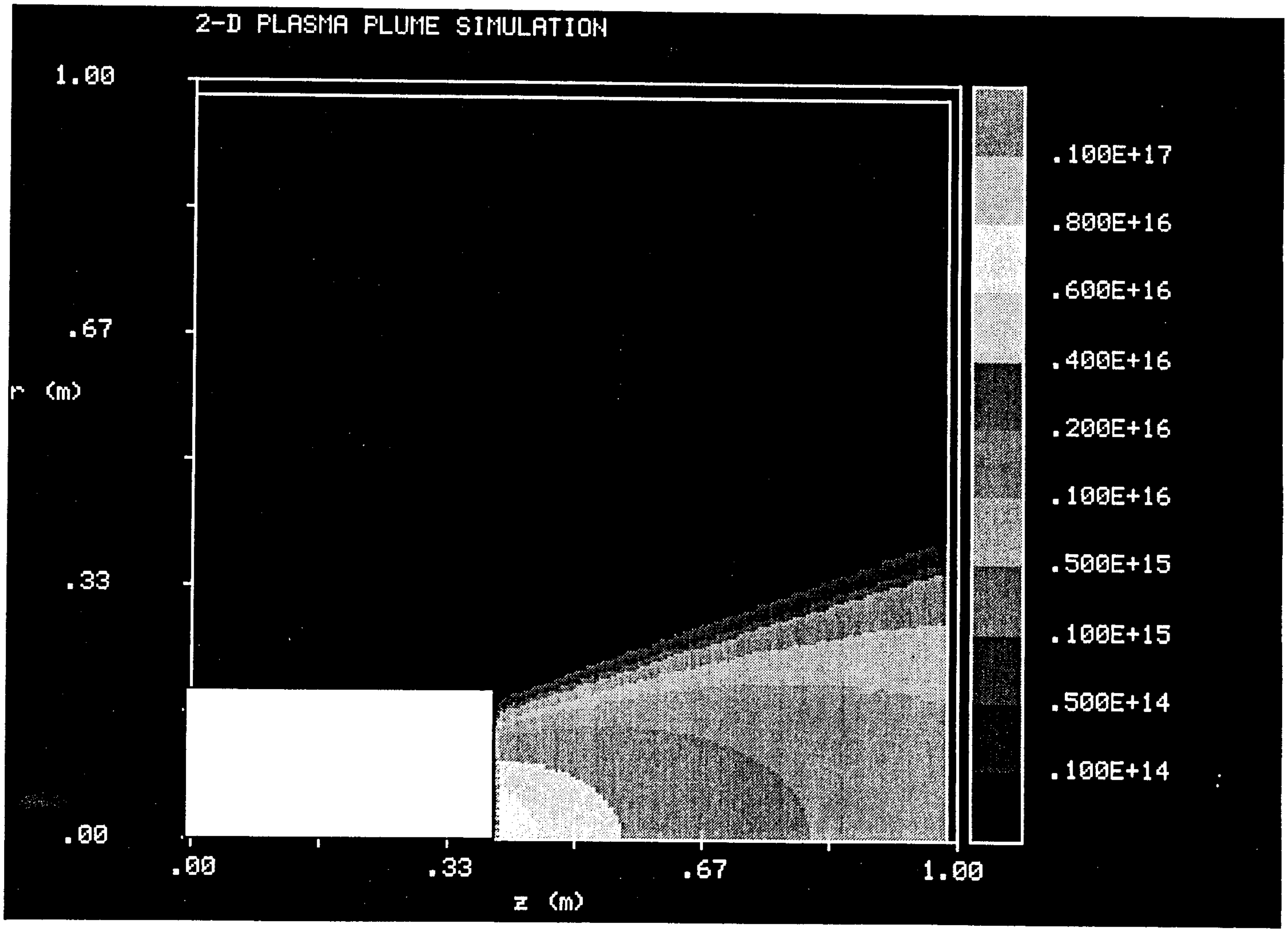
- Beam ion current density modelled by a parabolic axisymmetric profile:

$$j_{bi}(r,z) = \frac{2I_b}{\pi r_b^2}\left(1 - \frac{r^2}{r_b^2}\right) \qquad r_b = r_T + z \tan \theta_{div}$$

- Current is dominantly axial with constant beam velocity over length scales of interest:

$$n_{bi}(r,z) = \frac{j_{bi}(r,z)}{e\, v_{bi}}$$

Beam Ion Model



(Contours in m^-3)

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Propellant Neutral Effluent Model

- Unionized neutrals leave thruster in free molecular flow in equilibrium with thruster walls. Assume flow from a point source:

$$n_n(r,z) = \frac{n_{no}}{4} \frac{r_T^2 (z + r_T)}{\left[(z + r_T)^2 + r^2\right]^{3/2}}$$

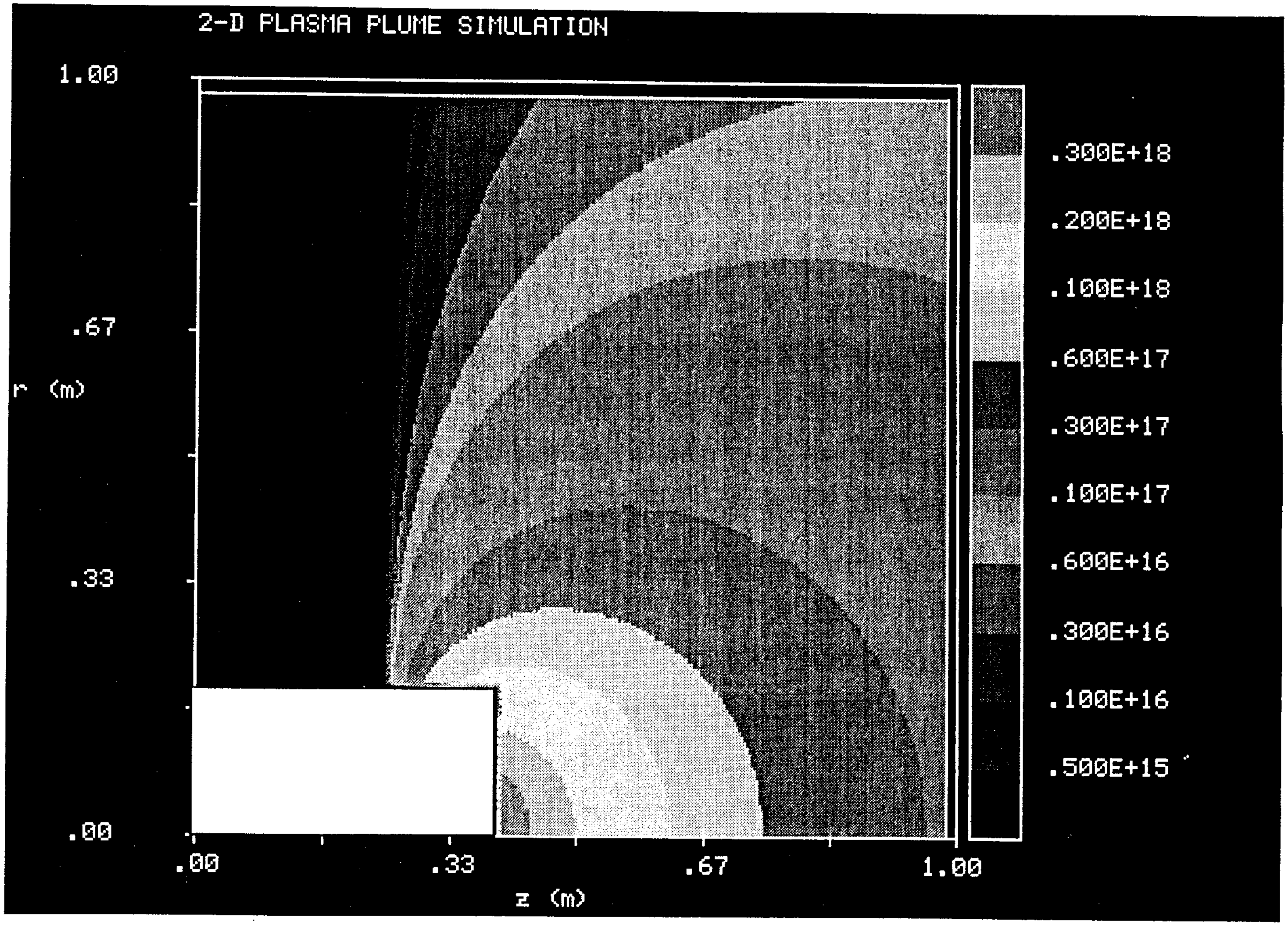
- Maximum neutral density:

$$n_{no} = \frac{4\, I_b}{e\, C\, A_n} \left(\frac{1 - \eta_p}{\eta_p} \right)$$

- Propellant utilization fraction based on total mass flow rate (incorporate neutralizer flow rate):

$$\eta_p = \frac{I_b}{\dot{m}_{total}} \left(\frac{m_i}{e} \right)$$

Propellant Neutral Effluent Model



(Contours in m^-3)

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CEX Plasma Production

- Produce slow CEX ions volumetrically -> create PIC ions based on this rate.

- Volumetric production rate:

$$\dot{n}_{cex}(r,z) = n_n(r,z)n_{bi}(r,z)V_{bi}\sigma_{cex}$$

- Computationally, $N_{p\,cell\,i} = \dfrac{\dot{N}_{cex\,i}\,V_{cell\,i}\,\Delta t}{Z_p}$

- Approach valid for:

$$\frac{I_{cex}}{I_b} = \frac{4}{3} r_T\, n_n\, \sigma_{cex} << 1$$

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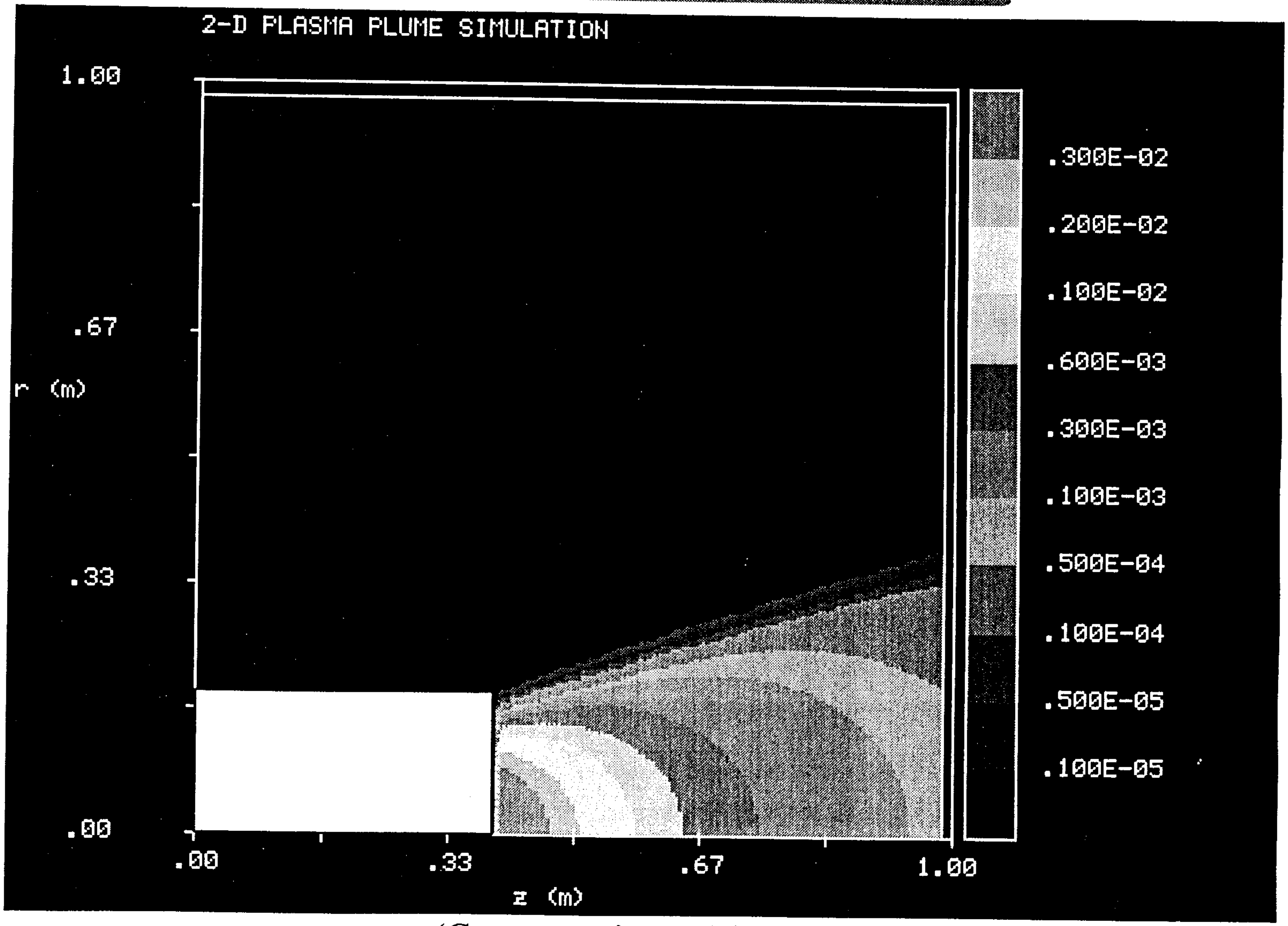
CEX Plasma Production



(Contours in mA/cm^3)

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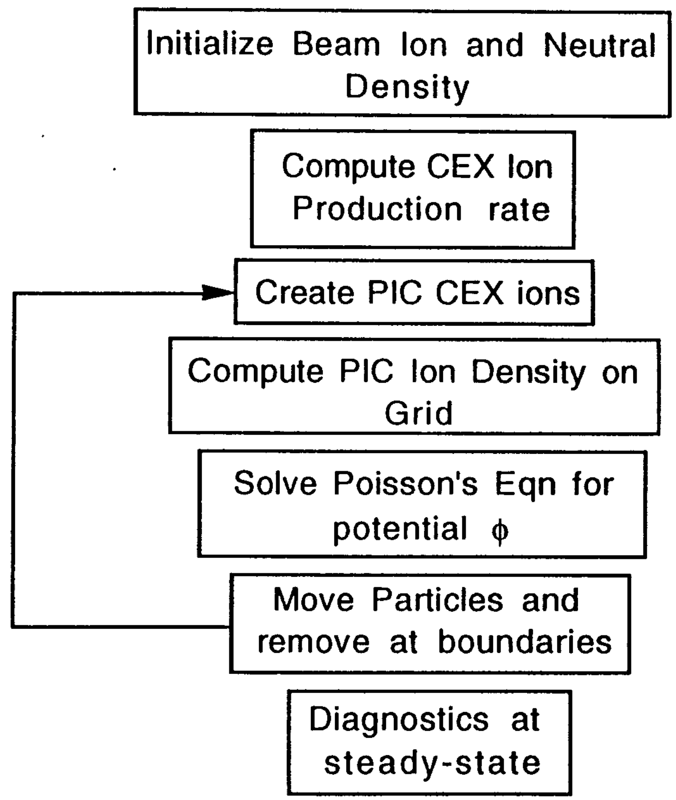
Numerical Methods

- Non-linear elliptic Poisson equation solved with SOR with Newton-Raphson
- Neumann BC on potential on all exterior boundaries; Dirichlet on spacecraft surfaces.
- Spacecraft potential floats at equilibrium value where net current is zero.

Simulation Flowchart



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Scope of Numerical Problem

Realistic 3-D Spacecraft Simulation: (half plane symmetry)

- ESEX spacecraft (1.5 m x 0.5 m x 1.0 m)
- Computational Domain (3.2 m x 4.5 m x 3 m)

  ~ 9.5 million grid points
- Up to 100 million particles

--> **Up to 5 GB of memory**

- 5,000 - 10,000 time steps to equilibrium

--> **T3D run performance: about 30 s per time step. So for 10,000 iterations-->about 3.5 days of CPU time.**

Availability is: 4 hr slots every night.

Parallel Computing

- **Enabling** for large-scale problems
- Message-passing and Domain decomposition approach

  -- Domain split into blocks; multiple blocks to a processor

  -- Particles created in beam and diffuse around; no. of particles grows with time until steady-state

  -- Dynamic load balancing important
- Use for a realistic 3-D problem for engineering predictive purposes.

Message-Passing PIC Algorithm

- Algorithm Structure:
  - **Initialize** a Block (grid, faces, B.C.'s, particles, at t=0)
  - **Compute** (density, E t>0, move particles t>0)
  - **Extract** (Get information to pass: densities and particles)
  - **Update** (incorporate received information)
  - **Solve field** (SOR) for some convergence criterion: **MP**
    - Get guard cell (GC) values to pass
    - Incorporate GC values and do one iteration
  - t = t + 1

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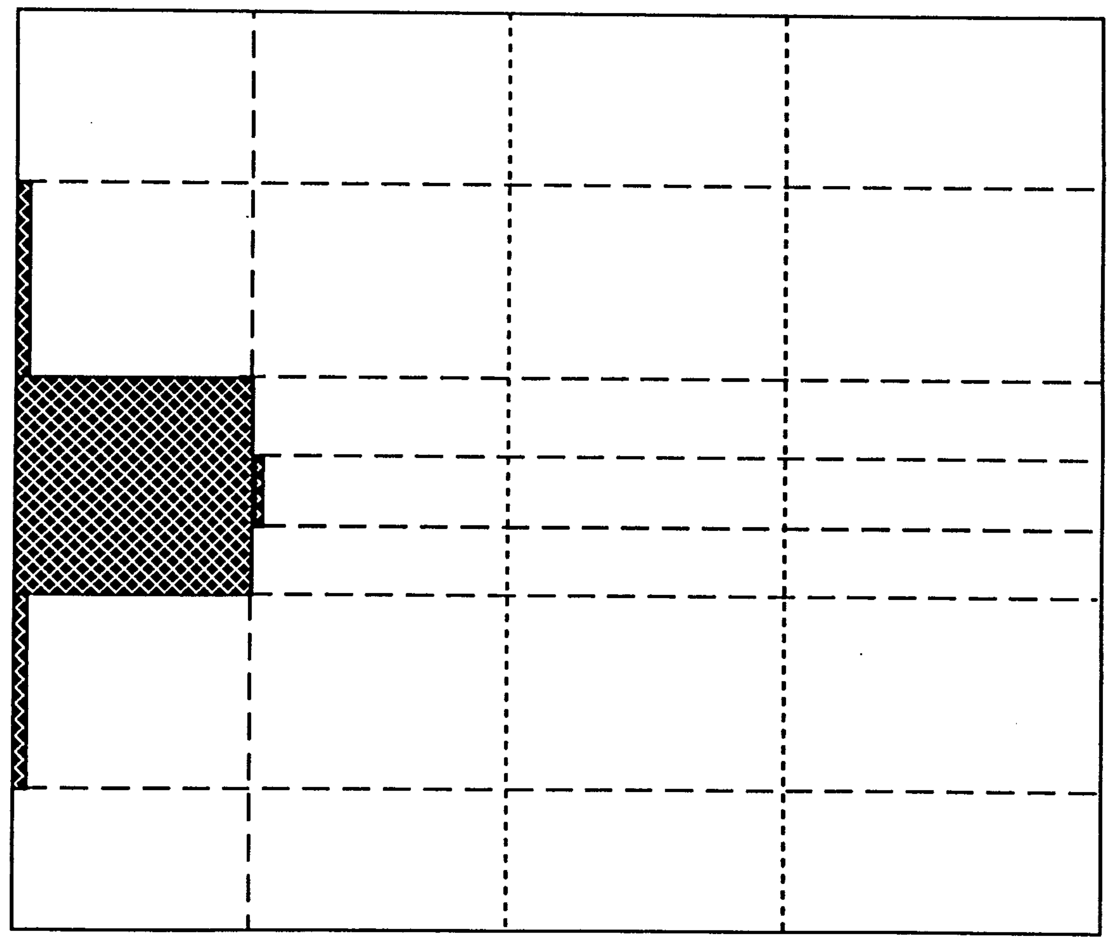
Domain Decomposition



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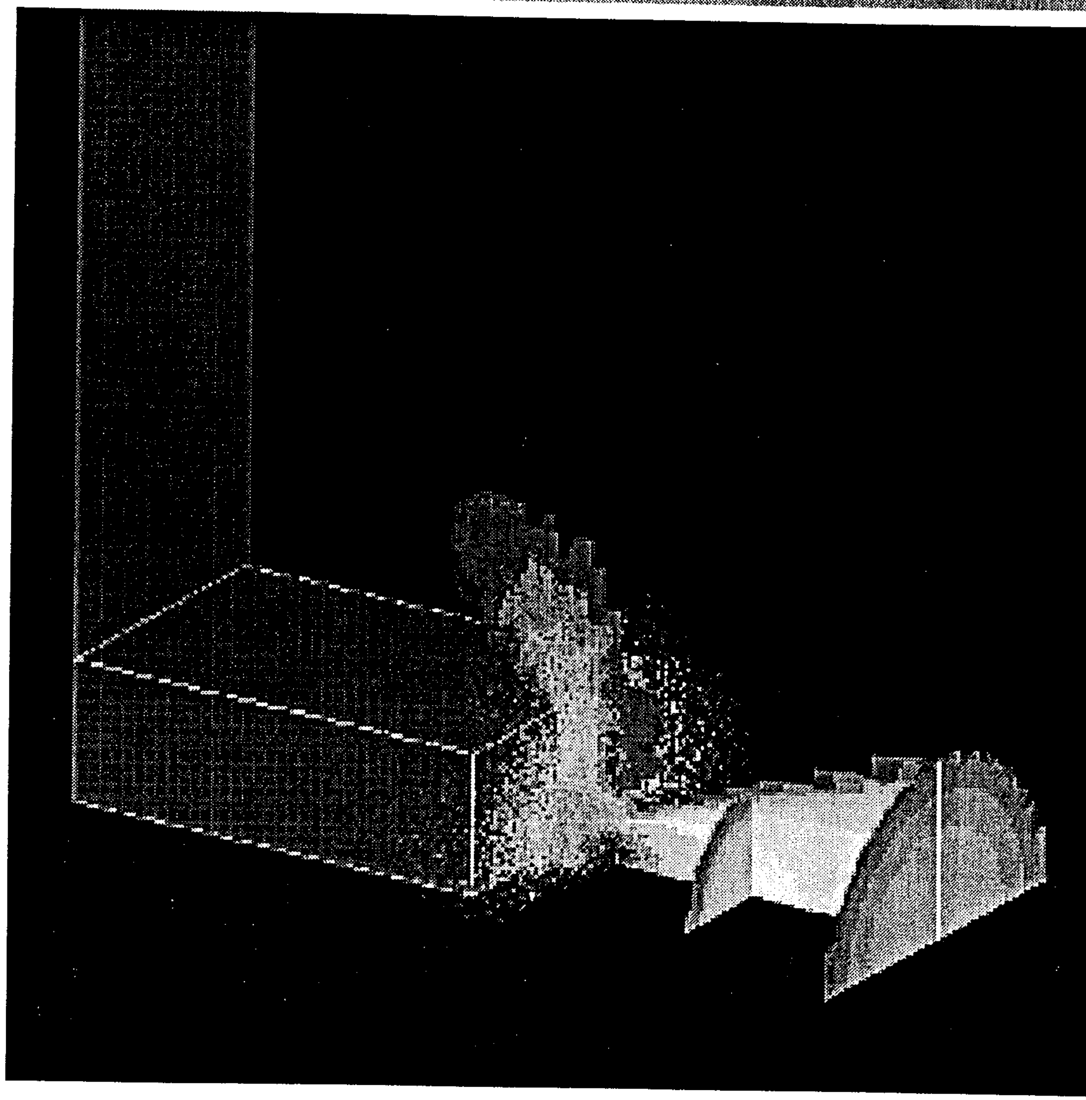
3-D Total Ion Density in Plume with Particles



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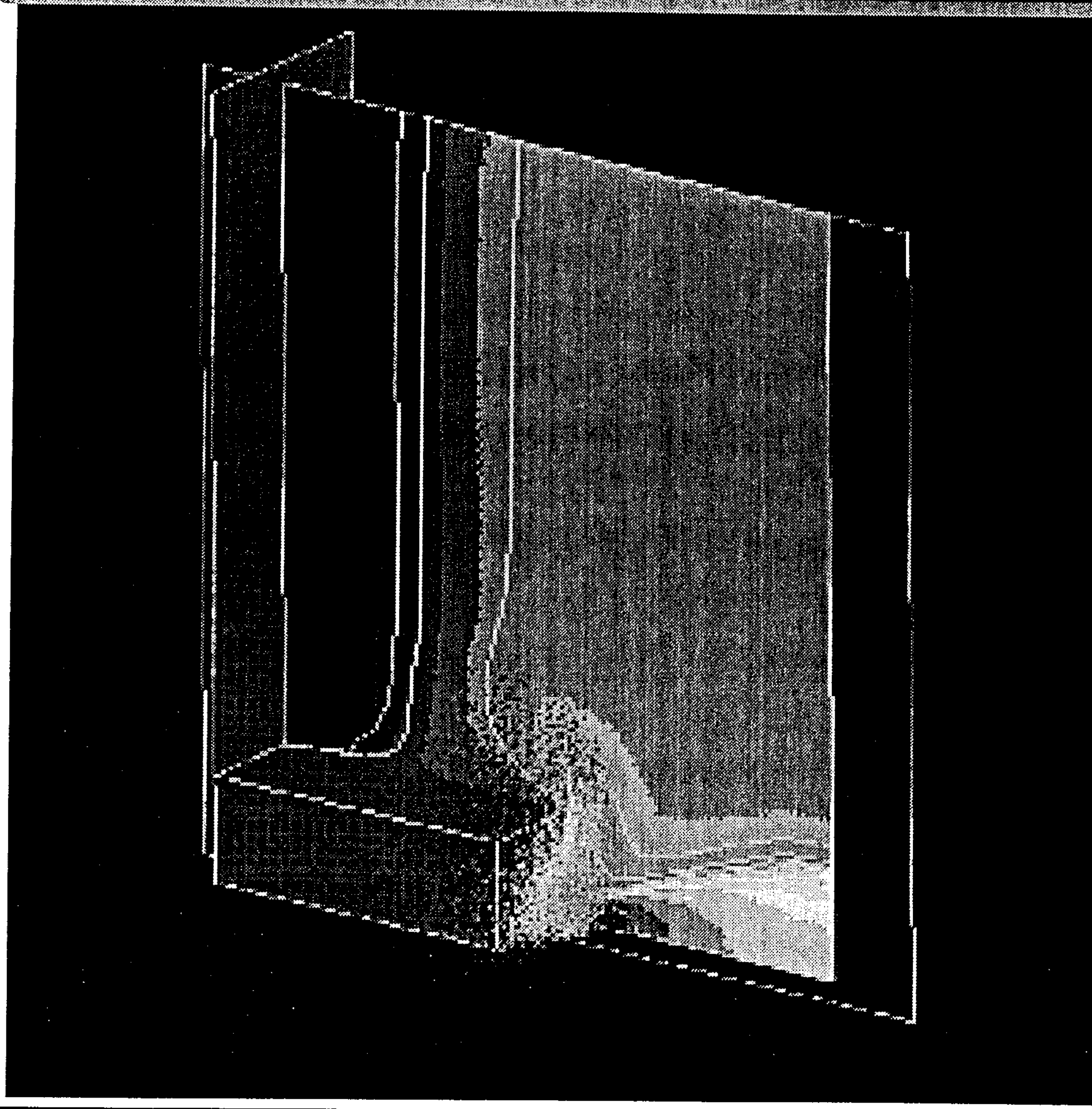
3-D Electric Potential Structure in Plume



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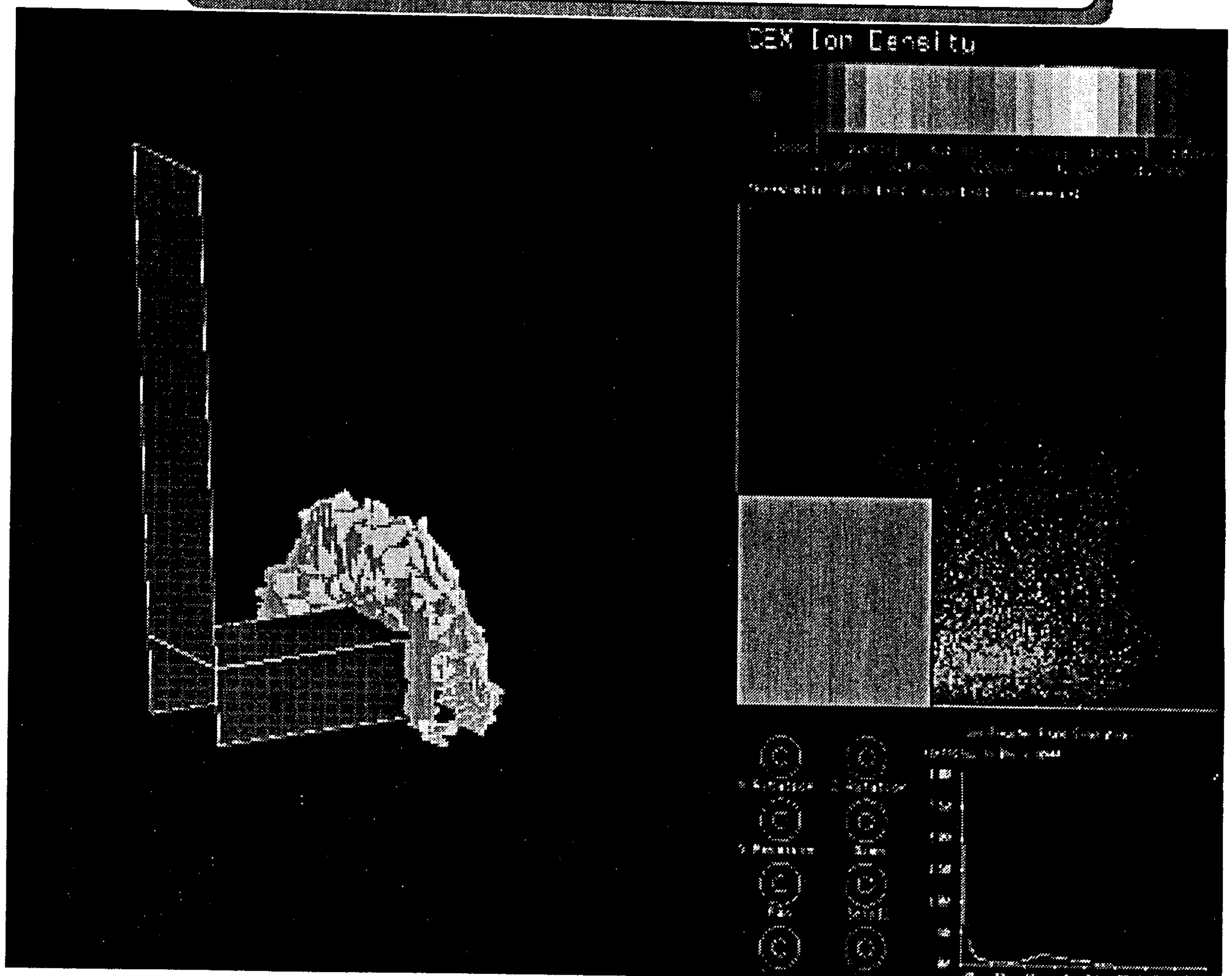
SPPL

3-D CEX Ion Backflow Isosurface with 2-D Particle Positions



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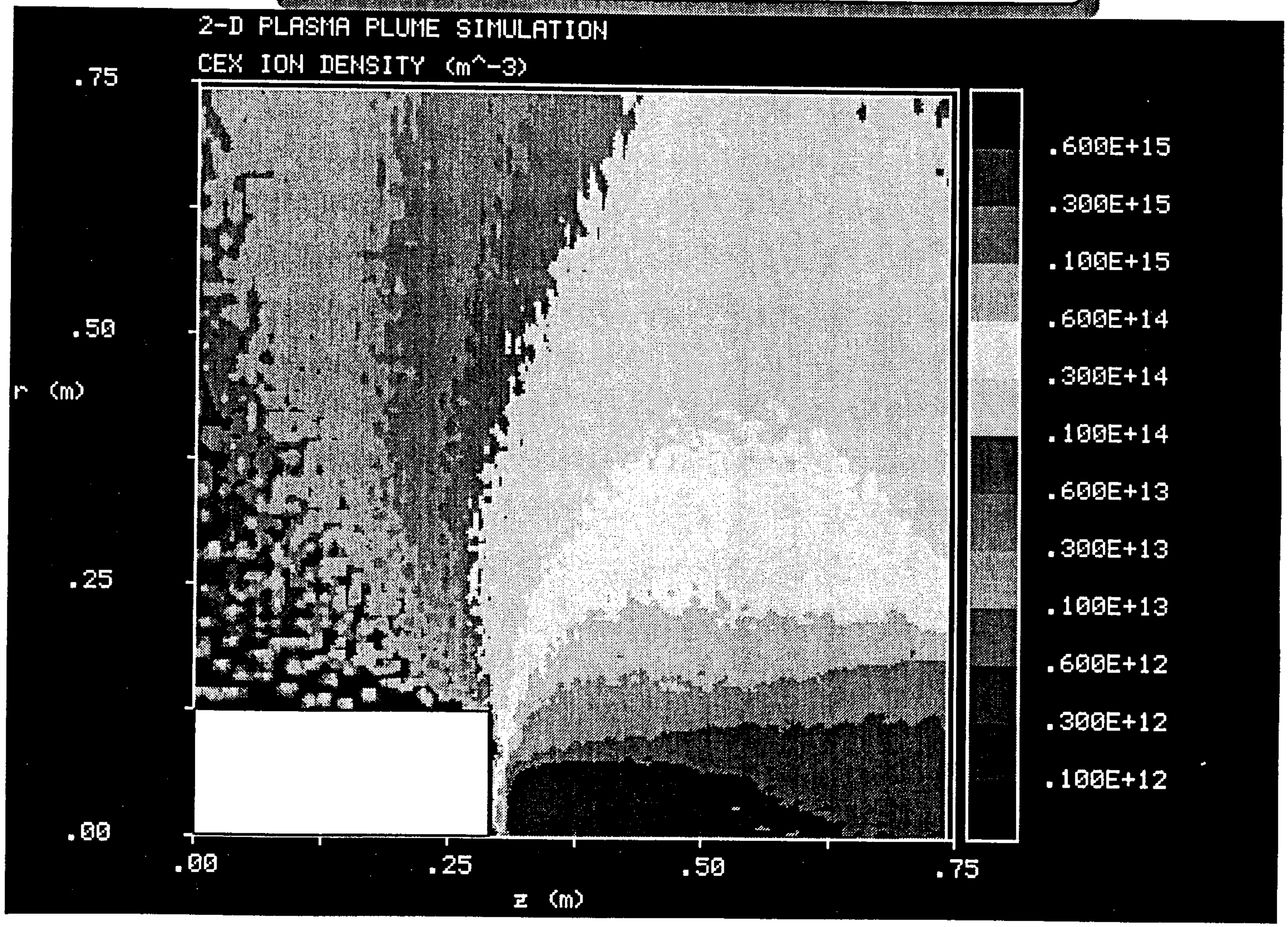
SPPL

2-D CEX Ion Backflow Density



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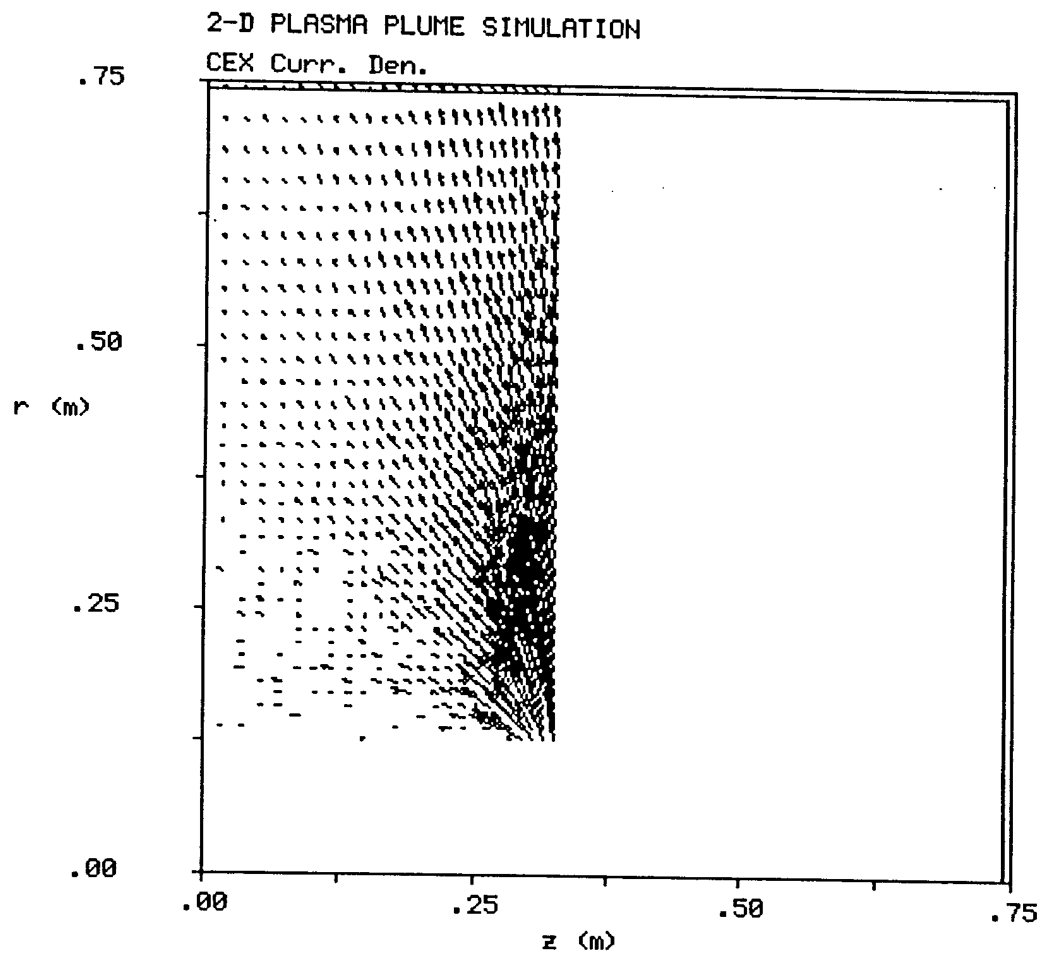
2-D CEX Ion Current Density



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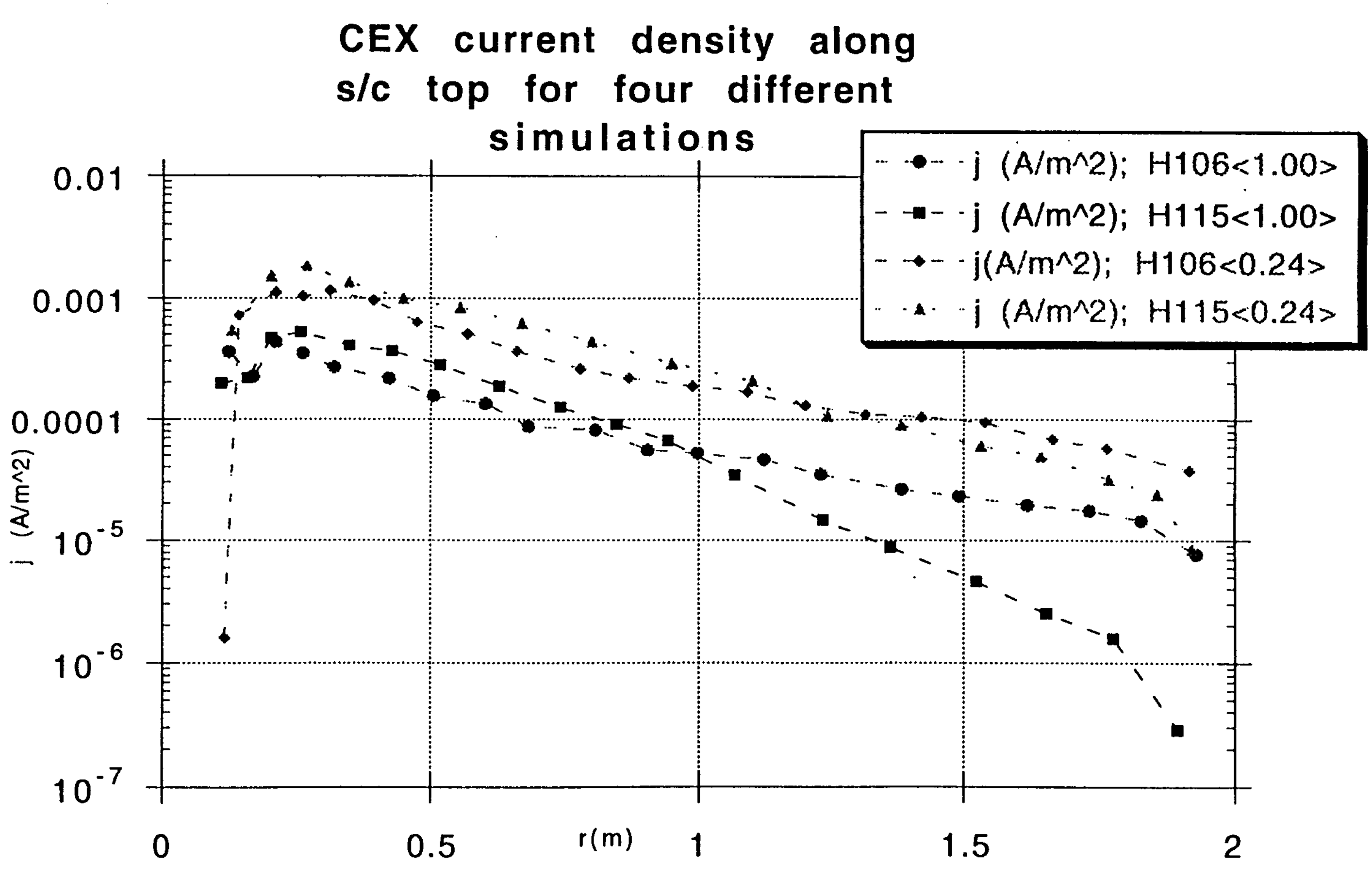
CEX Current Density on S/C Surface Indicates CEX Plasma Dominates Ambient Plasma



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Engineering Impact Issues Learned

- Contamination from EP thrusters is not a show stopper, but it must be included in a careful design of a satellite

- Lack of care can lead to significant changes in thermal radiator properties with concomitant satellite problems

Computational Issues Learned

- Use of a massively parallel computer has been **Enabling** for this large-scale problem
- Use of a development machine such as the Intel Touchstone Delta (512 nodes) has been frustrating due to:

  - lack of available CPU time for debugging and running simulations

  - frequent crashes of the hardware
- Use of the Cray T3D (256 nodes) has led to increased throughput (5x)
- It has been necessary to rethink the problem from the start and work closely with a computer scientist

Future Work

- We have developed a 3-D hybrid PIC code to simulate the plume of an ion thruster
- Detailed parametric studies are underway with Xe as well as C_{60}
- Model Non-Propellant-Efflux (Sputtered Grid Material)
- Effect of CEX plasma on floating SC potential

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Large Scale Data Acquisition and Processing in Turbulent Flows

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LARGE-SCALE DATA ACQUISITION AND PROCESSING IN TURBULENT FLOWS

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Department of Aerospace Engineering
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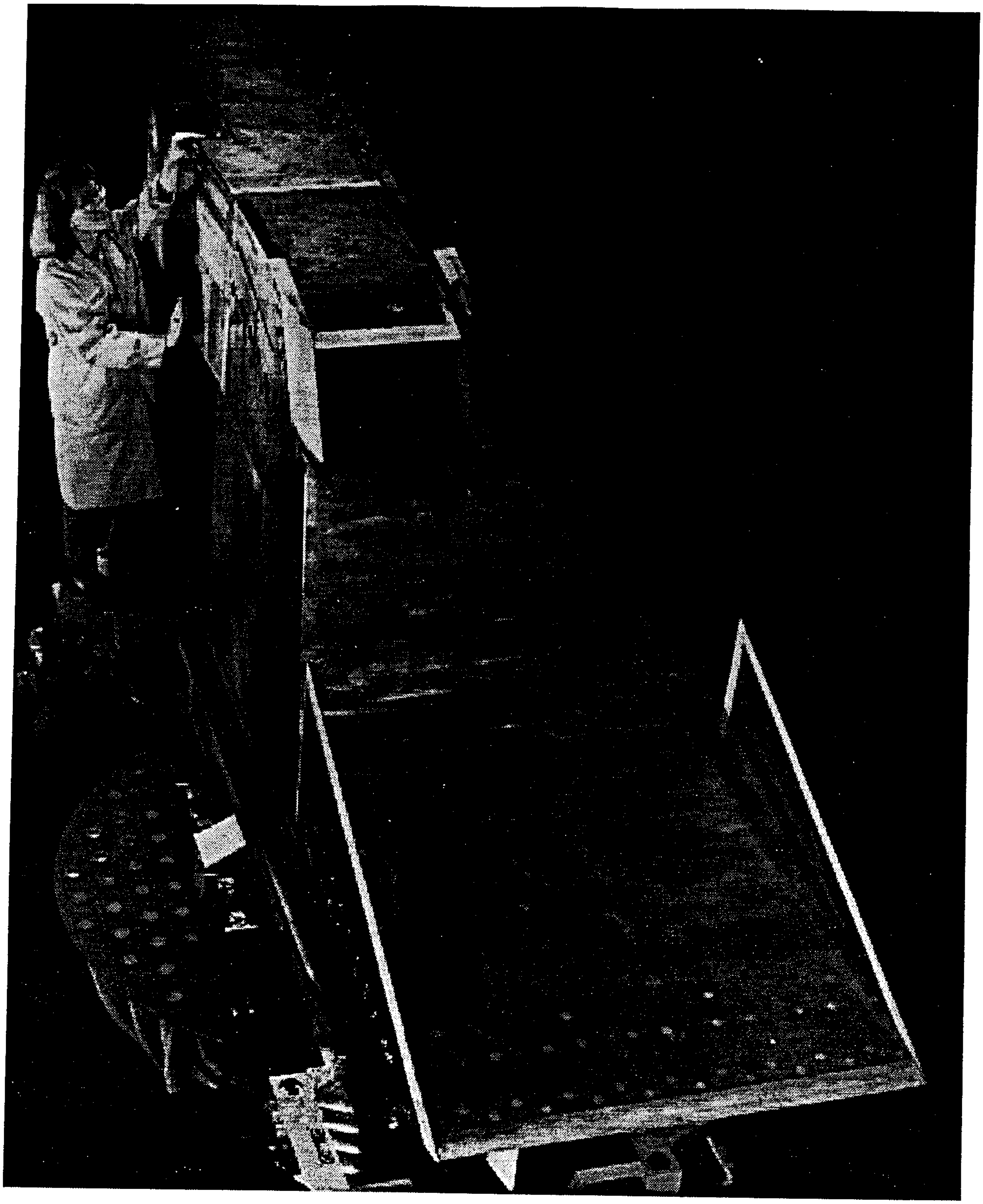
Ann Arbor, MI

Applications of Advanced and Innovative Computational Methods to Defense Science and Engineering

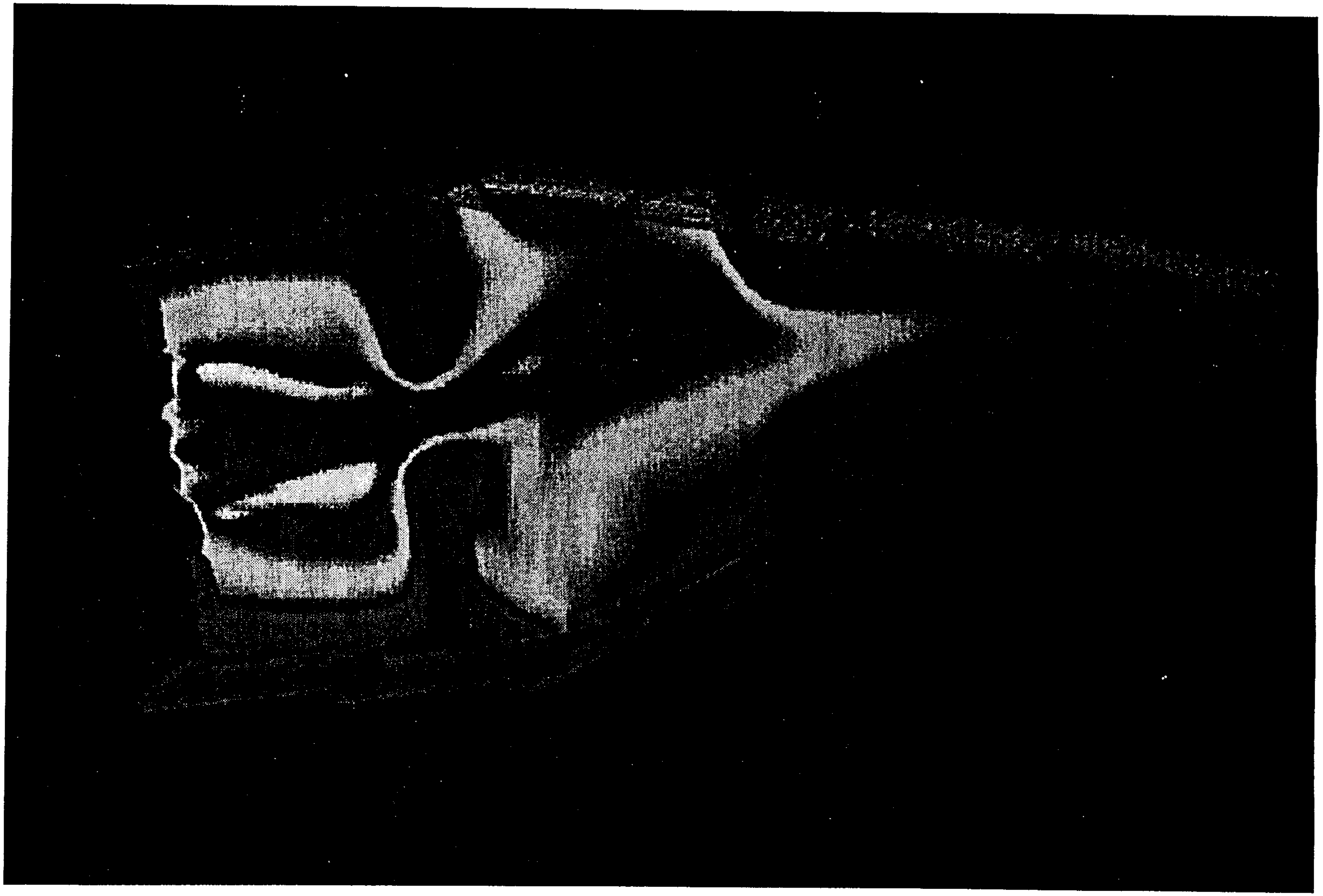
DSSG Alumni Symposium

October 31 – November 2
Institute for Defense Analyses

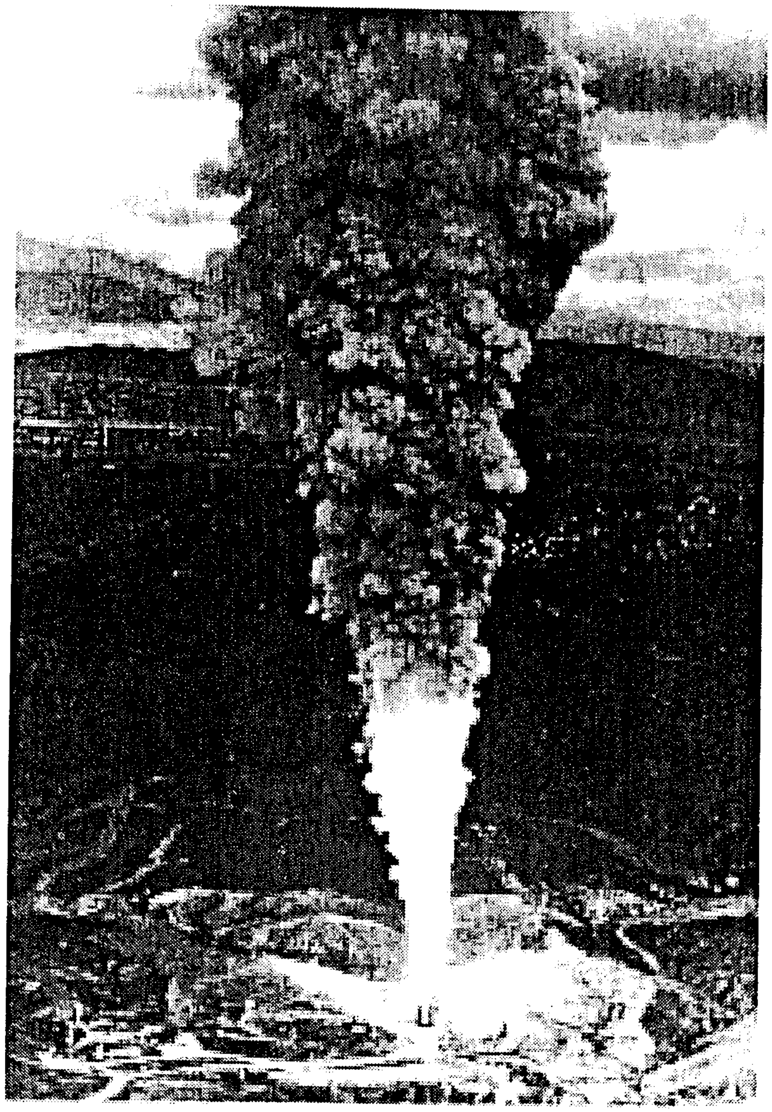
Scramjet Combustor Development



Aircraft Engine Emissions Reduction



Turbulent Shear Flows: Inner and Outer Scales



- Velocity Field $\underline{\mathbf{u}}(\underline{\mathbf{x}},t)$
- Conserved Scalar Field $\zeta(\underline{\mathbf{x}},t)$

- Outer scales are flow-specific
- Inner scales are <u>universal</u>

- Outer length scale δ
- Inner length scale λ

- Outer time scale (δ/u)
- Inner length scale (λ^2/ν)

- Outer scale Reynolds number

$$Re_\delta \equiv \left[\frac{u\,\delta}{\nu}\right]$$

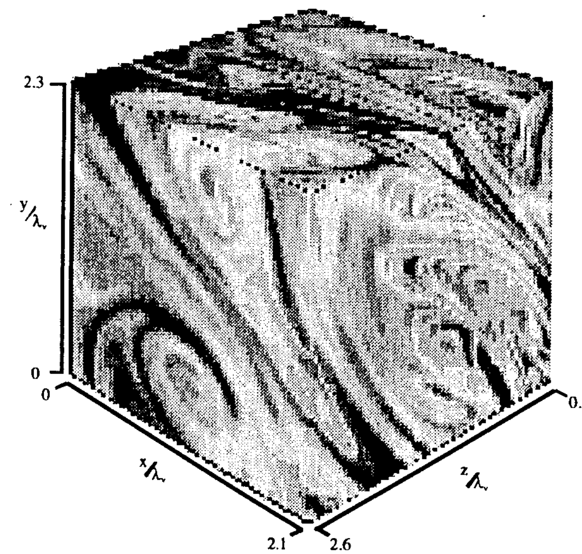
Microscales: Reynolds Number Scaling

- **Inner Scales**
  - **Length :** $\lambda \equiv$ **diffusion length scale**

    $$\lambda \sim \delta \cdot Re_\delta^{-3/4} Sc^{-1/2}$$

  - **Time :** $\tau \equiv$ **diffusion time scale**

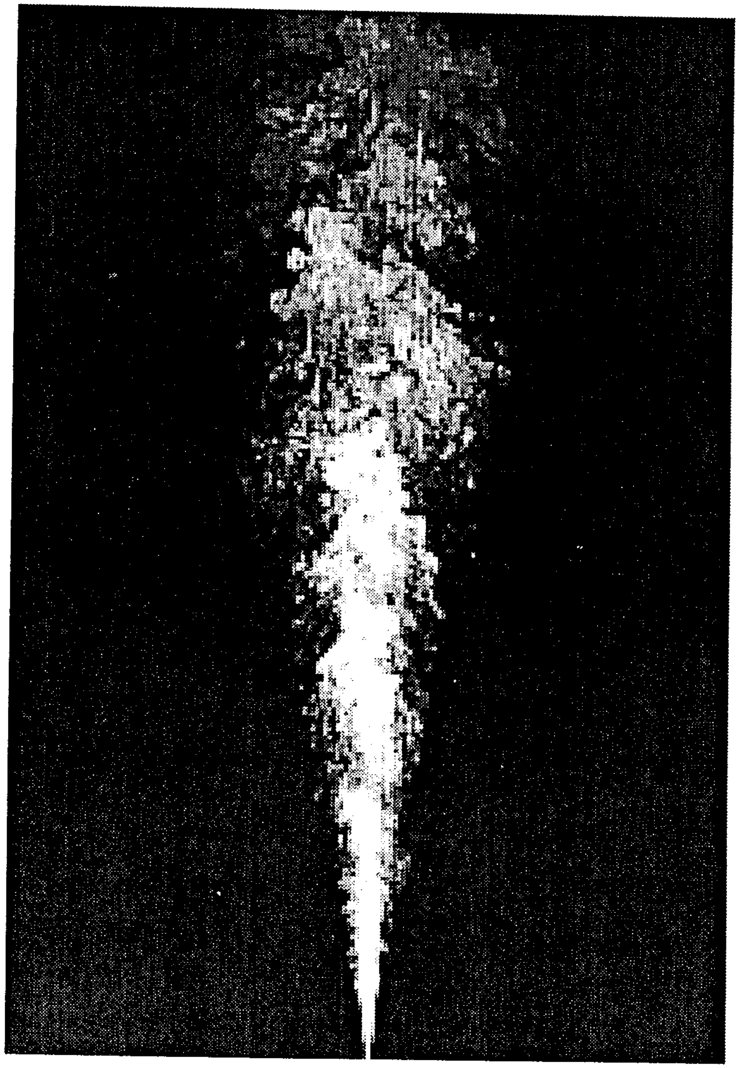
    $$\tau \sim (\delta/u) \cdot Re_\delta^{-1/2} Sc^{-1}$$

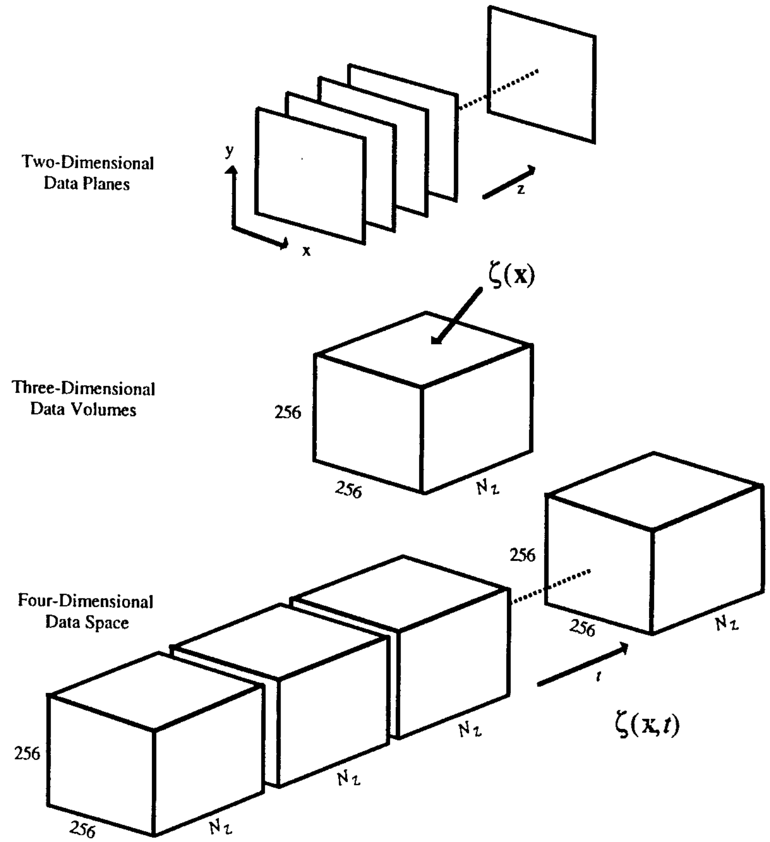


- **Space-Time Dynamic Range**
  - $$N_\lambda \sim \left(\frac{outer\ scale}{inner\ scale}\right)^3 \sim Re_\delta^{9/4} Sc^{3/2}$$
  - $$N_\tau \sim \left(\frac{outer\ scale}{inner\ scale}\right) \sim Re_\delta^{1/2} Sc$$

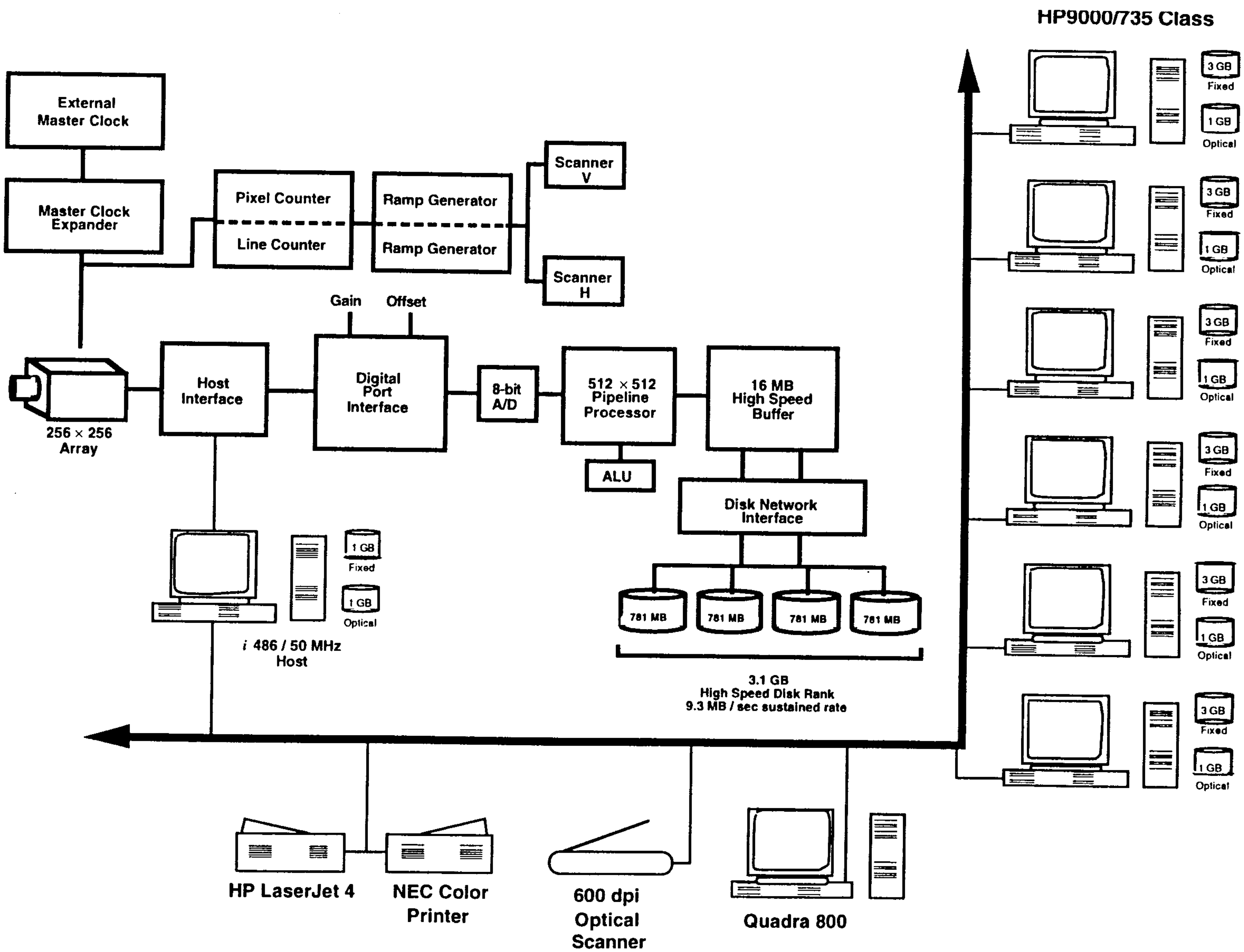
Re_δ	N_λ	N_τ	N
10^8	10^{18}	10^4	10^{22}
10^6	10^{13}	10^3	10^{16}
10^4	10^9	10^2	10^{11}

Four-Dimensional (*x-y-z-t*) Turbulence Measurements

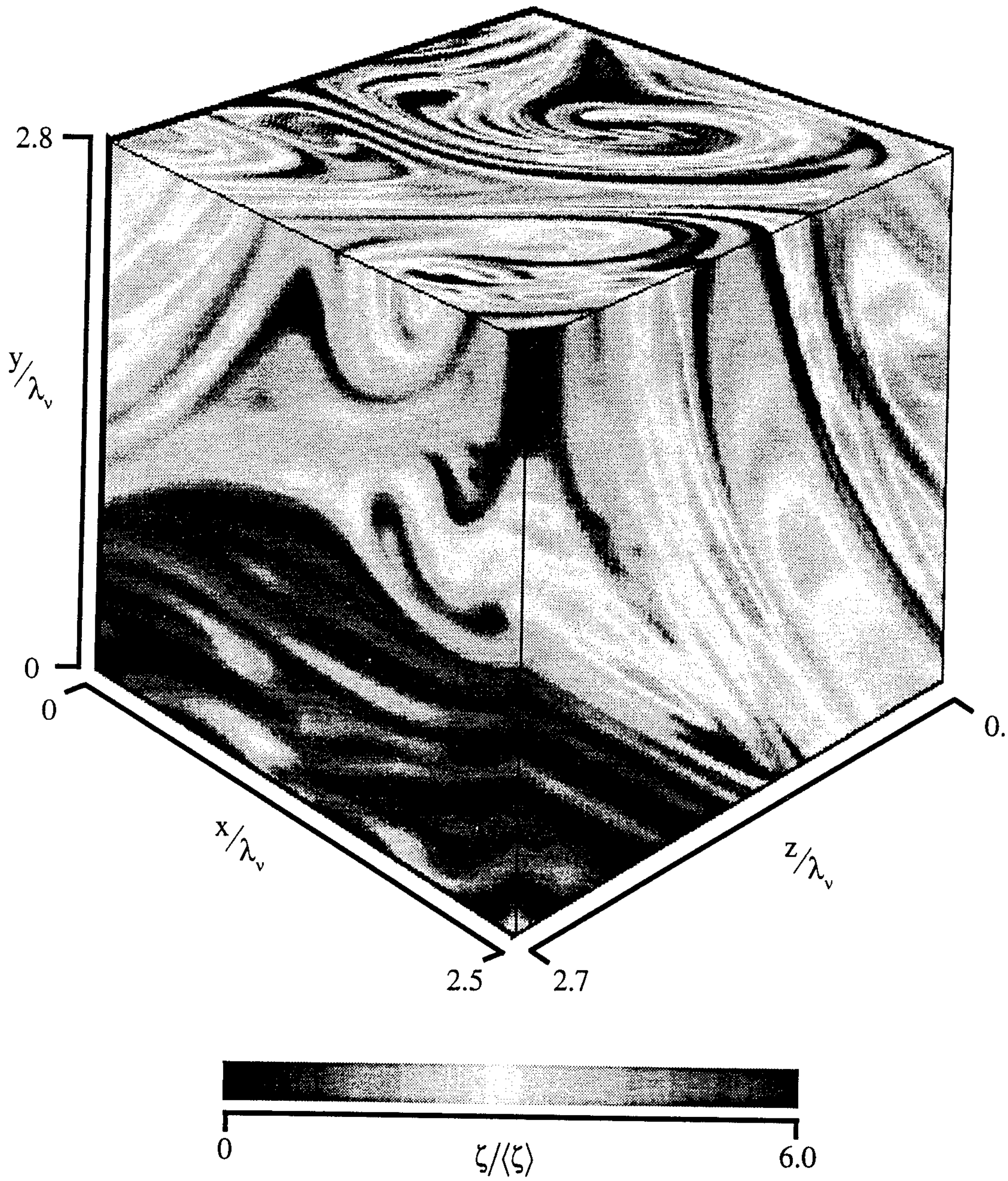




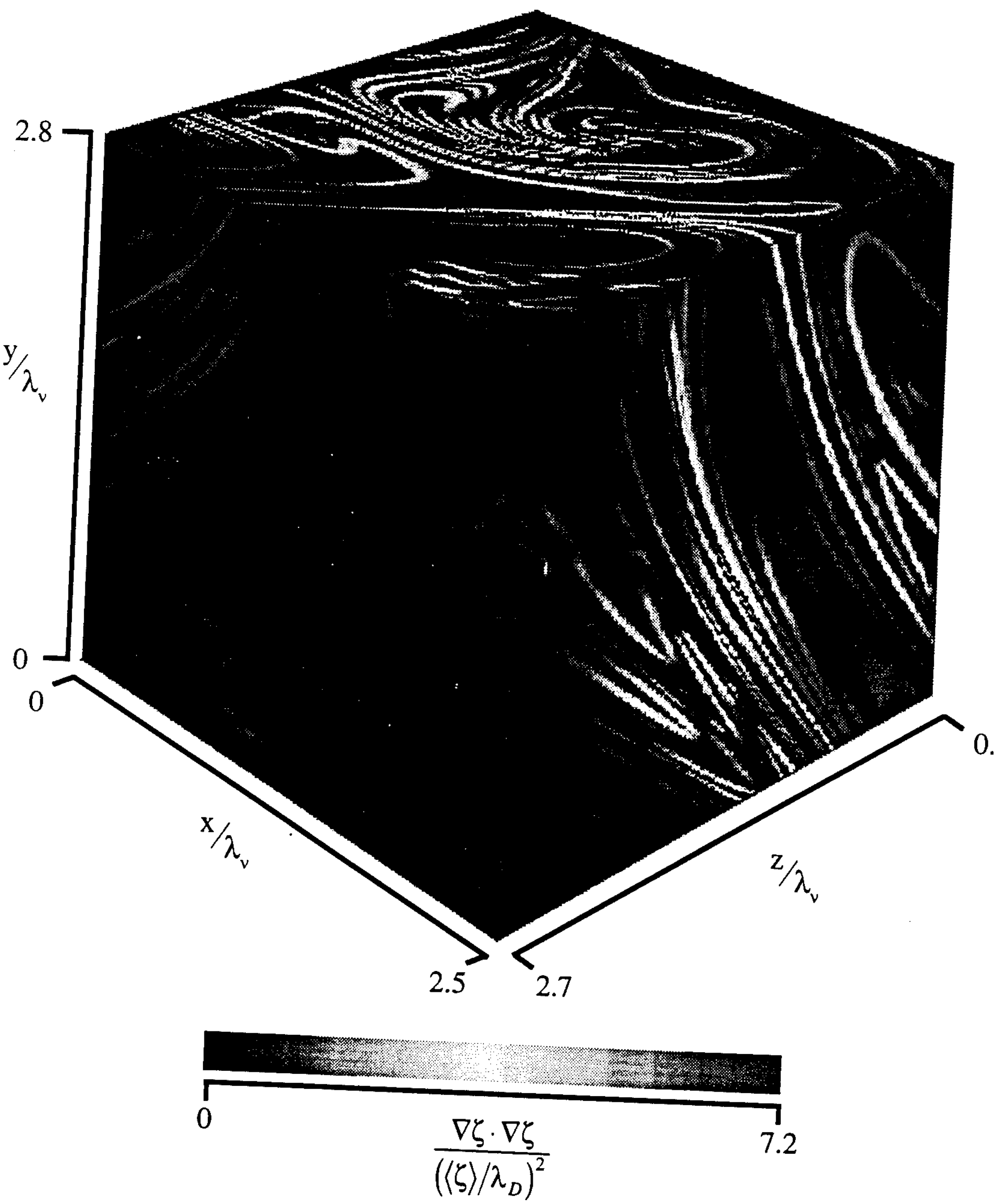
Four-Dimensional Spatio-Temporal LIF Imaging



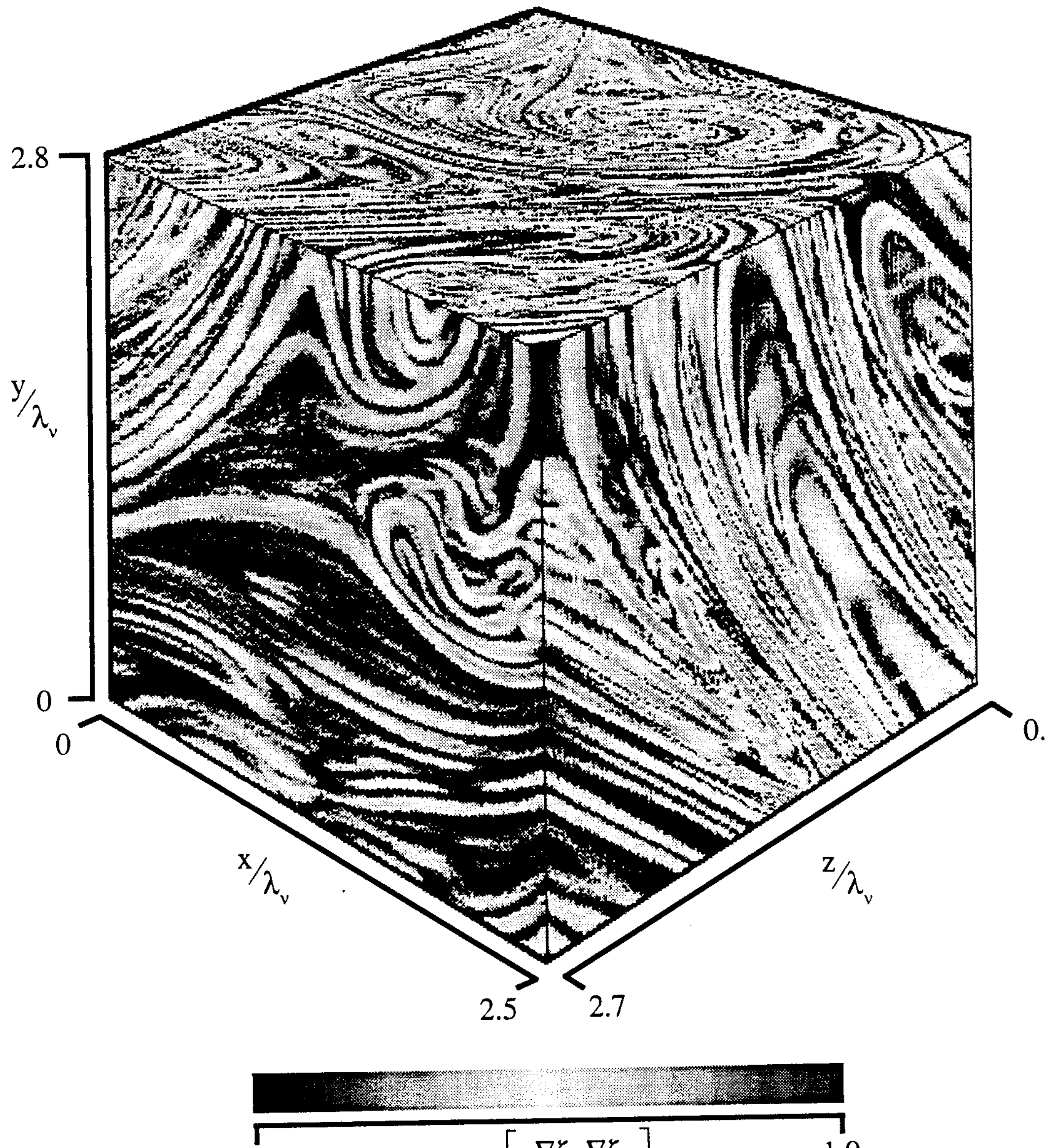
Conserved Scalar Measurement $\zeta(\underline{x},t)$ (256^3)



Scalar Energy Dissipation Field $\nabla\zeta \cdot \nabla\zeta(\underline{\mathbf{x}},t)$

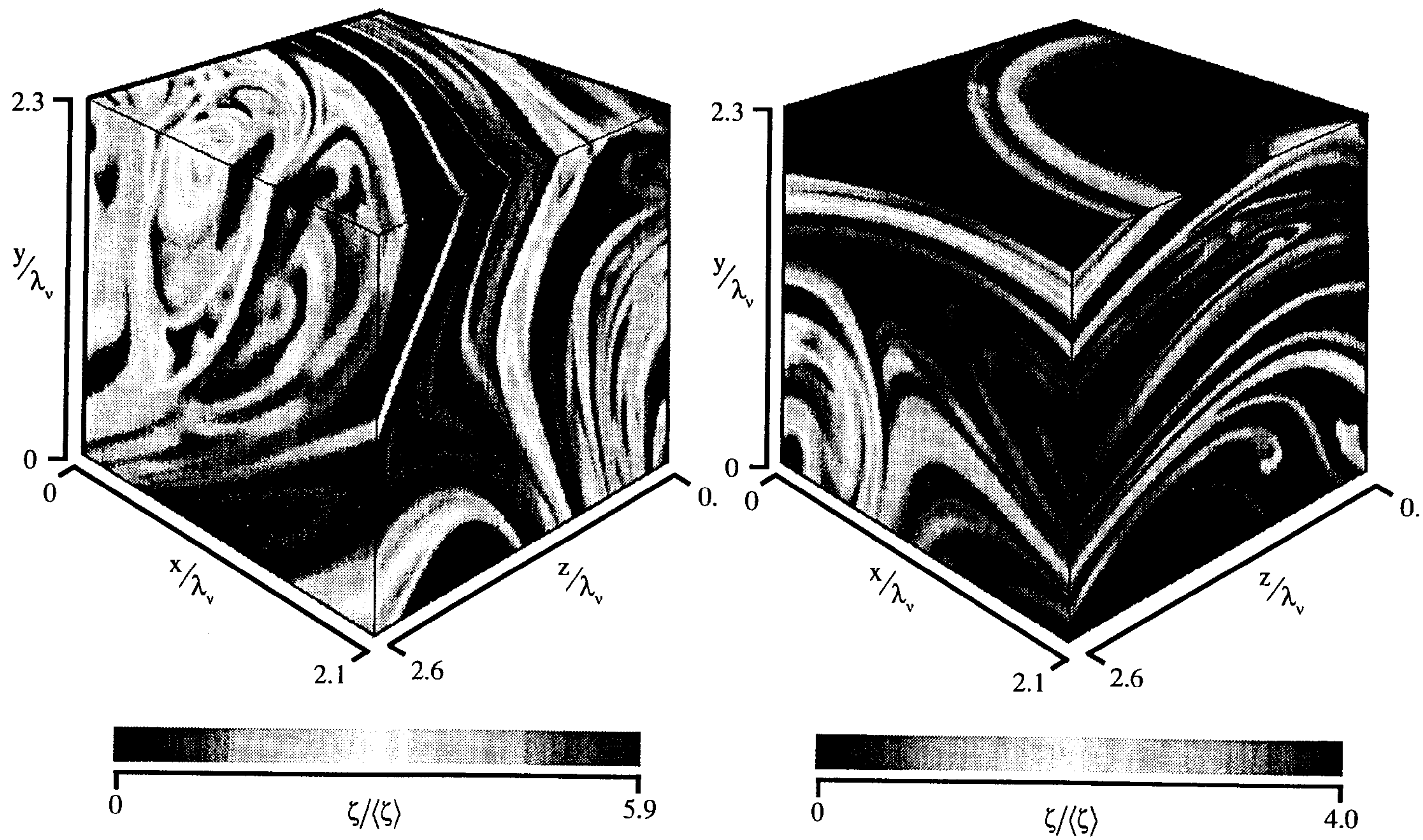


Scalar Energy Dissipation Field $log \nabla\zeta \cdot \nabla\zeta(\underline{\mathbf{x}},t)$

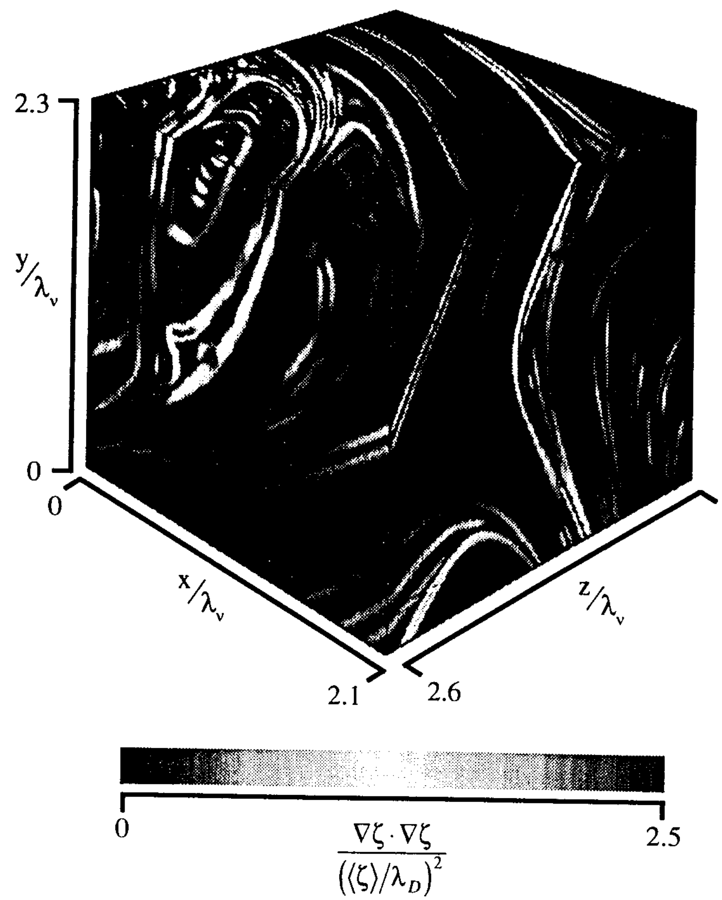


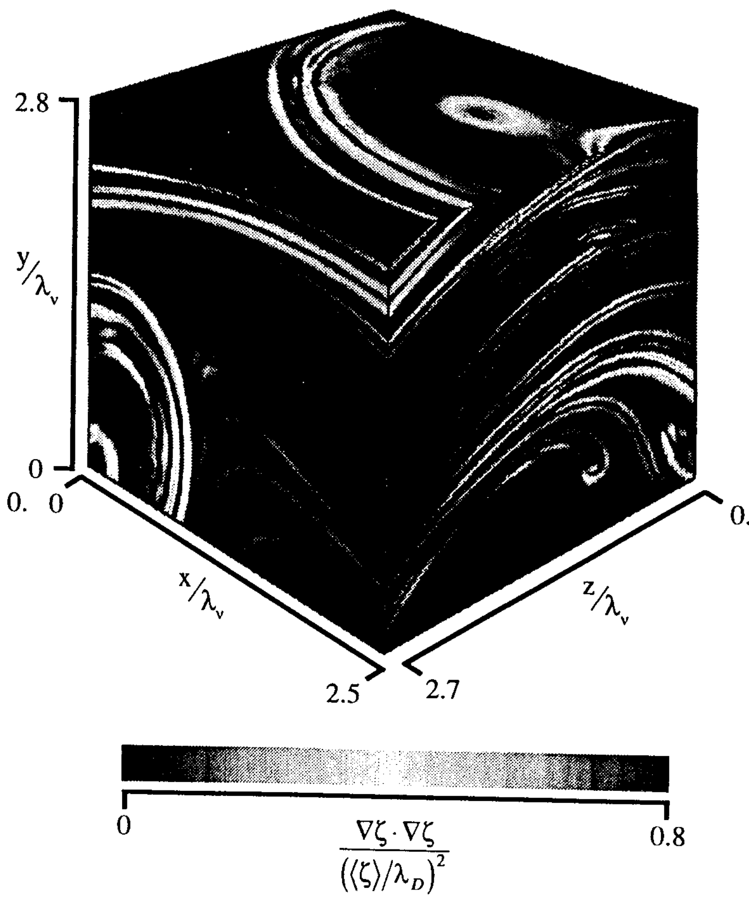
$\log_{10}\left[\frac{\nabla\zeta \cdot \nabla\zeta}{(\langle\zeta\rangle/\lambda_D)^2}\right]$

Conserved Scalar Measurement $\zeta(\underline{x},t)$ (256^3)

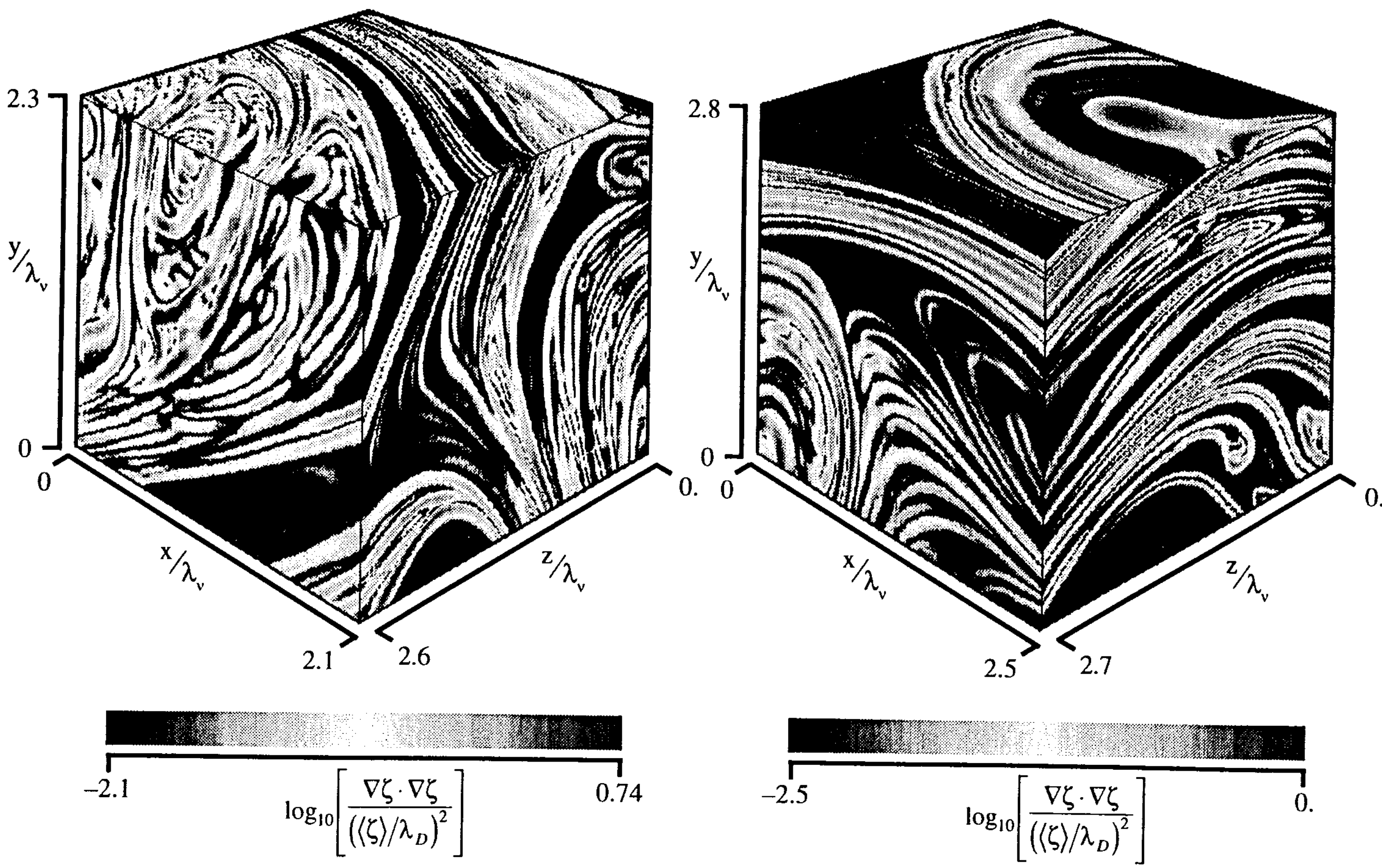


Scalar Energy Dissipation Field $\nabla\zeta \cdot \nabla\zeta(\underline{\mathbf{x}},t)$





Scalar Energy Dissipation Field $log \nabla\zeta \cdot \nabla\zeta(\underline{\mathbf{x}},t)$



Scalar Imaging Velocimetry (SIV)

Solution of an inverse problem gives the velocities $\underline{\mathbf{u}}(\underline{\mathbf{x}},t)$ from fully-resolved measurements of the scalar field $\zeta(\underline{\mathbf{x}},t)$

Variational formulation:

$$E_1 = \left(\frac{\partial}{\partial t} + \underline{\mathbf{u}} \cdot \nabla - \frac{1}{ReSc} \nabla^2 \right) \zeta(\underline{\mathbf{x}},t)$$

$$E_2 = \nabla \cdot \underline{\mathbf{u}}$$

$$E_3 = \nabla \underline{\mathbf{u}} : \nabla \underline{\mathbf{u}}$$

$$E^2 \equiv \iiint_{\underline{\mathbf{x}}} \left(E_1^2 + \alpha^2 E_2^2 + \beta^2 E_3^2 \right) \, d^3 \underline{\mathbf{x}}$$

Minimizing E^2 requires

$$\frac{\partial}{\partial u}\left(E^2\right) = 0 \quad \frac{\partial}{\partial v}\left(E^2\right) = 0 \quad \frac{\partial}{\partial w}\left(E^2\right) = 0$$

Scalar Imaging Velocimetry (SIV)

Discretizing in space puts these in matrix form as

$$\underline{\underline{\mathbf{A}}}\,\underline{\mathbf{u}} = \underline{\mathbf{b}}$$

$$\left.\begin{matrix}\underline{\underline{\mathbf{A}}} \\ \underline{\mathbf{b}}\end{matrix}\right\} \text{ elements are } \quad \frac{\partial \zeta}{\partial t}, \quad \frac{\partial \zeta}{\partial x_i}, \quad \frac{\partial^2 \zeta}{\partial x_i \partial x_j}$$

$256 \times 256 \times$ N volumes $\times$ 3 components requires

$\underline{\mathbf{b}}$ is 196,608 $\times$ N elements long

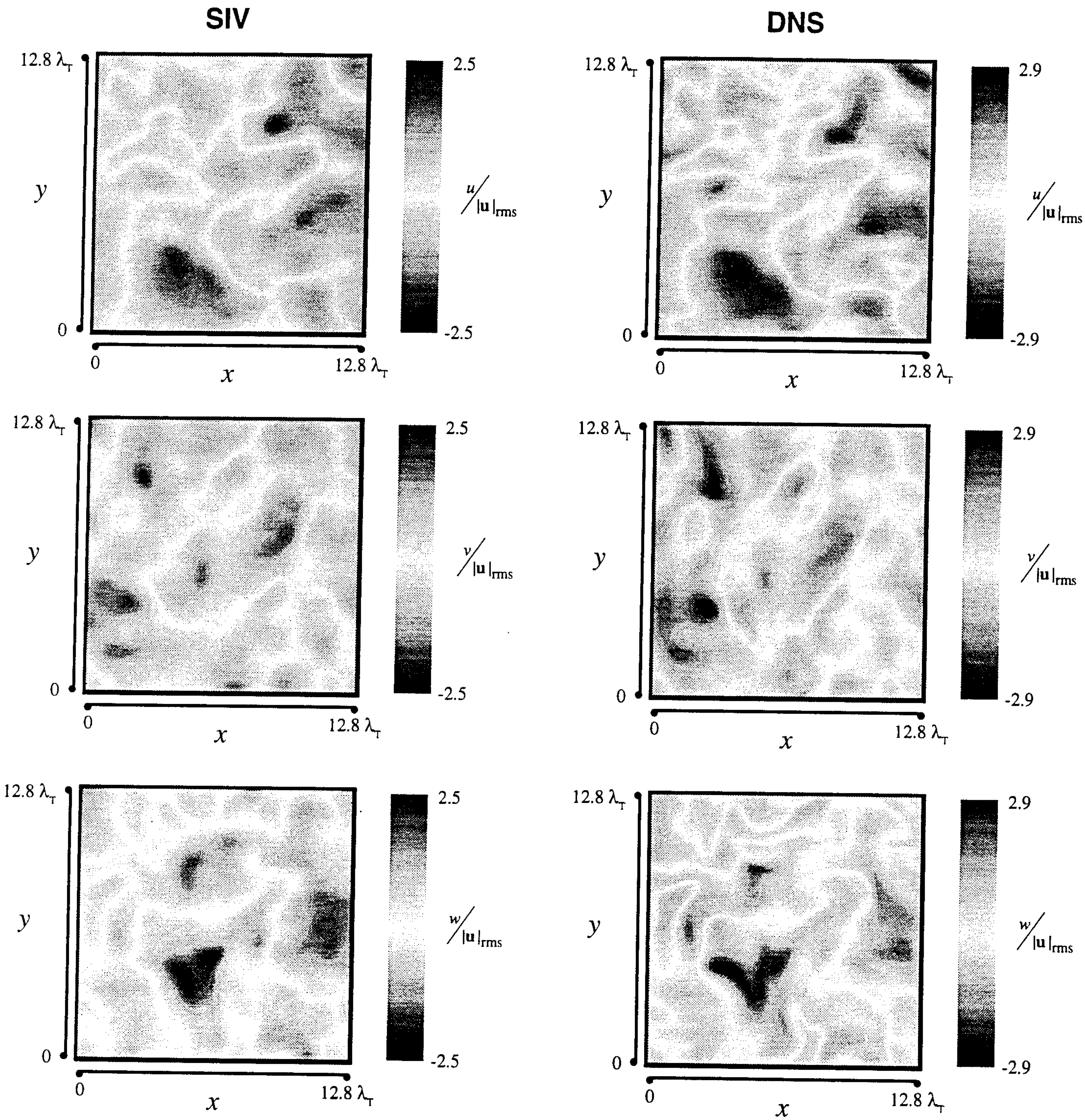
$\underline{\underline{\mathbf{A}}}$ is $3.87(10^{10}) \times N^2$ elements large

Direct solutions methods are out of the question

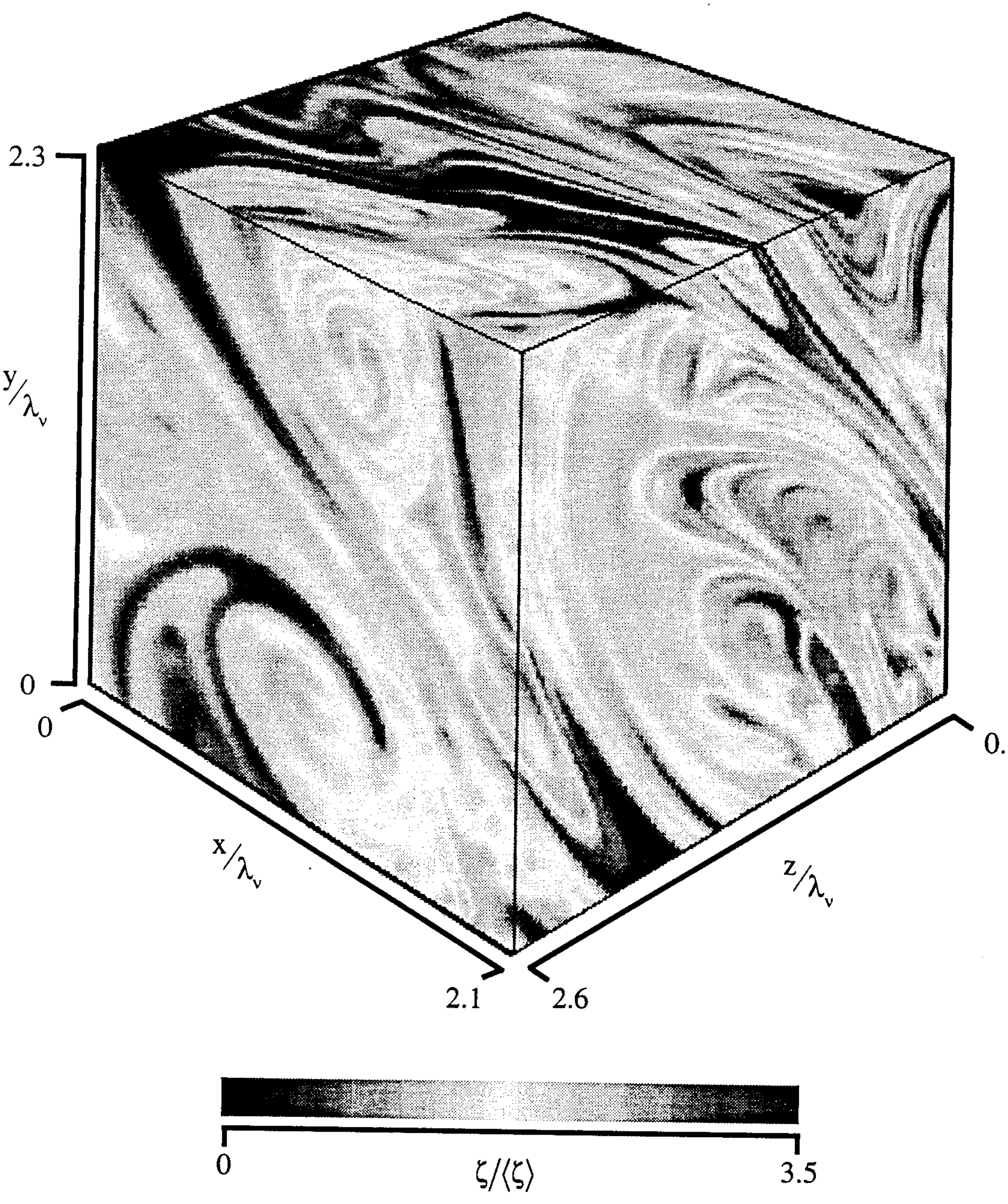
Linear Iterative methods are used

Diagonal dominance requirement restricts (α, β)

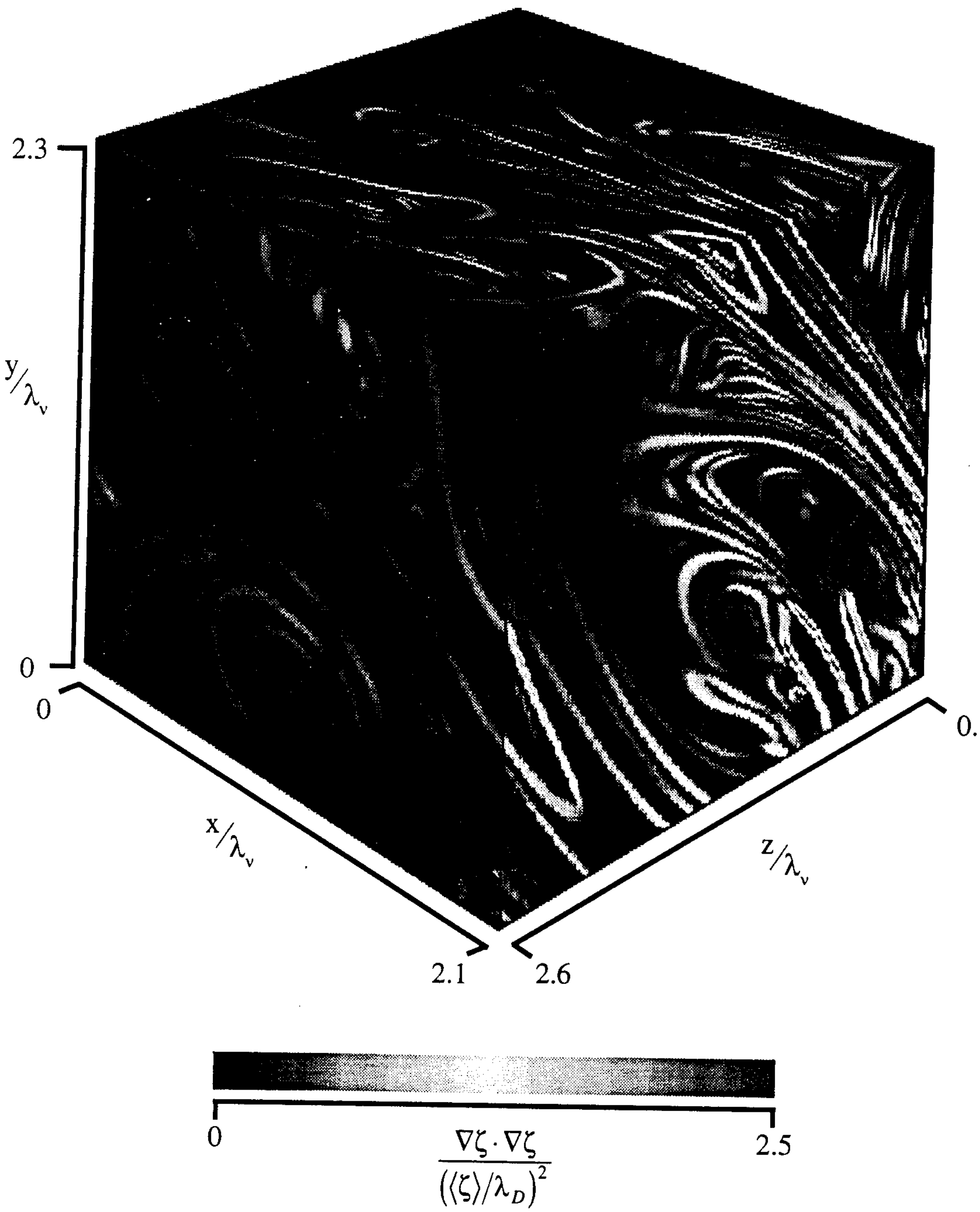
SIV / DNS Validation Study



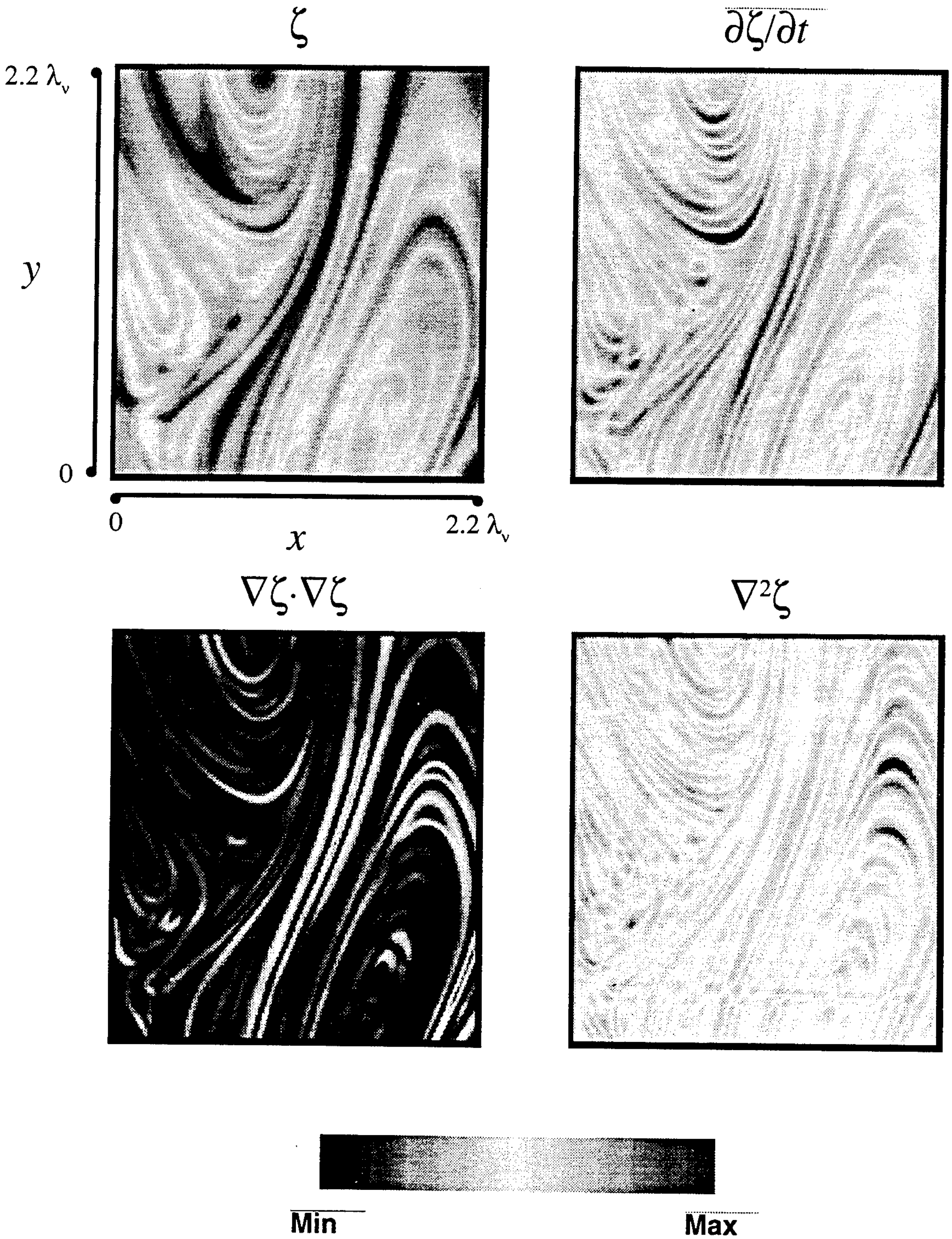
Conserved Scalar Measurement $\zeta(\underline{\mathbf{x}},t)$ (256³)



Scalar Energy Dissipation Field $\nabla\zeta\cdot\nabla\zeta(\underline{\mathbf{x}},t)$

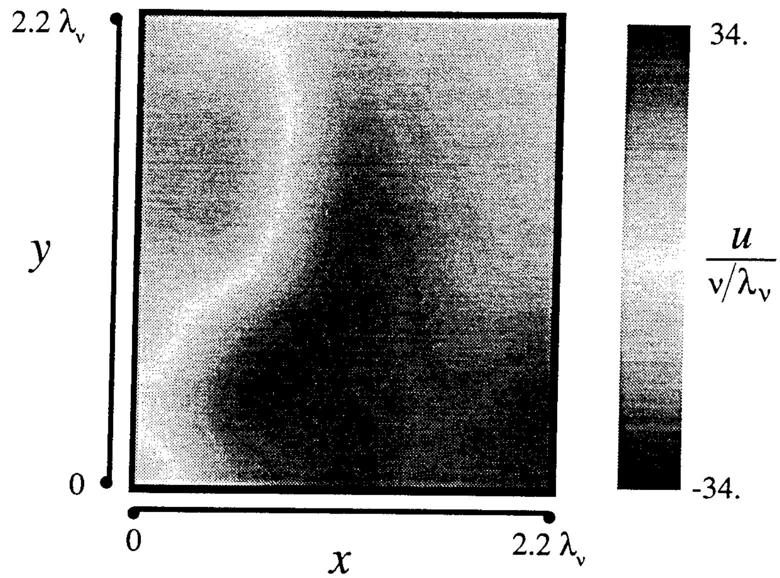


Scalar Imaging Velocimetry Measurements

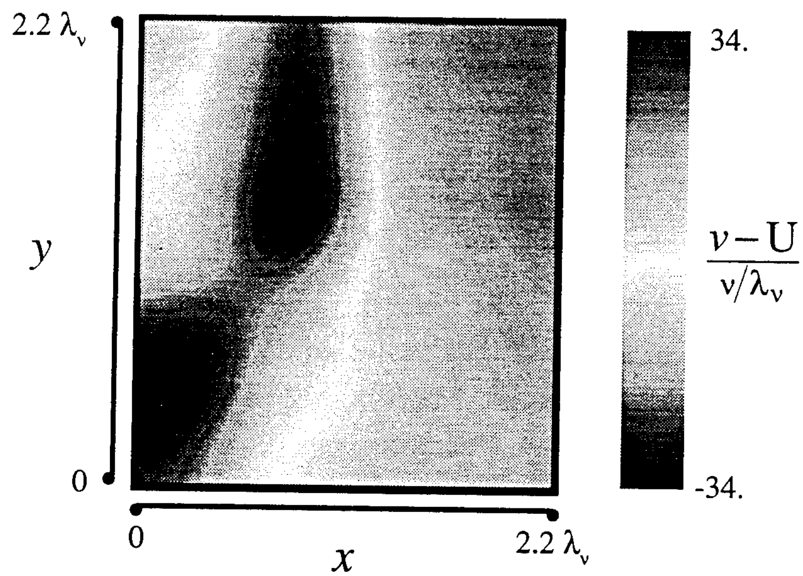


Scalar Imaging Velocimetry Computations

u

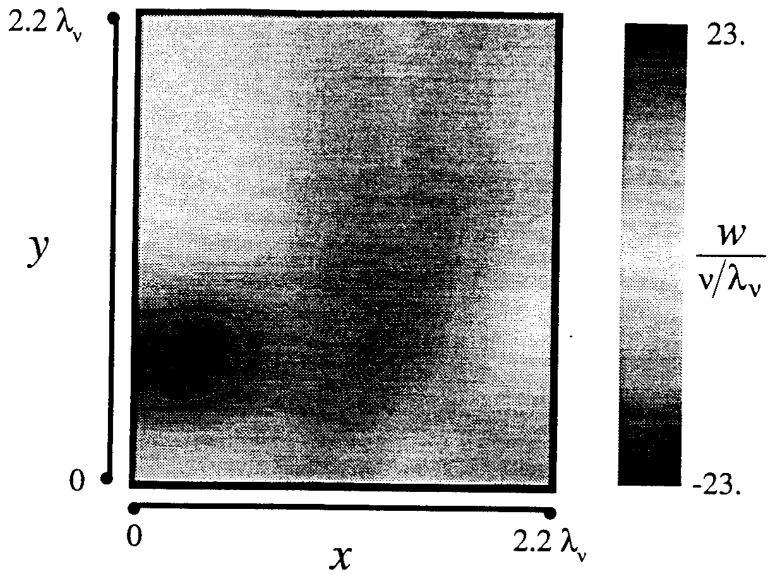


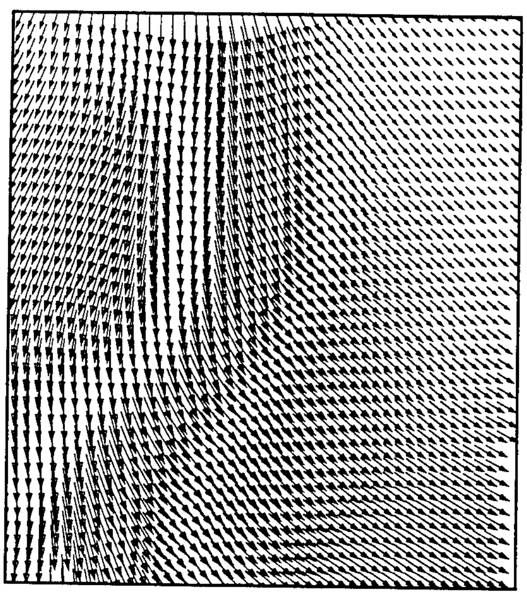
v



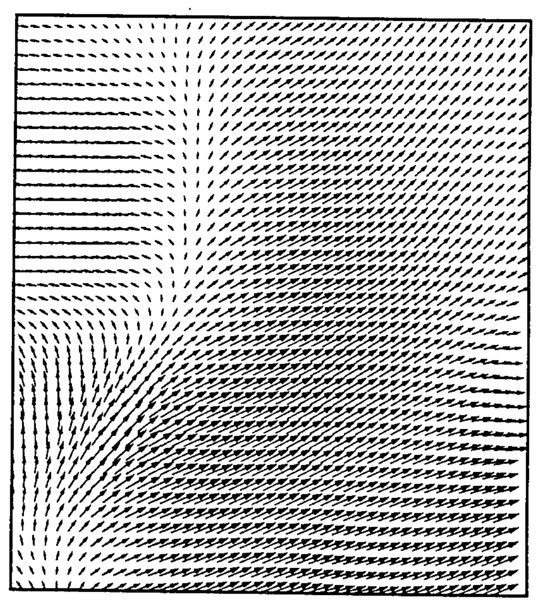
Scalar Imaging Velocimetry Computations

W

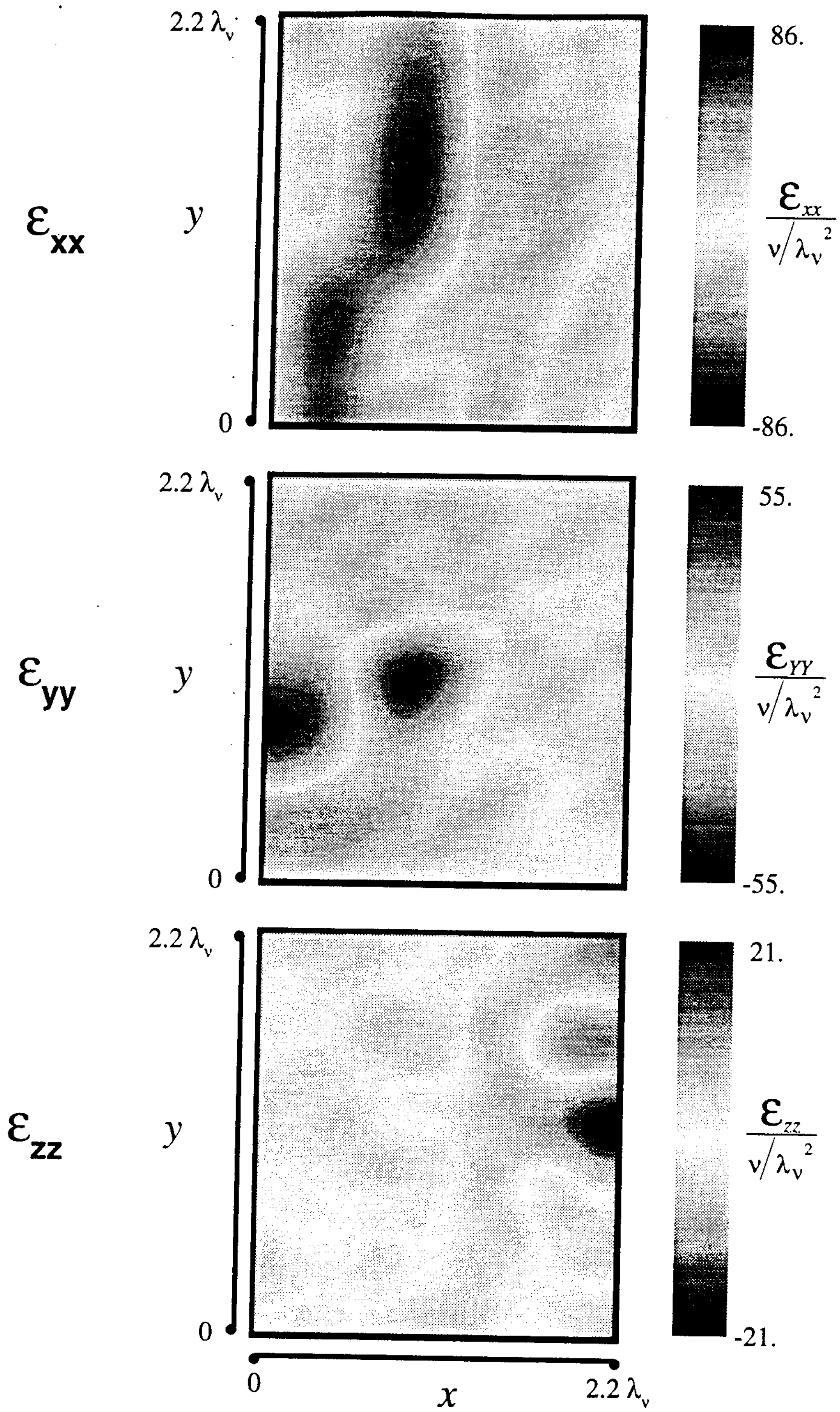




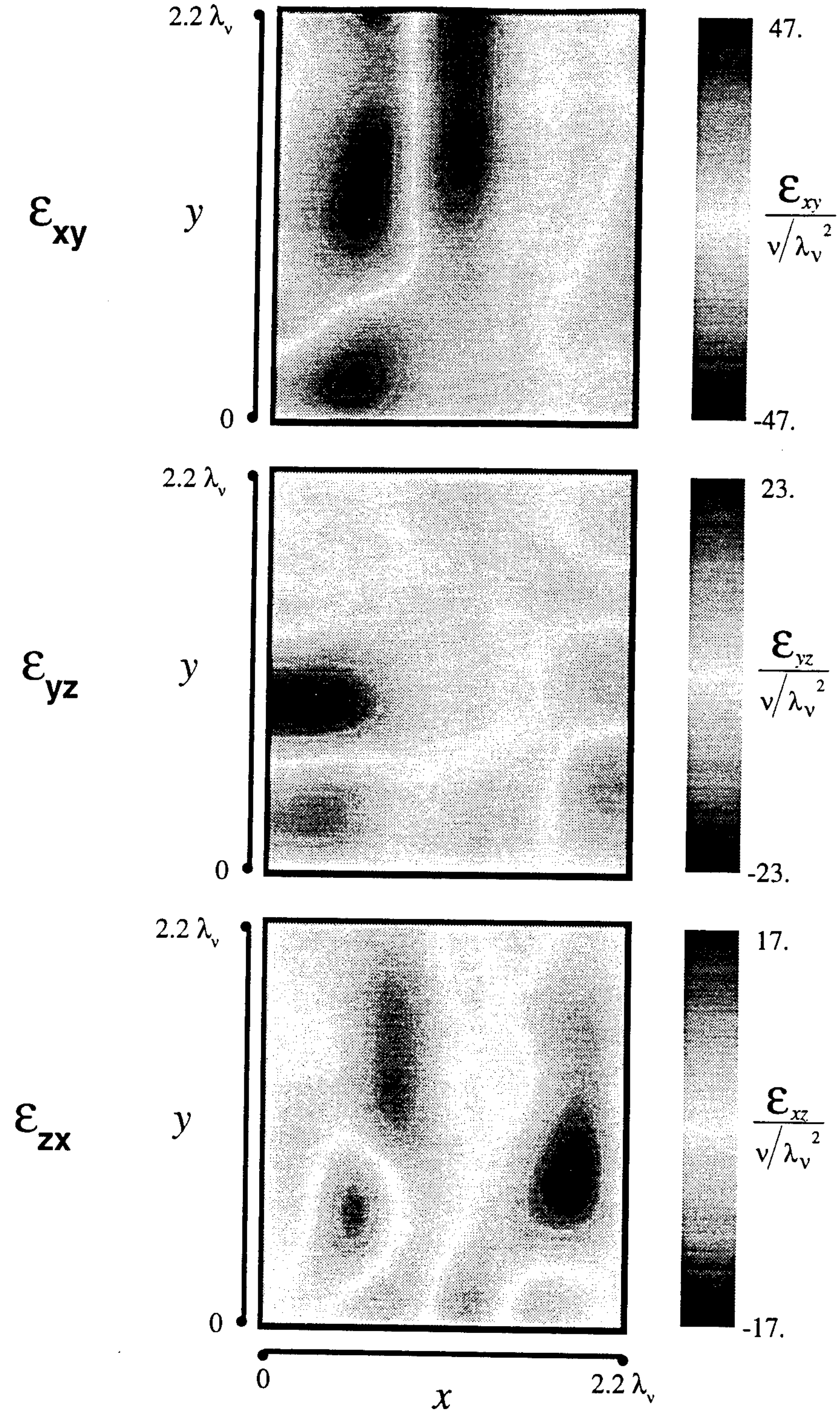
u-v

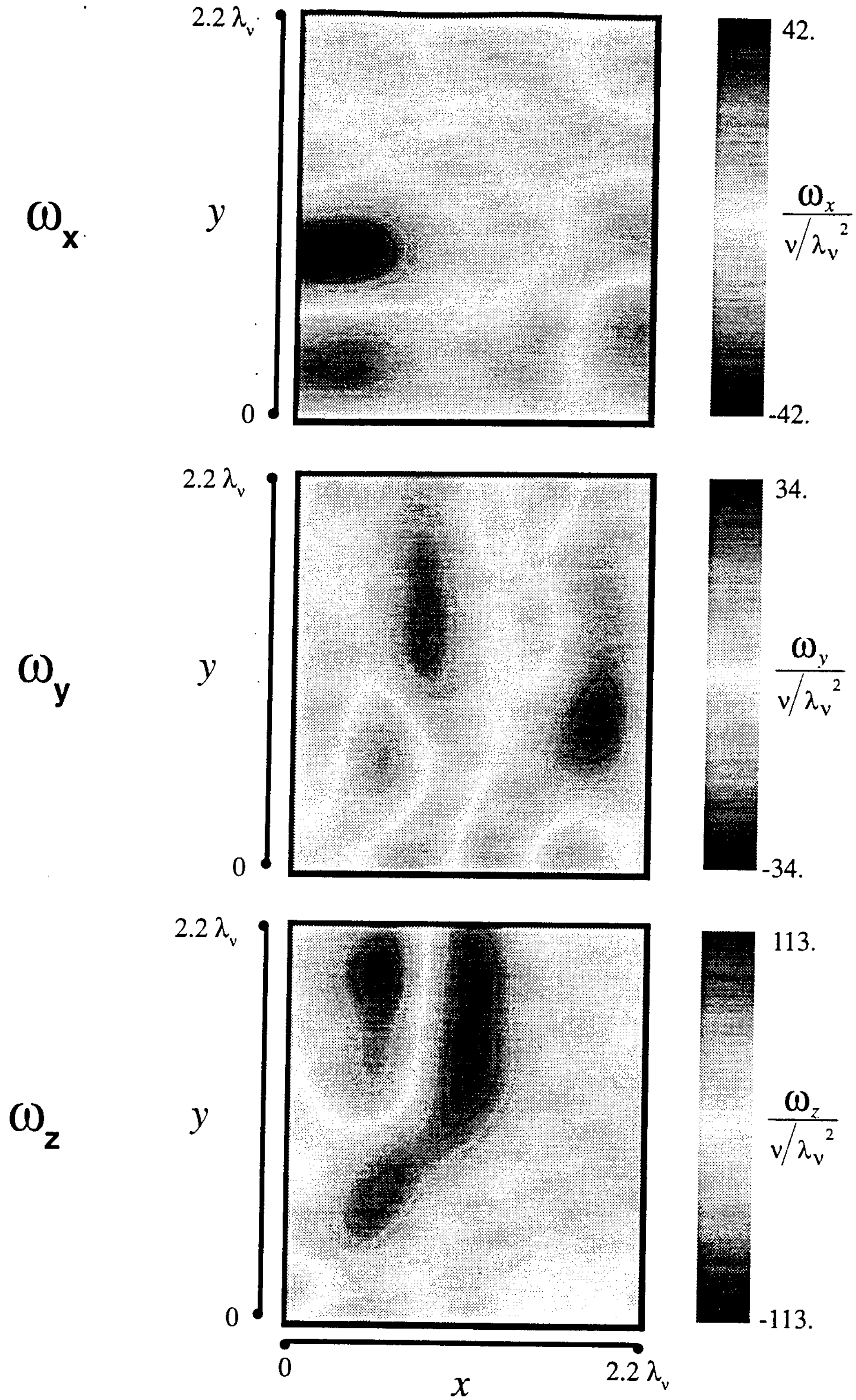


v-w



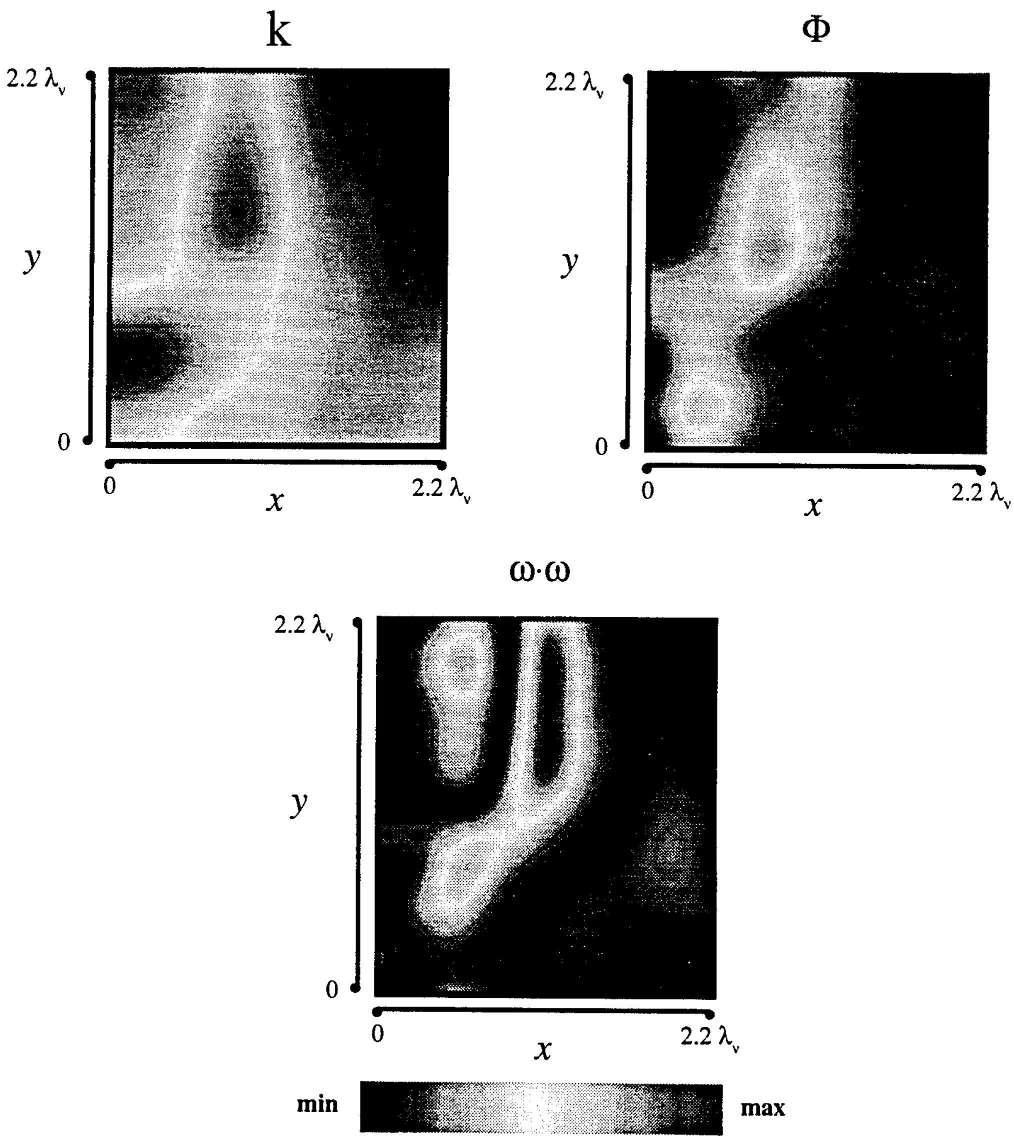
ε_{xx}
ε_{yy}
ε_{zz}
y
$2.2\,\lambda_v$
0
86.
-86.
$\frac{\varepsilon_{xx}}{\nu/\lambda_v^2}$
55.
-55.
$\frac{\varepsilon_{YY}}{\nu/\lambda_v^2}$
21.
-21.
$\frac{\varepsilon_{zz}}{\nu/\lambda_v^2}$
x


ε_{xy}
y
2.2 λ_v
0
47.
-47.
$\frac{\varepsilon_{xy}}{\nu/\lambda_v^2}$
ε_{yz}
y
2.2 λ_v
0
23.
-23.
$\frac{\varepsilon_{yz}}{\nu/\lambda_v^2}$
ε_{zx}
y
2.2 λ_v
0
17.
-17.
$\frac{\varepsilon_{xz}}{\nu/\lambda_v^2}$
0
x
2.2 λ_v

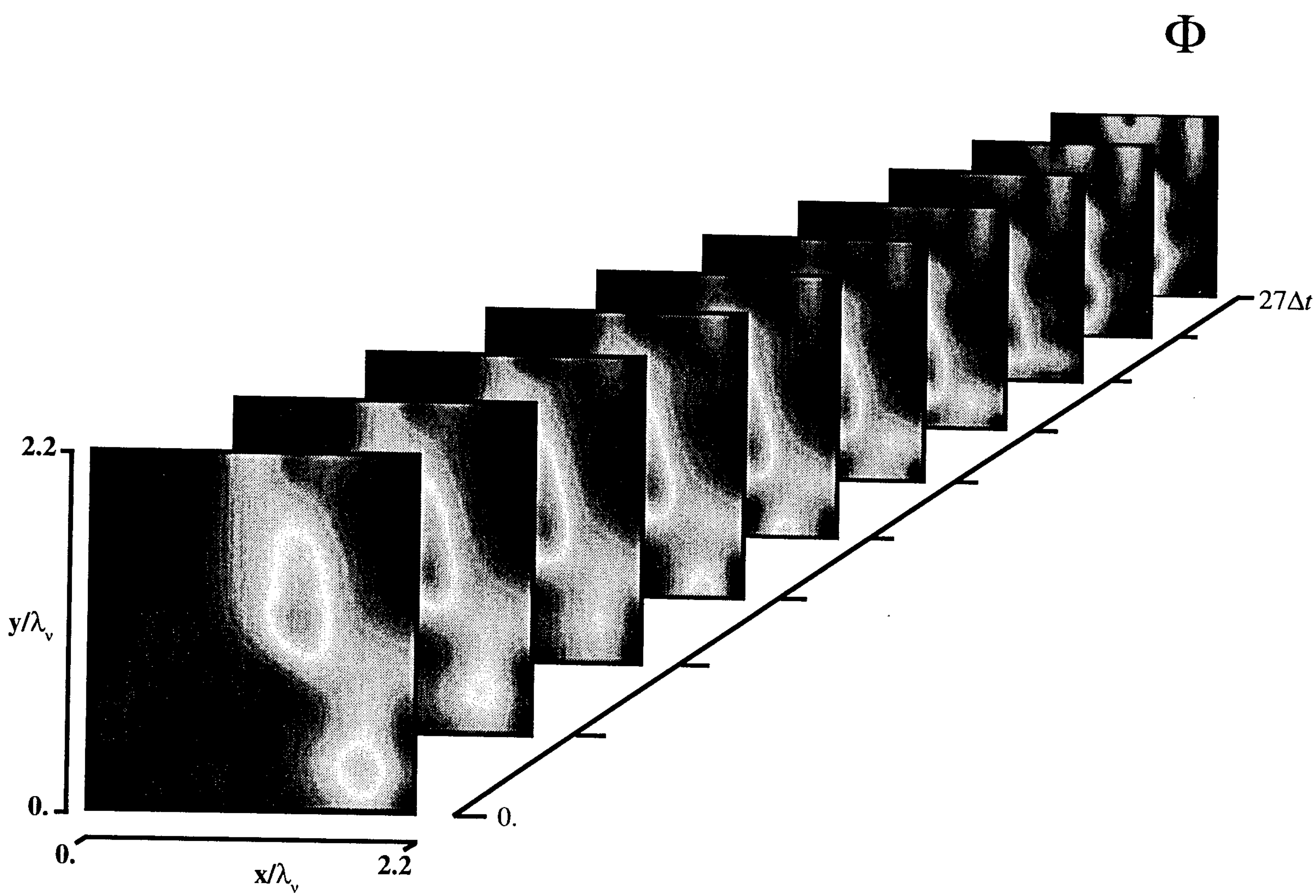


ω_x
y
$2.2\ \lambda_v$
0
42.
$\frac{\omega_x}{\nu/\lambda_v^2}$
-42.
ω_y
y
$2.2\ \lambda_v$
0
34.
$\frac{\omega_y}{\nu/\lambda_v^2}$
-34.
ω_z
y
$2.2\ \lambda_v$
0
113.
$\frac{\omega_z}{\nu/\lambda_v^2}$
-113.
0
x
$2.2\ \lambda_v$

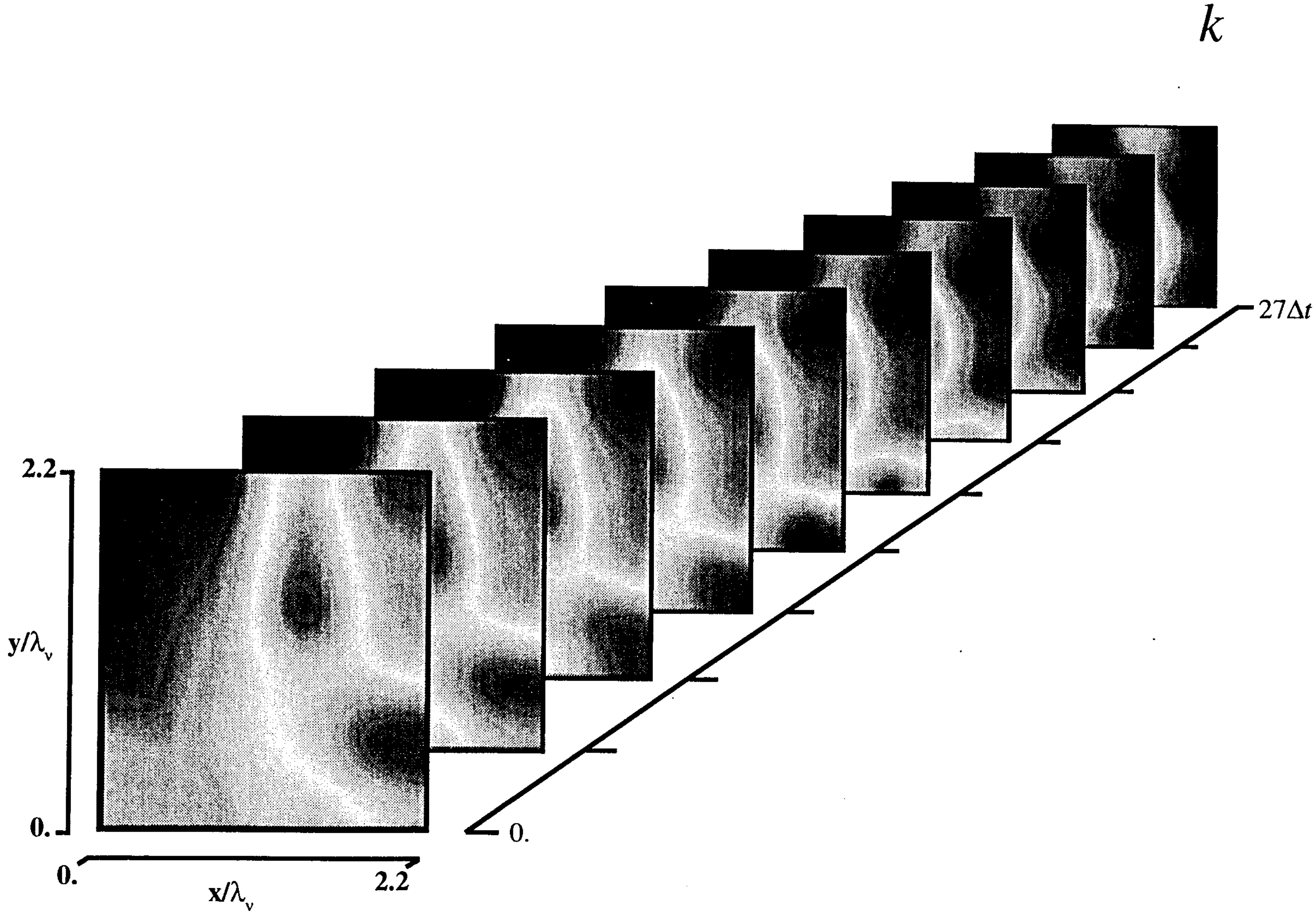
Dynamical Turbulence Quantities



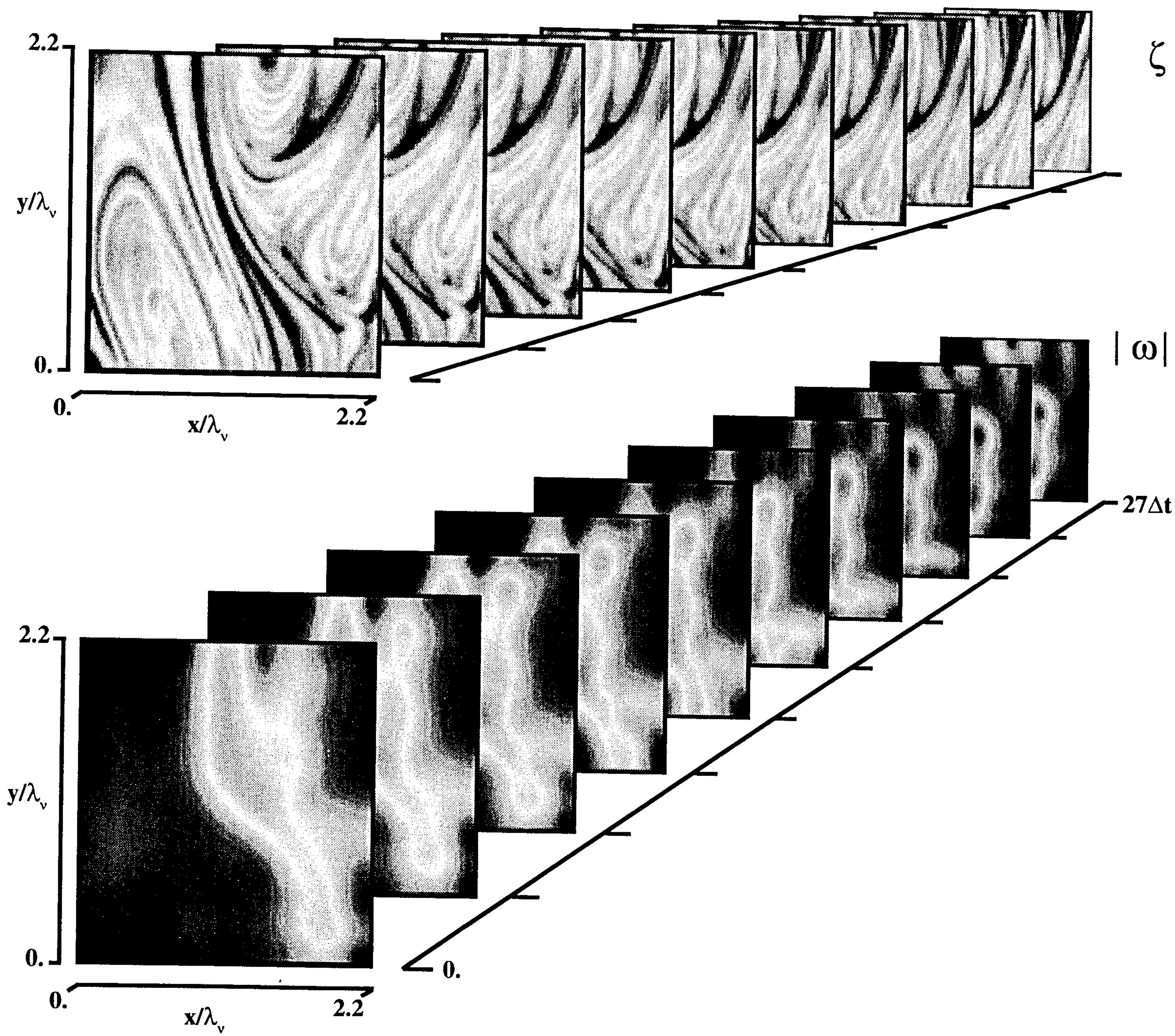
Spatio-Temporal Turbulence Data



Spatio-Temporal Turbulence Data



Spatio-Temporal Turbulence Data



Concluding Remarks

- Fully-resolved four-dimensional measurements of the small scales of turbulent shear flows have recently become possible, and are providing direct access to the dynamical foundations of turbulence

- These experimental measurement techniques are erasing many of the traditional boundaries between experimental and computational investigations

- Large scale acquisition and processing of turbulent flow data is providing remarkable new insights into
  - » the basic physics of turbulent flows and physical processes occurring in them
  - » physically-based submodels for turbulent transport and turbulence-chemistry interactions

High Performance CFD Simulation for Priority Real-Time Applications

Dr. Jay Boris

Naval Research Laboratory

High Fidelity CFD Simulation for Priority Real-Time Applications

Dr. Jay Boris, Chief Scientist
Laboratory for Computational Physics and Fluid Dynamics, NRL Code 6400

The IDA Alumni Symposium on
Applications of Advanced and Innovative Computational Methods to Defense Science and Engineering
Wednesday, 2 November [illegible]

NRL Laboratory for Computational Physics

Leaders in High Performance Computing

- Decade of parallel processing experience
- Developed/exploited GAPS parallel computer
- 1st reactive flow & BMCCC models on CM
- 32-node iPSC/860 in production in LCP&FD

Leaders in Detailed Simulation Technology

- Flux-Corrected Transport revolutionized CFD
- Complex geometry fluid/manybody dynamics
- Pioneered online, asynchronous graphics

Recognition in the Scientific Community

- Boards/fellows of APS, AIAA, CI, SNAME
- Numerous navy and national S&T awards

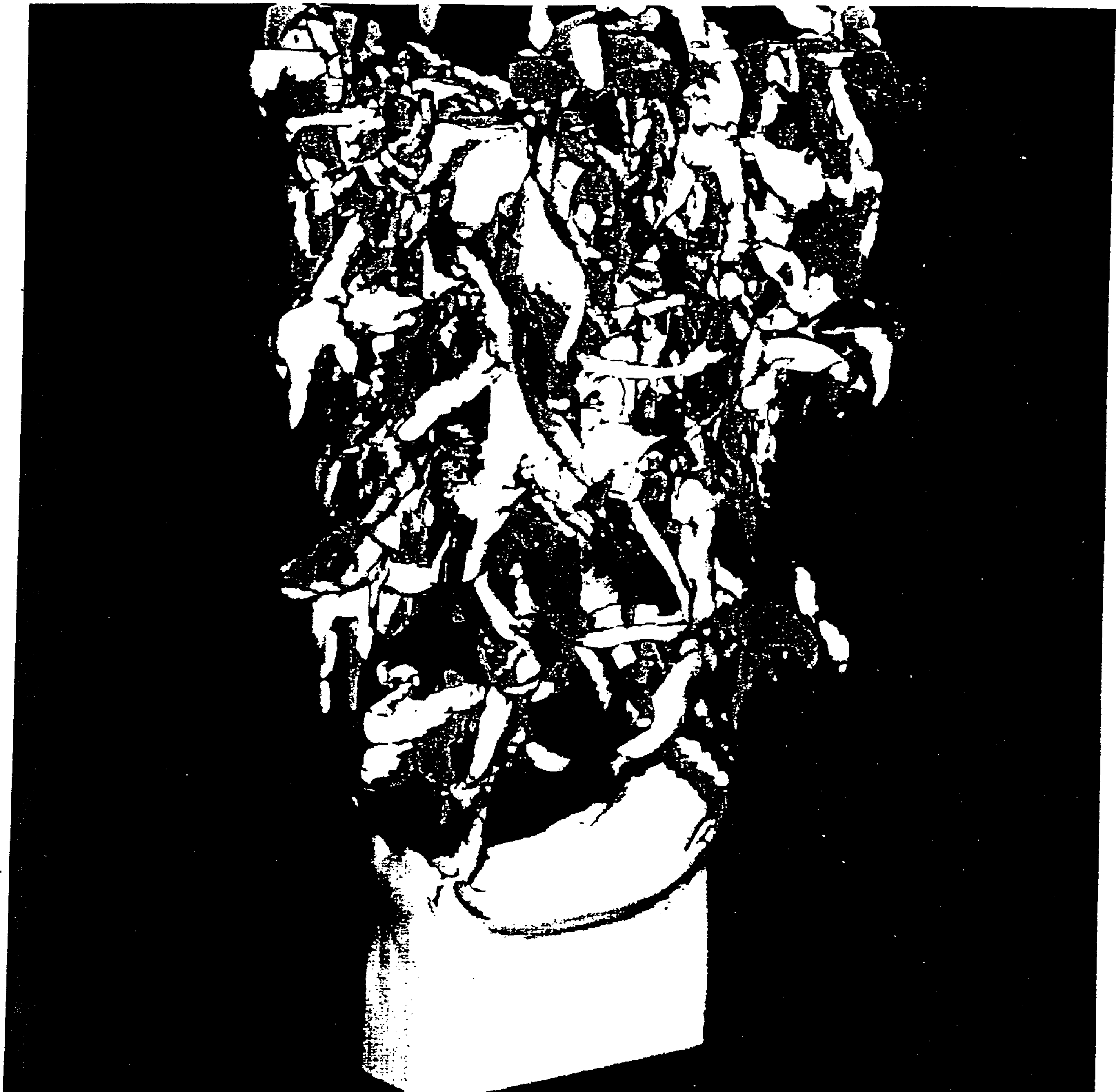
poc: boris@lcp.nrl.navy.mil

LCP&FD

LCP&FD MPP Success Stories

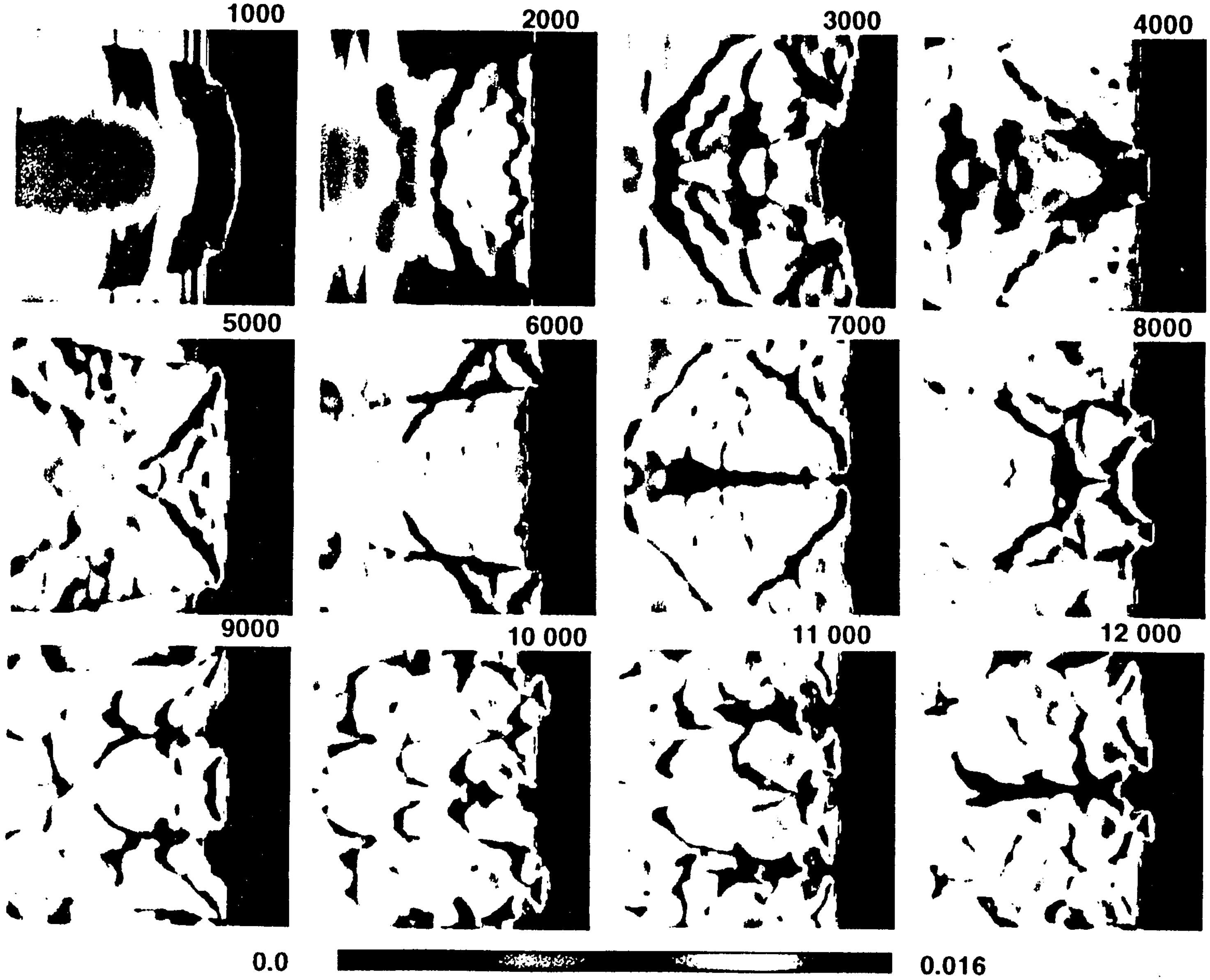
- Time dependent airwake simulation for shipboard landing
- Unsteady two-body torpedo launch & flapping foil studies
- Detonation dynamics & acceleration in the ram accelerator
- 3D radiation hydrodynamics for laser-pellet implosions
- Shock/detonation reactive flow boundary layer dynamics
- Simulations of jet exhaust noise modification for the HSCT
- Shock initiation dynamics in condensed phase explosives
- Correlation/tracking of 32,000 objects faster than real time

LCP&FD Laboratory for Computational Physics and Fluid Dynamics
U.S. Naval Research Laboratory Code 6400 202-767-3055

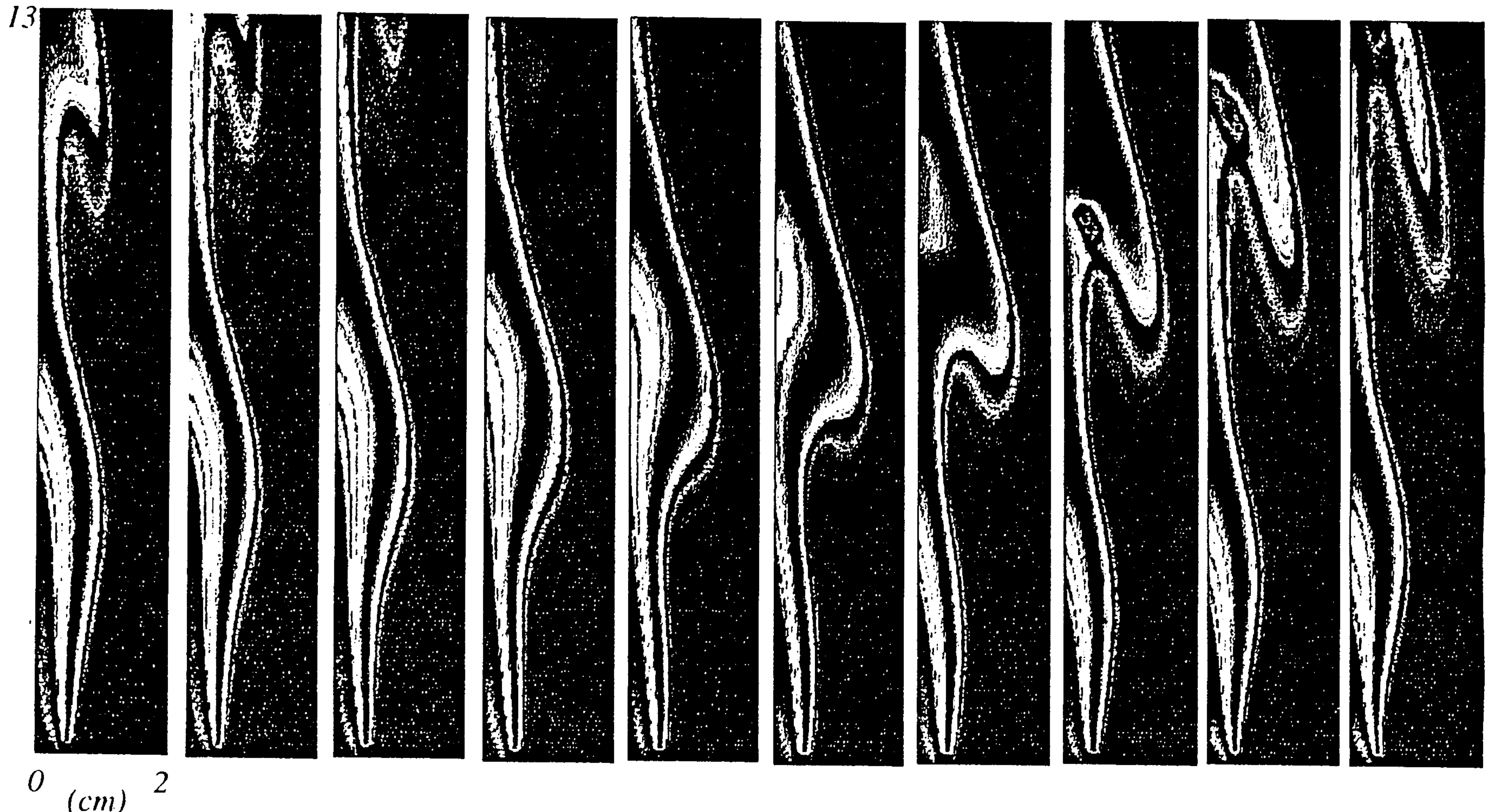


Time History of OH Mass Fraction

20% H_2 : 10% O_2 : 70% Ar Detonation Wave



Flickering Methane-Air Diffusion Flame



Sequence of temperature contours in time for a flickering methane-air flame shows clipped off portion. Interval between frames is 10 ms.

What Is the DoD Applications Software Problem?

- S&T Management expectations and process do not account for normal human limitations

  Warfare Centers emphasize near term problems and results
  The 'universal expert' is a practical impossibility

- Computational technology requirements do not respect the traditional 'ricebowl' societies

- Old 'production code' development paradigm wastes hardware and network advances

  Algorithms, implementations, and support software are obsolete by the time they reach the DoD end users

- External Expertise' - Part of the problem as much as part of the solution

Transferring Parallel Programming Technology

Provide A Library of Program Shells -
- Exploit data structures & communications
- Re-usable control and restart facilities
- Standard online, real-time graphics

Build Problem Solving Teams -
- Developer, application specialist & end user
- Pick a test problem of immediate significance
- Maintain fully compatible conventional model

People Are the Best Technology Transfer -
- Work where others have had similar problems
- Build your own model under expert tutelage
- Build and maintain professional contacts

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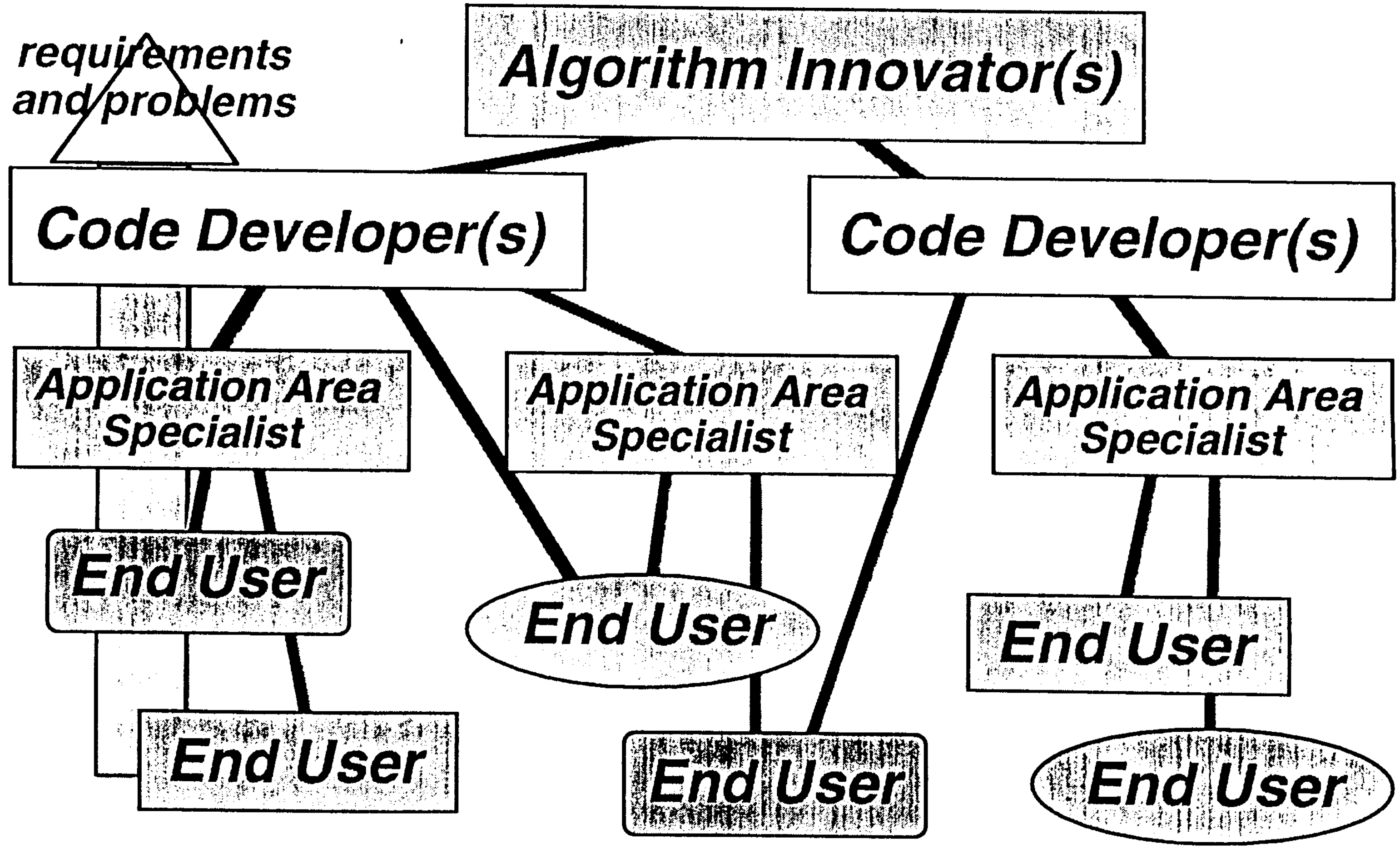
A Team for Multigeneration Scalable Software



Three Distinct Classes of Simulation

Simulation is the use of advanced computers and software to solve scientific, engineering and operational problems

- ***Scientific (Detailed) Simulation for Research***
  - Requires physically accurate detailed models
  - Uses extensive high performance computing resources
- ***Engineering Simulation and Modeling***
  - For design, interpretation, performance enhancement, and technology assessment - being mandated for procurements
  - Requires complex, quantitative, efficient predictive models
  - Multidisciplinary interactions & HPCC use are major issues
- ***Operational Simulation and Modeling***
  - Systems-level, wargaming, and real time performance
  - Distributed heterogeneous computing and networking
  - Problems with accuracy & calibration of underlying models

Computer Advances Blur These Classes!

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Identified Needs for Real Time Detailed Simulation

- *Real Time Manned Flight Simulation/Pilot Aids*
- *High Resolution Contaminant Transport Model*
- *Training Simulators for Large Ship Docking*
- *Accurate Simulation for Ship & Sub Maneuvering*
- *Shipboard & Confined Fire/Explosion Safety*
- *Monitor & Control Plasma Etch/CVD Processes*
- *Monitor & Control Thermal Curing Processes*

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Elements of a Real Time CFD Simulation Strategy

Computer Advances Enable Shorter Timescales

- Weather & environment real time are well understood uses
- Envelop of possible applications is growing

Several x Real Time Speed Often Required

- Tactics and strategy can be developed by test & evaluate
- Response on battle field, civil crisis, in manufacturing

Composite Solutions for Realtime Requirements

- Not all components of a solution need real time capability
- CFD interface technology, man and machine, need work
- Coupling HPC platforms enhances spectrum of uses

Human Scales Provide Short Time Cutoff

- Faster than human time may be fast enough in many cases
- Damage assessment of explosions against vehicles need only exceed human delay in interaction (1-2 seconds, not the microseconds or milliseconds of the physics)

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FAST3D

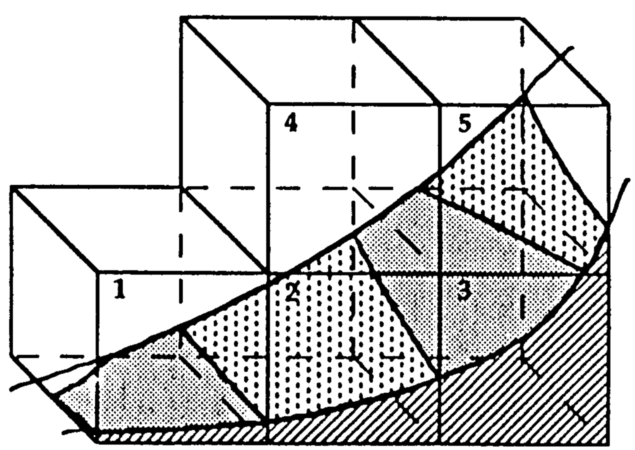
- Solves the unsteady 3-D convective transport equations using 4th order FCT algorithms and VCE methods representing complex geometry
- Produces accurate results verified by series of idealized 2-D and 3-D problems and calibrated against jet and turbulent mixing experiments
- Compatible scalar/vector/MPP versions use virtual nodes, architecture-independent data structures, explicit functional segregation via decomposition, cyclic block transpose communications, asynchronous online graphics

VIRTUAL CELL EMBEDDING (VCE) METHOD

- To cancel the staircasing effect, the VCE method was developed to allow smooth surfaces of complex bodies to cut cleanly through a rectilinear grid

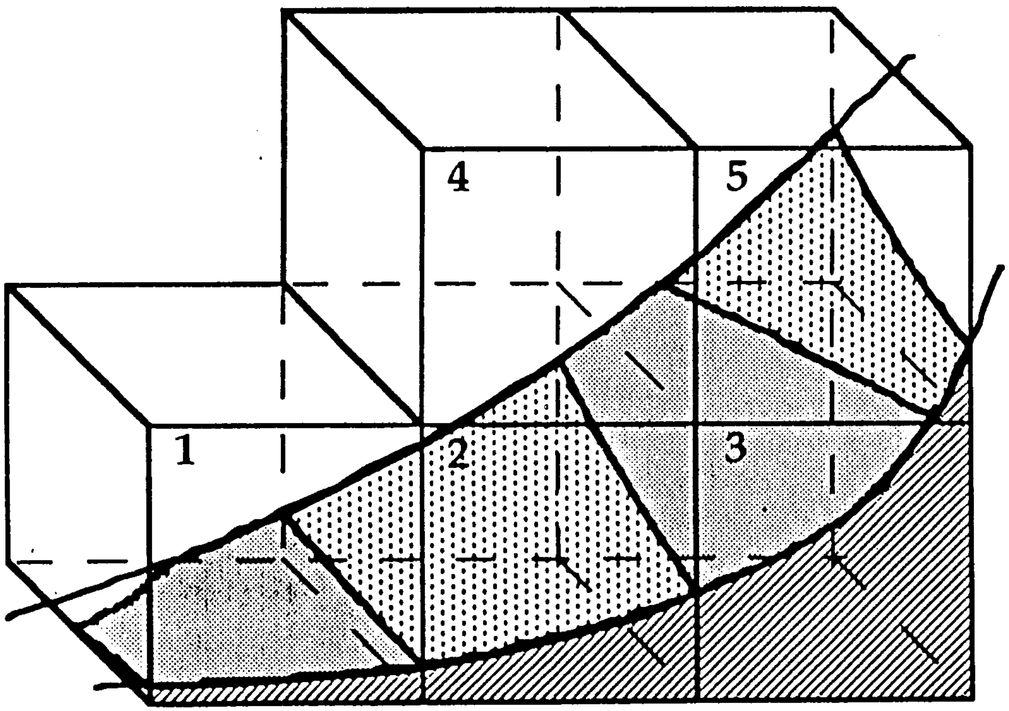
- Greatly improves the accuracy around complex geometries without much sacrifice in speed or memory

- Cells may be fully outside the body, fully inside the body or partitioned by the body

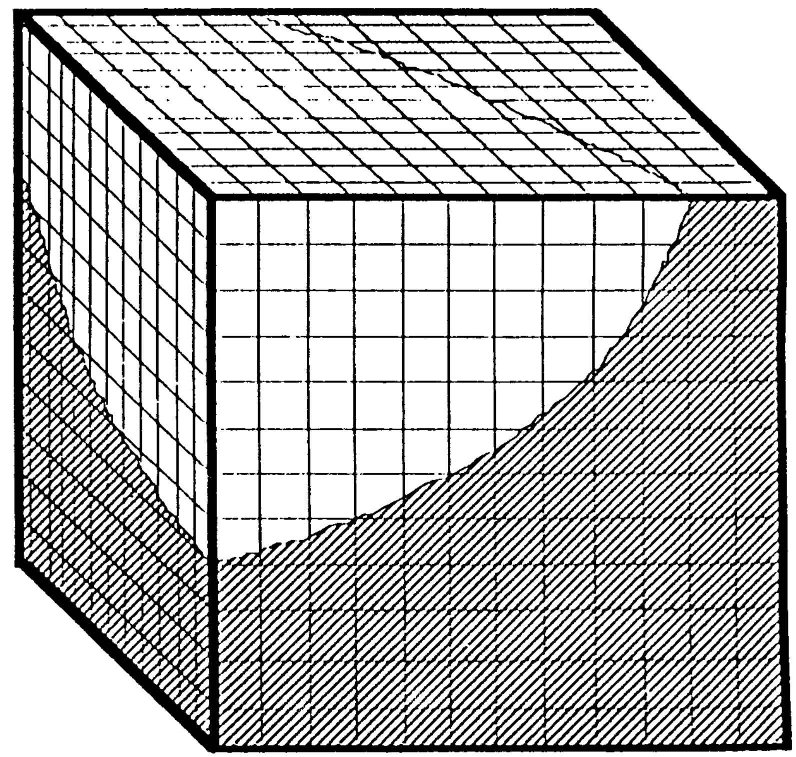


VCE Gridding

VIRTUAL CELL EMBEDDING (VCE) METHOD

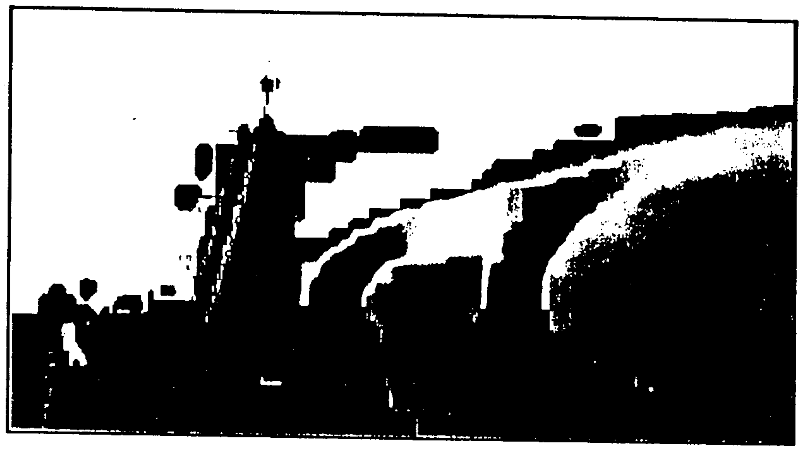


VCE Gridding

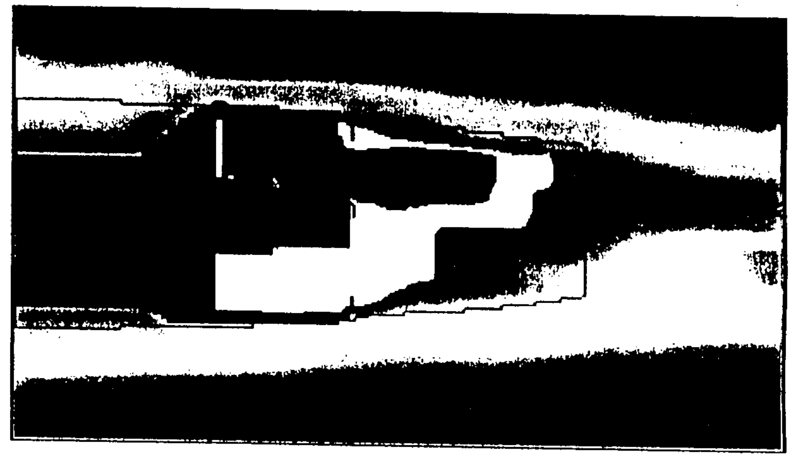


Cell Subdivision

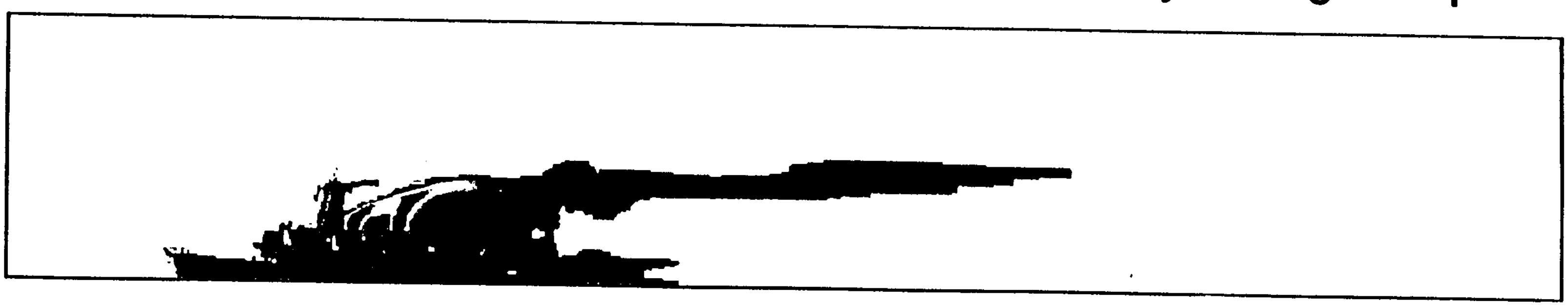
Unsteady Flow Calculations for the Navy DDG51



Temperature - Stack Vicinity



Axial Velocity - Hangars Open



Temperature - Entire Domain

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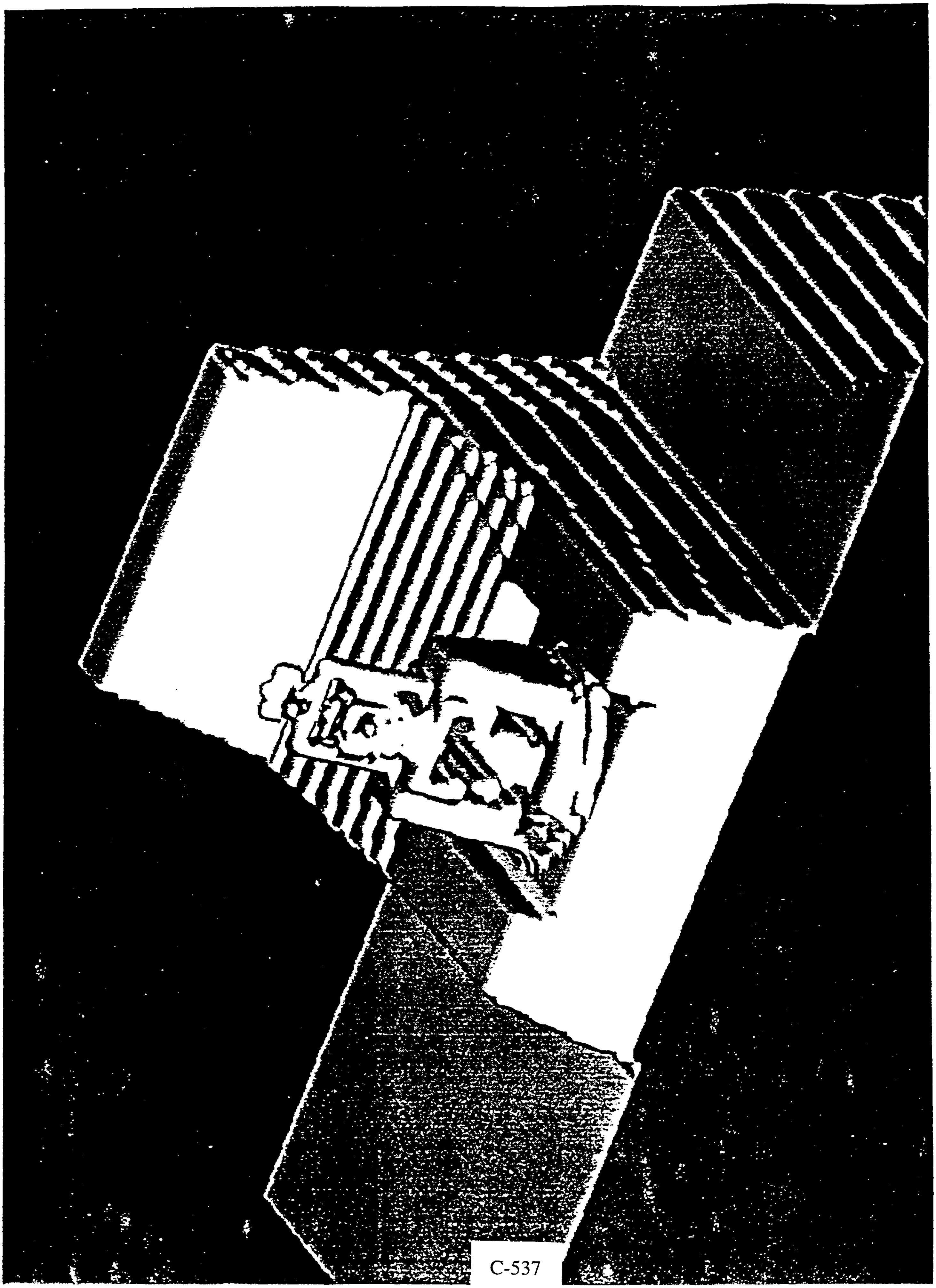
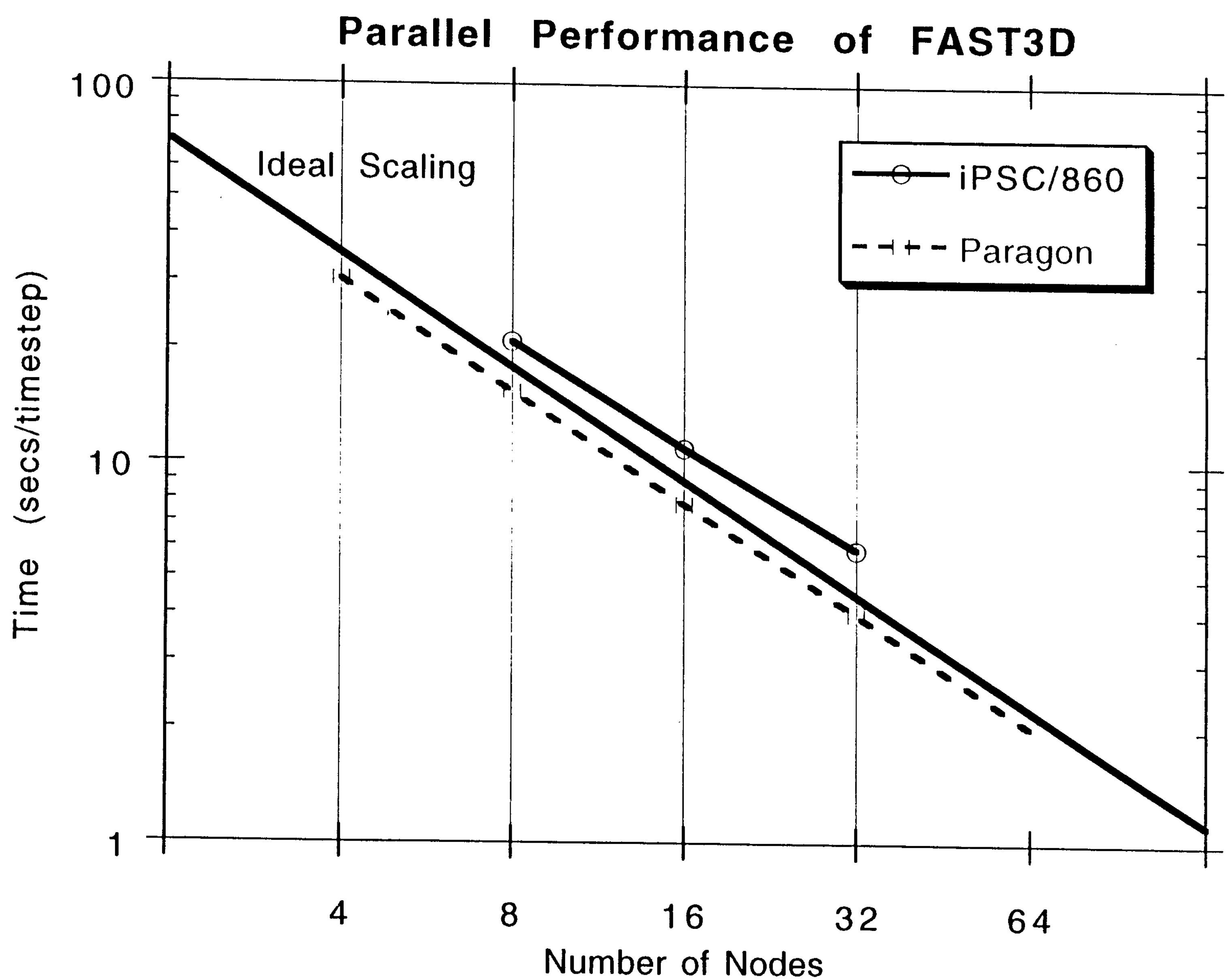
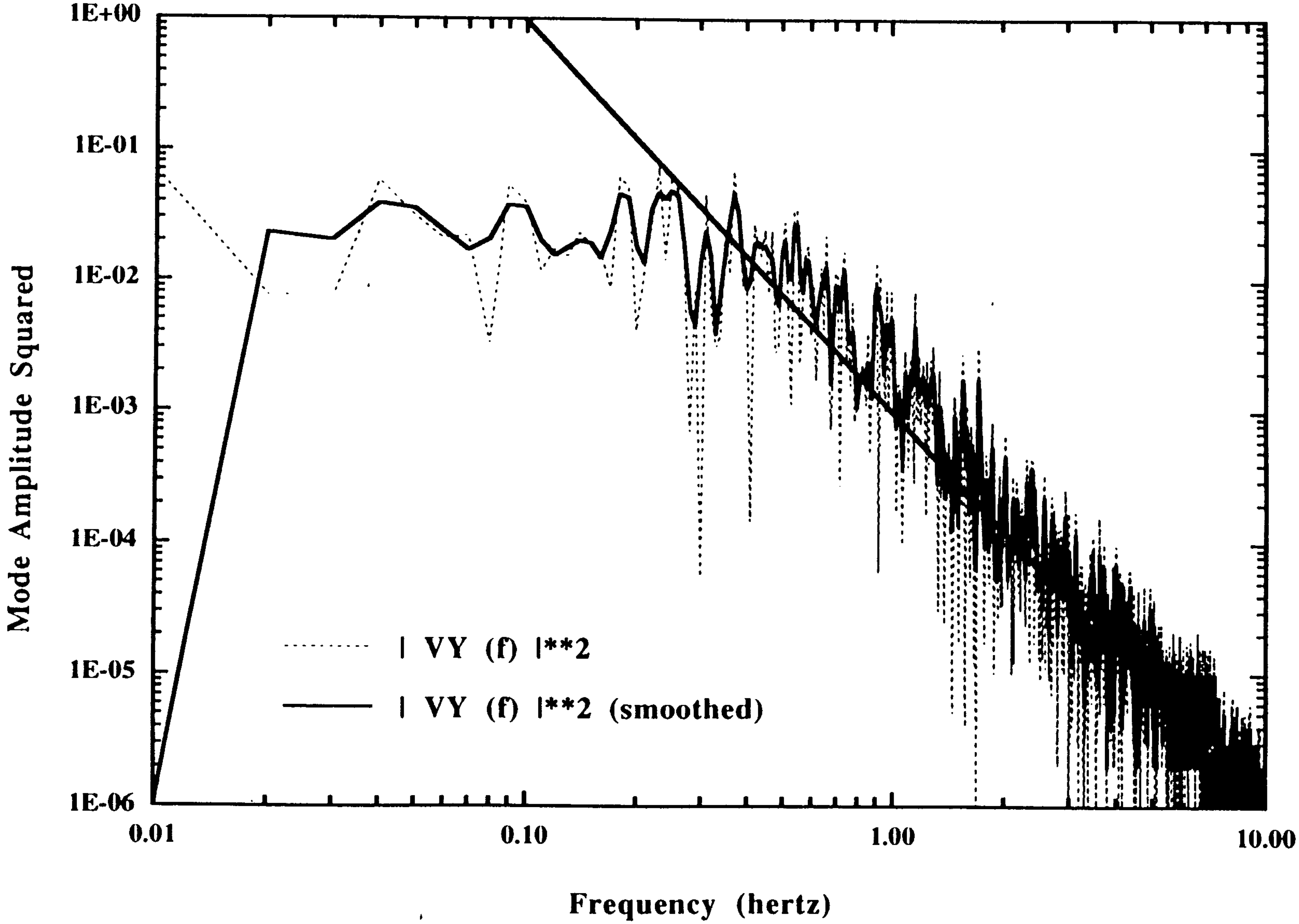



Parallel Performance of FAST3D
Ideal Scaling
iPSC/860
Paragon
100
10
1
Time (secs/timestep)
4
8
16
32
64
Number of Nodes

Time Series Power Spectrum of Vertical Velocity



Real Time Helo Landing Simulation: 3 Approaches

Phenomenology Based on Detailed Simulations

- Detailed simulations give 3D maps of varying vortex strength, orientation, range of frequencies, average flow properties
- Instantaneous flow at helicopter location in simulator taken stochastically from maps adding simple helo model
- Major Problems: gust phasing/correlation & helo feedback

Prerecord (Detailed Simulation) Ship Air Wakes

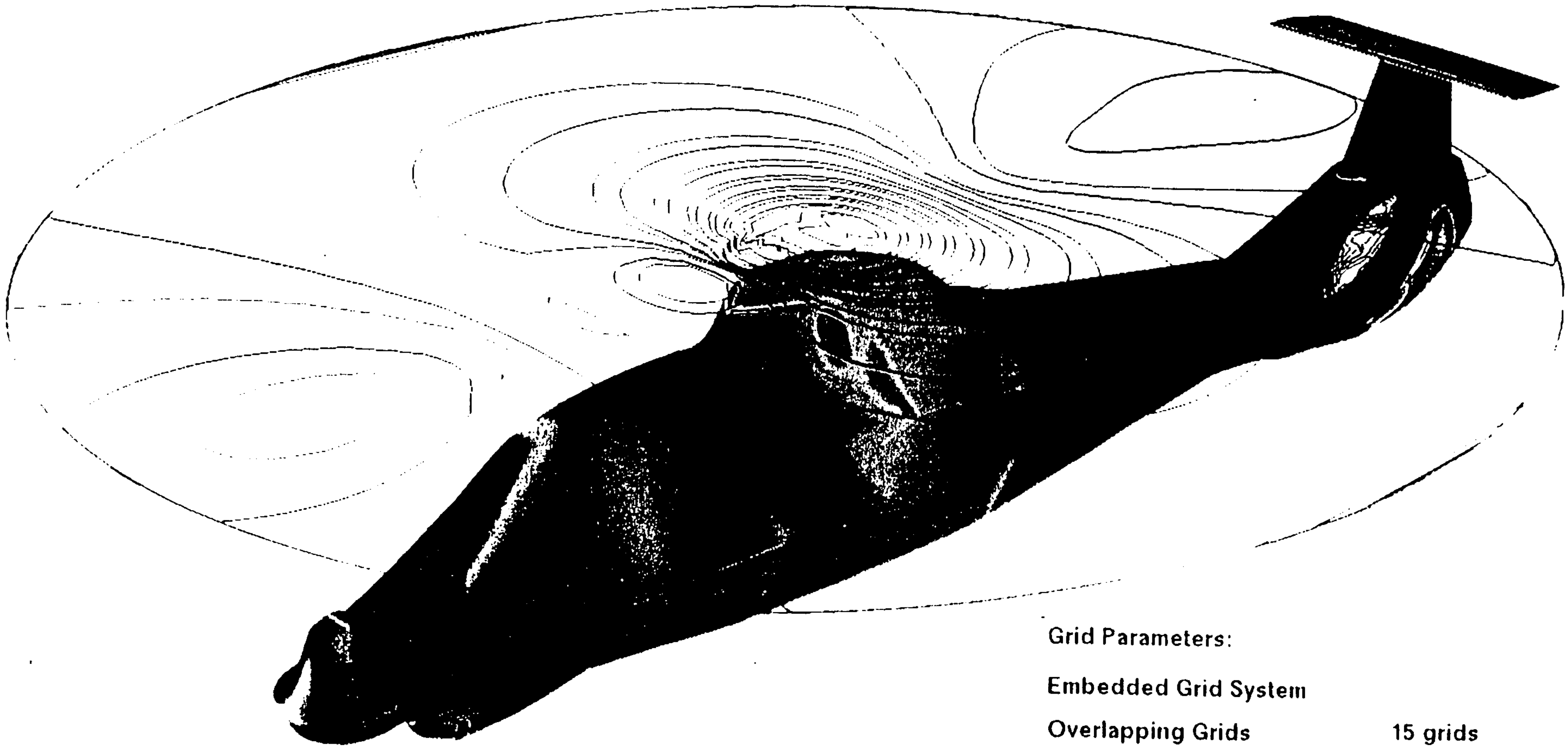
- Optical disks (or networked data bases) for ship air wakes
- Helo downwash and response models added by simulator
- Problems: nonlinear helo/flow field feedback & data set size

Detailed Simulation of Helicopter Region

- 50 x 30 x 30 region around helicopter simulated (10 GF)
- B.C.s from prerecorded ship air wakes simulations are determined interactively by simulator/pilot
- Problems: Distributed simulation requires dedicated HPC systems & large data transfer rates, also higher cost

Comanche

- Fuselage with Main and Tail Rotor Actuator Disks



Pressure Contours

Grid Parameters:

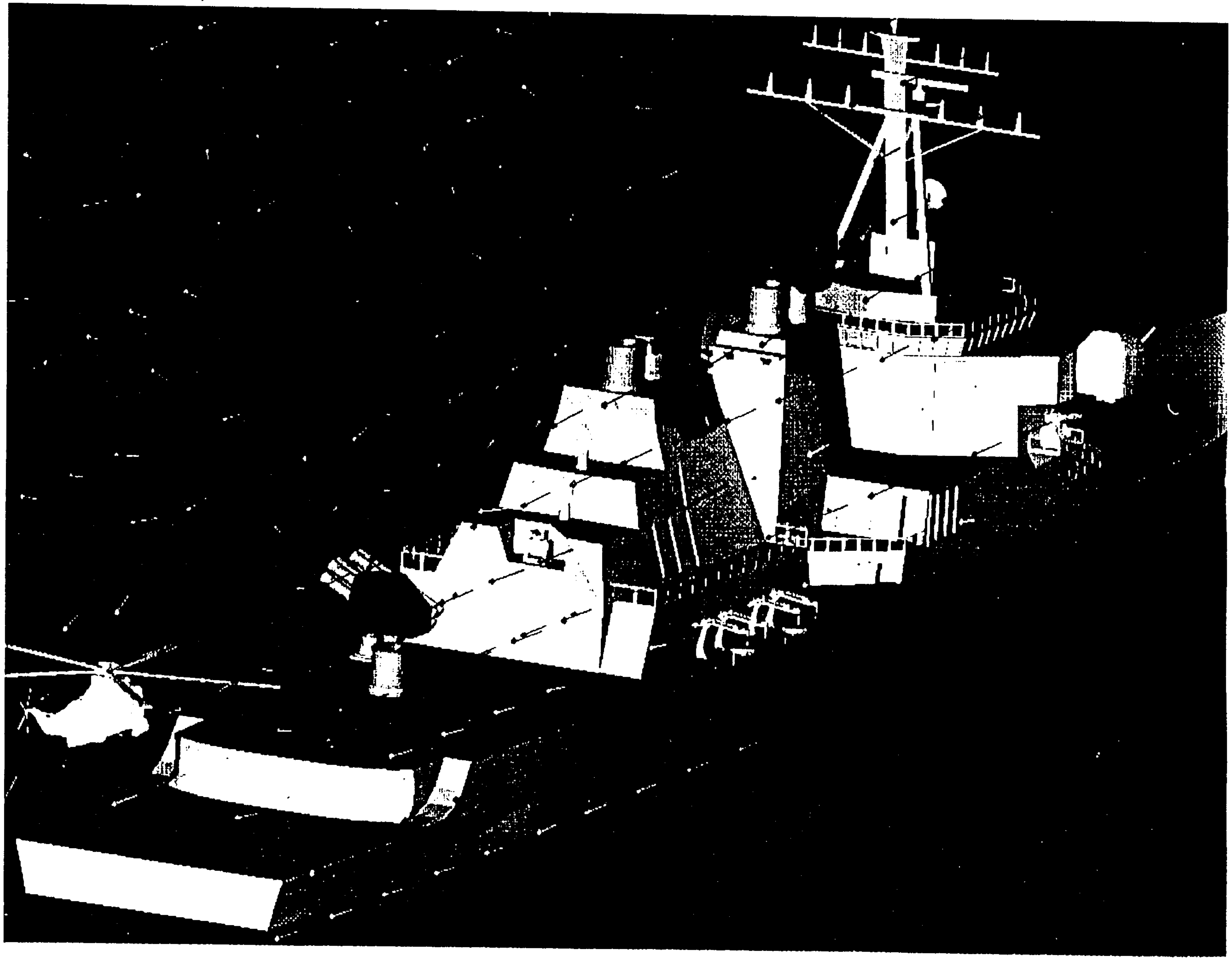
Embedded Grid System	
Overlapping Grids	15 grids
Grid Point Total	2,675,488 pts.

Flow Parameters:

Angle of Attack	0 deg.
Mach Number	0.26
Reynolds Number	14,000,000

By: A.C.B. Dimanlig and E.P.N. Duque

U.S. Army Aeroflightdynamics Directorate – ATCOM



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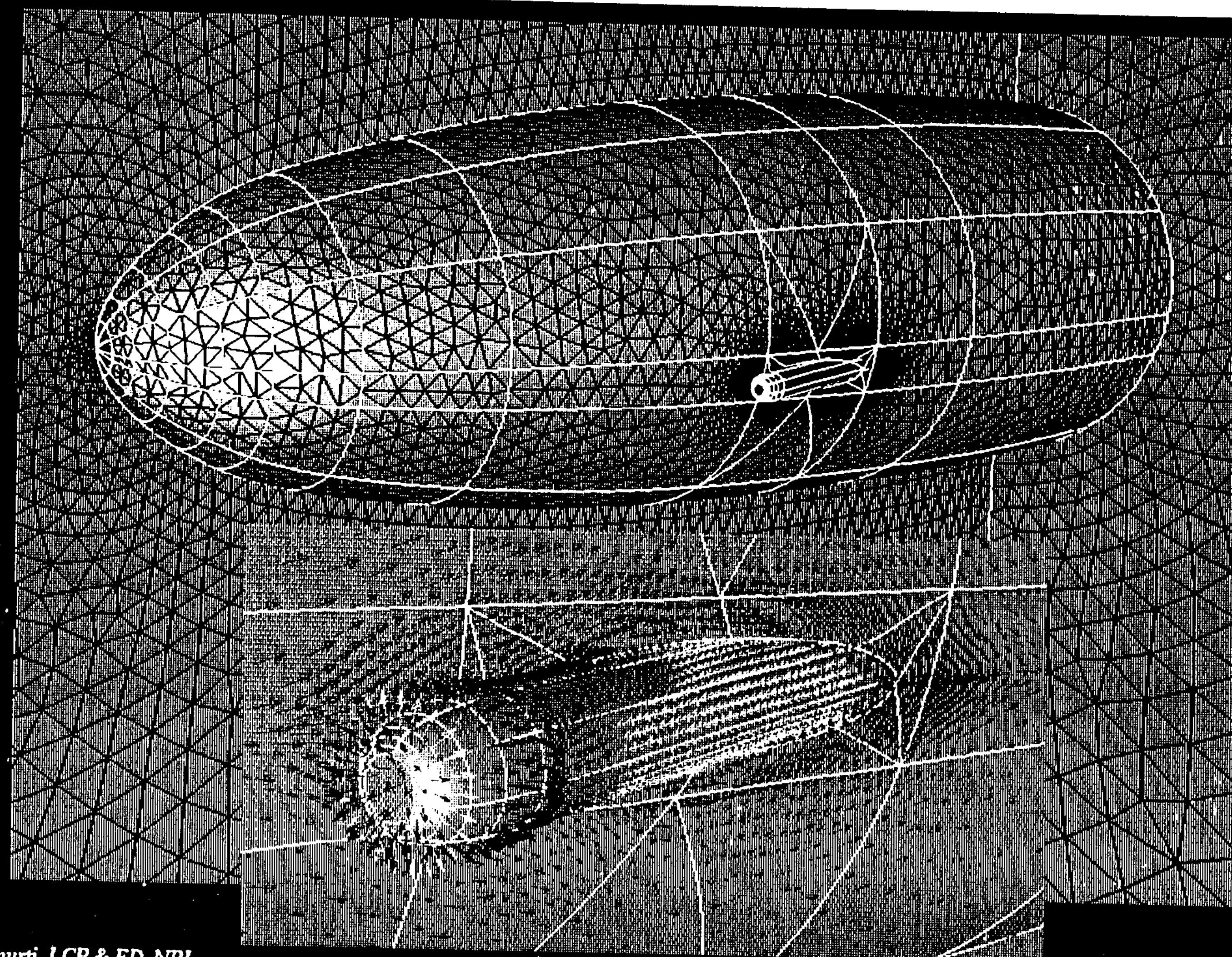
Other Real Time Simulation Opportunities

- ***High Resolution Contaminant Transport Model***
  - State-of-the-art high resolution CFD with environmental server
  - Implement as continuum field server for battlefield simulation
  - Technology can be extended to remove SIMNET bottlenecks
- ***Accurate Two-Body Simulation for Ship, Sub, & Unmanned Underwater Vehicle Dynamics***
  - Control of maneuvering submarines in shallow water
  - Ship docking simulator in currents and rough seas
  - Dynamics of torpedo launch and stores separation
  - Technology can be extended to fluids & structural mechanics
- ***Shipboard and Vehicle Fire/Explosion Safety***
  - Model spread of fire in connected enclosed compartments
  - Model explosions in confined, complex geometry regions
  - Dynamic "Heads Up" virtual reality displays for firefighters
  - Technology can be modified for propulsion system design

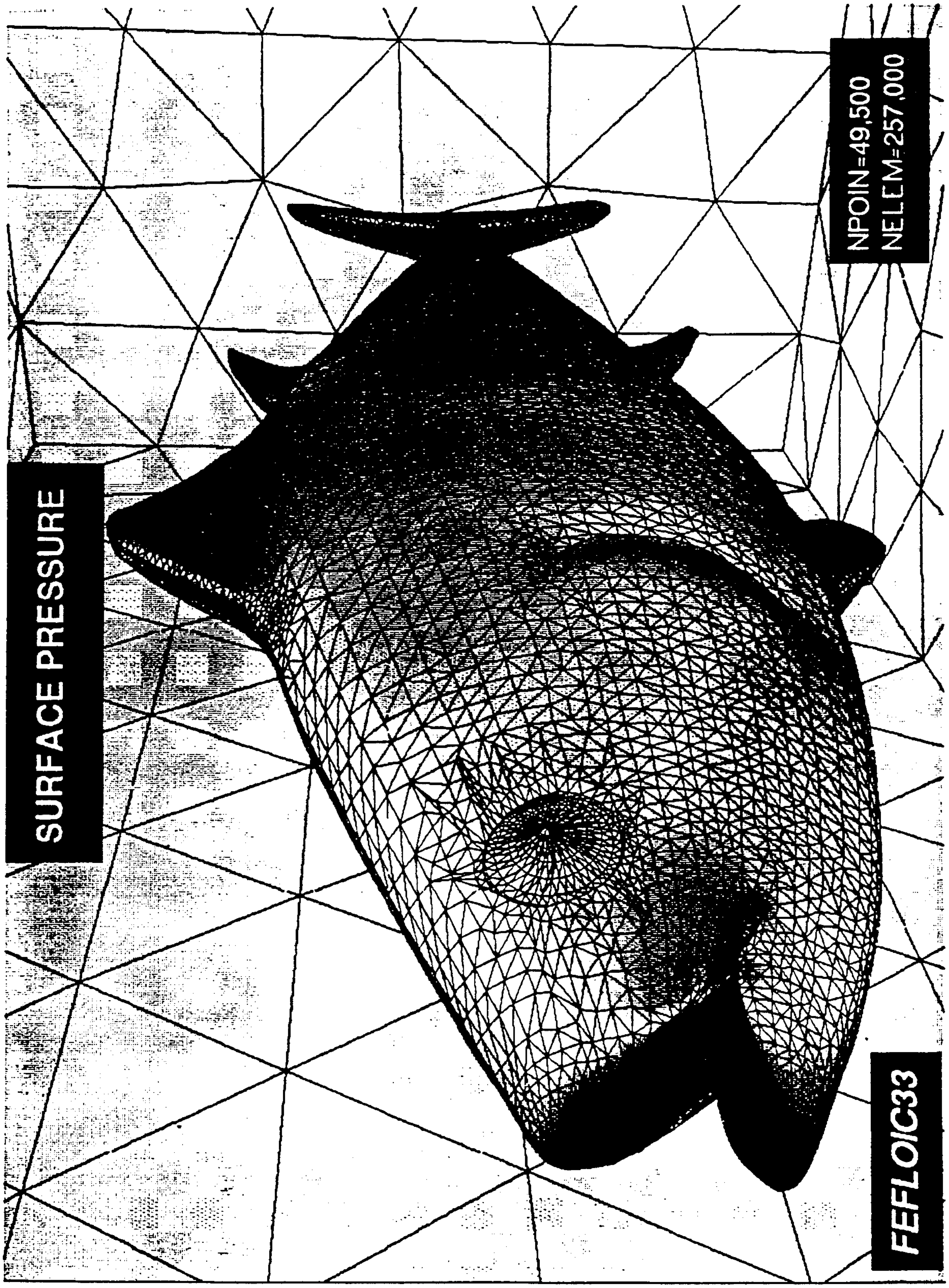
LCP&FD



Ravi Ramamurti, LCP & FD, NRL

Unsteady Flow Simulation of a Torpedo Launch from a Submarine

FEFL01C71


SURFACE PRESSURE
NPOIN=49,500
NELEM=257,000
FEFLOIC33

Applications for a

High Resolution Contaminant Transport Model

Simulations of Biological and Chemical Toxicity

- Real time toxicity level evaluations in warfare simulations
- Engineering and system studies of bio/chemical scenarios
- Smoke and particulate contamination from enclosed fires

Engineering Studies of Plumes & Exhaust Wakes

- Infrared and optical tracking of missiles and planes
- Surface ship stack wakes cause meteorological effects
- Evaluate possible mine detection via sediment "wakes"

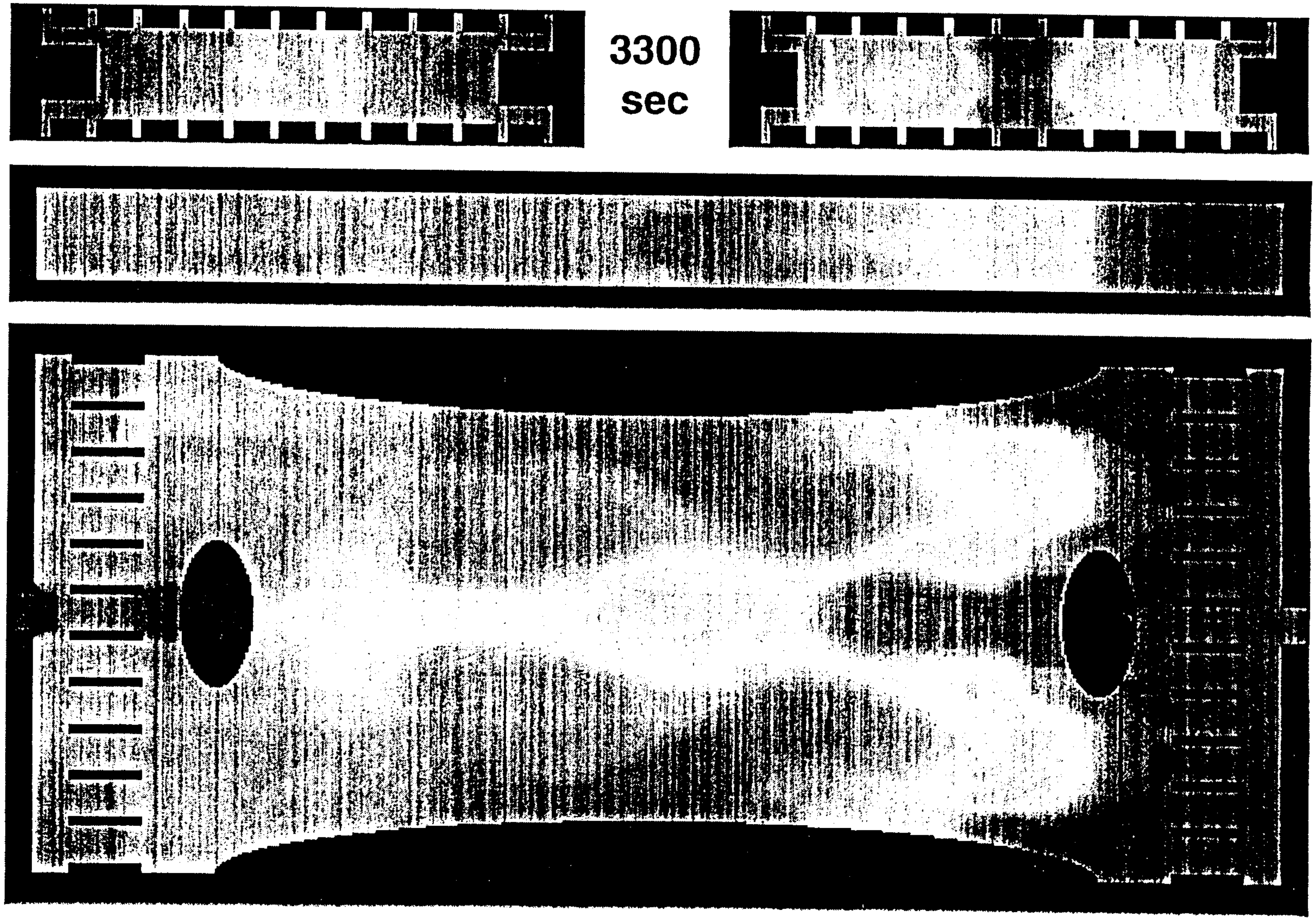
Environmental and Climatological Effects

- Pollutant concentrations and transport in the atmosphere
- Growth and dynamics of the benthic boundary layer
- Vorticity generation & transport to calculate oceanic drag

8/93 boris@lcp.nrl.navy.mil

LCP&FD

fast3d (vce & iPSC/860) LCP&FD 8/94



AUTOMATIC TARGET RECOGNITION

Automatic Target Recognition (ATR) for Wide Area Surveillance

Dr. Jonathan Schonfeld

Advanced Research Projects Agency

Automatic Target Recognition and Wide-Area Surveillance

Jonathan F. Schonfeld
Sensor Technology Office

Essence of STO Program

War Breaker

Surveillance & Targeting

- **Mission: Develop sensors and processing technology within an end-to-end sensor architecture**
  - Baseline: All-radar architecture

- **Priorities**
  - Make sensors and ATR best they can be
  - Make sensors and ATR achievable today
  - Put sensors and ATR in proper place in overall battlefield-wide Sensor/ Processor Architecture
  - Solve the Time-Critical Target problem
    - » In hide and in open
  - Revolutionize wide-area imagery analysis

STO Perspective

- Develop sensor and ATR technology to fill deficiencies in surveillance and targeting
- Work within the context of an <u>integrated, end-to-end, sensor architecture</u> evolving from today's infrastructure
- Prosecute targets around the clock throughout their operations, making their lives miserable

ARPA S&T Challenges

- Deep: Confront the fundamentals
- Broad: Develop <u>system technologies</u>, not just component technologies
- Far: Develop technology <u>for the long view</u>, as well as to make best use of what's available or emerging today

The Tier II Plus Unmanned Air Vehicle

War Breaker

Surveillance & Targeting

- This new ARPA/AF/Navy program holds the promise to revolutionize warfare
  - 40,000 sq nmi per day of SAR stripmap imagery at 1 m resolution
  - 1900 SAR spots/day at 1ft resolution
  - GMTI
  - 65,000 ft altitude, penetrating hostile airspace
  - $10M unit flyaway cost

- The low unit cost will make wide-area surveillance (WAS) a commodity rather than a "crown jewel"

The WAS Mission

- Fulfill full range of commander's information needs
  - Enemy disposition
  - Enemy courses of action
  - Enemy sustainability
  - Location and readiness of weapons of mass destruction
- Extends well beyond familiar ARPA War Breaker focus on time-critical targets (TCTs)
- Provides many transition opportunities for automatic target recognition (ATR) even when hardest job and lowest false-alarm rates are still out of reach

Requirements Analysis

Commander's Needs	Sensor Mode	Resolution (test)	Area Coverage Rate	Depth of Battlefield	Response Time	Acceptable FAR	Correct Classification Rate	% of Commander's Needs	Priority
WMD (Active)	MTI ISAR SAR	1-2 1-2	Large Small Small	Deep	Short	.001/km^2	0.9	Small	1
WMD (only stationary)	SAR	1-2	Large	Deep	Short	.001/km^2	0.9	Small	1
Deployment	MTI SAR	5-10 10-50	Large	Shallow to Medium	Medium	1/km^2	NA	Large	2
Composition	ISAR SAR	1-3 1-3	Small	Shallow to Medium	Medium	NA	0.5 to 0.7	Large	2
Movement	MTI	10-50	Large	Shallow to Medium	Short Medium	1/km^2	NA	Large	2
Follow on Forces	MTI ISAR SAR	10-50 1-2 1-2	Large to Small	Deep	Long	1/km^2	0.5 to 0.7	Medium	3

Note: Deployments, composition, etc. include ground, aviation, naval and electronic orders of battle; entries shown are for ground forces only.

ATR and wide-area surveillance

Prior Efforts in ATR and Wide-Area Imagery

War Breaker

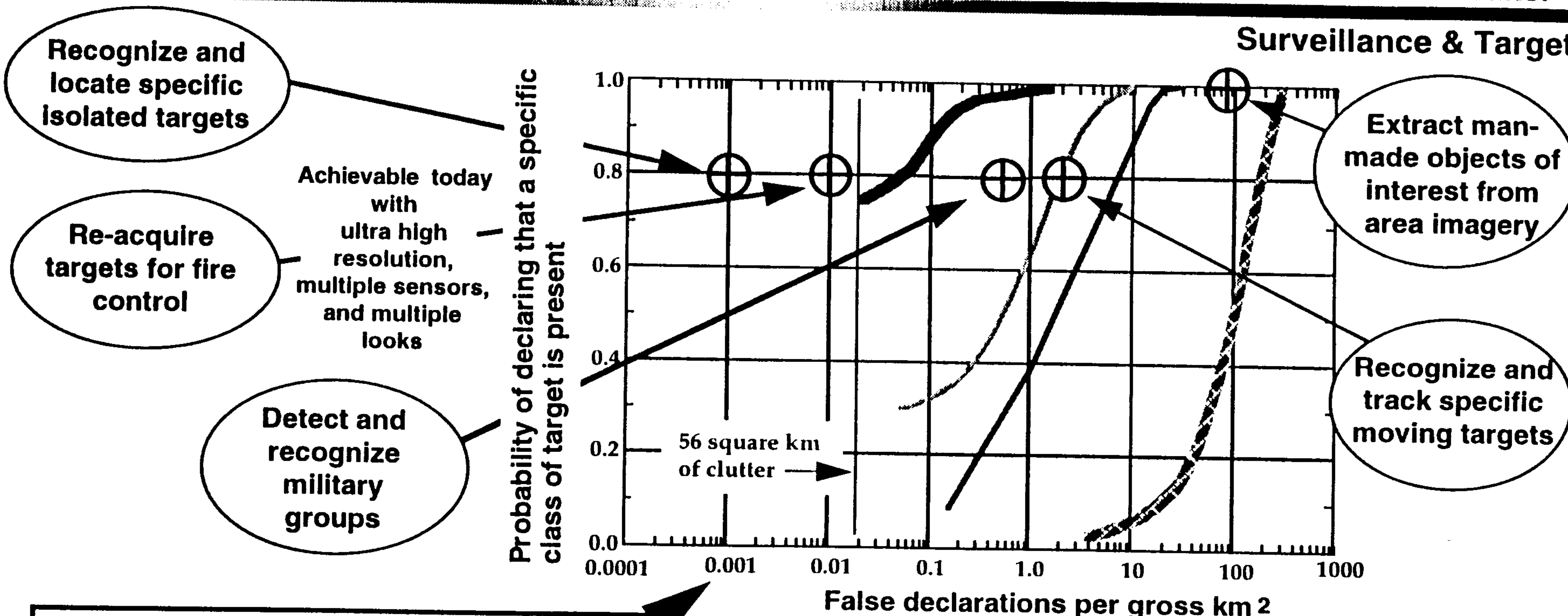
Surveillance & Targeting

- **MIT/LL: Search for SRT's and tactical targets in remote areas**
  - Pd = .9 with 0.1/km^2 against tactical camouflaged targets using 1/3m, fully polarimetric SAR
- **ADVL: Site monitoring in SAR imagery**
  - High P_d, low P_{fa} documented for airfields: highly organized sites, very large targets (bombers)
- **PROBE: Detection of man-made activity in broad-area, moderate-resolution optical imagery**
  - Suitable primarily for remote regions
  - Unacceptable false alarm rates (up to 40% at the required P_d of 90%) documented
- **Gold Pan: Detection of targets in broad-area, coarse-resolution SAR imagery**
  - Distractingly high false alarm rates reported
- **IES/BTI: Identification of tactical battlefield groupings in patterns of unresolved points**
  - Sidesteps target recognition per se
  - Presupposes that adversary positions forces according to known and unchanging doctrine
    - With known doctrine, 70% (approx.) correct ID documented in blind testing
  - Uses terrain analysis and collateral information
- **SNL/ARL: Focused search for TCT's with high resolution SAR**
  - High p_d demonstrated with limited target set

Sensor/ATR Performance

War Breaker

Surveillance & Targeting



Lincoln Lab. Baseline

- Single sensor, single look
- Tactical targets
- Stockbridge, NY
- Camouflaged deployments
- K_a-band SAR

Polarization	Resolution 1/3 m	Resolution 1 m
Full		
Single		

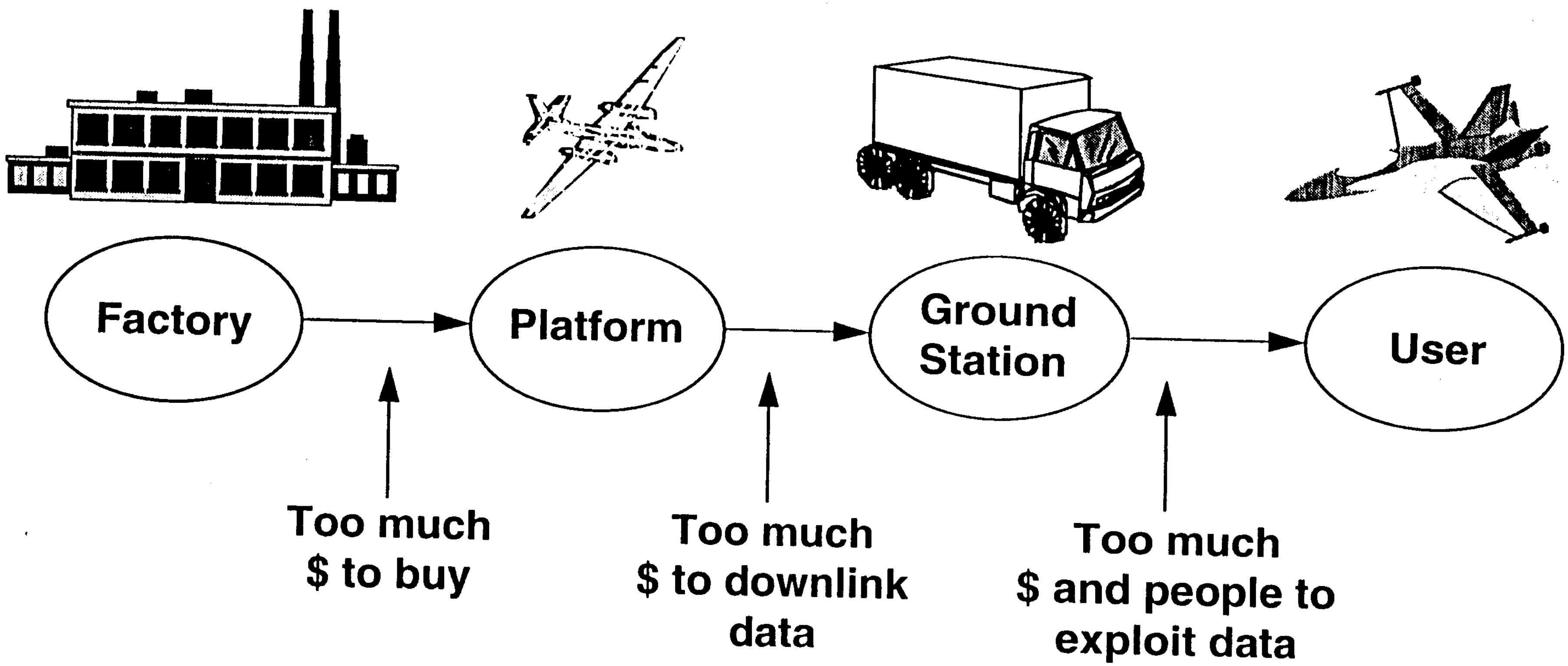
Conclusion: Some ATR requirements can be met now; others need more work.

=> Implement and demonstrate a <u>hierarchy</u> of sensor data exploitation system capabilities

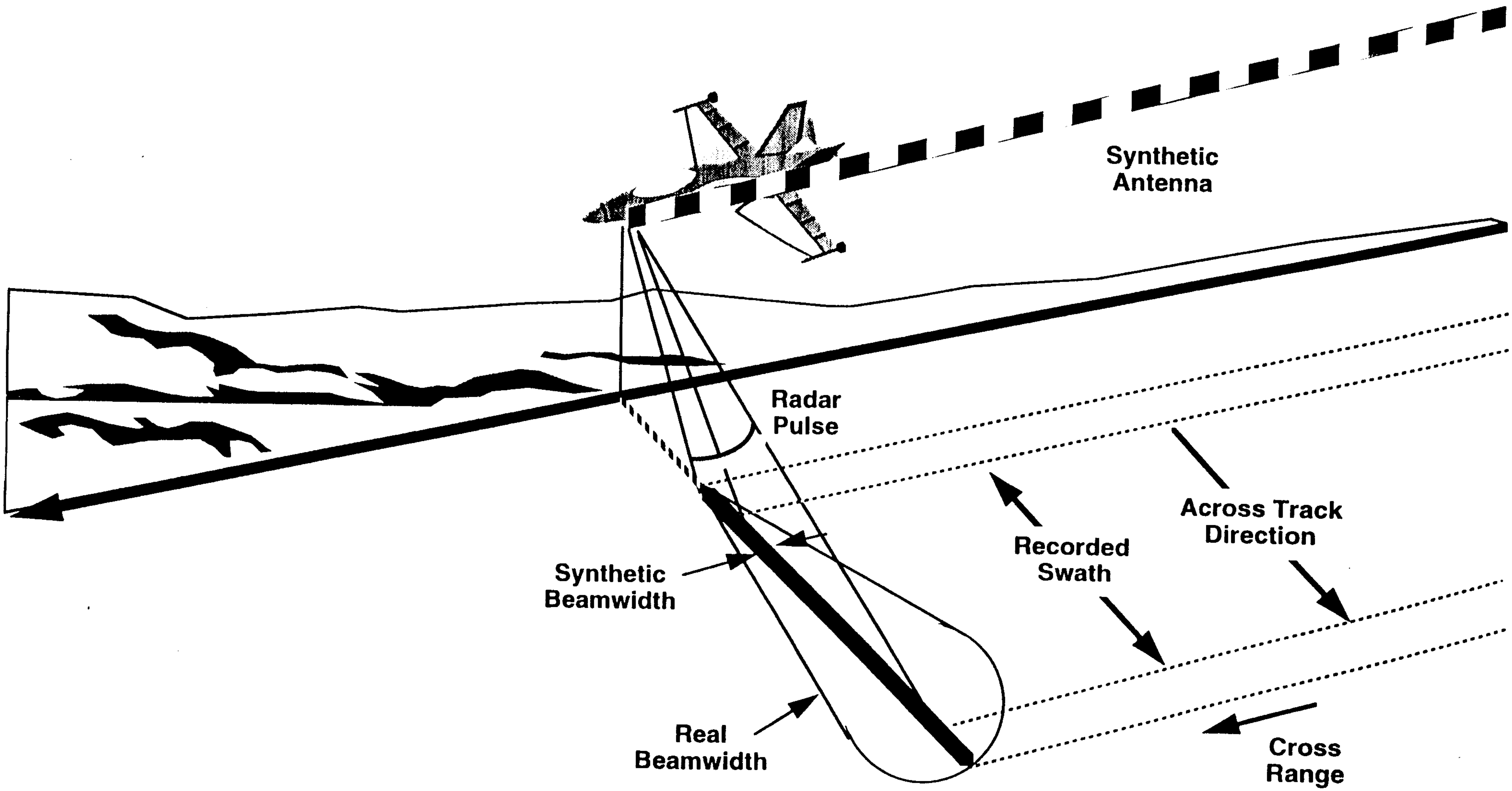
System Costs, End-To-End

War Breaker

Surveillance & Targeting

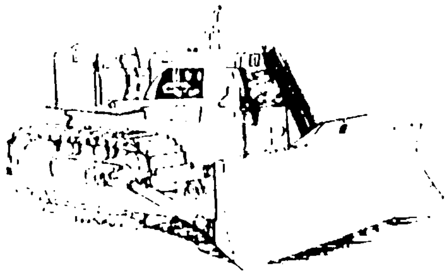


Synthetic Aperture Radar

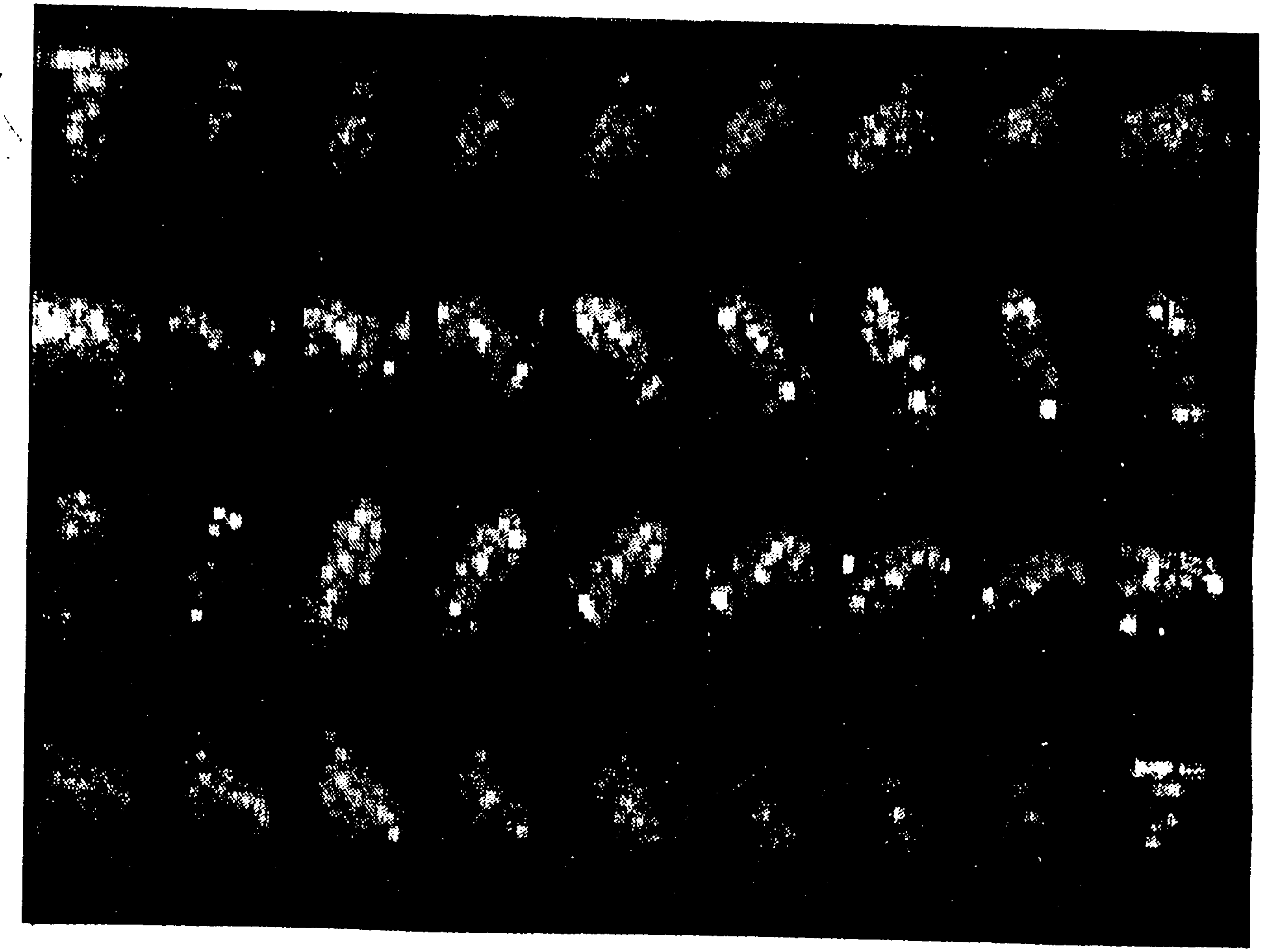


ISAR Target at Different Angles

STO



Color Map



1' x 1' Resolution, PWF Images, 10° Increments

High-Leverage ATR Application Program Candidates for Near-Term Transition

War Breaker

Surveillance & Targeting

- **Clipping Service -**
  - Onboard imagery screener to minimize downlink data rate
- **Dragnet -**
  - System for detecting, recognizing and tracking high-value moving ground targets in traffic, to avoid unaffordably rapid sensor revisit
- **Monitor -**
  - ATR combined with integrated suite of false-alarm mitigation strategies to dramatically reduce the information load on image analysts (IAs)

Clipping Service
Motivation

- **HAE UAV data rate vs. cost of wide-band satellite communications**
  - 40,000 sq nmi/day means at least 112 Mbps peak data rate
  - Compression to 7 Mbps is state of art
  - World-wide high-bandwidth SATCOM costs roughly $60M/year, for one UAV per theater
  - Need additional compression, to under 1.5 Mbps, for true affordability

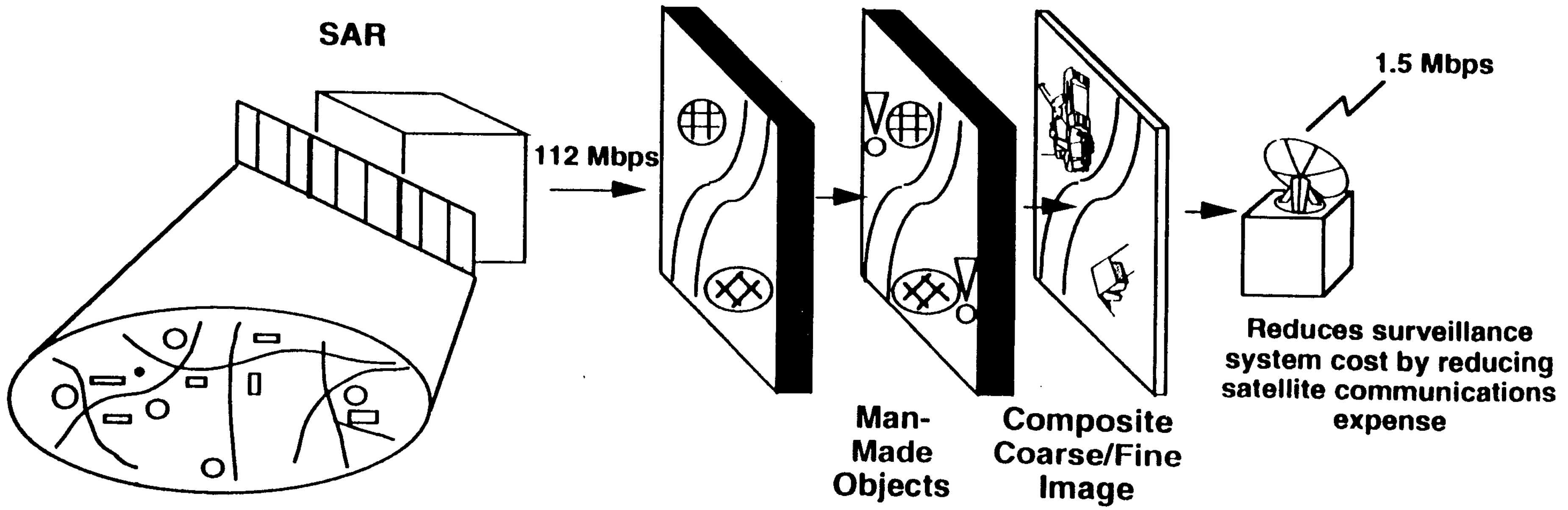
Clipping Service
Technical Concept

War Breaker

Surveillance & Targeting

- **Onboard imagery screening**
  - Onboard ATR detects likely vehicles by measuring "man-madeness"
  - Chips containing detections are downlinked at full resolution; remainder downlinked at coarse resolution

- **Application is inherently false-alarm tolerant; man-madeness detection and multiscale SAR image formation are maturing**



Dragnet Motivation

War Breaker

Surveillance & Targeting

- Mobility of time-critical targets vs. unaffordable cost of rapid revisit
  - Exposed TEL stands still for less than half hour, in transport for less than half hour
  - WAS SAR today can ID exposed stationary TEL but cannot support 30 min revisit
  - WAS MTI today can support very rapid revisit but can't ID anything

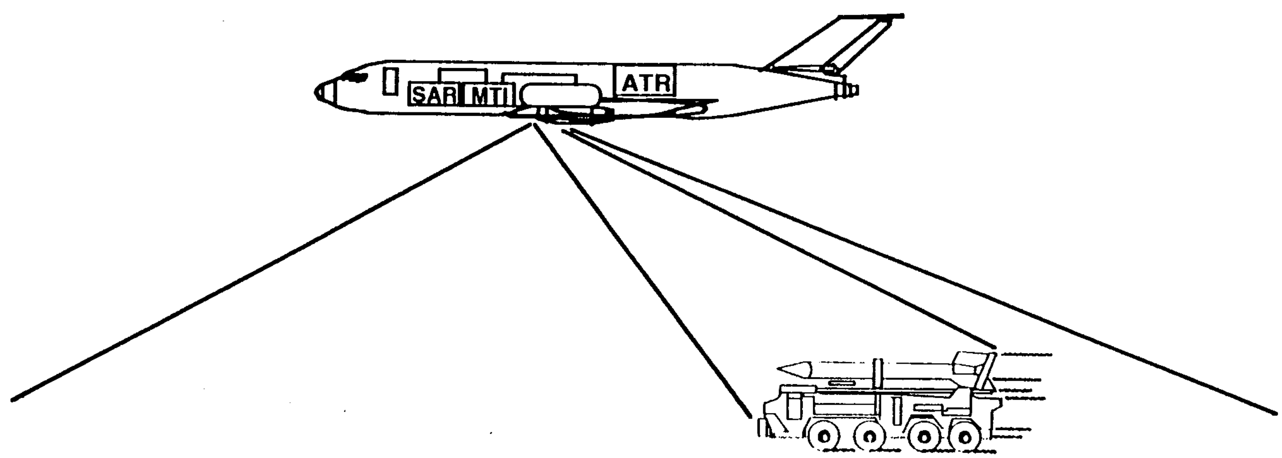
Dragnet
Technical Concept

War Breaker

Surveillance & Targeting

Autonomously detect, recognize, and track high-value moving ground targets in traffic by cueing moving target SAR image formation with high-resolution MTI

- Moving ground targets are much more amenable to ATR than stationary targets
  - Uncamouflaged
  - Doors closed, equipment stowed
  - MTI ideal for detection and aspect determination



War Breaker

Monitor Motivation

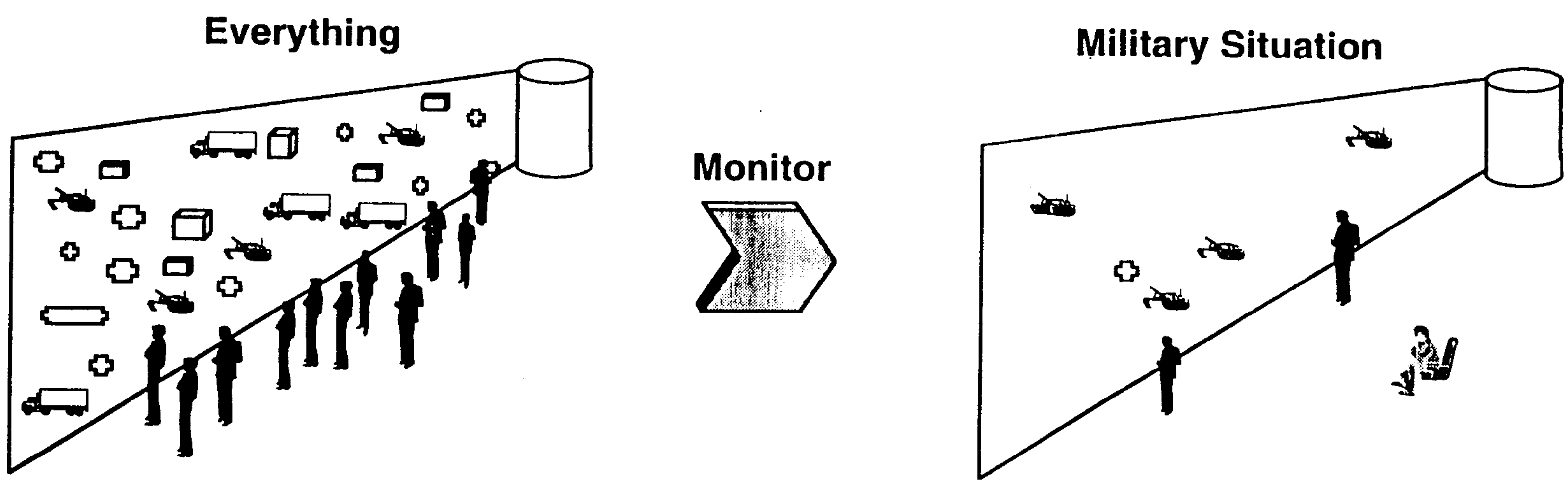
War Breaker

Surveillance & Targeting

- **Volume of HAE UAV data vs. shrinking image analyst (IA) population**
  - Low-cost commoditization of wide-area sensing requires low-cost commoditization of wide-area exploitation
  - Desired: Two IAs per platform, self-sufficient, and deployable at will

Monitor
Technical Concept

- Combine present-day ATR with an integrated suite of novel false-alarm-mitigation techniques to dramatically reduce information load on IAs
  - Image superresolution - to optimize ATR signatures
  - Object-level change detection - to eliminate recurrent false-alarms
  - Cluster enhanced ATR (doctrine-free) - to exploit tendency of most military vehicles to travel in packs
  - Structure modeling - to mitigate urban clutter



MSTAR Technology

(Moving and Stationary Target Acquisition and Recognition)

War Breaker

Surveillance & Targeting

- Vision: Target recognition with performance of $P_d = 0.9$ and 0.001 false alarms per km^2 against partially obscured targets with CC&D
- Program
  - Focused thrust in SAR model-based recognition
  - University ATD/R Initiative

ATR and wide area surveillance

Model-Driven Reasoning

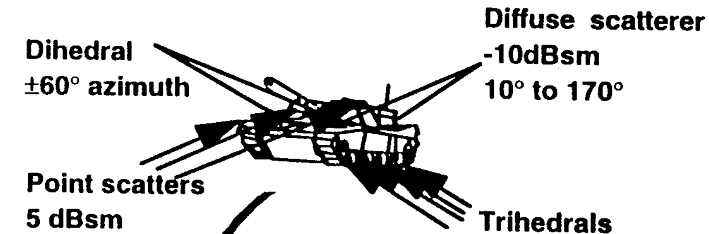
ARPA
War Breaker
Surveillance & Targeting

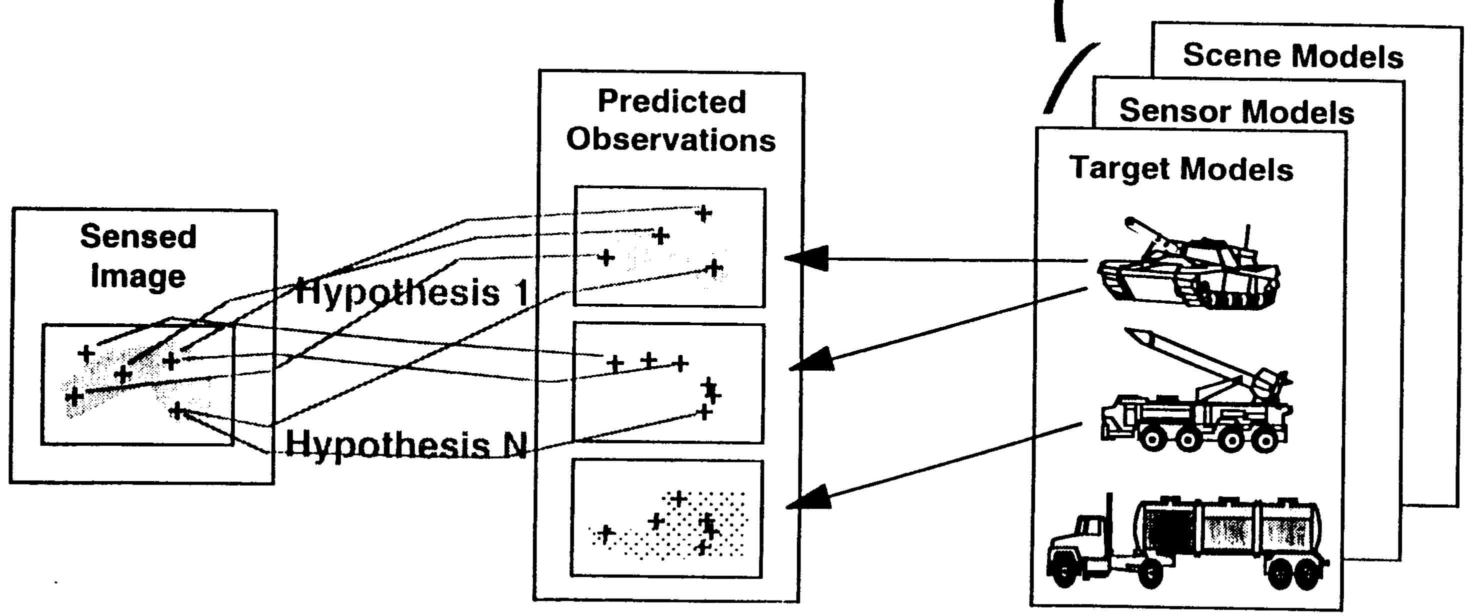
Data Sets

- CAD models
- EM theory
- EM codes
- Turntable measurements
- Rail SAR measurements
- Airborne sensor measurements

Model Development

Target Model





ATR and wide-area surveillance

The University ATD/R Initiative

War Breaker

Surveillance & Targeting

- **Motivation**
  - Open field to hitherto untapped source of creativity, experience and energy
  - Draw fresh talent into field at formative career stage
  - Spread appreciation of <u>military</u> ATR challenge through teaching
- **Demographics**
  - 20 projects, 17 universities/consortia, using common development environment, and data from <u>real</u> military operational/testbed sensors
- **Research Emphasis**
  - Application of novel techniques (e.g. wavelets, fractals) and understanding of fundamental limits
- **Accomplishments**
  - After less than one year, five university ATR component products evaluated on Lincoln Laboratory algorithm testbed
  - Two outperform existing Government-sponsored baseline

Profile of University ATR Projects

War Breaker

Surveillance & Targeting

- Conservative/evolutionary development and critical look at status quo (7)
- Novel end-to-end system development (4)
- Multiscale ATR (3)
- Novel wavelet techniques supporting ATR (3)
- ATR in novel combinations (2)

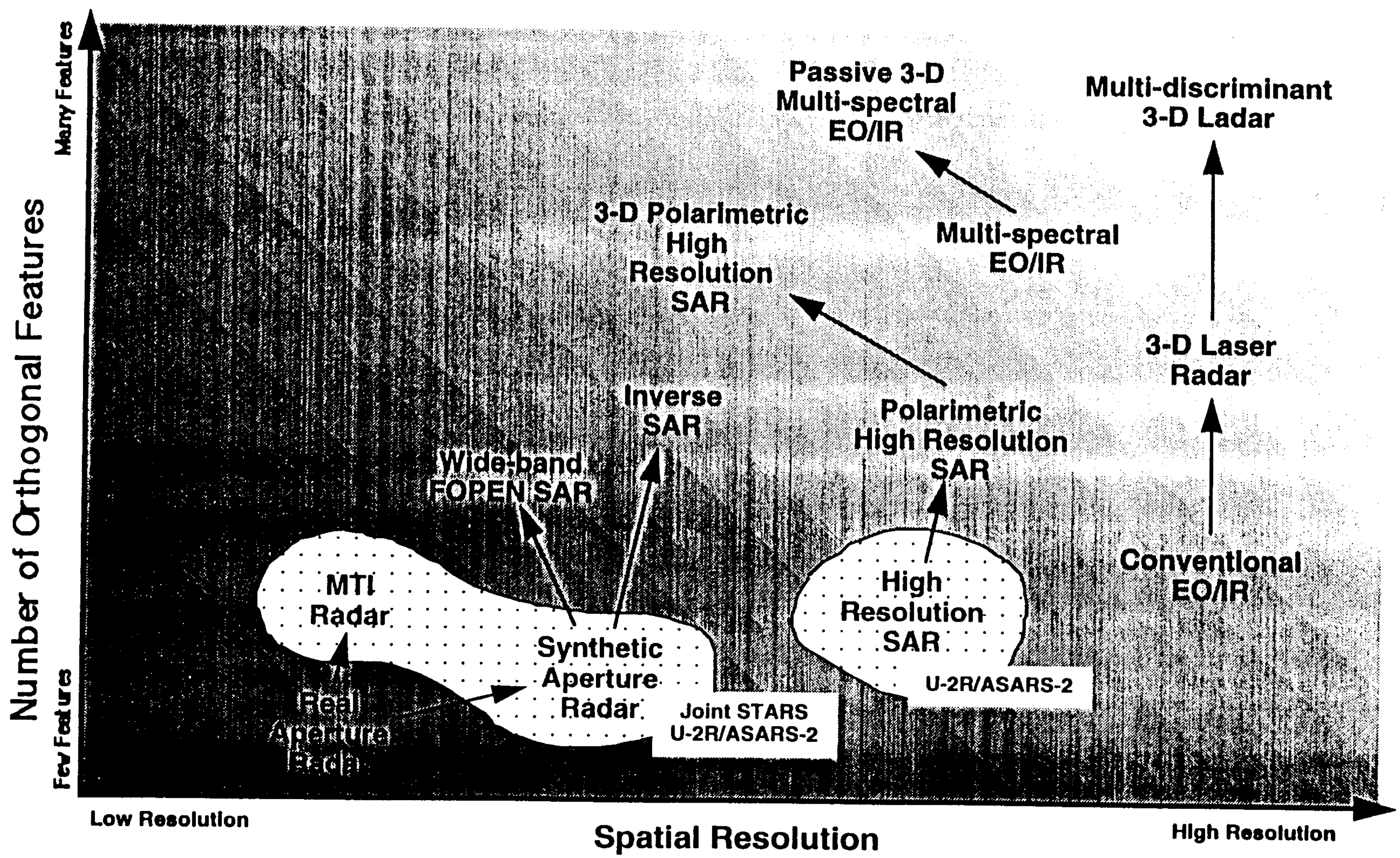
SAR ATR Processor Sizing
Tier II plus

- Image formation, search: 20 GFLOP/s peak
  - 1 m stip map, 40,000 nmi^2/ day, 50%daily cycle
- Prescreener for Tier II Plus search: 547 MFLOP/s peak
- Discriminator for Tier II Plus spot: 640 MFLOP/s
  - 0.3 m IPR
  - 2 km X 2 km spots
  - 100 spots/hour
- Classifier for Tier II Plus spot: 700 MFLOP/s

Future Data Processing Challenges

War Breaker

Surveillance & Targeting



ATR and wide-area surveillance

ATR Algorithm Development Using Khoros

Professor Robert A. Hummel

New York University

ATR Algorithm Development using Khoros

(1) Perspectives on ATR, and the concept of multisensor systems

(2) An ATR Project at NYU

Robert Hummel, NYU

Page 1

This talk is concerned with the use of simulation and computer modeling for ATR applications. We begin with some perspectives on ATR, both the need and the algorithmic underpinnings, and then discuss some of the methods that are being used in the NYU ATD/R project funded by Arpa in the MSTAR University Research Initiative.

Simulation impacts on ATR in three ways:

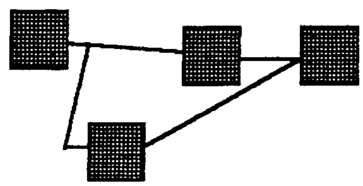
• In order to recognize a target, a system needs a model of the target, and must compute a comparison between the observed object and the targets as predicted by the models. The computation often requires supercomputer potential on an embedded system.

• In developing the ATR algorithms, researchers *simulate* an embedded system, using software tools that enable them to build a virtual ATR system. This aspect is more challenging than it seems, and is greatly facilitated by advanced software tools.

• ATR must be trained and tested against a large database of imagery. Since acquisition of sample images is expensive, it is imperitive to develop test scenes and realistic background clutter through simulation methods.

What is Khoros?

- A poor-person's AVS
- An image processing visualization system
- A visual programming system



An Arpa-funded project at Univ of NM

Now distributed by Khoral Research, Inc

Robert Hummel, NYU

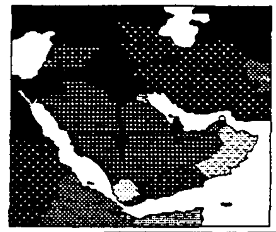
Page 2

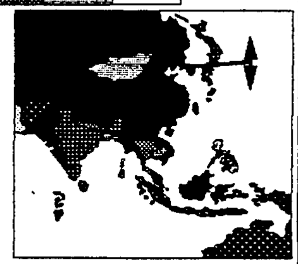
This talk is a call for advanced software tools for supporting research in ATR, especially in the aspect of simulating an embedded system by a laboratory system. Khoros is a visual programming language for image processing, funded by Arpa, that supports this goal, and can be considered a prototype model of software tool development.

An issue to consider in the development of software tools through government funding is the extent to which the publically-available software displaces commercial software that helps to drive a software industry.

ATR Challenges

- Find Mobile Missile Launchers, TELS
- Expose massed armor movements
- Separate true targets from confusers, decoys, even when counter-measures are applied
- Target munitions, submunitions, and provide surveillance aids





Iraq had hundreds of Scuds, shot over 80 during ODS, and effective opposition capabilities were, and remain, minimal

Robert Hummel, NYU

Page 3

ATR is experiencing a resurgence of support and military interest, in part motivated by the desire to locate missile launchers from platforms flying in combat air patrol missions.

However, ATR in general has many other potential applications.

To partly explain the level of interest, consider how different the world would be if the act of moving a tank or a missile launcher, or firing a mortar, constituted an extremely risky action. In order to deter hostile action, one needs information, and surveillance and detection requires analysis, which needs to be automated by ATR

ATR Sensors

- Sensors:
  - FLIR, Second Generation and FPA's
  - Multispectral E/O, "color" in multiple spectral bands
  - Radar: X band and MMW
    - High-resolution 1-D, polarimetric
    - Doppler beam sharpenned modes
    - SAR, spotlight and strip modes
    - Moving target detection
    - Vibration modes
  - Ladar
    - Time of flight ranging
    - Interferometric methods for ranging
  - Lidar
    - Chemical composition of effluents

Robert Hummel, NYU Page 4

ATR can make use of many different kinds of sensor inputs. The most common sensor systems for ATR include FLIR and SAR, but real-beam radar, LADAR, and even LIDAR (to, for example, examine exhaust characteristics of vehicles) can be included.

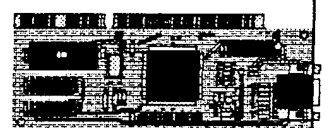
The most interesting and successful ATR systems will make use of multiple sensor inputs, and attempt to fuse the information, either by running separate ATR algorithms on each sensor modality and combining the decisions, or better, by combining features from different sensors.

It is important to model the sensor as well as modeling of the targets, since simulation of the imagery, as well as recognition of the targets, depends on an understanding of the sensors.

ATR Processors

- Processor Power is no longer a problem
  - On-board processor capabilities far exceed what the academic community normally expects
  - Typical architecture: Multiple Sparc SBC's, a MIMD or pipeline multiprocessor, and a SIMD mesh array computer
- Memory is no longer a problem
  - Hundreds of megabytes can be assumed, for a price
  - Rapid processing reduces memory needs

The challenge is in the "algorithms" for detection and recognition



Case Study: Aladin processors, 0.5 Gflops

Robert Hummel, NYU Page 5

One of the reasons that ATR is increasingly realizable is that processor power is now commensurate with the needs. Massive computer power (throughput) is required, but processing needs are highly parallel. Further, by making the ATR system hierarchical (proceding from detection to recognition and identification), processing power can be concentrated on small regions.

An example program to develop processors for ATR application is the Aladdin program, funded by Arpa and administered by NVL-ESD. This program has developed two different form-fitted half-gigaflop multiprocessors, and especially notable for developing large-scale wafer microprocessor manufacturring. The processors are small (four inch diameter), and the biggest problem is heat dissipation. Increasingly, the recognition processing can be combined with the image formation (as in processing raw radar return as opposed to image formation). Unique algorithmic methods are as important as processor capabilities.

Operational Algorithms in ATR Systems

- ATR systems are now being built!
- What are the embedded algorithmic methods?
  - Statistical pattern recognition
    - Radar CFAR algorithms, Quadratic classifiers on multiple simple features
  - Matched filtering
    - Often on edge images
    - Carefully constructed filters, whittenning filters
  - Logical matched filtering
    - Same as matched filtering, but using AND and OR's in place of weighted sum
    - E.g., Hausdorff measure; Hierarchical Generalized Hough Transform

Examples: MUSTRS and DAMOCLES

Comanche has a planned multisensor ATR !

There have been a number of prototype ATR systems built and tested. The ATR algorithms are still wanting, but there has been some level of performance. The algorithmic methods tend to be simple, and rely heavily on matched filtering (convolution-based matching) using edge maps (edges extracted from the literal imagery). More sophisticated methods involving model-based vision are similar, but use logical connectives (and's and or's) instead of the convolutions in matched filtering, which means that FFT methods cannot be used for processing.

We mention the MUSTRS project, which developed an embedded ATR system for the advanced cruise missile (now cancelled), which developed a multi-sensor multi-look system that combines decisions from SAR and FLIR ATR's to improve ATR performance. The on-board processor includes a 196 by 480 SIMD 2-D mesh of processors, as well as quad i860 boards for SAR processing.

The DAMOCLES project is wild. This submunition, being developed by Textron, includes an Aladdin processor (using C40's instead of C30's) and high throughput to detect targets using real-beam radar and FLIR. The scenario includes launching an ATACM, dropping the DAMOCLES submunition, which parachutes toward the target, with a rotating body used to scan the region, and a "hockey-puck" munition tossed from the DAMOCLES body. The intended fielded cost of the submunition is $25K per unit.

The key to ATR is stable feature extraction

- Geometric hashing, and any matching scheme, depends on stable features
- Features must be rich, descriptive, and discriminative of the object
- In order for the Bayesian result to work, features should be *independent*
  - This means that under the assumption of the presence of a model, knowledge of a particular feature provides no support for presence or lack of presence of other features
  - Features for the model are already known to be present
  - E.g., line edgels are not independent
    - Bad news for many systems
    - But corners, with angle bisectors, are independent

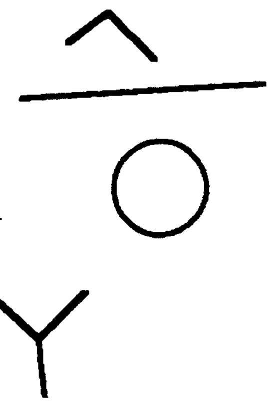
The NYU ATR project is emphasizing the development of advanced features for matching target models against images. The matching techniques need to be efficient, but the key to ATR is in the use of descriptive features. Whereas edges are currently the main source of features, we believe that corners, blobs, tricorners, and other features offer promise for using internal detail of targets in order to enhance the recognition capabilities.

In order to develop useful feature extractors, software tools are needed and simulation facilities must be disseminated in order to develop and test different kinds of ATR algorithms. Likewise, databases of example images, both synthetic and real, need to be made available.

Robert Hummel, NYU Page 7

Feature operator design is facilitated by the use of Khoros

- Corner detection
- Edge detection
- Circle detection
- Multicorner detection

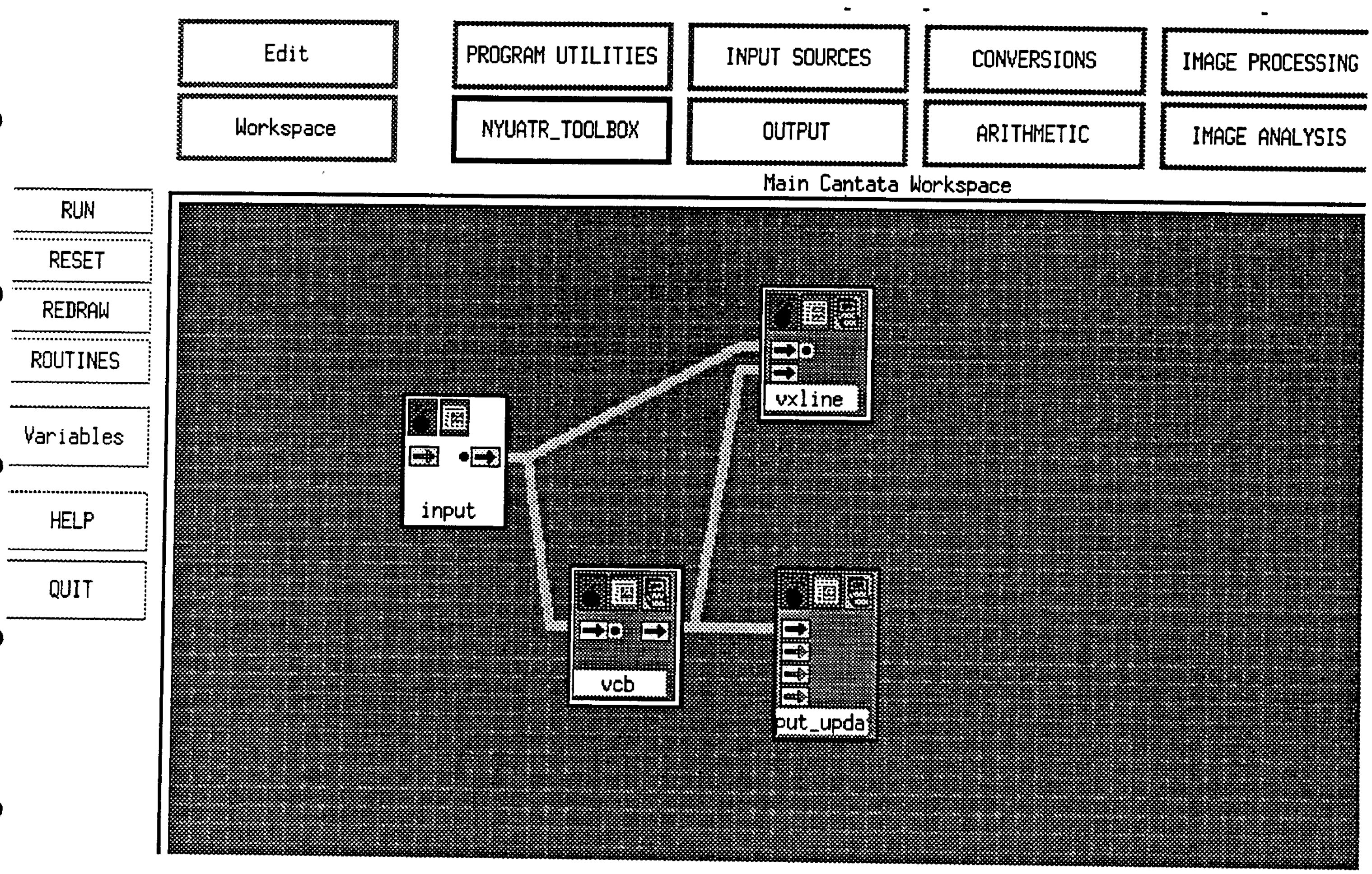


Robert Hummel, NYU Page 8

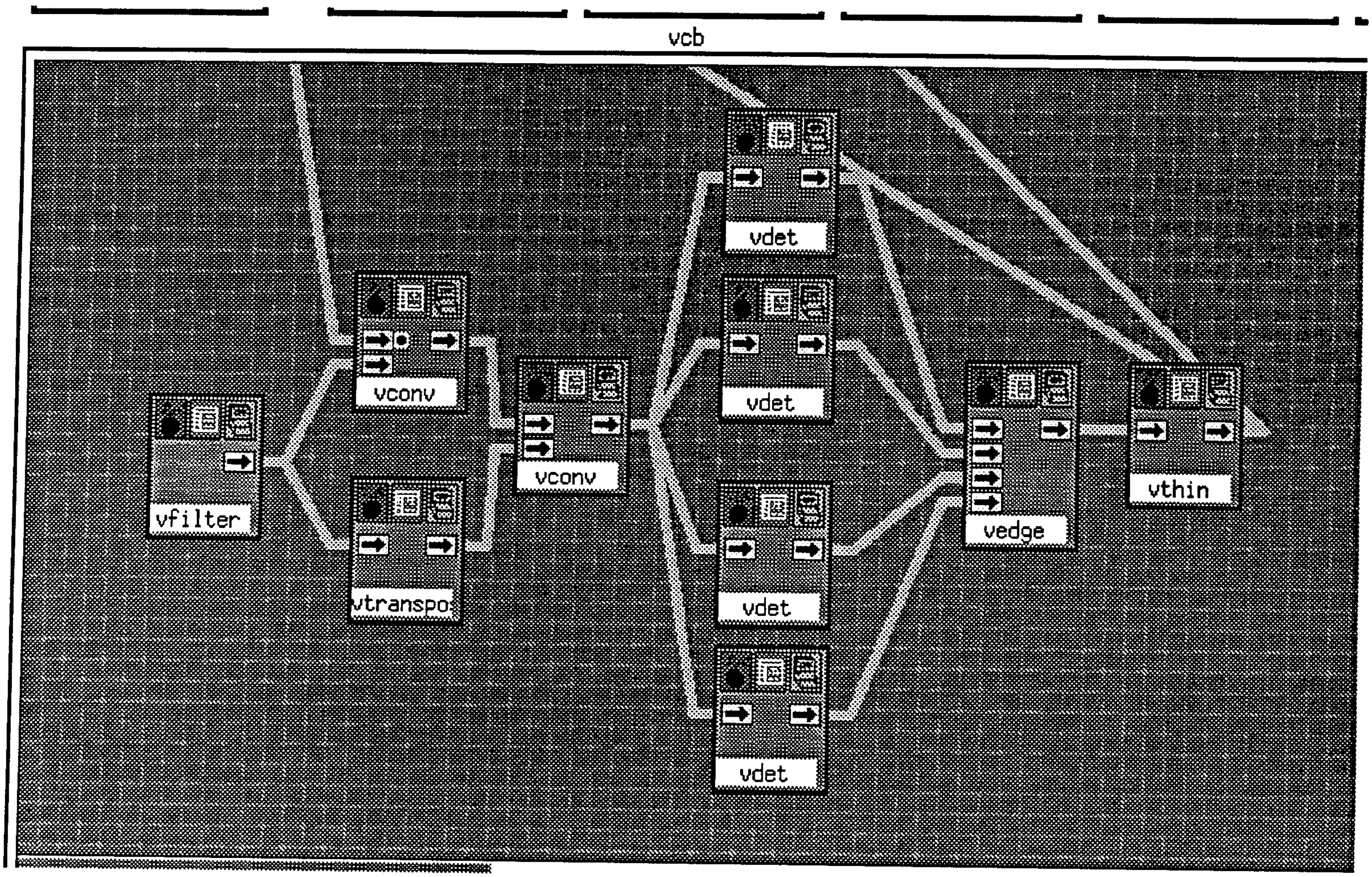
The remainder of this presentation demonstrates the use of the software system Khoros for the development of feature extraction methods, together with preliminary results of object recognition.

We first show some example Khoros "workspaces" containing multiple glyphs, which are the programming modules of Khoros (in a visual display system called "cantata"). We also show some example FLIR imagery, and an example of simple experimental enhancement, facilitated by the use of Khoros modules. We demonstrate feature extraction, showing circle extraction, corners, edges (represented by midpoints), and an image whose magnitude gives the curvature magnitudes of isocontours, which should be useful for corner detection that is independent of edge extraction. The recognition result is based on using color EO imagery (from a TV camera), and models of an M60 tanks.

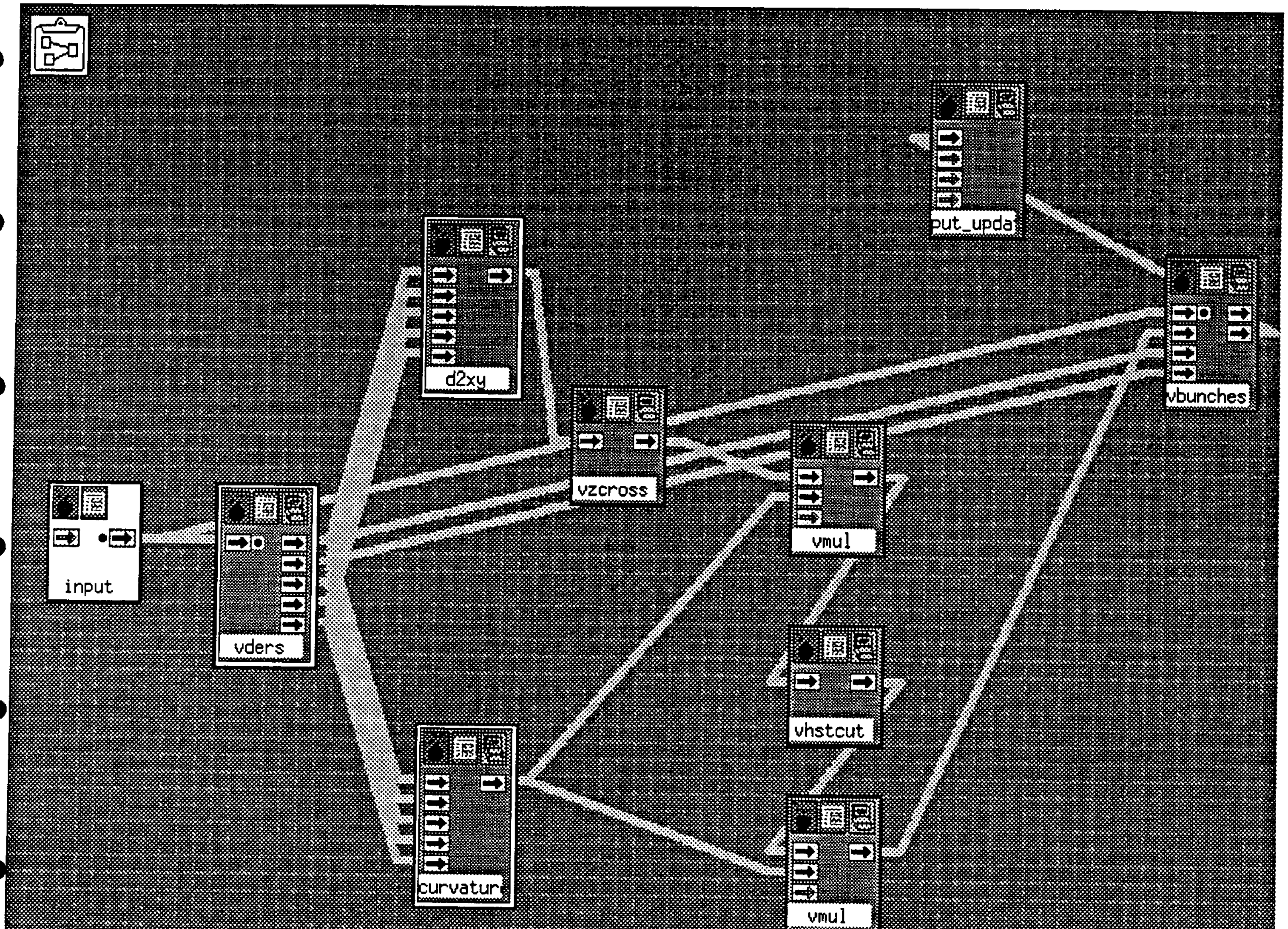
Most of the results and work represented by these examples were produced by NYU graduate student Jyhjong Liu.



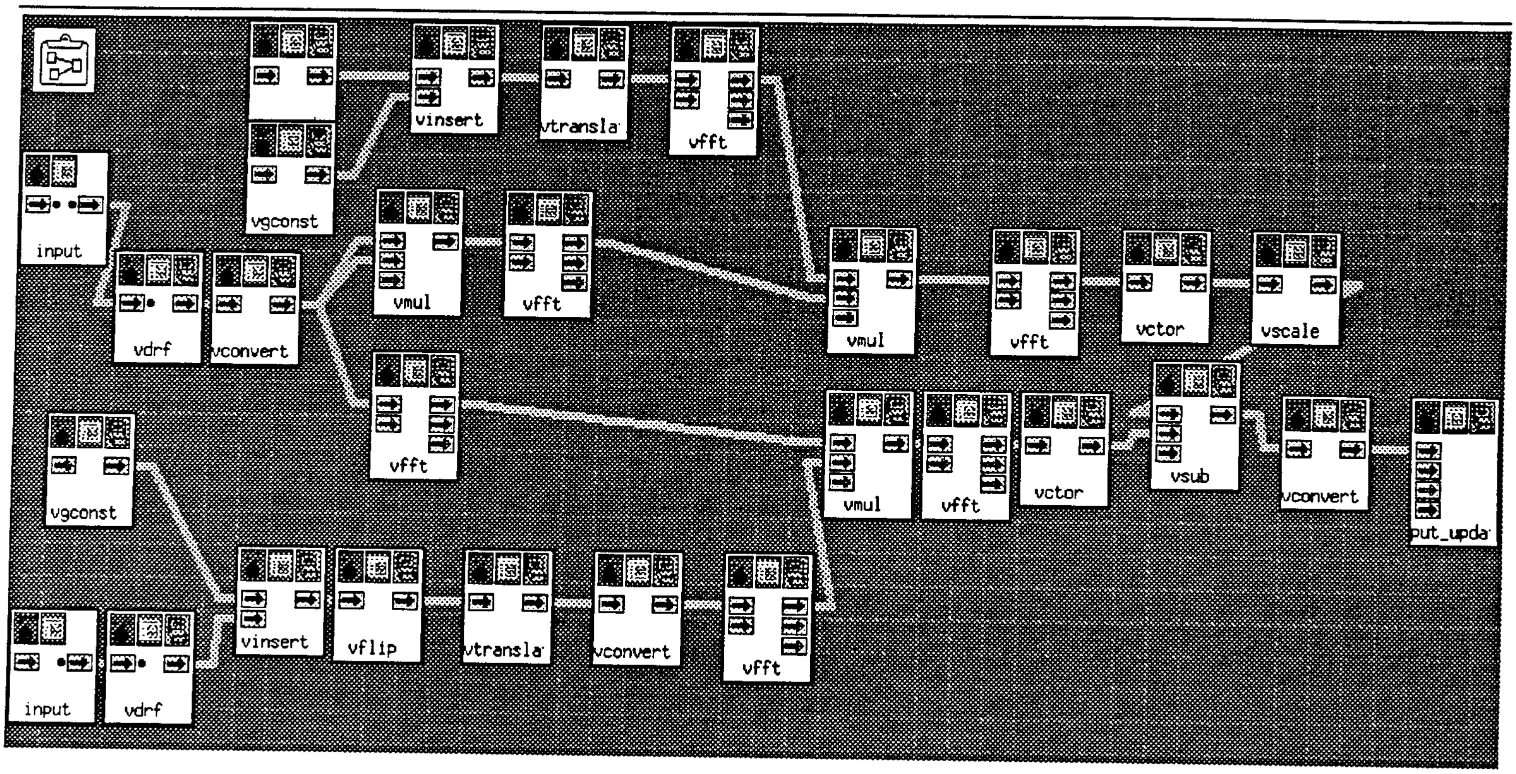
This is an example of the Cantata workspace with a number of glyphs, used to extract edges. The glyph at the left is an image input, and the other glyphs extract edges, fit lines, and display results.



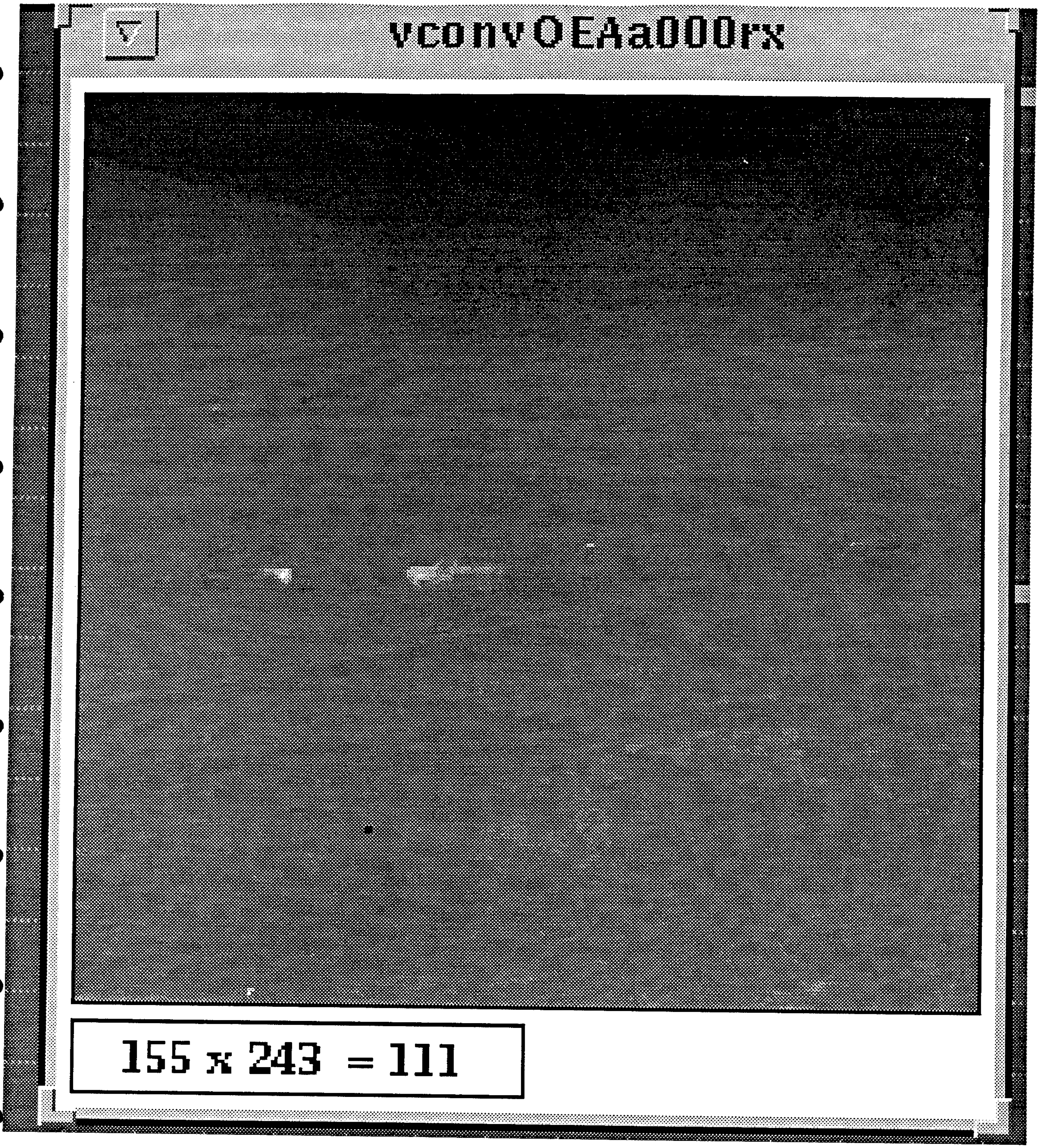
Glyphs are hierarchical. This workspace is an expansion of the vcb glyph from the previous workspace.



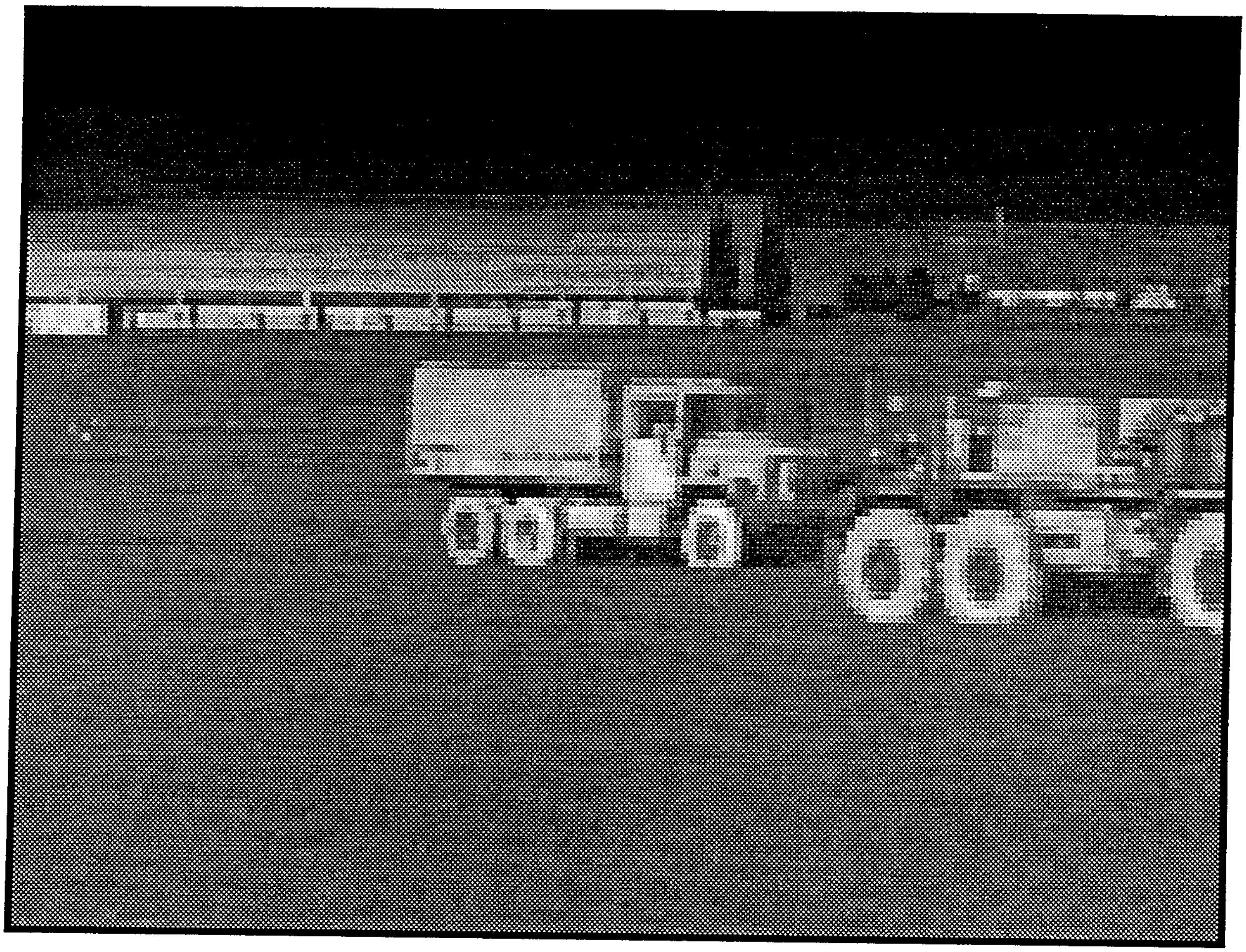
This workspace is used to compute and display points of high curvature computed as large magnitudes of the curvature of isocontours.



This set of glyphs is used to compute a normalized convolution. Note the use of the fft in order to perform the convolution in a reasonable amount of time.

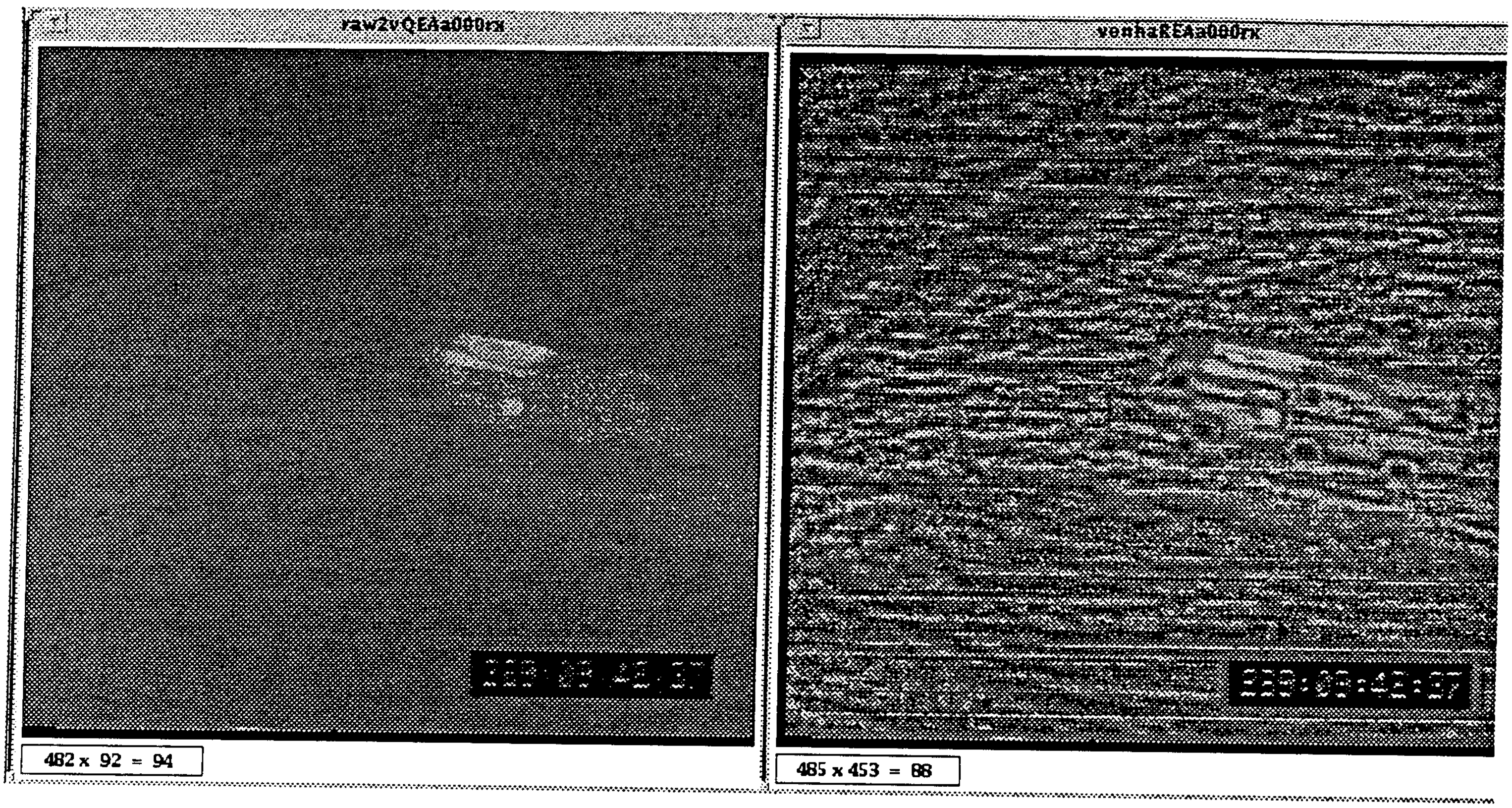


This is a first-generation FLIR image of some trucks. Note that the engine compartments show up more brightly than the rest of the vehicles.

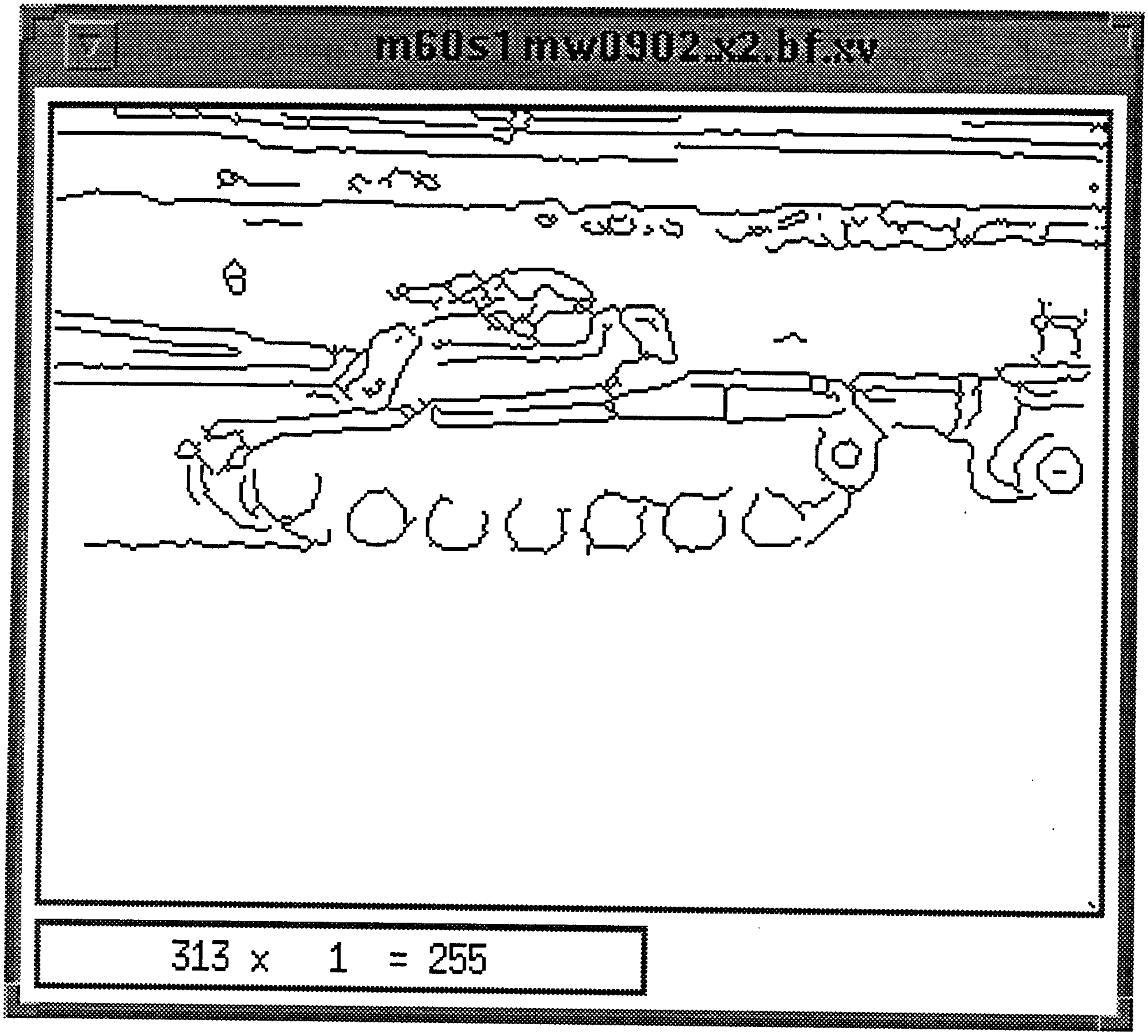


These M35 trucks are viewed in short wave (3-5 mm.) FLIR, in low resolution. In this spectral region, the objects are less emmissive and more reflective.

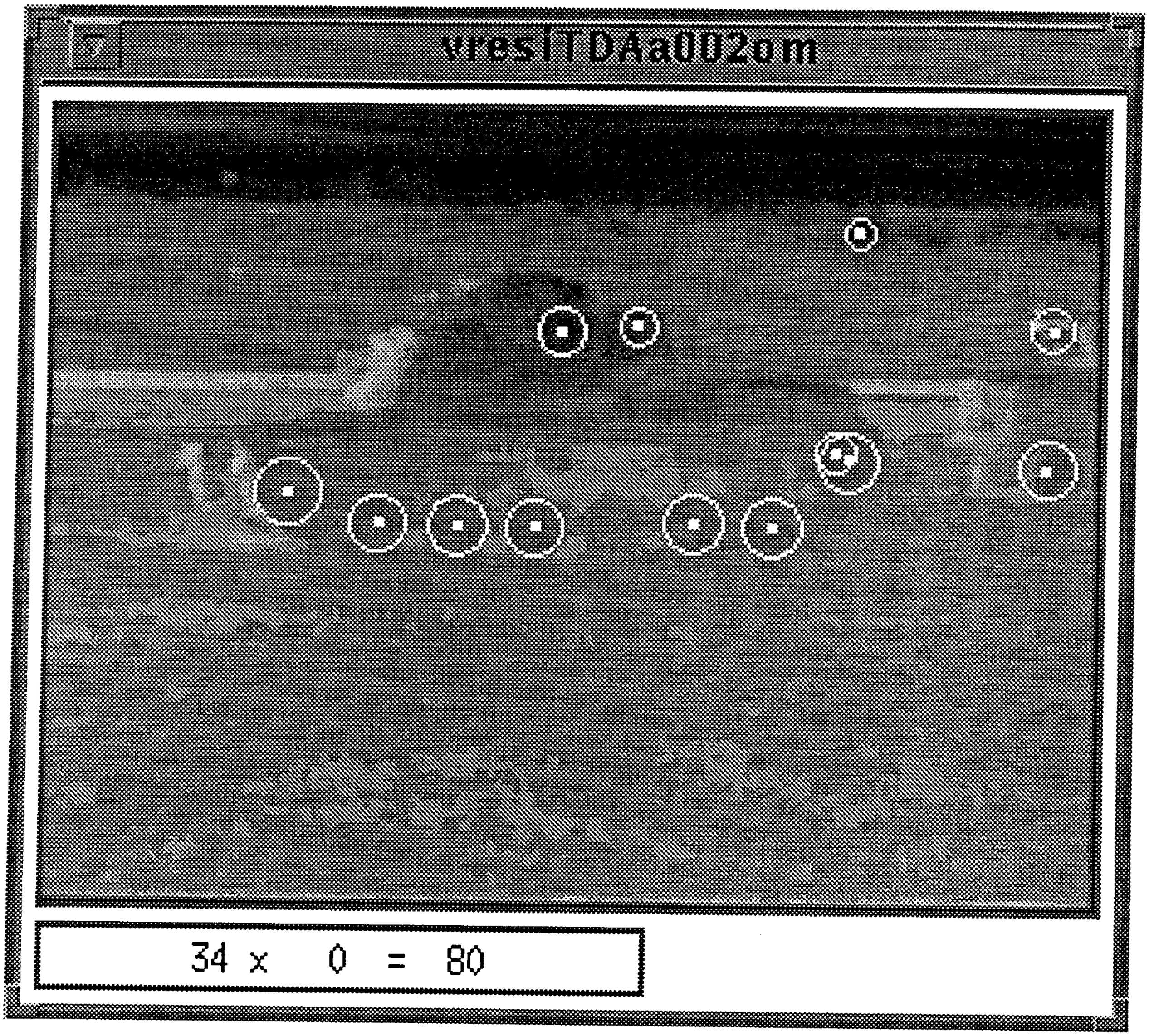
This is a mobile missile launcher, viewed with a second-generation FLIR. Note how the target is washed out due to the lack of temperature variations.



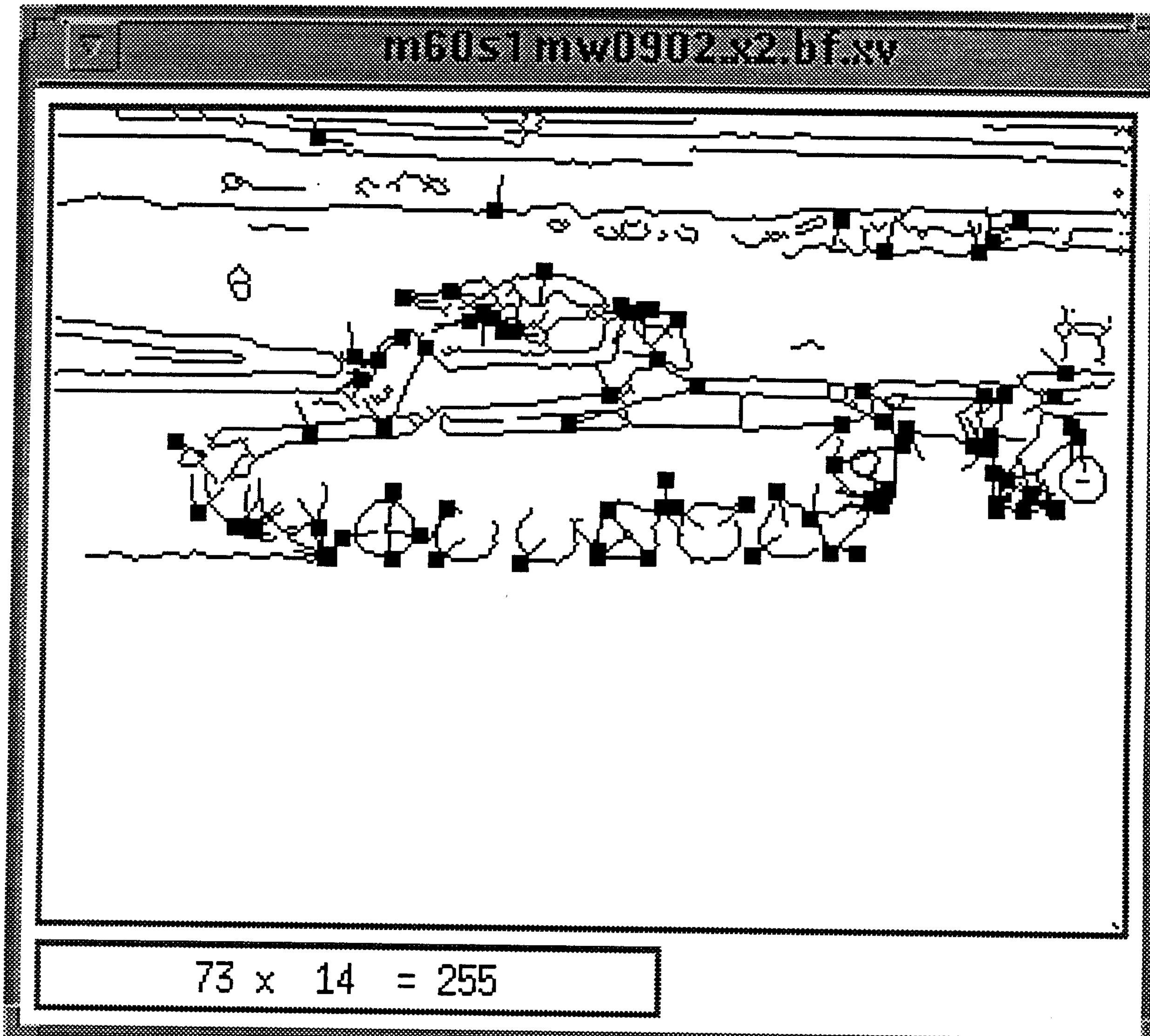
This view of a mobile missile launcher, which is slightly different than the previous, has been subjected to a simple enhancement algorithm, available as a single glyph in the Khoros module set.



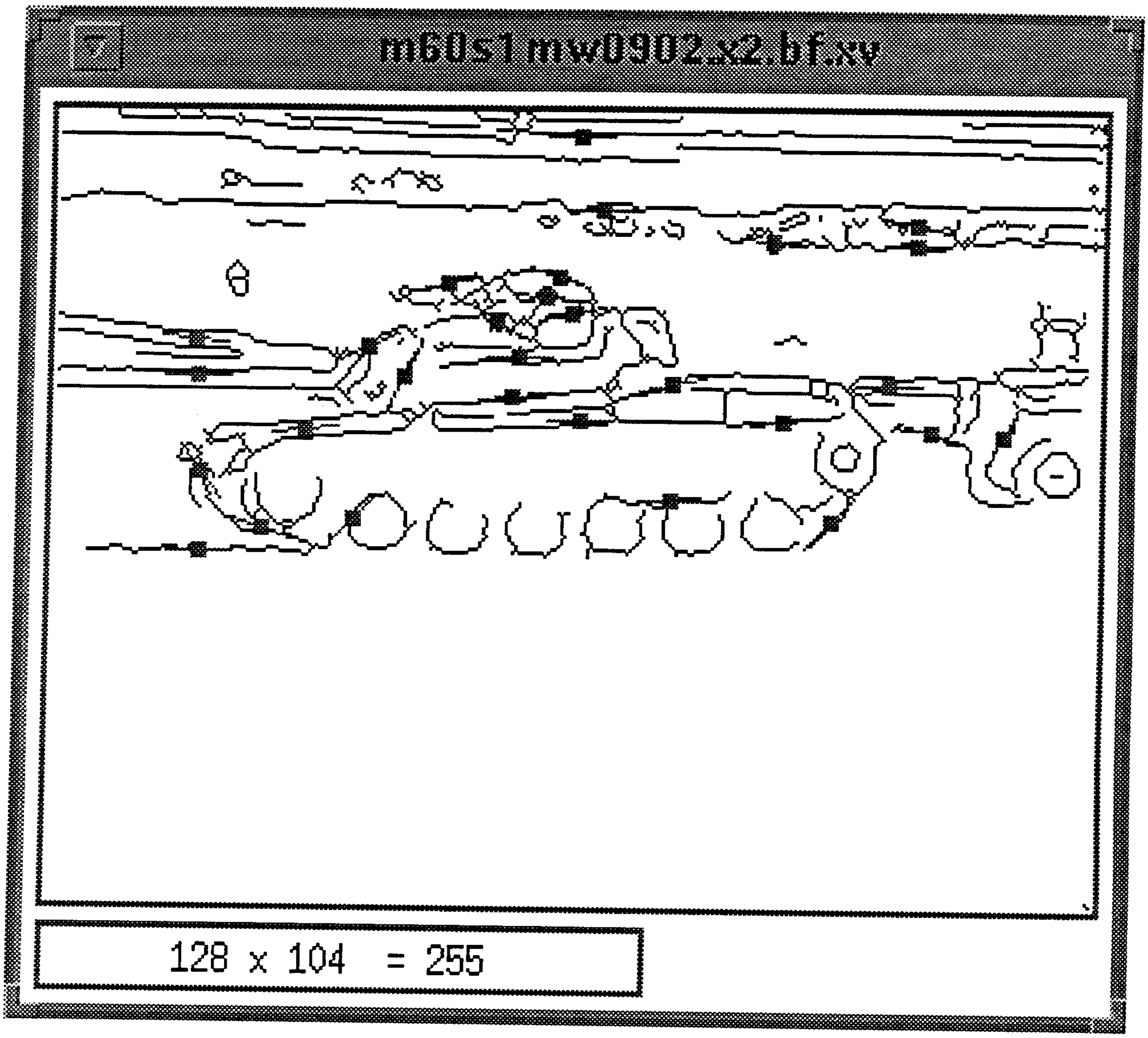
These are the edges extracted from a FLIR image of an M60 tank.



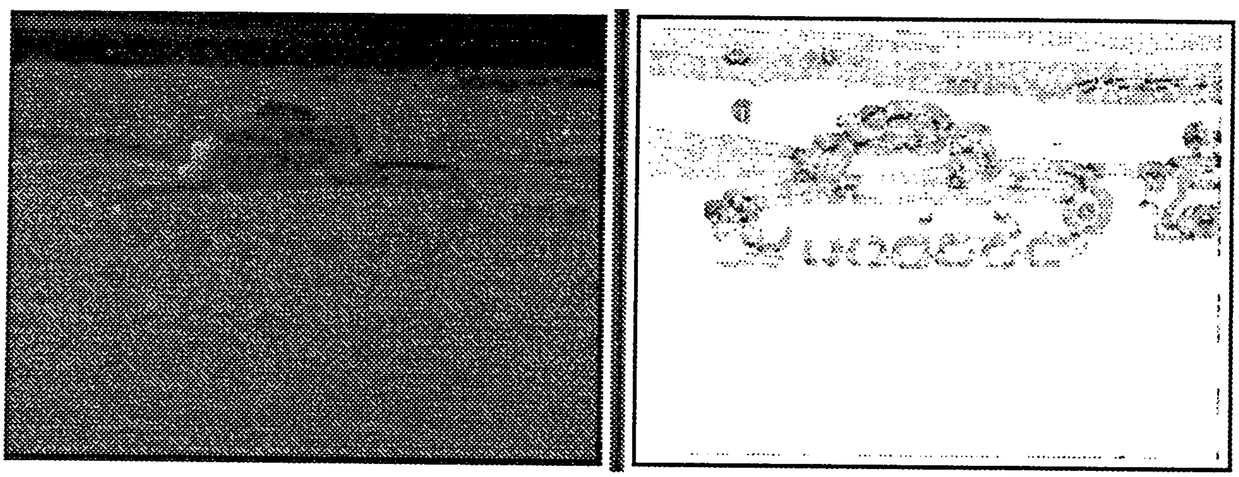
The results of a circle detection algorithm, based on the Hough transform, are shown here.



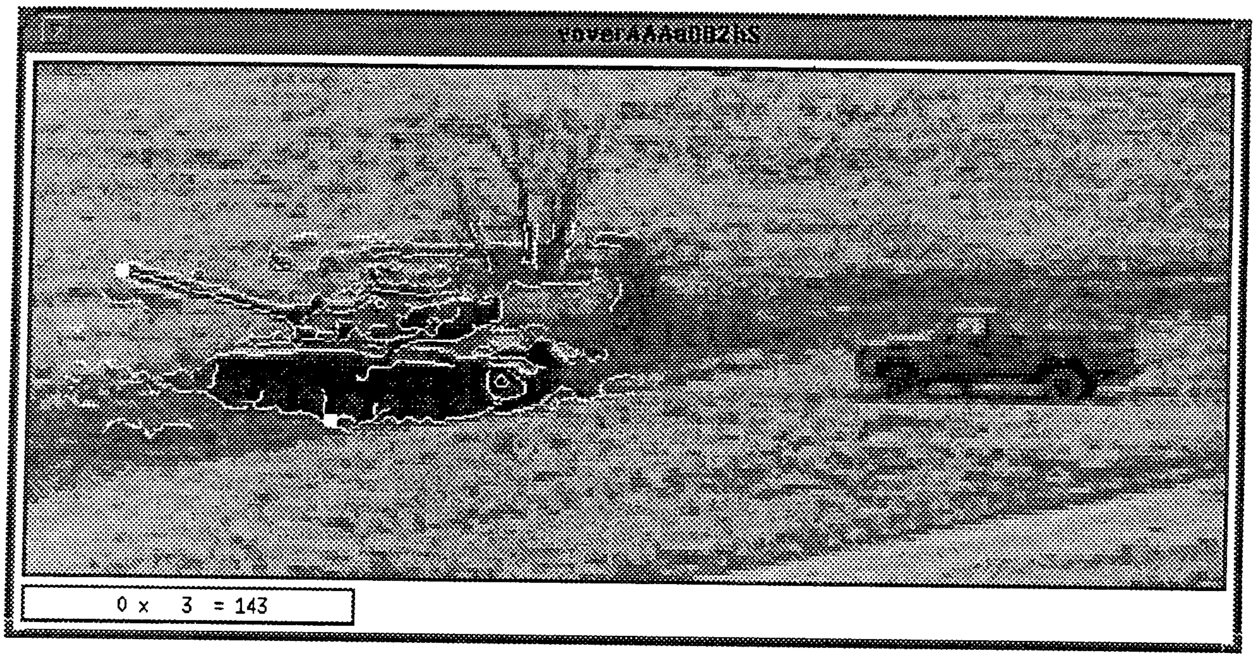
The points mark the locations of corners, with the bisectors of the corner indicated by short lines, representing oriented corner features.



The points and lines mark the midpoints and orientations of straight line segments fitted to the edge detection results.



The darkness of the pixels on the right represent the magnitude of the curvature of the isocontour passing through the point in the image on the left.



This is a preliminary recognition result based on matching of edges to a tank model.

Appendix D

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This document summarizes a symposium whose purpose was to use more fully the talents of the alumni of the Defense Science Study Group (DSSG) to help ensure that DoD was benefiting to the fullest extent possible from the use of advanced computational methods in academic research. The participants were the alumni of the DSSG, other key academics, and members of the DoD and DOE. The alumni and other academics presented briefings on advanced and innovative ways that computers are being used in academic research, while the members of DoD and DOE presented briefings on their related research. The participants believe that the DoD should continue to reach out to the commercial world and to academia for expertise that could aid the DoD in finding the best ways to implement the use of parallel computing for applications related to scientific and engineering research. They agreed that new techniques of visualizing the results of many of the various applications discussed are needed. The document should help the DoD in continuing its work with the commercial world and academia.

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