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MEMORANDUM FOR PRS (In-House/Contractor Publication)

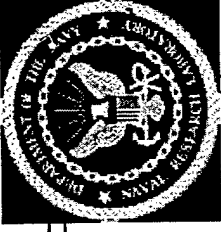
FROM: PROI (TI) (STINFO)

07 Aug 2000

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-TP-2000-162**
I. J. Wysong (AFRL/PRSA); D. C. Wadsworth, D. B. VanGilder (ERC); C. Kaplan, D. Mott
(NRL/LCPFD), "SUPREM-DSMC (CHSSI CFD-8) Software Acceptance Test Review (Draft)"

HPCMO CHSSI Software Acceptance Test Review
(Washington DC, 11 Aug 00) (Submission Deadline: 10 Aug 00)

(Statement A)



SUPREM-DSMC (CHSSI CFD-8)

Software Acceptance Test Review

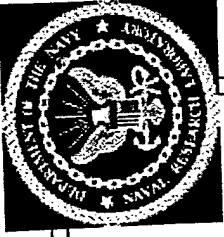
Agenda:

- Introduction and Overview: I. Wysong
- Software Design: D. Wadsworth
- Grid and Geometry: C. Kaplan
- Particle Movement: C. Kaplan
- Gas/Chemistry: D. Wadsworth
- Boundary Conditions: D. Wadsworth
- Status and Conclusions: I. Wysong

HPCMO/NRL
Washington, D.C.

11 August, 2000

Approved for public release; distribution unlimited



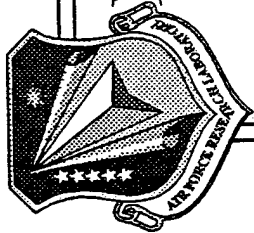
Computational Fluid Dynamics CTA
(Computational Technology Area)
CTA Leader: Dr. Jay Boris

CFD-8: SUPREM DSMC

Scalable, Parallel, Reacting, Multidimensional Direct
Simulation Monte Carlo Flow Code

Awarded: November, 1999

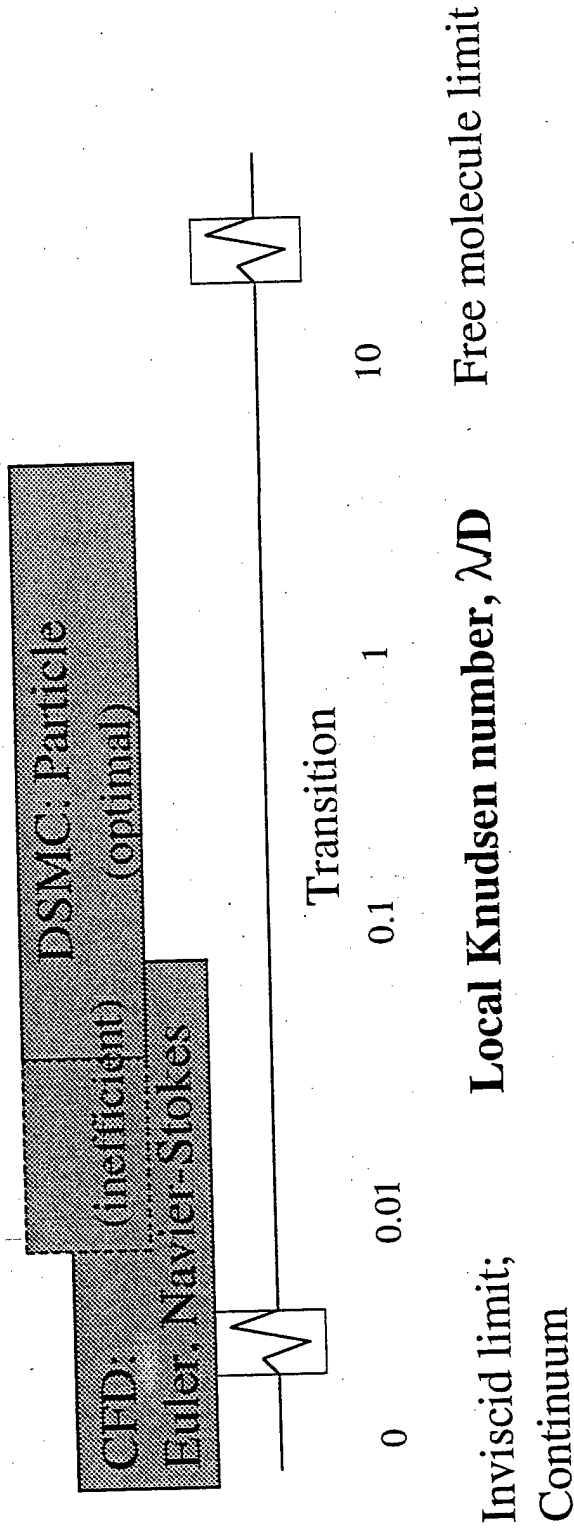
Start Date: January, 2000



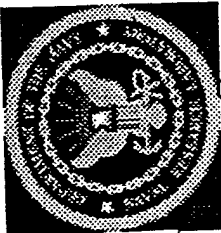
Direct Simulation Monte Carlo method (DSMC)

- Reduced number of model particles represent real gas
- Moved in a grid covering physical space
- Inter-molecular collisions selected statistically from particles in grid cell; physics and chemistry of collisions modeled directly (but phenomenologically)
- No assumption of equilibrium (e.g. N-S eqns.)

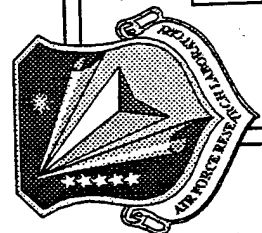
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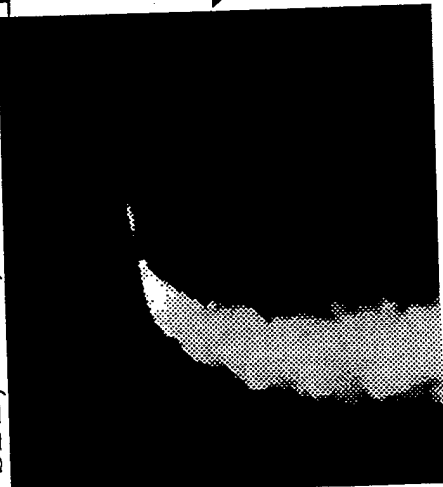
Based on G.A. Bird, "Molecular Gas Dynamics and the Direct Simulation of Gas Flows"



DoD Need for DSMC Simulation Capability:



BattleSpace Environment
Simulation codes:
NTW, THAAD, NMD,
SBL, ABL, SBIRS

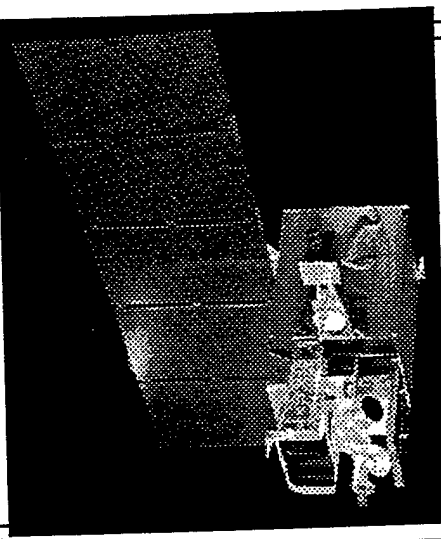


Plasma Processing (etching,
deposition, wafer yield):
Intel, Watkins-Johnson

Micropropulsion, MEMS
(microfluidics):
AF, NASA (JPL), DARPA



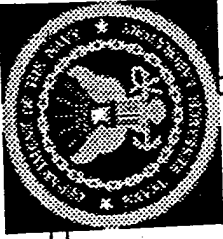
Spacecraft Contamination
(lifetime on orbit):
AF (SBIRS, SBL), NASA



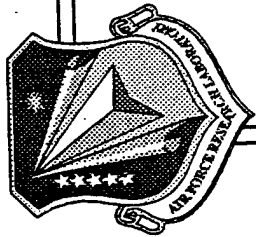
Hypersonic Re-entry Vehicles
(heat transfer, drag...):
NASA (planetary probes, shuttle),
AF(HyTech, Military Aerospace
Vehicle)

insert space

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Integration into HPCMO CHSSI Program



CCM

Molecular Dynamics
Quantum Models

Surface Interactions
Chemical Reactions

PET

CFD

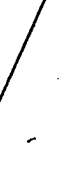
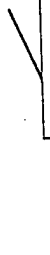
Continuum CFD
Codes

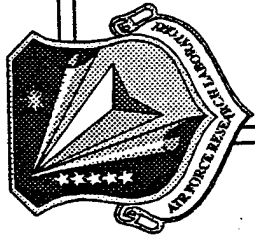
DSMC
Codes

SUPREM

GUI Support
Grid Generation
Post-processing
Data Mgmt?

Fast3D
COBALT
FEFLO
OVERSET
MERCURY-^{3D}NS
ARL Zonal NS
NPARC Alliance
CFD





SUPREM Team:

AFRL/PRSA (Edwards AFB, CA):

Dr. Ingrid Wysong
Dr. Dean Wadsworth
Dr. Douglas VanGilder
Dr. David Campbell

NRL/LCP (Washington, DC):

Dr. Carolyn Kaplan
Dr. Elaine Oran
Dr. David Mott

Grid

Code architecture

User Interface, automation

Particle collisions

Boundary Conditions, Sampling

Chemical reaction & species

databases

Geometry

Particle movement through grid

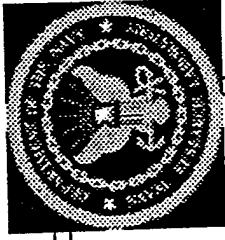
Parallelization

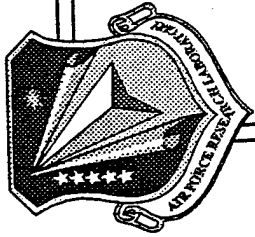
Consultants: International Team of DSMC Experts:

Prof. Graeme Bird (Sydney, Australia)

Prof. Mikhail Ivanov (Inst. Theor. Appl. Mech., Novosibirsk, Russia)

Prof. Iain Boyd (Univ. Michigan)



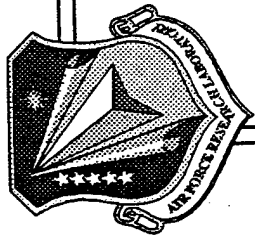


SUPREM Team: Project Management

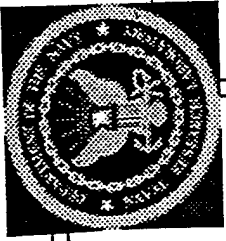


- Geographically distributed:
 - inter-service team brings greater range of experience and breadth of DoD resources.
 - Real-time interaction limited: face-to-face meetings ^{remove extra space} infrequent. Thus, use of email, video and telephone conferences important.
- Software configuration management:
 - Problems:
 - Not a mature process (No HPC MSRC Provision)
 - Single vs. multiple distributed repositories
 - DSMC is "toolbox", i.e., complex input, many models
 - Solution: Aegis (Gnu)
 - 1 version of code
 - changes undergo development, build, test, review, integration
 - each site has repository, synchronized weekly

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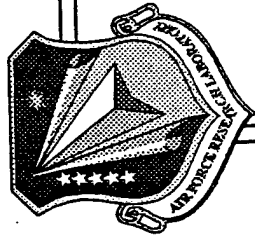
DSMC Code Availability



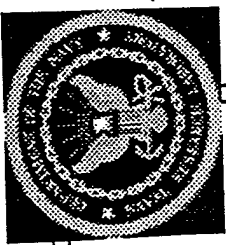
- Number of research & specialized application codes exist.
- None optimized for DoD RDT&E community.

Code: Funding	Ser/ Par.	Geom.	Grid	Lang.	User Interface	Documen- tation
Socrates: AF/BMDO	S	3D	Cartesian Static	F77	Text/ Windows	User, Theory
Bird: COTS	S	2D/3D	Cartesian Adaptive	F77	Windows	(user), (theory)
SMILE:	P	2D/3D	Cartesian Adaptive	F77/C	Text/GUI	(user), (theory)
Monaco: Univ.	P	2D/3D	Unstruct. Static	F77/C	Text files	(user)
DAC: NASA	P	3D	Cartesian Static	F77	Text	-
SUPREM: HPCMO	P	3D/2D	Cartesian Adaptive	F90	Text/GUI	User, Theory, & Prog.

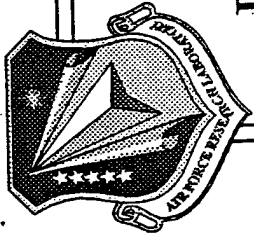
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SUPREM: Capability Assessment/Feedback



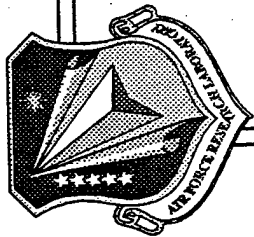
- Detailed DoD User Requirements:
Questionnaire emailed to users, potential users and
DSMC researchers
- Direct Discussions and Input from Users:
AIAA Reno, Jan 00; JANNAAF, May 00; AIAA Denver
June 00
- Direct Discussions with consultants:
AIAA, Reno, Jan 00; AIAA Denver, June 00



SUPREM Approach

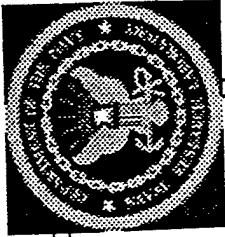
Primary requirements: Robust, reliable performance and results for non-expert users (efficiency secondary)

- HPC
 - Language: Fortran 90 + MPI [possibly HPF-2]
 - dynamic memory & portable
 - Platforms: Initial version to be demonstrated on SGI-Origin, IBM-SP. Then portable to other platforms.
- Software
 - Structured, Modular, Modern code and coding practices to enable flexibility and upgradability (supplemented by documentation)
 - Hierarchical design:
 - input/interface
 - data structures

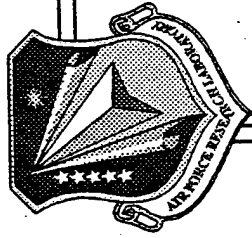


SUPREM: Risk Mitigation

- Build on DSMC core modules and experience of AFRL and NRL teams.
- Input from expert advisory panel.
- Use thoroughly established and tested algorithms.
- Validation of results against established data sets, analytical cases and extent research codes.
- Frequent input from DoD users to ensure product will meet requirements (Tech. transitions/ leveraging)

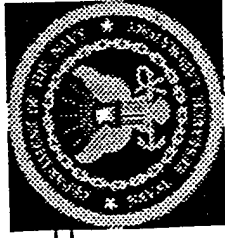


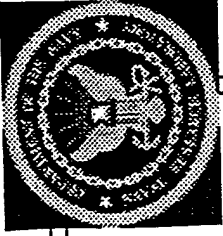
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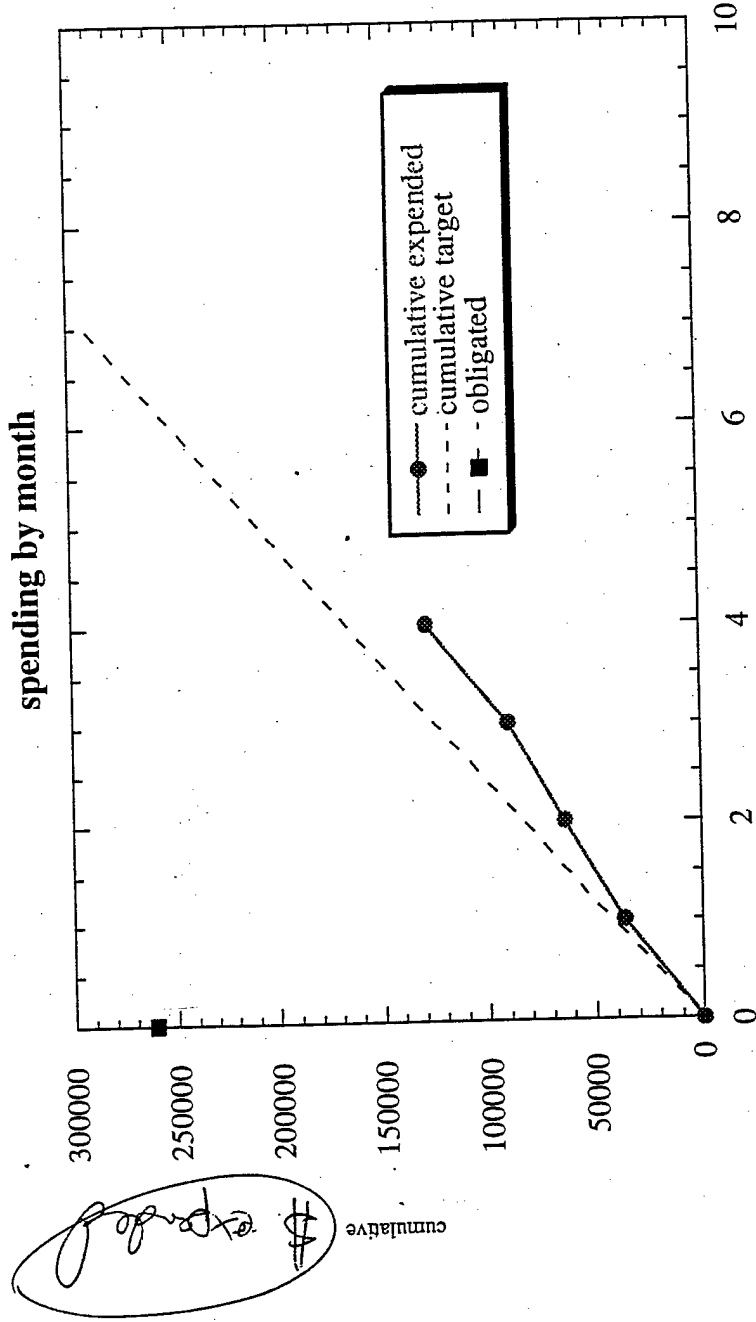
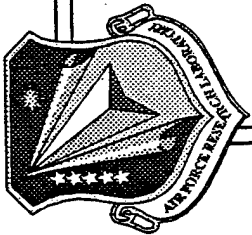
SUPREM: Leveraging

- BMDO -- plume simulation expertise, potential additional funding for radiation module
- NRL DARPA-funded MEMS-flow computations
- AFRL AFOSR-funded research into DSMC collision models and validation cases
- Spectral Sciences SBIR project: comparison case runs for molecular beam simulation, unsteady flowfield computational techniques





CFD-8 Spending Profile



expended

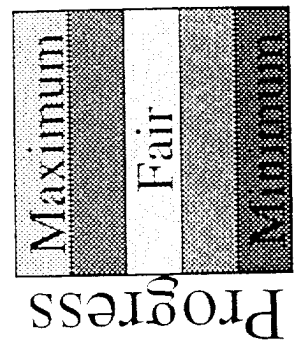
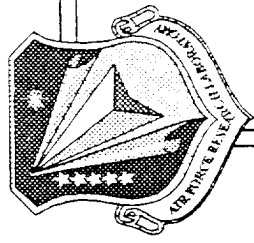
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Month after Jan 00

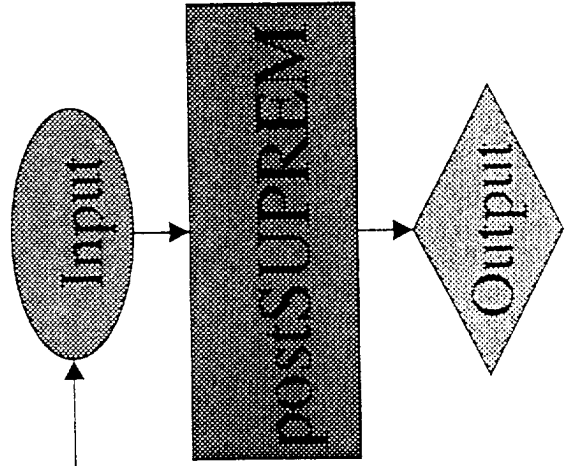
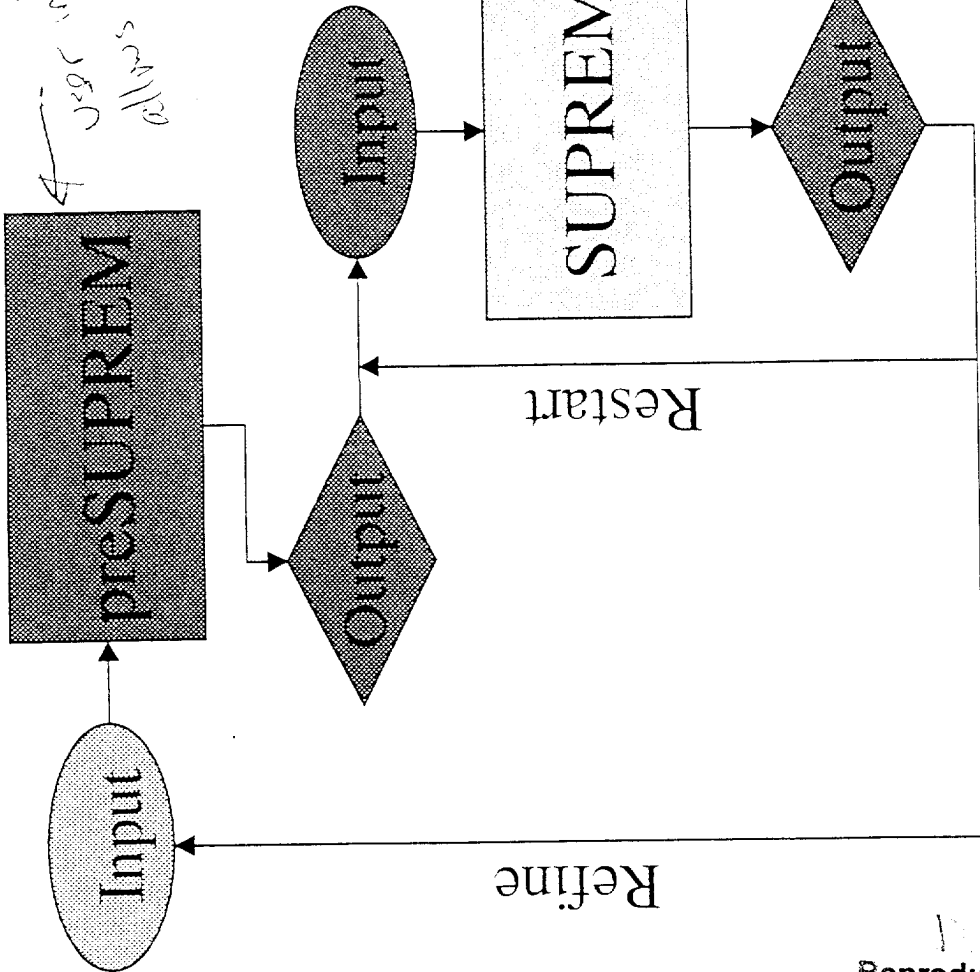
update



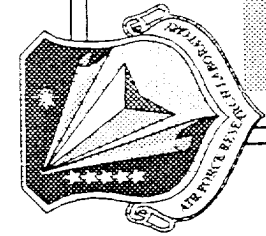
SUPREM-DSMC Overview & Status



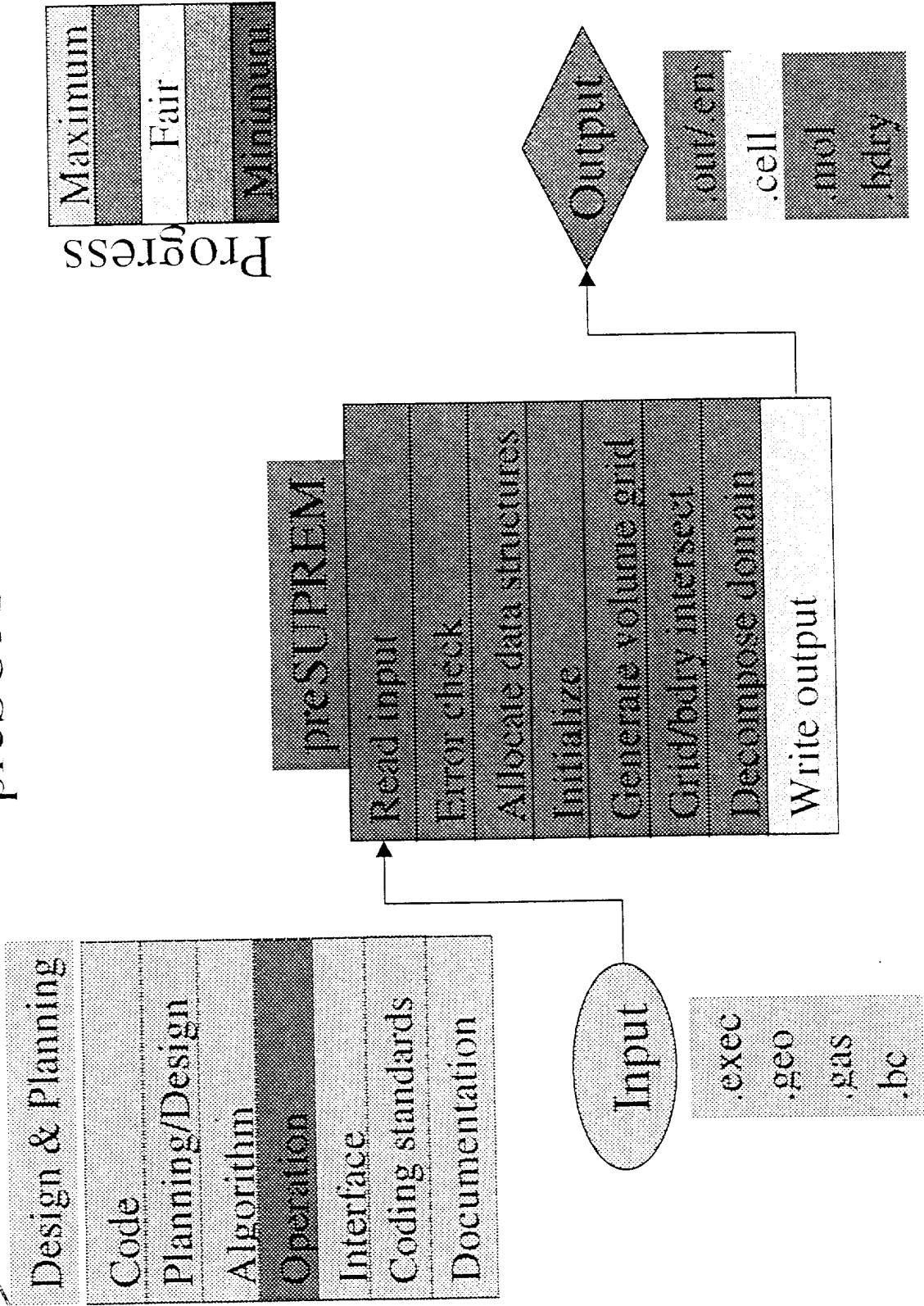
allows non-experts to use info for HS



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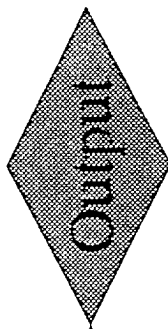
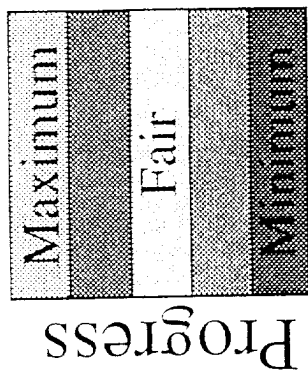
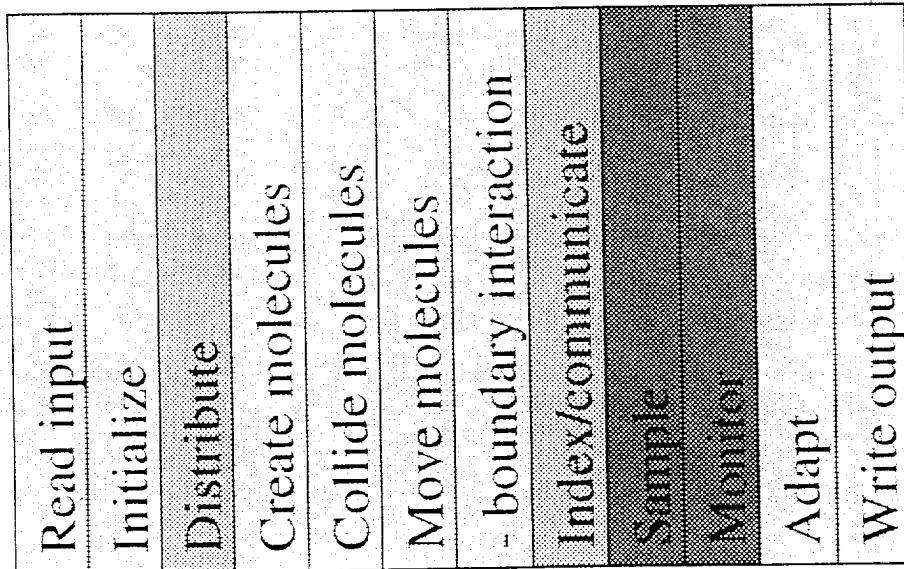
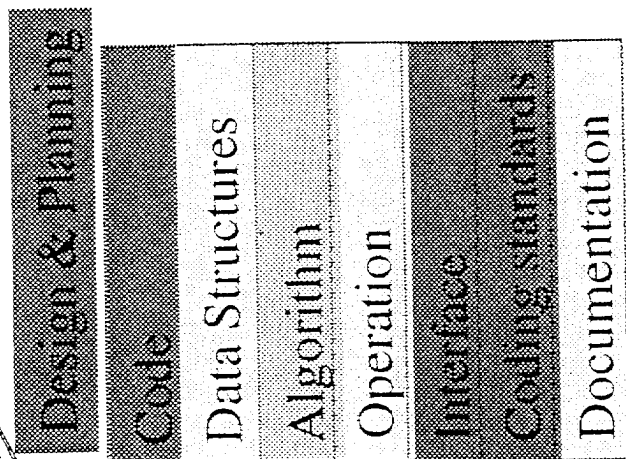
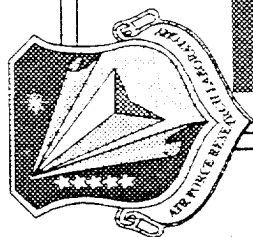
Code Overview & Status: preSUPREM





Code Overview & Status:

SUPREM



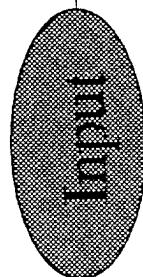
.out,.err

.smpl

.cell

.mol

.bdry



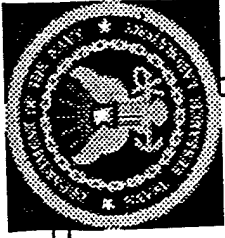
(.exec)

.cell

.mol

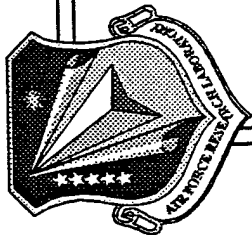
.bdry

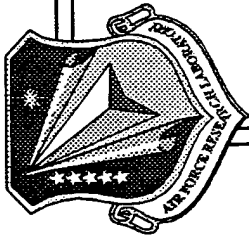
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Software Design

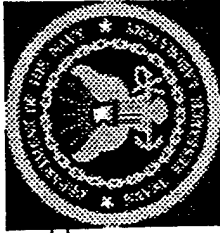
- Configuration Management
- User Interface / Code Operation
- Automation / Adaption

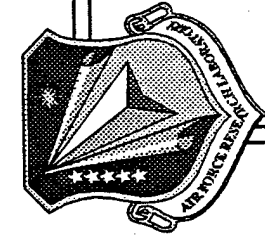




Configuration Management

- One Active, Validated Version of Code (Baseline)
- Configuration Management Process:
 - At Minimum: Source Code Version Control
 - Develop / Modify / Build / Test / Review ...
 - Integrate Changes into Baseline
 - Distribute
 - Track Bugs / Fixes
- Desire to Leverage HPC/CHSSI/PET in this Area
 - No CHSSI/PET/MSRC Process Identified
 - MSRC Serves as Repository of Application Codes (Executables)
 - Need “Standards” - Repository of Software Development / Maintenance Expertise

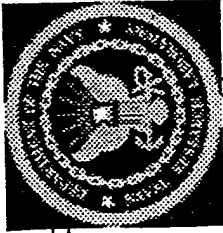
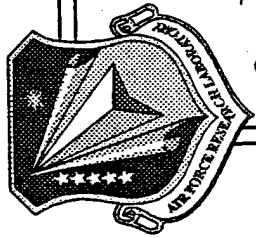




Configuration Management (cont.)

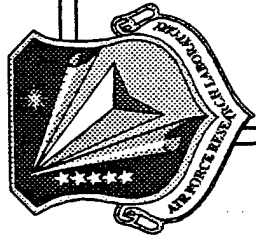


- Aegis (GNU) Selected as C.M. Tool (and C. M. Process)
 - Multiple Architecture Support
 - Full Regression Testing is Integral
- Multiple Local Repositories (ARFL, NRL)
- Changes “Pushed” Weekly
- Repository Includes (& Aegis Controls):
 - Source code, etc,
 - Documentation
 - Databases (Gas, Chemistry, etc.)
 - Test, Demonstration, Validation Cases & Results



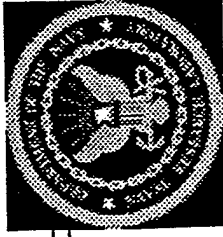
Coding Standards

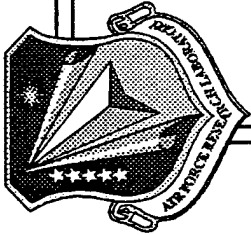
- Modularity / Extensibility of Source Code and Data Structures is Key Objective *check spacing between lines*
 - Object-Oriented
 - Data-Hiding
 - Data-Proximity
- Exploit Fortran90 [HPF-2?] Features
 - Modules
 - Interfaces
 - Data Structures (TYPE)
 - Parallel Portability / Maintainability (HPF-2)
- Establish Templates for Key Modules / Routines
 - Standardization
 - Re-use
- Data Management?
 - Database Format (HDF/CGNS?) / Interface to External Tools



User Interface

- DSMC as Toolbox
 - Grows in Complexity with Time (“Feature Creep”)
 - No Single or Optimal Approach / Algorithm / Model
 - Robustness Makes Maintenance / Control Difficult
- Provide / Enforce Standardized Interface
 - Scalable Physics - Models Classed by Complexity
 - Restrict Features Based on User Expertise
 - Very Complex Input - Automate or Guide Problem Setup
- Control Size / Contents / Usage of Toolbox

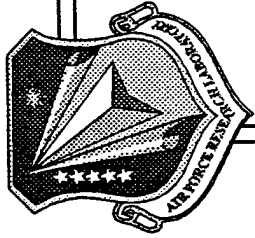




User Interface (cont.)



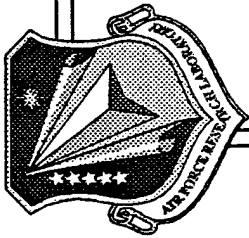
- Hierarchical / Extendable Input
- User Expertise versus Code Features
 - Novice: Restricted Access, Limited Control (Automatic, Conservative Defaults)
 - Intermediate
 - Expert: Full Access, Full Control
- “Problem Type” versus Setup and Model Availability
 - Dominant Flowfield Characteristics (Shock Layer, etc.) can be used to Guide Selection of Models (Gas, Chemistry, Boundary Conditions, Grid, etc.)



Automation

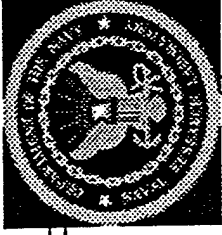
- User Defines Problem, but Code Should Control How Solution is Obtained
- Are the Results Accurate?
 - Satisfy DSMC Algorithm
 - Time Step, Cell Size, Nearest-Neighbor Collision Partners
 - Satisfy Physics of Problem
 - Gas Representation, Chemistry, Boundary Conditions
- Is the Simulation Efficient?
 - Memory, CPU, Load Balance
- Primary Objective: Accuracy, Generality, Scalability, and Robustness of Physics and Algorithm

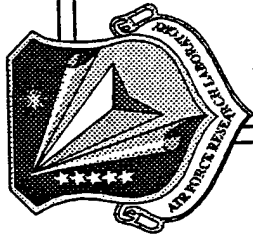




Automation (cont.)

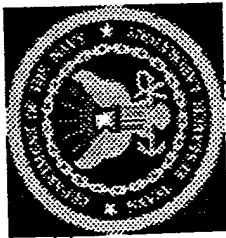
- Very Limited Existing DSMC Work in this Area - Far Short of Conventional CFD
- Plan:
 - Quality / Accuracy Constraints Represented via Metrics
 - Global (Average)
 - Local (Worst Case)
 - Expert User (Only) Can Tradeoff Quality for Efficiency
 - Interpretation of Results Facilitated by Feedback & Output
 - Desired vs. Achieved Quality and Accuracy Metrics
 - Refinement / Adaptation Results

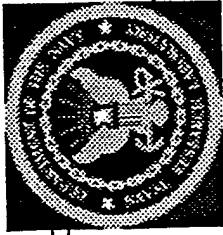
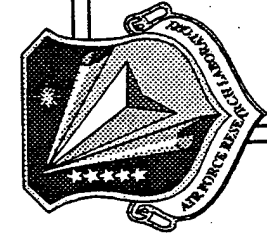




Gas / Chemistry Description

- Representation
- Models
- Algorithms
- Data Structures
- User Access
 - Input
 - Initialization
 - Sampling/Output

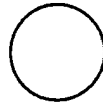




Gas Model

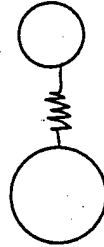
- Multiple Species
- Arbitrary Complexity of Each (Scalable)
 - Number of Independent Internal Modes
 - Representation of Mode (Continuous or Quantized)
 - Each Mode is a Scalar Quantity Stored for Each Molecule

Atom



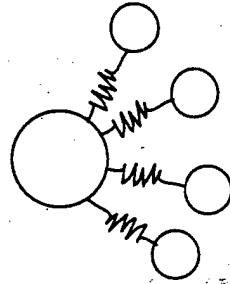
Ar (ϵ_t)

Diatom

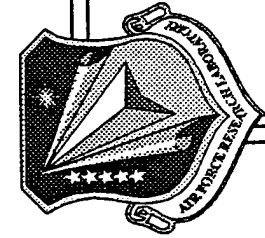


NO ($\epsilon_t, \epsilon_r, \epsilon_v$)

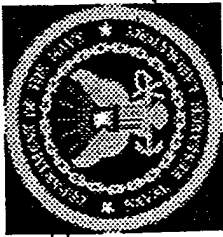
Polyatom



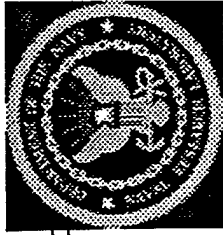
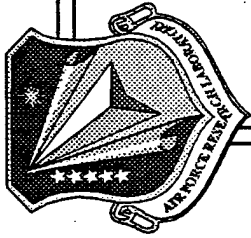
CH₄ ($\epsilon_t, \epsilon_r, \epsilon_{v1}, \dots, \epsilon_{vn}$)



Gas Model



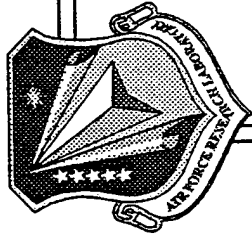
- **Predefined Common Modes are Available**
 - Rotation -- Rigid Rotor: Quantized, Bounded
 - $\epsilon_j = k_B \theta_j(j+1)$ gives ϵ_r for level j
 - Vibration -- Simple Harmonic Oscillator: Quantized, Bounded
 - Anharmonic Oscillator: Quantized, Bounded
- **Allow Fictitious or Simplified Representation**
 - Lumped -- Combine (Lump) "Real" Modes Together
 - Arbitrary Subset of Levels in a Quantized Mode



Databases Provided for Common Applications

- Completeness/Complexity Parameterized by Flow Energy Content (e.g. Temperature, Velocity, Average Collision Energy) Relative to Characteristic Mode Energy
- Simple Monatomics
 - e.g., Ar
- Common laboratory species
 - N₂
 - Room Temperature / Thermal
 - Weak or Strong Shock Layers
- Air
 - N₂, O₂
 - N₂, O₂, O, N, NO
- Propellents, Combustion Products
 - CO, CO₂, CH, H₂O

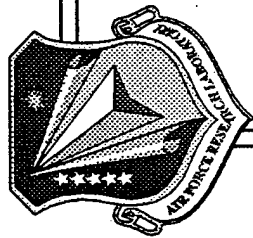
X



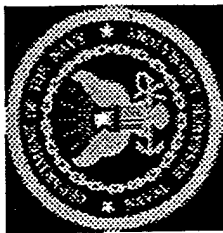
Access to Molecules / Species



- Input: Compact, Self-contained Definition Section; 1 for Each Species
- Initialization: Molecule of a Given Species can be Assigned an Arbitrary Velocity & Energy in any mode
 - Sampled from Equilibrium (e.g., Temperature)
 - Sampled from Nonequilibrium Distribution (e.g., Discrete Mode Energy Population)
- Sampling/ Output:
 - Default: Mean Properties per Mode in ALL Cells
 - “Detail”: Distribution Function of Any Mode of Any Species (at Any Location) -- Vital for “Microscopic” Interpretation



Molecule and Species Data Structures



Molecule

- Species_ID ispec
- XYZ(:)
- VEL(3)
- Mode_energy(:)
- etc.

- Name
- Composition
- Mass
- Num_modes
- Modes(1..Num_modes)

Species (1..Num_species)

Mode

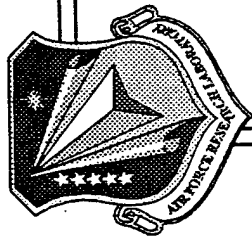
- Name
- Max_energy
- Rep(resentation)
 - Cont(inous)
 - or
 - Quant(ized)

Cont

- DOF

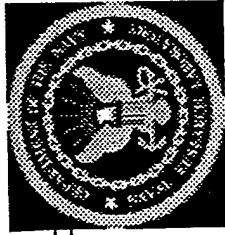
Quant

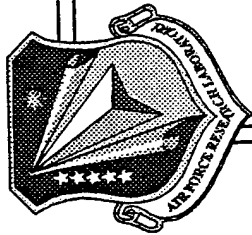
- Num_levels
- Energy(1..nlvls)



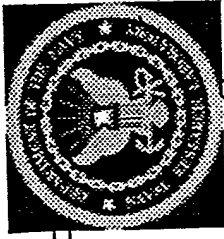
Chemistry (Intermolecular Collision) Model

- Bimolecular [Trimolecular & Unimolecular also Available]
- Arbitrary Complexity of Collision for Each Species Pair (Scalable)
 - Number of Independent Processes
 - Complexity of Each Process
- Collision Description is INPUT (Self-Documenting)
 - 1) Chemical Equation:
 - Defines Species and Modes that Participate
 - 2) Process Keyword Description:
 - Type (Elastic, Inelastic, Reaction)
 - Model Used to Calculate Cross Section σ and Model Parameters

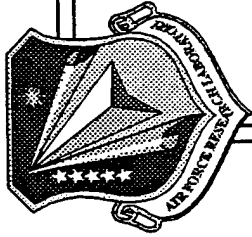




Chemical/ Collision Equations



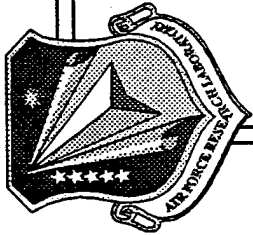
- $NO + O \rightarrow NO + O$
 - PROCESS: ELASTIC
 - VHS, VSS Model Used to Calculate $\sigma_e = \sigma_e(\mathcal{E}_t)$
 - Isotropic Scattering
- $NO(\mathcal{E}_r) + O \rightarrow NO(\mathcal{E}_r') + O$
 - PROCESS: INELASTIC
 - Collision Number "Z" Model $\sigma_i = \sigma_i(\mathcal{E}_t) \approx \frac{1}{Z} \sigma_e(\mathcal{E}_t)$
 - Borgnakke-Larsen Redistribution (\mathcal{E}_r')
- $NO(\mathcal{E}_r, \mathcal{E}_v) + O \rightarrow N + O_2(\mathcal{E}_r', \mathcal{E}_v')$
 - PROCESS: REACTION
 - Total Collision Energy (Arrhenius-based) Model
 - Borgnakke-Larsen Redistribution/Initialization ($\mathcal{E}_r', \mathcal{E}_v'$)



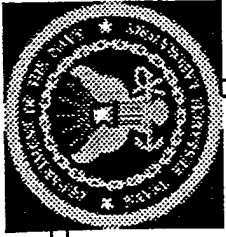
Collision Representation - Issues



- DSMC Collision Models are Wholly Phenomenological
 - Microscopic/ Kinetic Description Required, but is Nominally Based on Macroscopic Data
 - No Real Cross Sections are Used
- Complex, Real Coupled Processes are Necessarily Decoupled
- Statistical Process: Detailed Balance Achieved by Uncorrelating Pre- & Post- States
- Continued Research into Collision Physics & DSMC-Representation Required
 - SUPREM team
 - CCM

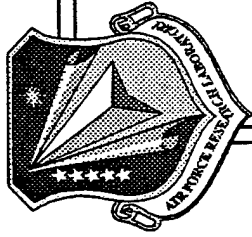


Collision Algorithm - Implementation



- Pair Selection is Cell-Local
 - Nearest-Neighbor Approximated via Bird Transient Adaptive Subcell Procedure
- Pair & Pair-Process Acceptance
 - Independent of Process Type or Input Order
 - Depends ONLY on (Abstract) Physical Parameter σ
- Null Collision Method
 - Probability of Process

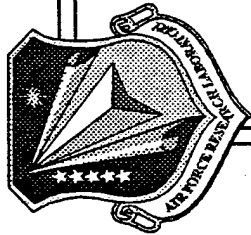
$$P_i = \frac{\sigma_i}{N \sum_{j=1} \sigma_j}$$



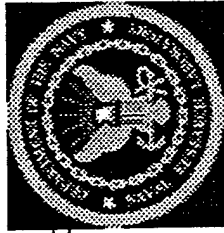
Collision Description - User Issues



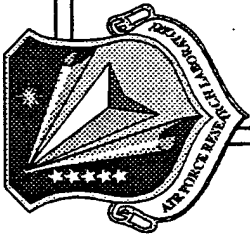
- Databases Provided for Common Gases
- User (NOT Black-Box Code) Determines Complexity of Gas & Collision Processes
- Extensive Diagnostics & Feedback from Code
 - DSMC Constraints (e.g., Nearest-Neighbor)
 - Model Realism / Accuracy / Range [Limits] of Applicability



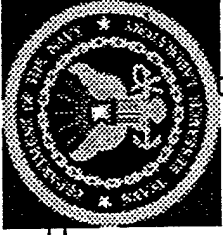
User Access to Collision Processes



- Input: Compact, Self-Documenting for Each Pair / Process
- Initialization: N/A
- Sampling / Output
 - Default: Mean Properties (e.g., Collision Frequencies) Per Pair (& Per Process)
 - Detail: Distribution Function of Any Mode of Any Species (Pre- and/or Post- Collision) -- Vital for Improvement of DSMC Models & Interpretation of Results



Collision Pair Data Structures



Colln Pair(ispec,jspec)

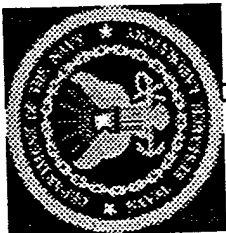
space?

- Weight
- Num_processes
- Process(1..Num_processes)

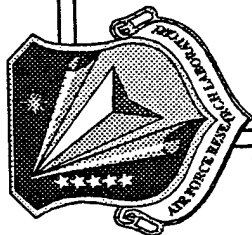
Process

- Type/name
 - Modes_involved
 - Model
- Parameters(1..N)

X

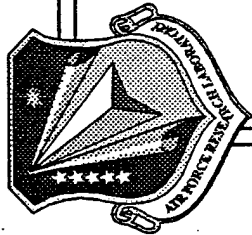


Gas/ Chemistry Example Input File (Ar-N₂)

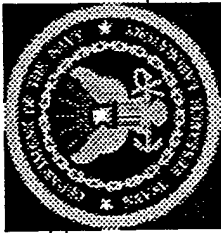


1) Species Definition

```
SPECIES_NAME Ar  
COMPOSITION Ar-1  
NUM_INTL_MODES 0  
SPECIES_NAME NO  
COMPOSITION N-1 O-1  
NUM_INTL_MODES 2  
MODE_NAME ROT  
MODE_REP CONTIN  
DOF 2  
MAX_ENERGY 1.04E-17  
MODE_NAME AHOVIB  
MAX_ENERGY 1.04E-17  
NUM_DUNHAM_TERMS 3  
DUNHAM_COEFFS 0.1 0.2 0.3
```

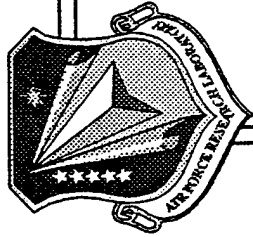


Gas/ Chemistry Example Input (cont.)

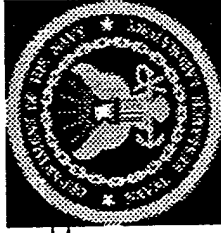


2) Collision Definition

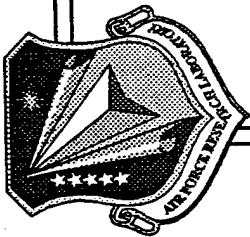
```
BIMOLECULAR TRUE
SPECIES_PAIR Ar ANY
  Ar + ANY -> Ar + ANY
  PROCESS ELASTIC MODEL VHS NUM_PARAMS 3
    DIAM_REF 4.185e-10
    VISC_EXPON 0.80
    TEMP_REF 273.
    COMMENT ref: Bird 1994, App. A, avg(NO+Ar) "
SPECIES_PAIR NO NO
NO + NO -> NO + NO
  PROCESS ELASTIC MODEL VHS NUM_PARAMS 3
  ...
NO(ROT) + NO -> NO(ROT') + NO
  PROCESS INELASTIC MODEL COLLN_NUM NUM_PARAMS 2
    COLLN_NUM 5.0
    TEMP_REF 300.
SPECIES_PAIR NO Ar
  ...
```



Boundary Conditions



- Describe:
 - 1 Interaction of Molecule with Boundary During Molecular Movement Stage
 - 2 Spontaneous Creation of Molecules at Boundary (e.g., Inflow)
- Allow Arbitrary Complexity (Scalable)
 - Define Several Basic Types or Classes (General Characteristics)
 - Each Type has Several Subtypes
 - Simple to Complex
 - Highly Constrained to General / Arbitrary
 - Constant or Prescribed Variation in Space or Time

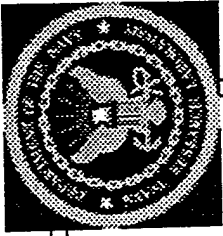
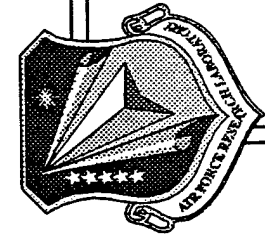


Boundary Conditions

Handwritten note: (x,y,z) = 0

Type	Subtype	Interaction	Creation
SOURCE	MACRO	Delete	Constant, Equilibrium
	MSIS90	Delete	Constant, Equilibrium
	MANUAL	Delete	Arbitrary (f(x,y,z), Noneq.)
	MOL_LIST	Delete	[Externally Supplied]
	ITERATIVE	Delete	Adjustable Rate, Equilibrium
SINK	VACUUM	Delete	N/A
	PUMP	Possible Reflection	N/A
WALL	OUTGAS DESORB	Reflection/Reaction	N/A
		Reflection/Reaction	Constant, Equilibrium
		Reflection/Reaction	Coverage-Dependent, Equilibrium
SYMMETRY		Specular Reflection	N/A
FLUXPLANE		No Change	N/A
PERIODIC	LINEAR	Linear Displacement	[Displ. from matching bdry]
	AZIMUTHAL	Rotational Displ.	[Displ. from matching bdry]

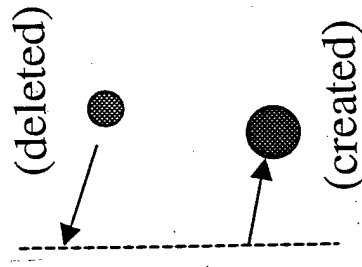




X

Source Boundary Condition ?

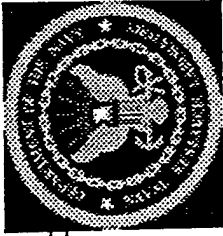
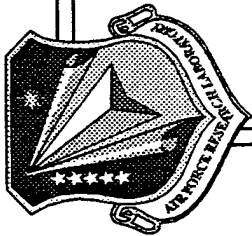
- Typical Case: Constant Inflow, Known Freestream Macroscopic Properties ($n_\infty, p_\infty, T_\infty, u_\infty$)
- General Case: Arbitrary Spatial Variation (e.g., U Profile), Inter-species, Inter-mode, Intra-mode Nonequilibrium



$\rho_\infty, T_\infty, u_\infty \rightarrow$

- Sample u, E_{mode} (Equilibrium)
- u_∞, T_∞ (Equilibrium)
- $f(u), f(\epsilon_r), f(\epsilon_v)$ (Nonequilibrium)

- Issues:
 - Subsonic vs. Supersonic (Directed Fluxes)
 - Macroscopic vs. Microscopic Description



Source / MACRO

- Constant Incoming (Created) Flux
- Incoming Flux Independent of Outgoing Flux
- Strictly Valid Only for High Supersonic Speeds
- Molecule Properties Sampled from Analytical Equilibrium Kinetic Flux

$$\text{Flux} = n \overline{Q u_n} = n \int Q u_n f dv; \quad f \propto \exp\left(\frac{-mc^2}{2k_B T}\right)$$

Flux:

$Q =$

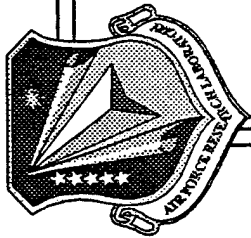
Mass

$m \vec{v}$

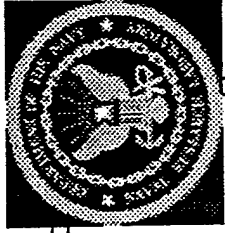
Momentum

$m |v|^2$

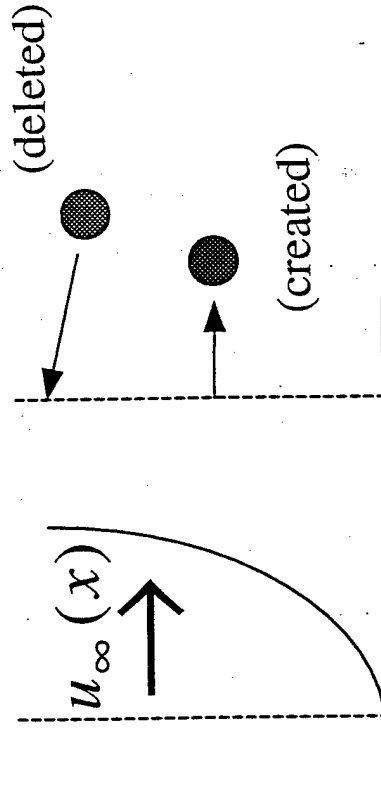
Energy
(Trans.)

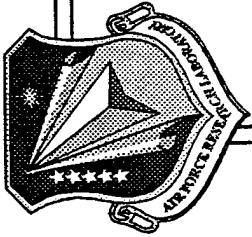


Source / MANUAL



- Generalized Spatial Variation of ρ_∞ , T_∞ , u_∞
- Independent Properties for Each Species
- Independent Properties for Each Mode
 - $T_{\infty \text{ mode}}$ or Distribution/Population
 - (Also $T_{\infty x,y,z}$ or $f(u,v,w)$)
- Incoming Flux Uncoupled from Outgoing

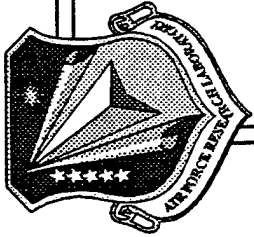




Source / MSIS90

- Flight in Earth Atmosphere
 - MSIS90 Model Calculates Freestream Properties from Given Flight Parameters
 - Remainder Equivalent to Source / Macro
- Source / Iterative
- Couple Incoming & Outgoing Fluxes
 - Update Incoming Flux Parameters to Recover Desired Net Flux
 - Approximate Subsonic Boundary
 - Still Based on Equilibrium, Macroscopic Parameters

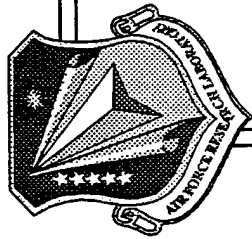




Wall Boundary Condition



- Typical Case: Constant Temperature Engineering Surface (Diffuse, Fully Accommodating Reflection)
- General Case:
 - $T_w(x,y,z)$
 - Species & Mode-Dependent Reflection & Reaction
 - Spontaneous Creation (Outgassing, Desorption)
- Two Components to Description:
 - Properties Associated with Wall Surface
 - Material
 - Temperature, Velocity, Coverage, Spatial Variation
 - Properties Associated with Interaction
 - Process, Model, Parameters

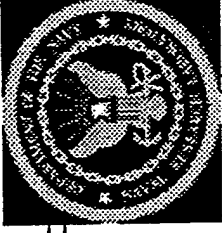
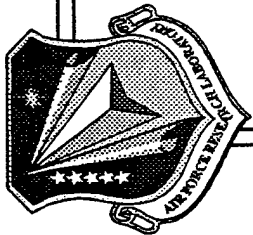


Wall Interaction Processes

- Analogous to Chemistry/Collision Process -
 - Probability (cross-section) of Post-interaction State
- Arbitrary Number and Type of Processes for Each Incident Species / Material Pair (Scalable)
- Interaction Description is Input
 - Chemical Equation - Species & Mode
 - Process Definition
 - Type / Model / Model Parameters

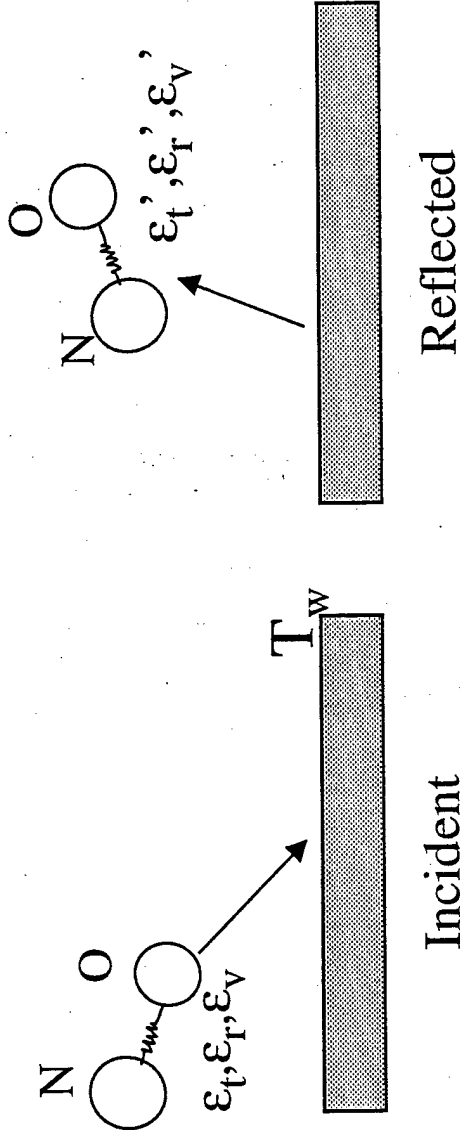


X



Wall Interaction Equations

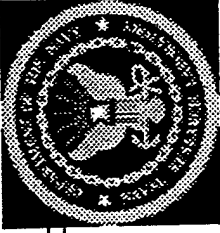
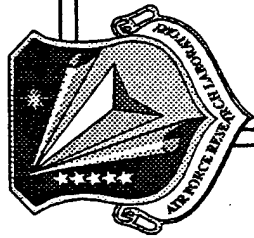
Example - Reflection



PROCESS RELECTION MODEL MAXWELL NUM_PARAMS 2

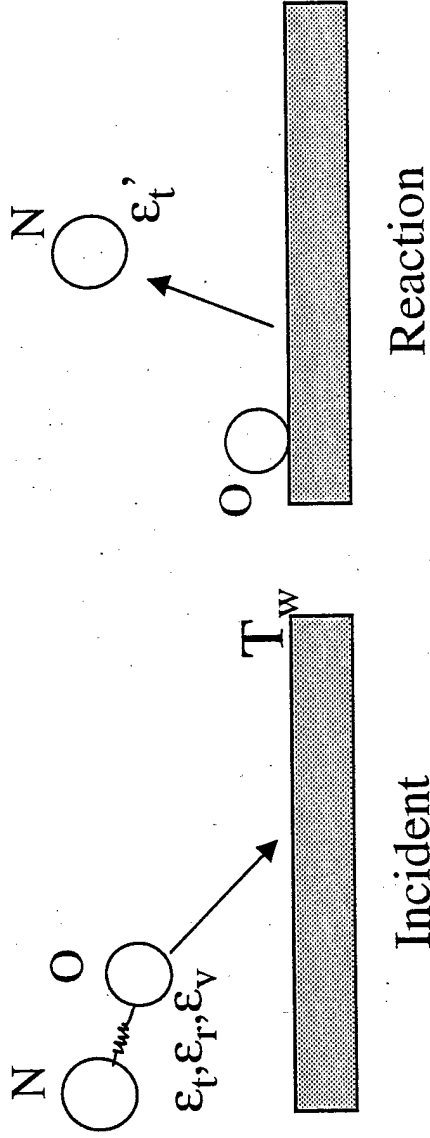
PROB_DIFF 0.5

TEMP_REF 300.0



Wall Interaction Equations

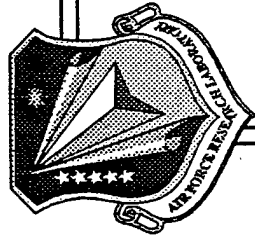
Example - Reaction



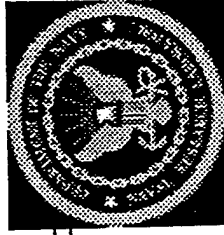
PROCESS REACTION MODEL CATALYTIC NUM_PARAMS 2

PROB_CATALYTIC 0.9

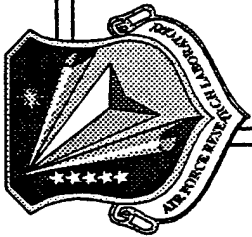
TEMP_REF 1000.0



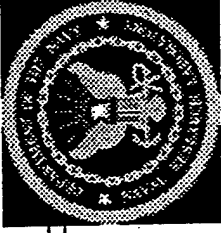
Wall Interaction Representation Issues



- DSMC Interaction Models are Wholly Phenomenological
 - Microscopic/Kinetic vs. Macroscopic
 - Typically *Independent* of Collision Energy
 - Decoupled from Wall Response
 - Less Sophisticated than Gas-Gas Collision Models
- Much More Research Required
- Present Approach:
 - Implement Available Models
 - Standardize Input & Algorithm
 - Provide Feedback (Accuracy / Realism)

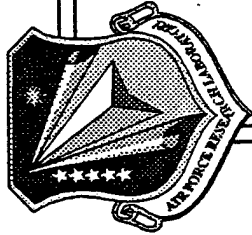


Wall Interaction Algorithm



- Movement Routine Provides:
 - Incident Molecule
 - Boundary Element Involved
- Combination of Serial & Null Collision Schemes
 - Event Probability Independent of Input Order
 - Reflection: Serial, Independent for Each Mode
 - Reaction: Null Collision Evaluation of:

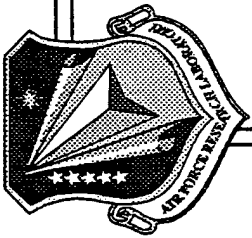
$$\text{Event } i = \frac{P_i}{\sum_{j=1}^N P_j}$$



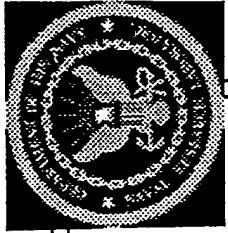
Wall Interaction Description - User Issues



- Very Limited Data for any but “Fully Accommodating, Diffuse Reflection” Process
- User Defines / Controls Complexity of Interaction
- Extensive Feedback
 - DSMC Constraints (Surface Element Size, Sample Size)
 - Model Realism / Accuracy



User Access to Interaction



- Input: Compact, Self-Documenting For Each Species & Process
- Initialization: N/A
- Sampling / Output:
 - Default: Mean Incident and Reflected Species Properties (Fluxes)
 - Detail: Distribution Function of Any Mode of Any Species (Pre- & Post-interaction)
 - Macroscopic: Surface Pressure, Shear
 - Integrated: Forces & Moments on a Component
- (Long Term:) Couple to Material / Surface Response Model