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62 Separate items are enclosed

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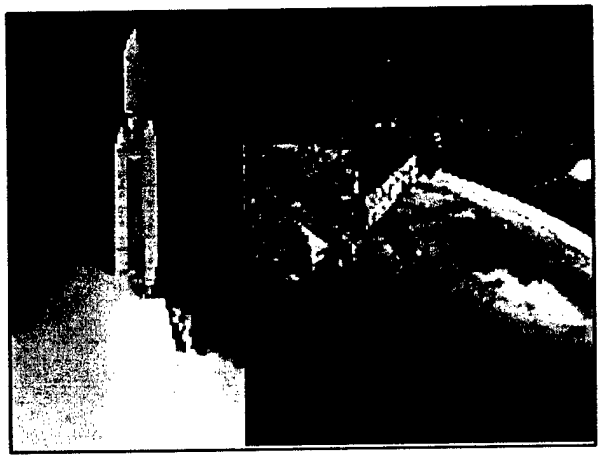
MEMORANDUM FOR PRS (~~Contractor~~/In-House Publication)

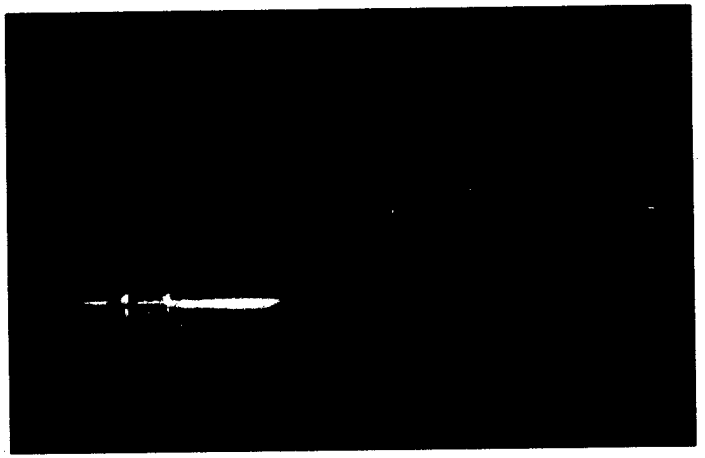
FROM: PROI (TI) (STINFO)

2 July 1999

SUBJECT: Authorization for Release of Technical Information, Control Number: AFRL-PR-ED-TP-FY99-0162
Dr Perkins, "Computational Chemistry and Material Science for Rocket Propulsion"
Defense S&T Presentation **(Statement A)**

Computational Chemistry and Materials Science for Rocket Propulsion





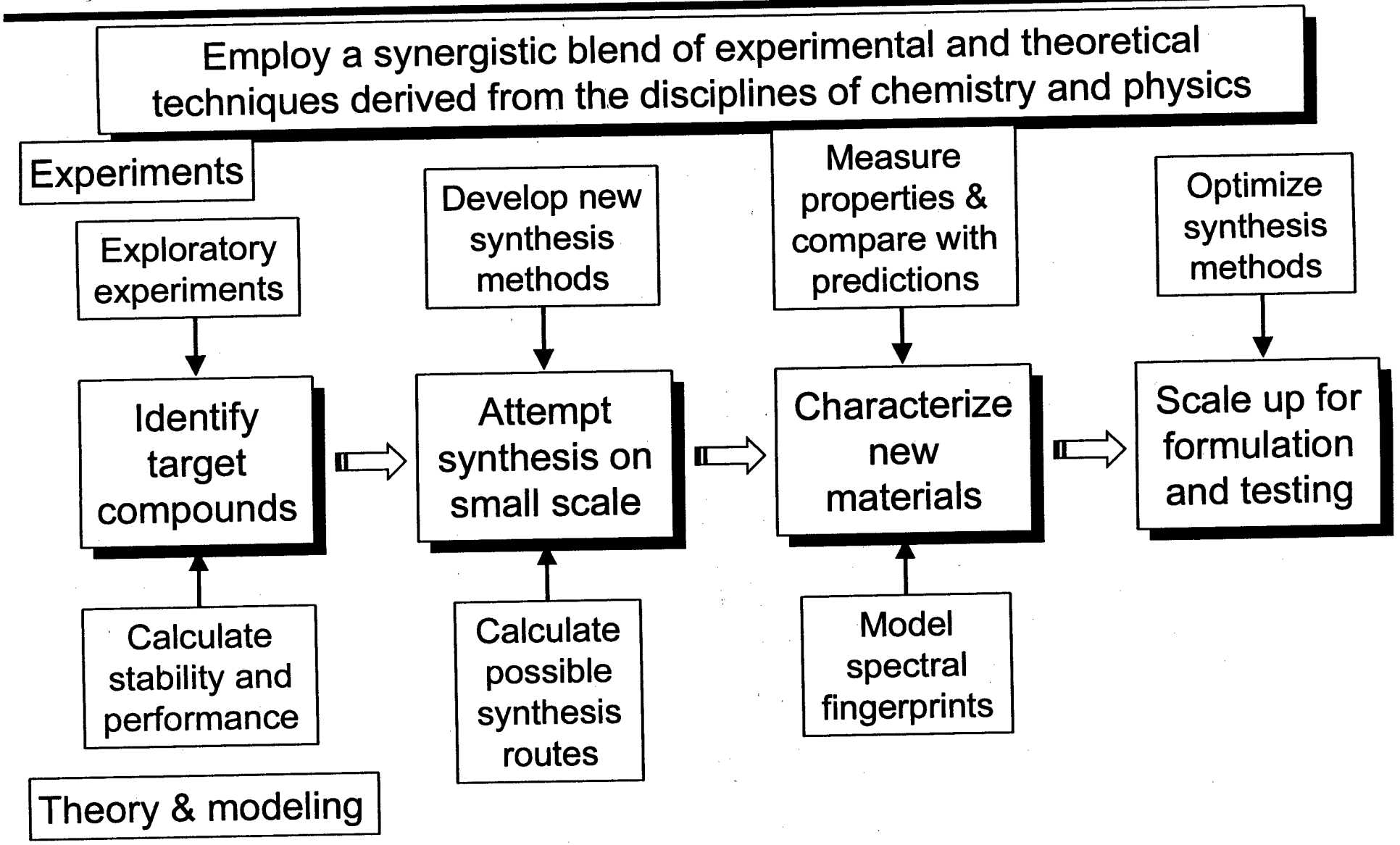
Dr. Leslie S. Perkins
Propulsion Directorate
Air Force Research Lab
Edwards AFB CA 93524

High Performance Computing is **Vital** to Materials Development in Rocket Propulsion!

- Identifies material improvements for liquid engines and solid motors
  - Decide which proposed materials are worthwhile to pursue: **Months** rather than years!
- Reduces the long process to synthesize new materials.
  - Eliminate unlikely pathways for making a new material

Approach to Developing Advanced Materials

Employ a synergistic blend of experimental and theoretical techniques derived from the disciplines of chemistry and physics



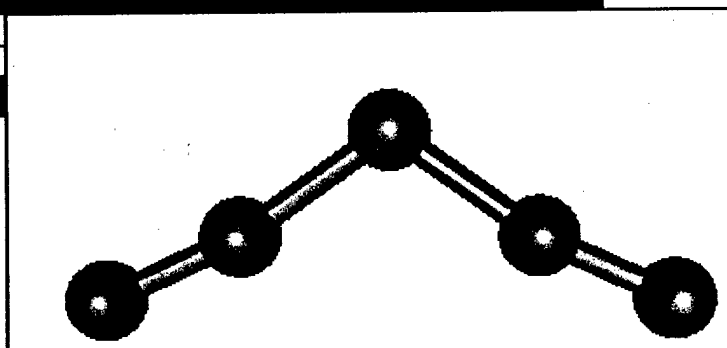
New Energetic All-Nitrogen Compound

From *Chemical and Engineering News*, 25 Jan 99

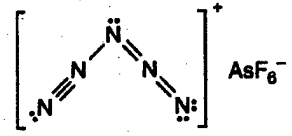
news of the week

N_5^+ CATION MAKES EXPLOSIVE DEBUT

High-energy ion is first new all-nitrogen species in 100 years



It wasn't in his abstract, but Karl O. Christe, a chemist who studies high-energy materials at the Air Force Research Laboratory at Edwards Air Force Base in California, had a little something extra to offer last week in his plenary presentation at the American Chemical Society's Winter Fluorine Conference in St. Petersburg Beach, Fla. Along with colleague William W. Wilson, Christe has synthesized and characterized a salt containing the N_5^+ cation. The cation is the first new all-nitrogen species to be synthesized in isolable quantities in more than a century, and only the third ever to be produced.



Although species that contain only ni-

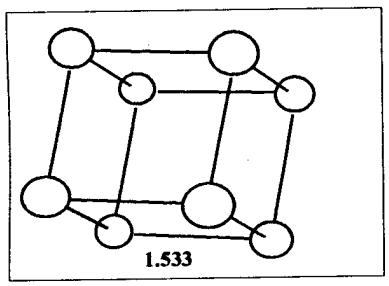
taking," says Gary J. Schrobilgen, a professor of chemistry at McMaster University, Hamilton, Ontario. "This synthesis could only be done in a very few laboratories in the world, and certainly Christe's is one of them." The work is supported by the Air Force Research Laboratory's propulsion directorate as well as by the Defense Advanced Research Projects Agency and the

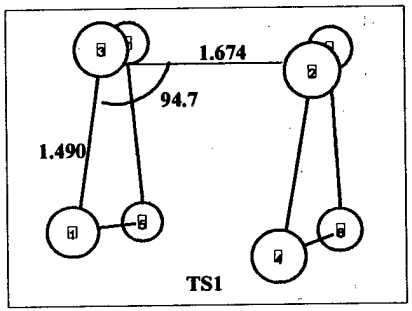
be theoretical chemists who are initially most interested in the new cation. "It's going to be of incredible interest to theoreticians who, perhaps, thought that compounds like this would be too unstable to isolate at all," Strauss says.

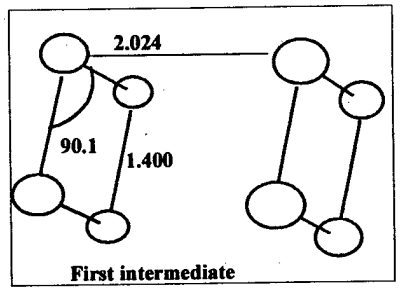
The salt is surprisingly stable, considering its huge calculated positive heat of formation of more than 350 kcal per mol, Christe points out. Vibrational spectroscopy and theoretical calculations by his coworkers Jeffrey A. Sheehy and Jerry A. Boatz show the cation to have a V shape in which resonance structures increase its stability.

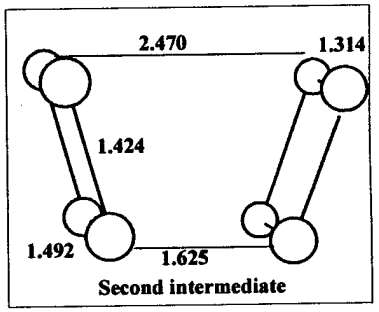
Christe and his group envision other N_5^+ salts—such as $N_5^+SbF_6^-$—that might have even more thermal stability. They also would like to use the cation to pre-

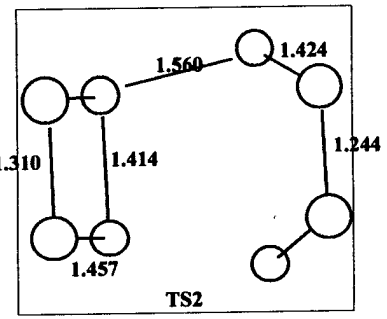
Evaluation of N_8 for stability

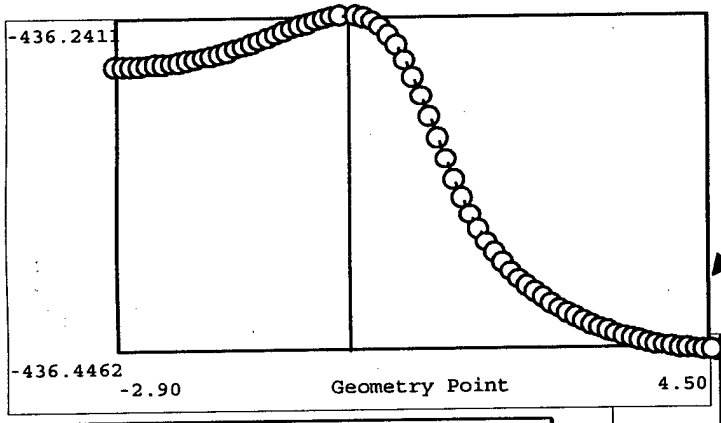


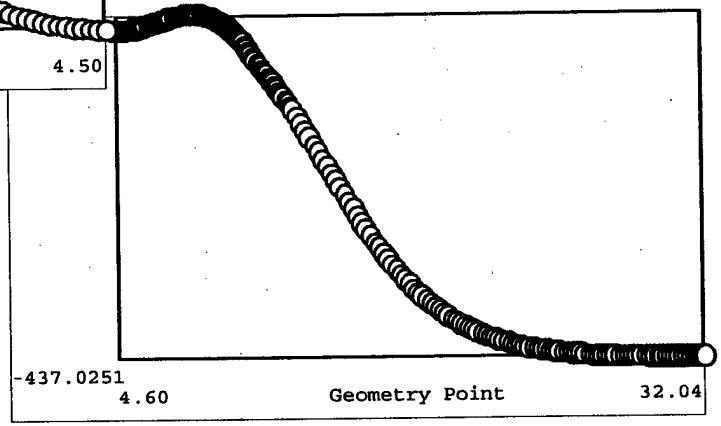








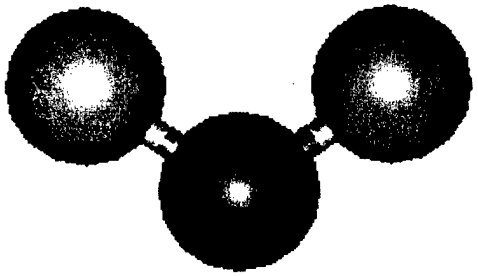




N_8 does not meet stability requirements!!

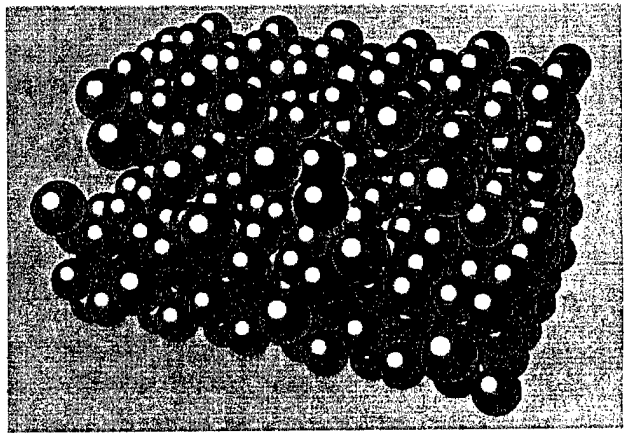
$4N_2$
-473 kcal

HPC aids in identifying future propellants



In 1987, a single calculation would take over 1 week.

Software & Hardware



Software

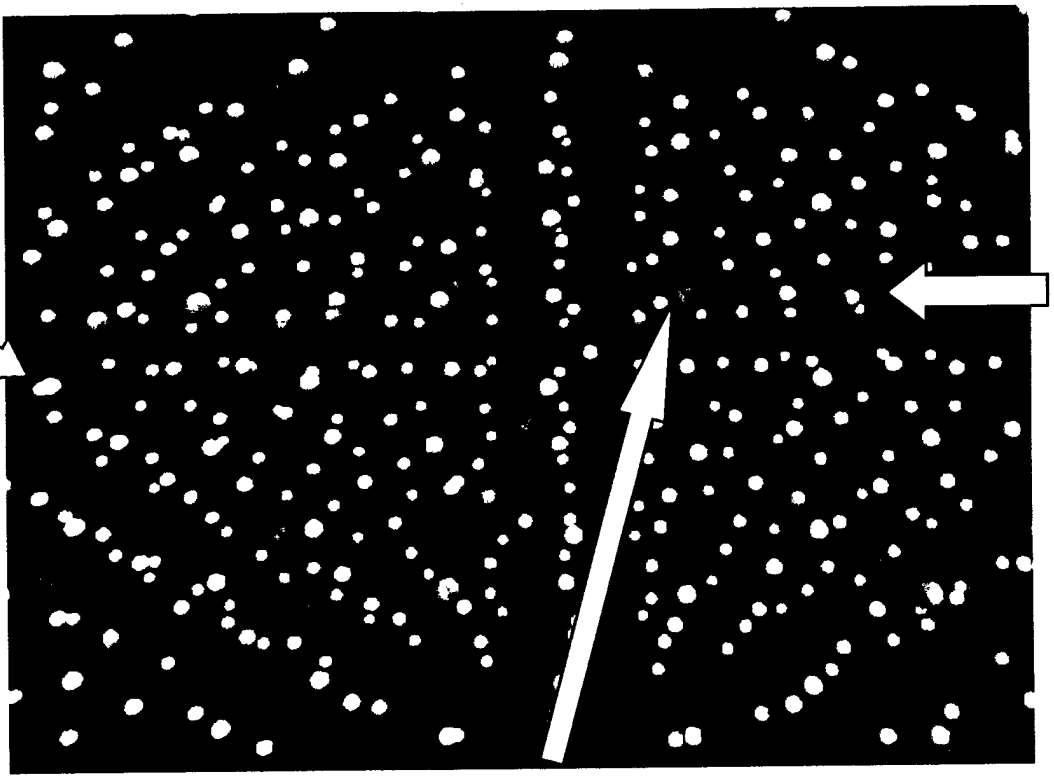
GAMESS calculation on a workstation: 8 hours!!

B in *para*-H_2: 200 times the number of atoms in 5 weeks on IBM SP!! (This would require *4 YEARS* on a workstation)

Future Solid Propellants

6.25% boron atoms in solid *para*-hydrogen

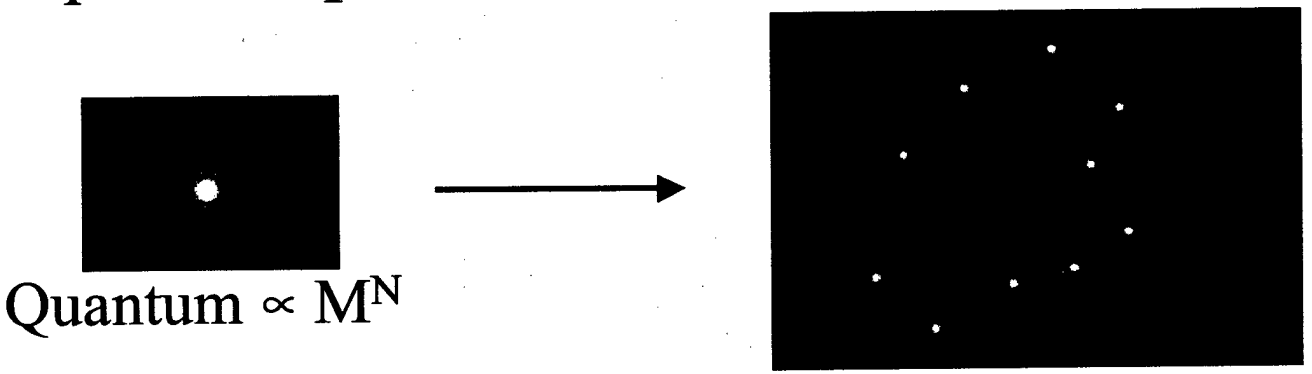
(64 nodes on an IBM SP at Maui - 5 weeks)



After reaction: Only local recombination of impurities!

CMD: Quantum Particles and Classical Dynamics

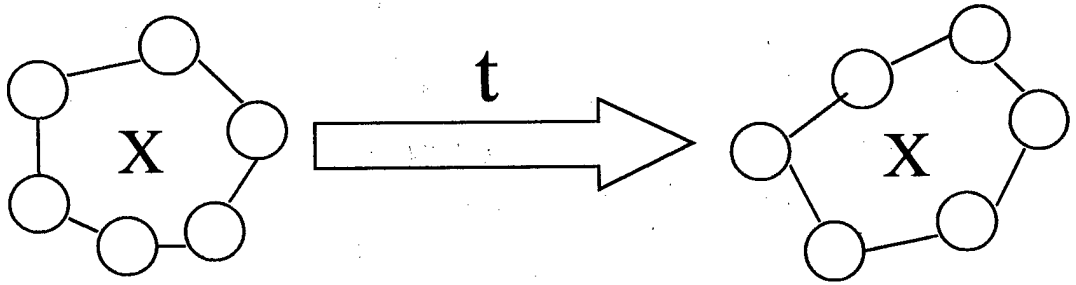
1. Treat the quantum particles as a "ring" of classical particles



Quantum $\propto M^N$

Classical $\propto N$ to N^2

2. The dynamics of the "ring" is calculated for each time step.



$q_c(0)$ $q_c(t)$

CMD on HPC Architectures

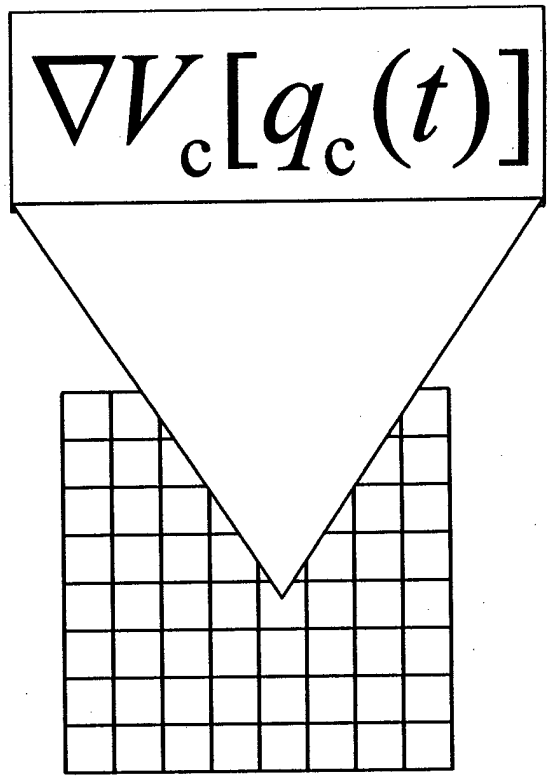
Compute the movement of particles using:

$$m \bullet \frac{d^2 q_c(t)}{dt^2} = -\vec{\nabla} \mathrm{V_c}[q_c(t)]$$

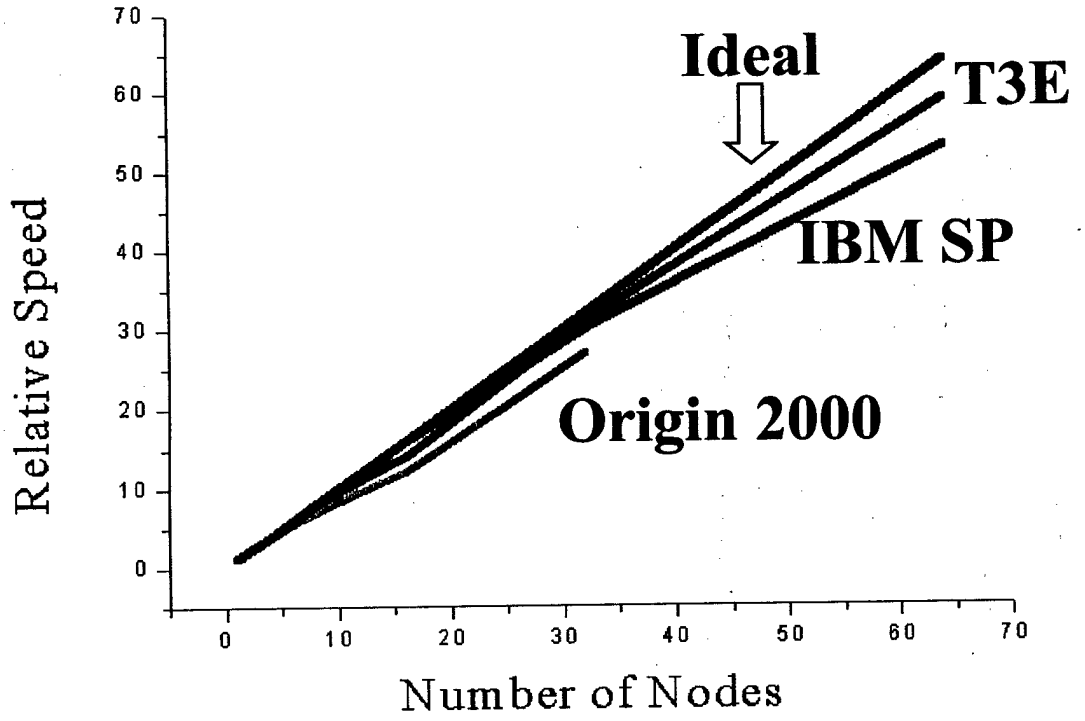
where

$$\mathrm{V_c}(q_c) = -k_B T \ln[\rho_c(q_c)]$$

The largest part of the work is solution of the forces. It is equally balanced onto 64 nodes.



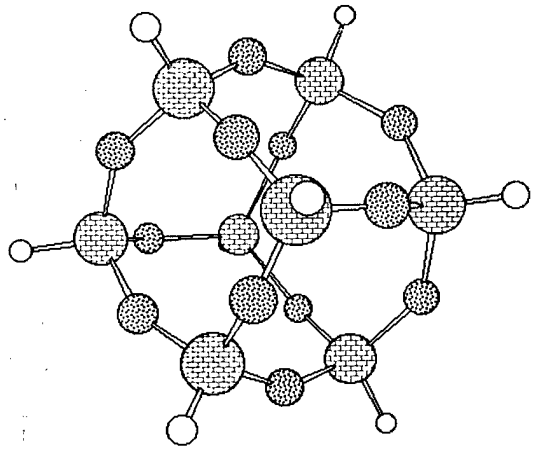
How does CMD perform on HPC machines?



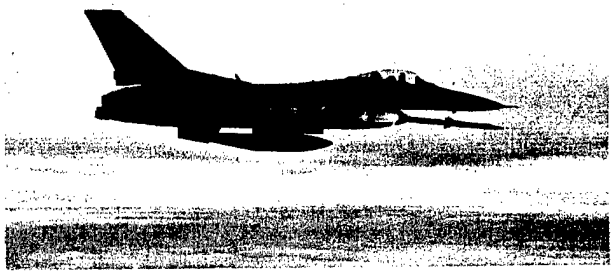
CMD shows different performance curves on the three machines.

Parallel coding is not a "one-size fits all" procedure

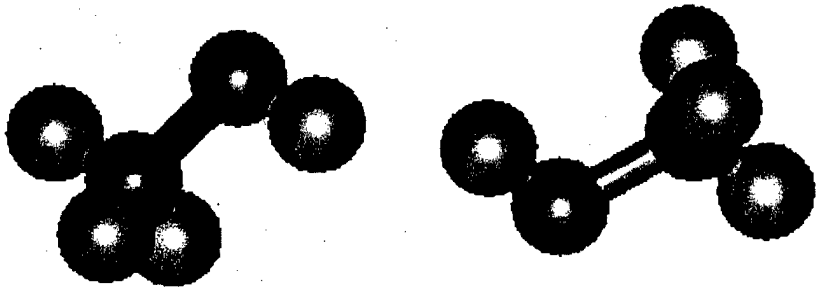
HPC in Materials Design and Synthesis

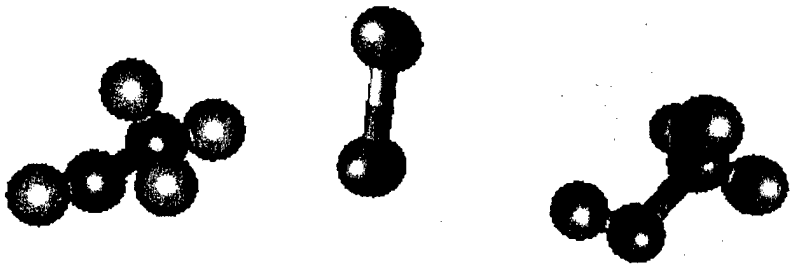


Polyhedral Oligomeric Silsesquioxane (POSS)



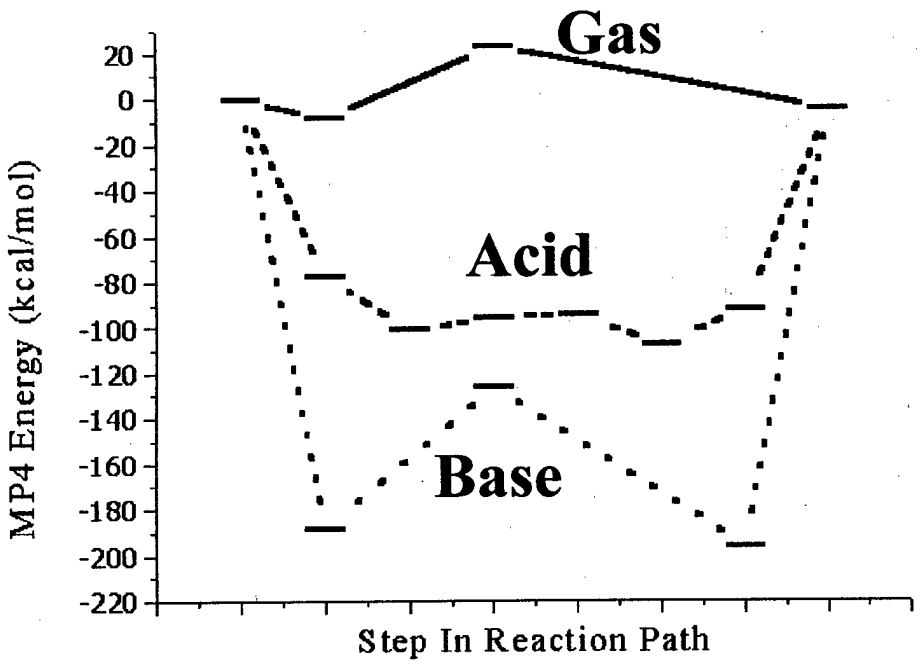
Significant barrier to initial condensation - 20 kcal/mol





In a basic solution, the condensation pathway is more favorable!

Condensation of POSS



- There are different reaction pathways with different liquid environments
- Aids in experimental design to get to end product
- UNABLE to accomplish prior to HPC!!!

Computational Chemistry and Materials Science - Future Directions

- Simulations of "real" sized systems
  - Material simulations consisting of billions of atoms with a volume of *at least* 1 cubic centimeter
- Dynamic and static simulations that include ~~a~~ quantum effects *without* a significant turn-around time for results
  - Software development that incorporates quantum mechanics in an ingenious manner

HPC - What has it done for Rocket Propulsion?

- HPC has identified likely candidates (N_5^+, B in solid H, POSS) and rejected unlikely prospects (H_4,N_8) in the AFRL/PR Rocket Propellant and Rocket Component Materials programs
- HPC has identified likely routes to achieve the creation of new rocket materials