

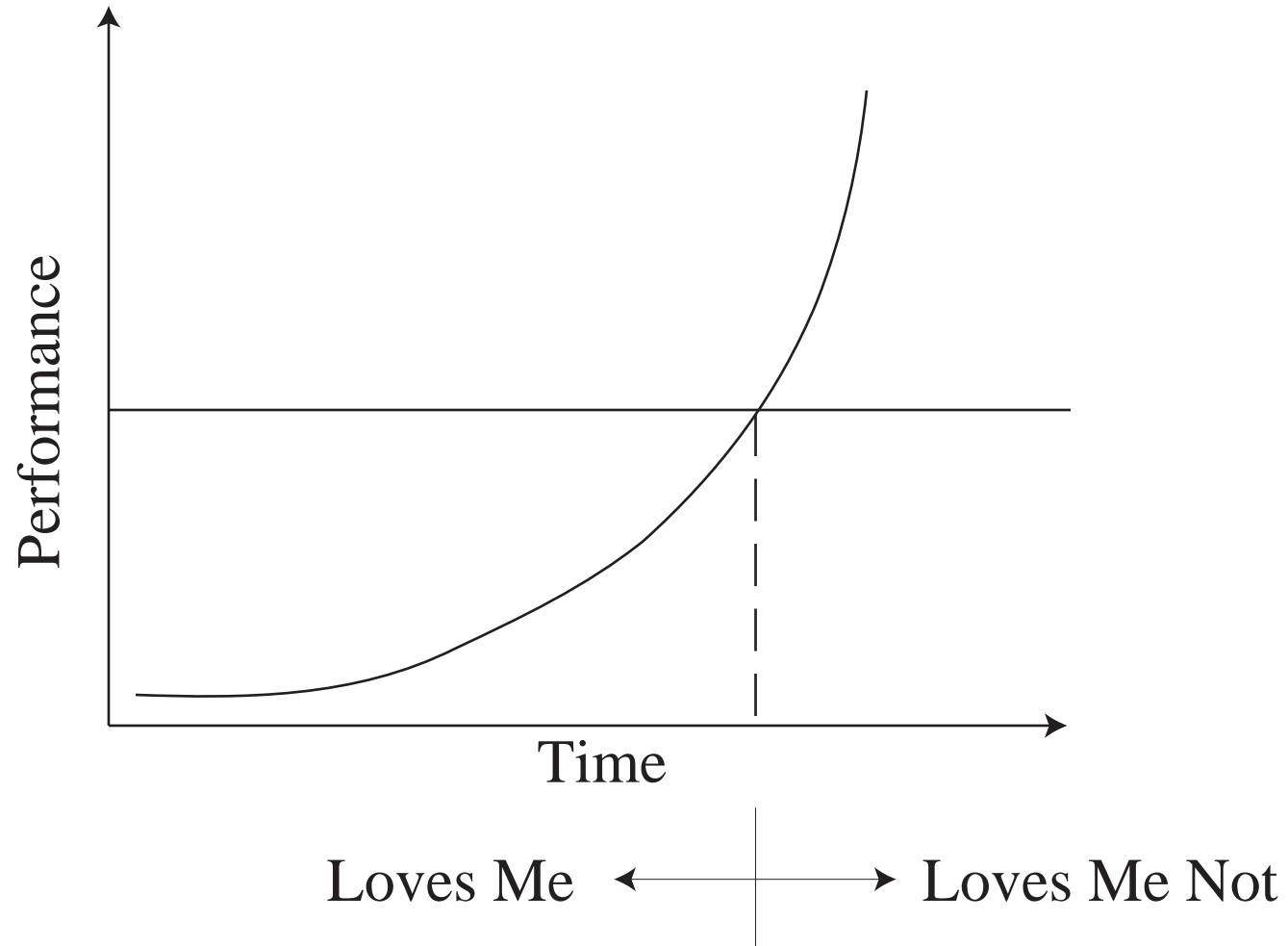
# High Performance Electronic Structure Calculations<sup>1</sup>

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<sup>1</sup>Work supported by DOE contract DE-AC04-94AL85000.



# The Teraflop Blues



# Examples of Applications

**Transition Metal Nanoclusters:** Turnover of icosahedral to bulk terminated structures

**Al<sub>2</sub>O<sub>3</sub> Surfaces:** Unusually deep surface relaxations

**Al<sub>2</sub>O<sub>3</sub> Metal Surfaces:** Unusual non-polar non-bulk film structure for nominally polar surface

**CO, NH<sub>3</sub>/Pt Surfaces:** Interaction between molecules adsorbed on surfaces

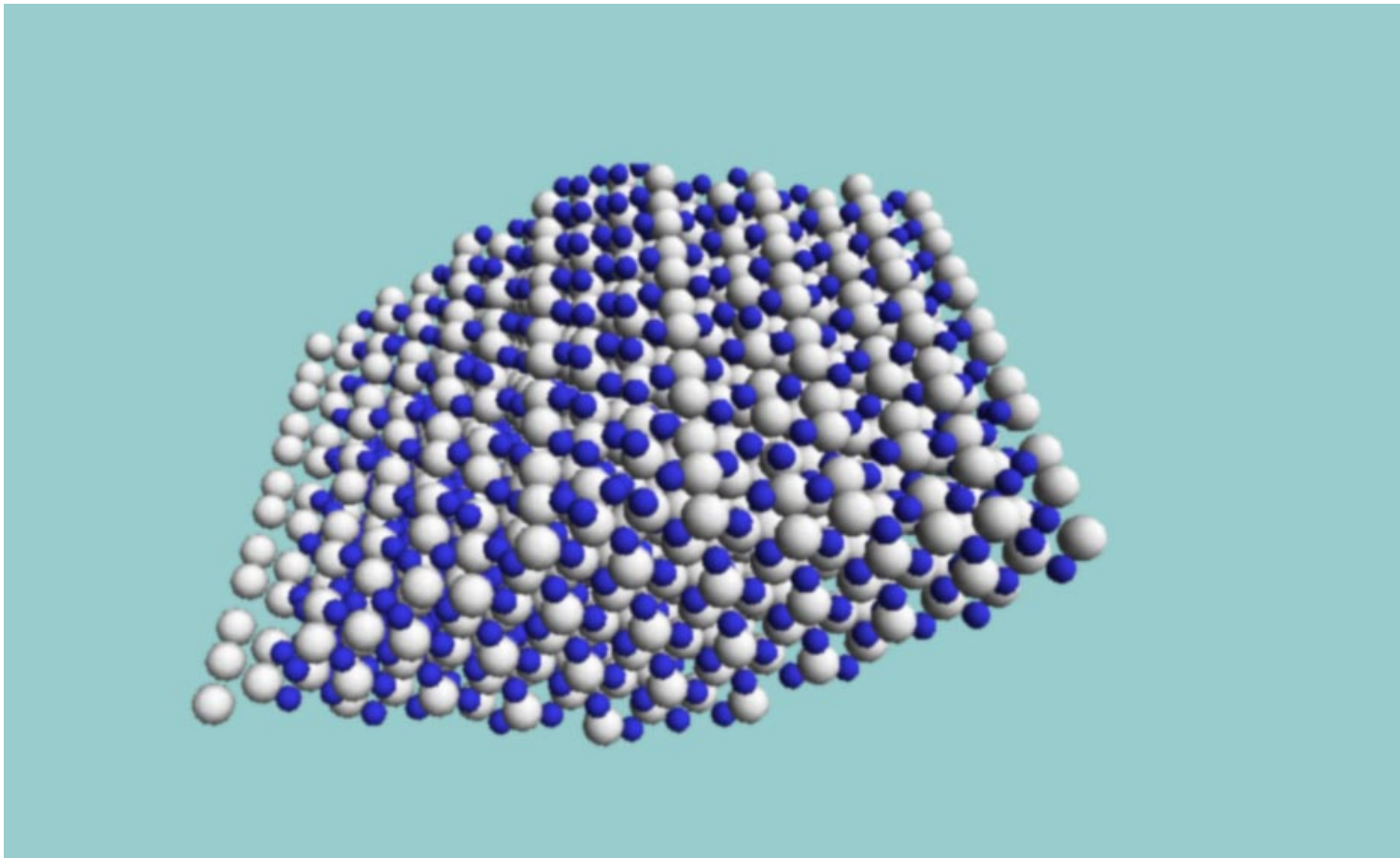
**Pt Stepped Surfaces:** Equilibrium island shapes; chemistry at steps

**Amorphous Tetrahedral Carbon:** Structural properties of amorphous materials

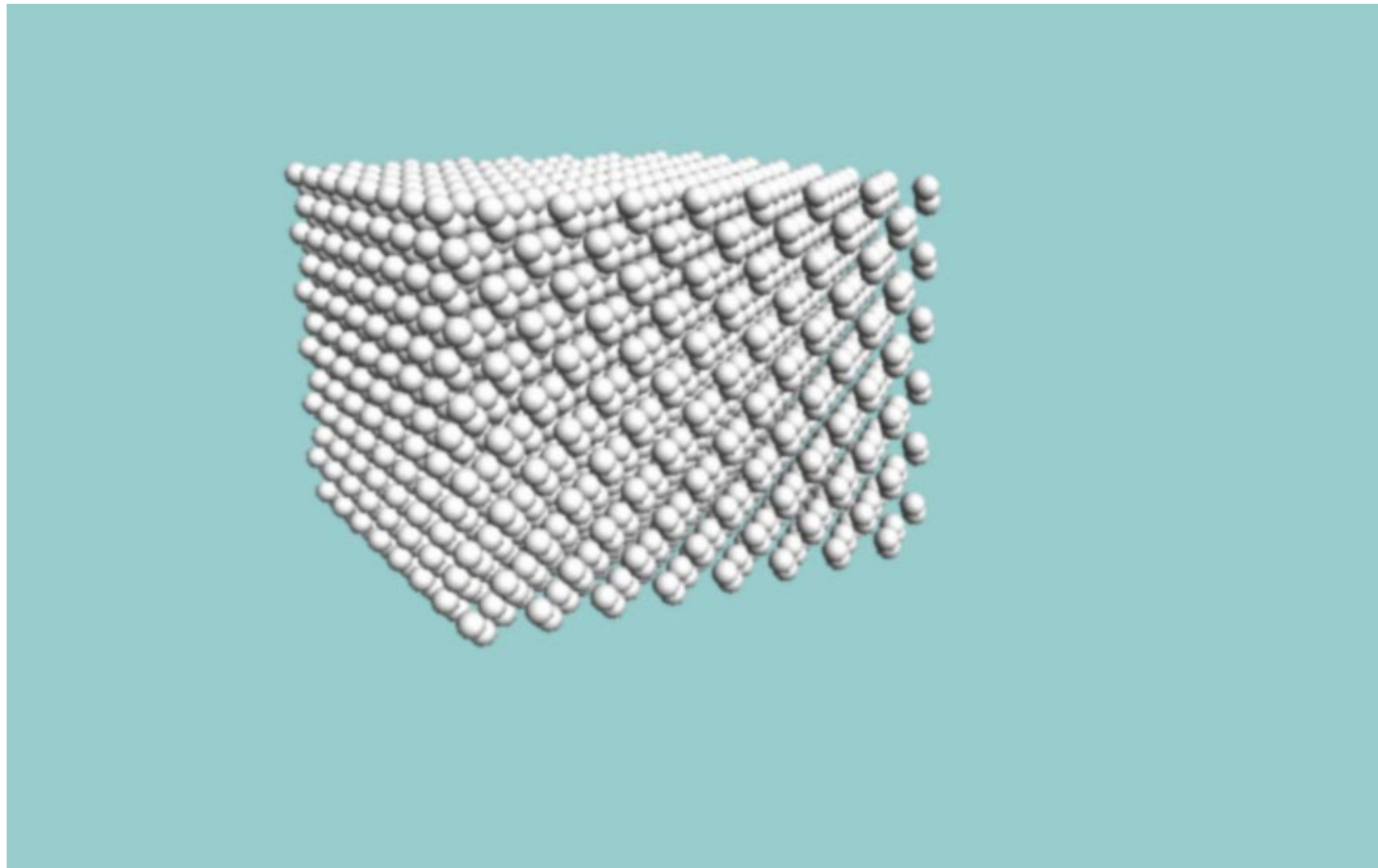
**Rare Earths in Glasses:** La in Al<sub>2</sub>O<sub>3</sub>; unusually large relaxation

**PZT:** Structural transformation as function of composition

# $\text{Al}_2\text{O}_3$ 0001 Surface Unit Cell



# $\text{Si}_{3072}$ Bulk Unit Cell



# MP-Quest Highlights

General purpose code

Molecules, slabs, bulk systems

Energies, forces, geometries

Large problems

Accurate LDA

Ab-initio relativistic pseudopotentials.

Basis sets for many atoms (Schultz).

Gaussian LCAO basis with DZP.

Efficient algorithms

Mixed analytic/numerical integrations (Feibelman).

$O(N)$  scaling for Hamiltonian and forces.

$O(N^3)$  scaling for eigensolver.

Portable and scalable (to  $P > 10^3$ ).



# Computational Procedure

Compute initial density:  $\rho = \sum \rho_{\text{at}}$

Construct Hamiltonian:  $H_{ij} = \langle \phi_i | H[\rho] | \phi_j \rangle$

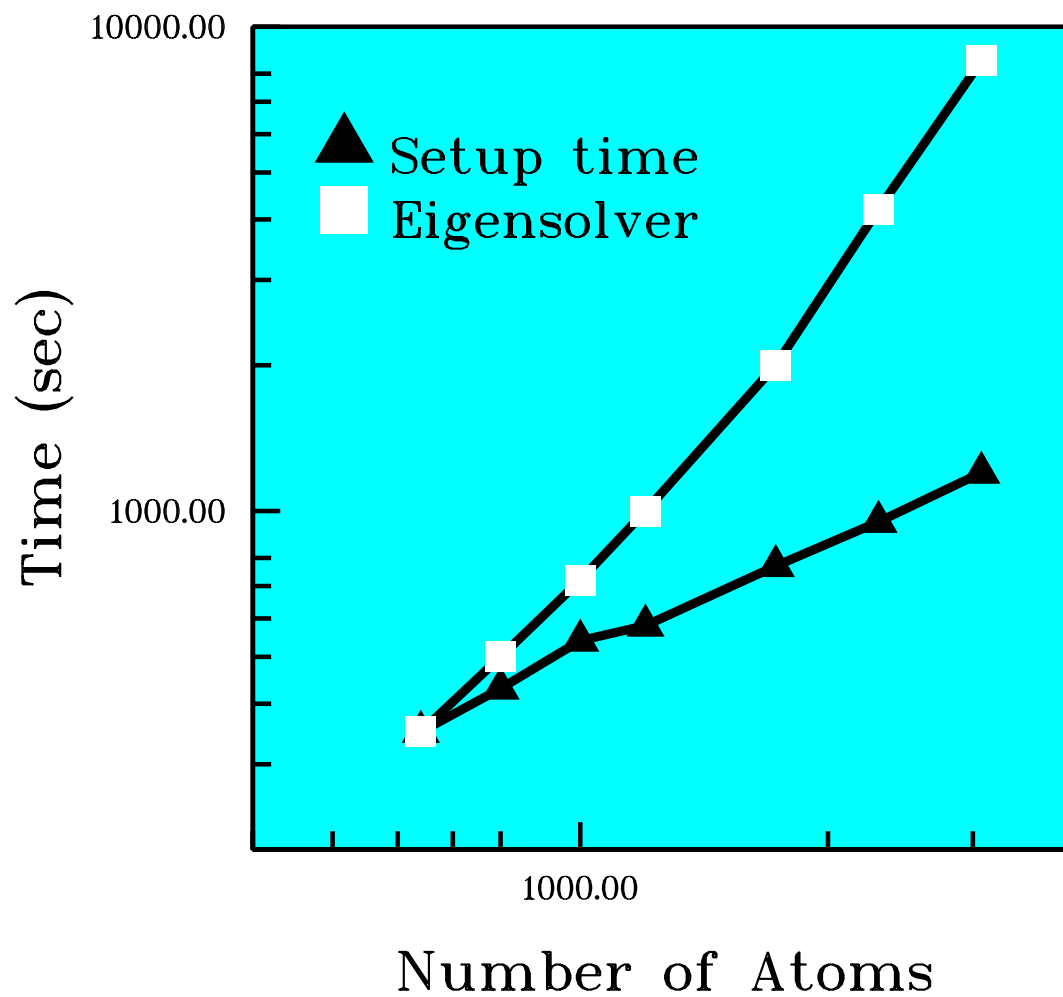
$$H = T + V_{\text{nuc}} + V_{\text{coulomb}}[\rho] + V_{\text{xc}}[\rho].$$

Solve for wavefunctions:  $\psi_i : H\psi_i = E_i\psi_i$ .

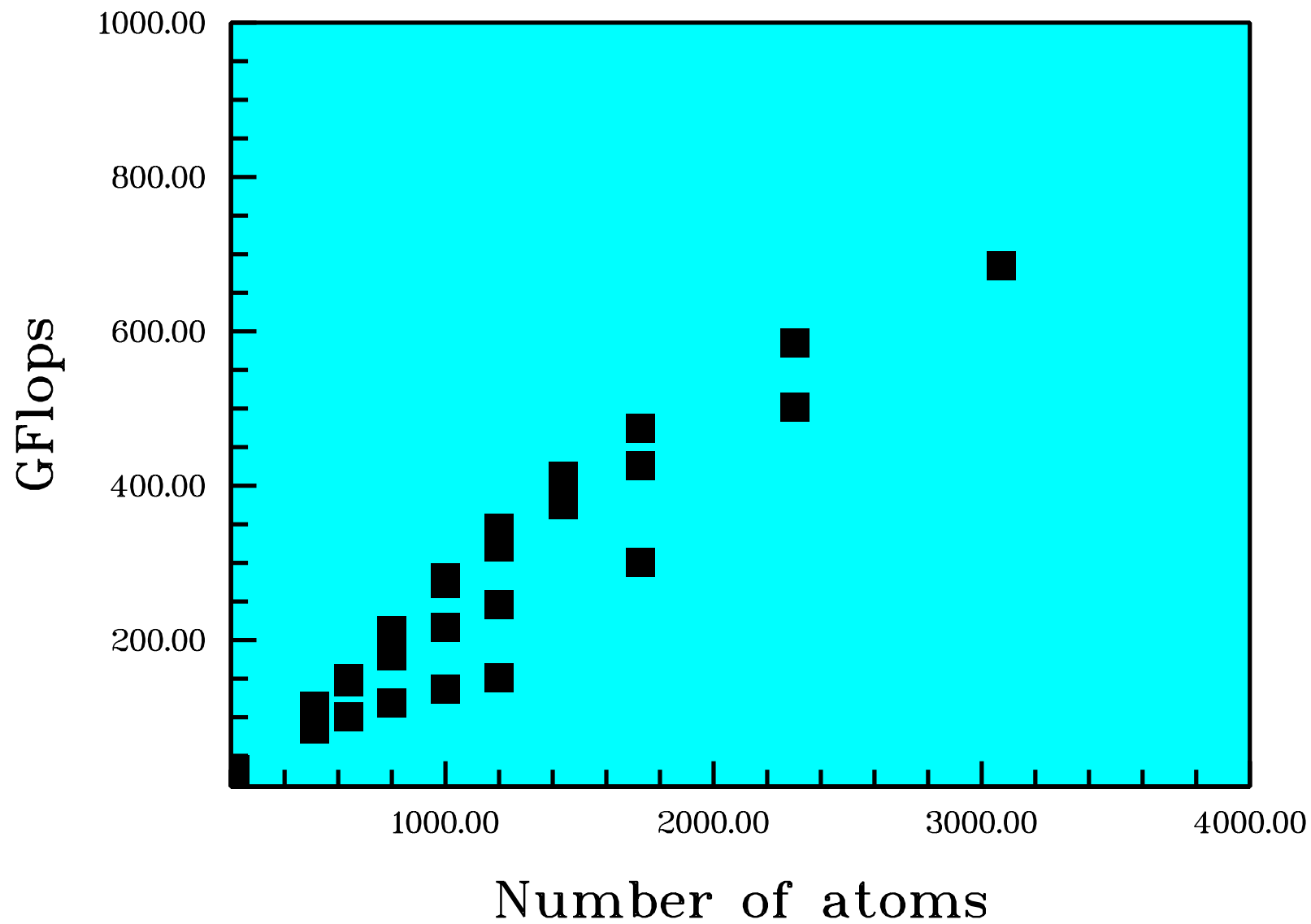
Compute new density:  $\rho = \sum f_i |\psi_i|^2$ .



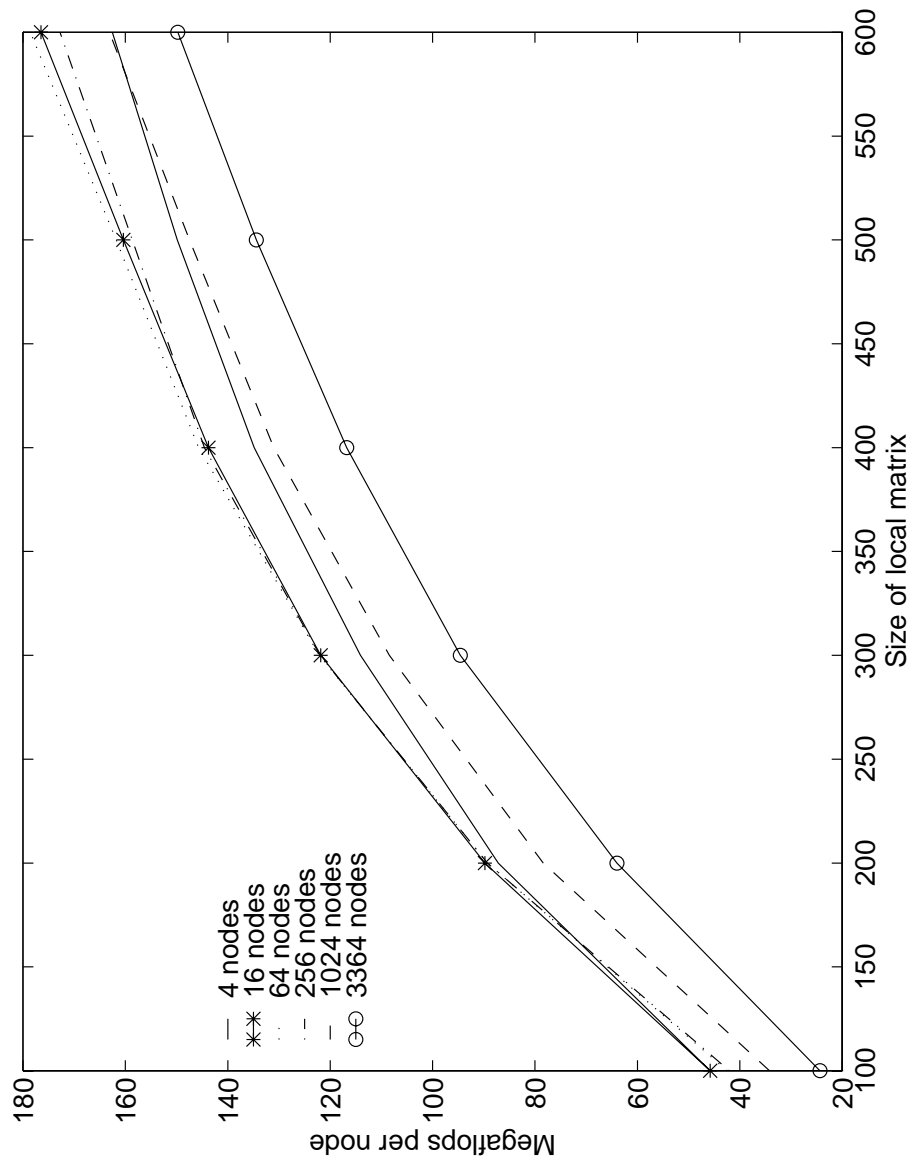
# Scaling of MP-Quest



# Eigensolver performance



# Eigensolver performance



# Summary

- MP-Quest probably at upper limit of 1-person project.
- Not feasible to develop large amounts of code for threaded model; easier to write pure message-passing code.
- Need to develop algorithms for mixed project environment: fast local comm., slower high-latency non-local comm.
- Too much latency!
  - ASCII-Red:  $50\mu\text{s}$  @ 200 MHz x 2=20000 cycles
  - OS Bypass
  - Smarter NIC

# Summary, cont.

- Back to the Future: Current cache architectures are too crude. Too often “How can I kludge my program so the compiler will generate the right code”?
- Compilers:
  - 30 years ago: Fortran 3x slower than hand code
  - Today: **The same**
- Proprietary Software:
  - OS
  - Compilers
  - A funding/reward mechanism needed for certain non-proprietary software needed.