Towards Petacomputing in Nanotechnology

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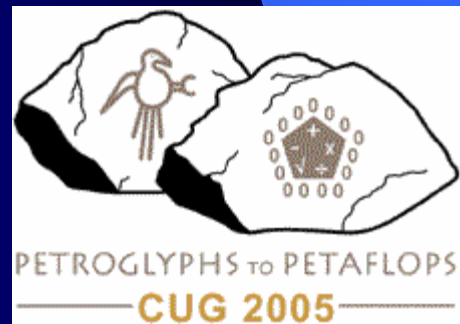


Nanotechnology and Nanomaterials

- Precision manufactured at sizes less than 100nm
  - 1nm = 10^{-9}m = 10Å, about 4 to 5 bonded atoms long
- Making of nanomaterials
  - Buckyballs, Nanotubes, Nanowires, Nanoparticles, etc.
- Novel properties because of size confinement effects
  - optical, mechanical, thermal, electrical, magnetic, etc.
- Commercial applications
  - Adhesives, sealants, coatings, anti-microbial materials, and many more

How can high performance computing help to understand and design nanomaterials?

Outline

- Theoretical approach to materials science

  Empirical, semi-empirical, and *ab initio* methods
  - *Ab initio* approach to the electronic structure
- Locally self-consistent multiple Scattering (LSMS) method and Petaflop computing
  - Algorithm, Parallel implementation, and Performance
- Applications of LSMS method
  - Electronic and magnetic structure of nanoparticles
- Future development and challenges

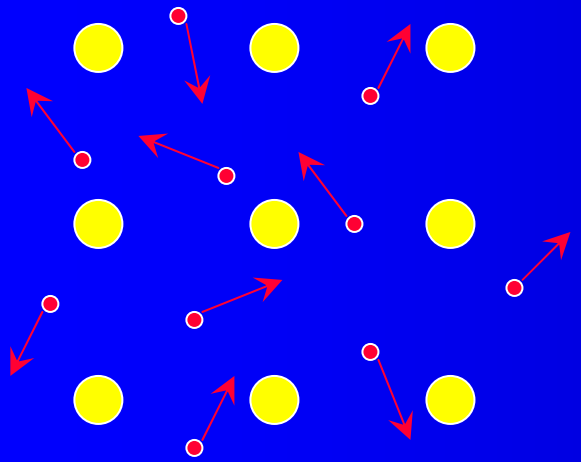
Theoretical Approach

- Empirical
  - Model potentials for inter-atomic interactions
  - Less accuracy and poor predictability
- Semi-empirical
  - Parameters in the model potential are determined quantum mechanically
  - Better accuracy and reasonable predictability
- Quantum mechanical (*ab initio*)
  - No models
  - The best accuracy and predictability

Quantum Mechanical Solution of Materials Science Problems

Electron: **Nucleus:**

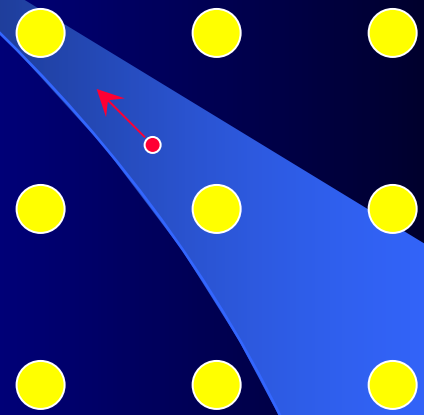
Many-electron problem



electron-electron interaction
electron-nucleus interaction
many-electron Schrödinger equation

Density Functional Theory

One-electron problem

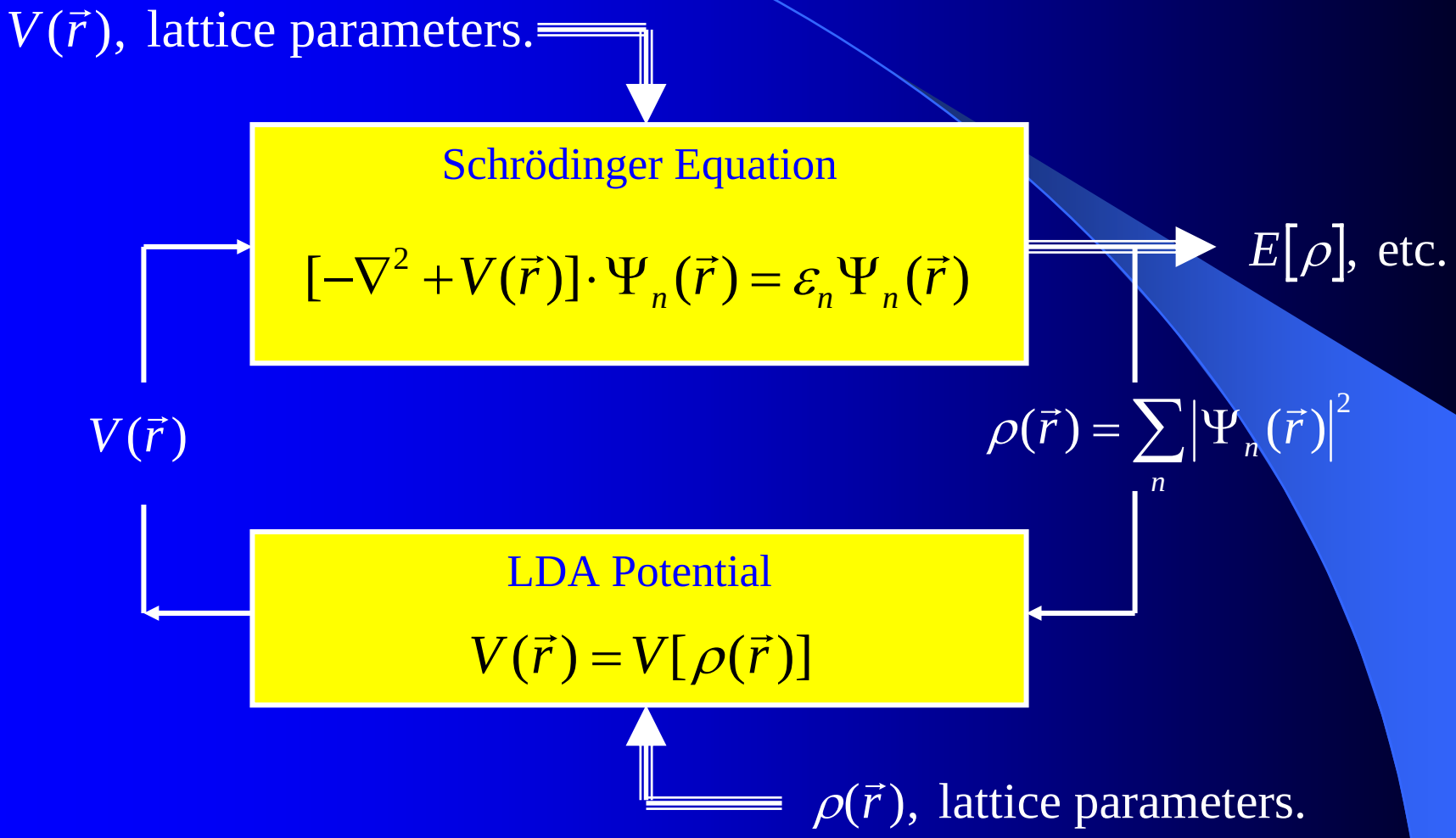


non-interacting electrons move in the potential: $V[\rho]$
one-electron Schrödinger equation

Local (Spin) Density Approximation

Calculation of $V[\rho]$ becomes feasible: $V[\rho] = V(\vec{r}) = \sum_n v_n(\vec{r} - \vec{R}_n)$

Self-consistent Process



Bottlenecks of Conventional *ab initio* Electronic Structure Methods

- N^3 scaling in computational requirement
- N^2 scaling in memory requirement
- Dominated by global operations
- Lack of efficient parallel implementation scheme
- Simulation size is limited to 100s atoms

Locally Self-consistent Multiple Scattering (LSMS) Method

- Real space multiple scattering approach

Electron Density → $$\rho_i(\vec{r}) = -\frac{1}{\pi}\,\mathrm{Im}\,Tr\int_{-\infty}^{\varepsilon_F} dz\cdot \underline{G}_i(\vec{r},\vec{r};z)$$

Moment Density → $$\vec{m}_i(\vec{r}) = -\frac{1}{\pi}\,\mathrm{Im}\,Tr\int_{-\infty}^{\varepsilon_F} dz\cdot \left[\underline{G}_i(\vec{r},\vec{r};z)\cdot\vec{\underline{\sigma}}\right]$$

Moment Orientation → $$\vec{e}_i = \int_{\Omega_i} d^3\vec{r}\cdot\vec{m}_i(\vec{r}) \Big/ \left|\int_{\Omega_i} d^3\vec{r}\cdot\vec{m}_i(\vec{r})\right|$$

- Solve the multiple scattering equations associated with atom ***i*** and compute the Green's function $\underline{\boldsymbol{G}}_{\boldsymbol{i}}$, which depends on the single scattering ***t***-matrix and the location of the atoms in the local region.

- Order-***N*** scaling in time and space complexity

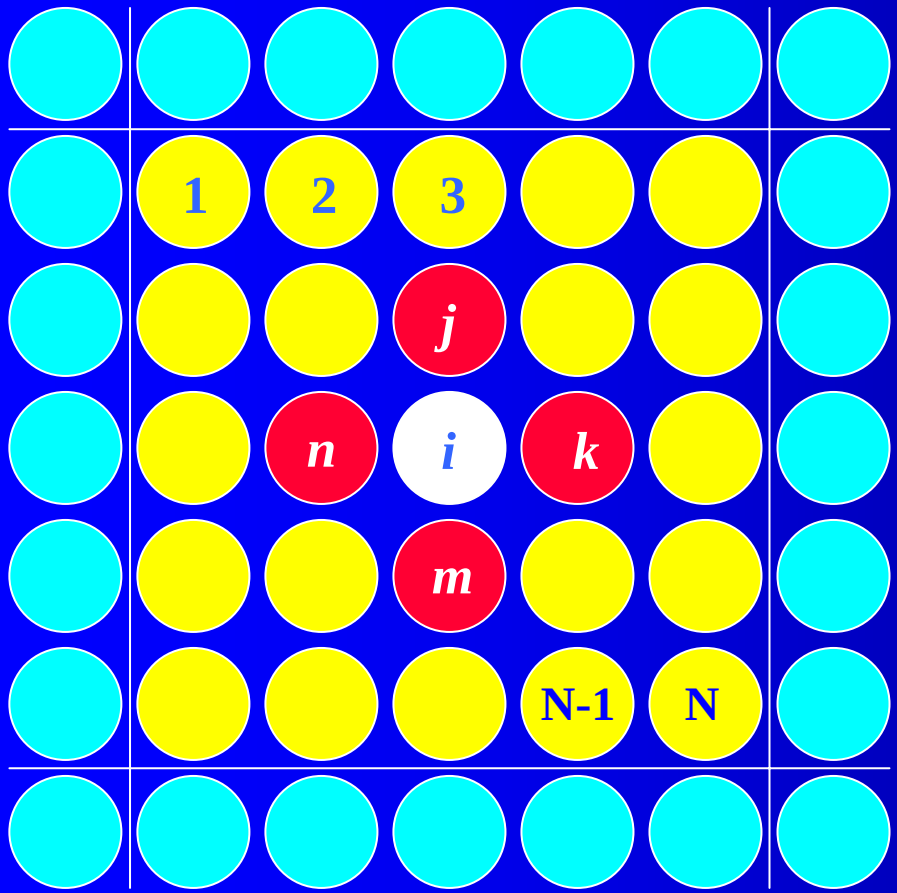
Major Floating-Point Operations

To obtain the Green's function $\underline{\underline{G}}_i$ for atom ***i***, one needs to compute:

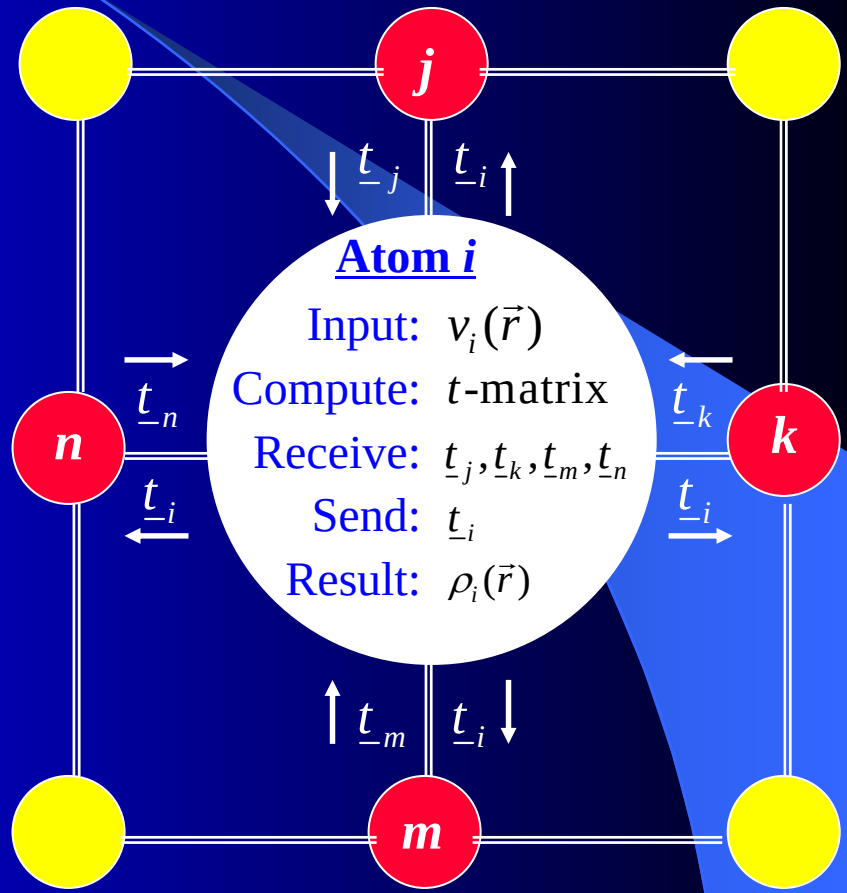
$$\underline{\underline{\tau}}^{ii}(\varepsilon) = \left[\begin{array}{ccccc} \underline{\underline{t}}_i^{-1}(\varepsilon) & \underline{\underline{g}}_{ij}(\varepsilon) & \underline{\underline{g}}_{ik}(\varepsilon) & \underline{\underline{g}}_{in}(\varepsilon) & \underline{\underline{g}}_{im}(\varepsilon) \\ \underline{\underline{g}}_{ji}(\varepsilon) & \underline{\underline{t}}_j^{-1}(\varepsilon) & \underline{\underline{g}}_{jk}(\varepsilon) & \underline{\underline{g}}_{jn}(\varepsilon) & \underline{\underline{g}}_{jm}(\varepsilon) \\ \underline{\underline{g}}_{ki}(\varepsilon) & \underline{\underline{g}}_{kj}(\varepsilon) & \underline{\underline{t}}_k^{-1}(\varepsilon) & \underline{\underline{g}}_{kn}(\varepsilon) & \underline{\underline{g}}_{km}(\varepsilon) \\ \underline{\underline{g}}_{ni}(\varepsilon) & \underline{\underline{g}}_{nj}(\varepsilon) & \underline{\underline{g}}_{nk}(\varepsilon) & \underline{\underline{t}}_n^{-1}(\varepsilon) & \underline{\underline{g}}_{nm}(\varepsilon) \\ \underline{\underline{g}}_{mi}(\varepsilon) & \underline{\underline{g}}_{mj}(\varepsilon) & \underline{\underline{g}}_{mk}(\varepsilon) & \underline{\underline{g}}_{mn}(\varepsilon) & \underline{\underline{t}}_m^{-1}(\varepsilon) \end{array} \right]^{-1}$$

$$\text{LIZ Size} \times (l_{\max}+1)^2 \qquad 11$$

Algorithm



N-atom Unit Cell

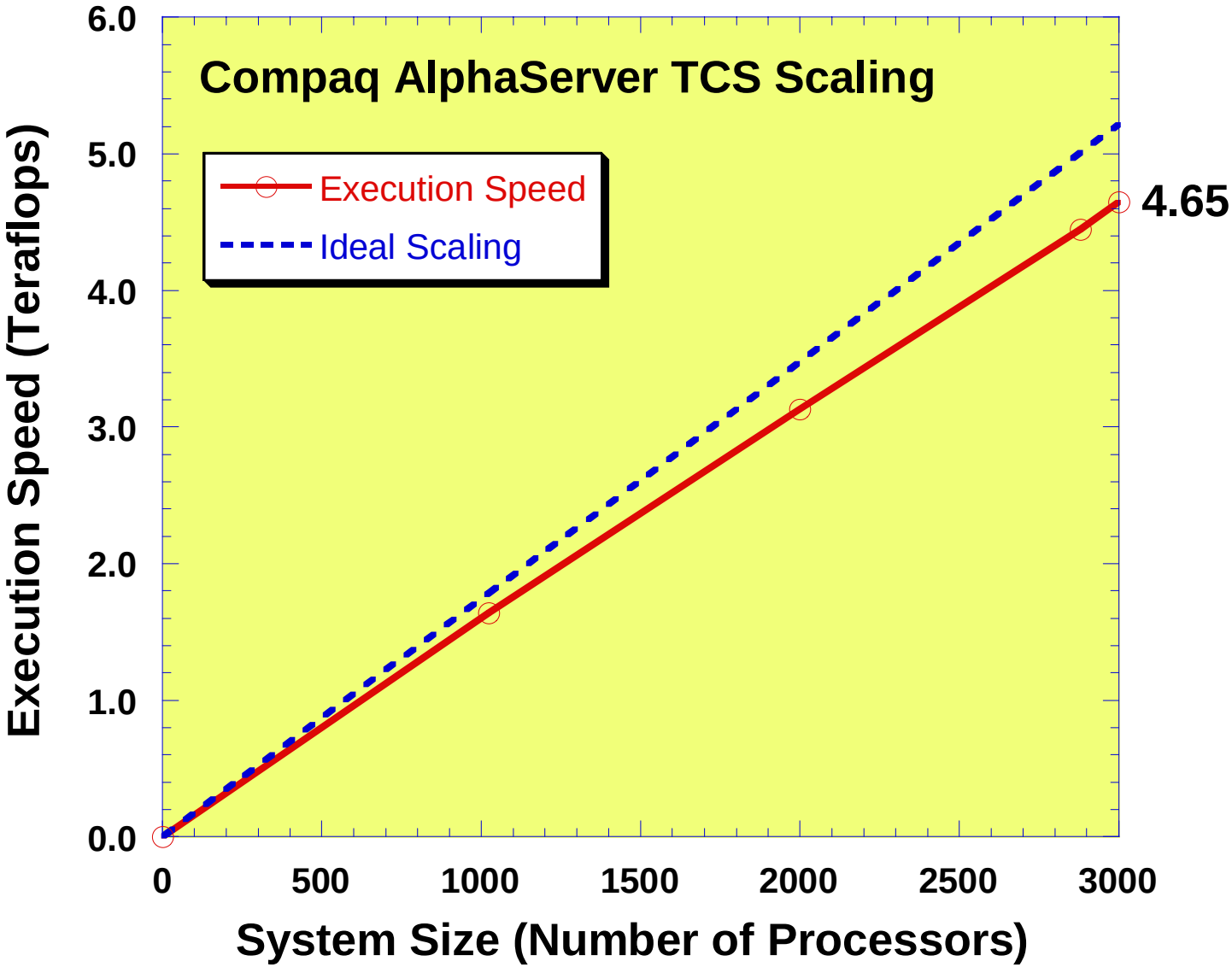


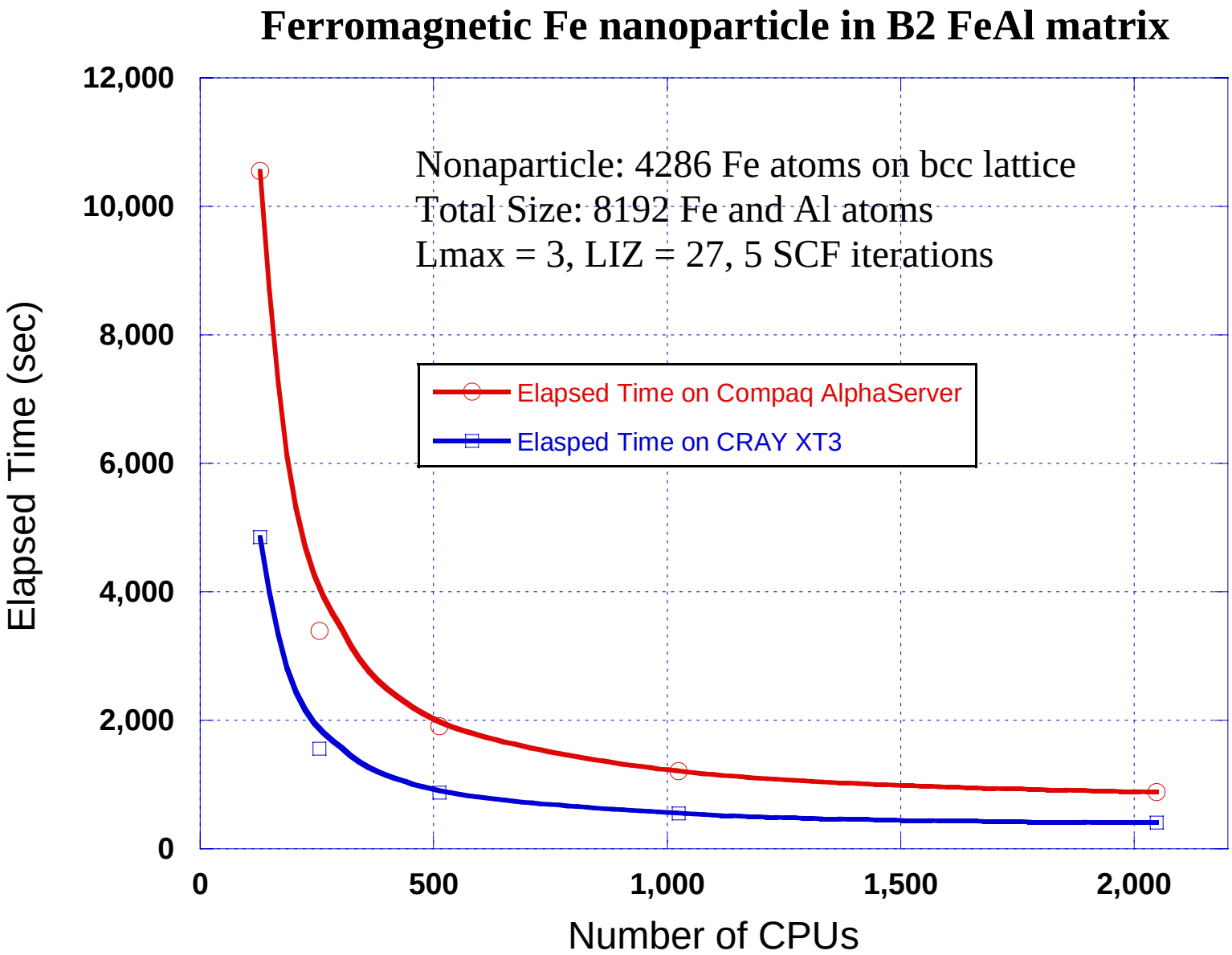
Local Interaction Zone (LIZ)

Parallel Implementation

- Intrinsic parallelism:
  - the atoms in the unit cell
  - the energy points along the complex energy contour
- Atoms are distributed evenly among CPUs, and, unlike the previous version, the code allows multiple atoms mapped onto each CPU
- One-sided communications are used for getting the ***t***-matrix from those neighboring atoms that are mapped onto other CPUs

Linear Scaling



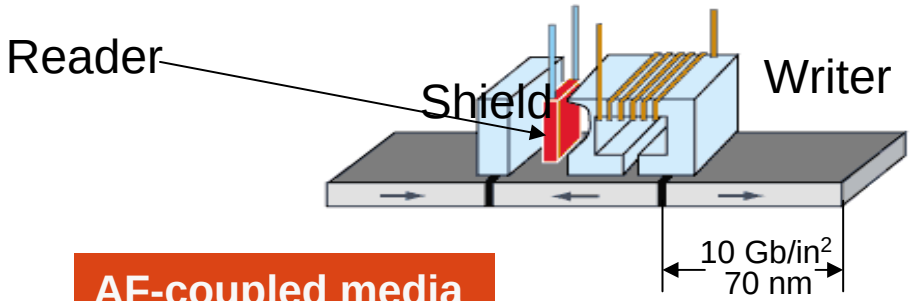

Ferromagnetic Fe nanoparticle in B2 FeAl matrix
Nonaparticle: 4286 Fe atoms on bcc lattice
Total Size: 8192 Fe and Al atoms
Lmax = 3, LIZ = 27, 5 SCF iterations
Elapsed Time on Compaq AlphaServer
Elasped Time on CRAY XT3
Elapsed Time (sec)
12,000
10,000
8,000
6,000
4,000
2,000
0
0
500
1,000
1,500
2,000
Number of CPUs

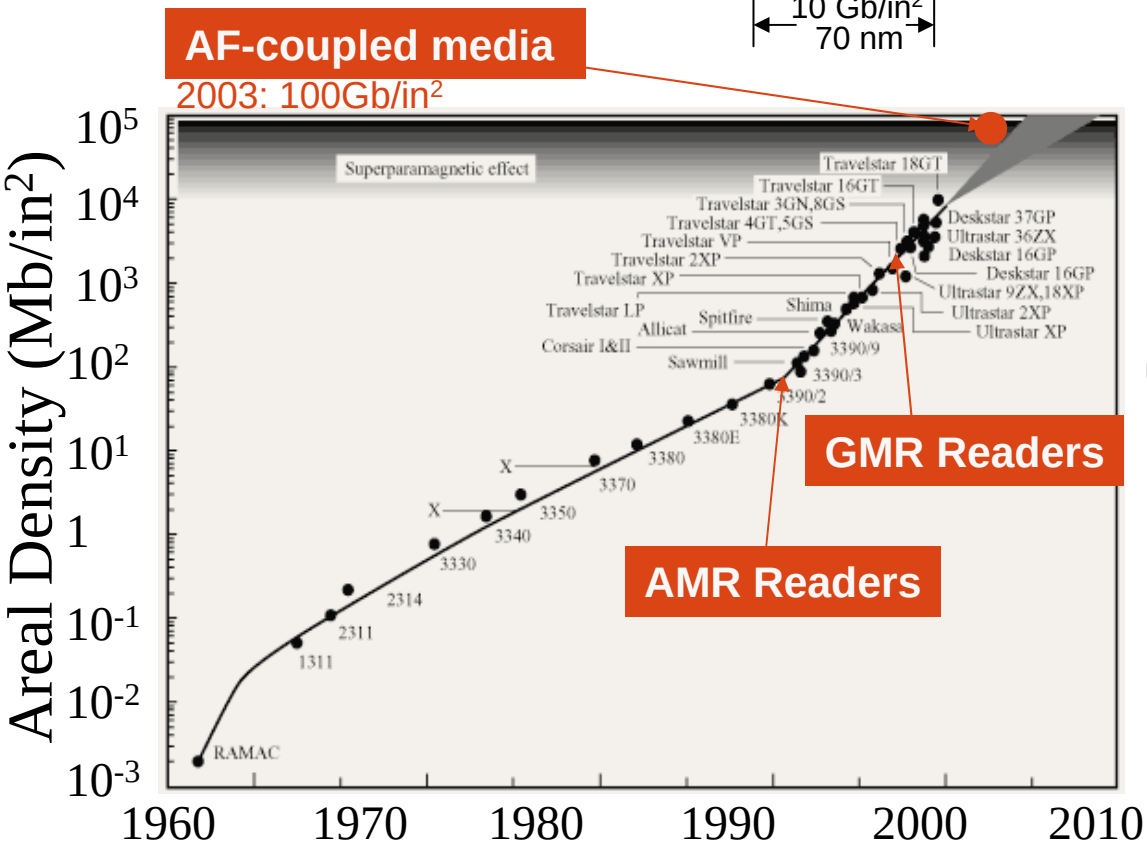
Magnetic Nanoparticles

Nanoscale magnetic crystallites in an amorphous or crystalline matrix

- Properties: with nanostructured materials, physical parameters such as coercivity can be adjusted selectively.
  - Cobalt nanoparticles possess a higher permeability, curie temperature and electrical resistance than conventional ferrite materials due to quantum coupling effects between neighbouring nanoparticles.
  - Iron nanoparticles possess TMR (tunnel magnetoresistance) properties.
- The advantages: an increased sensitivity to detect changes of magnetic field and a higher working temperature range.
- Potential applications: miniaturized and energy-saving microwave antennas, inductors, sensors, data memories, MRI contrast enhancing reagents, smart drugs, etc.

Science of Drives: Magnetic Nanostructures





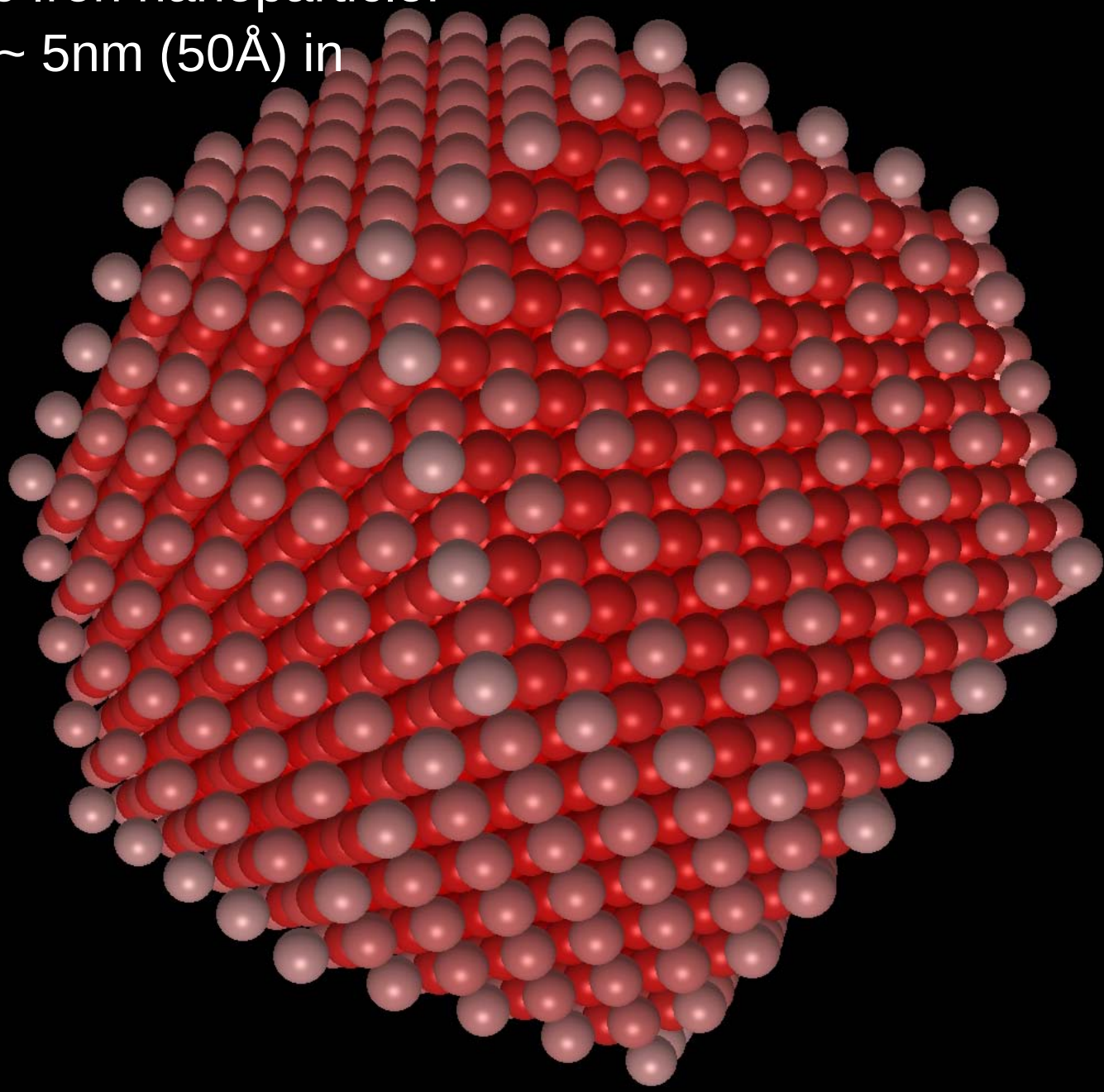
- Disk Storage
  - Historic storage density growth rate ~60%/yr [Early '90s]
  - GMR read head based on advances in basic science
    - Oscillatory exchange coupling
    - Giant Magneto-Resistance
    - Exchange Bias
  - Discovery 1998
  - Application 1998
    - Boosts growth rate ~100%/yr
- Future challenges
  - Stability
    - Anisotropy too low magnetic moment thermally unstable
      - Super paramagnetic limit
  - Switching
    - Anisotropy too high – can't switch

Applications of LSMS Method

Electronic Structure of Magnetic Nanoparticles

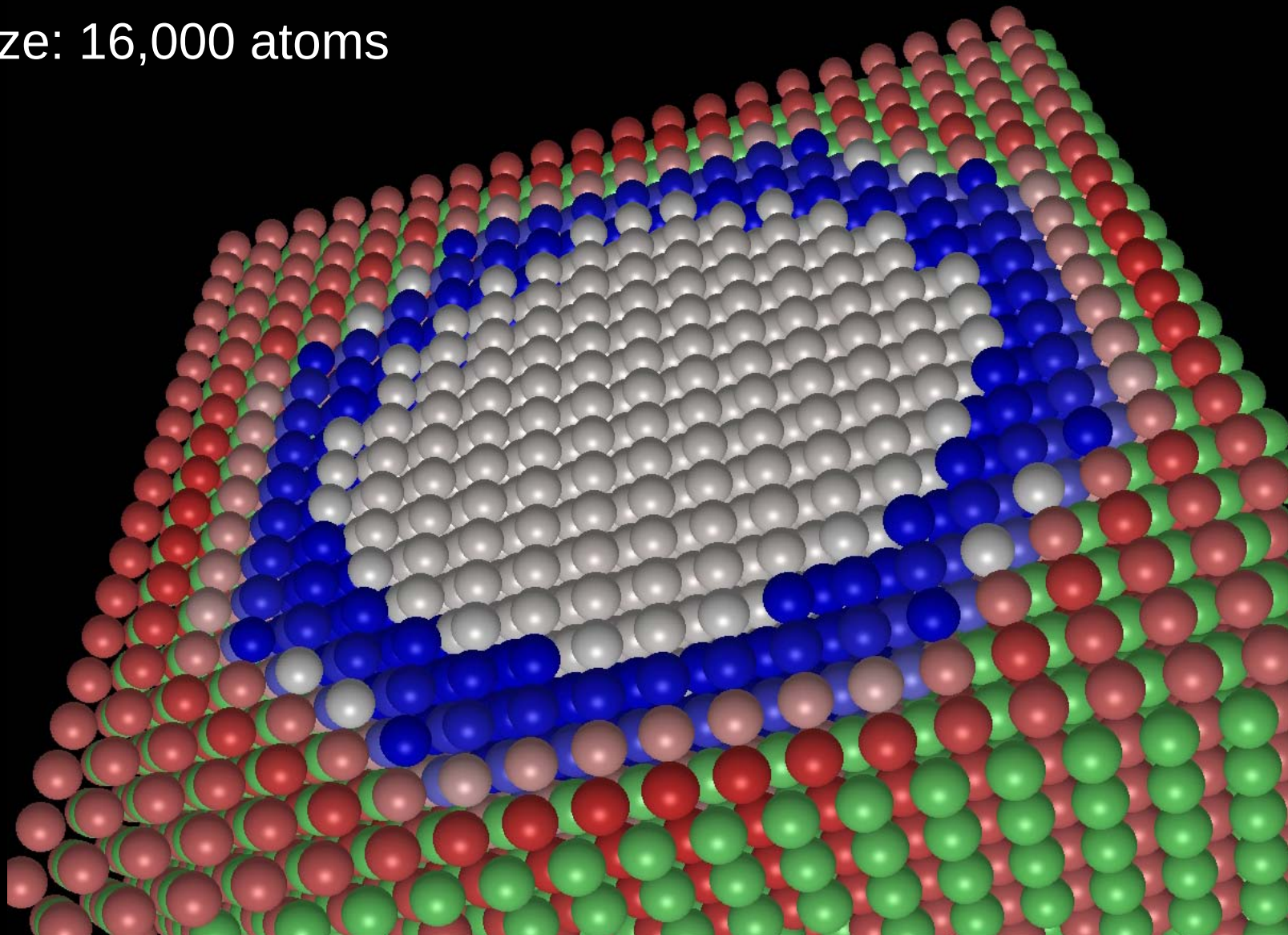
- Fe nanoparticle (body-centered cubic structure) embedded in FeAl (B2 structure) matrix
- Spin-polarized LSMS calculations are applied to the unit cell sample simulating the nanoparticle in a media
- The Fe nanoparticle contains 4,409 Fe atoms, which is about 5nm along the diagonal
- All together, there are 16,000 Fe and Al atoms in the unit cell sample

Ferromagnetic Iron nanoparticle:
4,409 atoms, ~ 5nm (50Å) in diagonal

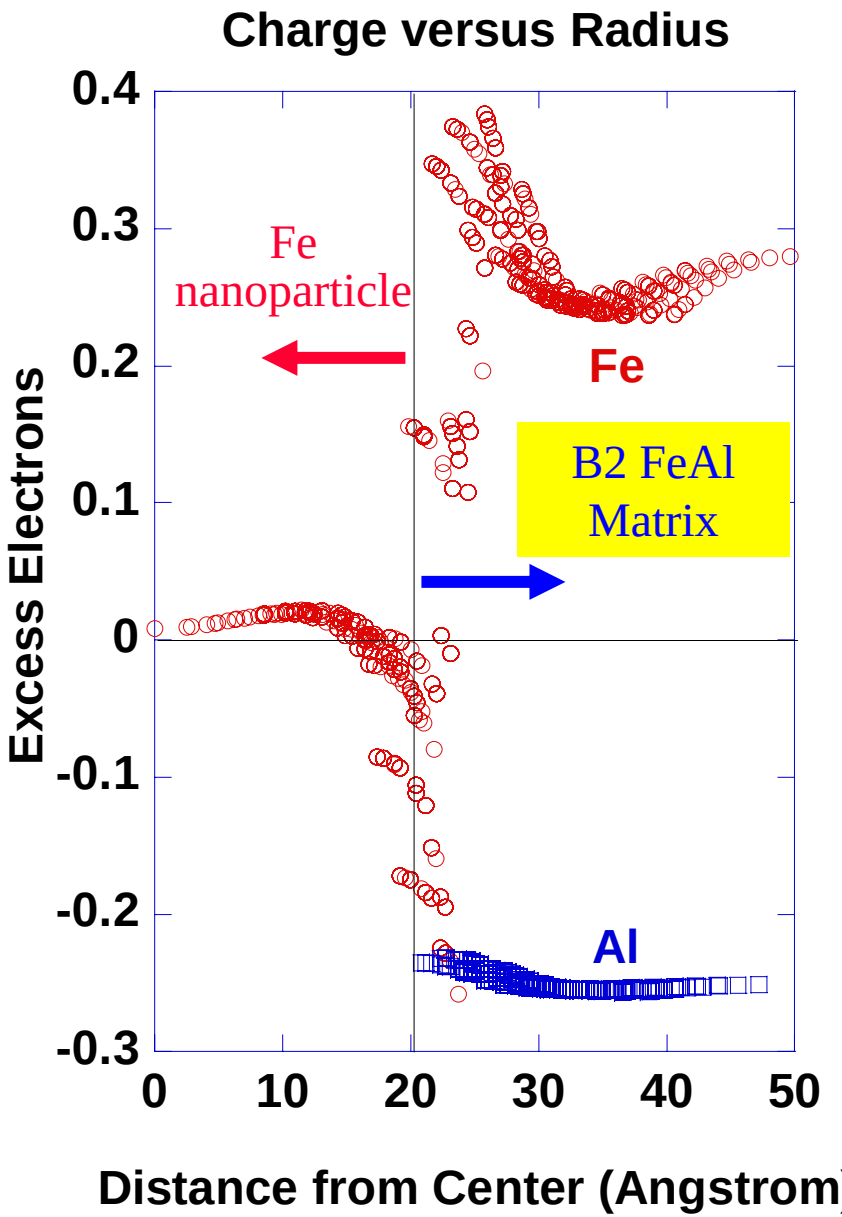


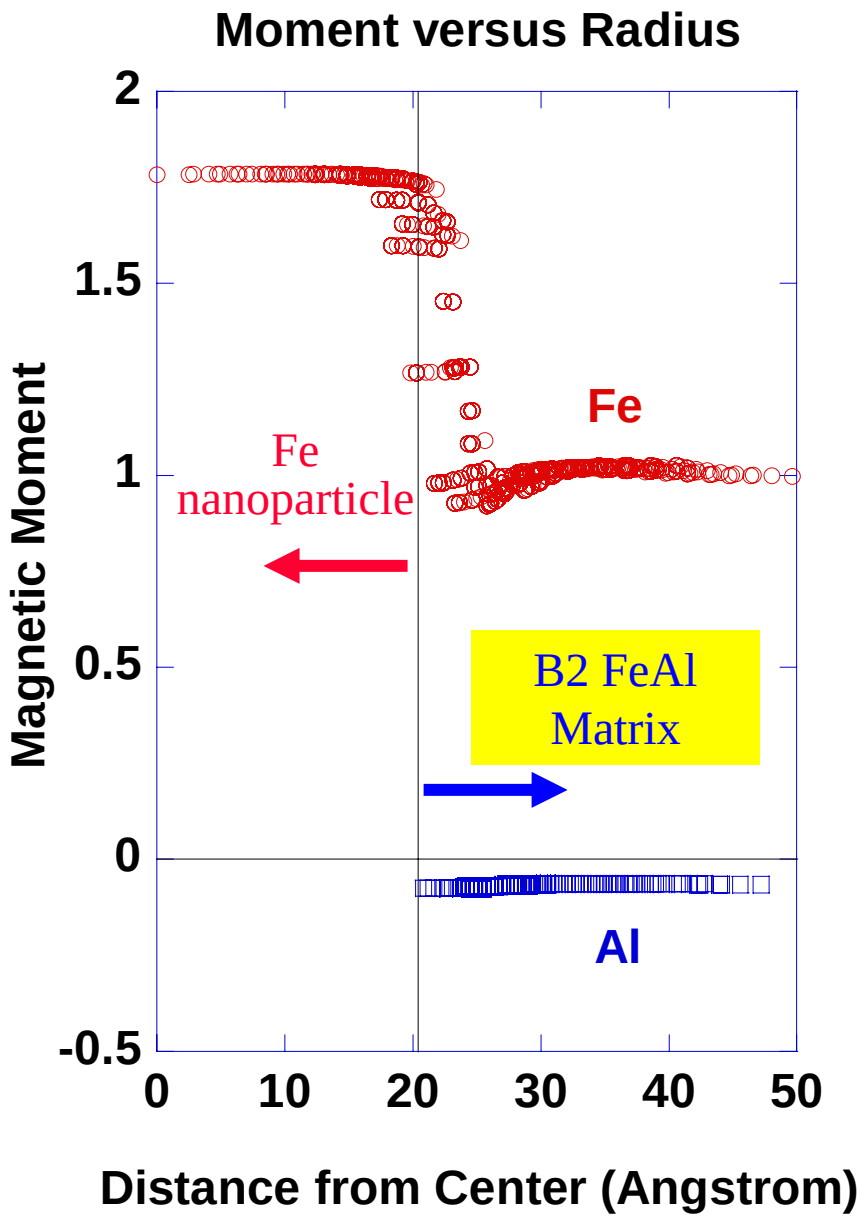
Charge distribution of Iron nanoparticle (4,409 atoms) in FeAl matrix

Total size: 16,000 atoms



Electronic and Magnetic Structure of Fe nanoparticle in B2 FeAl Matrix





Petaflop Computing and Simulation of Nanomaterials

- With linear-scaling *ab initio* code and teraflop machine, we can perform electronic structure calculations for nanoparticles of ~ 5nm (~ 5,000 atoms) in size
- It requires a petaflop machine to perform electronic structure calculations for nanoparticles of ~ 50nm (~ 5,000,000 atoms) in size, and other nanomaterials such as nanowire and nanotubes.

Current Feature of LSMS 2.0

- Full-potential
- Multiple atoms per CPU
- ***k***-space methods
- Muffin-tin potential, ASA potential, and Muffin-tin ASA potential
- Non-relativistic and scalar-relativistic
- Spin-polarized and spin-canted

Future Development and Challenges

- Layered LSMS
- Force field calculation
- Spin-dynamics
- Fully-relativistic
- Non-uniform atom distribution and CPU load balancing

How to?

Task:

Distribute a large pile of apples to 1000s of baskets.

Requirement:

The weight of the apples in each basket is the same!