ITAMIT Meeting August 2004

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Lisboa PORTUGAL

INESC-MN

What is INESC-MN

- Private non-profit association
- Created January 2002 (before solid state group of INESC)
- 4 Senior researchers, 5 post-docs, 10 PhD students

What are the research interests

- Magnetism
- Thin film MEMS
- Simulation of Materials
- Biological applications

Instituto Superior Técnico

- Engineering school in Lisbon
- 7000 students
- 45 physics student/year

Recent Research

- Micromagnetism (with Paulo Freitas and Liu Yaowen)
- First principles Monte Carlo (with Jorge Pacheco)
- Pseudopotential with explicit core states (with Jorge Pacheco and C.S.Loia)
- Silicates (with R.M.Wentzcovitch and Liu Yaowen)

Motivation

- Miniaturization in magnetic recording technology and MRAMs
- Devices made at INESC-MN, group of Paulo Freitas
- Need of simulation of magnetic domains as a function of applied field
- Disagreement between simulation codes when the project was started

Micromagnetic Simulations

Basic equations: Maxwell

Assumptions: $\vec{E}=\vec{0}$ $\partial/\partial t \to 0$ $\vec{j}=\vec{0}$

$$\nabla \cdot \vec{B} = 0 \qquad \vec{B} = \mu\left(\vec{M}+\vec{H}\right)$$

$$\nabla \times \vec{H} = 0 \qquad \vec{H} = \vec{H}_a + \vec{H}_D$$

Phenomenology

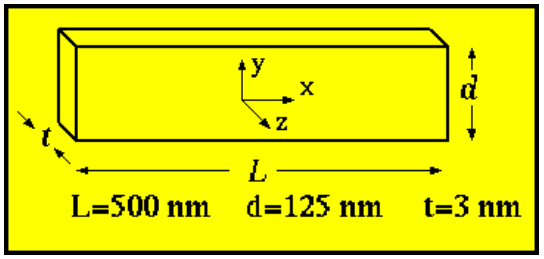
- Ferromagnetism $|\vec{M}| = \vec{M}_S$
- Thermodynamics $E_Z = \iiint \mu \vec{H}_a \cdot \vec{M}\, dr$ $E_D = \frac{1}{2}\iiint \mu \vec{H}_D \cdot \vec{M}\, dr$

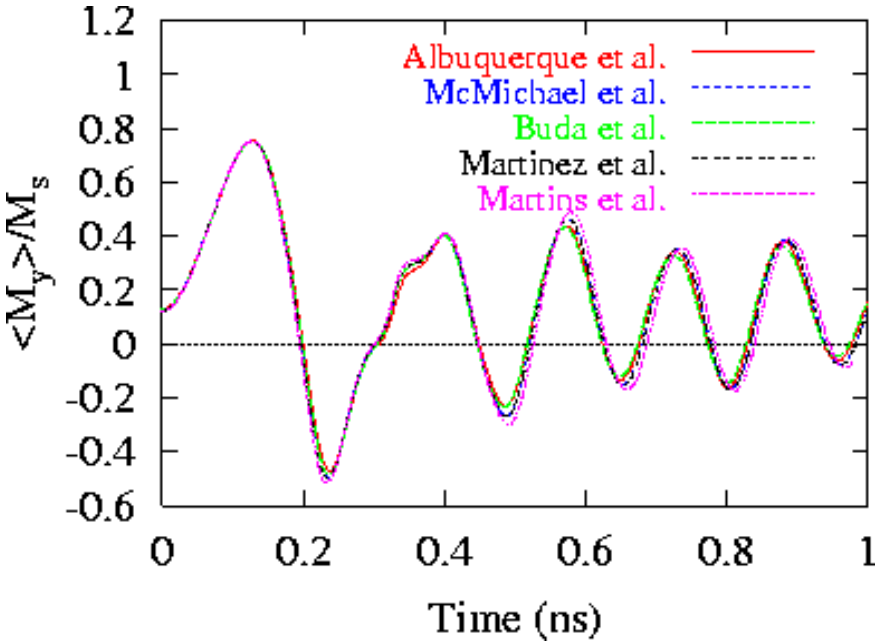
$$E_x = A \iiint \left(\nabla \frac{\vec{M}}{M_S}\right)^2 dr$$

Solving the equations of micromagnetism

- From $\nabla \cdot \vec{B} = 0$ we have $\nabla \cdot \vec{H} = -\nabla \cdot \vec{M}$
- From $\nabla \times \vec{H} = \vec{0}$ we have $\vec{H} = -\nabla V$
- The result is a Poisson equation $\Delta V = \nabla \cdot \vec{M}$
- The “magnetic charge” is mostly a surface charge
- Solving Poisson equation on a simple grid
  - SOR relaxation
  - Multigrid
- We use low order formulas that preserve the integral form of Maxwell equations

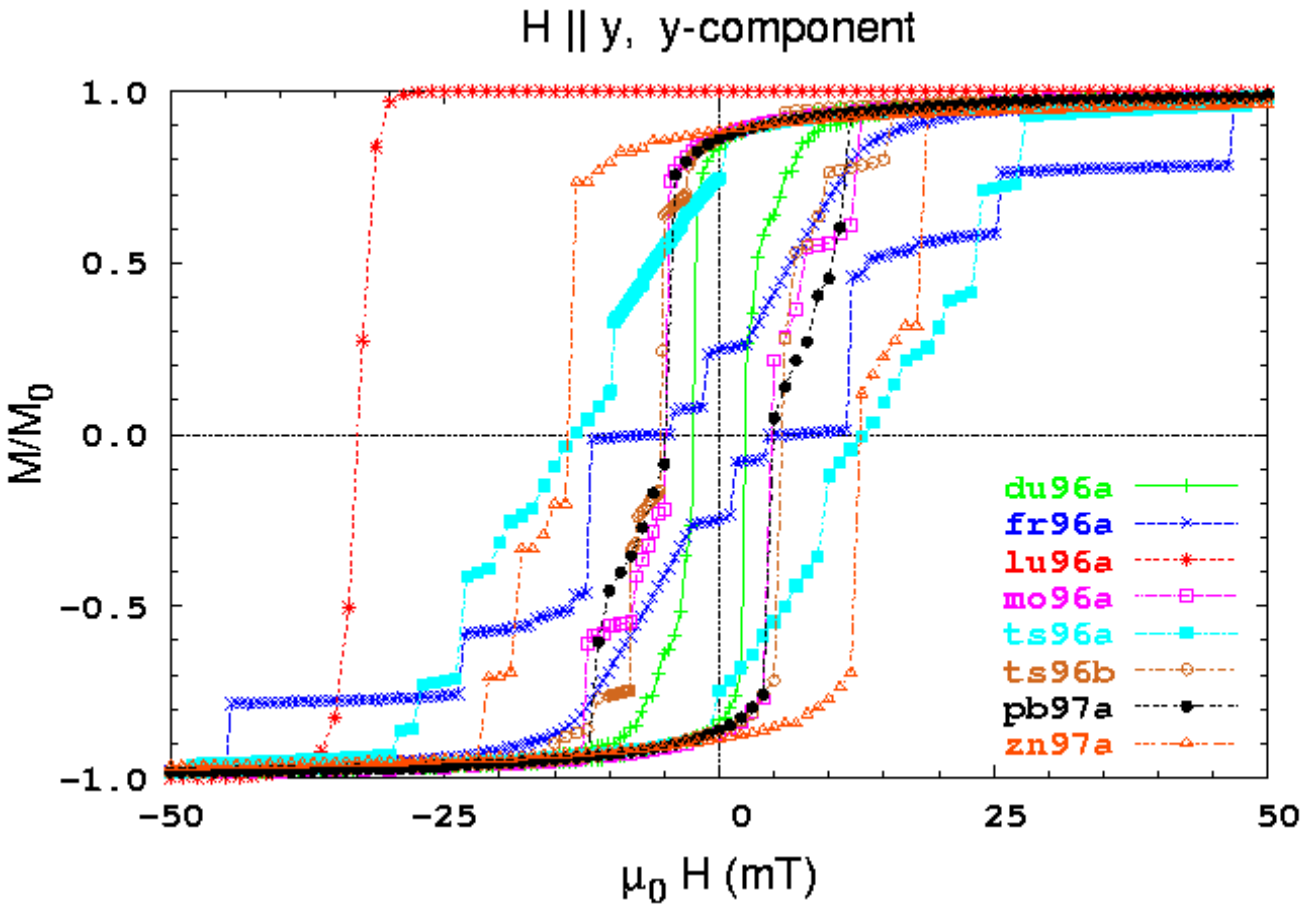
Comparison with other codes





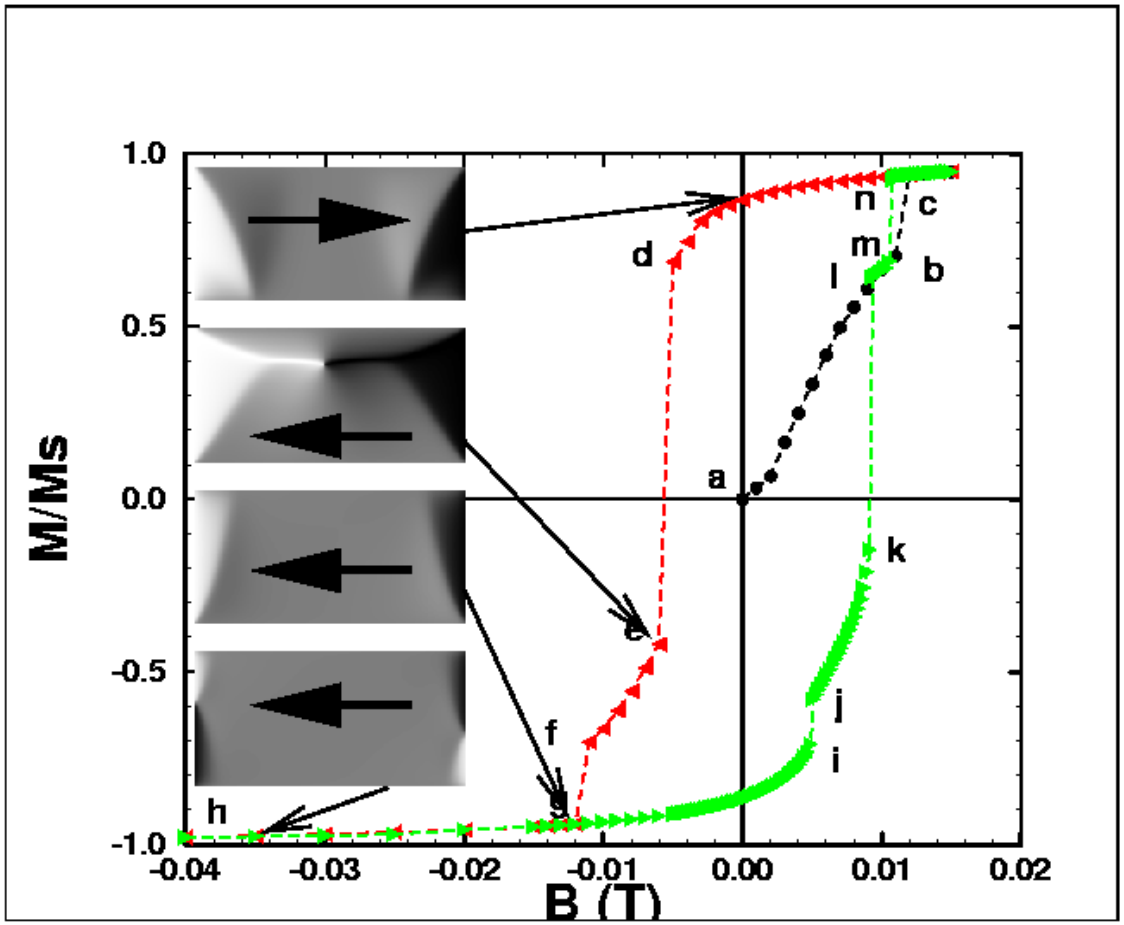
- There is a collection of standard problems used to compare codes
- Currently most codes agree with each other
- Problem 4 simulates the reversal of the magnetization of a small permalloy thin film

Comparison with other codes

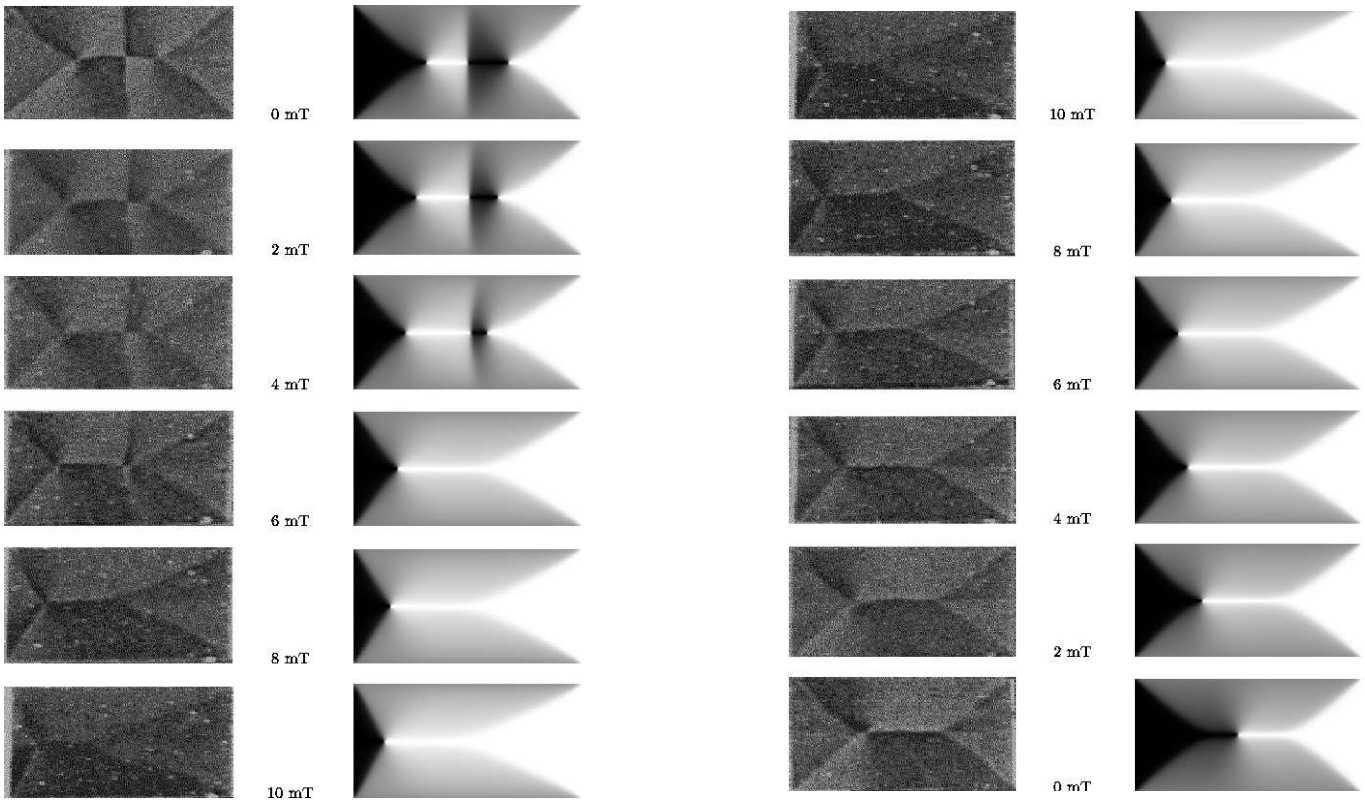


In the original number one problem nobody agreed

Our solution to first problem



Comparison with magnetic force microscopy



The hysteresis loop is well described

Recent micromagnetic simulation work

- Tunnel junctions (multilayers)

  Y. Liu et al, JAP 91, 8296 (2002)
- Current induced magnetization switching

  Y. Liu et al, APL 82, 2871 (2002)

  Y. Liu et al, JAP 93, 8385 (2003)
- Low resistance spin dependent tunnel junctions

  Y. Liu et al, JAP 93 8367 (2003)

Combined theory experiment papers

First Principles Monte Carlo

- Two methods are widely used in statistical mechanics: Monte Carlo and Molecular Dynamics. However only molecular dynamics is used with first principles forces (Car-Parrinelo or Born-Oppenheimer dynamics).
- In classical simulations Monte-Carlo is competitive because it does not need the expensive calculation of forces
- First principles forces are cheap to calculate compared with the determination of the wavefunctions
- First principles Monte Carlo only makes sense if we have a "trick" to speed up the calculations

Pacheco, Martins, Lecture Notes in Computer Science 1981, 230 (2001)

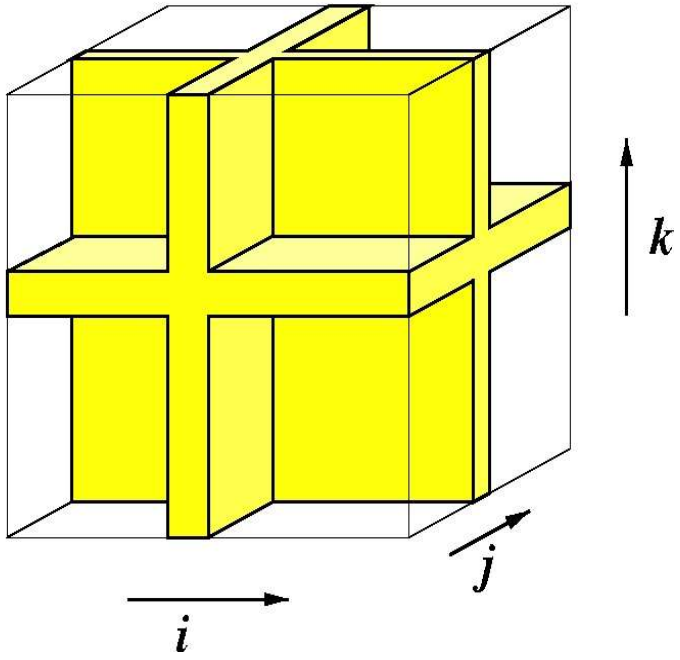
Martins, Pacheco, AIP Proceedings 577, 166 (2001)

Kohn-Sham equations in atom centered basis

- In LCAO and other localized basis sets we can also expand the self-consistent potential and charge density in localized functions
  - We expand the wavefunctions in atom centered gaussians $\varphi(\vec{r})$
  - We expand the potential in other atom centered gaussians $g(\vec{r})$
- We will have to calculate a lot of integrals of the type

$$B_{ijk} = \iiint \varphi_i(\vec{r})\, g_j(\vec{r})\, \varphi_k(\vec{r})\, d\,r$$

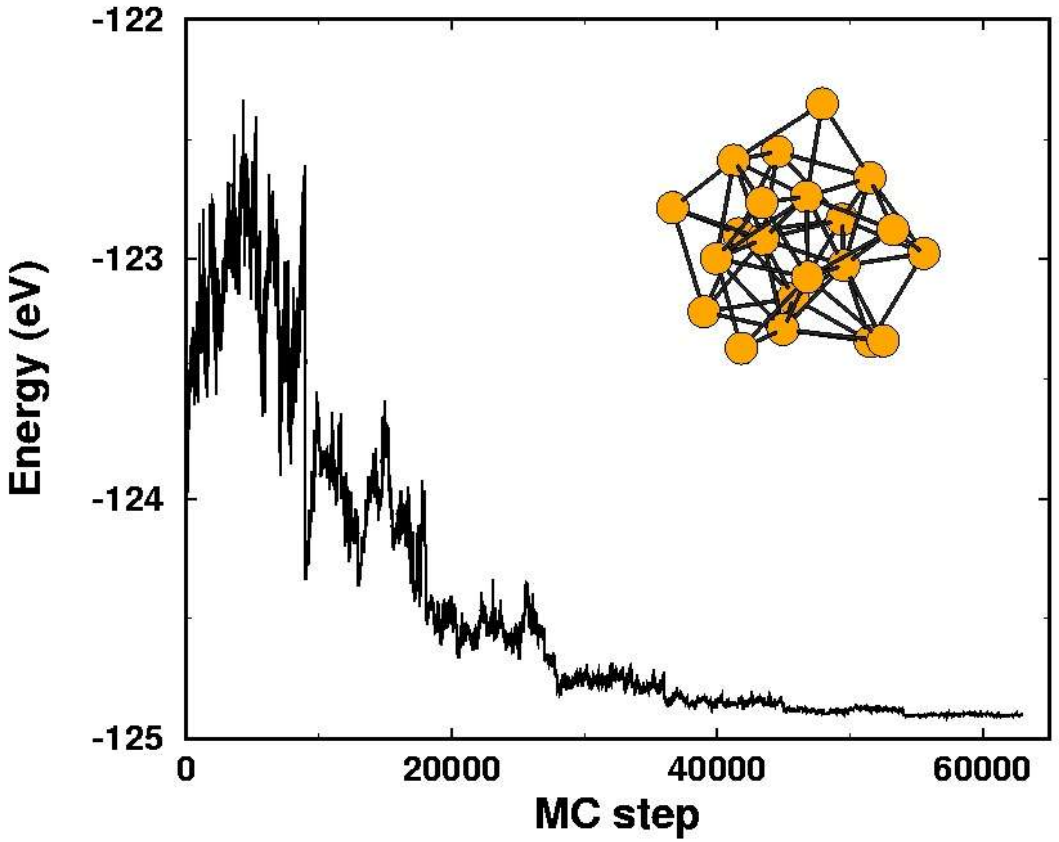
Integrals after a Monte-Carlo move



- In a typical Monte Carlo move only one atom changes position
- Only the integrals that contain basis functions attached to that atom must be recalculated
- For *n* atoms we have to recalculate only 1/*n* integrals of the type

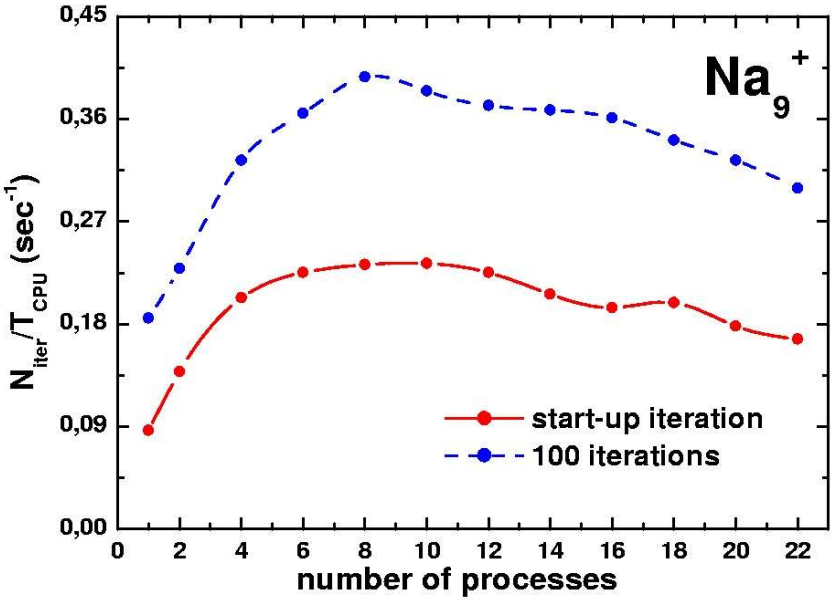
$$B_{ijk}$$

Example for Na_{21}^{+}



- With our method we can perform first principles Monte-Carlo simulations
- Parallel for a few machines
- Limited by memory...

Parallelization of First Principles Monte Carlo



- The calculation of integrals is easy to parallelize
- The calculation of integrals is speeded up by a factor of *n* the number of atoms

– The rest of the program that is still sequential reduces the gains of parallelization (diagonalization, can be parallelized!)

– Parallelization in Markov chains and temperature (J-walk)

Pseudopotential with explicit incorporation of semicore states

- For certain extreme cases (early transition metals, alkali or alkaline-earth ions) the semi-core states (2s and 2p for transition metals) may be relevant for the chemical bonding
- We have modified the Troullier-Martins recipe to generate a multi reference pseudopotential (MRPP)
- Applied to 3d transition metals

Loia, Pacheco, Martins, PRB 68, 155111 (2003)

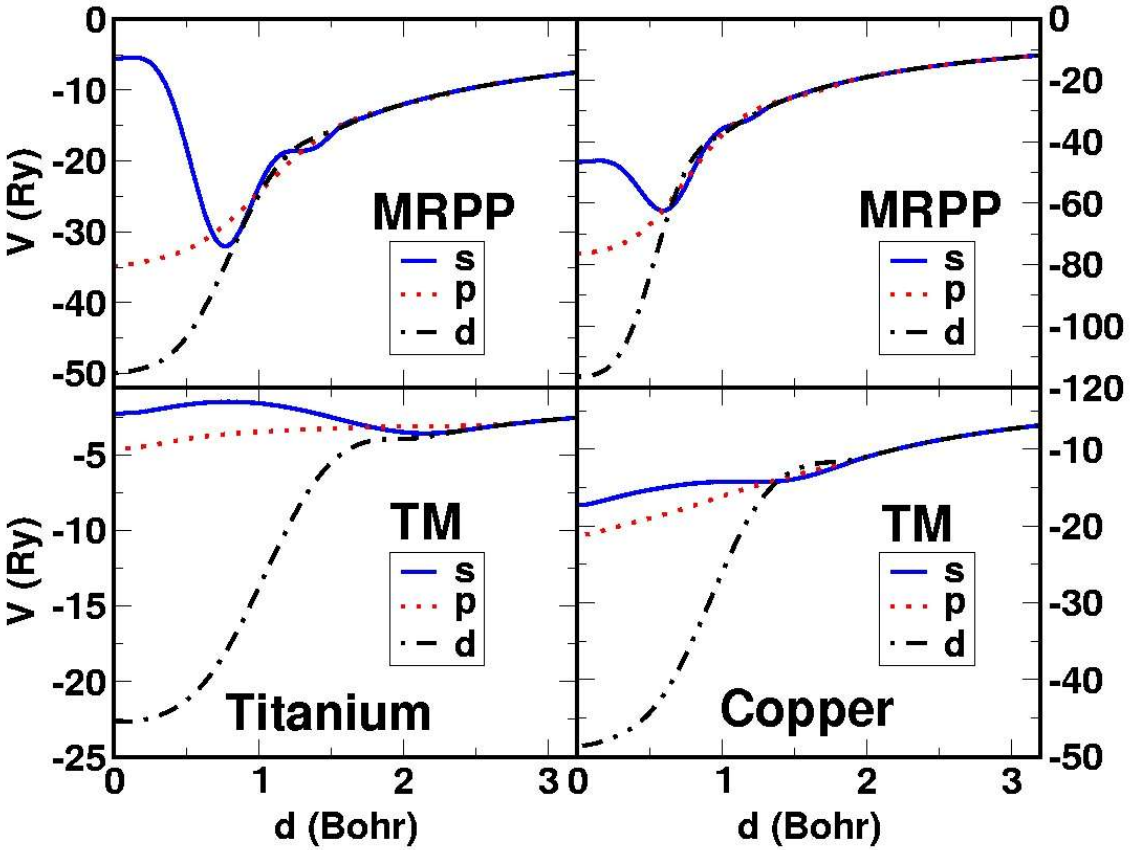
The MRPP recipe (for 3d transition metals)

- We include 2s, 2p, 3s, 3p, 3d in the valence
- We generate the all-electron wavefunctions
- For the 3d we follow the TM recipe
  - Wavefunction is $e^{p(r^2)}$ inside core radius (p 6th order polynomial)
  - Norm conservation
  - Continuity of pseudo-wavefunction up to fourth derivative
  - Zero curvature of screened pseudopotential at origin
  - Same eigenvalue

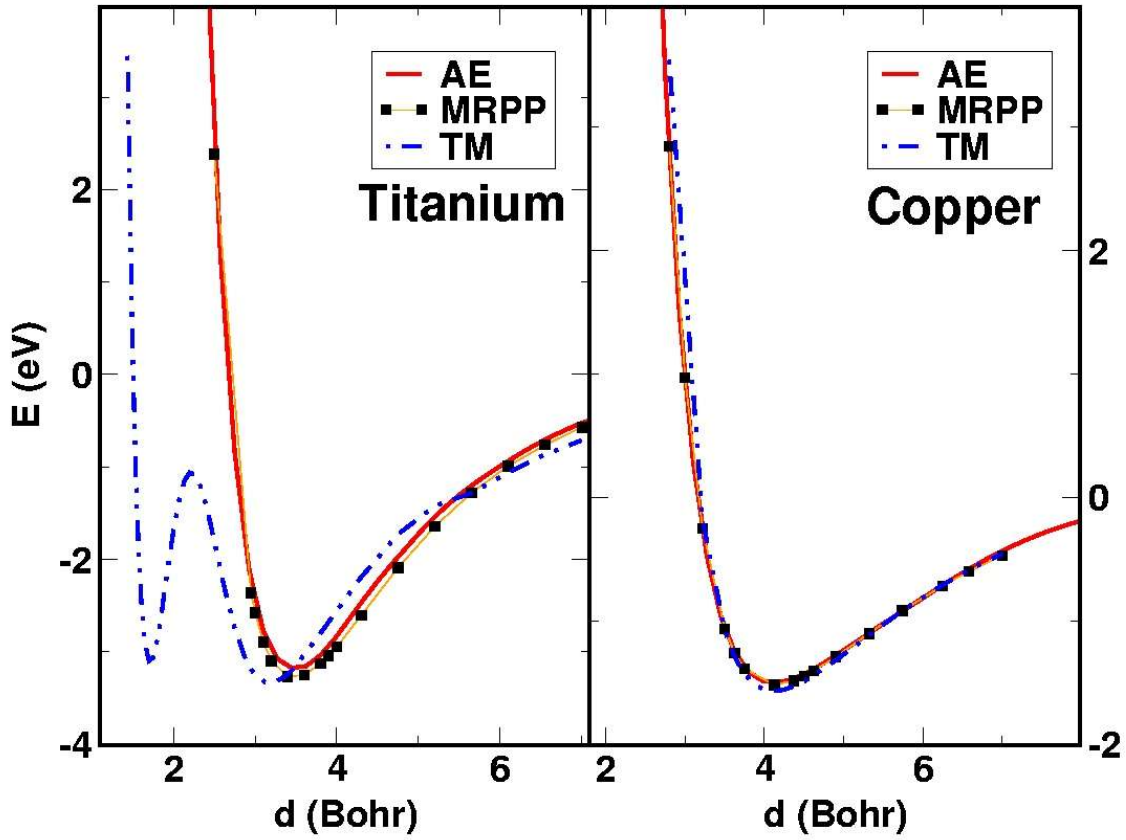
The MRPP recipe (for 3d transition metals)

- For the 2s (and 2p) we modify the TM recipe
  - Wavefunction is $e^{q(r^2)}$ inside core radius (q 9th order polynomial)
  - Norm conservation of 2s AND 3s
  - Continuity of 2s pseudo-wavefunction up to fourth derivative
  - Zero curvature of screened pseudopotential at origin
  - Same eigenvalue of 2s AND 3s
  - Continuity of 3s wavefunction

MRPP and TM pseudopotentials



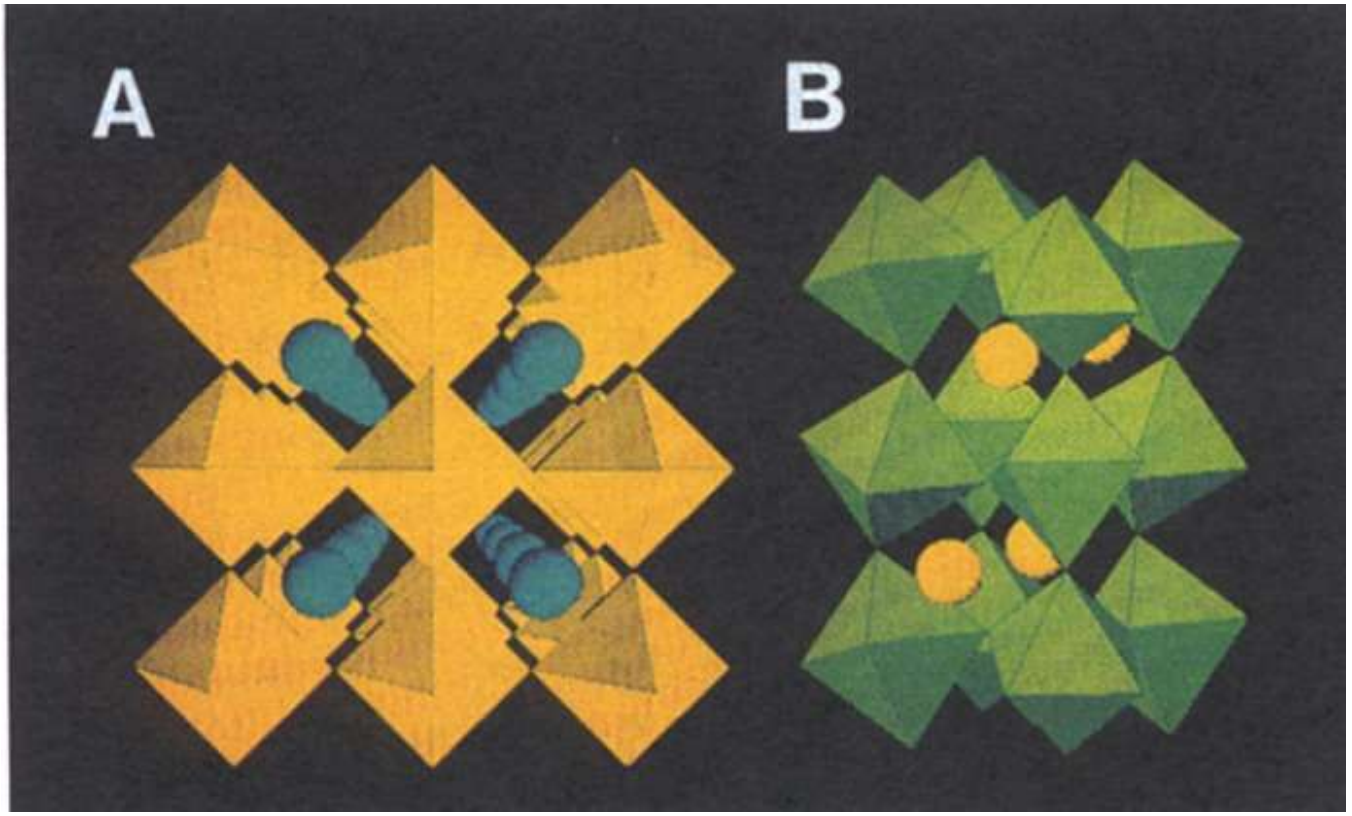
Titanium and copper dimers with MRPP and TM



Magnesium Silicates under pressure

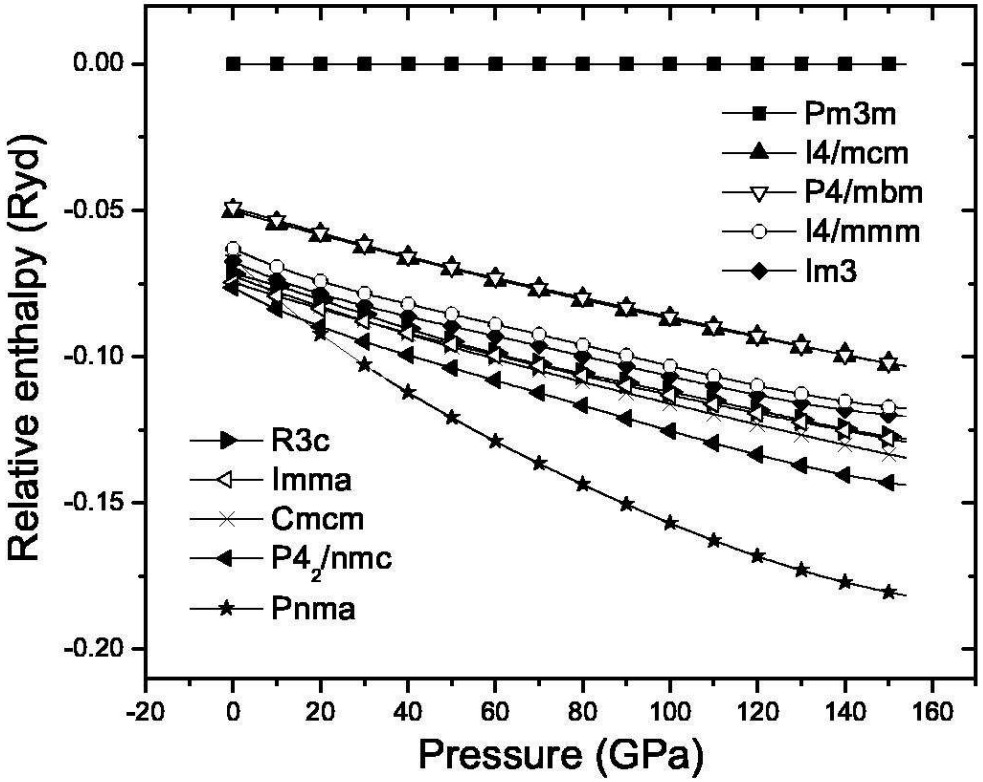
- Collaboration with R.M. Wentzcovitch, U of Minn.
- Pressures relevant to Earth's mantle
- Comparison of the enthalpies of several perovskite phases of $MgSiO_3$
  - Plane wave pseudopotential
  - Constant pressure structural minimization (including cell shape)

Distorted Perovskite structures



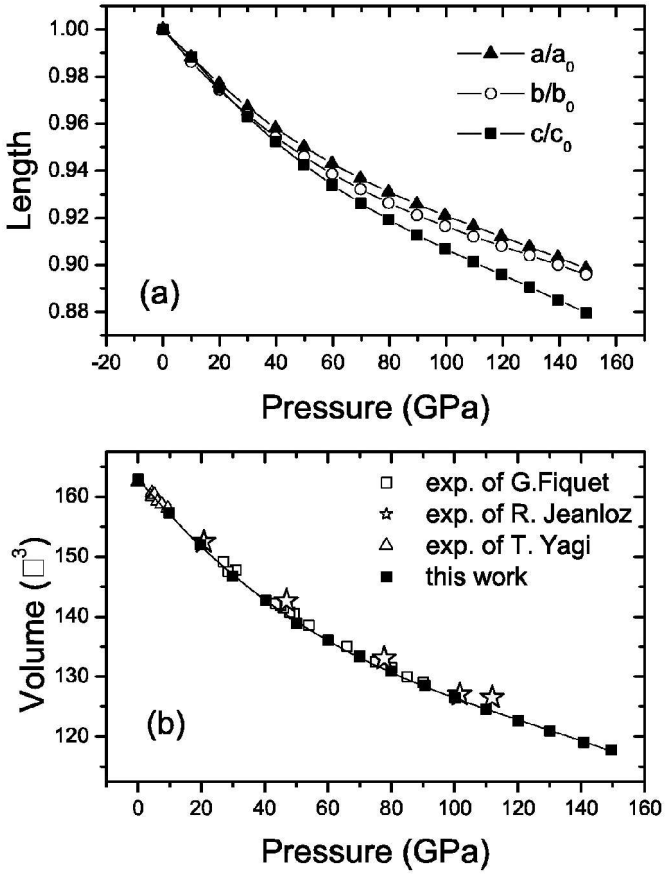
The ideal perovskite (A) and the Pmna/Pbnm distorted structure (B)

Enthalpy versus pressure of perovskite phases



The most stable structure among the distorted perovskites is the Pnma/Pbnm

Experimental and calculated lattice constants



- The experimental lattice constants are well reproduced

Conclusions

Future Work:

- Micromagnetic simulations in cooperation with experimentalists
- High pressure silicates (temperature?)
- Methodological developments (for cheap computers)