Implementation of a scalable parallel finite element package for micromagnetic simulations

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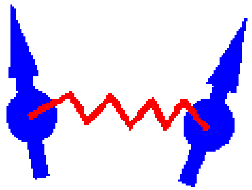
http://magnet.atp.tuwien.ac.at/scholz/magpar/

Outline

- Finite element micromagnetics
- Parallelization
- Static and dynamic solvers
- Performance
- Implemented features
- System/software requirements, licenses

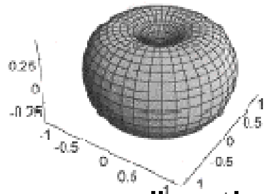
Finite Element Micromagnetics

exchange



⇨ parallel spins

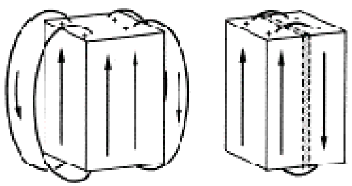
anisotropy



⇨ easy directions

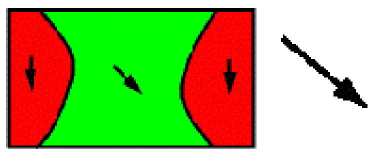
$$\frac{\partial \boldsymbol{J}}{\partial t} = -|\gamma| \boldsymbol{J} \times \boldsymbol{H}_{\text{eff}} + \frac{\alpha}{J_s} \boldsymbol{J} \times \frac{\partial \boldsymbol{J}}{\partial t}$$

magnetostatics



⇨ domains

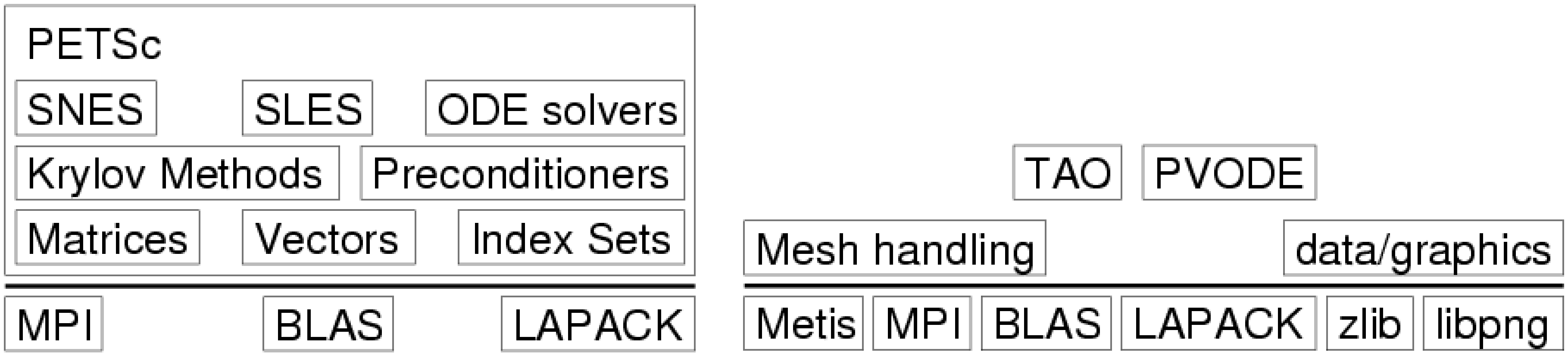
external field



⇨ rotation

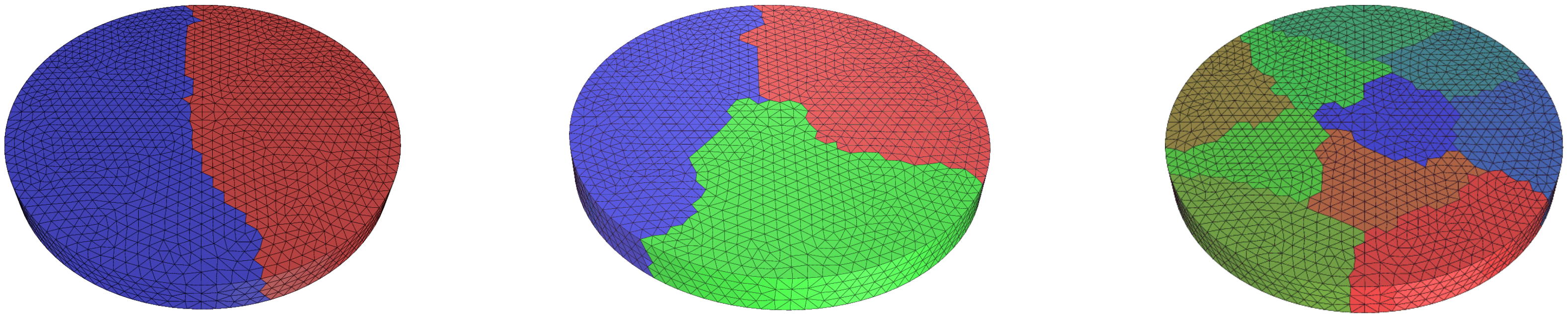
magpar - Software Modules

- **Preprocessing: AutoCAD, Patran, GiD**
- **PETSc library**
  Portable, Extensible Toolkit for Scientific Computation
- **MPI library**
- **METIS: Multilevel partitioning**
- **TAO library – energy minimization**
- **SUNDIALS (PVODE) – LLG time integration**
  SUite of Nonlinear and DIfferential/ALgebraic equation Solvers
- **Postprocessing: PNG snapshots, GeomView, (Micro)AVS**

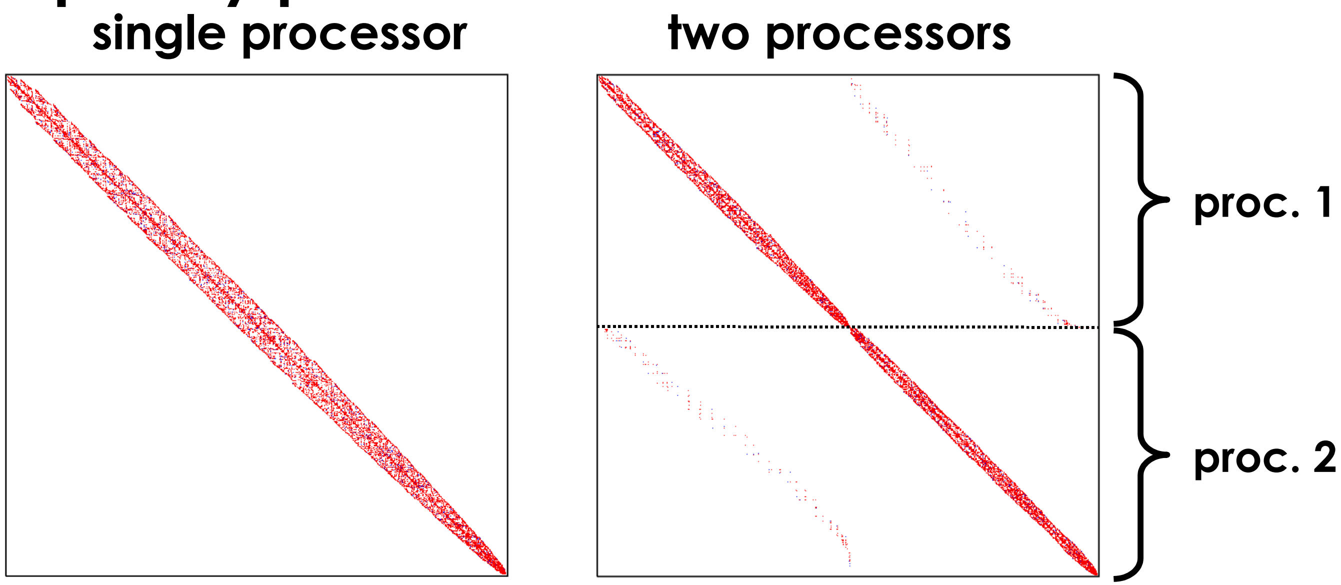


Mesh Partitioning

Partitioning pattern for 2, 3, and 10 processors



Sparsity pattern of the stiffness matrix



Energy Minimization using TAO

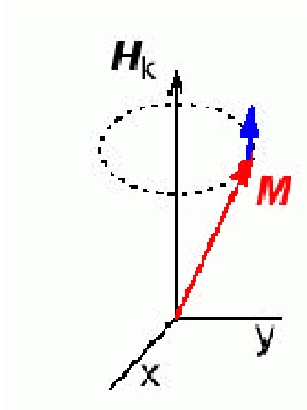
$$E_{tot} = E_{exch} + E_{ani} + E_{mag} + E_{Zee}$$

- **Magnetization given in Cartesian coordinates**
- **Energy gradient calculated in spherical coordinates**
- **TAO provides several solvers**
- **LMVM (limited memory variable metric) quasi-Newton method**
- **requires only energy and gradient (no Hessian)**
- **second-order information approx. by FD**

LLG Integration using PVODE

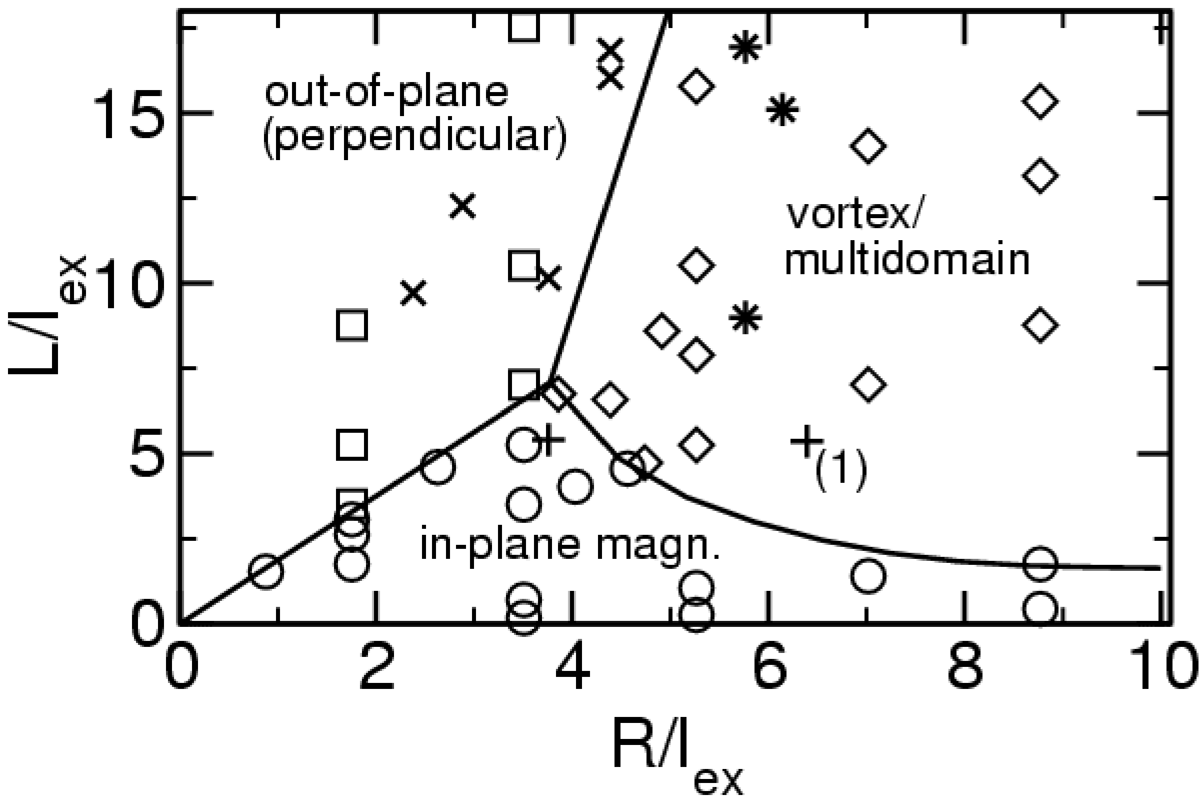
$$\frac{\partial \mathbf{J}}{\partial t} = -|\gamma| \mathbf{J} \times \mathbf{H}_{\mathrm{eff}} + \frac{\alpha}{J_s} \mathbf{J} \times \frac{\partial \mathbf{J}}{\partial t}$$

$$\mathbf{H}_{\mathrm{eff}} = -\frac{\delta E_{tot}}{\delta \mathbf{m}}$$



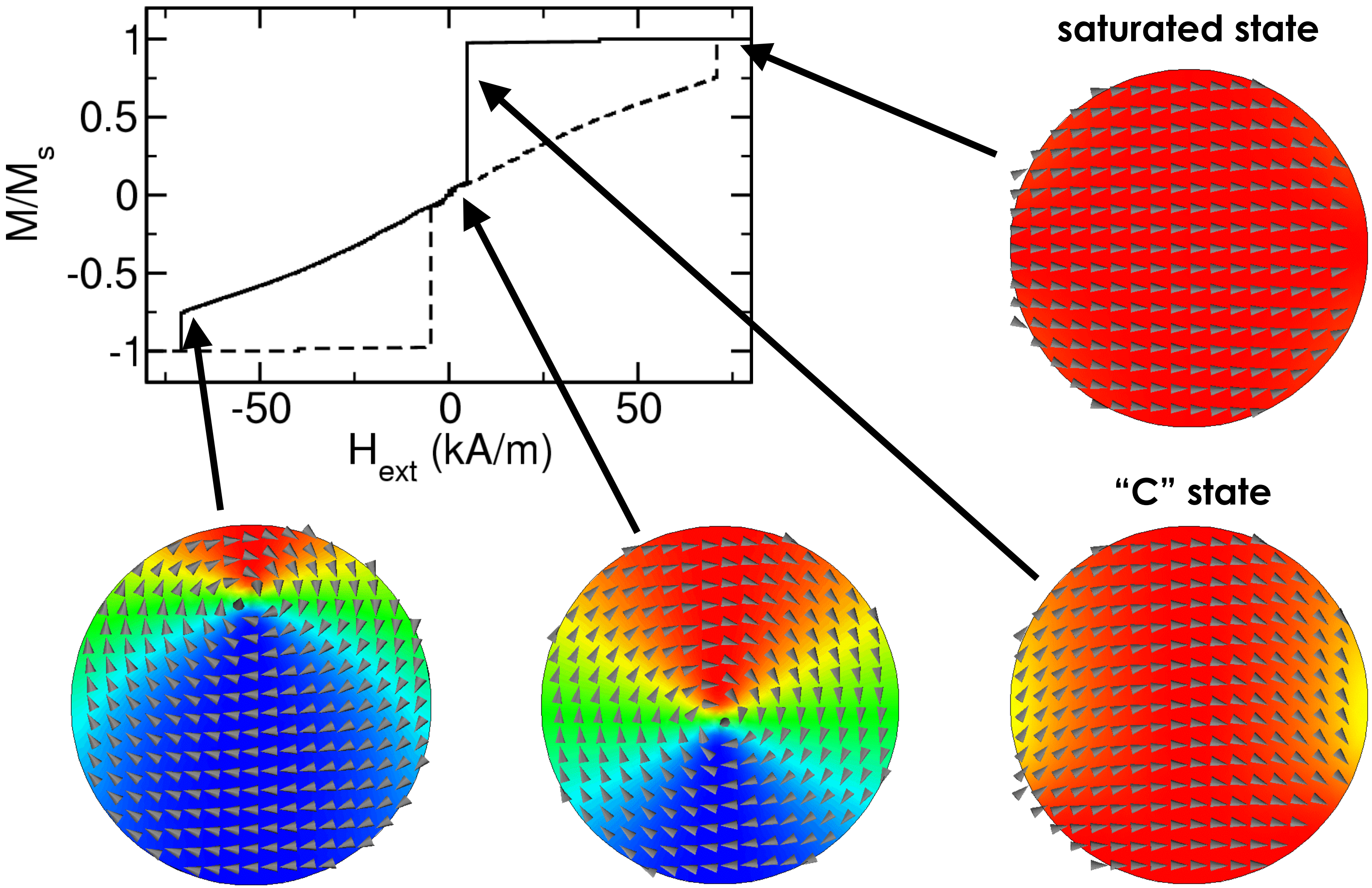
- Integration using ODE solver PVODE
- BDF and Adams-Moulton formulas
- variable step size, variable order
- varied automatically and dynamically
- preconditioning

Phase Diagram



W. Scholz et al., “Transition from single-domain to vortex state in soft magnetic cylindrical nanodots”, J. Magn. Magn. Mater. 266 (2003) 155-163.

Hysteresis Loop

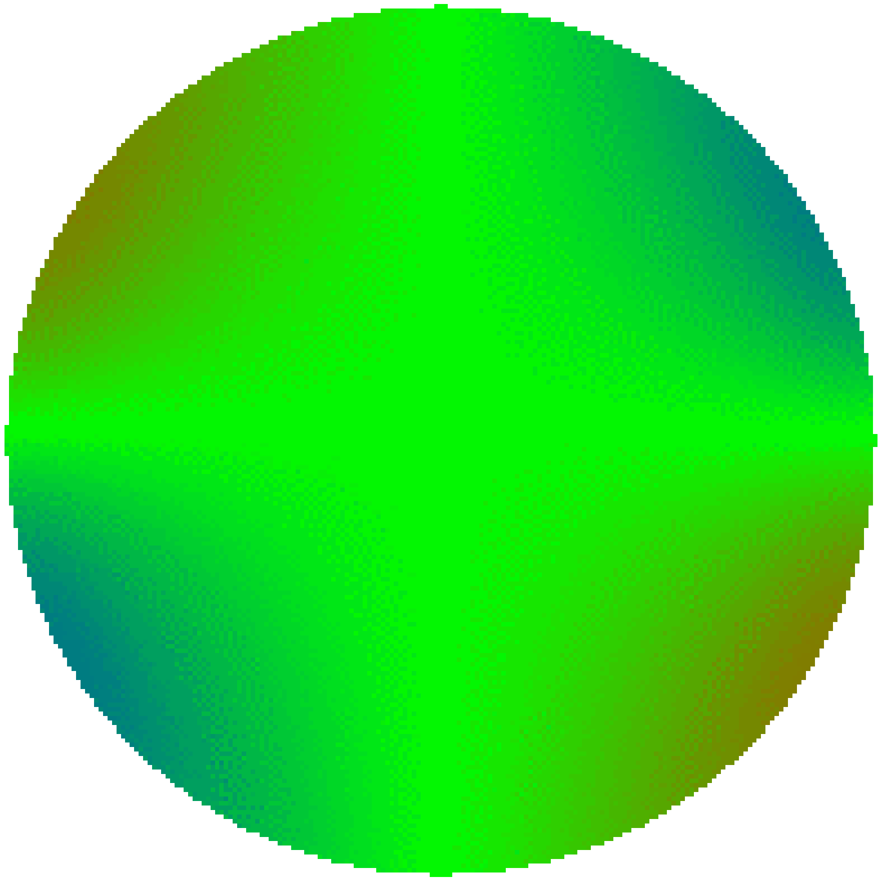


annihilation field:
70 kA/m = 880 Oe = 88 mT

Equilibrium in zero field

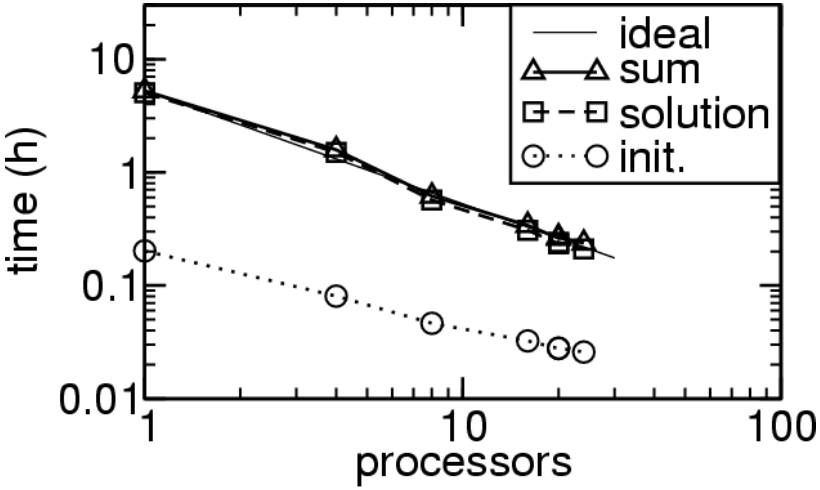
nucleation field:
5 kA/m = 62 Oe = 6.2 mT

Vortex nucleation



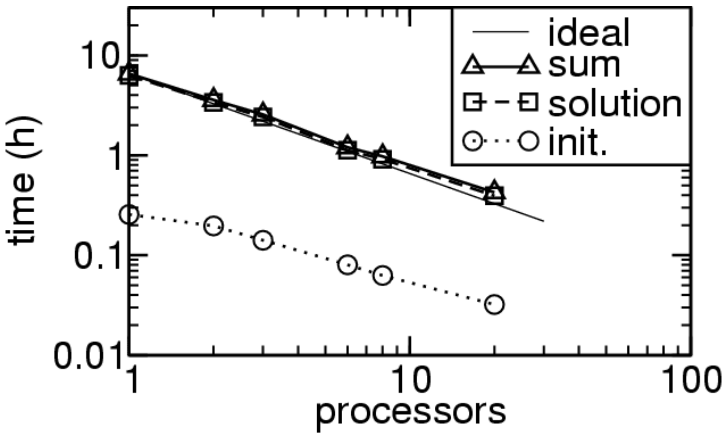
Parallel Efficiency

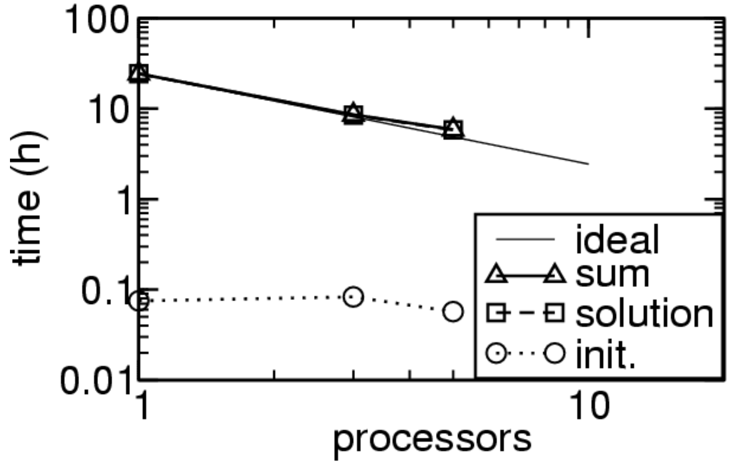
TAO (energy minimization)



- TAO:
  speedup 23.9 on 24 processors
  superlinear behavior on 8 processors
  (caching effects)
- PVDODE:
  speedup 16 on 20 processors

PVODE (dynamic LLG integration)





Implemented features 1

- **Debugging and optimized compilation**
- **Easy activation of optional components**
- **Consistency checking**
  assert statements
- **Memory allocation tracking**
  PetscMalloc, PetscFree, memory usage statistics
- **C++ compatible**
  required by TAO
- **Problem independent parallelization**
- **Profiling**
  timing in every subroutine
- **Performance evaluation**
  timing, FLOP count (PVODE missed!)

Implemented features 2

- **Mesh import**
  - MSC/Patran neutral file (no surface triangles)
  - AVS inp file (Patran neutral file <u>not</u> required)
  - GiD
- **Mesh analysis**
  - element and node volumes (max,min,avg)
  - edge lengths (max,min,avg)
  - element quality check
  - model bounding box
  - volume by property id
- **Mesh distortion**
  mimic surface/interface roughness
- **Mesh refinement**
  full regular refinement before partitioning:
  x 8^n number of nodes and elements

Implemented features 3

- **Micromagnetics**
  - Uniaxial anisotropy
  - Exchange
  - Magnetostatic field (hybrid FEM/BEM)
  - External field (quasistatic, sweeping, rotating)
- **Dynamic LLG integration using PVODE**
- **Static energy minimization using TAO**
- **Data output**
  - Geomview output
  - Log file
  - PNG files
  - “sampling line”

System/software requirements

- **Hardware/Software platform, which is supported by PETSc**
  http://www-fp.mcs.anl.gov/petsc/docs/machines.html
  IBM RS6000 including IBM SP, SGI running IRIX, 64 bit SGI including Origin and PowerChallenge, Convex Exemplar running HPUX, HP running HPUX, Sun Sparcstations running Solaris, Cray T3D/E, DEC Alpha OSF (Tru64), Intel processors running Linux, FreeBSD, Windows, Mac OS X, PC Running BeOS
- **MPI library**
  The Message Passing Interface (MPI) standard
  http://www-unix.mcs.anl.gov/mpi/mpich/
- **PETSc library**
  Portable, Extensible Toolkit for Scientific Computation
  http://www-fp.mcs.anl.gov/petsc/
- **GNU make**
  http://www.gnu.org/software/make/make.html
- **C/C++ compiler**
  http://www.gnu.org/software/gcc/
- **METIS**
  Multilevel partitioning
  http://www-users.cs.umn.edu/~karypis/metis/

Optional components

- **TAO library – energy minimization**
  Toolkit for Advanced Optimization
  http://www-fp.mcs.anl.gov/tao/
- **SUNDIALS (PVODE) – LLG time integration**
  SUite of Nonlinear and DIfferential/ALgebraic equation Solvers
  http://acts.nersc.gov/pvode/main.html
  http://www.llnl.gov/CASC/sundials/
- **zlib – compression of output data**
  A Massively Spiffy Yet Delicately Unobtrusive Compression Library
  http://www.gzip.org/zlib/
- **libpng – output of graphics files**
  The official PNG reference library
  http://www.libpng.org/pub/png/libpng.html

Licenses

- **MPICH:** free
  http://www-unix.mcs.anl.gov/mpi/mpich/mpich-license.txt
- **PETSc library:** free
  http://www-fp.mcs.anl.gov/petsc/docs/copyright.html
- **GNU make, GNU C:** free: GPL
  http://www.gnu.org/licenses/licenses.html
- **METIS:** free
  http://www-users.cs.umn.edu/~karypis/metis/metis/faq.html#distribute
- **TAO:** unknown (same as PETSc ? – also ANL tool)
- **SUNDIALS:** free (BSD style license)
  http://www.llnl.gov/CASC/sundials/download/cvode_par_agree.html
- **zlib:** free (OSI approved license)
  http://www.gzip.org/zlib/zlib_license.html
- **libpng:** free (OSI approved license)
  http://www.libpng.org/pub/png/src/libpng-LICENSE.txt

Summary

- Finite element micromagnetics: easy to formulate with matrix-vector operations
- Suitable for parallelization
- magpar - efficient implementation and parallelization using free open source software packages
- PETSc library compiles and runs on a variety of hardware platforms ranging from simple clusters of PCs to massively parallel supercomputers
- Excellent speed up measured
- Universal tool: soft and hard magnets, inhomogeneous microstructures, static and dynamic solvers
- Free open source package

Acknowledgement

- Josef Fidler
- Thomas Schrefl
- Dieter Suess, Rok Dittrich, Vassilios Tsiantos, Hermann Forster
- Roy Chantrell

References

- **WWW (download, documentation): http://magnet.atp.tuwien.ac.at/scholz/magpar/**
- **email: magpar@magnet.atp.tuwien.ac.at**
- **mailing-lists: majordomo@magnet.atp.tuwien.ac.at**

- **Papers:**
  - dissertation: Werner Scholz, “Scalable Parallel Micromagnetic Solver for Magnetic Nanostructures”
  - W. Scholz, J. Fidler, T. Schrefl, D. Suess, R. Dittrich, H. Forster, V. Tsiantos, Comp. Mat. Sci 28 (2003) 366-383.
  - W. Scholz, D. Suess, R. Dittrich, T. Schrefl, V. Tsiantos, H. Forster, J. Fidler, "Implementation of a high performance parallel finite element micromagnetics package", J. Magn. Magn. Mater. (2003), submitted.