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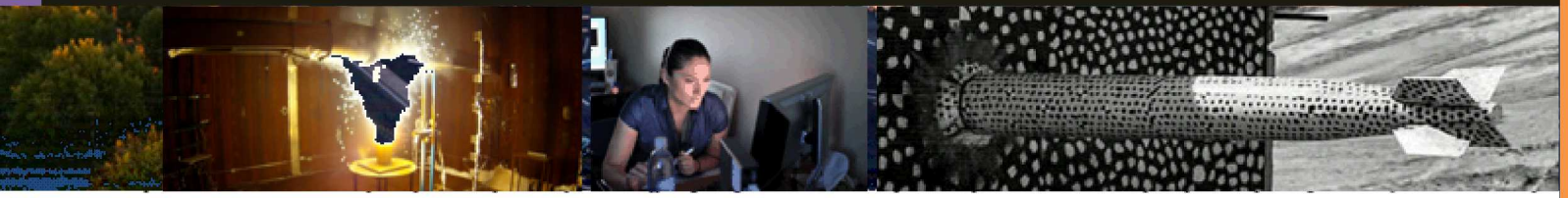

Coupled Magnetic Spin Dynamics and Molecular Dynamics in a Massively Parallel Framework

PRESENTED BY

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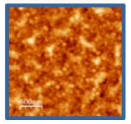
A computational model coupling micro-structure and magnetic properties

Fabrication process

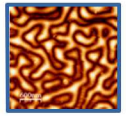
Learning cycles

Micro-structure



- Defects
- Inhomogeneity
- Composition
- Phase-change (inter-metallic)

Properties



- Magneto-elasticity
- Spin-lattice relaxation
- Magnetization dynamics
- Spin textures

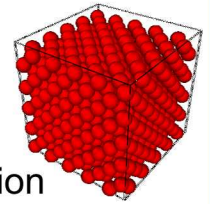
Applications

- Energy (magneto-calorics devices, efficient data storage),
- Multiferroic materials,
- Quantum computing.

Development of a model enhancing those learning cycles, and enabling the study of magnetoelastic effects and of the influence of the micro-structure on the magnetic properties.

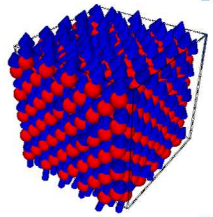
Molecular dynamics (MD)

- Enables: defects, inhomogeneity, phase-change
- ✖ Limitations: do not account for magnetization



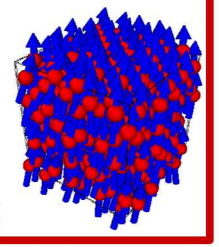
Spin dynamics (SD)

- Enables: magnetization dynamics, spin textures
- ✖ Limitations: structural defects, fixed lattice



Coupled SD - MD

- Coupled lattice and magnetic spins
- Enables: magneto-elasticity, s-l relaxation, coupled s-l phenomena



Pictures from MFM measurements performed by T-M Lu, org. 1867

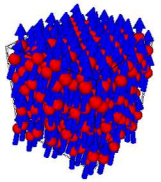
Methodology, first successes, and some current limitations

Methodology

:

Coupled SD - MD

$$\begin{cases} \frac{\partial \boldsymbol{r}_i}{\partial t} = \boldsymbol{v}_i \\ \frac{\partial \boldsymbol{v}_i}{\partial t} = \boldsymbol{F}_i\left(\boldsymbol{r}_{ij}, \boldsymbol{s}_{i,j}\right) \\ \frac{\partial \boldsymbol{s}_i}{\partial t} = \boldsymbol{\omega}_i \times \boldsymbol{s}_i \end{cases}$$



$$\boldsymbol{H}_{sl} = \underbrace{\sum_{i=1}^{N} \frac{|\boldsymbol{p}_i|^2}{2m_i} + \sum_{i,j=1}^{N} V\left(r_{ij}\right)}_{\text{MD Hamiltonian}} \underbrace{- \sum_{i,j,i\neq j}^{N} J\left(r_{ij}\right) \boldsymbol{s}_i \cdot \boldsymbol{s}_j - \mu_B \mu_0 \sum_{i=0}^{N} g_i \boldsymbol{s}_i \cdot \boldsymbol{H}_{ext}}_{\text{Spin-lattice coupling}}$$

First successes:

- Simulation of magneto-caloric effects
  - Ma, P. W., & Dudarev, S. L. (2014). Dynamic magnetocaloric effect in bcc iron and hcp gadolinium. Physical Review B, 90(2), 024425.
- Influence of defects on the magnetism of bcc iron
  - Mudrick, M., et al. Combined molecular and spin dynamics simulation of bcc iron with lattice vacancies. In Journal of Physics: Conference Series (Vol. 921, No. 1, p. 012007).
  - Wen, H., Ma, P. W., & Woo, C. H. (2013). Spin-lattice dynamics study of vacancy formation and migration in ferromagnetic BCC iron. Journal of Nuclear Materials, 440(1-3), 428-434.

Some current limitations:

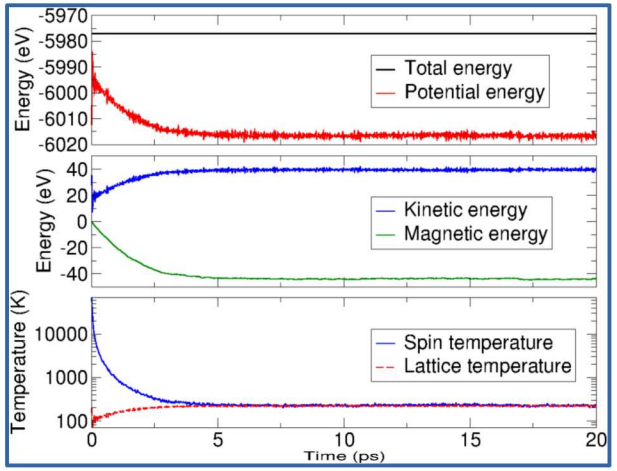
- ✖ No release in an open-source MD code
  - preventing from the development of a large user base
- ✖ Insufficient level of parallelization
  - does not allow the simulation of large magnetic devices
- ✖ Simulation of the spin-orbit coupling
  - fundamental importance for the simulation of magnetoelasticity
- ✖ Simulation of the long-range dipolar interaction
  - Unable to stabilize the domain structure of actual magnets

A scalable implementation of SD-MD in LAMMPS

http://lammps.sandia.gov/

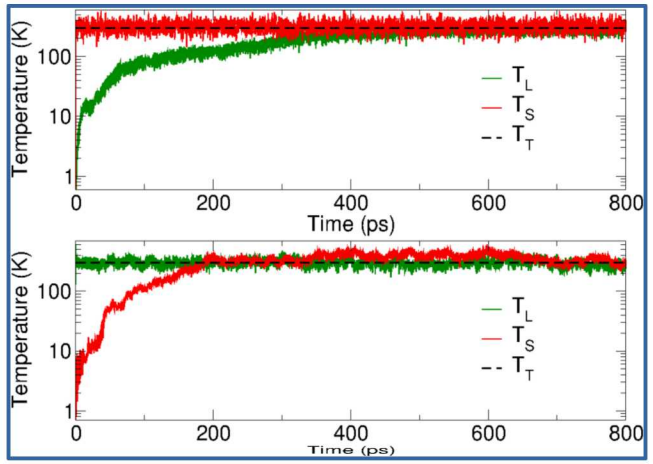
- A symplectic SD-MD sectoring algorithm was implemented in LAMMPS.
- The current version accounts for six magnetic interactions:
  - Exchange interaction,
  - Zeeman interaction,
  - Uniaxial anisotropy,
  - Magneto-electric interaction,
  - Spin-orbit coupling:
    - Dzyaloshinskii-Moriya,
    - Néel pair anisotropy.

Spin-lattice relaxation, NVE calculation



- Parameters of fcc-cobalt
- Energy preservation
- Equilibration of the spin and lattice temperatures

Spin-lattice relaxation, NVT calculation

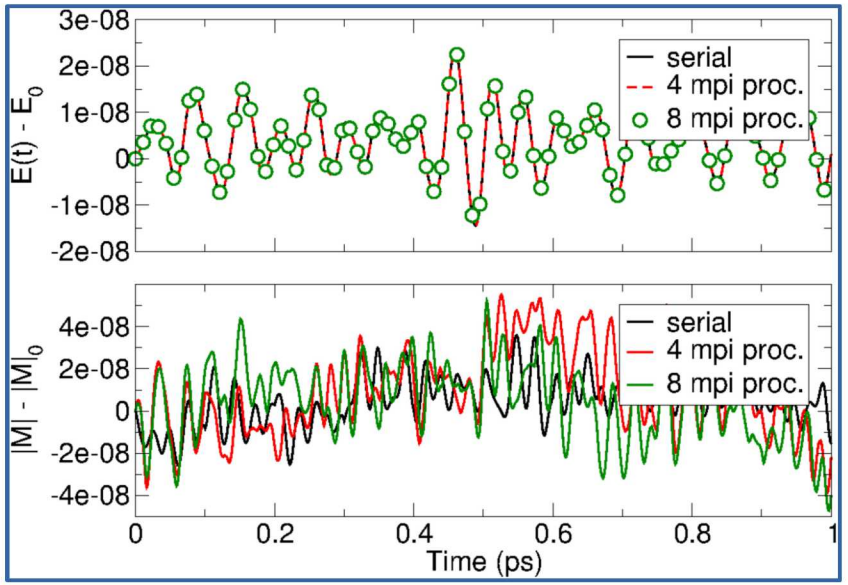


- Parameters of fcc-cobalt
- Langevin thermostat applied to the spins, and to the lattice
- Equilibration of the spin and lattice temperatures

Tranchida, J., Plimpton, S. J., Thibaudeau, P., & Thompson, A. P. (2018). Massively parallel symplectic algorithm for coupled magnetic spin dynamics and molecular dynamics. arXiv preprint arXiv:1801.10233, submitted to Journal of Computional Physics.

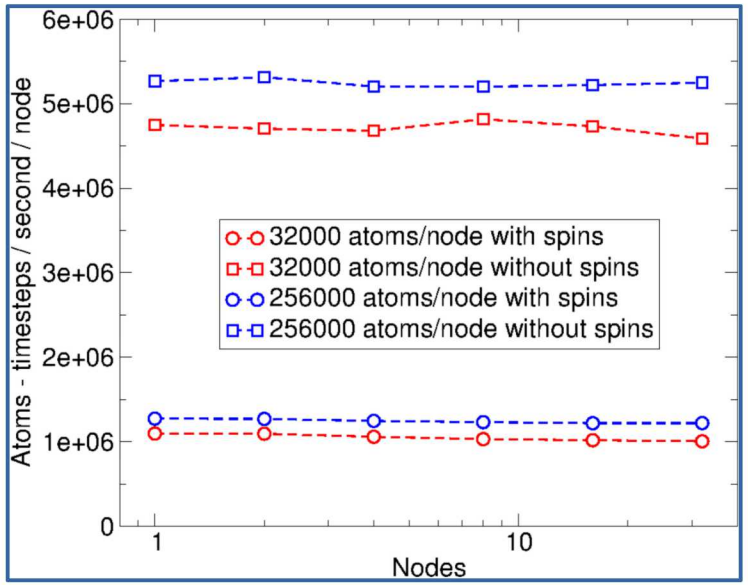
A scalable implementation of SD-MD in LAMMPS

Accuracy of the parallel algorithm



- Error for the total energy and the norm of the magnetization preservation.
- Different trajectories, but nor accuracy loss with the number of precesses.

Parallel efficiency: weak scaling



- From 1 to 32 Broadwell nodes, with 36 processes per node (1024 processes for the last point).
- Spin-lattice calculations only 5 times slower than an EAM calculation.

Tranchida, J., Plimpton, S. J., Thibaudeau, P., & Thompson, A. P. (2018). Massively parallel symplectic algorithm for coupled magnetic spin dynamics and molecular dynamics. arXiv preprint arXiv:1801.10233, submitted to Journal of Computional Physics.

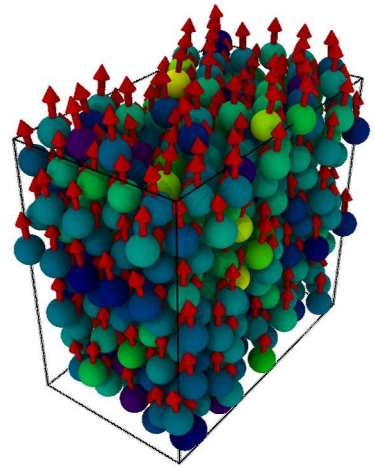
Example: magnetoelasticity of hcp cobalt

- Exchange interaction and EAM potential;

$$\mathcal{H}_{\mathrm{hcp-Co}} = \sum_{i=1}^{N} \frac{|\boldsymbol{p}_i|^2}{2m_i} + \underbrace{\sum_{i,j=1}^{N} V(r_{ij})}_{\text{EAM potential} \Rightarrow (1)} - \underbrace{\sum_{i,j,i\neq j}^{N} J(r_{ij})\, \boldsymbol{s}_i \cdot \boldsymbol{s}_j}_{\text{Exchange interaction} \Rightarrow (2)}$$

1 Pun, G. P. et al.. (2012). Phys. Rev. B, 86(13), 134116.

2 Sabiryanov, R. F. et al.. (1999). Phys. Rev. Lett., 83(10), 2062.



- Spin-orbit coupling and magneto-elastic effects with Néel dipolar and quadrupolar functions:

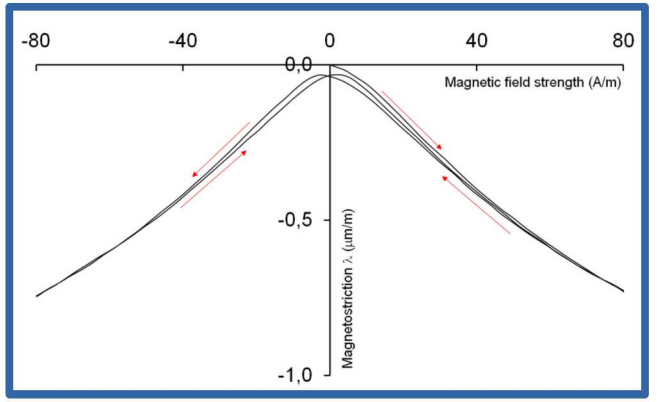
$$\mathcal{H}_{N\acute{e}el} = -\sum_{i,j=1,i\neq j}^{N} g_1(r_{ij}) \left((\boldsymbol{e}_{ij}\cdot\boldsymbol{s}_i)(\boldsymbol{e}_{ij}\cdot\boldsymbol{s}_j) - \frac{\boldsymbol{s}_i\cdot\boldsymbol{s}_j}{3}\right) + q_1(r_{ij}) \left((\boldsymbol{e}_{ij}\cdot\boldsymbol{s}_i)^2 - \frac{\boldsymbol{s}_i\cdot\boldsymbol{s}_j}{3}\right)\left((\boldsymbol{e}_{ij}\cdot\boldsymbol{s}_i)^2 - \frac{\boldsymbol{s}_i\cdot\boldsymbol{s}_j}{3}\right) + q_2(r_{ij})\Big((\boldsymbol{e}_{ij}\cdot\boldsymbol{s}_i)(\boldsymbol{e}_{ij}\cdot\boldsymbol{s}_j)^3 + (\boldsymbol{e}_{ij}\cdot\boldsymbol{s}_j)(\boldsymbol{e}_{ij}\cdot\boldsymbol{s}_i)^3\Big)$$

Pair model from the magnetostriction constants

- Following Cullen's approach, magnetostriction constants can be expressed as functions of g1, q1, and q2.
- Knowing the experimental values of λ_i, one can fit the constant g1, q1 and q2.
- Using spin-dependent DFT to check the obtained energy surface.

$$\begin{aligned}
\lambda_1^{\alpha} &= \frac{-B_1^{\alpha}\left[g_1(r_{ij}), q_1(r_{ij}), q_2(r_{ij})\right]}{C_1^{\alpha}} \\
\lambda_2^{\alpha} &= \frac{-B_2^{\alpha}\left[g_1(r_{ij}), q_1(r_{ij}), q_2(r_{ij})\right]}{C_2^{\alpha}} \\
\lambda^{\epsilon} &= \frac{-B^{\epsilon}\left[g_1(r_{ij}), q_1(r_{ij}), q_2(r_{ij})\right]}{C_{44}} \\
\lambda^{\gamma} &= \frac{-B^{\gamma}\left[g_1(r_{ij}), q_1(r_{ij}), q_2(r_{ij})\right]}{C_{11}-C_{22}}
\end{aligned}$$

Target result



*Cullen, J. R. (1995). Pair model of magnetostriction for hexagonal close-packed crystals. Phys. Rev. B, 52(1), 57.

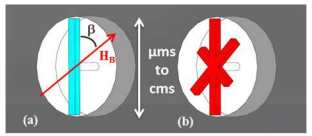
Perspectives, future work and conclusions

Models of spin-orbit coupling

- Current model: pair Néel anisotropy, fitted for hcp cobalt:

$$\mathcal{H}_N = \sum_{i,j,i\neq j}^{N} g_1(r_{ij}) \left((\boldsymbol{e}_{ij} \cdot \boldsymbol{s}_i)(\boldsymbol{e}_{ij} \cdot \boldsymbol{s}_j) - \frac{1}{3} \boldsymbol{s}_i \cdot \boldsymbol{s}_j \right)$$

- Second approach: using spin-dependent DFT to fit g1, q1 and q2, and check the obtained magnetostriction constants.
- Next steps: test this model and develop new ones for cubic crystals => magnetostriction in FeCo resonator devices.

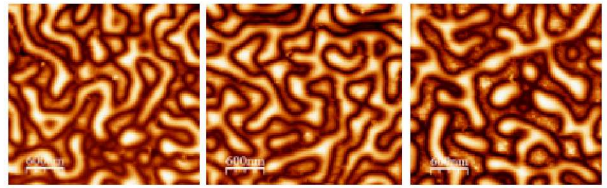


Single- (a) and multi-frequency (b) resonators

Long-range interaction

$$\mathcal{H}_{Mag} = \underbrace{-\sum_{i,j,i\neq j}^{N} J_{ij}(r_{ij})\, \boldsymbol{s}_i \cdot \boldsymbol{s}_j}_{\text{exchange interaction}} \underbrace{-\frac{\mu_0 \mu_b^2}{4\pi} \sum_{i,j,i\neq j}^{N} \frac{g_i g_j}{r_{ij}^3} \left((\boldsymbol{s}_i \cdot \boldsymbol{e}_{ij})(\boldsymbol{s}_j \cdot \boldsymbol{e}_{ij}) - \frac{1}{3}(\boldsymbol{s}_i \cdot \boldsymbol{s}_i) \right)}_{\text{long-range dipolar interaction}}$$

- A direct calculation of this long-range Hamiltonian would scale as N^2
- We want to adapt a P3M to magnetic dipoles will be performed (scaling of N.log(N)).



MFM measurements by T-M Lu, Sandia Labs

Conclusions:

- A scalable implementation of spin-lattice dynamics was implemented into LAMMPS (open release within the next months).
- The model adds new physics into LAMMPS, is accurate, scales very well with the number of processes, and only 5 times slower than usual MD – EAM calculations.
- Open to collaborations, feel free to contact us (jtranch@sandia.gov).