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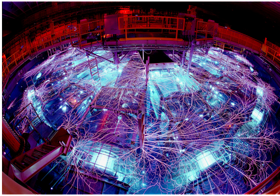

Spin–lattice simulations with LAMMPS

LAMMPS Workshop and Symposium

Julien Tranchida (jtranch@sandia.gov), Steve Plimpton, Aidan Thompson

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U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

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Introduction

Objective: developing a LAMMPS package for spin–lattice simulations.

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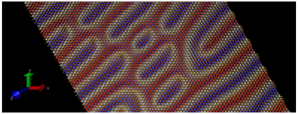
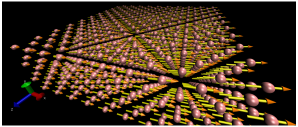
Enable study of:

- Magnetostriction,
- Spin–lattice relaxation,
- Spin dynamics,
- Topological spin structures,
- Spin liquids, ...





Simulations of bismuth oxide and fcc colbalt.

EOMs for the spin dynamics

- From the DFT formalism, Antropov *et* al. derived equations for the dynamics ot atomic spins [2]:

$$\frac{d\boldsymbol{s}_i}{dt} = \frac{1}{1+\lambda^2}\left((\boldsymbol{\omega}_i + \boldsymbol{\eta}_i) \times \boldsymbol{s}_i + \lambda\, \boldsymbol{s}_i \times (\boldsymbol{\omega}_i \times \boldsymbol{s}_i)\right)$$

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Magnetic interactions:

$$\boldsymbol{\omega}_{\mathrm{i}} = -\frac{1}{\hbar}\frac{\partial \mathcal{H}_{\mathrm{Mag}}}{\partial \boldsymbol{s}_i}$$

- Spin Hamiltonian:

$$\mathcal{H}_{\mathrm{Mag}} = \sum_{\mathrm{i,j,i\neq j}}^{\mathrm{N}} \mathrm{J_{ij}}\left(r_{\mathrm{ij}}\right) \boldsymbol{s}_{\mathrm{i}} \cdot \boldsymbol{s}_{\mathrm{j}} + g\mu_B\mu_0 \sum_{\mathrm{i=0}}^{\mathrm{N}} \boldsymbol{s}_{\mathrm{i}} \cdot \boldsymbol{H}_{\mathrm{ext}}$$

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Connection to a random bath:

$$\begin{aligned}\langle \boldsymbol{\eta}_{\mathrm{i}} \rangle &= 0 \quad \text{and} \\ \langle \boldsymbol{\eta}_{\mathrm{i}}^{\alpha}(t)\boldsymbol{\eta}_{\mathrm{j}}^{\beta}(t') \rangle &= 2\mathrm{D}\delta_{ij}\delta_{\alpha\beta}\delta(t-t')\end{aligned}$$

- Fluctuation–dissipation relation:

$$D = \frac{2\pi\lambda \mathrm{k_B T}}{\hbar}$$

[2] Antropov, V. P. *et al.* (1996). Phys. Rev. B, 54(2), 1019.

EOMs for spin–lattice dynamics

- Spin–lattice Hamiltonian [3]:

$$\mathcal{H}_{\mathrm{sl}} = \sum_{\mathrm{i}=1}^{N} \frac{m_{\mathrm{i}} |\boldsymbol{v}_{\mathrm{i}}|^2}{2} + \sum_{\mathrm{i,j}}^{N} V(r_{\mathrm{ij}}) + \sum_{\mathrm{i,j,i}\neq\mathrm{j}}^{\mathrm{N}} \mathrm{J}_{\mathrm{ij}}\left(r_{\mathrm{ij}}\right) \boldsymbol{s}_{\mathrm{i}} \cdot \boldsymbol{s}_{\mathrm{j}} + g\mu_B\mu_0 \sum_{\mathrm{i}=0}^{\mathrm{N}} \boldsymbol{s}_{\mathrm{i}} \cdot \boldsymbol{H}_{\mathrm{ext}}$$

[3] Beaujouan, D., *et al.*. (2012). Phys. Rev. B, 86(17), 174409.

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- The associated spin–lattice equations of motion are given by [3]:

$$\begin{aligned}
\frac{\partial \boldsymbol{r}_i}{\partial t} &= \boldsymbol{v}_i \\
\frac{\partial \boldsymbol{v}_i}{\partial t} &= \boldsymbol{F}_i(\boldsymbol{r}_{ij}, \boldsymbol{s}_{i,j}) = \sum_{j,i\neq j}^{N} \left[-\frac{dV(r_{ij})}{dr} + \frac{dJ(r_{ij})}{dr} \boldsymbol{s}_i \cdot \boldsymbol{s}_j \right] \\
\frac{\partial \boldsymbol{s}_i}{\partial t} &= \boldsymbol{\omega}_i \times \boldsymbol{s}_i
\end{aligned}$$

[3] Beaujouan, D., *et al.*. (2012). Phys. Rev. B, 86(17), 174409.

Numerical integration

- Advance operators are not commuting, a Suzuki–Trotter decomposition has to be used [4]:

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ST decomposition:

$$\begin{tikzcd}
\boxed{\boldsymbol{v} \leftarrow \boldsymbol{v} + L_v.\Delta t/2} \arrow[d] & & \boxed{\boldsymbol{s}_0 \leftarrow \boldsymbol{s}_0 + L_{s_0}.\Delta t/2} \arrow[d, dotted] \\
\boxed{\boldsymbol{r} \leftarrow \boldsymbol{r} + L_r.\Delta t/2} \arrow[d] & & \boxed{\boldsymbol{s}_{\mathrm{N}-1} \leftarrow \boldsymbol{s}_{\mathrm{N}-1} + L_{s_{\mathrm{N}-1}}.\Delta t/2} \arrow[d] \\
\boxed{\boldsymbol{s} \leftarrow \boldsymbol{s} + L_s.\Delta t} \arrow[d] \arrow[uurr, dotted] \arrow[ddrr, dotted] & & \boxed{\boldsymbol{s}_{\mathrm{N}} \leftarrow \boldsymbol{s}_{\mathrm{N}} + L_{s_{\mathrm{N}}}.\Delta t} \arrow[d] \\
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$$\boldsymbol{s}_{\mathrm{N}-1} \leftarrow \boldsymbol{s}_{\mathrm{N}-1} + L_{s_{\mathrm{N}-1}}.\Delta t/2$$
$$\boldsymbol{s}_{\mathrm{N}} \leftarrow \boldsymbol{s}_{\mathrm{N}} + L_{s_{\mathrm{N}}}.\Delta t$$
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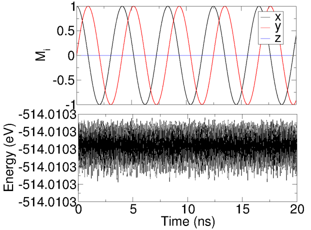
$$\boldsymbol{s}_0 \leftarrow \boldsymbol{s}_0 + L_{s_0}.\Delta t/2$$

Numerical results:

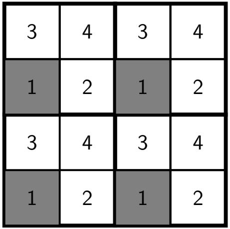


Sim. param.: $\lambda = 0$, $\mathrm{H}_{\mathrm{ext}} = 10\mathrm{T}$ along $\boldsymbol{e}_{\mathrm{z}}$, J_{Co}

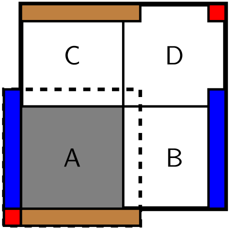
[4] Omelyan, I. P. *et al.* (2001). Phys. Rev. Lett., 86(5), 898.

Parallel implementation

- A sectoring method, respecting the symplectic properties of the spin–lattice algorithms, was implemented [5]:



Sectoring operations for a two dimensional system with four processors.

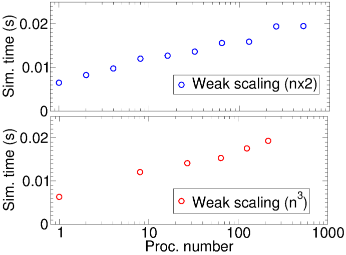


Communication between four sectors for periodic boundary conditions.

[5] Amar, J. G. *et al.* (2005). Phys. Rev. B, 71(12), 125432.

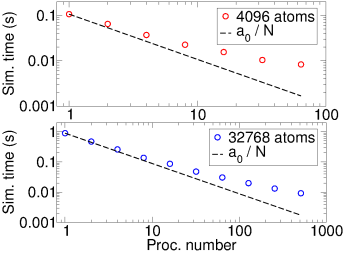
Results

- Weak and strong scaling results for the sectoring algorithm:



<u>Simulation conditions</u>: $\lambda = 0$, $J_{Co} > 0$,

Δ t $= 10^{-4}$ ps, $H_{ext} = 10$T along $\boldsymbol{e}_z$



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- The 50 % efficiency of the algorithm is reached between 250 and 300 atoms per process.

Conclusions

Summary:

- A package allowing spin lattice simulations has been developed,
- Mathematically rigorous integration algorithms were implemented (magnetization and energy preservation),
- A sectoring algorithm was implemented and tested.

Future work:

- Take the long range dipolar interaction into account:

$$\mathcal{H}_{\mathrm{Mag}} = \sum_{\mathrm{i,j,i\neq j}}^{\mathrm{N}} \mathrm{J_{ij}}\left(\boldsymbol{r}_{\mathrm{ij}}\right) \boldsymbol{s}_{\mathrm{i}} \cdot \boldsymbol{s}_{\mathrm{j}} - \frac{\mu_0 \mu_b^2}{4\pi} \sum_{\mathrm{i,j,i\neq j}}^{\mathrm{N}} \frac{g_{\mathrm{i}} g_{\mathrm{j}}}{\boldsymbol{r}_{\mathrm{ij}}^3} \left((\boldsymbol{s}_{\mathrm{i}} \cdot \boldsymbol{e}_{\mathrm{ij}})(\boldsymbol{s}_{\mathrm{j}} \cdot \boldsymbol{e}_{\mathrm{ij}}) - \frac{1}{3} (\boldsymbol{s}_{\mathrm{i}} \cdot \boldsymbol{s}_{\mathrm{i}}) \right)$$

- Find experiments to compare with.

Appendix 1: Magnetic interactions

Spin Hamiltonian:

$$\mathcal{H}_{\mathrm{Mag}} = \mathcal{H}_{\mathrm{Ex}} + \mathcal{H}_{\mathrm{Zee}} + \mathcal{H}_{\mathrm{An}} + \mathcal{H}_{\mathrm{DM}} + \mathcal{H}_{\mathrm{ME}} + \mathcal{H}_{\mathrm{Dip}}$$

- Magnetic anisotropy:

$$\mathcal{H}_{\mathrm{An}} = K_{\mathrm{a}} \sum_{\mathrm{i}=0}^{\mathrm{N}} (\boldsymbol{s}_{\mathrm{i}} \cdot \boldsymbol{n}_{\mathrm{a}})^2$$

- Magneto-electric interaction:

$$\mathcal{H}_{\mathrm{ME}} = \sum_{\mathrm{i,j,i}\neq\mathrm{j}}^{\mathrm{N}} (\boldsymbol{E} \times \boldsymbol{r}_{\mathrm{ij}}) \cdot \boldsymbol{s}_{\mathrm{i}} \times \boldsymbol{s}_{\mathrm{j}}$$

- Zeeman interaction:

$$\mathcal{H}_{\mathrm{Ze}} = g\mu_B\mu_0 \sum_{\mathrm{i}=0}^{\mathrm{N}} \boldsymbol{s}_{\mathrm{i}} \cdot \boldsymbol{H}_{\mathrm{ext}}$$

- Dzyaloshinskii-moriya:

$$\mathcal{H}_{\mathrm{DM}} = \sum_{\mathrm{i,j,i}\neq\mathrm{j}}^{\mathrm{N}} \boldsymbol{D}_{\mathrm{ij}} \cdot \boldsymbol{s}_{\mathrm{i}} \times \boldsymbol{s}_{\mathrm{j}}$$

Appendix 2: Poisson bracket for spin–lattice systems

- Considering $f(t, \boldsymbol{r}_\mathrm{i}, \boldsymbol{p}_\mathrm{i}, \boldsymbol{s}_\mathrm{i})$ and $g(t, \boldsymbol{r}_\mathrm{i}, \boldsymbol{p}_\mathrm{i}, \boldsymbol{s}_\mathrm{i})$, one has:

$$\{f, g\} = \sum_{\mathrm{i}=1}^{\mathrm{N}} \left[\frac{\partial f}{\partial \boldsymbol{r}_\mathrm{i}} . \frac{\partial g}{\partial \boldsymbol{p}_\mathrm{i}} - \frac{\partial f}{\partial \boldsymbol{p}_\mathrm{i}} . \frac{\partial g}{\partial \boldsymbol{r}_\mathrm{i}} + \frac{\boldsymbol{s}_\mathrm{i}}{\hbar} . \left(\frac{\partial f}{\partial \boldsymbol{s}_\mathrm{i}} \times \frac{\partial g}{\partial \boldsymbol{s}_\mathrm{i}} \right) \right]$$

[] Yang, K. H. *et al.* (1980). Phys. Rev. A, 22(5), 1814.

Appendix 3: Parametrization of the exchange interaction

- Bethe–Slater model for the parametrization:

$$J(\mathrm{ij}) = 4\alpha \left(\frac{r_{\mathrm{ij}}}{\delta}\right)^2 \left(1 - \gamma \left(\frac{r_{\mathrm{ij}}}{\delta}\right)^2\right) \exp\left(-\left(\frac{r_{\mathrm{ij}}}{\delta}\right)^2\right) \Theta\left(r_{\mathrm{c}} - r_{\mathrm{ij}}\right) \quad (1)$$

with:

- α an energy in eV,
- δ a characteristic distance in Å,
- γ an adimensional coefficient,
- r_{c} a cutoff distance.