Coupling magnetic and mechanical phenomena with LAMMPS

PRESENTED BY
Julien Tranchida

Contact: jtranch@sandia.gov
Molecular dynamics

- Enables: defects, inhomogeneities, phase-transitions, ...

- Limitations: do not account for magnetization.
A computational model coupling micro-structure and magnetic properties

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- **Enables**: defects, inhomogeneities, phase-transitions, ...
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**Spin dynamics**
- **Enables**: magnetization dynamics, spin textures, ...
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SPIN package, coupled SD - MD

\[ \begin{align*}
\frac{\partial r_i}{\partial t} &= \mathbf{v}_i \\
\frac{\partial \mathbf{v}_i}{\partial t} &= \mathbf{F}_i (r_{ij}, s_{i,j}) \\
\frac{\partial s_i}{\partial t} &= \omega_i \times \mathbf{s}_i
\end{align*} \]

\[ H_{SL} = \sum_{i=1}^{N} \frac{|p_i|^2}{2m_i} + \sum_{i,j=1}^{N} V(r_{ij}) - \sum_{i,j \neq j}^{N} J(r_{ij}) \mathbf{s}_i \cdot \mathbf{s}_j - \mu_B \mathbf{H}_0 \sum_{i=0}^{N} g_i s_i \cdot \mathbf{H}_{ext} \]

MD Hamiltonian

Spin–lattice coupling


- Resolution of spin-waves, magnon modes.
- Adiabatic approximation: electronic dynamics frozen.
- Atomic spin: time average of the spin density over V atom.

- Enables: magneto-elasticity, spin-lattice relaxation, magnon-phonon scattering, magneto-structural phase-transitions, ...
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NVE and NVT ensembles

- Geometric integration algorithms enable NVE calculations.
- Langevin thermostat on the spins for NVT calculations.
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Three spin minimizers
- Damped dynamics with adaptive timestep, CG and LBFGS.
- Minimization on the energy, or on the total or per-atom torque.
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Eight different magnetic interactions
- Five pairs: exchange, DMI, Neel, Magneto-electric, dipolar.
- Three fixes: Zeeman, cubic and uniaxial anisotropies, and setforce.
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- Output per-atom spin, per-atom and total mag energy, magnetic temperature, ...
- Read/restart from generated magnetic configurations.
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Long-range dipolar fields
- Ewald and P3M implemented to calculate long-range magnetic dipolar interactions.
- Nucleate and stabilize magnetic domains and domain-walls.
Chiral magnetic textures in multiferroics

Collaboration with M. Viret, J.-Y. Chauleau and T. Chirac at CEA

- Material: Bismuth ferrite BiFeO$_3$ (prototypical multiferroic, AF and ferroelectric at room temperature)
- Simulation of chiral magnetic textures at ferroelectric domain-walls.
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**Simulation details**

\[ H_{\text{BFO}} = - \sum_{i,j; i \neq j} J_{ij}^{(1,2)} s_i \cdot s_j + \sum_{i,j; i \neq j} \left( P^{(A,B)} \times e_{ij} \right) \cdot (s_i \times s_j) - \sum_{i=1}^{N} K_i (s_i \cdot n_i)^2 \]

- Ferroelectric domains simulated by alternating the polarization vector \( \mathbf{P} \) in the ME interaction.
- Simulation box of about 200k magnetic atoms
- Configuration relaxed in about 2 days on a 40 core-workstation
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Results were compared with experimental measurements (performed by NV center). Very good agreement was recovered.
Thermal transport in magnetic materials


- Abnormal behavior: drop of the lattice thermal conductivity at T_c.
- Development of a Green-Kubo equilibrium atomic and spin dynamics (GK-EASD) approach in LAMMPS.
- Development of better exchange models and statistics could greatly improve the accuracy.

**Lattice thermal conductivity**


**Norm of total magnetization**

Magnetic dipole-dipole interaction

Long-range SD - MD

\[
\begin{align*}
\frac{\partial r_i}{\partial t} &= \mathbf{v}_i \\
\frac{\partial \mathbf{v}_i}{\partial t} &= \mathbf{F}_i (r_{ij}, s_{ij}) \\
\frac{\partial s_i}{\partial t} &= \omega_i \times \mathbf{s}_i
\end{align*}
\]

\[
\mathcal{H}_{\text{long}} = -\frac{\mu_0 (\mu_B)^2}{4\pi} \sum_{i,j,i\neq j}^N \frac{g_i g_j}{r_{ij}^3} \left( 3(e_{ij} \cdot s_i)(e_{ij} \cdot s_j) - s_i \cdot s_j \right)
\]

\[
\mathbf{F}_i = \frac{\mu_0 (\mu_B)^2}{4\pi} \sum_j \frac{g_i g_j}{r_{ij}^4} \left[ \left( (s_i \cdot s_j) - 5(e_{ij} \cdot s_i)(e_{ij} \cdot s_j) \right) e_{ij} + \left((e_{ij} \cdot s_i)s_j + (e_{ij} \cdot s_j)s_i \right) \right]
\]

\[
\omega_i = \frac{\mu_0 (\mu_B)^2}{4\pi \hbar} \sum_j \frac{g_i g_j}{r_{ij}^3} \left( 3(e_{ij} \cdot s_j)e_{ij} - s_j \right)
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Magnetic dipole-dipole interaction

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\]

\[
\omega_i = \frac{\mu_0 (\mu_B)^2}{4\pi \hbar} \sum_j \frac{g_i g_j}{r_{ij}^3} \left(3(e_{ij} \cdot s_j)e_{ij} - s_j\right)
\]

- Two methods implemented: Ewald and P3M (P3M also implemented for electric dipoles).
### Magnetic dipole-dipole interactions

#### Long-range SD - MD

\[
\begin{align*}
\frac{\partial r_{ij}}{\partial \tau} &= \mathbf{v}_i \\
\frac{\partial \mathbf{v}_i}{\partial \tau} &= \mathbf{F}_i (r_{ij}, s_{ij}) \\
\frac{\partial s_i}{\partial \tau} &= \omega_i \times \mathbf{s}_i
\end{align*}
\]

\[
\mathcal{H}_{\text{long}} = -\frac{\mu_0 (\mu_B)^2}{4\pi} \sum_{i,j,i \neq j}^N \frac{g_i g_j}{r_{ij}^3} \left( 3(e_{ij} \cdot s_i)(e_{ij} \cdot s_j) - s_i \cdot s_j \right)
\]

\[
\mathbf{F}_i = \frac{\mu_0 (\mu_B)^2}{4\pi} \sum_j \frac{g_i g_j}{r_{ij}^4} \left[ ((s_i \cdot s_j) - 5(e_{ij} \cdot s_i)(e_{ij} \cdot s_j)) e_{ij} + ((e_{ij} \cdot s_i)s_j + (e_{ij} \cdot s_j)s_i) \right]
\]

\[
\omega_i = \frac{\mu_0 (\mu_B)^2}{4\pi \hbar} \sum_j \frac{g_i g_j}{r_{ij}^3} \left( 3(e_{ij} \cdot s_j)e_{ij} - s_j \right)
\]

- Two methods implemented: Ewald and P3M (P3M also implemented for electric dipoles).

**Scaling results**

- From 1 to 32 Broadwell nodes, with 36 processes per node (1024 processes for the last point).
- Spin-lattice Ewald has the same scaling as Ewald/disp (reference in LAMMPS).
- Spin-lattice PPPM faster and much better scaling.
Magnetic dipole-dipole interaction

\begin{align*}
\frac{\partial \mathbf{r}_i}{\partial t} &= \mathbf{v}_i \\
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\[\mathcal{H}_{\text{long}} = - \frac{\mu_0 (\mu_B)^2}{4\pi} \sum_{i,j,i \neq j} g_i g_j \frac{3 (\mathbf{e}_{ij} \cdot \mathbf{s}_i)(\mathbf{e}_{ij} \cdot \mathbf{s}_j) - \mathbf{s}_i \cdot \mathbf{s}_j}{r_{ij}^3}\]

\[\mathbf{F}_i = \frac{\mu_0 (\mu_B)^2}{4\pi} \sum_j \frac{g_i g_j}{r_{ij}^4} \left[ \left((\mathbf{s}_i \cdot \mathbf{s}_j) - 5(\mathbf{e}_{ij} \cdot \mathbf{s}_i)(\mathbf{e}_{ij} \cdot \mathbf{s}_j) \right) \mathbf{e}_{ij} + (\mathbf{e}_{ij} \cdot \mathbf{s}_j) \mathbf{s}_j + (\mathbf{e}_{ij} \cdot \mathbf{s}_i) \mathbf{s}_i \right] \]

\[\mathbf{\omega}_i = \frac{\mu_0 (\mu_B)^2}{4\pi \hbar} \sum_j \frac{g_i g_j}{r_{ij}^3} \left( 3 (\mathbf{e}_{ij} \cdot \mathbf{s}_j) \mathbf{e}_{ij} - \mathbf{s}_j \right)\]

Domain-wall nucleation

- Allows the simulation of nucleation and motion of magnetic domains and domain-walls.
- Goal: bridging ab initio and continuum scale magnetic calculations.
Conclusions

- SPIN package available in LAMMPS.
- Enables massively parallel spin-lattice dynamics to be performed with LAMMPS.
- 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.
- Accounts for a lot of magnetic interactions. Models for the spin-orbit coupling are currently being developed.
- Open to collaborations, feel free to contact us (jtranch@sandia.gov).

Thanks to the LAMMPS group at Sandia: Aidan, Steve, Mitch, Stan, Mary-Alice.


And at CEA: Pascal Thibaudeau, Michel Viret, Jean-Yves Chauleau, Theophile Chirac.

Thank you for hosting me and for your attention.

http://lammps.sandia.gov

https://github.com/lammps/lammps
**Potential improvements, ongoing developments**

- **Pressure and temperature effects**
  - Need to account for longitudinal spin fluctuations.
  - Example: magneto-structural phase transitions (alpha → epsilon in iron)

- **Electronic degrees of freedom in MD**
  - TD-DFT parametrization of a 3-temperature model.
  - Longitudinal spin fluctuations parametrized on Te.

- **Phase-transition and defects in metals**
  - Irradiation-based defects in bcc iron:
    - Vacancies.
    - Interstitial sites.
  - Need Ab initio exchange parameters.

- **Kinetic of magnetism**
  - Visit of Hannes Jonsson's group in January.
  - Implementation of a magnetic NEB, and begin development of a spin-lattice version.

- **Simulation of multiferroics**
  - Example: bismuth oxide
  - Magnetic (AF) and ferroelectric orders.

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**Magnetostriction**

- Models for effects of the SOC
- Example: cobalt, gadolinium, uranium dioxide


**Simulation of multiferroics**

- Example: bismuth oxide

## Accounting for the spin-lattice interactions

The current version accounts for six magnetic interactions:

### Exchange interaction:

\[
H_{\text{exchange}} = - \sum_{i,j, i \neq j}^N J(r_{ij}) \hat{s}_i \cdot \hat{s}_j
\]

- Simulation of ferromagnetism, antiferromagnetism, ferrimagnetism, ...

### Uniaxial anisotropy:

\[
H_{an} = - \sum_{i=1}^N K_{an}(r_i) (\hat{s}_i \cdot \hat{n}_i)^2
\]

- Simulation of magnetocrystalline anisotropy or shape anisotropy.
- Poor lattice dependence.

### Dzyaloshinskii-Moriya:

\[
H_{dm} = \sum_{i,j=1, i \neq j}^N \tilde{D}(r_{ij}) \cdot (\hat{s}_i \times \hat{s}_j)
\]

- Simulation of an effect of the spin-orbit coupling
- Very trendy (chiral magnetism, skyrmions...)

### Zeeman interaction:

\[
H_{\text{Zeeman}} = -\mu_B \mu_0 \sum_{i=0}^N g_i \hat{s}_i \cdot H_{\text{ext}}
\]

- Interaction with an external magnetic field (constant or time dependent).

### Magneto-electric interaction:

\[
H_{me} = - \sum_{i,j, i \neq j}^N \left( \vec{E} \times \vec{e}_{ij} \right) \cdot (\hat{s}_i \times \hat{s}_j)
\]

- Interaction between spins and electric dipoles.
- Simulation of multiferroic materials.

### Néel pair anisotropy:

\[
H_{\text{Néel}} = - \sum_{i,j=1, i \neq j}^N g_1(r_{ij}) \left( (\hat{e}_{ij} \cdot \hat{s}_i)(\hat{e}_{ij} \cdot \hat{s}_j) - \frac{\hat{s}_i \cdot \hat{s}_j}{3} \right)
\]

- Other way to account for effects of the spin-orbit coupling.
- Simulation of magnetocrystalline anisotropy and magneto-elasticity.
