



Contribution ID: 69

Type: **Contributed Oral**

Speeding up Simulations of Magnetic Nanoparticles

Friday 5 December 2025 11:55 (15 minutes)

Magnetic nanoparticles are used in biomedicine to treat and image cancer. This is because of their ability to generate heat within an alternating magnetic field and to track cells, respectively. Thus, it is important that their response to a magnetic field is simulated accurately to predict and understand their behaviour. However, simulations can be computationally expensive, so it is necessary to minimise the computational power used to generate results.

There are two ways that nanoparticles change their magnetisation direction under the influence of a magnetic field: (i) particles physically rotate and the magnetization moves with the particle (so-called Brownian motion), and (ii) the particle does not move, but the internal magnetic moments rotate (so-called Néel motion).

Of, course the real motion is a mixture of these two cases.

The goal of this work is to average over the faster Néel dynamics, to speed up simulations. This is done by stochastically moving the internal magnetic moment inside nanoparticles every nanosecond, according to their thermodynamics. In comparison, full simulations usually involve integrating equations of motion forward in time. This requires timesteps that are at least 1000 times smaller.

Here, we detail computer simulations that simultaneously model both Brownian and Néel dynamics. These simulations are rigorously tested by comparing the Brownian and the Néel behaviour to literature results. To show its validity, we compare results of our stochastic, approximate method to treat the Néel dynamics with those from full time-integration of equations of motion.

Author: Mr CRAMER, Samuel (University of Newcastle)

Co-authors: Dr LIVESEY, Karen (University of Newcastle); Prof. CAMLEY, Robert (University of Colorado - Colorado Springs); Mr HOWARD, Jake (University of Colorado - Colorado Springs)

Presenter: Mr CRAMER, Samuel (University of Newcastle)

Session Classification: Condensed Matter & Materials

Track Classification: Topical Groups: Condensed Matter & Materials