Application of established heuristic solvers to physics problems

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Introduction

Optimisation problems that are computationally difficult can be addressed using heuristic solvers, which are pieces of software which apply one or many algorithms to find a "good estimate" of a solution when exact methods are too slow. These solvers find a lot of use in commercial applications, but this project studied their use in physics problems. Code was written to model a two-dimensional lattice of interacting spins and a range of solvers were tested for their efficiency at solving the problem. Then the most efficient solver was chosen for further tests of three-dimensional models.

Software packages

Solvers were used from three different software packages: Pyomo, pyOpt and SciPy, all based in Python. Between them, 15 solvers were tested.

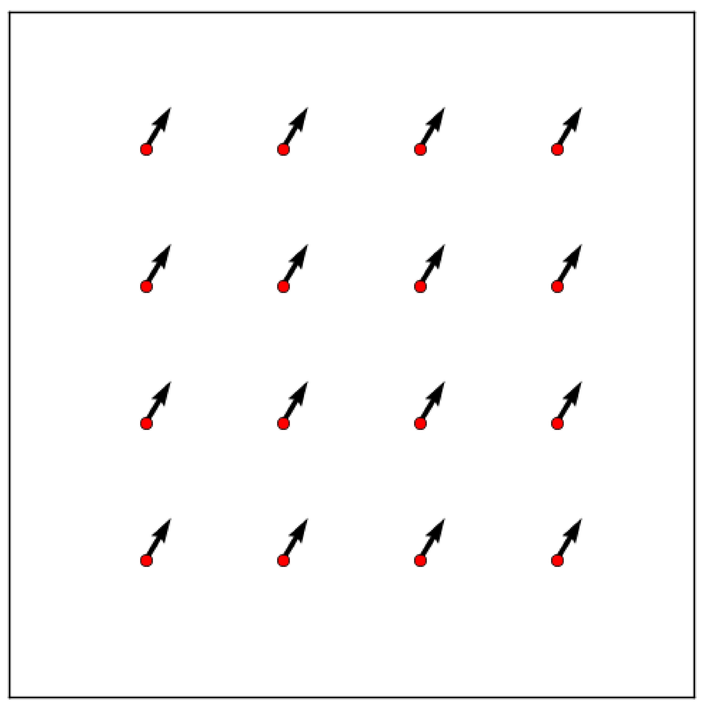
Physics problem

Atoms in a magnetic material have spin-angular-momentum vectors, and how these align determines the magnetic properties of the lattice. The problem was modelling how these spins interact and align on a lattice according to given parameters.
This was modelled using the Classical Heisenberg model, which involves changing the spin vectors to minimise the Hamiltonian:

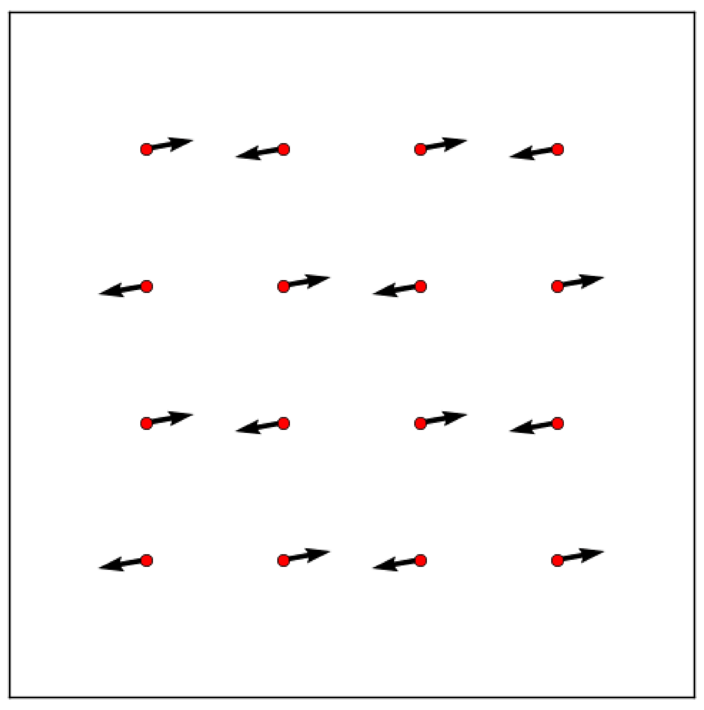
$$\mathcal{H} = -\sum_{i,j} J_{i,j}\mathbf{S}_i \cdot \mathbf{S}_j$$

2D model

The problem was formulated as a two-dimensional lattice of spins, which were then plotted. The arrows are the spin vectors and dots are positions on the lattice.



Ferromagnet



Anti-ferromagnet

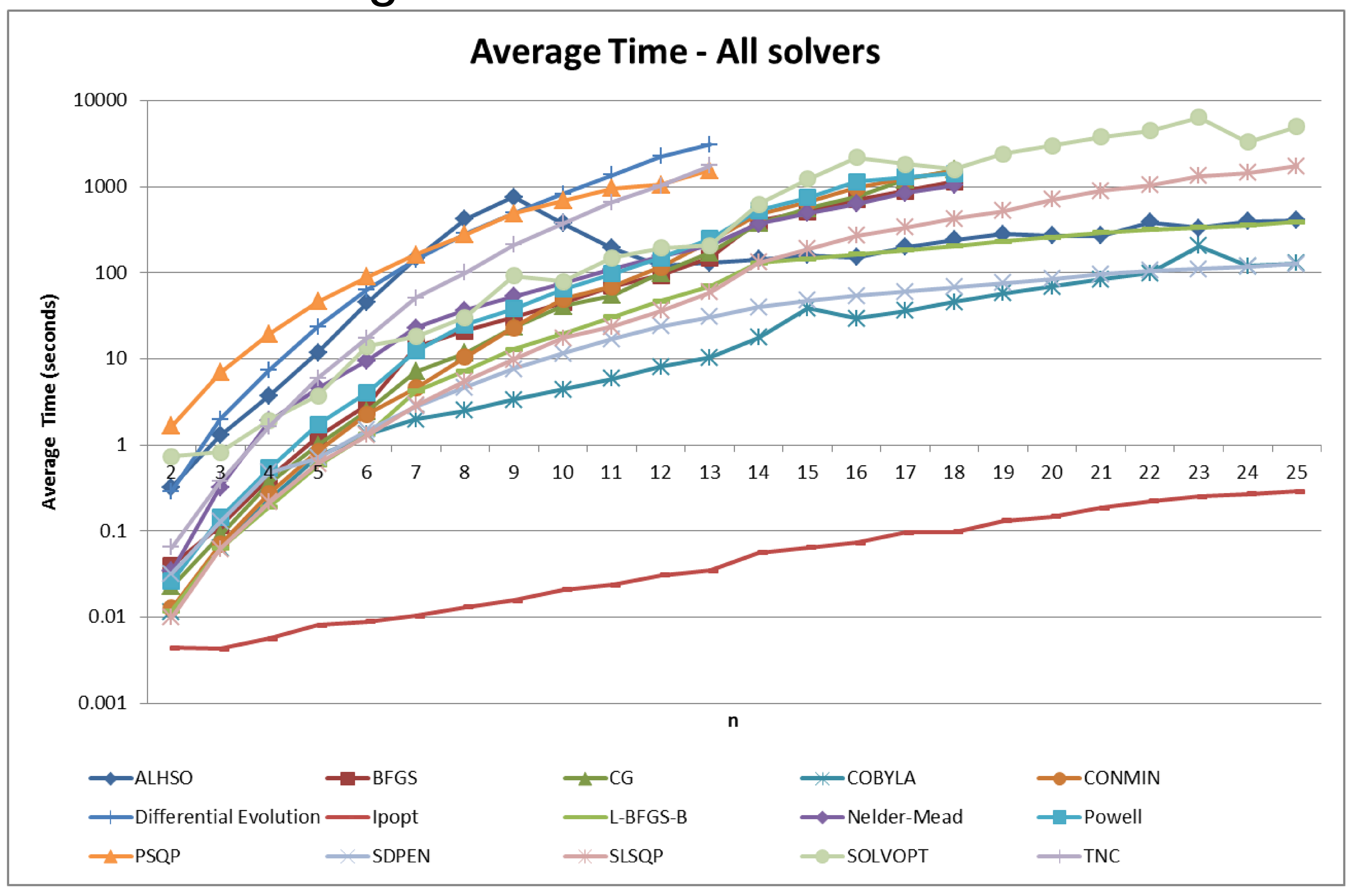
Further work

- Test the other 14 solvers in 3D
- Test more Pyomo solvers (the fastest solver, Ipopt, was the only Pyomo solver
- Investigate different physics problems

Report and code: https://github.com/MNegus/SpinModel3D

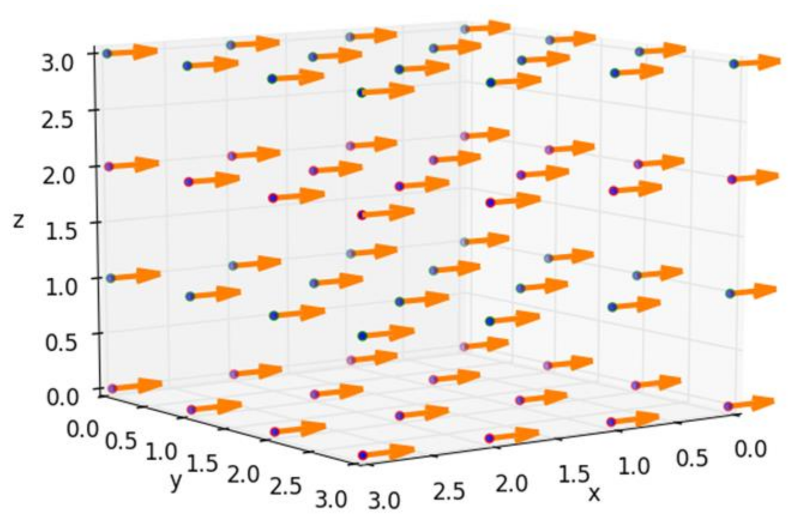
Testing

The 15 solvers were tested at solving the two-dimensional problem in the ferromagnetic case, and the time it took to solve at different grid sizes was measured.



3D model

The same problem was then formulated in 3D using the faster solver, with terms for a magnetic field, single-ion-anisotropy and Dzyaloshinskii-Moriya interactions.



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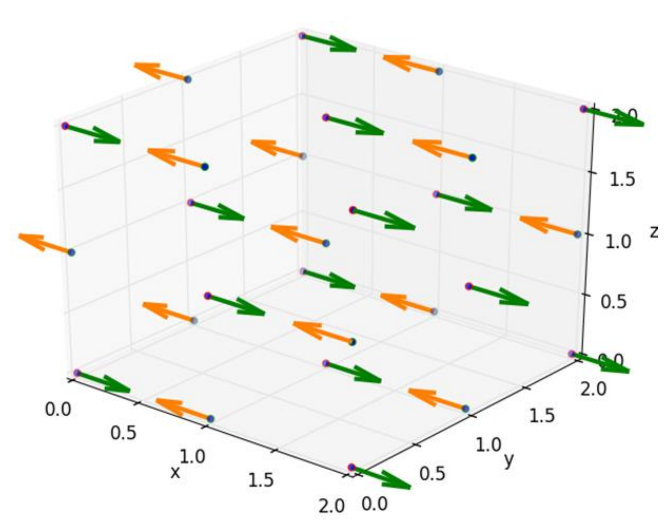
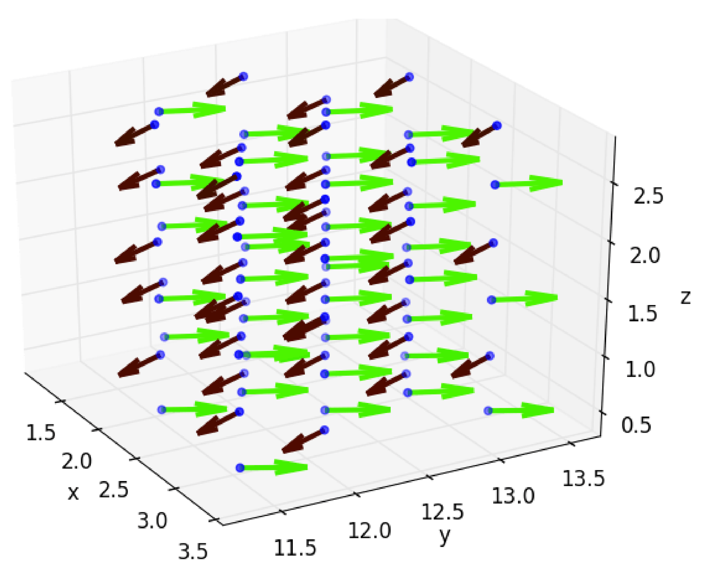
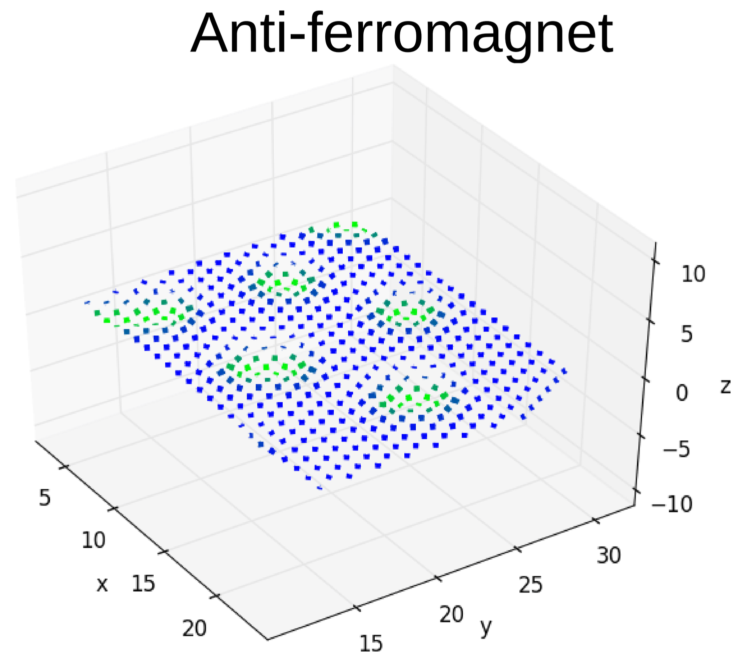


Anti-ferromagnet



$FeBO_3$



Magnetic skyrmions

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