Working with Magnetite

Requirements

- Input file:
  - Lattice constant 8.397 A
  - System dimensions
  - Program
  - Output
- New parameter for spinel materials
  - `create:crystal-structure=spinel`
- `If using a unitcell file this parameter is not used`

Requirements

- Material File: 3 materials
  - FeA
  - FeB
  - O (non-magnetic)
- Each magnetic material requires exchange matrices and anisotropy values
- `material[x]:unit-cell-category = x`
- Oxygen can use parameter:
  - `material[3]:non-magnetic = remove`

Unitcell file

- Contains the unit cell information
- As well as the exchange interactions
- Usually has to be made for each complex crystal structure
  - Requires some coding by the user

Unitcell file structure

- Lattice parameters and crystal orientation (always cubic)
- Atom position list
  - Number of atoms
  - id, fractional coordinates, material information
- Exchange list
  - Number of interactions, type
  - Interaction id, $atom_{[i]}$ id, $atom_{[j]}$ id, unit cell location, exchange value

Making it easier

- New input file parameter
  - `create:crystal-structure = spinel`