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A Multiscale Modelling environment for magnetism and spintronics

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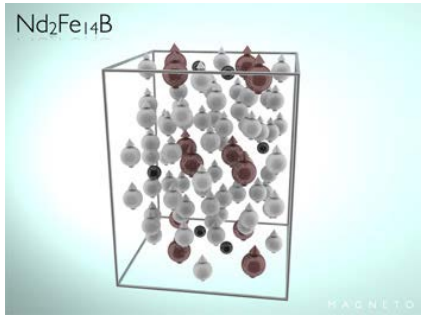
New electronic devices based on electron spin rather than charge



Atoms to technology – multiscale calculations underpin magnet developments for hybrid cars.
Strategic drive to reduce Rare-Earth content

- Electronic structure calculations.
  - Difficult because magnetic quantities are rather small energy contributions.
  - Many separate codes, VASP, SIESTA, CASTEP, WIEN2k
- Atomistic calculations. VAMPIRE (York) and UPP ASD (Uppsala) the only open source code
- Mesoscopic calculations
  - Continuum formalism (Micromagnetics)
  - Open source code OOMMF (NIST), MagPar (Scholz)

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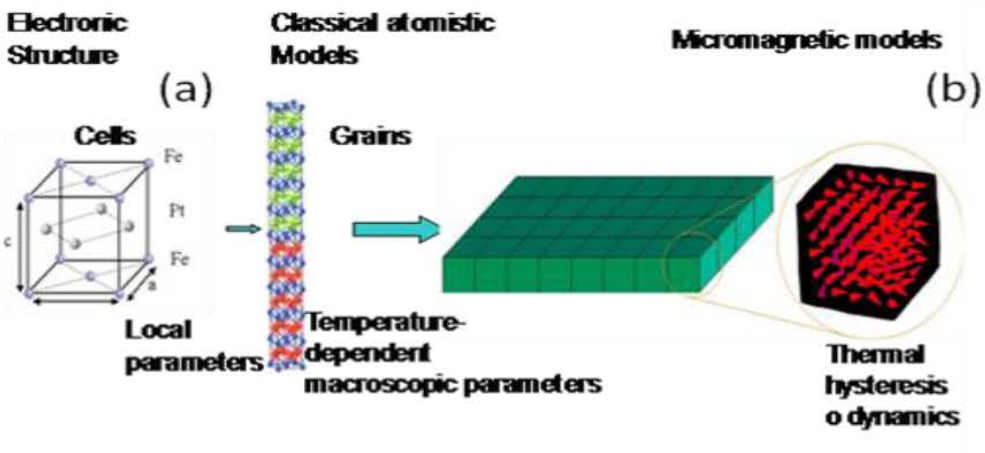
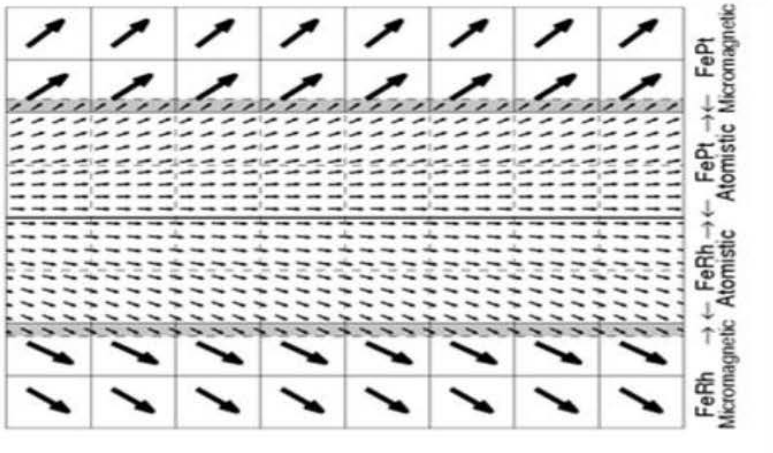
Grand Challenge





- To develop an environment capable of linking all lengthscales and creating mesoscopic models *with specific materials parameters*
- Multiscale modelling of spin systems is difficult and is at an early stage.
- Necessary to support vital industrial needs

Challenges

- Improved information from electronic structure calculations
- Mapping information from electronic structure calculations to atomistic models
  - Mapping of information to spin Hamiltonian
  - Each material is unique and so is the mapping
- Mapping atomistic to mesoscopic models
  - Requires temperature dependence of magnetic properties
  - Cell size scaling is also important
- Database needs
  - Database of magnetic parameters from electronic structure calculations
  - Database of spin Hamiltonian parameters
  - Both updated by users
  - Need to engage whole community
- Flexible approach, producing linking structures independent of CPU platform; Applicable to Local, National and Cloud-based systems

Modular approach

1. **Interfacing module linking ab-initio and atomistic models:** including a database for materials and interfaces of interest with layer-resolved ab-initio parameters; standardized input for future users to include any specified material from external ab-initio codes.
2. **Modules for interfacing to commercial codes**
3. **Atomistic module**: thermal atomistic approach for evaluation of macroscopic parameters based on Hamiltonians, parameterized from ab-initio (with input from module 1) yielding the necessary input for the mesoscopic models.
4. **Module for atomic structure:** molecular dynamics for modeling the lattice structure including the atomistic structure of interfaces to properly model multilayer materials. Links to 3).
5. **Spin accumulation module:** this will use (where appropriate) ab-initio information (module 1) and input from magnetisation structures for a self-consistent solution of the spin accumulation and magnetization dynamics as necessary to model spintronics devices.
6. **Heat transport module:** Important for device simulations

Summary

- New technology developments in magnetism and spintronics require support from multiscale models
- Need for Collaborative environment for software development linking formalisms (open source and commercial)
- Need to develop user community via workshops
- Good opportunities for EU/US collaboration
  - EU groups (arguably) pioneering the basic developments
  - Numerous US Universities interested
  - Initial ‘ad-hoc’ approaches already used in industry