What is simulation

Simulant (German) = Malingerer

History: Horse simulator (Wikipedia)

Simulation is the imitation of the operation of a real-world process or system over time.

The act of simulating something requires a model.

Model

Occupation

A model, is a person with a role either to promote, display, or advertise commercial products or to serve as a visual aide for people who are creating works of art. Wikipedia

Median pay (annual): 18,750 USD (2012)
Median pay (hourly): 9.02 USD (2012)
Entry level education: Less than high school
Projected 10-year growth: 15% (2012)
Number of jobs: 4,800 (2012)
Similar professions: Child Actor, Fashion Designers

Modelling (Wikipedia)

Modelling: A scientific activity, the aim of which is to make a particular part or feature of the world easier to understand, define, quantify, visualize, or simulate by referencing it to existing and usually commonly accepted knowledge

Philosophy

experiments

parameters, methods

intuition

Model → Simulation

© P. Rekacewicz
Our model

\[ i \gamma^{\mu} \left( \partial_{\mu} + ie A_{\mu} \right) - m \psi = 0 \]

Modeling and simulation

The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved.

(Paul Dirac)

All of condensed matter theory is modelling and simulation!

The fundamental–applied divide

academic

industrial

Contents

• Modelling and simulation: a physicists point of view

Part 1

I. M&S of electronic structure
II. M&S of magnetization
III. M&S of spin and charge transport
IV. M&S of MRAM elements

Part 2

• Case study: heterostructures with magnetic insulators

I. M&S of electronic structure

Many-body problem

• Exact solutions (hydrogen molecule, 1D systems, 2D Ising model)
• Many-body perturbation theory, Green's functions, diagrammatic methods (also for alloys)
• Configuration interaction (chemistry)
• Coupled cluster expansions (chemistry)
• Quantum Monte-Carlo approaches
• Density functional theory
• Lattice gauge theory
• Quantum tensor network theory
• Numerical renormalization group
• AdS-CFT (string theory)
### “Mean-field” Theory

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### Density Functional Theory

The ground state energy $E[\rho]$ is a functional of the electron (spin) density $\rho(\mathbf{r})$ (Hohenberg & Kohn, 1964):

$$E[\rho] = \min_{\psi} \left\{ \sum_{\alpha} \epsilon_{\alpha}(\mathbf{r}) \psi_{\alpha}(\mathbf{r})^2 + \sum_{\alpha \beta} \int d\mathbf{r} \mathbf{r}_1 \mathbf{r}_2 \psi_{\alpha}(\mathbf{r}_1) \psi_{\beta}^{*}(\mathbf{r}_2) V_{\alpha \beta}(\mathbf{r}_1, \mathbf{r}_2) \right\} + E_{xc}[\rho] + E_{\text{corr}}[\rho]$$

#### Kohn-Sham Equations

Variational principle: ground state energy is minimal for the ground state density. The variation under particle number constraint $N = \int \rho(\mathbf{r}) d\mathbf{r}$ is stationary:

$$\frac{\delta E[\rho] - \mu N}{\delta \rho(\mathbf{r})} = 0 \Rightarrow \frac{\delta E[\rho]}{\delta \rho(\mathbf{r})} = \mu$$  \hspace{1cm} $\mu$ chemical potential

$$\frac{\delta (E[\rho] - \mu N)}{\delta \rho(\mathbf{r})} = 0 \Rightarrow H_{\text{KS}}\psi(\mathbf{r}) = \epsilon_{\alpha}(\mathbf{r}) \psi(\mathbf{r})$$

$$H_{\text{KS}} = -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{xc}}(\mathbf{r}) + V_{\text{loc}}[\rho](\mathbf{r})$$

$$\rho_{\alpha}(\mathbf{r}) = \int \rho(\mathbf{r}) d\mathbf{r}$$  \hspace{1cm} local density approximation

### Spin Density-Functional Theory

Spin-polarized Kohn-Sham equations:

$$\rho_{\alpha}(\mathbf{r}) = \sum_{\alpha} \rho_{\alpha}(\mathbf{r})$$

$$H_{\alpha}^{\rho}(\mathbf{r}, \rho_{\alpha}) = H_{\text{loc}}^{\rho}(\mathbf{r}, \rho_{\alpha}) + H_{\text{exc}}^{\rho}(\mathbf{r}, \rho_{\alpha})$$

Starting density matrices:

$$\rho_{\alpha}(0) = \frac{1}{\sqrt{N}} |\phi_{1}(\mathbf{r}), \cdots, \phi_{N}(\mathbf{r})\rangle$$

### Band Structure and Fermi Surfaces of Co

Zwierzycki et al. (2008)

### DMFT

Fe spin-up and Fe spin-down

Lichtenstein et al. (2003)
Transition metals and s-d hybridization

\[ \Delta E_{sd} -10eV \Rightarrow \Delta E_{sd} - \frac{\hbar}{\Delta E_{sd}} - fs \]

sp and d- electrons are strongly hybridized and cannot be distinguished on electron transport time scales.

Stoner metallic ferromagnet

\[ \tilde{H}^{(c)} = -\frac{\hbar^2}{2m} \psi^2 - (+) \Delta \]

\( \Delta \): exchange(-correlation) potential that reflects the energy splitting between majority and minority spin states.

II. M&S of magnetization (dynamics)

Simulated magnetic vortex switching © G. Schütz

Magnetic dipole in a magnetic field

\[ U = -\mathbf{M} \cdot \mathbf{B} \]
\[ \mathbf{F} = (\mathbf{M} \cdot \mathbf{B}) \]
\[ \frac{d\mathbf{L}}{dt} = \mathbf{T} = \mathbf{M} \times \mathbf{B} \]
\[ \frac{d\mathbf{M}}{dt} = -\gamma \frac{d\mathbf{L}}{dt} = -\gamma \mathbf{T} = -\gamma \mathbf{M} \times \mathbf{B} \]

Magnetization dynamics

Spin equation of motion

Heisenberg spin-operator equation of motion:

\[ \frac{d}{dt} \mathbf{s} = \frac{i}{\hbar} [\mathbf{s}, \mathbf{H}] = \frac{i}{\hbar} \sum_i B_i [\mathbf{s}, \mathbf{s}_i] \]
\[ = -\gamma \mathbf{s} \times \mathbf{B} \]

\[ \langle \mathbf{s} \rangle = \langle \psi | \mathbf{s} | \psi \rangle = \langle \langle s_x, s_y, s_z \rangle \rangle \]
\[ \mathbf{m} = -\gamma \langle \mathbf{s} \rangle \]

Spin-vector (Landau-Lifshitz) equation of motion:

\[ \frac{d}{dt} \mathbf{m} = -\gamma \mathbf{m} \times \mathbf{B} \]
Magnetism, statics and dynamics

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Landau-Lifshitz-Gilbert equation

\[
\frac{d \mathbf{m}(t)}{dt} = -\gamma \mathbf{m} \times \left( \mathbf{B}_{\text{eff}}(t) - \frac{\alpha}{\gamma} \frac{d \mathbf{m}(t)}{dt} \right) \\
\mathbf{m} = \frac{\mathbf{M}}{M_s}; \quad \mathbf{M}_s = |\mathbf{M}|
\]

Landau-Lifshitz-Gilbert equation; Gilbert damping constant \(\alpha\)

Landau-Lifshitz-Gilbert equation

\[
\frac{d \mathbf{m}(t)}{dt} = -\gamma \mathbf{m} \times \left( \mathbf{B}_{\text{eff}}(t) - \frac{\alpha}{\gamma} \frac{d \mathbf{m}(t)}{dt} \right) \\
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\]

Landau-Lifshitz-Gilbert equation; Gilbert damping constant \(\alpha\)

Micromagnetism (static)

Course grain minimization of magnetostatic energy with \(\mathbf{M} = 0\):

\[
\mathcal{F} \left[ \mathbf{M} \right] = \int \left[ -\mathbf{M}(r) \cdot \mathbf{B}_{\text{eff}} \left[ \mathbf{M}(r) \right] + \frac{C}{2} \left| \mathbf{M}(r) \right| \right] \, dr \\
\mathbf{B}_{\text{eff}} (\mathcal{F}) = \mathbf{B}_{\text{app}} + \frac{1}{2} \mathbf{B}_{\text{dipole}} \left[ \mathbf{M} \right] + \frac{\mathbf{B}_{\text{inst}}}{2M_s} \quad C \text{ spin-wave stiffness}
\]

transverse magnetic head-to-head domain wall

Spin waves or magnons

Plane wave solution of LL equation:

William Fuller Brown, Jr. (1904–1983)

FATHER OF MICROMAGNETICS

Thermal Fluctuations of a Single-Domain Particle
William Fuller Brown, Jr.
Phys. Rev. 130, 1677 – Published 1 June 1963

The Center for Microscopy and Image Information Technology
**Thermal magnetization noise**

- **Thermal equilibrium:**
  \[ M(T) = M_s \int f_{\text{eq}}(\mathbf{Q}) d\Omega \rightarrow M_0 \left( 1 - \frac{kT}{2\mu_s H_{\text{eff}}} \right) \]

- **Stochastic field:**
  \[ \mathbf{m} = \mathbf{m} \times (-\gamma (\mathbf{H}_{\text{eff}} + \mathbf{h}(t)) + \alpha \mathbf{m}) \]

- **Fluctuation-dissipation theorem:**
  \[ \langle h_i(t) h_j(t') \rangle = \frac{2\alpha k_T T}{\gamma M_s^2} \delta(t - t') \delta_{ij} \]

- Fokker-Planck equation for probability distribution function \( P(\mathbf{m}, t) \)

**LL(Gilbert) vs. LLB(loch) Garanin (1997)**

- **LLG:** \( M_s = |\mathbf{m}| = \text{const.} \)
- **LLB:** \( \mathbf{m} = M_s(T) \)

**LLG:**

\[
\frac{d\mathbf{m}}{dt} = -\mathbf{m} \times \mathbf{B}_{\text{eff}} - \alpha \mathbf{m} \times \left( \mathbf{m} \times \mathbf{B}_{\text{eff}} + \mathbf{b}(t) \right) + \alpha \mathbf{m} (\mathbf{m} \cdot \mathbf{B}_{\text{eff}}) + \mathbf{b}(t)
\]

- **Transverse dynamics**
- **Longitudinal dynamics**
+ FD theorem

**Atomistic spin simulations for localized spins**

\[
\mathbf{S}_i = -\gamma \mathbf{S} \times \mathbf{B}^{\text{eff}} + \alpha \mathbf{S} \times \mathbf{S}_i
\]

\[
\mathbf{B}^{\text{eff}} = -\frac{\partial E_j}{\partial \mathbf{S}_j} + \mathbf{b}(t)
\]

\[
E_j = -\frac{1}{2} \sum_{j=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_j
\]

- Garanin (1997)

**III. Transport**

- Spin-wave dispersion in the (1, 1, 1) direction of the reciprocal space for LaTiO3 measured by neutron-scattering experiment. The line is the fitting curve by using the Heisenberg model with isotropic \( j \) of 15.5 meV on the cubic lattice (Keimer et al., 2000)

- **Micromagnetism:**

\[ E_x = -J \sum_{j=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_j \]
Charge and spin transport

- Green function methods
  - Diagrammatic, Kubo formula, Keldysh
- Scattering theory of transport
- Semiclassical methods
  - Kinetic, Boltzmann, diffusion (Valet-Fert)
- Numerical (first principles and model)
  - Recursive GF, Kwant
- Hybrid methods
  - circuit theory, Continuous-RMT

Regimes dictate the models and methods

- Linear vs. non-linear transport
- Ballistic vs. diffuse transport
- Bulk vs. interfaces
- Zero vs. finite temperature
- Relativistic vs. non-relativistic
- Metals vs. insulators
- Qualitative vs. predictive

Atomic scale interfaces + disorder

Diffusion in bulk 3D metal

- Ohm’s Law
- Disorder
- Multilayers
- Noise
- Spin Hall effect
- YIG
- material design

Mesoscopic physics

- Quantum point contacts
- Quantum wires
- Break junctions

Interface conductance

- Landauer-Büttiker formula
- Sharvin conductance
Metallic interface

Specular metallic interface

Disorder

Interfaces

Spin valve and giant magnetoresistance (GMR)

Two spin-channel model

Disorder

Interface alloying and roughness

Bulk disorder scattering

Spin valve and giant magnetoresistance (GMR)

Two spin-channel model

Ohm’s Law

spin relaxation

spin-flip diffusion

Equivalent circuit

Equivalent circuit

spin diffusion length

averaged diffusion constant
Spin accumulation and spin current

\[ \tau_{sf} = \sqrt{D \tau_r} \]

- \( \tau_{sf} \) spin-flip diffusion length
- \( D \) diffusion constant
- \( \tau_r \) spin-flip relaxation time

F|N|F spin valves

- \( \ell_{sf} \ll L \)
- \( \ell_{sf} \gg L \)
- \( \ell_{sf} \approx L \)
F|N|F spin valves: non-collinear

Electron spin vector operator
\[
\mu = g_s \frac{\hbar}{2m} = -g_s \mu_B \frac{\sigma}{2} \quad \mu_B = \frac{\hbar}{2m} \text{ Bohr magneton}
\]
\[
s = \frac{\hbar}{2} \sigma
\]
\[
\sigma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\]
\[
\begin{align*}
\mathcal{X} & = -\mathbf{B} \cdot \frac{\hbar}{2} \sigma \\
& = \frac{\hbar}{2} \sigma \\
& = \hbar \omega_0
\end{align*}
\]
When \( \mathbf{B} \perp \mathbf{s} \) the system oscillates with Larmor frequency \( \omega_0 \).

Rotation in quantum mechanics
Rotation of a state \(|\psi\rangle\) by an angle \( \theta \) around an axis with unit vector \( \mathbf{n} \):
\[
|\psi\rangle_* = \hat{R}_n (\theta) |\psi\rangle
\]
Electron spin:
\[
\hat{L}_z = \frac{\hbar}{2} \sigma_z
\]
\[
\hat{R}_n (\theta) = e^{i \mathbf{n} \cdot \mathbf{\sigma} \theta / 2}
\]
With \( \mathbf{n} = (\cos \varphi, \sin \varphi, 0) \)
\[
|\psi\rangle_* = \hat{R}_n (\theta) |\psi\rangle
\]
generates all possible spin states. Example:
\[
|\psi\rangle_* = \hat{R}_n (\theta) |\psi\rangle
\]
Check:
\[
\langle \psi | \hat{R}_n (\theta) |\psi\rangle = \frac{\hbar}{2} (1, 0, 0)
\]

2013 Oliver E. Buckley Condensed Matter Physics Prize

Luc Berger
Carnegie Mellon University

John Slonczewski
IBM Research Staff Emeritus

Citation:
"For predicting spin-transfer torque and opening the field of current-induced control over magnetic nanostructures."

Rotation in quantum mechanics
Finite rotation:
\[
\hat{R}_n (\varphi) = \lim_{n \to \infty} \left[ 1 + i \frac{\varphi}{\hbar} \hat{L}_z \right] = e^{i \varphi \hat{L}_z / \hbar}
\]

Spins on the Bloch sphere
\[
\hat{R} \left( \frac{\pi}{2} \right) = e^{i \frac{\pi}{2} \sigma_y / 2} = \sum_{m=0}^{1} \left( \begin{array}{c} 0 \\ 1 \end{array} \right) \left( \begin{array}{c} 0 \\ -1 \end{array} \right) (\theta)_{m}^\pi
\]
\[
= \left( \begin{array}{cc} \cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{array} \right)
\]
\[
\hat{R} \left( \frac{\pi}{2}, 2\pi \right) = \left( \begin{array}{c} 0 \\ 1 \end{array} \right)
\]

Spin-up state in x-direction is obtained by rotation about \( \sigma_y \)-axis with \( \theta = \pi / 2 \).
\[
|\psi\rangle_+ = \hat{R} \left( \frac{\pi}{2}, \varphi \right) |\psi\rangle
\]
Check:
\[
\langle \psi | \hat{R} \left( \frac{\pi}{2}, \varphi \right) |\psi\rangle = \frac{\hbar}{2} (1, 0, 0)
\]
**Slonczewski torque and Andreev reflection**

Normal \[ \rightarrow \text{HMF} \]

\[ |\uparrow\rangle = (|+\rangle + |\rangle) / \sqrt{2} \]

Longitudinal spin current

\[ |\downarrow\rangle / \sqrt{2} \]

Transverse spin current = torque

\[ \tau = \hat{m} \]

\[ \theta = \frac{\pi}{2} \]

\[ N e / 2\pi \langle V_i - V_j \rangle \]

\( N \) = number of incoming channels

**Spin-mixing conductance**

\[ \tau (m = \hat{x}) = \hat{x} \frac{e^2}{\hbar} (V_1 - V_2) \]

\[ G_{\text{Shravin}} = \frac{2e^2}{h} \sum \frac{\epsilon_i}{k} = \frac{2e^2}{h} N \]

\( k \) = incoming wave vector

Scattering theory:

\[ \tau(m = \hat{x}) = \frac{2e^2}{h} \langle V_i - V_j \rangle \Re G_{\text{Shravin}} \]

Spin mixing conductance:

\[ G_{\text{Shravin}} = \frac{e^2}{h} \sum \left( 1 - \frac{\epsilon_k}{\epsilon_{k_0}} \right) = \frac{e^2 N}{h} \]

**Switching by spin transfer**

**Current-induced magnetization reversal**

Electrical currents can controllably reverse the magnetization in small (< 200 nm) magnetic devices (Slonczewski, Berger):

Kiselev et al. (2003)

**Ohm’s and Kirchhoff’s Laws**

Charge current:

\[ I_{j+2} = G_{j+2} (V_j - V_{j+1}) \]

\( G_{j+2} \) conductance

\[ G = \frac{e^2}{h} \sum \frac{\epsilon_i}{k} \]

Landauer formula

\[ \sum I_{j+2} = 0 \]

Charge conservation
Spin currents

\[ I_{s,z} = 2\text{Re}G_{zz}(\mathbf{m} \times \mathbf{V}_s \times \mathbf{m}) + 2\text{Im}G_{zz}(\mathbf{V}_s \times \mathbf{m}) \]

\[ \tau = \frac{\hbar}{2e}I_{s,z} \]

Pauli matrix notation

\[ \hat{\mathbf{k}} = \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} = X_s \hat{\mathbf{1}} + \mathbf{X} \hat{\boldsymbol{\sigma}} \]

\[ \hat{G} = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix}, \quad (\mathbf{I} \hat{\boldsymbol{\sigma}}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \]

Angular magnetoresistance

\[ c\text{MR}(\theta) = \frac{\text{Re}G^{zz} = 0.5 \times 10^4 \Omega^{-1} \text{m}^2}{0.1 \text{nm} \text{Py}} \]

Exp: S. Urazhdin et al. (2005)

III. M&S of MRAM elements

Dynamics of bilayers

\[
\dot{m} = -\gamma m \times B + \alpha_0 m \times \frac{\dot{m}}{\tau} + \frac{h \gamma}{4\pi M_s} m \times \left[ (1 + \eta) \dot{m} + \eta \dot{m} \right] \times m
\]

Re \( g_{\text{m}} = g \), Im \( g_{\text{m}} = 0 \)

Spin oscillators

Macrospin simulation of nanopillar

Continuous random matrix theory [Waintal c.s.]

Exchange-only theory is complete

SpinFlow3D (Thierry Valet)

- integration of current dynamics with micromagnetics (including Oersted fields)

Additional topics and challenges

- Current induces torques in magnetization textures (domain wall motion, emf due texture dynamics, topological Hall effect)
- Thermally induced spin currents (spin-dependent Seebeck effect, spin Seebeck effect)
- Spin Hall and related effects
- Spin orbit torques (field-like vs. damping-like)
- Magnetic insulators (YIG)
- Antiferromagnets
- Skyrmions