Ultrafast tutorial in Ultrafast Magnetism

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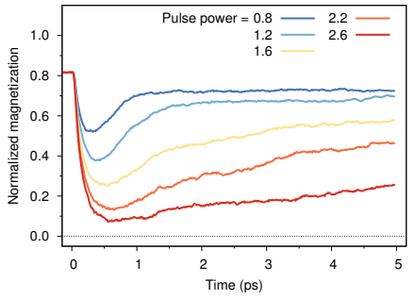
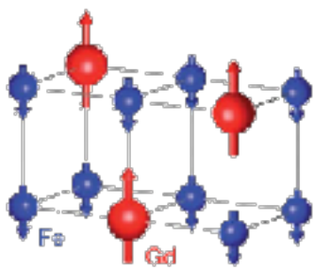
Overview

Running VAMPIRE

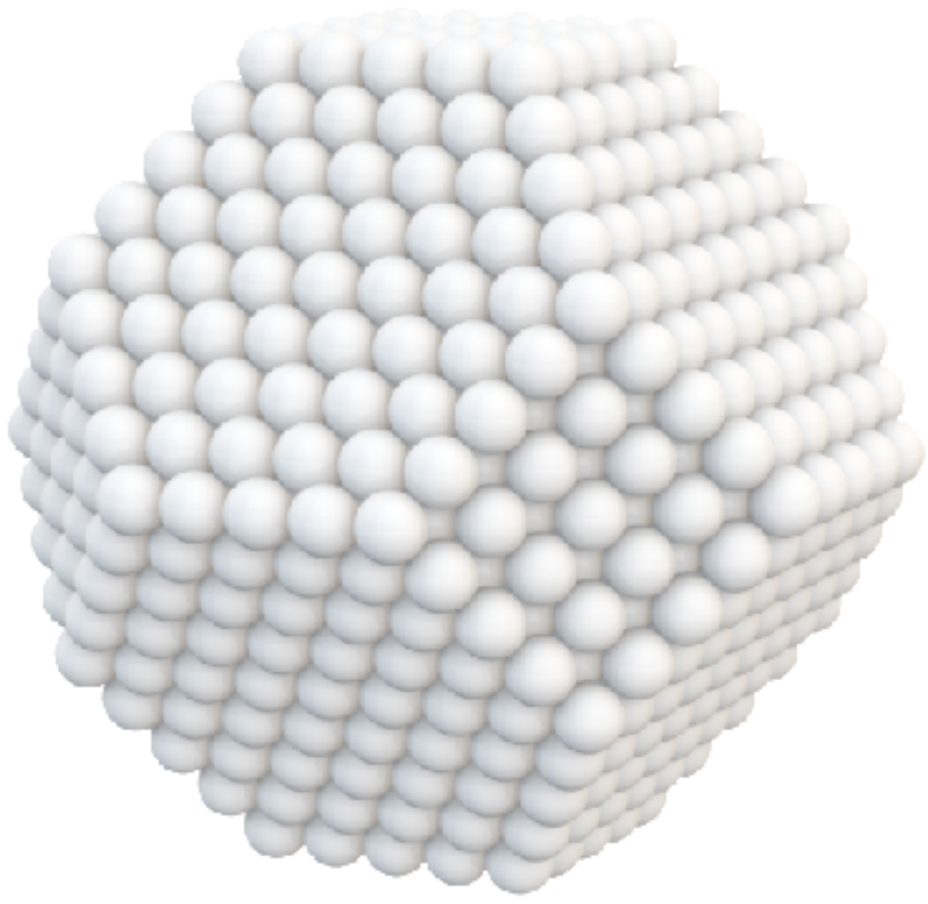


Demagnetization dynamics in Ni



Ultrafast thermally induced magnetic switching

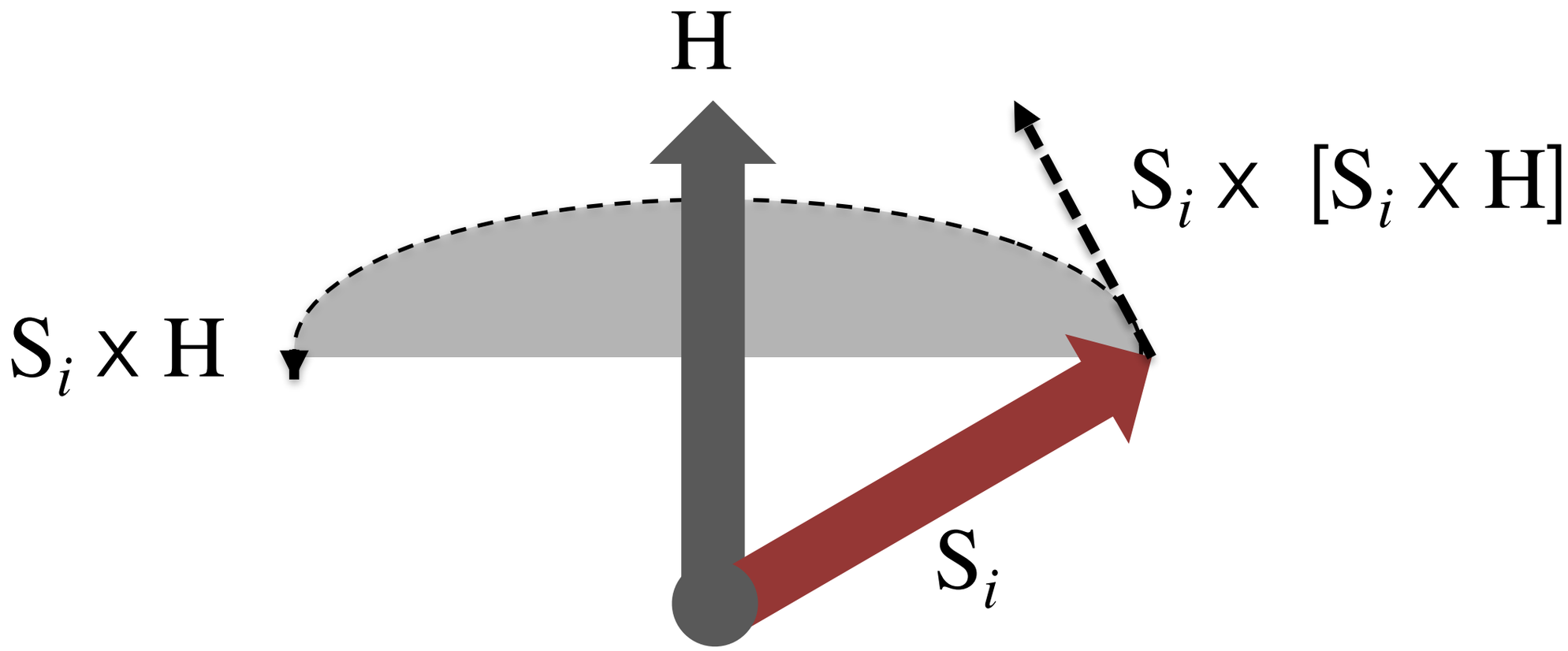
Spin Hamiltonian



$$\mathcal{H} = \mathcal{H}_{\mathrm{exc}} + \mathcal{H}_{\mathrm{ani}} + \mathcal{H}_{\mathrm{app}}$$

Describes the energetics of a complete system

Spin dynamics



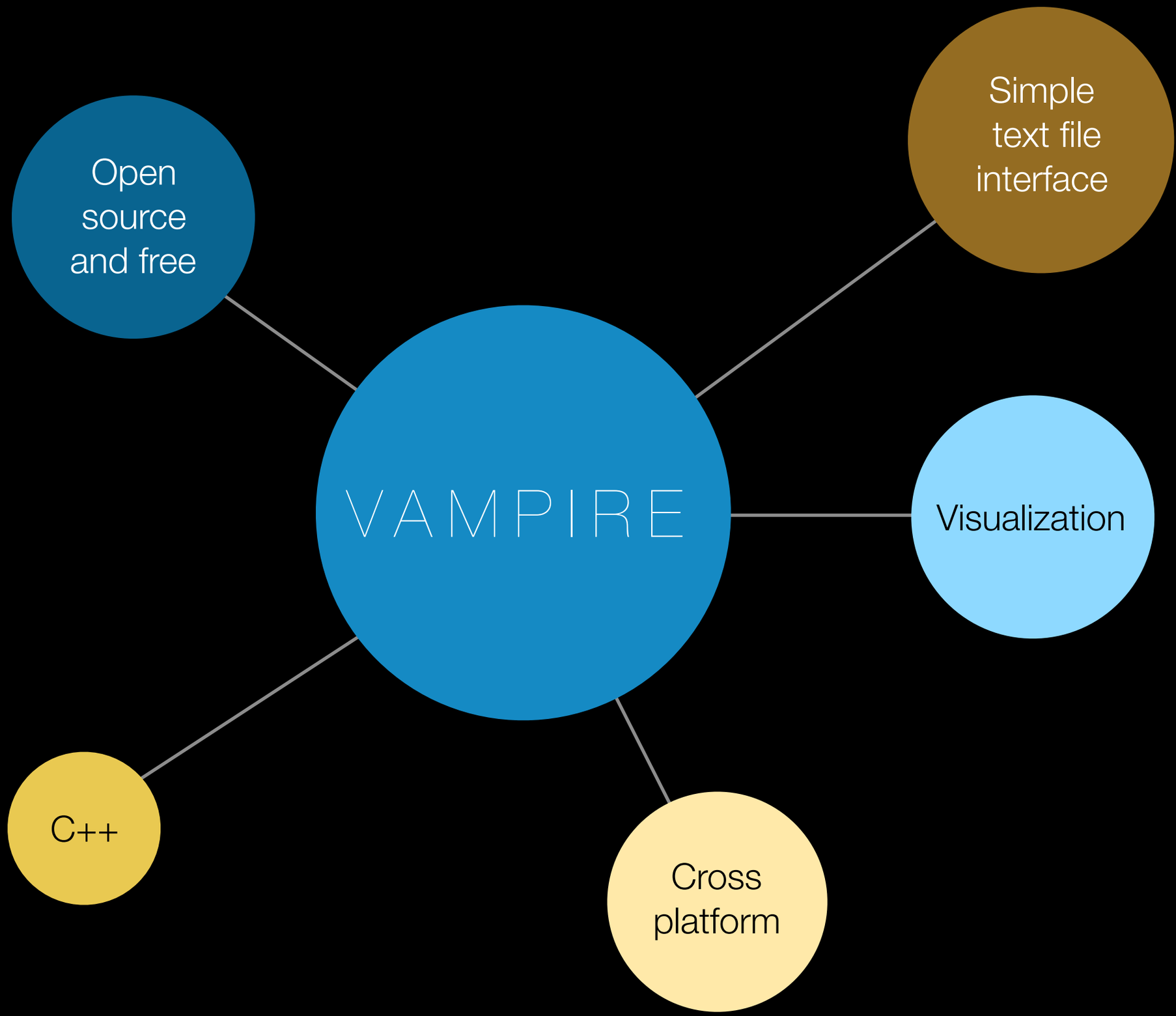
$$\frac{\partial \mathbf{S}_i}{\partial t} = -\frac{\gamma}{(1+\lambda^2)}[\mathbf{S}_i \times \mathbf{H}^i_{\text{eff}} + \lambda \mathbf{S}_i \times (\mathbf{S}_i \times \mathbf{H}^i_{\text{eff}})]$$

Stochastic Landau-Lifshitz-Gilbert

$$\mathbf{H}_{\mathrm{eff}}^{i} = -\frac{1}{\mu_{\mathrm{s}}}\frac{\partial \mathcal{H}}{\partial \mathbf{S}_i} + \mathbf{H}_{\mathrm{th}}^{i,\delta}.$$

$$\mathbf{H}_{\mathrm{th}}^{i} = \mathbf{\Gamma}(t)\sqrt{\frac{2\lambda k_{\mathrm{B}} T}{\gamma \mu_{\mathrm{s}} \Delta t}}$$

vampire.york.ac.uk



Tutorial resources

www-users.york.ac.uk/~rfle500/teaching/ultrafast-magnetism/

Setting up a simulation in Vampire

input file
(program control)

```
#-----------------------------------------
# Creation attributes:
#-----------------------------------------
create:crystal-structure=fcc
create:periodic-boundaries-x
create:periodic-boundaries-y
create:periodic-boundaries-z
#-----------------------------------------
# System Dimensions:
#-----------------------------------------
dimensions:unit-cell-size = 3.524 !A
dimensions:system-size-x = 4.0 !nm
dimensions:system-size-y = 4.0 !nm
dimensions:system-size-z = 4.0 !nm
…
```

material file
(material properties)

```
#-------------------------------------------------
# Number of Materials
#-------------------------------------------------
material:num-materials=1
#-------------------------------------------------
# Material 1 Nickel Generic
#-------------------------------------------------
material[1]:material-name=Ni
material[1]:damping-constant=0.01
material[1]:exchange-matrix[1]=2.757e-21
material[1]:atomic-spin-moment=0.606 !muB
material[1]:uniaxial-anisotropy-constant=0.0
material[1]:material-element=Ni
```

Spin Hamiltonian for Ni

$$\mathscr{H} = -\sum_{i<j} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j - \sum_i k_{\mathrm{u}} S_{i,z}^2$$

Ni.mat

```
#-------------------------------------------------
# Number of Materials
#-------------------------------------------------
material:num-materials=1
#-------------------------------------------------
# Material 1 Nickel Generic
#-------------------------------------------------
material[1]:material-name=Ni
material[1]:damping-constant=0.01
material[1]:exchange-matrix[1]=2.757e-21
material[1]:atomic-spin-moment=0.606 !muB
material[1]:uniaxial-anisotropy-constant=5.47e-26
material[1]:material-element=Ni
```

input

```
#-----------------------------------------
# Creation attributes:
#-----------------------------------------
create:crystal-structure=fcc
create:periodic-boundaries-x
create:periodic-boundaries-y
create:periodic-boundaries-z
#-----------------------------------------
# System Dimensions:
#-----------------------------------------
dimensions:unit-cell-size = 3.524 !A
dimensions:system-size-x = 4.0 !nm
dimensions:system-size-y = 4.0 !nm
dimensions:system-size-z = 4.0 !nm
#-----------------------------------------
# Material Files:
#-----------------------------------------
material:file=Ni.mat
#-----------------------------------------
# Simulation attributes:
#-----------------------------------------
sim:temperature=300
sim:minimum-temperature=0
sim:maximum-temperature=800
sim:temperature-increment=25
sim:time-steps-increment=1
sim:equilibration-time-steps=1000
sim:loop-time-steps=1000
```

```
#-----------------------------------------
# Program and integrator details
#-----------------------------------------
sim:program=curie-temperature
sim:integrator=monte-carlo
#-----------------------------------------
# Data output
#-----------------------------------------
output:real-time
output:temperature
output:magnetisation
output:magnetisation-length
output:mean-magnetisation-length
```

Getting and compiling vampire

- Need to get code from source repository

```
git clone https://github.com/richard-evans/vampire.git
```

- This creates a directory ‘vampire

```
cd vampire
```

- Checkout release version of the code

```
git checkout release
```

- Compile

```
make serial
```

Running vampire

- Each simulation should be in a separate directory

```
cd ..
mkdir Co
cd Co
```

- Copy in the input files and executable

```
cp ../vampire/Co.mat .
cp ../vampire/input .
cp ../vampire/vampire-serial .
```

- Now run the executable

```
./vampire-serial
```

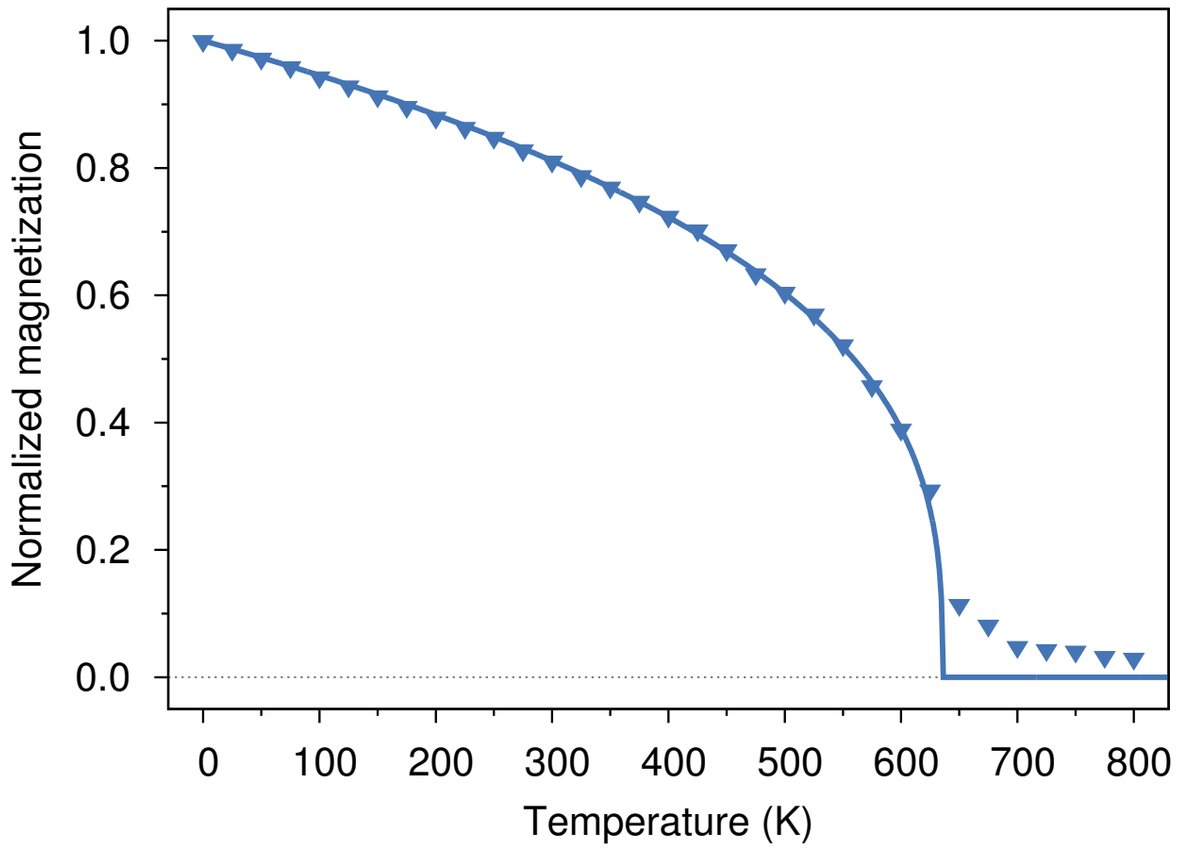
Curie temperature calculation

Calculate phase transition in Ni

Essential temperature dependent property of a magnetic material

$$\mathscr{H} = -\sum_{i<j} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j$$

$$J_{ij} = \frac{3k_B T_c}{\gamma z}$$



input

```
#------------------------------------------
# Creation attributes:
#------------------------------------------
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create:periodic-boundaries-x
create:periodic-boundaries-y
create:periodic-boundaries-z
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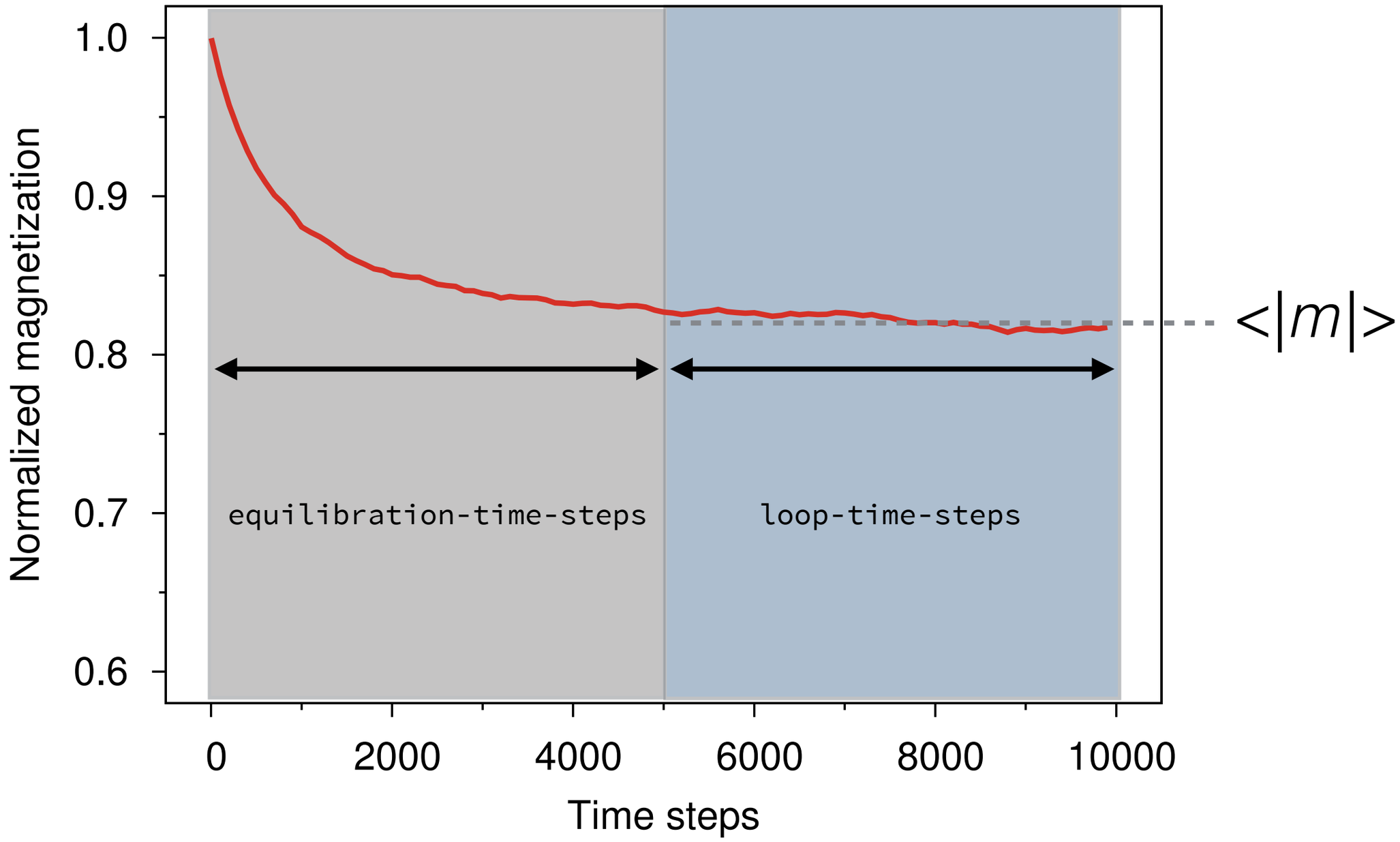
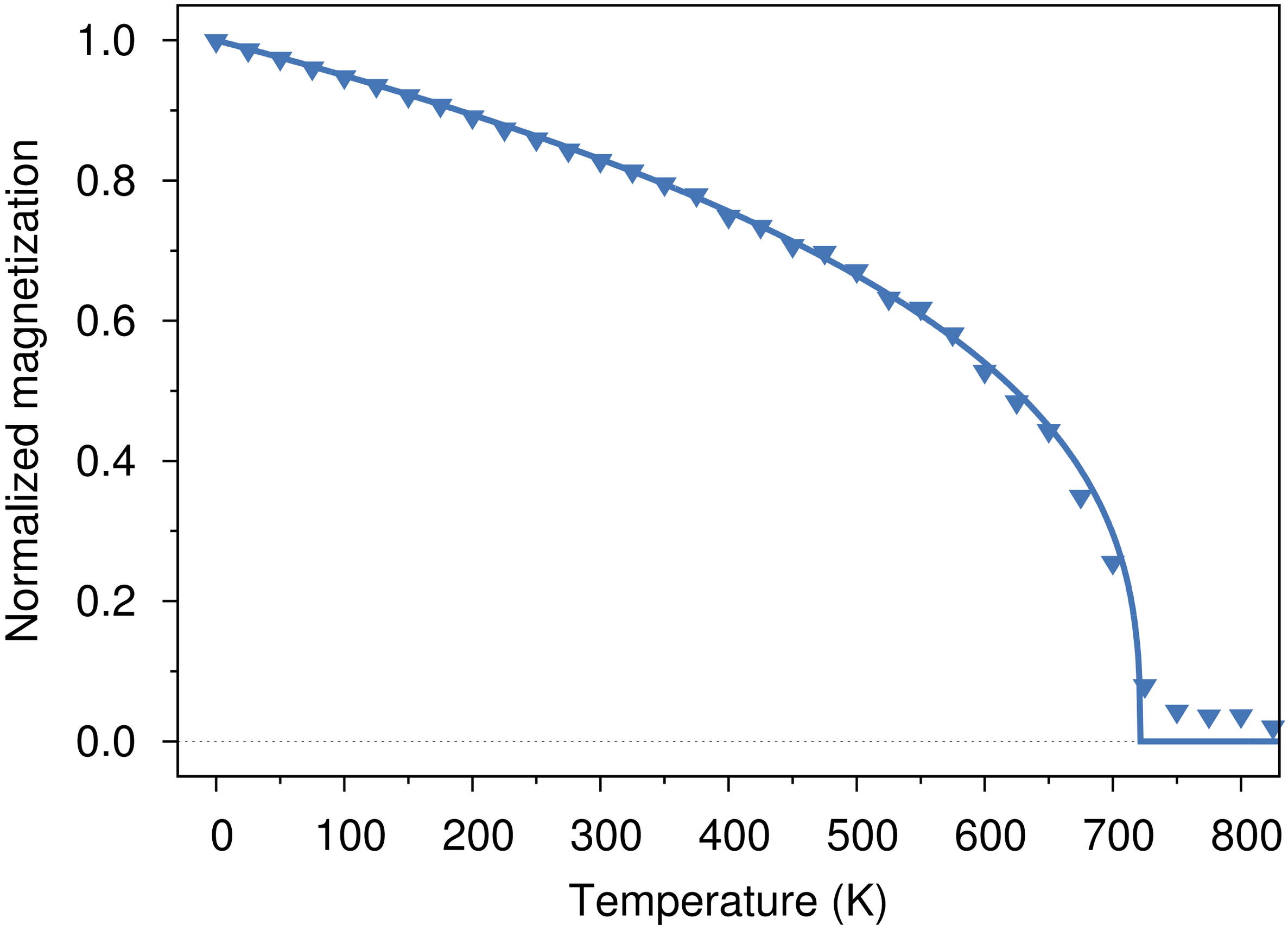
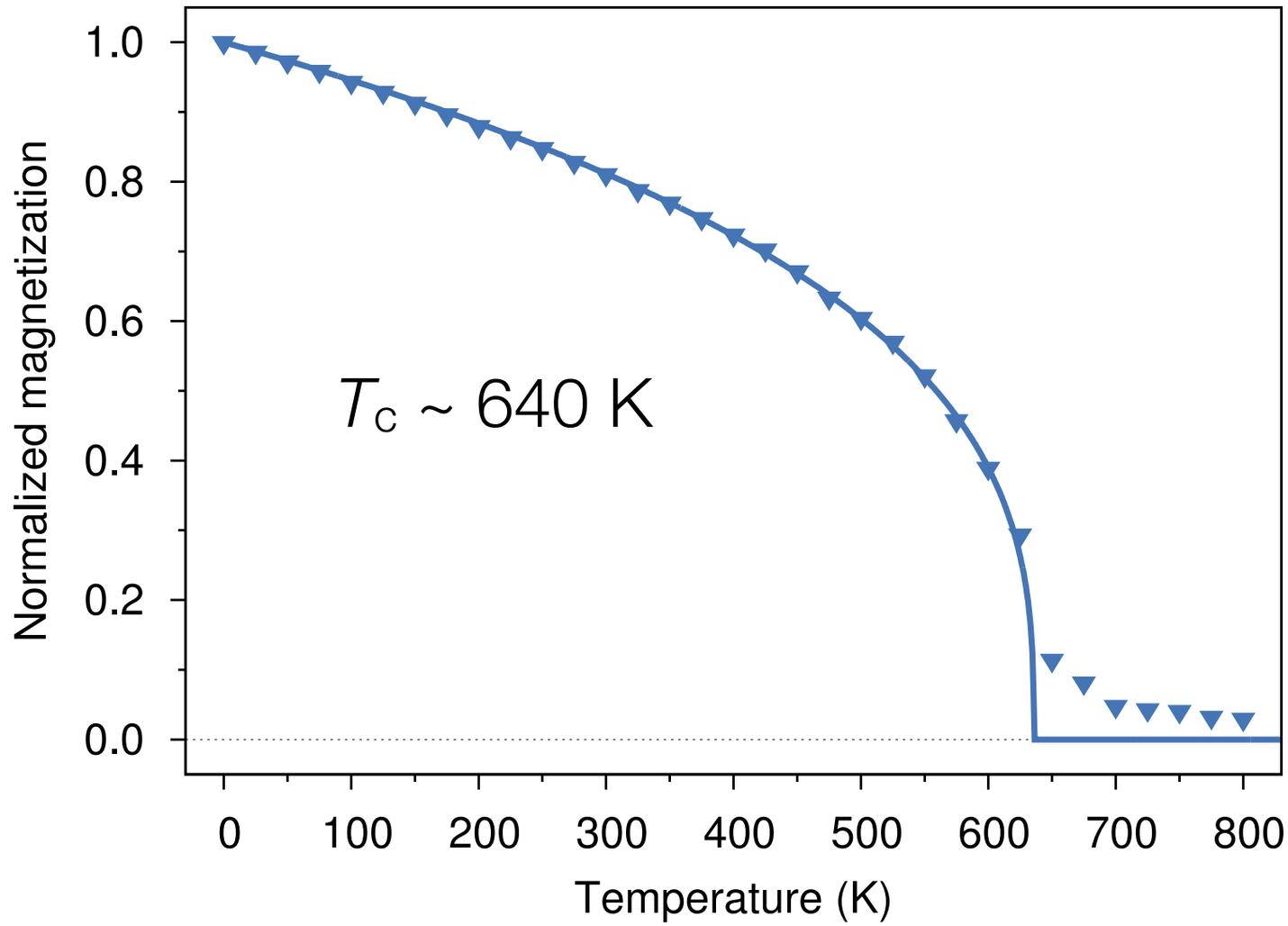
Curie temperature calculation




Normalized magnetization
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400
500
600
700
800
Temperature (K)

Curie temperature calculation



$$m(T) = \left[1 - \left(\frac{T}{T_c}\right)\right]^{\beta}$$

Gnuplot for plotting data and curve fitting

Start the gnuplot interactive plotting program on the command line:

```
gnuplot
```

```
p “output” u 2:7 w lp
```

plot

file name

using columns

2 and 7

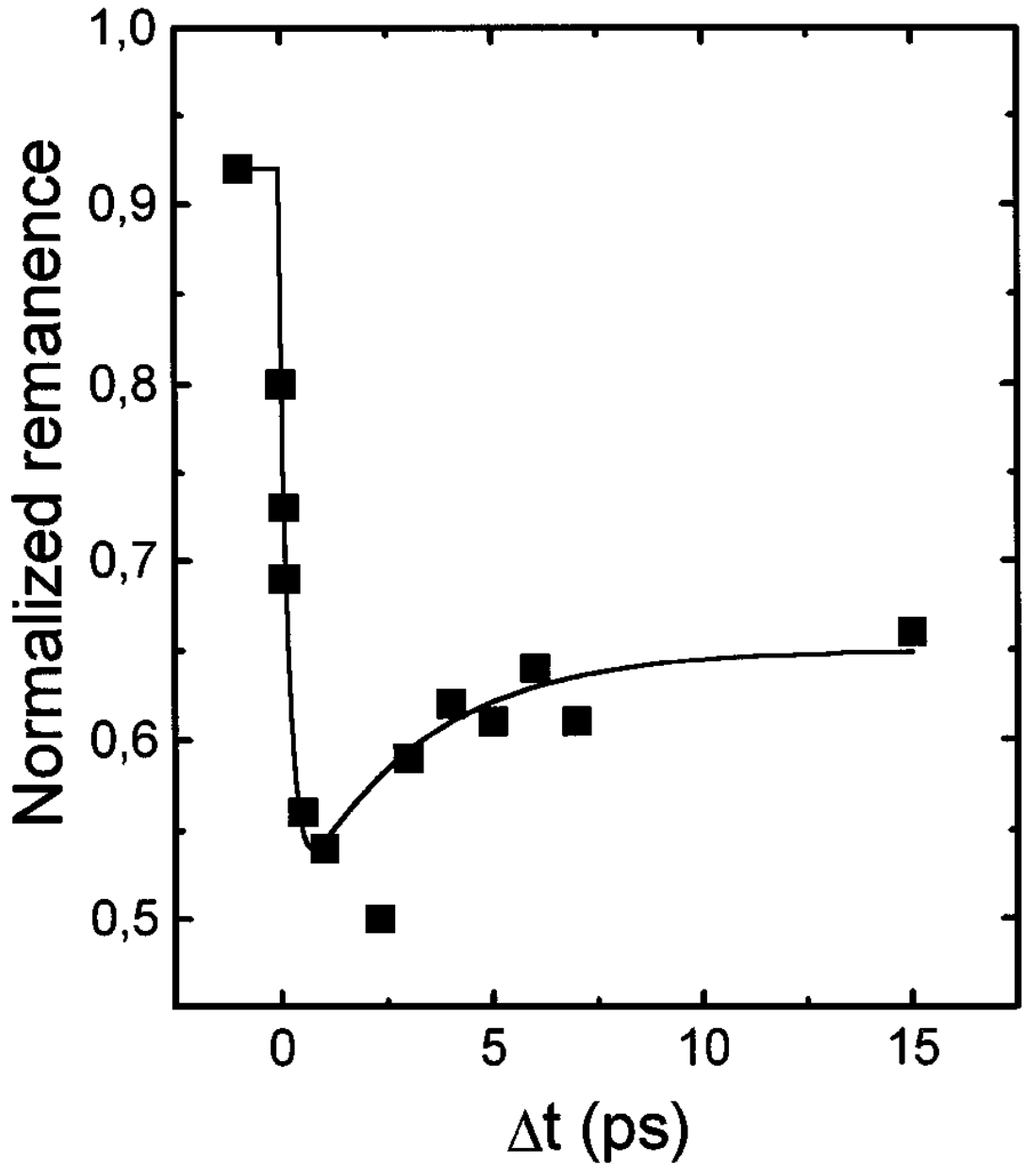
with

lines and points

Gnuplot for plotting data and curve fitting

```
m(x) = (1-x/Tc)**beta
Tc = 500.0
beta = 0.4
fit [0:Tc] m(x) “output” u 2:7 via Tc, beta
p “output” u 2:7 w p ti “data”, m(x) w l
```

Ultrafast demagnetization in Ni

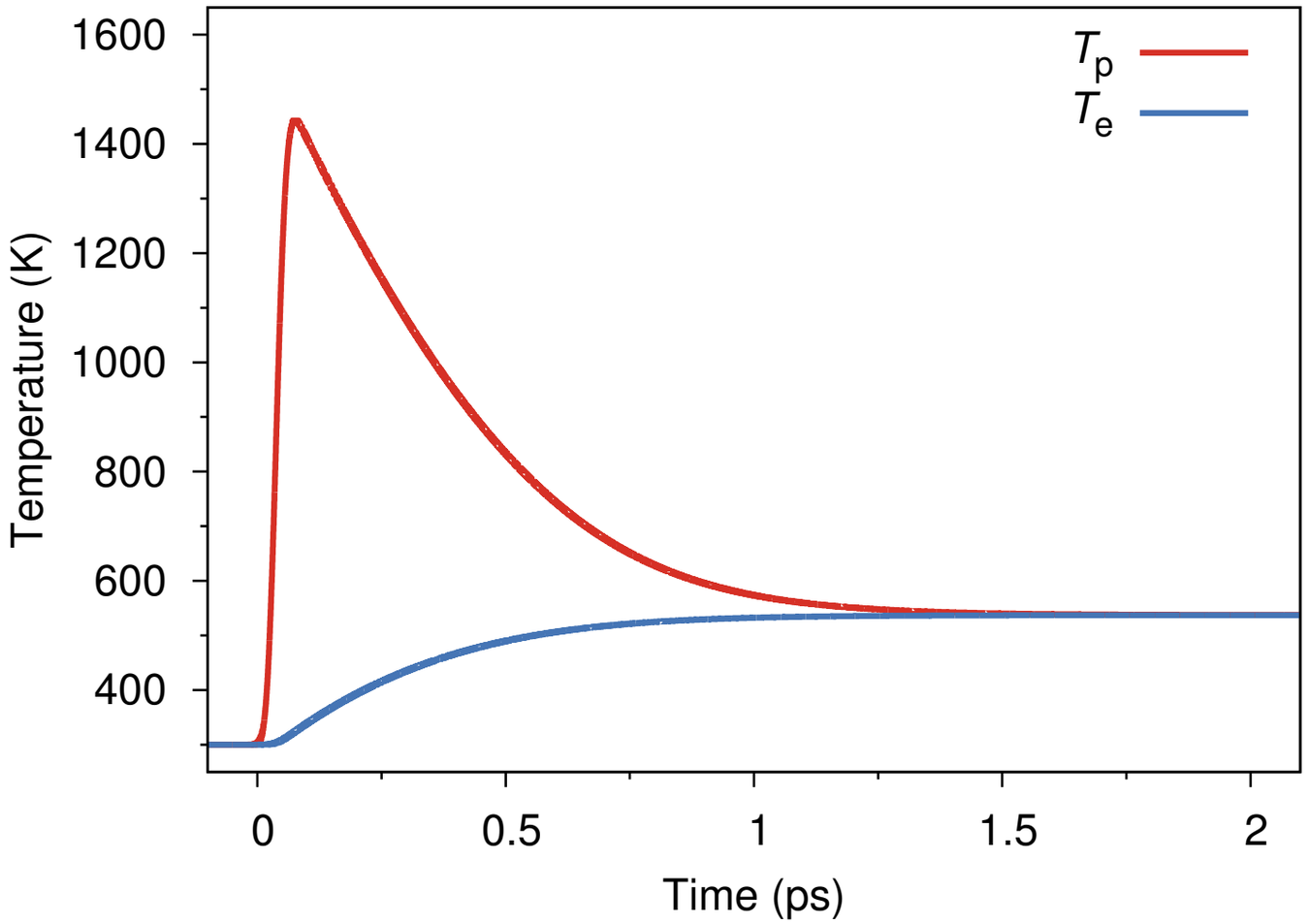


E. Beaurepaire et al, Phys. Rev. Lett. **76** 4250 (1996)

Two temperature model

$$C_e \frac{\partial T_e}{\partial t} = -G(T_e - T_l) + S(t)$$

$$C_l \frac{\partial T_l}{\partial t} = -G(T_l - T_e)$$



Free electron approximation

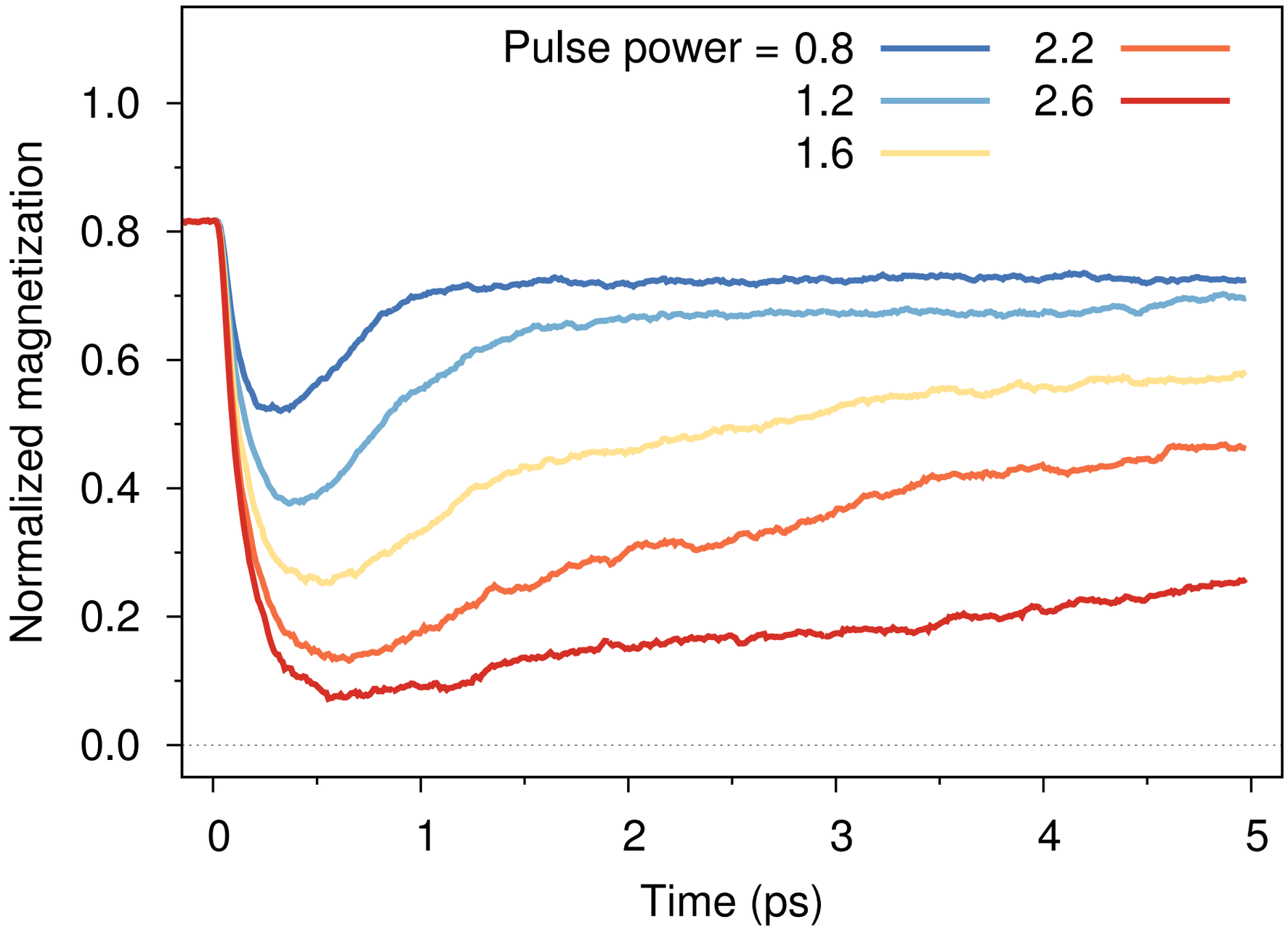
$C_e \propto T_e$

Input file for simulated laser pulse

```
sim:equilibration-time-steps=10000
sim:total-time-steps=50000
sim:laser-pulse-power=5.0
sim:laser-pulse-temporal-profile=two-temperature
sim:program=laser-pulse
sim:integrator=llg-heun
sim:time-step=1.0e-16

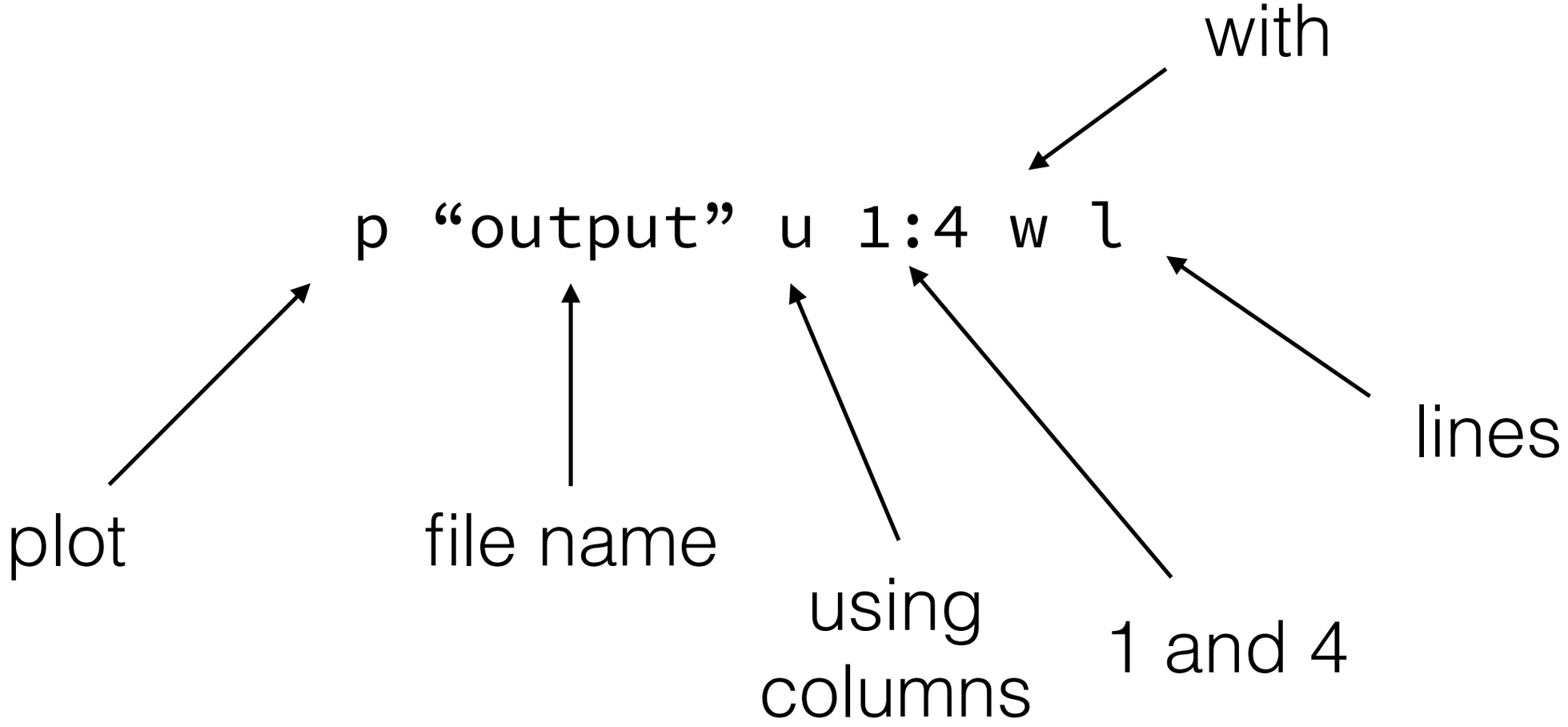
output:real-time
output:electron-temperature
output:phonon-temperature
output:magnetisation-length
```

Effect of pulse power in Ni

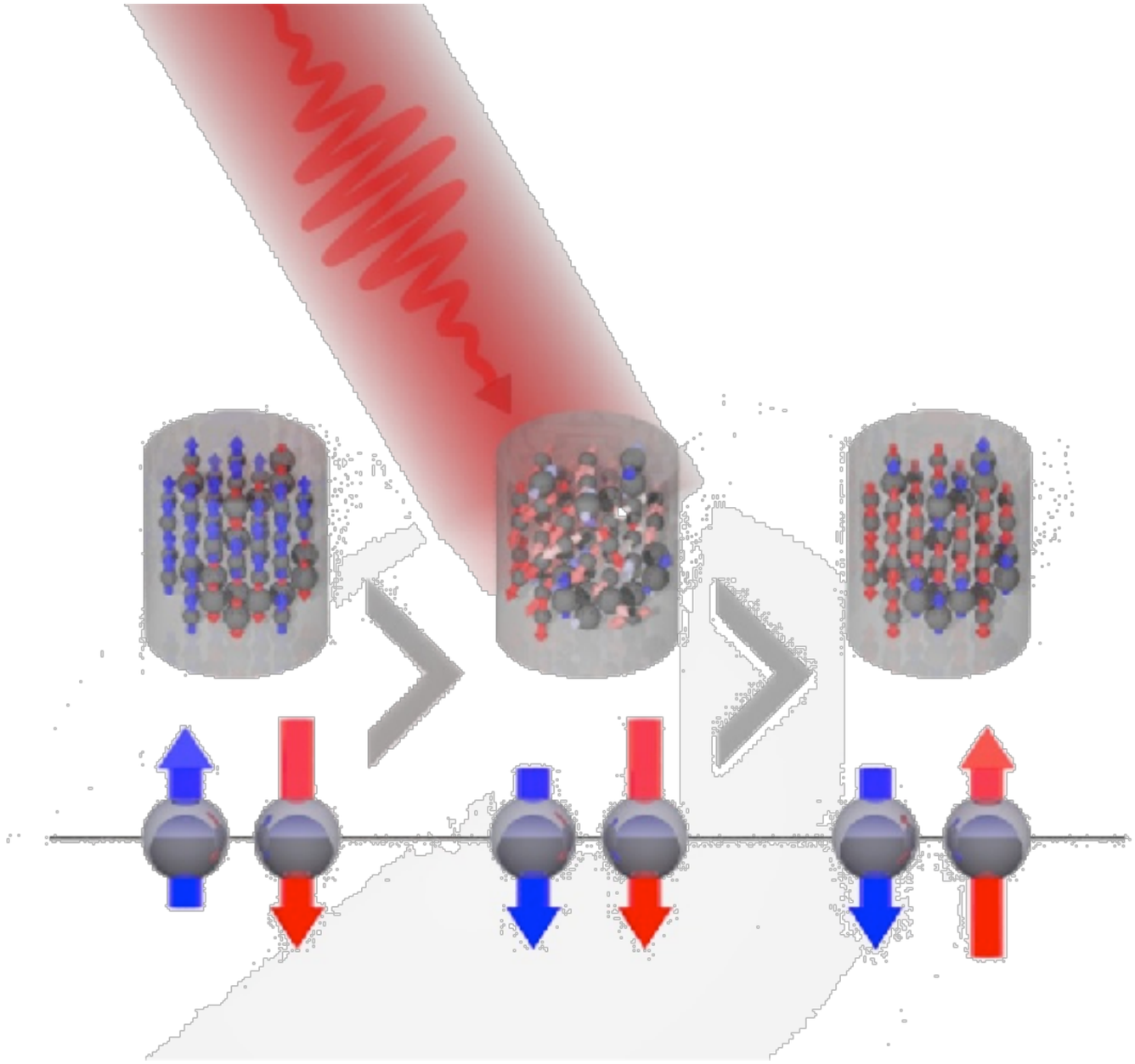


Stronger laser pulses show more demagnetization and slower recovery

Plot |m| vs time with gnuplot

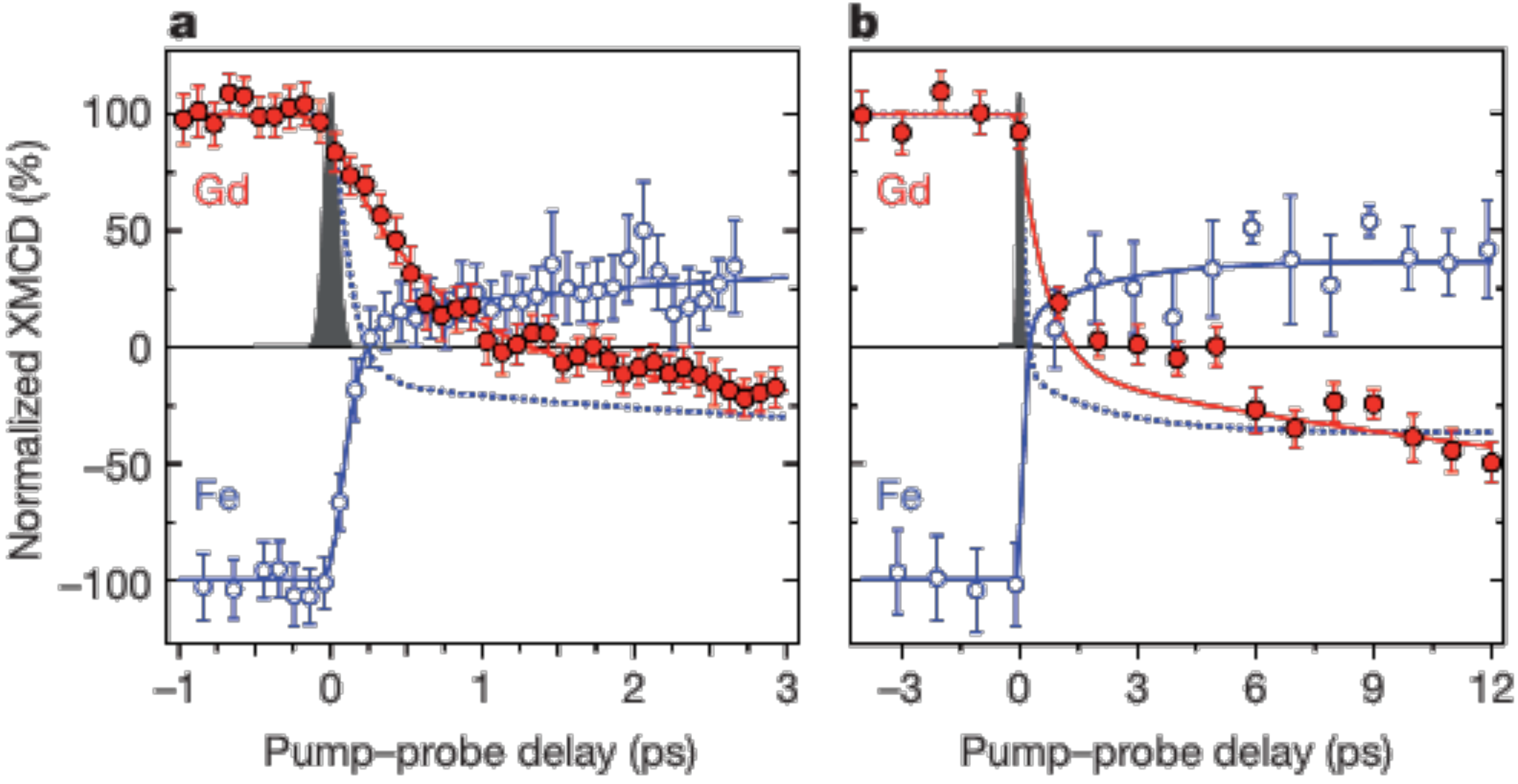


Thermally induced magnetic switching



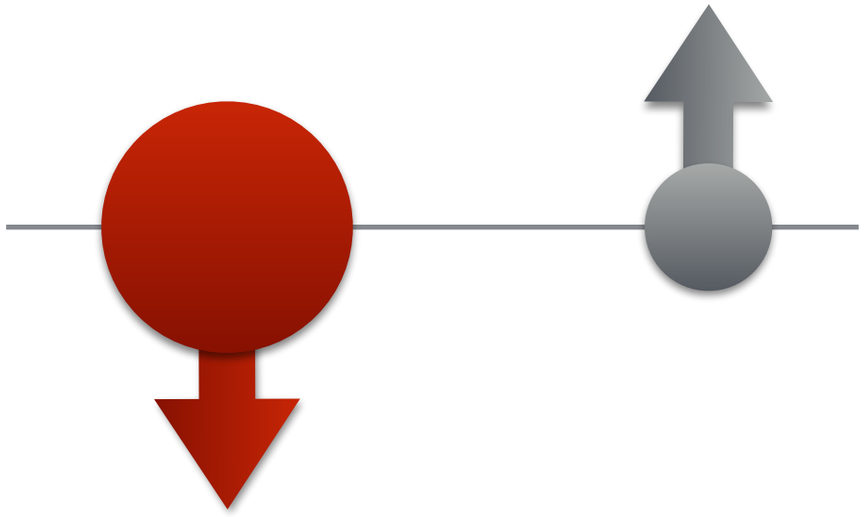
T. Ostler *et al*, Nat. Commun.(2012)

Sublattice magnetization dynamics

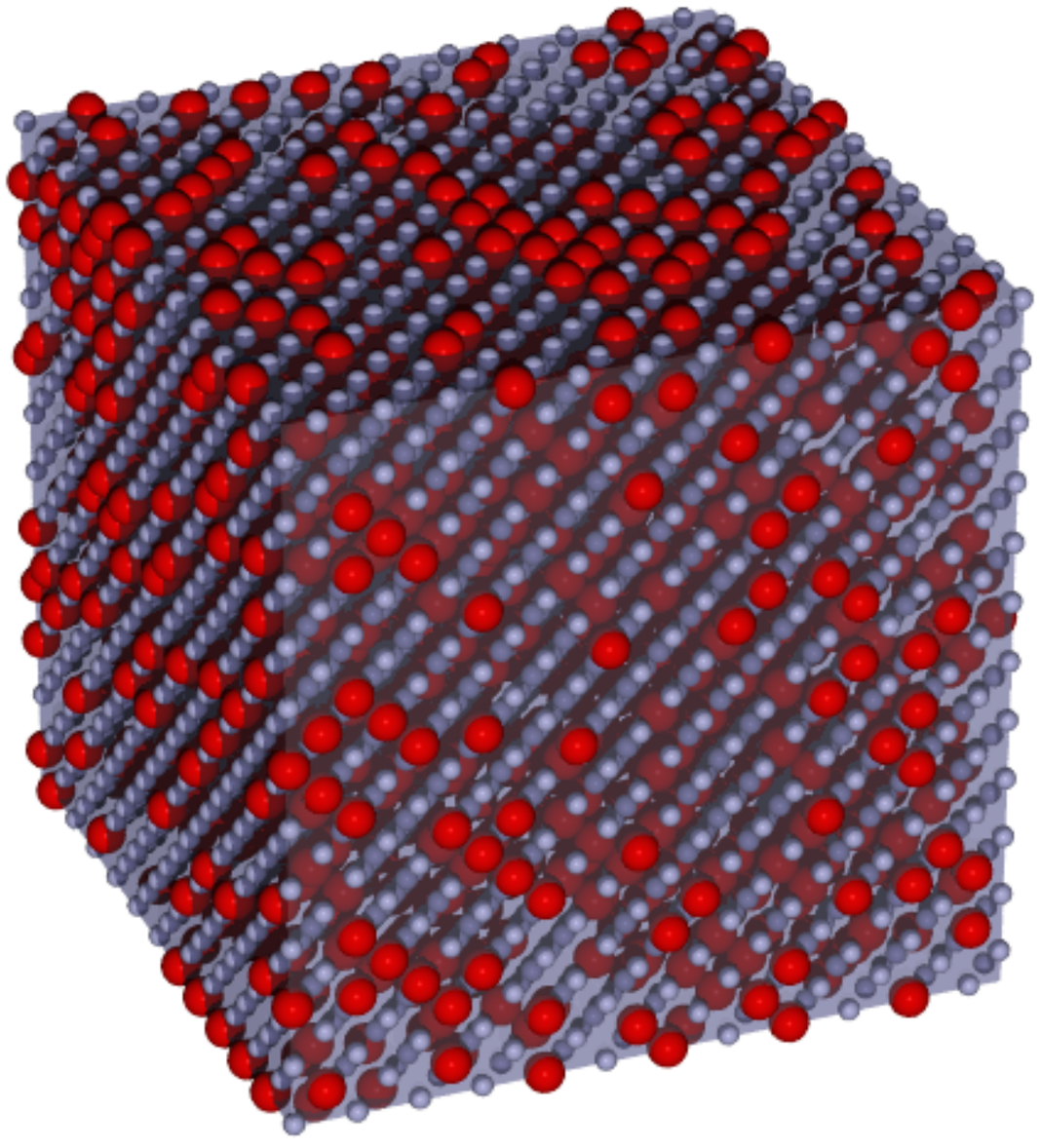


I. Radu *et al*, Nature (2011)

GdFe ferrimagnet



Gd Fe



GdFe.mat

```
#-----------------------------------------------------
# Number of Materials
#-----------------------------------------------------
material:num-materials=2
#-----------------------------------------------------
# Material 1 Fe (TM)
#-----------------------------------------------------
material[1]:material-name=TM
material[1]:damping-constant=0.02
material[1]:exchange-matrix[1]=2.835e-21
material[1]:exchange-matrix[2]=-1.09e-21
material[1]:atomic-spin-moment=1.92 !muB
material[1]:uniaxial-anisotropy-constant=8.07246e-24
material[1]:material-element=Fe
material[1]:minimum-height=0.0
material[1]:maximum-height=1.0
material[1]:alloy-host
material[1]:alloy-fraction[2]=0.25
material[1]:initial-spin-direction=0,0,1
#-----------------------------------------------------
# Material 2 Gd (RE)
#-----------------------------------------------------
material[2]:material-name=RE
material[2]:damping-constant=0.02
material[2]:exchange-matrix[1]=-1.09e-21
material[2]:exchange-matrix[2]=1.26e-21
material[2]:atomic-spin-moment=7.63 !muB
material[2]:uniaxial-anisotropy-constant=8.07246e-24
material[2]:material-element=Ag
material[2]:minimum-height=0.0
material[2]:maximum-height=0.0
material[2]:initial-spin-direction=0,0,-1
```

input file

```
sim:equilibration-time-steps=20000
sim:total-time-steps=50000
sim:temperature = 300.0
sim:equilibration-temperature = 300.0
sim:temperature-increment=25
sim:time-steps-increment=10
sim:preconditioning-steps = 200
sim:equilibration-time-steps=1000
sim:total-time-steps=50000

sim:two-temperature-electron-heat-capacity=2.25e2
sim:two-temperature-phonon-heat-capacity=3.1e6
sim:two-temperature-electron-phonon-coupling=2.5e17

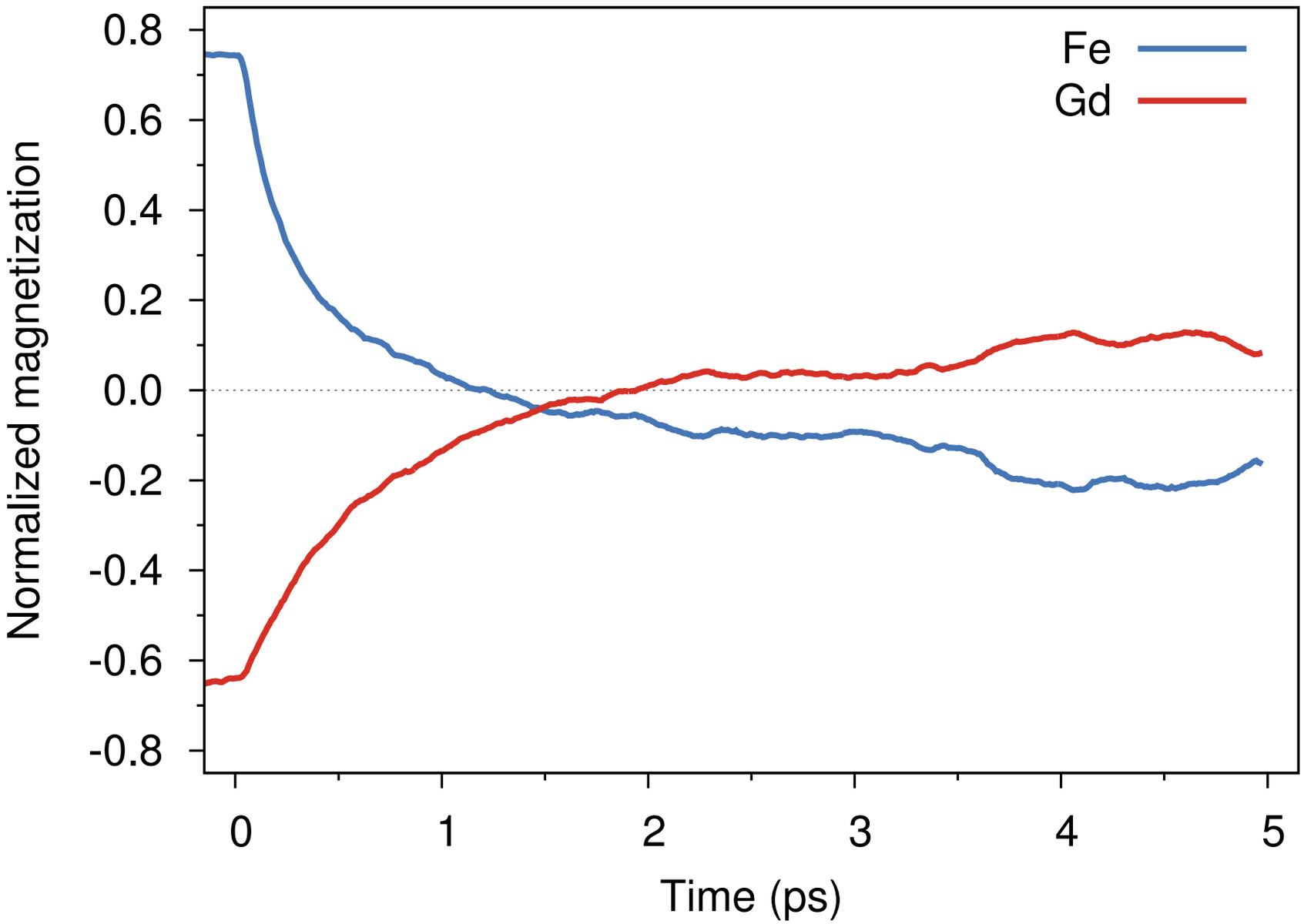
sim:laser-pulse-temporal-profile = two-temperature
sim:laser-pulse-time = 50 !fs
sim:laser-pulse-power = 16.70
```

input file (pt2)

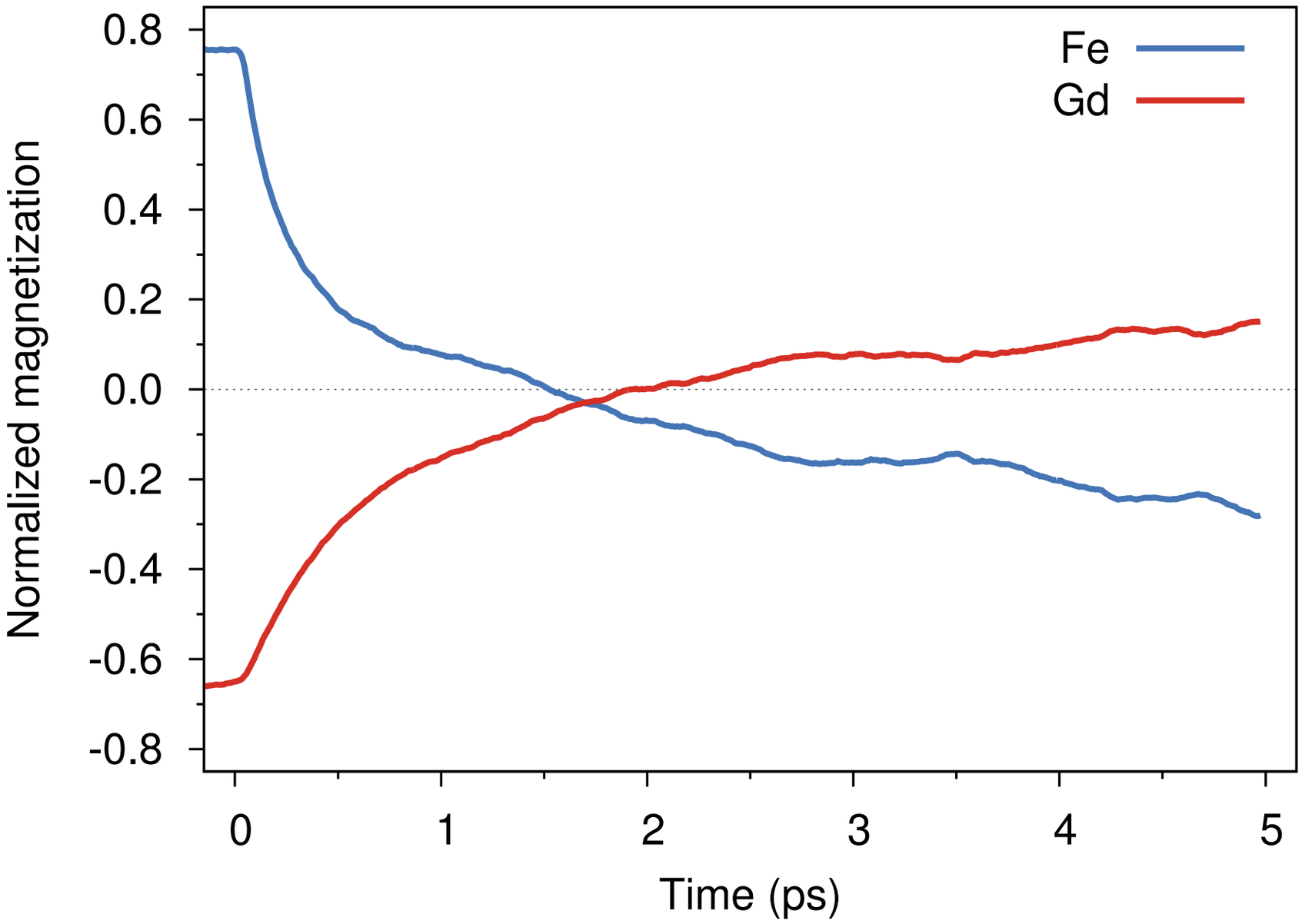
```
sim:integrator=llg-heun
sim:time-step=1.0e-16

output:real-time
output:electron-temperature
output:phonon-temperature
output:material-magnetisation
```

Calculated magnetization dynamics



Dynamics for 7nm^3 GdFe



Summary

Simulated Curie temperature and demagnetization dynamics in Ni

Simulated TIMS in GdFe

Many different types of simulations possible (materials, alloys, multilayers…)

VAMPIRE

vampire.york.ac.uk