Introduction to VAMPIRE

A practical course

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THE UNIVERSITY of York

CCP MAGNETISM

EPSRC

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Overview

9:00 - 9:30	Introduction to linux and editor basics
9:30 - 10:30	Getting started with VAMPIRE
10:30 - 10:50	Coffee break
10:50 - 12:00	Ultrafast magnetisation dynamics
12:00 - 13:00	Lunch
13:00 - 13:45	System generation
13:45 - 14:30	Hysteresis properties
14:30 - 15:00	Vampire Q&A and future development requests
15:00	Close

Tutorial resources

www-users.york.ac.uk/~rfle500/teaching/vampire-tutorial/

Introduction to linux and the command line

What is linux?

Free operating system with similar aims to Windows/ Mac

Clone of UNIX operating system, with wide range of command line utilities and tools

Simplistic GUI with a range of free software

What is the command line?

Simple text interface to a range of built-in tools

A bit like computers from the 80’s

But - very powerful and precise. Common programming tasks are much easier in a UNIX-like system

Still used extensively on supercomputers for this reason!

How does the command line work?

Typing a ‘command’ and return executes that command

command <options>

Command name

Options or ‘arguments’

Examples for directory management

ls	list files and folders in current directory
cd name	change directory into existing subfolder called *name*
mkdir name	makes a new folder called *name*
cd ..	change into directory above
rm name	remove file called *name* **permanently**
rm -r name	remove file/folder called *name* **permanently**

Other useful commands

gedit name	Open file called name in gedit GUI editor
emacs -nw *name*	Open file called *name in emacs editor*
	(Ctrl+X+S to save, Ctrl+X+C to quit)
gnuplot	Simple plotting program
rasmol -xyz file.xyz	Open file.xyz with atomic structure viewer
./vampire	Run a local executable file called vampire
[tab][tab]	Autocomplete command (tab key)

Getting started with VAMPIRE

Create a separate directory for all your vampire related stuff

```
cd ~

mkdir vampire

cd vampire
```

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
```

Running Vampire

```
rfle500@MacPro:~$ vampire
                                                 _
                                                (_)
          __   _____ _ _ __ ___  _ __  _ _ __ ___
          \ \ / / _` | '_ ` _ \| '_ \| | '__/ _ \
           \ V / (_| | | | | | | |_) | | | |  __/
            \_/ \__,_|_| |_| |_| .__/|_|_|  \___|
                               | |
                               |_|

                  Version 3.0.3 Aug  4 2014 21:00:13

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                Compiled with:  GNU C++ Compiler
                Compiler Flags:

================================================================================
Mon Aug  4 21:56:21 2014
================================================================================
Initialising system variables
Creating system
```

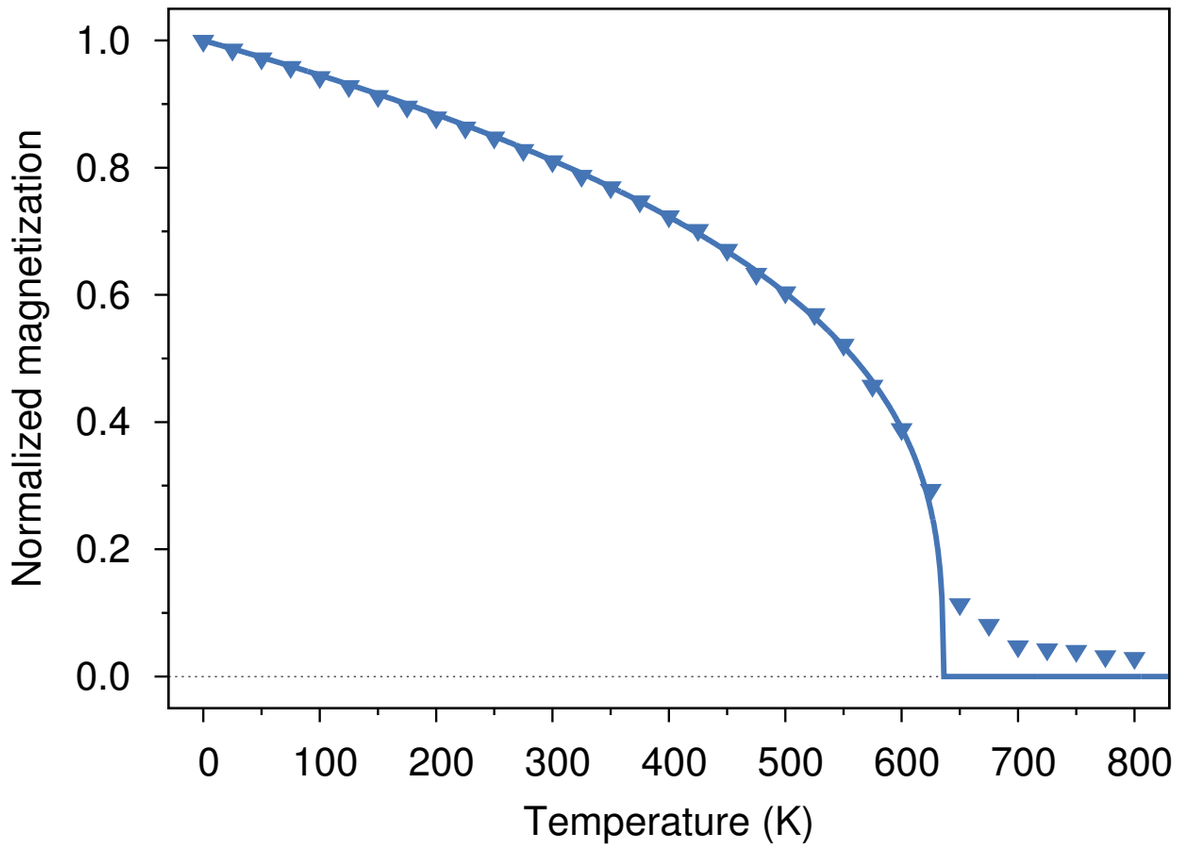
Curie temperature calculation

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:
#-----------------------------------------
create:crystal-structure=fcc
create:periodic-boundaries-x
create:periodic-boundaries-y
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# System Dimensions:
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```
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output:real-time
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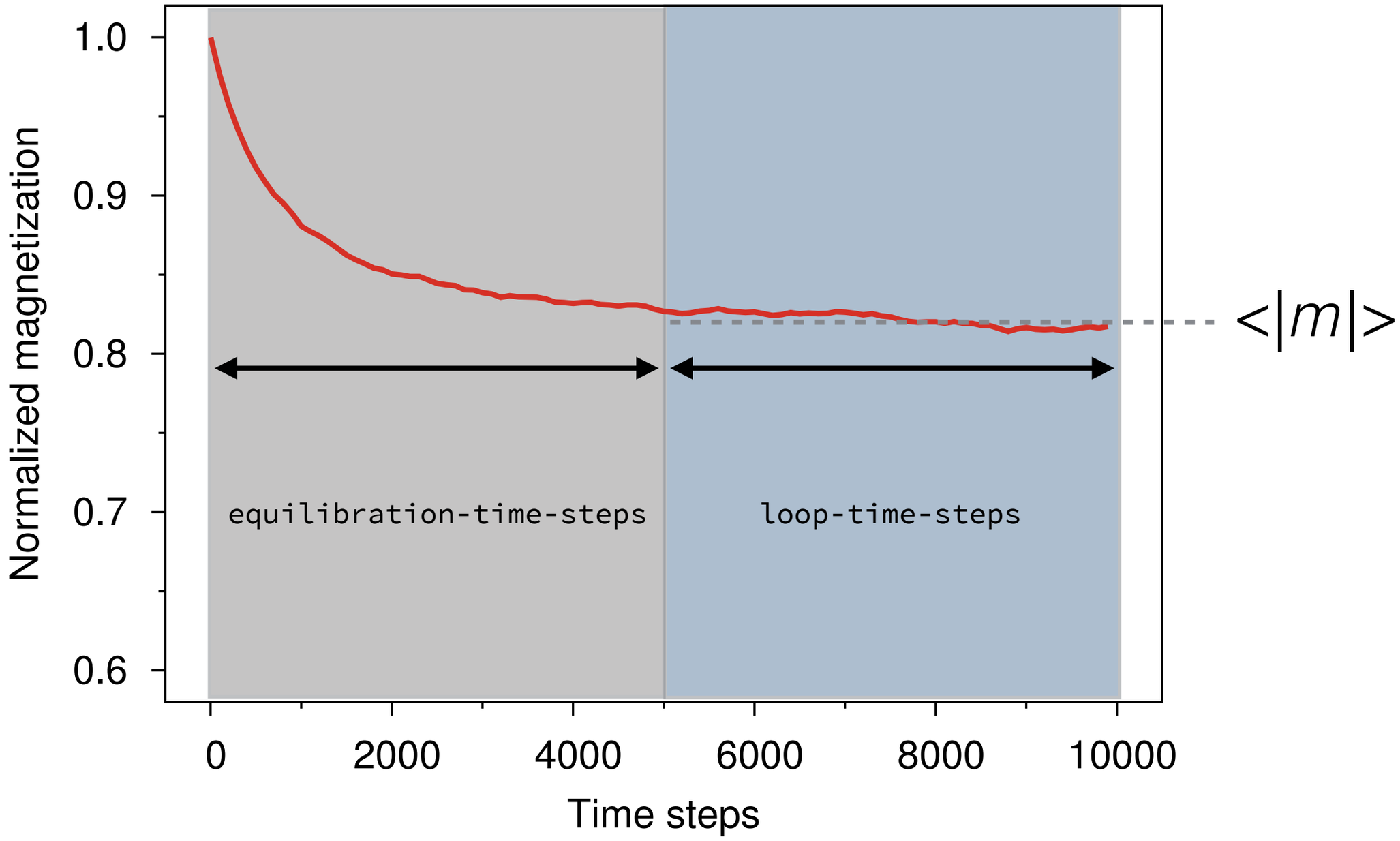
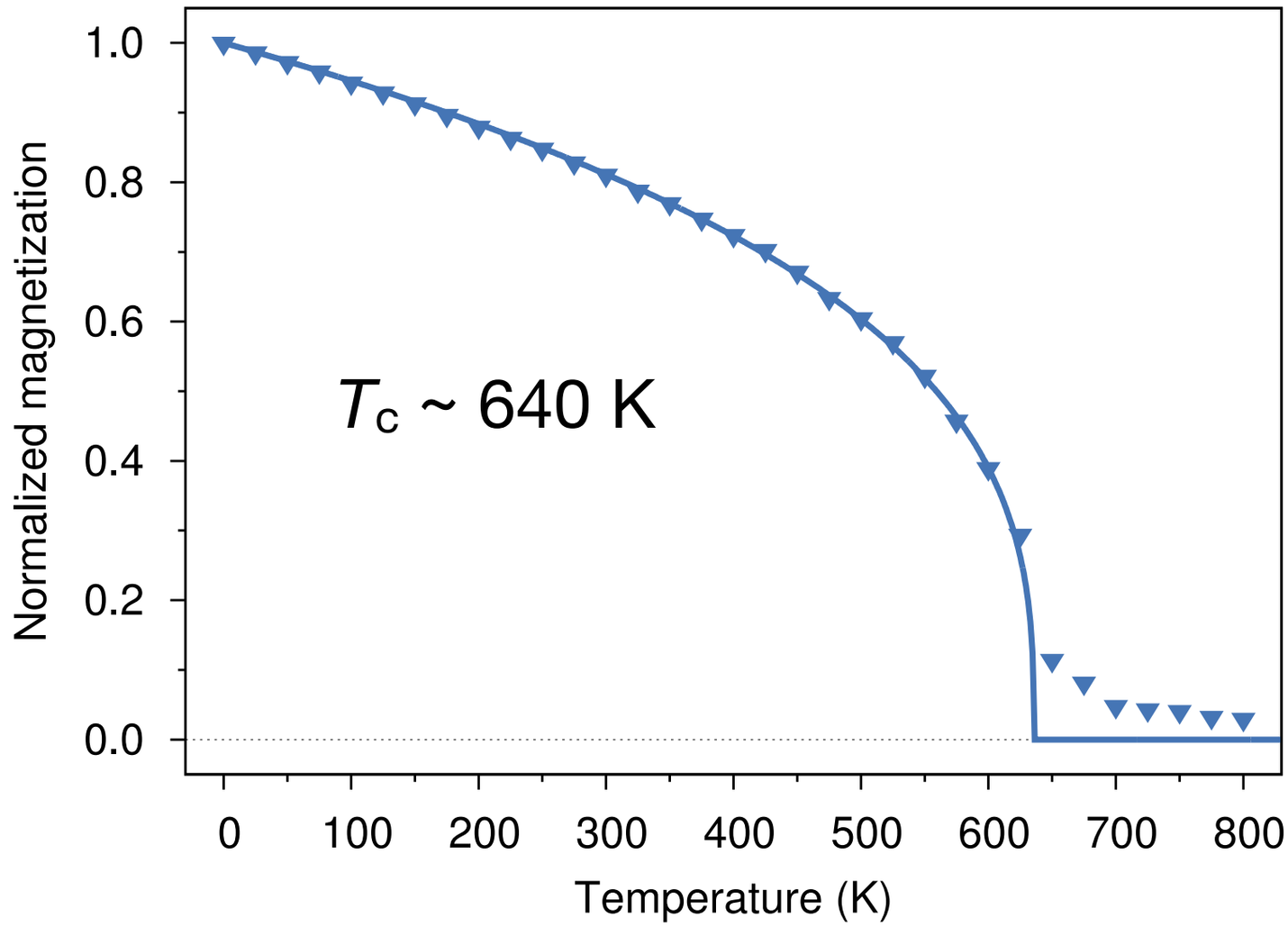
output:magnetisation
output:magnetisation-length
output:mean-magnetisation-length
```

Curie temperature calculation

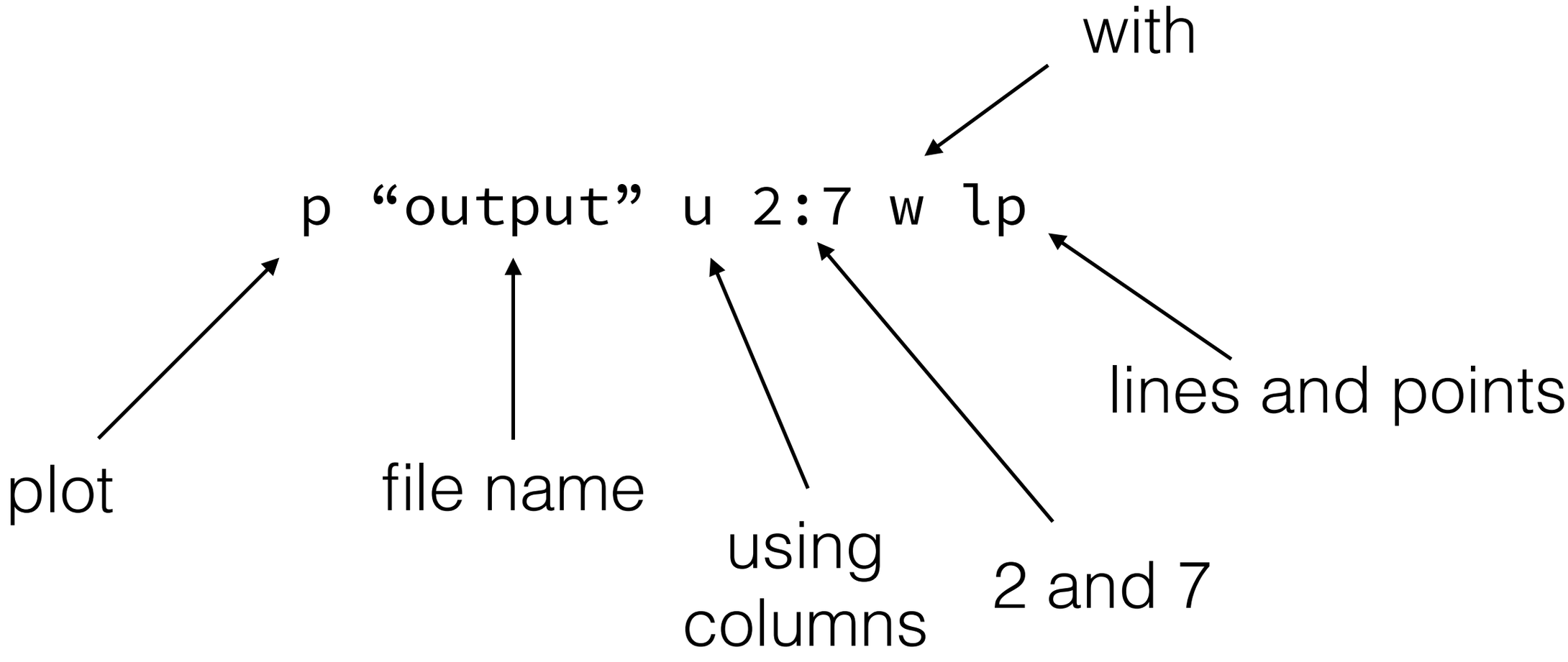


Curie temperature calculation



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

Gnuplot for plotting data and curve fitting

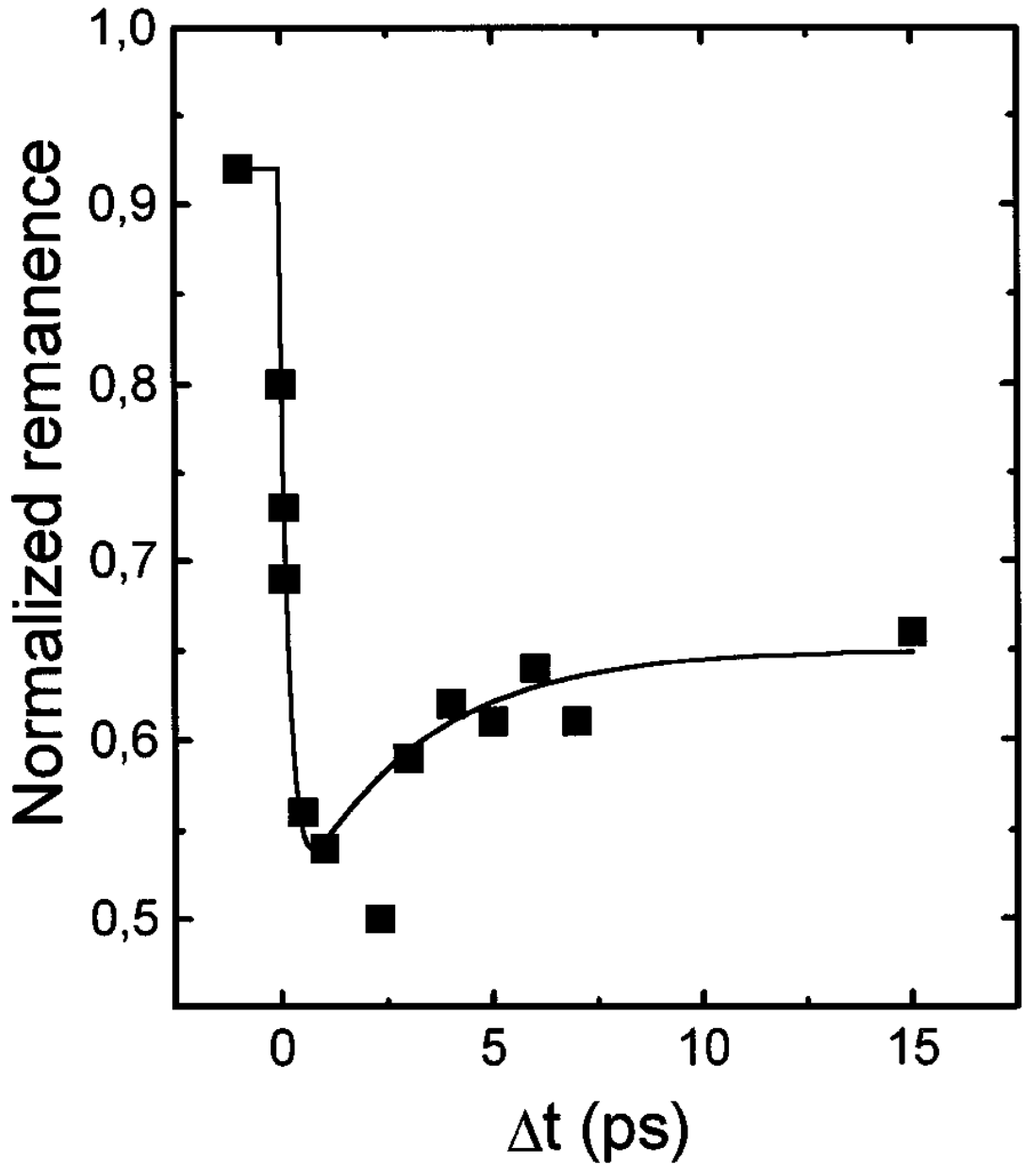


Gnuplot for plotting data and curve fitting

```
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 magnetisation dynamics

Ultrafast demagnetization in Ni



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

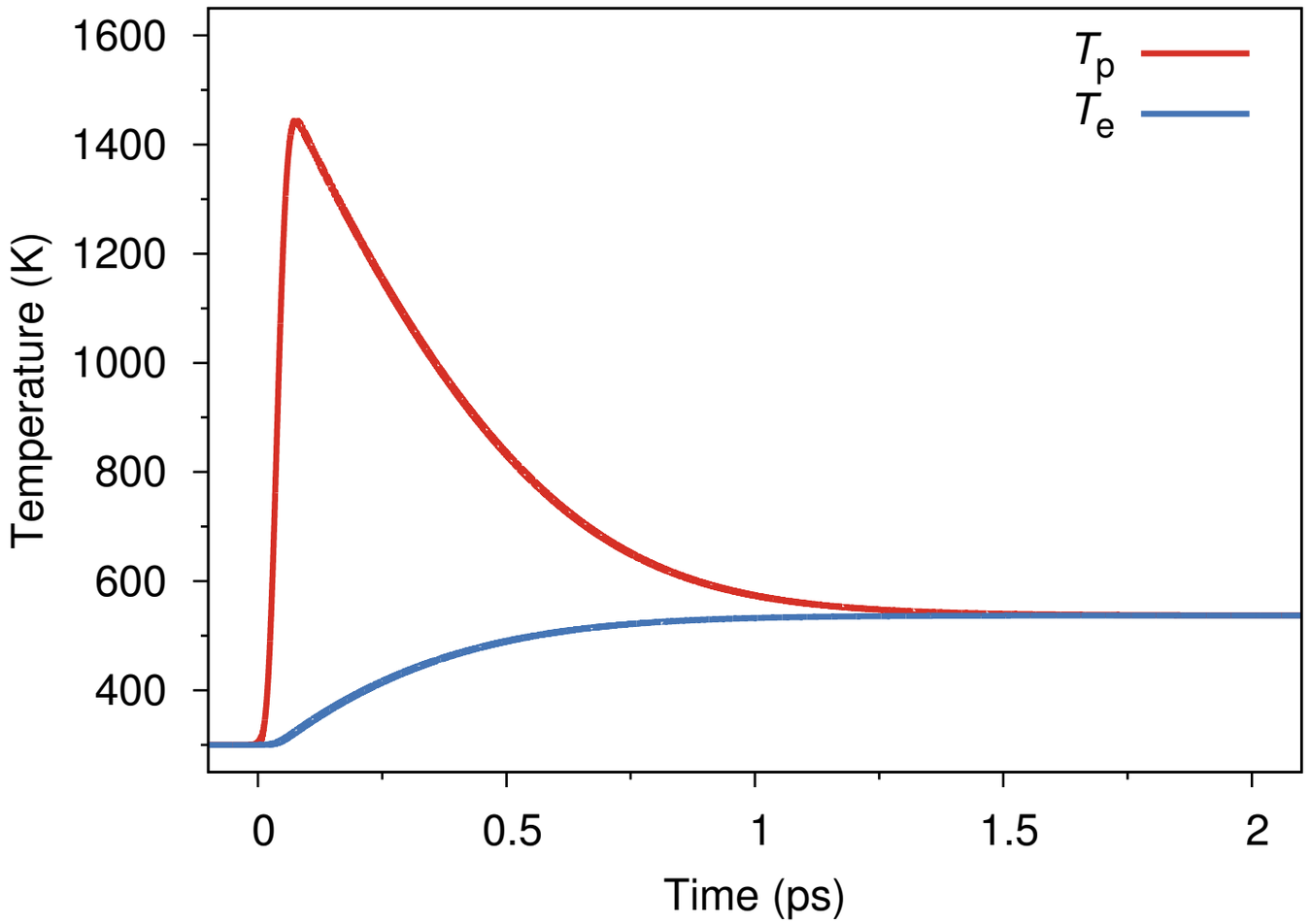
“If you put two condensed matter physicists in a room, you get two theories of ultrafast demagnetisation, unless one of them is a magnetician, in which case you get three”

(Winston Churchill)

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

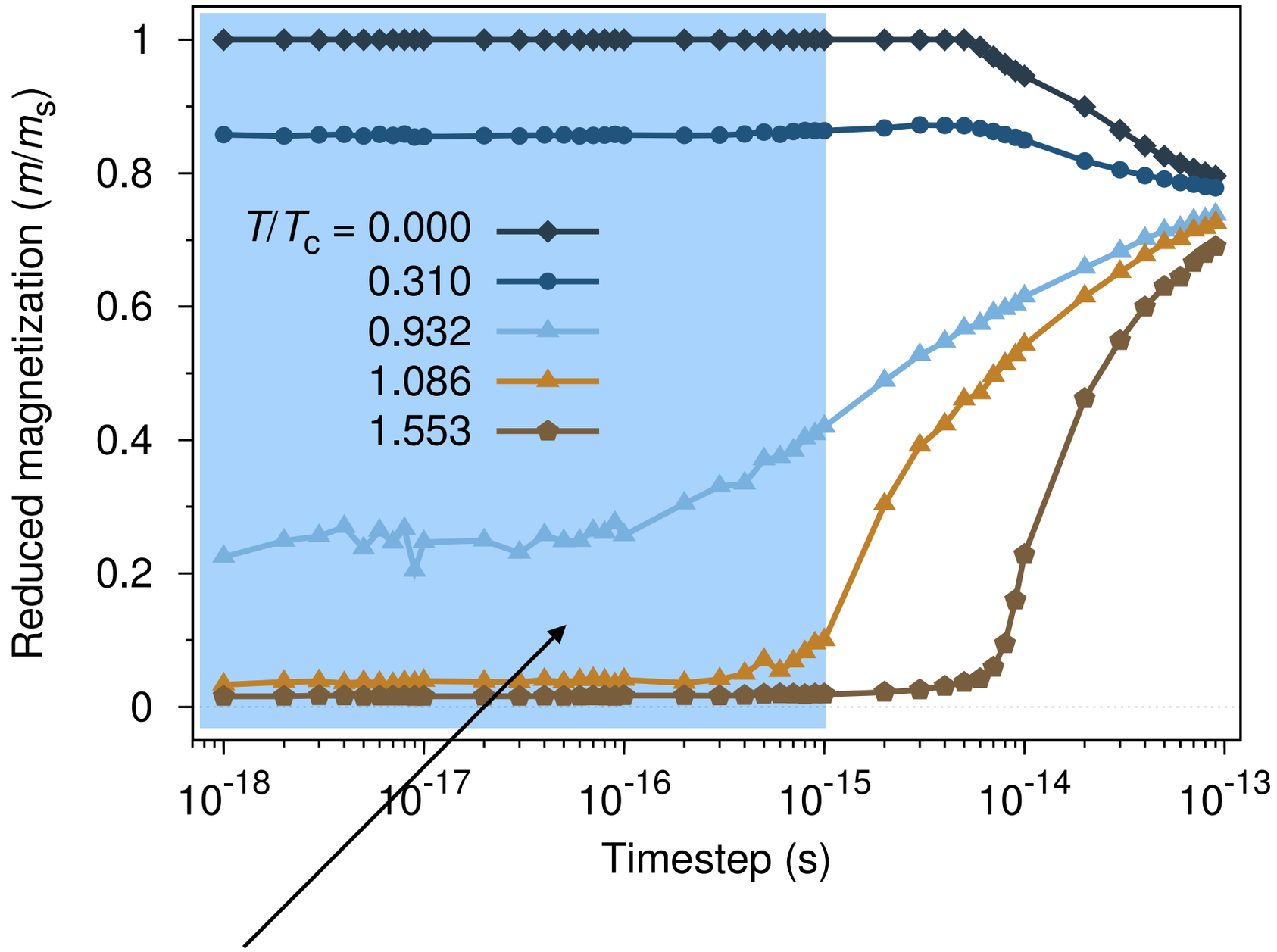
$C_e \propto T_e$

Input file for simulated laser pulse

```
sim:equilibration-time-steps=10000
sim:total-time-steps=50000
sim:laser-pulse-power=2.2e22
sim:laser-pulse-temporal-profile=two-temperature
sim:program=laser-pulse
sim:integrator=llg-heun
sim:time-step=1.0e-16

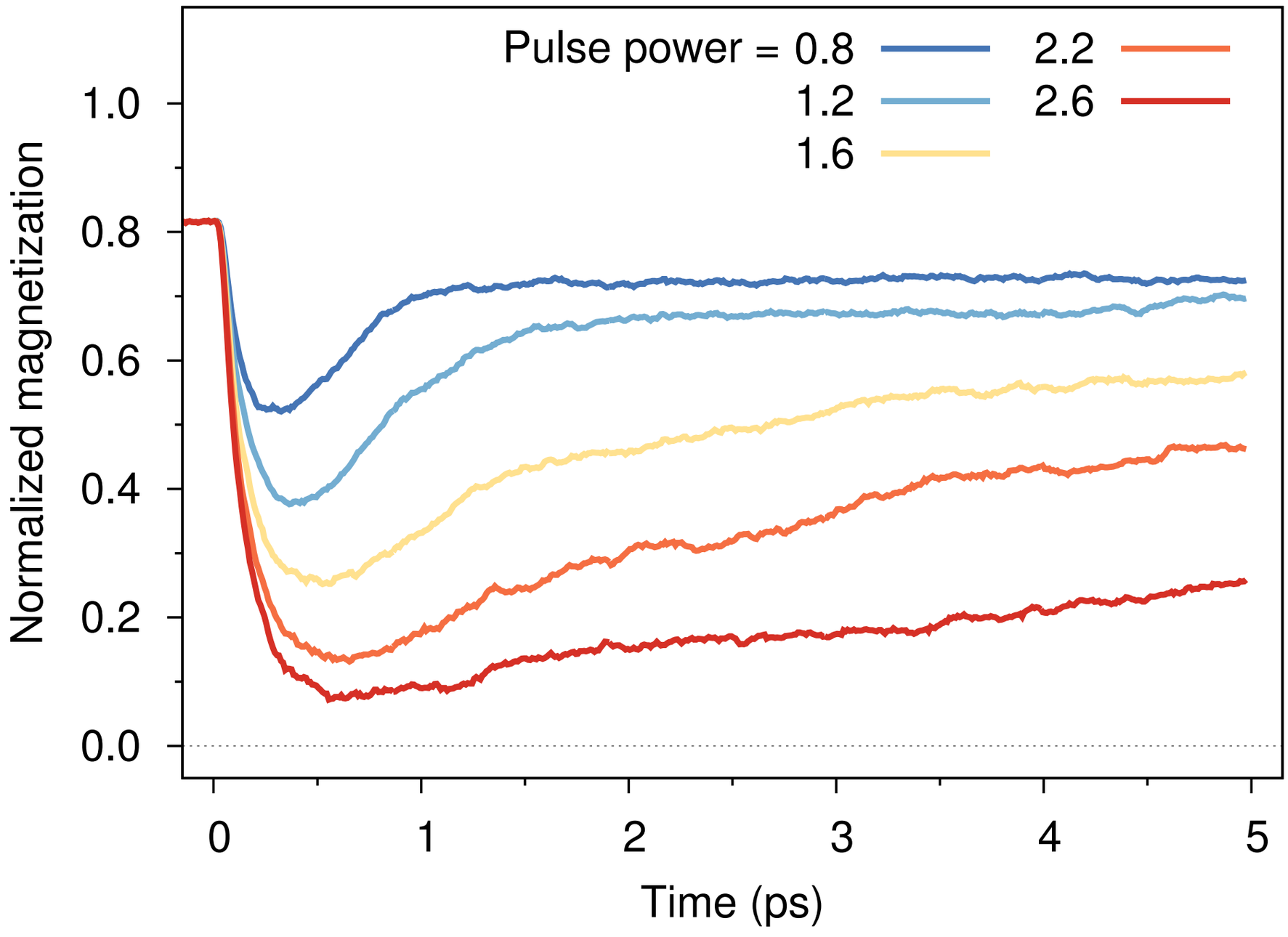
output:real-time
output:electron-temperature
output:phonon-temperature
output:magnetisation-length
```

Note strong time-step dependence of properties



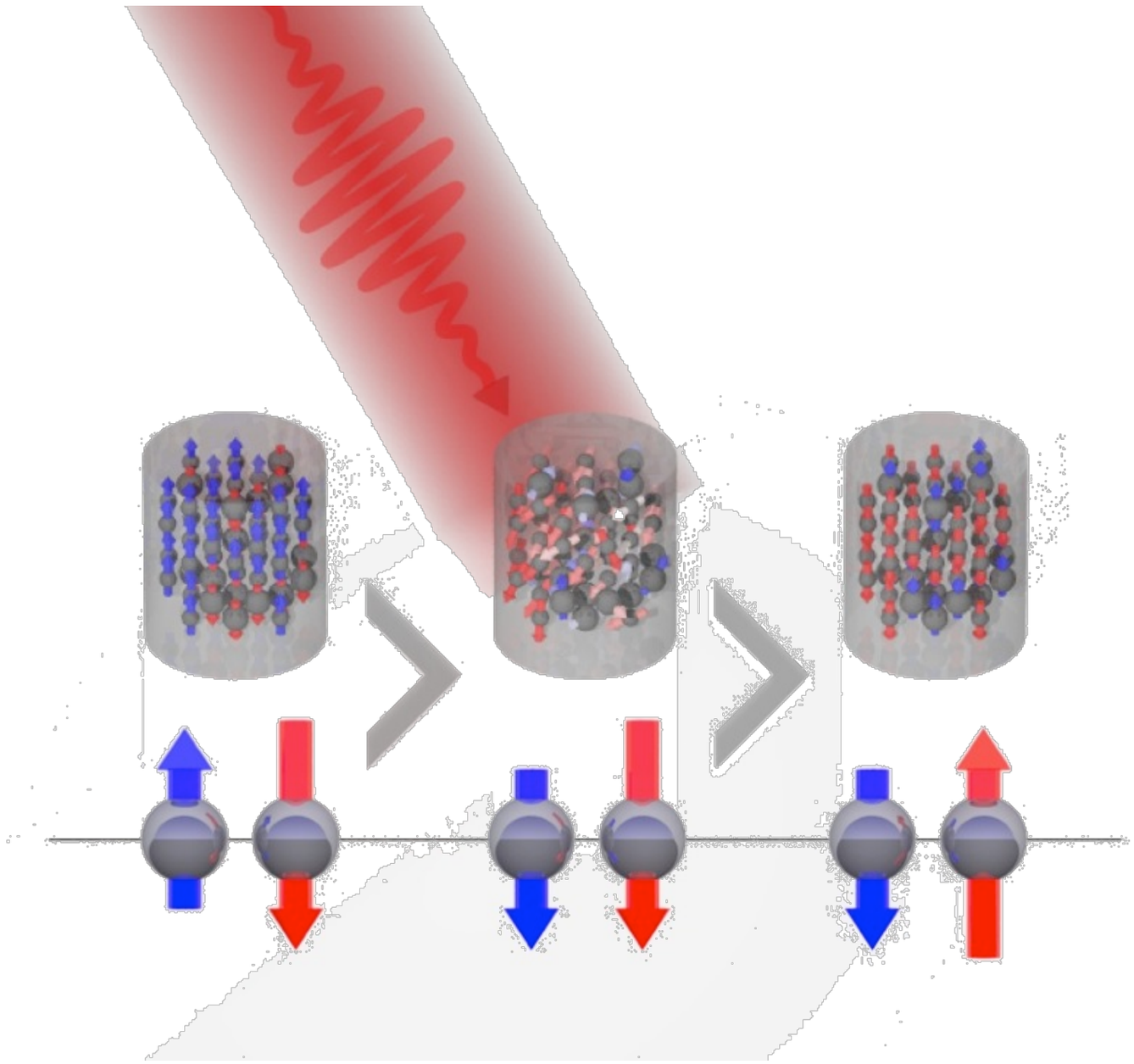
Safe region (depending on T/T_C)

Effect of pulse power in Ni



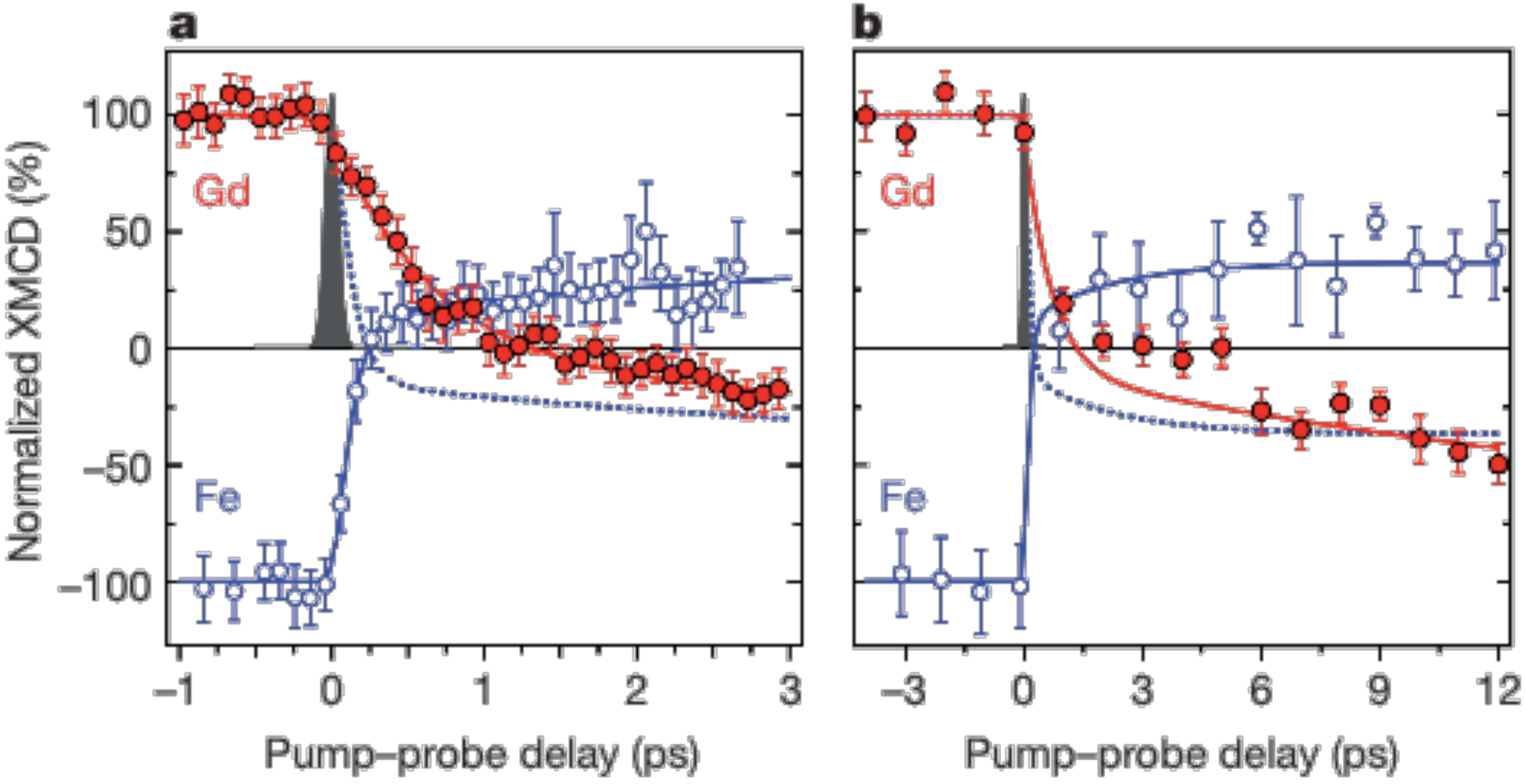
Stronger laser pulses show more demagnetization and slower recovery

Thermally induced magnetic switching



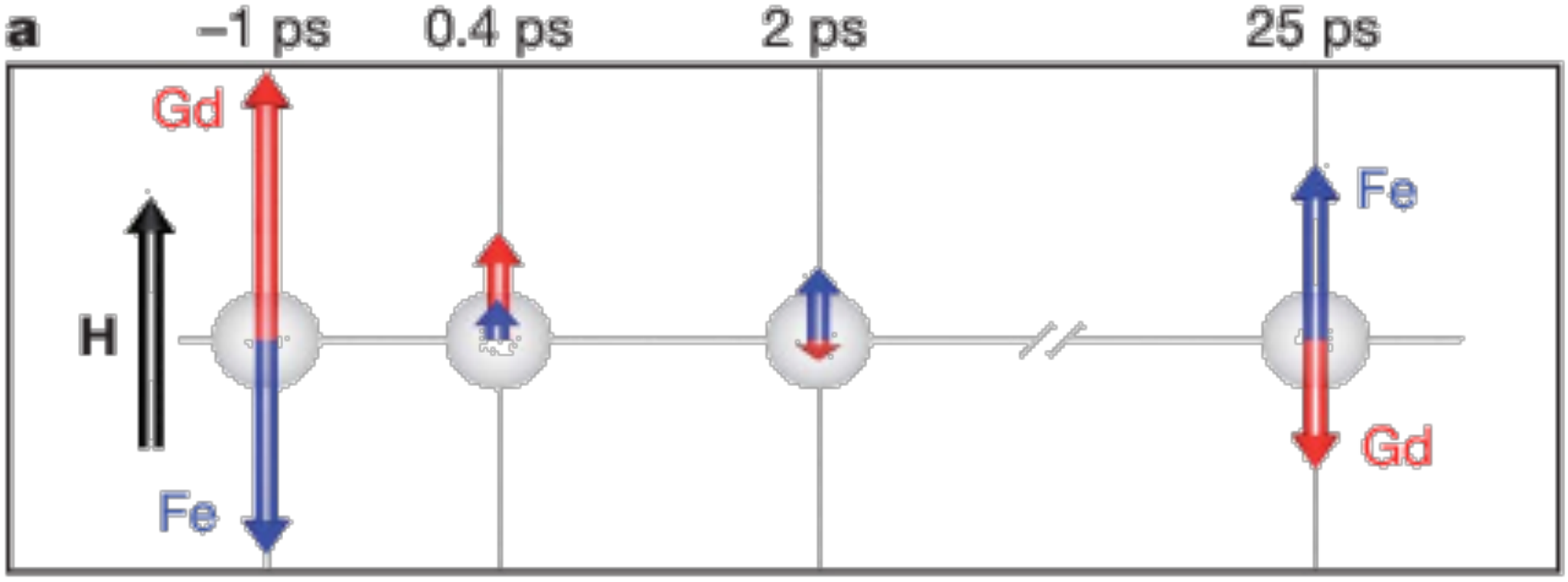
T. Ostler *et al*, Nat. Commun.(2012)

Sublattice magnetization dynamics



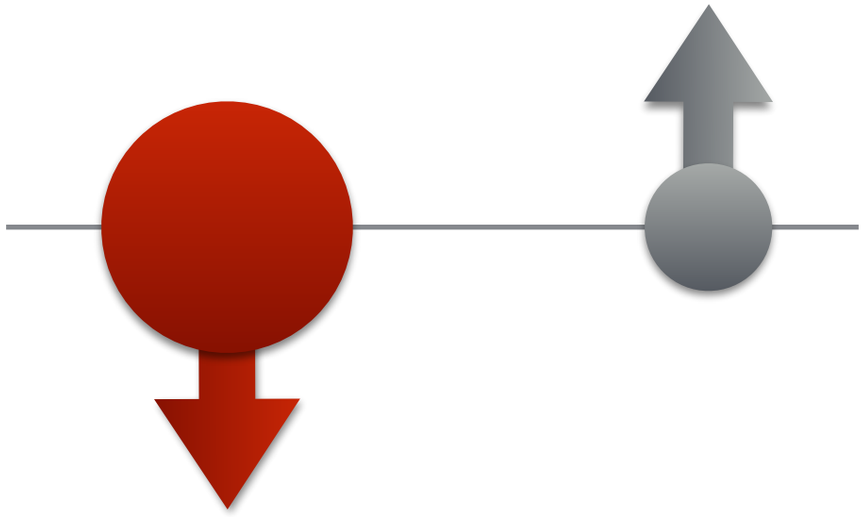
I. Radu *et al*, Nature (2011)

Transient ferromagnetic state

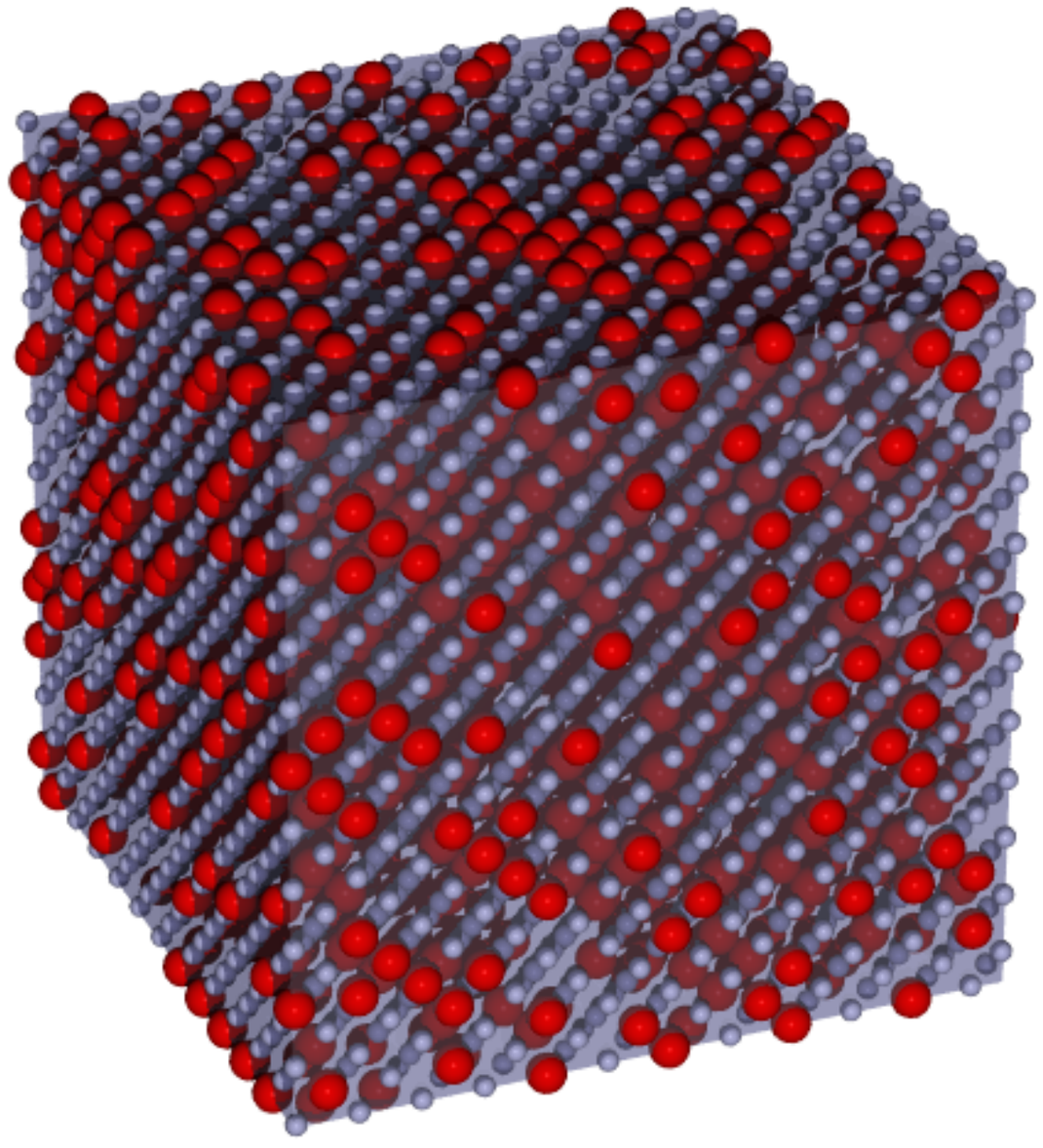


I. Radu *et al*, Nature (2011)

GdFe ferrimagnet



Gd Fe



GdFe.mat

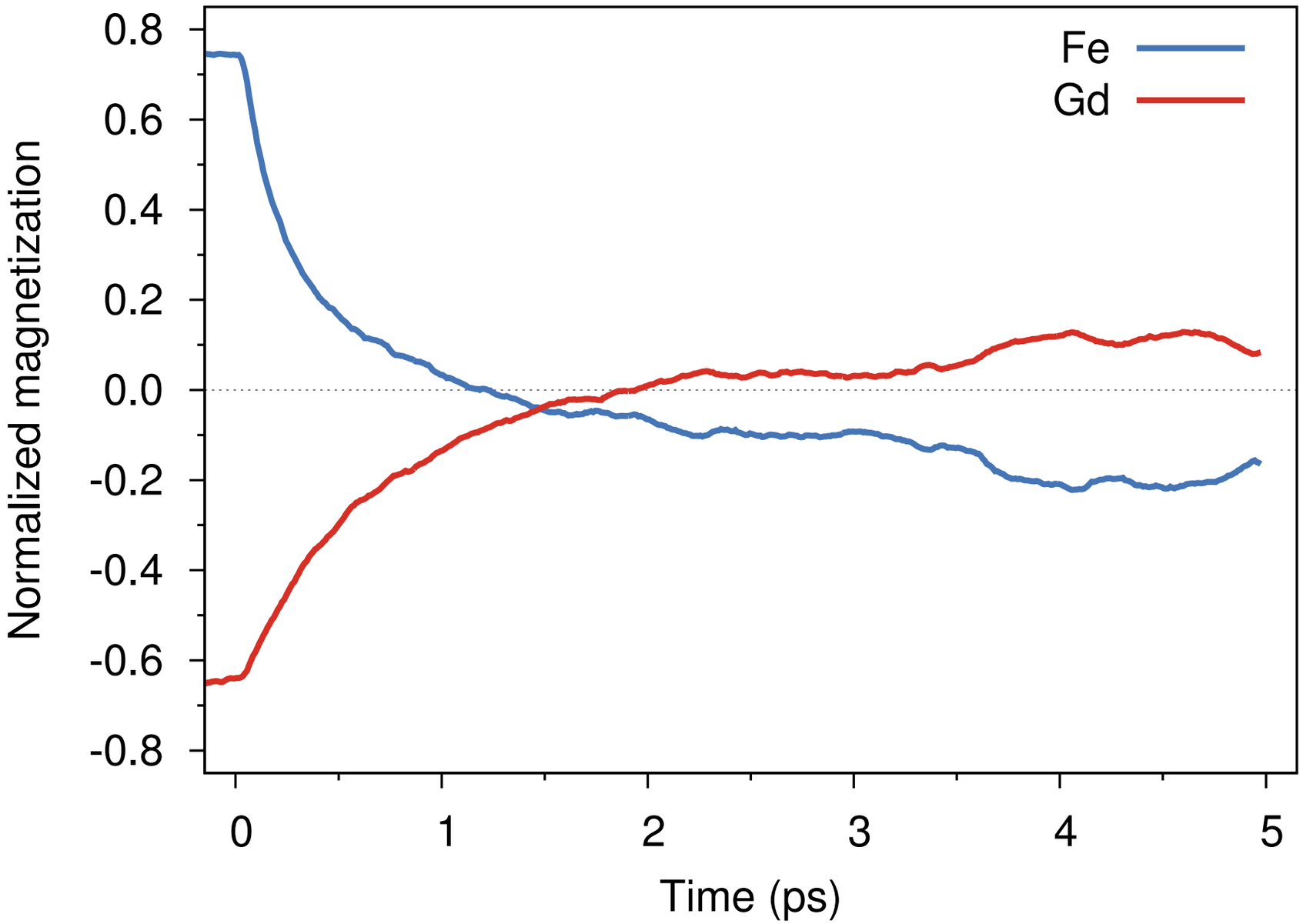
```
#-------------------------------------------------
# Number of Materials
#-------------------------------------------------
material:num-materials=2
#-------------------------------------------------
# Material 1 Fe (TM)
#-------------------------------------------------
material[1]:material-name=TM
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

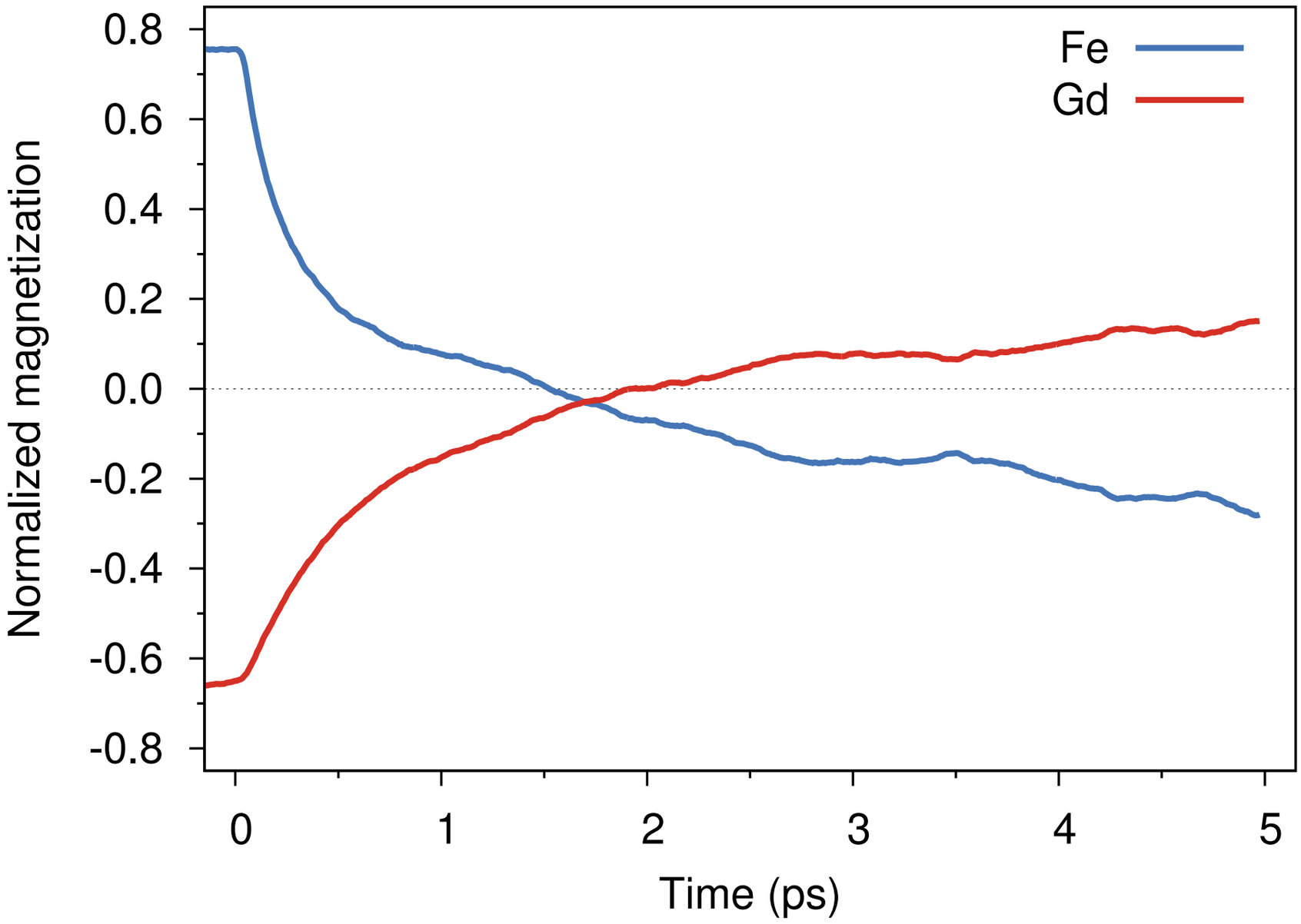
```
sim:equilibration-time-steps=20000
sim:total-time-steps=50000
sim:laser-pulse-power=1.6e22
sim:laser-pulse-temporal-profile=two-temperature
sim:program=laser-pulse
sim:integrator=llg-heun
sim:time-step=1.0e-16

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

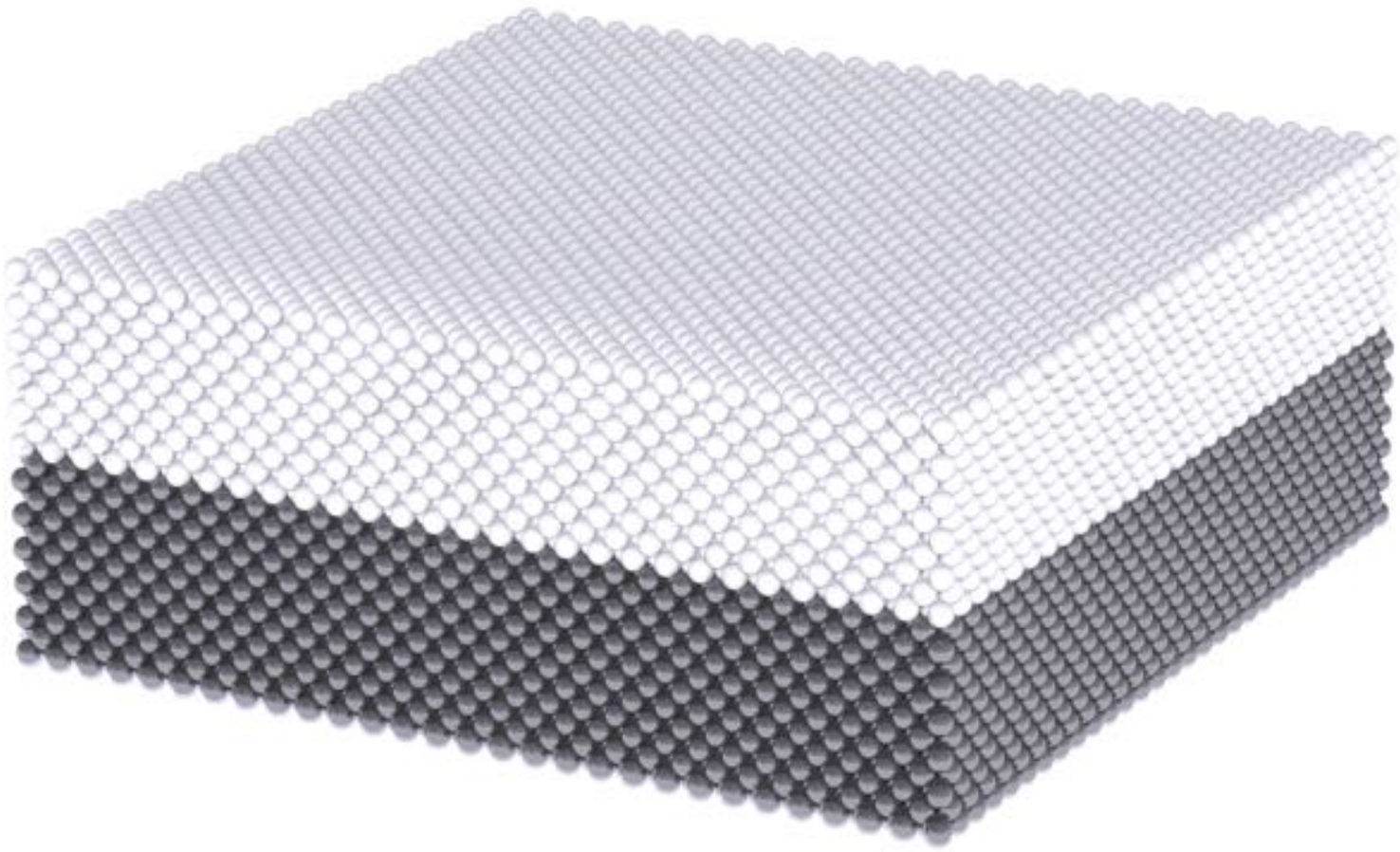
Calculated magnetization dynamics for $(4\ \mathrm{nm})^3$



Dynamics for $(7\ \mathrm{nm})^3$ GdFe



System generation



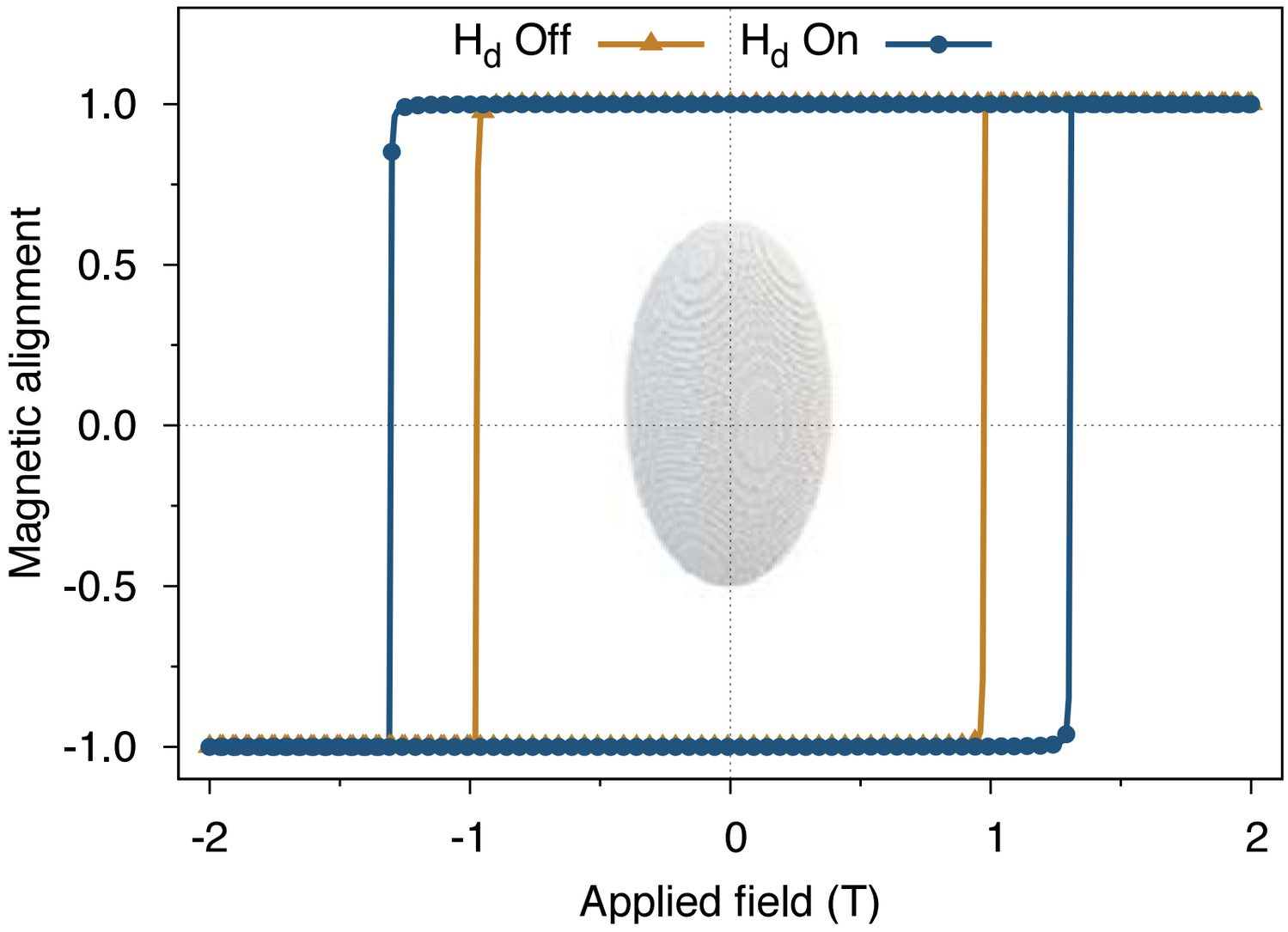
http://vampire.york.ac.uk/tutorials/

View your structures with rasmol

```
cfg2rasmol

rasmol -xyz crystal.xyz
```

Hysteresis properties



Hysteresis calculations

Generally a ‘slow’ process - typically 10s of nanoseconds

For comparison with experiment, use high damping limit, $\lambda = 1$

Coercivity **strongly** field rate dependent - slower is better!

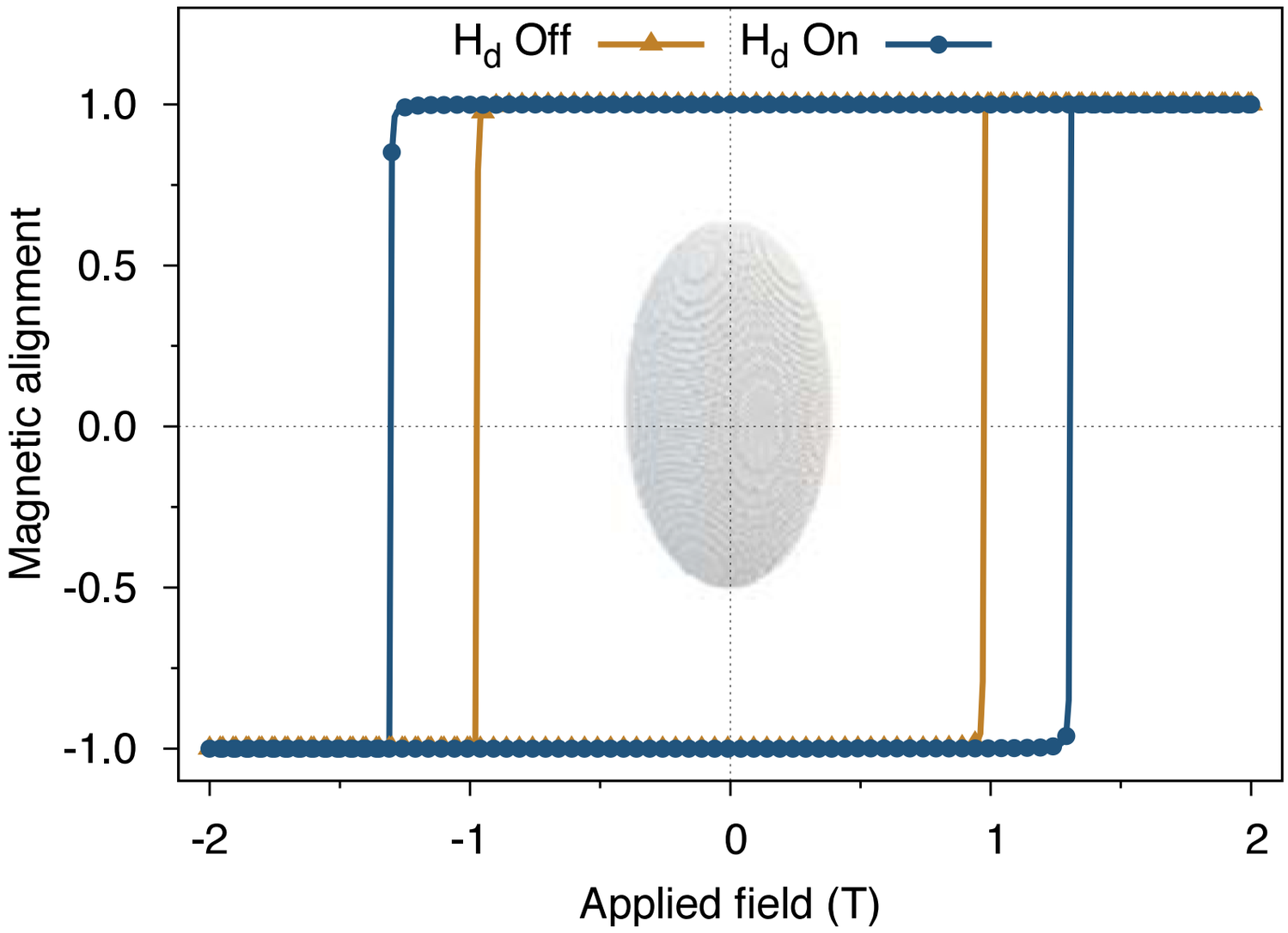
input file

```
create:single-spin

sim:loop-time-steps=100000
sim:program=hysteresis-loop
sim:integrator=llg-heun
sim:time-step=1.0e-15
sim:temperature = 0
sim:equilibration-applied-field-strength = 2.0 !T
sim:maximum-applied-field-strength = 2.0 !T
sim:applied-field-increment = 0.01 !T
sim:applied-field-angle-phi = 0.1 # (degrees from z)

output:real-time
output:applied-field-strength
output:applied-field-alignment
output:magnetisation
```

hysteresis-loop program



Cycles field from H_{max} to $-H_{max}$ in a user defined increment

Calculates dynamic response of the magnetisation to the field

Questions

What happens to the hysteresis loop if you change loop-time?

How many steps (field rate) do you need to reach the limit $H_c = 2k_u/\mu_s$

What effect does changing the field angle have?

Save and email your files

```
cd ~

tar -cjf myfiles.tar.gz vampire
```

(tar -xjf myfiles.tar.gz to extract)