Scale transitions in magnetisation dynamics

M. Poluektov[1]
G. Kreiss[1]
O. Eriksson[2]

1 – Uppsala University
Department of Information Technology
Division of Scientific Computing
2 – Uppsala University
Department of Physics and Astronomy
Division of Materials Theory

presentation at eScience academy 2015
October 14-15, 2015, Sweden

Multi-scale modelling of spin dynamics

- Materials Theory (Department of Physics and Astronomy)
  Olle Eriksson
  Anders Bergman
  …

- Scientific Computing (Department of Information Technology)
  Gunilla Kreiss
  Mikhail Poluektov
  Doghonay Arjmand

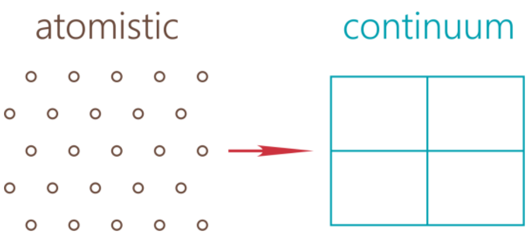
Introduction

- variety of applications
  - magnetic storage media
  - magnetic RAM
  - nanowires
  - etc.
- continuum modelling: micromagnetics
  - can handle relatively large spatial and time scales
- atomistic modelling: spin dynamics
  - precise treatment of singularities
  - material defects

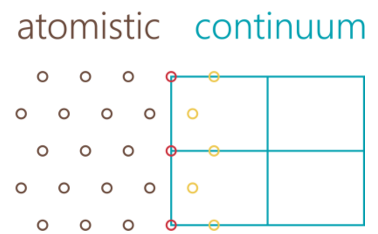
- combine advantages – multi-scale approach

Multi-scale modelling

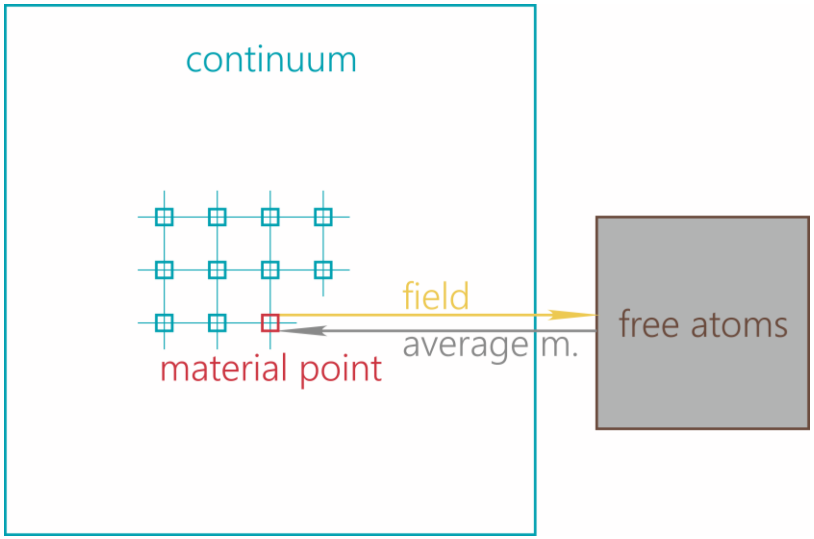
1. “information passing”



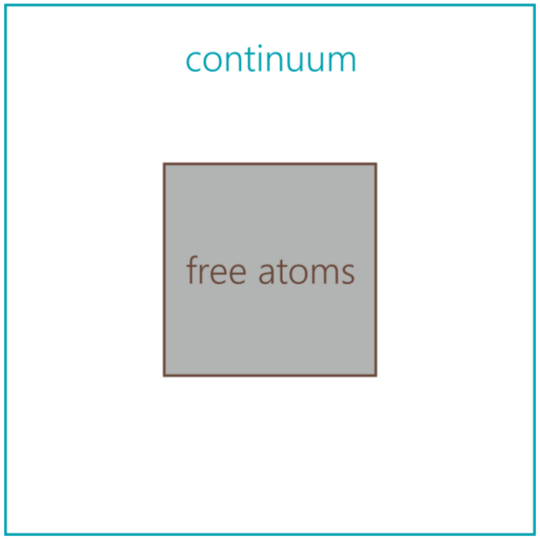
2. “direct coupling”



2a:

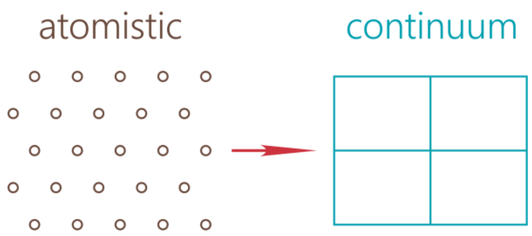


2b:

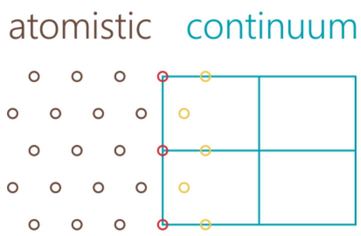


Multi-scale modelling

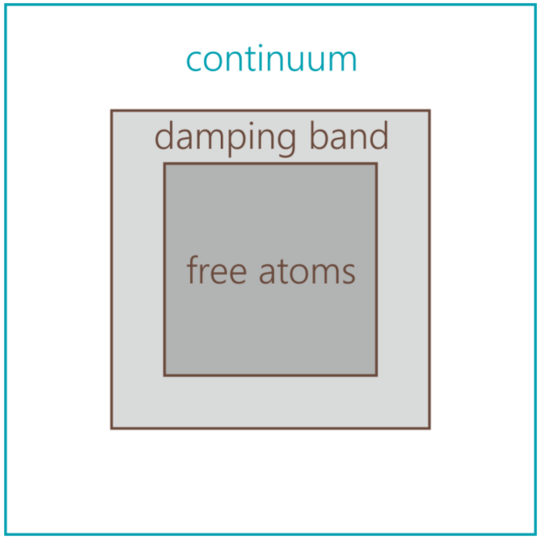
1. "information passing"



2. "direct coupling"



- static and dynamic methods
- wave reflections at the interface
  - not an issue of coupling methods
- approach: stadium damping region
  - wave-absorbing layer
  - thermostatting

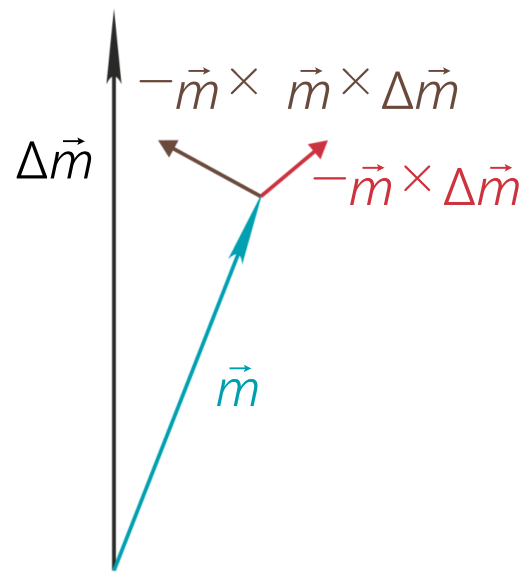


Micromagnetics

- magnetisation – density of magnetic dipole moments

- Landau-Lifshitz equation

$$\frac{\partial \vec{m}}{\partial t} = -\beta_{\text{L}} \vec{m} \times \Delta \vec{m} - \alpha_{\text{L}} \vec{m} \times \ \vec{m} \times \Delta \vec{m}$$

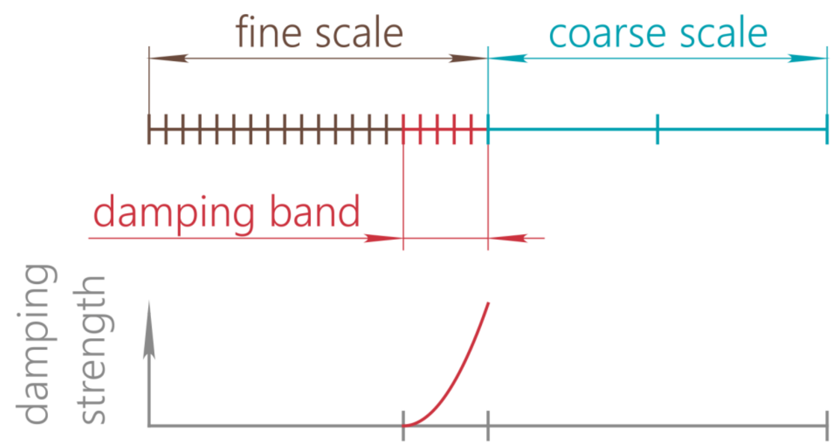


Damping band

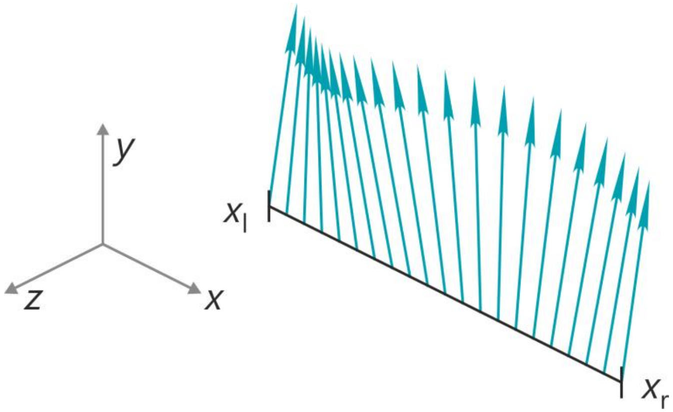
- atomistic and continuum descriptions are based on LL equation
- modify LL equation, test in continuum case

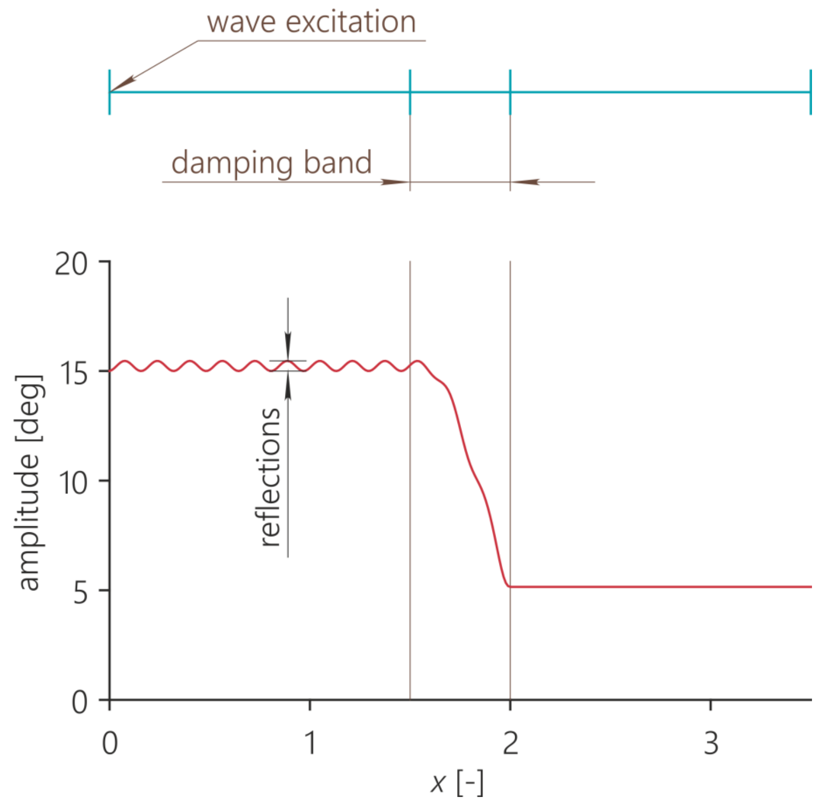
$$\frac{\partial \vec{m}}{\partial t} = -\beta_{\mathrm{L}} \vec{m} \times \Delta \vec{m} - \alpha_{\mathrm{L}} \vec{m} \times \; \vec{m} \times \Delta \vec{m} \; - \vec{m} \times \; \vec{m} \times \vec{f}$$

- 1D case
- choice of parameters?
- possible issues:
  - wave damping
  - influence of the boundary
  - size dependence
  - temperature stability



Spin waves

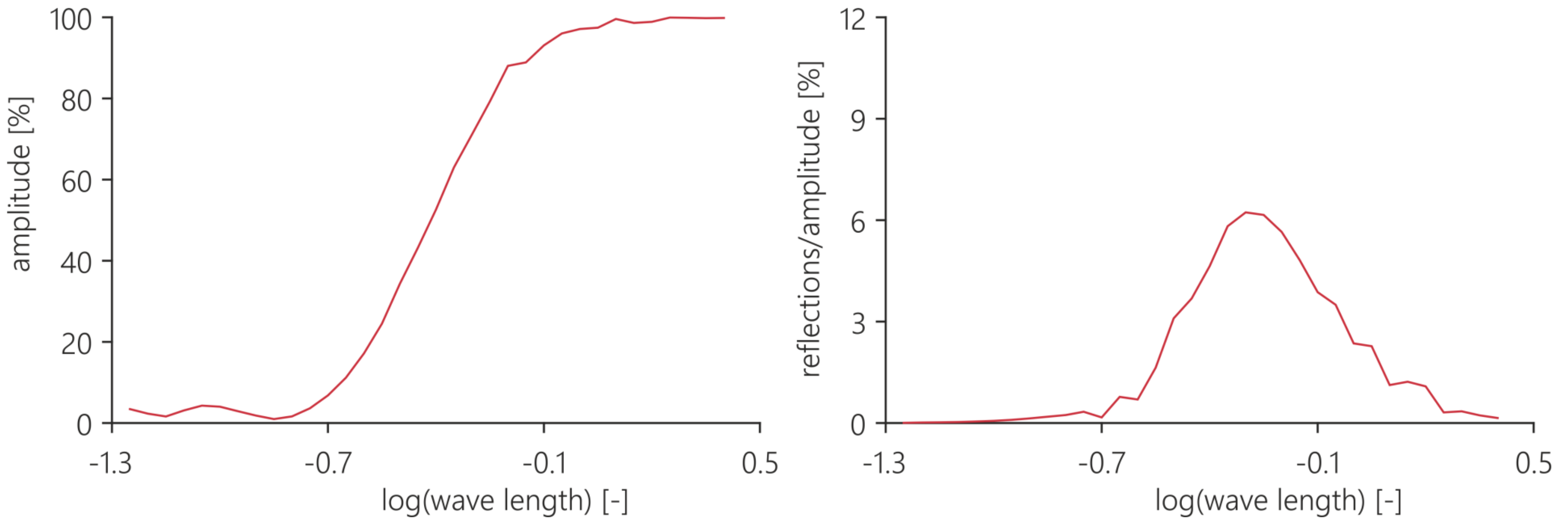




1D wave propagation analysis
(small amplitudes):

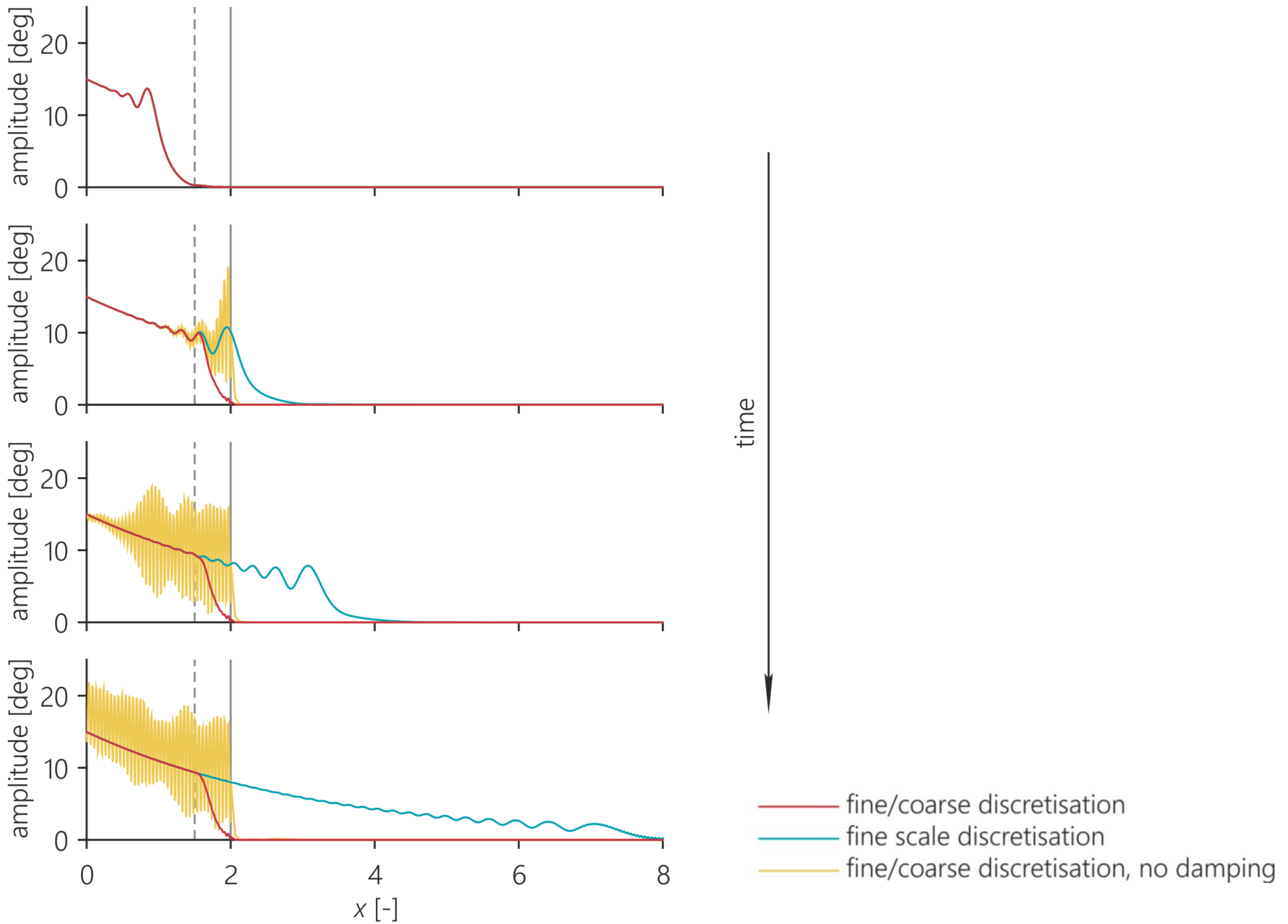
- damping strength should be proportional to time derivative of magnetisation
- width of damping band determines scale of reflections from it
- average magnetisation

Amplitude–frequency

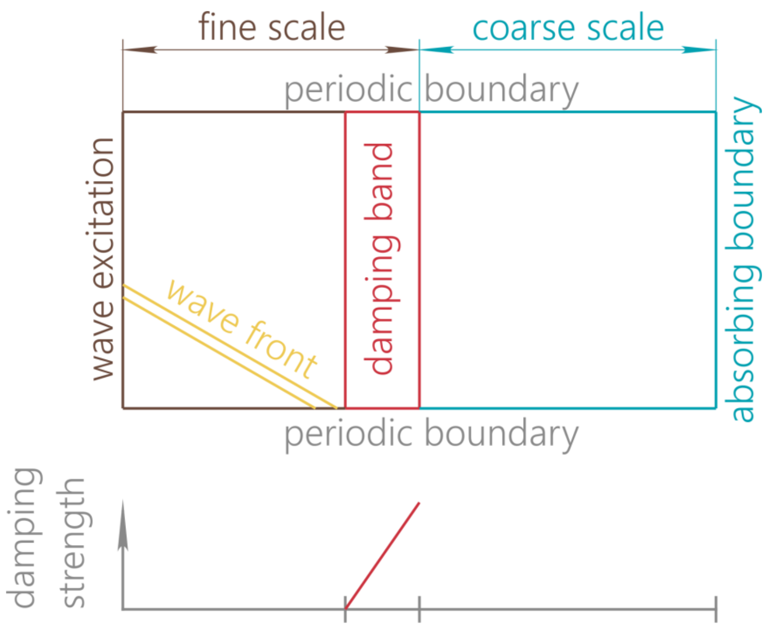


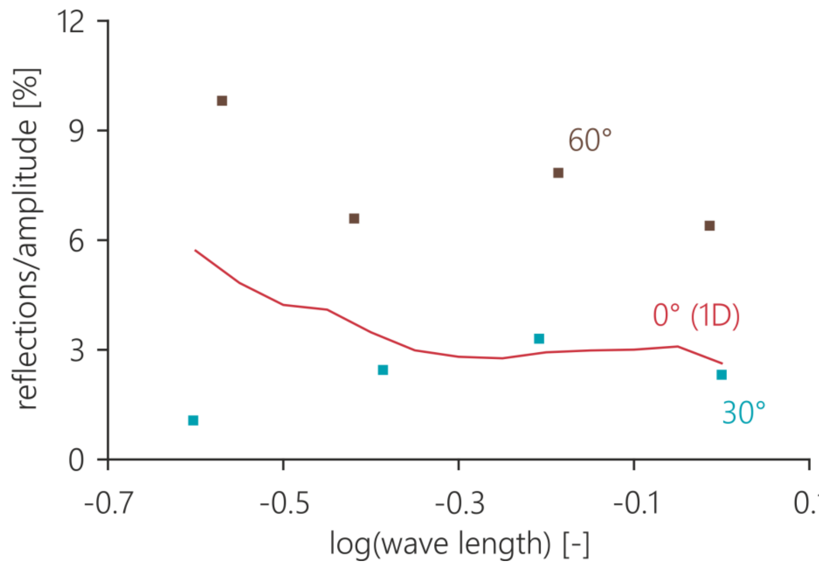
- uniform fine scale
- attenuation of small wave lengths
- finite error due to reflection from damping band
- size of averaging window determines cutoff wave length

Spin waves, example



Spin waves in 2D (preliminary results)





issues in 2D:

- local timestepping in case of implicit numerical methods
- large angle between wave front and interface: relatively high reflections

approach in 2D:

- borrow idea from damping of acoustic waves, perfectly matched layer

Conclusions

- damping zone at the interface eliminates wave reflections
- finite width (depends on desired accuracy)
- optimal values of damping parameters can be obtained numerically

Future work

- further investigation of damping in 1D continuum case
  - finite temperature (stochastic terms in LL eq.)
- further investigation of 2D continuum case
  - extensive testing of PML concept
  - domain wall motion
- transition form continuum fine scale to atomistic