Coupling atomistic and continuum modelling of magnetism

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Centre for Scientific Computing and Centre for Predictive Modelling seminar
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research profile: computational methods with focus on PDEs

- analysis of mathematical models: shock dynamics, boundary closures, …
- discrete approximations: finite differences, finite elements, radial basis functions, …
- numerical linear algebra: parallel iterative solvers, pre-conditioners, …
- parallel and large-scale computing: load balancing, memory architecture, …
- optimisation: global optimisation, design optimisation, …

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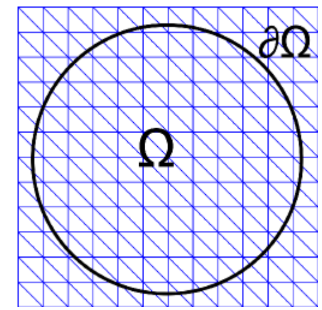
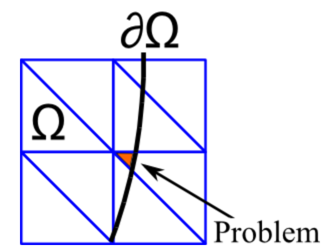
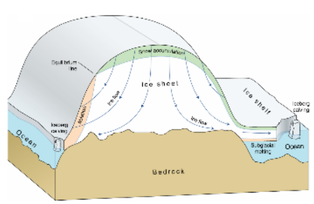
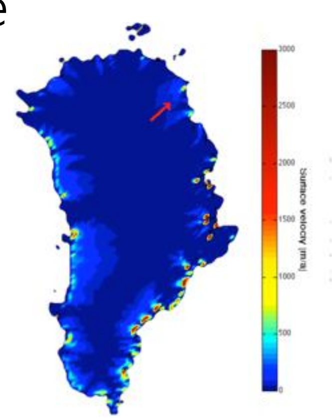
Department of Information Technology Division of Scientific Computing

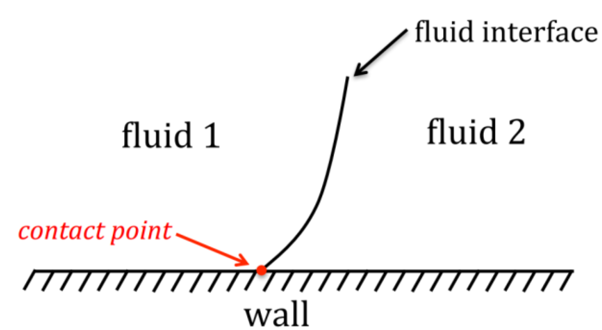
- wave propagation
  - finite differences, non-conforming grids
  - immersed finite elements
  - perfectly matched layers
- computational fluid dynamics
  - near-wall models for large eddy simulation
  - multiphase flow
- computational systems biology
- computational finance
- ice sheet modelling









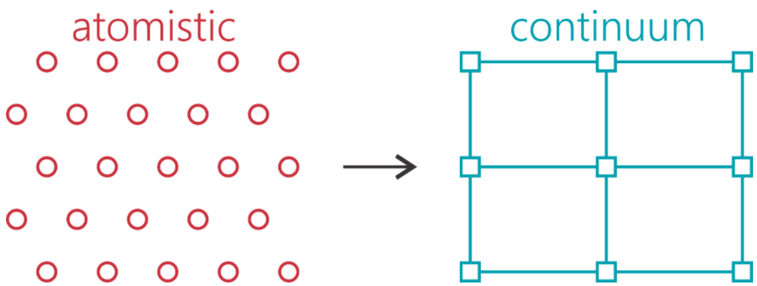


Outline

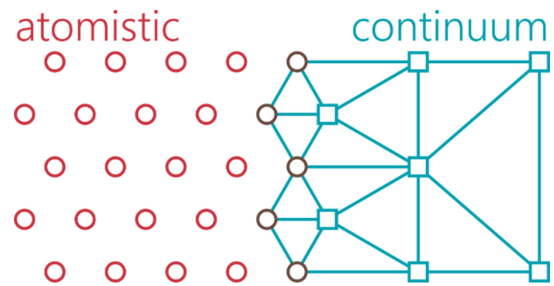
- research group
- multiscale modelling
- **mechanics:** coupling local and nonlocal models
  - **statics:** dealing with the interface error
  - **dynamics:** dealing with high-frequency waves
- **magnetism:** statics and dynamics
  - examples
- **magnetism:** finite temperatures
  - dealing with nonlinearities
- challenges and open problems

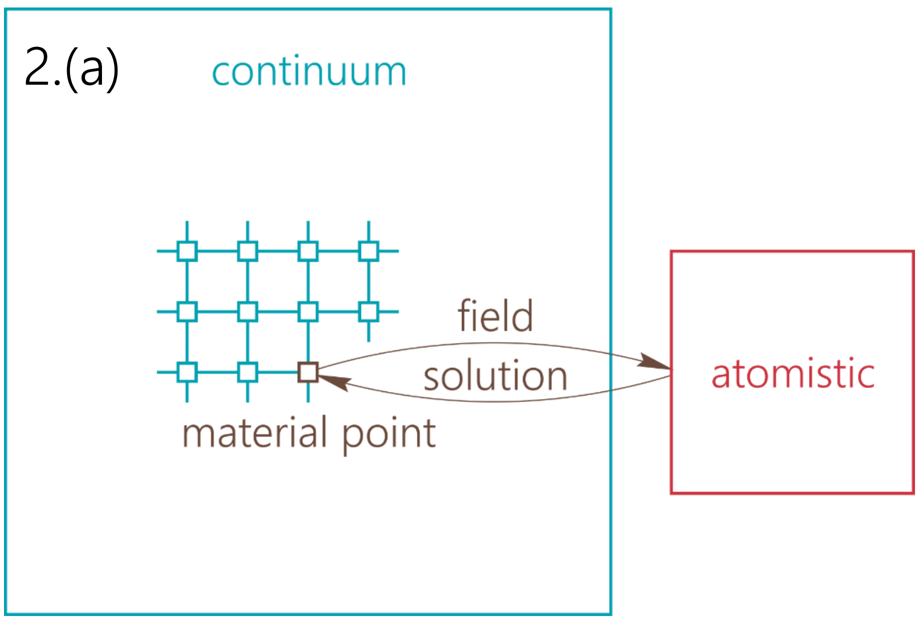
Atomistic-continuum methods

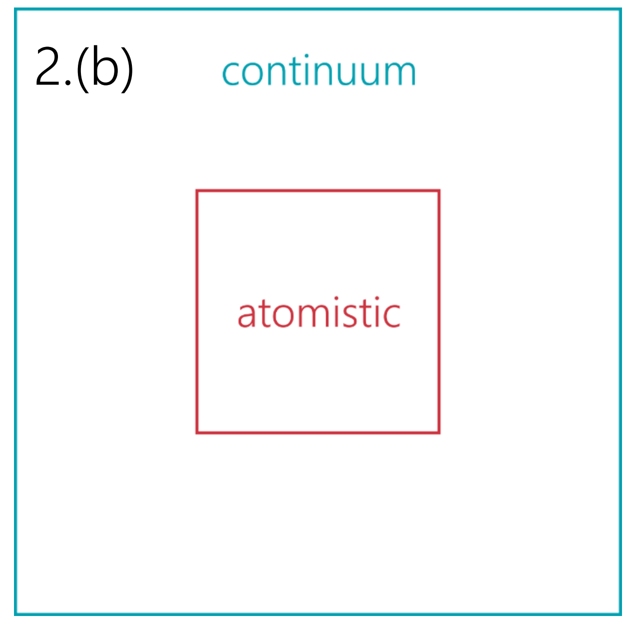
1. sequential



2. concurrent







Mechanics, statics

Statics, atomistic description

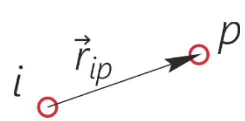
- goal: obtain minimum energy configuration
- total atomistic energy

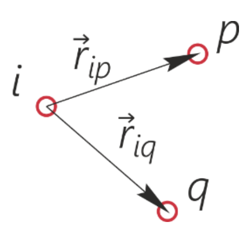
$$E = \sum_{i} E_i^{\mathrm{A}}$$

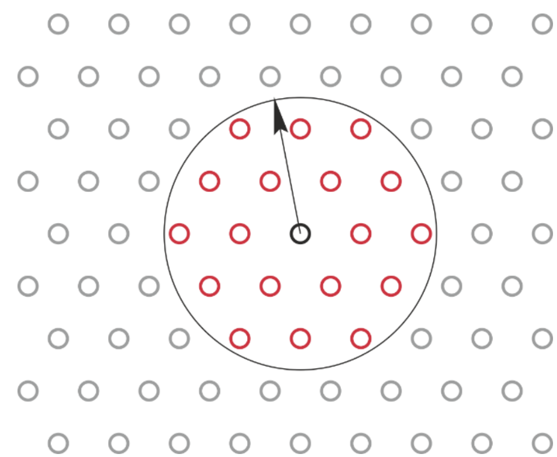
$$E_i^{\mathrm{A}} = \frac{1}{2} \sum_{p \neq i} \Pi_{ip}^{(2)} \left(\vec{r}_{ip} \right) + \frac{1}{6} \sum_{p \neq i} \sum_{q \neq p,i} \Pi_{ipq}^{(3)} \left(\vec{r}_{ip}, \vec{r}_{iq} \right)$$

$$\vec{f}_i = -\frac{\partial E}{\partial \vec{r}_i} = 0$$

- nonlocal interatomic interaction





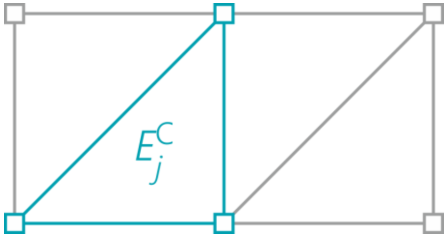


Statics, continuum description

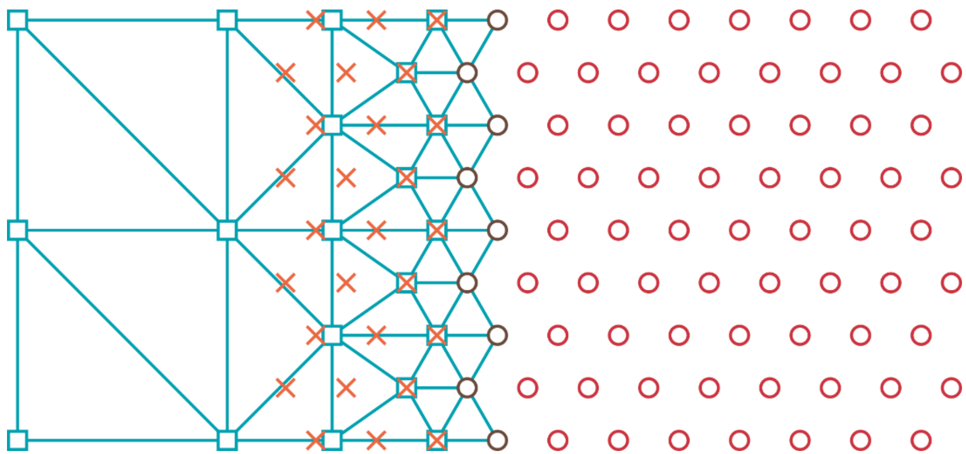
- goal: obtain minimum energy configuration
- continuum energy
  - local energy density e^C
  - finite-element representation

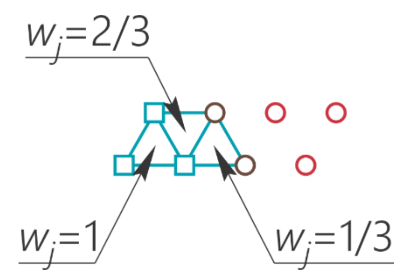
$$E = \sum_j E_j^C$$

$$E_j^C = \int_{V_j} e^C \mathrm{d}V_j$$



Coupling

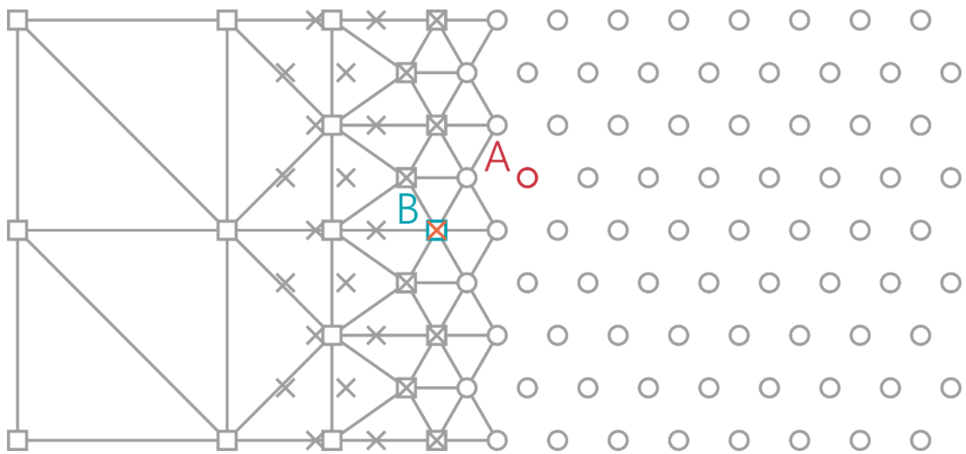


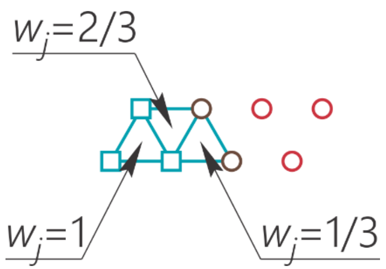


- introduce pad atoms (×), finite range of interatomic interaction
- all coupling methods differ in treatment of total energy

$$E = \sum_i E_i^A + \sum_j w_j E_j^C$$

Coupling



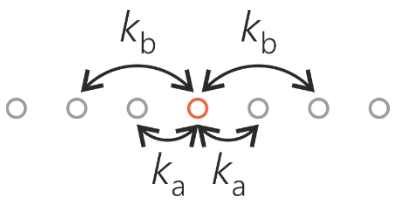


- introduce pad atoms (×), finite range of interatomic interaction
- all coupling methods differ in treatment of total energy

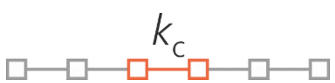
$$E = \sum_i E_i^A + \sum_j w_j E_j^C$$

- minimisation of total energy, **ghost forces**

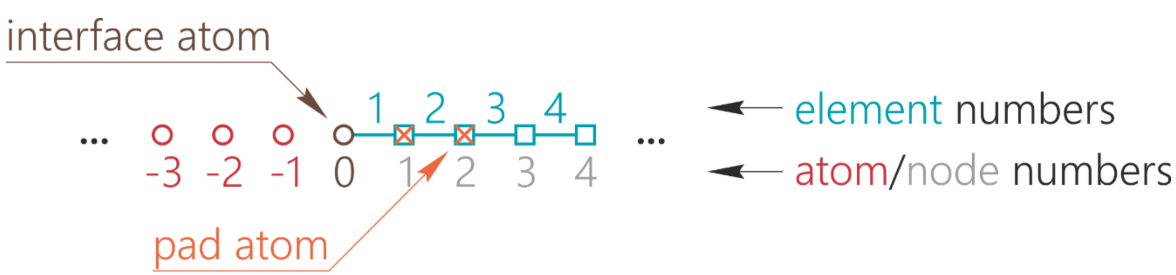
Illustrative 1D example



$$E_i^A = \frac{1}{2}\left(\frac{1}{2}k_a\left(u_i - u_{i-1}\right)^2 + \frac{1}{2}k_b\left(u_i - u_{i-2}\right)^2 + \right.$$
$$\left. + \frac{1}{2}k_a\left(u_i - u_{i+1}\right)^2 + \frac{1}{2}k_b\left(u_i - u_{i+2}\right)^2\right)$$



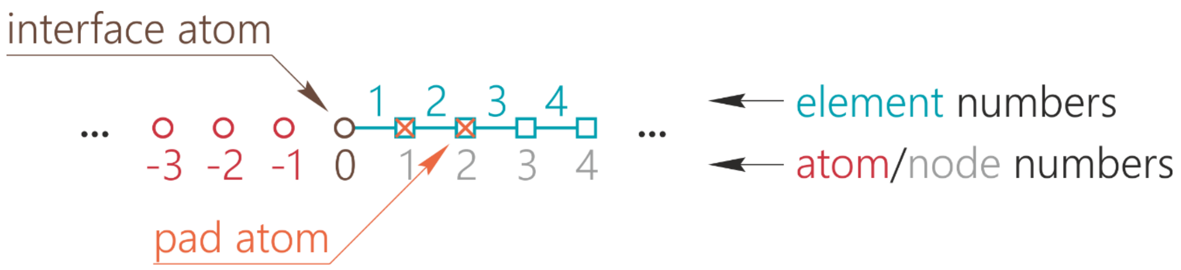
$$E_j^C = \frac{1}{2}k_c\left(u_j^R - u_j^L\right)^2 \quad u_{j+1}^L = u_j^R \quad k_c = k_a + 4k_b$$



$$E^T = \ldots + E_{-2}^A + E_{-1}^A + E_0^A + \frac{1}{2}E_1^C + E_2^C + E_3^C + \ldots$$

$$u_i - u_{i-1} = \varepsilon a$$

Illustrative 1D example



$$E^{\mathrm{T}} = \ldots + E^{\mathrm{A}}_{-2} + E^{\mathrm{A}}_{-1} + E^{\mathrm{A}}_{0} + \frac{1}{2}E^{\mathrm{C}}_{1} + E^{\mathrm{C}}_{2} + E^{\mathrm{C}}_{3} + \ldots$$

$$u_i - u_{i-1} = \varepsilon a$$

$$f_{-2} = -\frac{\partial E^{\mathrm{T}}}{\partial u_{-2}} = 0$$

$$f_{-1} = -\frac{\partial E^{\mathrm{T}}}{\partial u_{-1}} = -k_{\mathrm{b}}\varepsilon a$$

$$f_{0} = -\frac{\partial E^{\mathrm{T}}}{\partial u_{0}} = k_{\mathrm{b}}\varepsilon a$$

$$f_{1} = -\frac{\partial E^{\mathrm{T}}}{\partial u_{1}} = k_{\mathrm{b}}\varepsilon a$$

$$f_{2} = -\frac{\partial E^{\mathrm{T}}}{\partial u_{2}} = -k_{\mathrm{b}}\varepsilon a$$

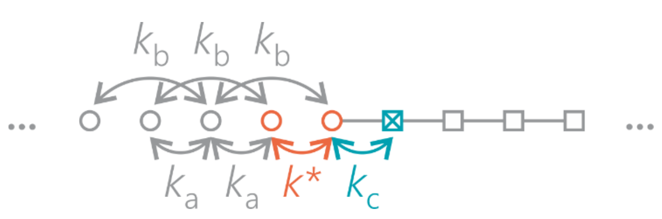
$$f_{3} = -\frac{\partial E^{\mathrm{T}}}{\partial u_{3}} = 0$$

Methods

- energy-based coupling methods (E)
  - ghost-force reduction techniques
  - quasi-nonlocal (QNL) atoms
- force-based coupling methods (E^{A}, E^{C})

$$E^{\mathrm{A}} = \sum_i E_i^{\mathrm{A}} + \sum_k E_k^{\mathrm{P}} \qquad E^{\mathrm{C}} = \sum_j E_j^{\mathrm{C}}$$

- many variations of these methods
  - overlapping and non-overlapping regions
  - review [Miller Tadmor 2009 *Modelling Simul. Mater. Sci. Eng.* **17** 053001]
- our approach (similar to QNL) – modify atoms at the interface

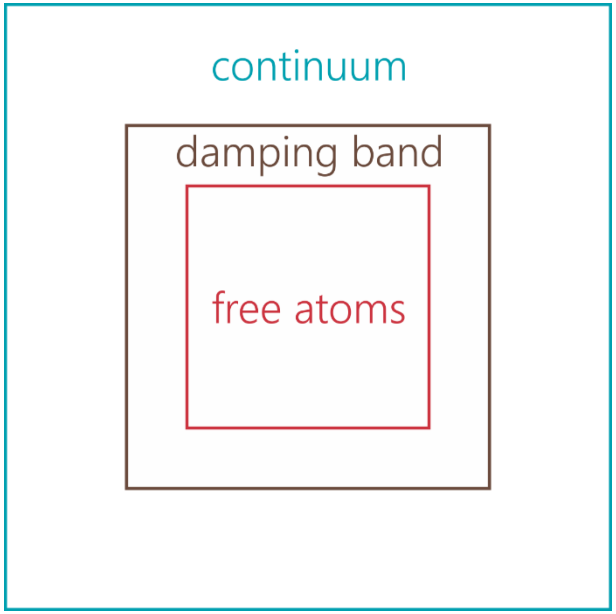


Mechanics, dynamics

Dynamics

- main problem: treatment of scale coarsening
  - wave reflections – not an issue of coupling methods

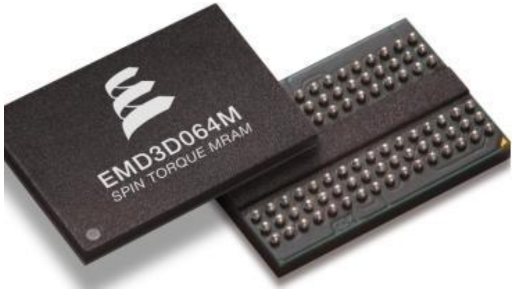
- approach: stadium damping region
  - wave-absorbing layer
  - thermostatting



Magnetism

Magnetic materials

- 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 – multiscale approach



Magnetism, statics

Spin statics

- discrete set of spin magnetic moments of atoms $\qquad |\vec{m}_k| = 1, \quad \forall k$
- fixed lattice positions

$$E = -\frac{1}{2}\sum_i \sum_{j\neq i} J_{ij}\vec{m}_i \cdot \vec{m}_j + \frac{1}{2}\sum_i \sum_{j\neq i} \vec{G}_{ij} \cdot (\vec{m}_i \times \vec{m}_j) - \frac{1}{2}\sum_i K(\vec{p}\cdot \vec{m}_i)^2 - \mu \sum_i \vec{H}_e \cdot \vec{m}_i$$

Spin statics

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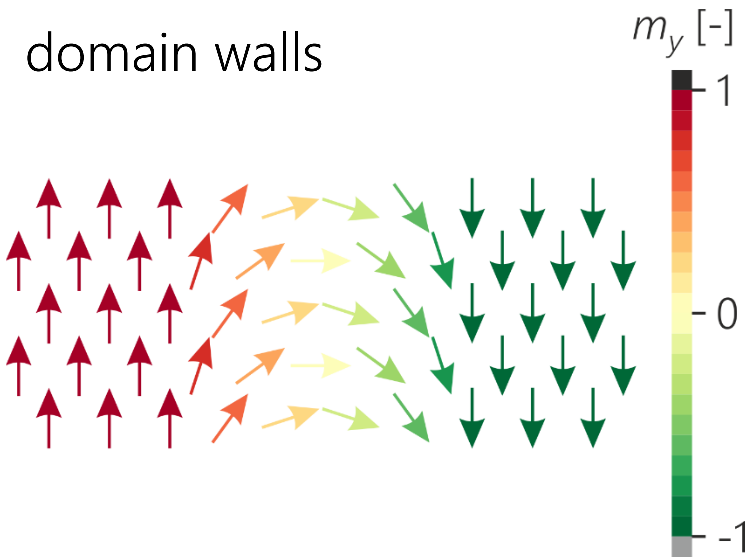
domain walls



Spin statics

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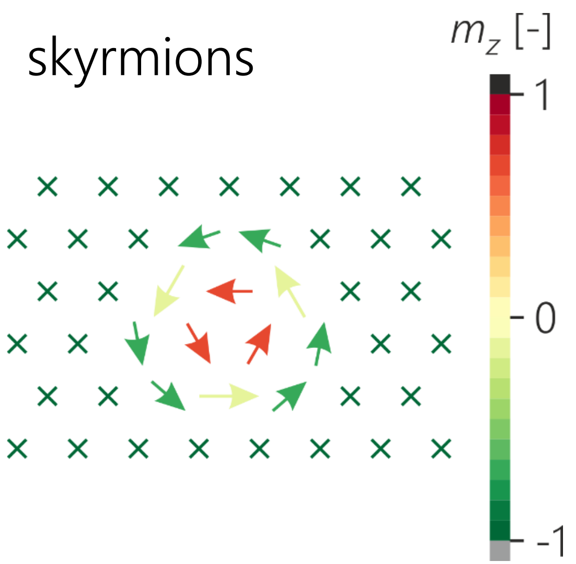
skyrmions



Analogy with mechanics

- mathematically equivalent to molecular statics
- spherical coordinates – two d.o.f. per atom

$$\vec{m}_k = \vec{e}_x \sin\theta_k \cos\phi_k + \vec{e}_y \sin\theta_k \sin\phi_k + \vec{e}_z \cos\theta_k$$

$$\vec{u}_k = \vec{e}_1\theta_k + \vec{e}_2\phi_k$$

$$E = \sum_i E_i^{\mathrm{A}}$$

$$E_i^{\mathrm{A}} = \Pi^{(1)}\left(\vec{R}_i,\ \vec{u}_i\right) + \frac{1}{2}\sum_{j\neq i}\Pi^{(2)}\left(\vec{R}_{ij},\ \vec{u}_j - \vec{u}_i,\ \vec{u}_j + \vec{u}_i\right)$$

- energy represented via potentials
  - R_i – atomic position vectors (not d.o.f.)
  - R_{ij} – vectors connecting atoms i and j (not d.o.f.)

Coarse-graining

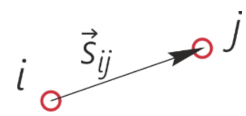
- matching energies
- atomistic description

$$E = -\frac{1}{2}\sum_{i}\sum_{j\neq i} J_{ij}\vec{m}_i \cdot \vec{m}_j + \ldots$$

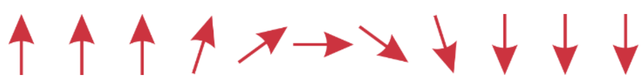
- continuum description

$$E = \frac{1}{2V_0}\int_V A_\mathrm{e}\left(\left|\nabla m_x\right|^2 + \left|\nabla m_y\right|^2 + \left|\nabla m_z\right|^2\right)\mathrm{d}V + \ldots$$

$$A_\mathrm{e} = \frac{1}{2}\sum_{j\neq i} J_{ij}\left(\vec{s}_{ij}\cdot\vec{e}_x\right)\left(\vec{s}_{ij}\cdot\vec{e}_x\right)$$

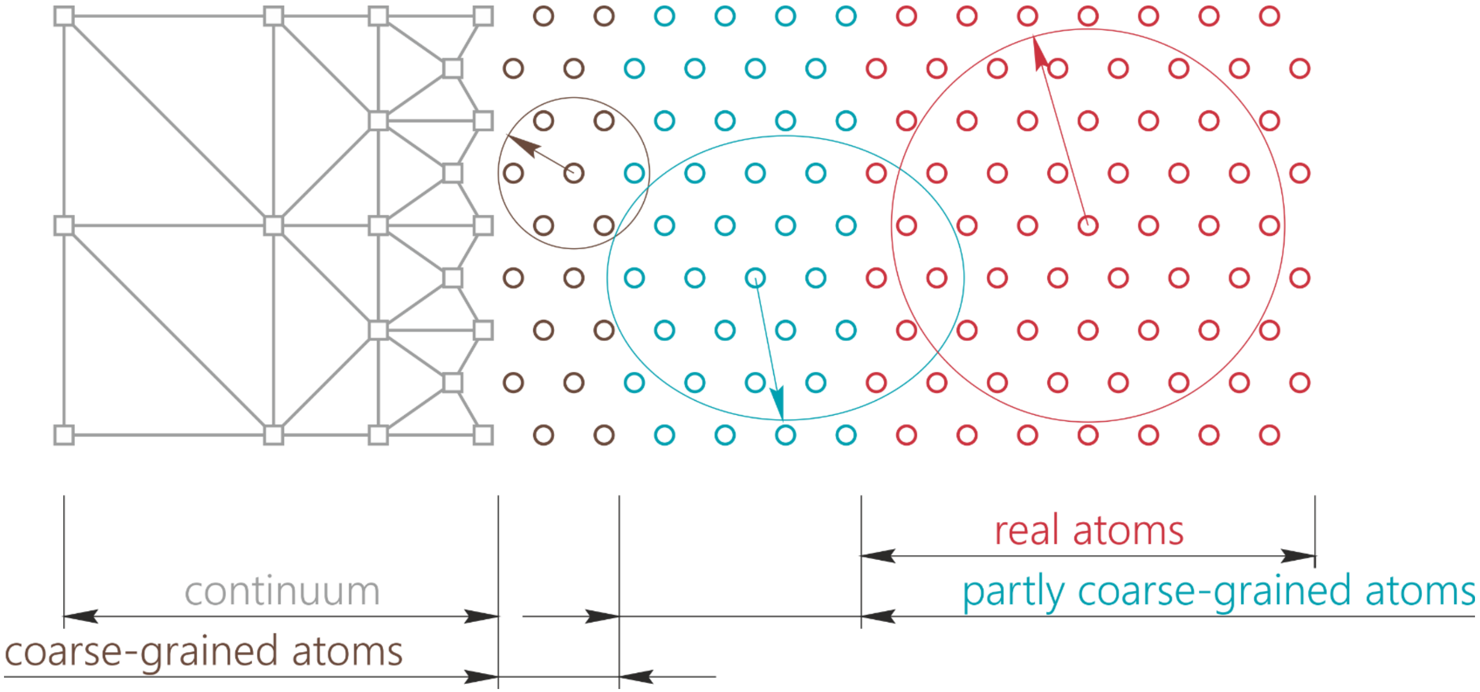


- mismatch between descriptions



Coupling

transition zone: modify atoms at the interface (J_{ij})



[Poluektov Eriksson Kreiss 2016 *Submitted*]

Coupling

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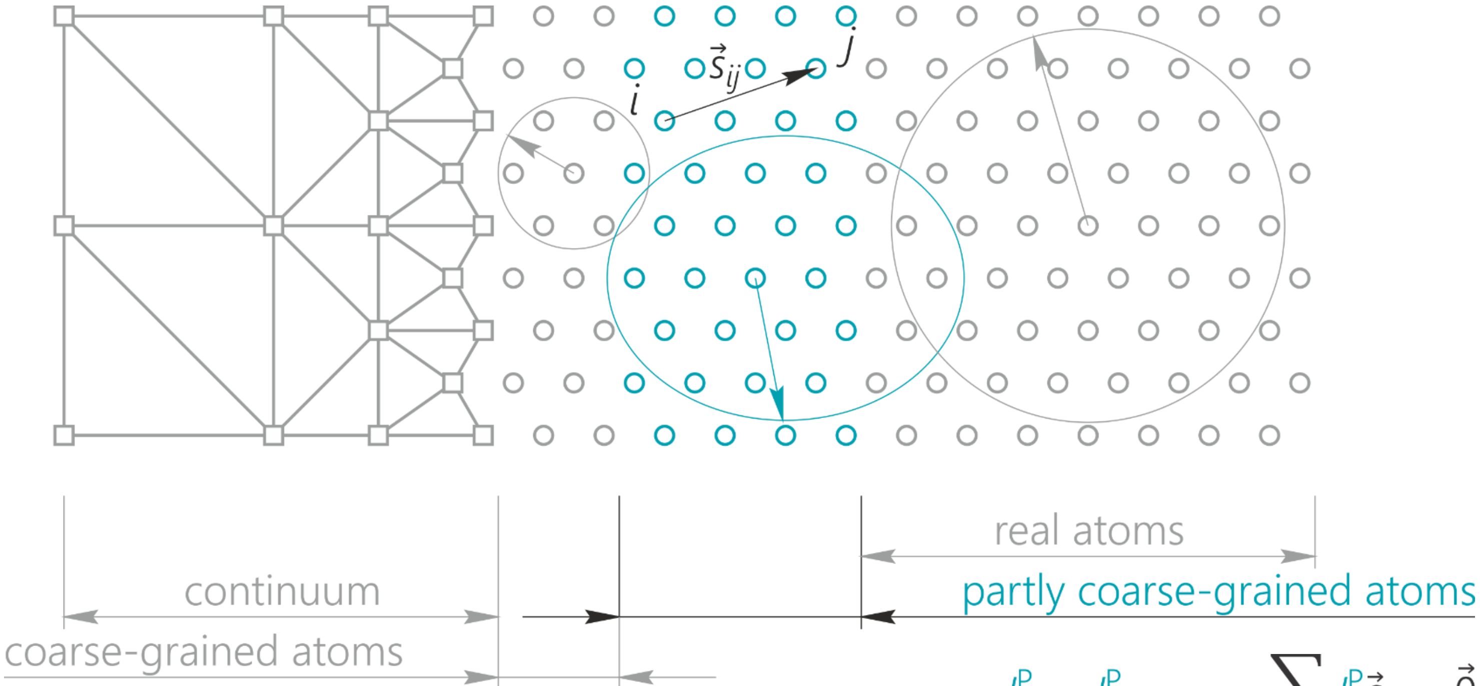


$$J_{ij}^{\mathrm{P}} = J_{ji}^{\mathrm{P}} \qquad \sum_{j \neq i} J_{ij}^{\mathrm{P}} \vec{s}_{ij} = \vec{0}$$

[Poluektov Eriksson Kreiss 2016 *Submitted*]

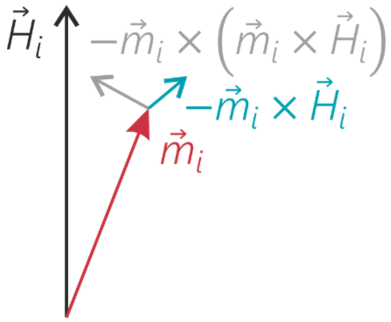
Magnetism, dynamics

Spin dynamics

- atomistic spin dynamics: discrete set of spin magnetic moments
- fixed lattice positions
- Landau-Lifshitz-Gilbert equation

$$\frac{\partial}{\partial t}\vec{m}_i = -\beta_L \vec{m}_i \times \vec{H}_i - \alpha_L \vec{m}_i \times \left(\vec{m}_i \times \vec{H}_i\right)$$

$$\vec{H}_i = \sum_j J_{ij}\vec{m}_j + \ldots$$



- micromagnetics: continuum vector field

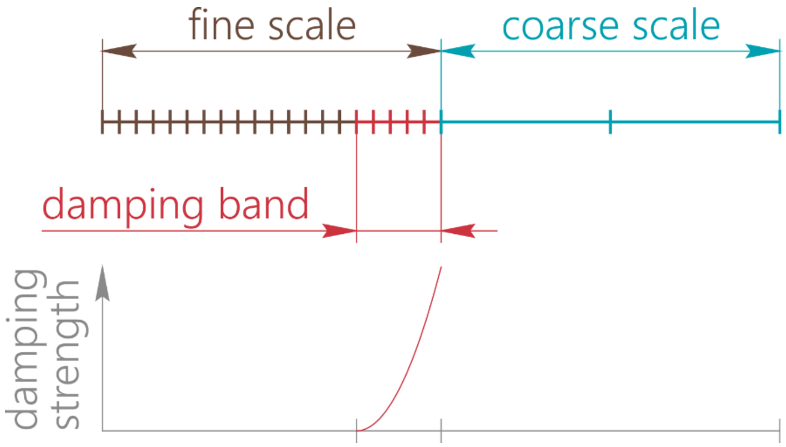
$$\vec{m}_i \longrightarrow \vec{m}\,(x)$$

Damping band

modify LLG equation, test in 1D continuum case

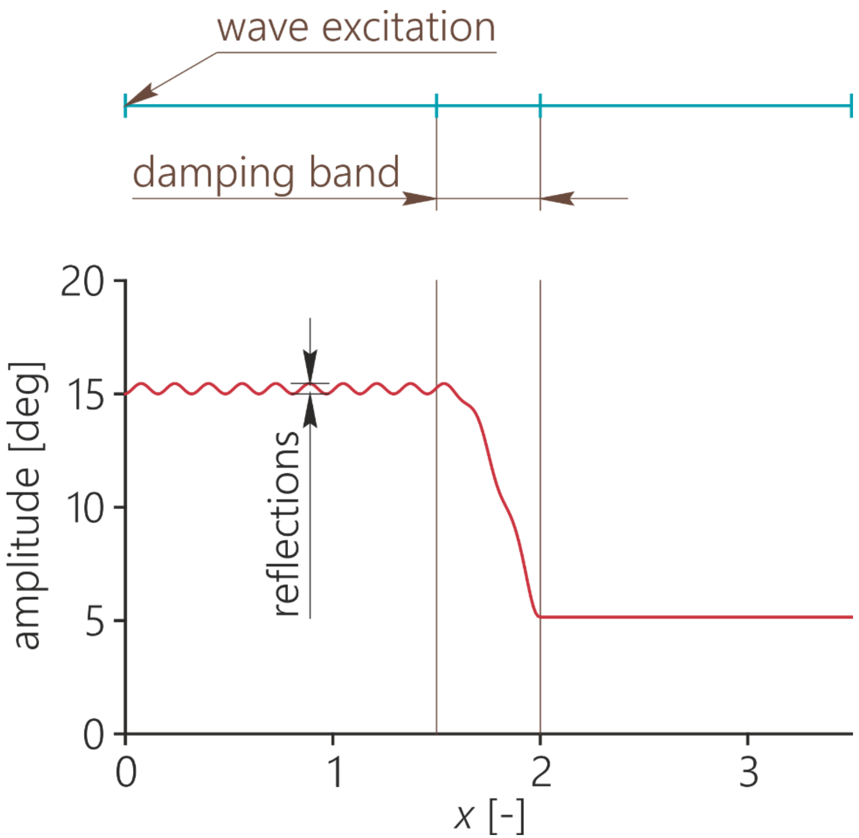
$$\frac{\partial}{\partial t}\vec{m} = -\beta_L \vec{m} \times \vec{H} - \alpha_L \vec{m} \times \left(\vec{m} \times \vec{H}\right) - \vec{m} \times \left(\vec{m} \times \vec{f}\right)$$

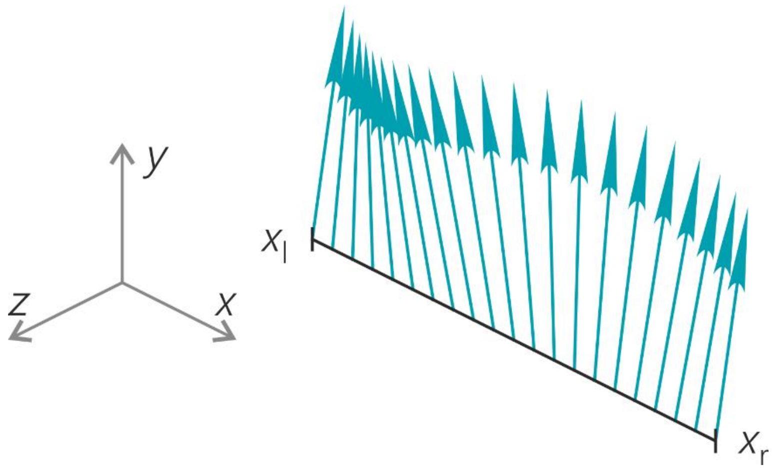
$$\vec{f} = g(x)\, \vec{m}_A \sqrt{\left|\frac{\partial}{\partial t}\vec{m}\right|}$$



[Poluektov Eriksson Kreiss 2016 *Commun. Comput. Phys.* **20** 969–988]

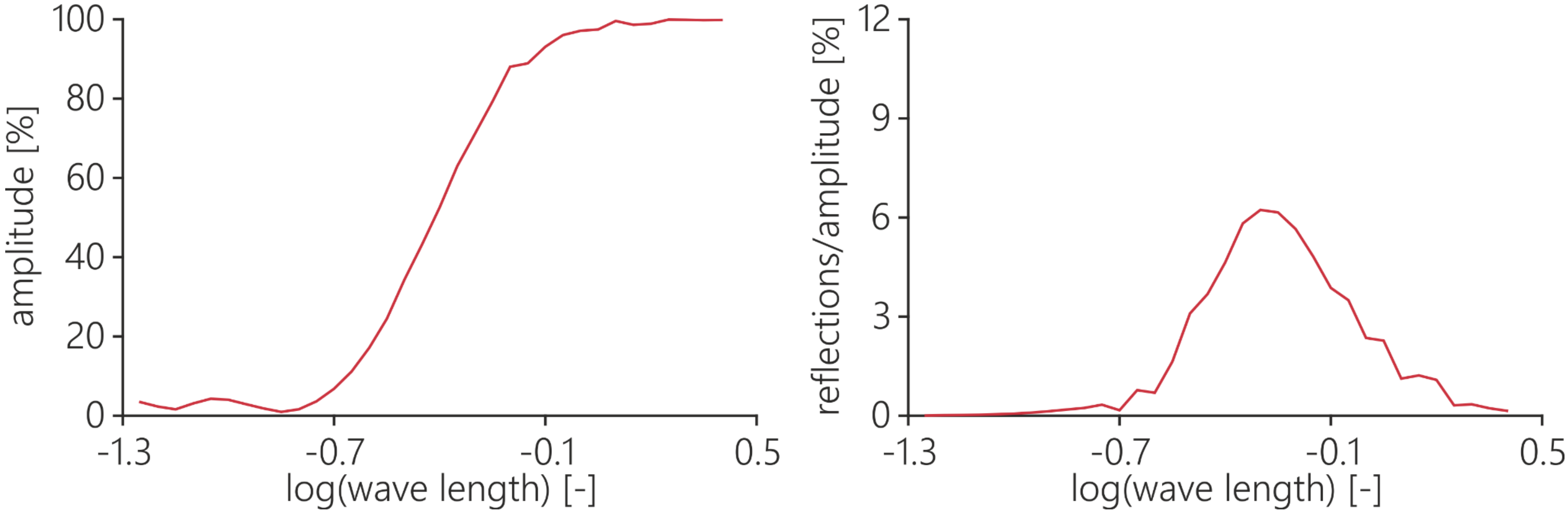
Spin waves





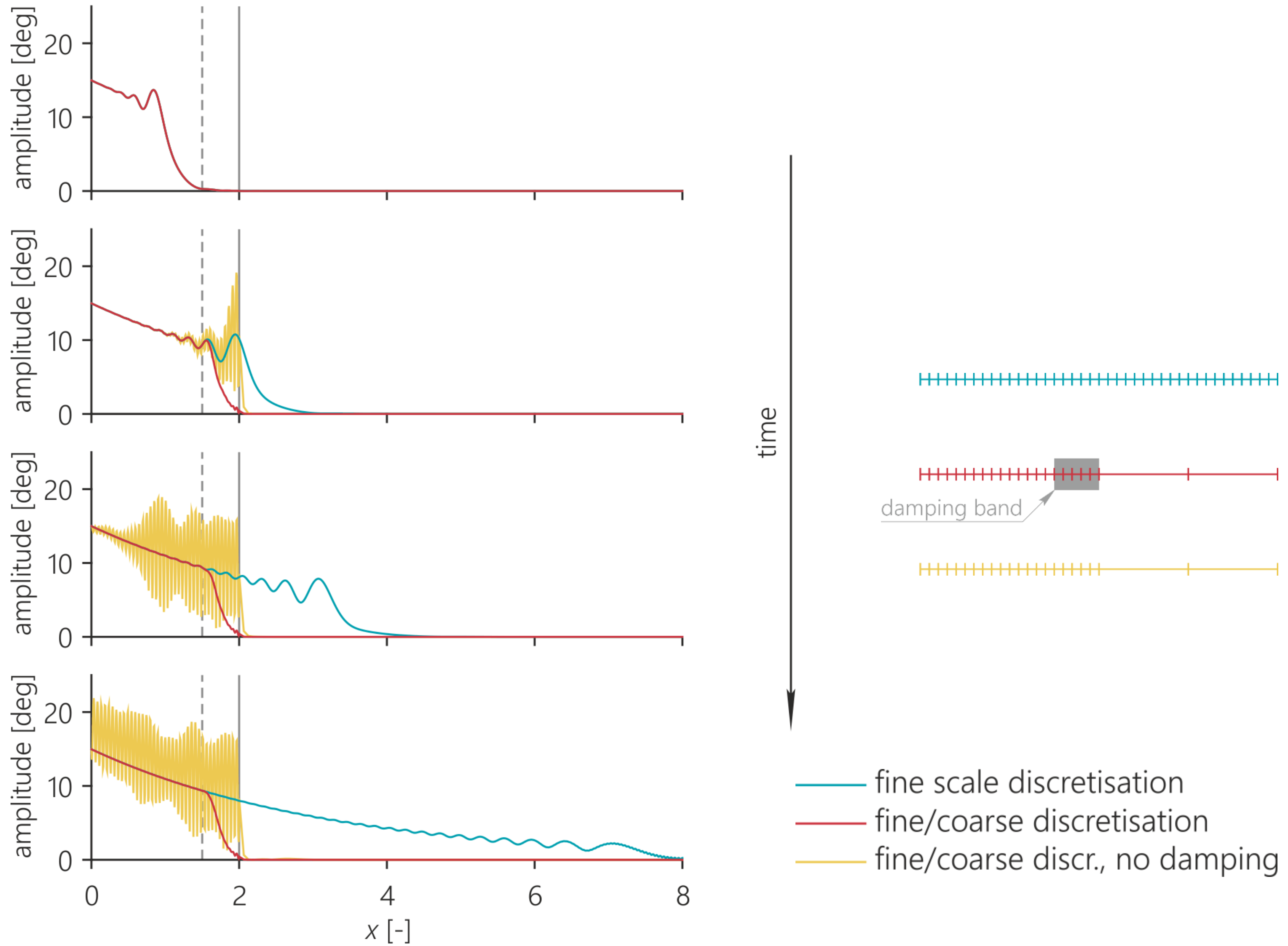
width of the damping band determines the scale of reflections from it

Amplitude–frequency

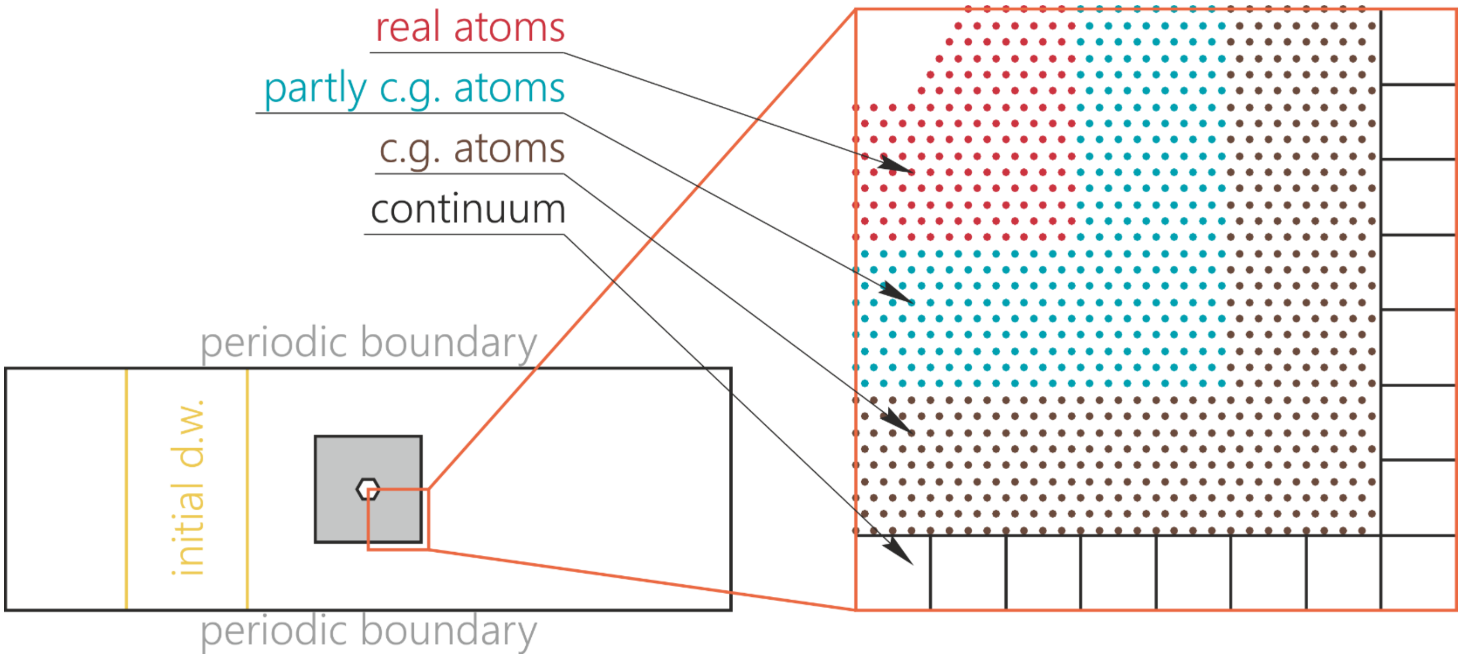


- uniform fine scale
- attenuation of small wave lengths, low-pass filter
- finite error due to reflections from the damping band
- the size of averaging window determines the cutoff wave length

Spin waves, 1D example

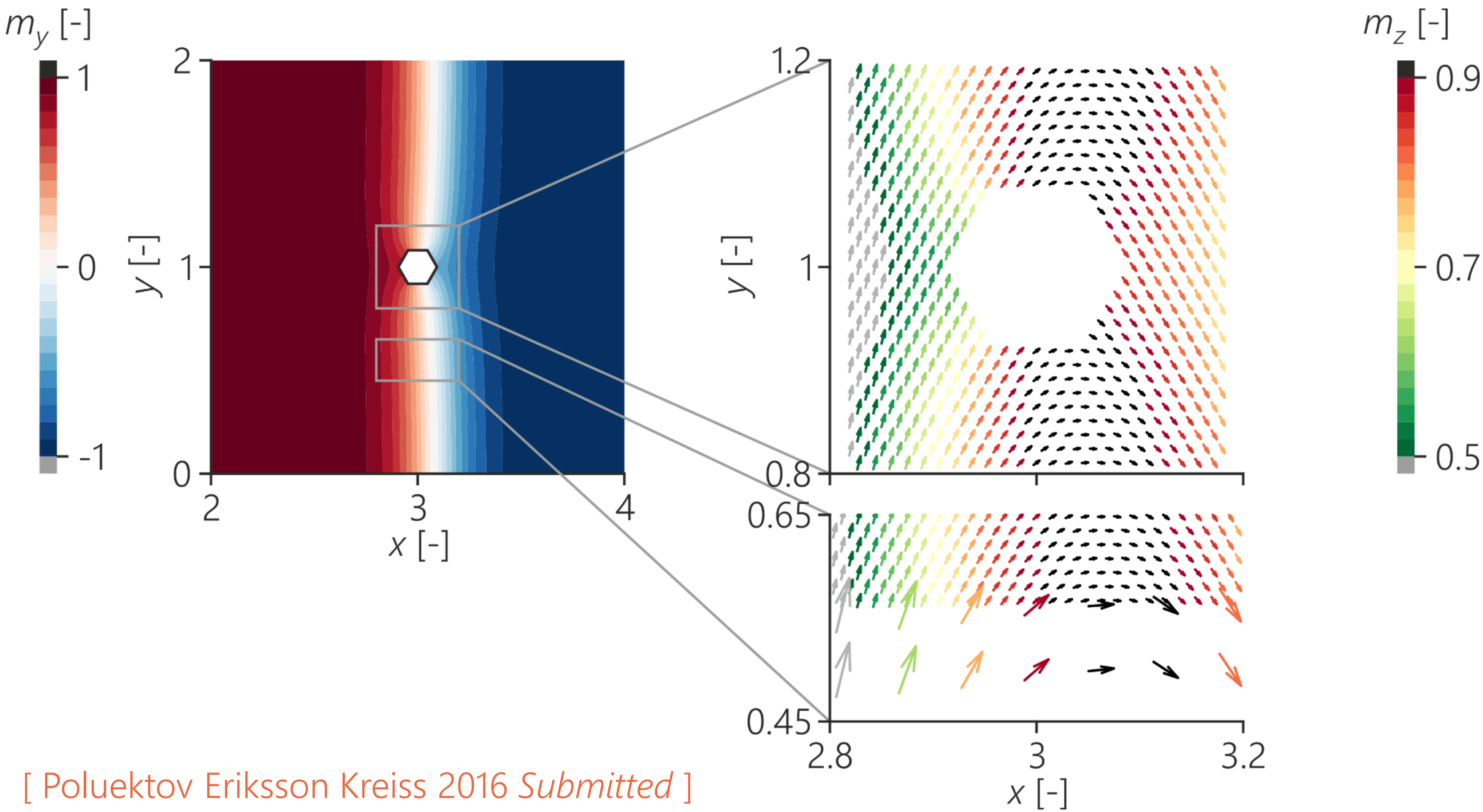


Material with the void



- magnetic field-induced movement of the domain wall
- layer of numerically-damped atoms
- non-refined mesh at the interface

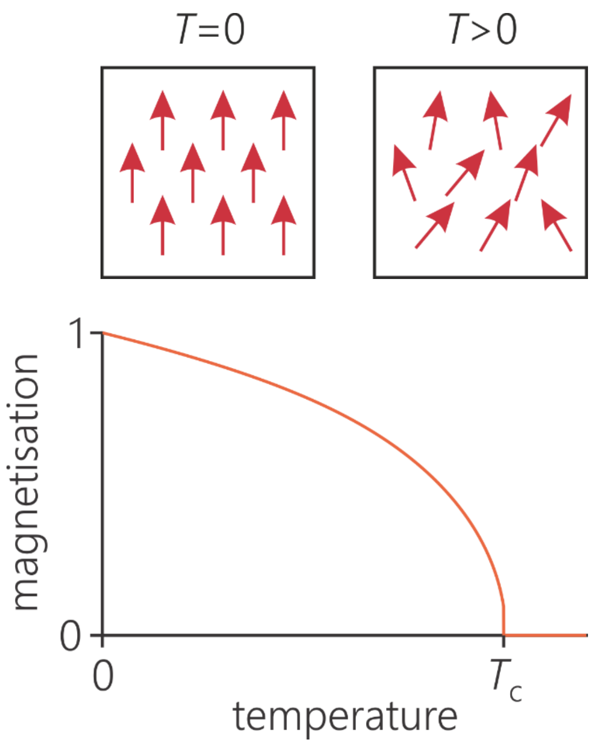
Domain wall around the void



[Poluektov Eriksson Kreiss 2016 *Submitted*]

Magnetism, finite temperatures

Finite temperatures



- additional noise term

$$\frac{\partial}{\partial t}\vec{m}_i = -\beta_L \vec{m}_i \times \vec{H}_i - \alpha_L \vec{m}_i \times \left(\vec{m}_i \times \vec{H}_i\right)$$

$$\vec{H}_i = [\text{deterministic terms}] + \vec{h}_i$$

$$\langle h_{i\rho}(t)\rangle = 0, \quad \langle h_{i\rho}(t)\, h_{j\nu}(s)\rangle = 2D\delta_{ij}\delta_{\rho\nu}\delta(t-s)$$

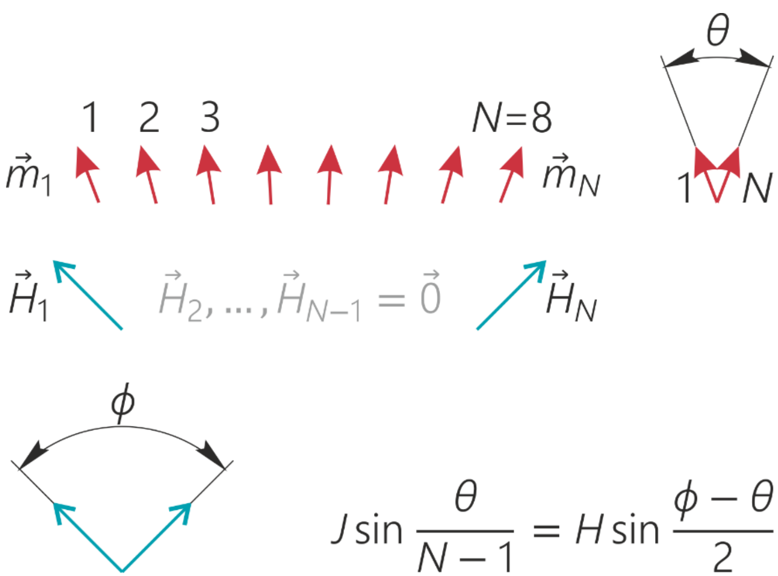
$$D = k_B T \frac{\alpha_L}{\beta_L \mu \gamma}$$

- decreasing magnetisation length
  - volume-average
- assumption: deterministic continuum description is applicable
  - other models (stochastic PDEs) are available

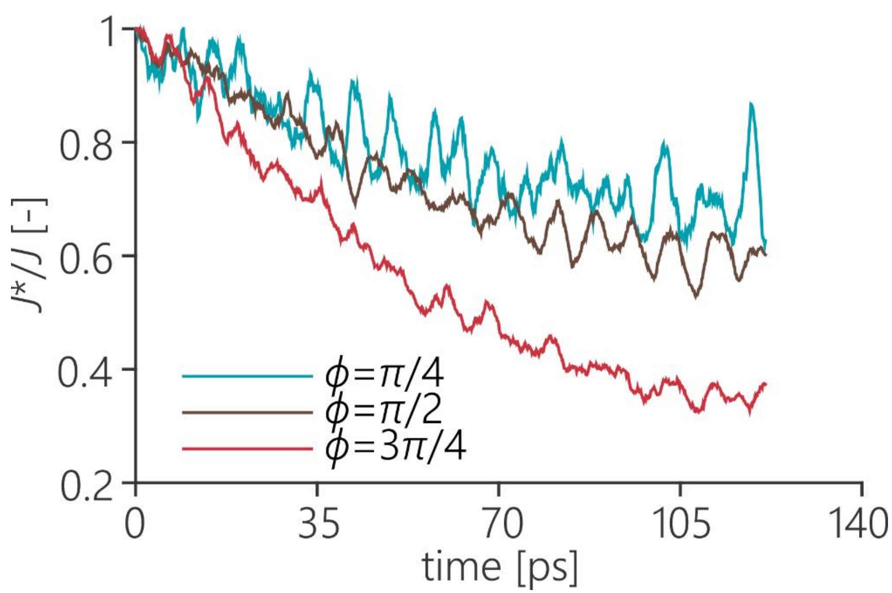
$$\vec{m} = \vec{m}^* s, \quad s = s(T), \quad \left|\vec{m}^*\right| = 1$$

Nonlinear effective exchange

- this assumption is not always correct, example: chain of 8 spins
- replace spins at $T>0$, which have exchange constant J, with spins at $T=0$, which have exchange constant J^*



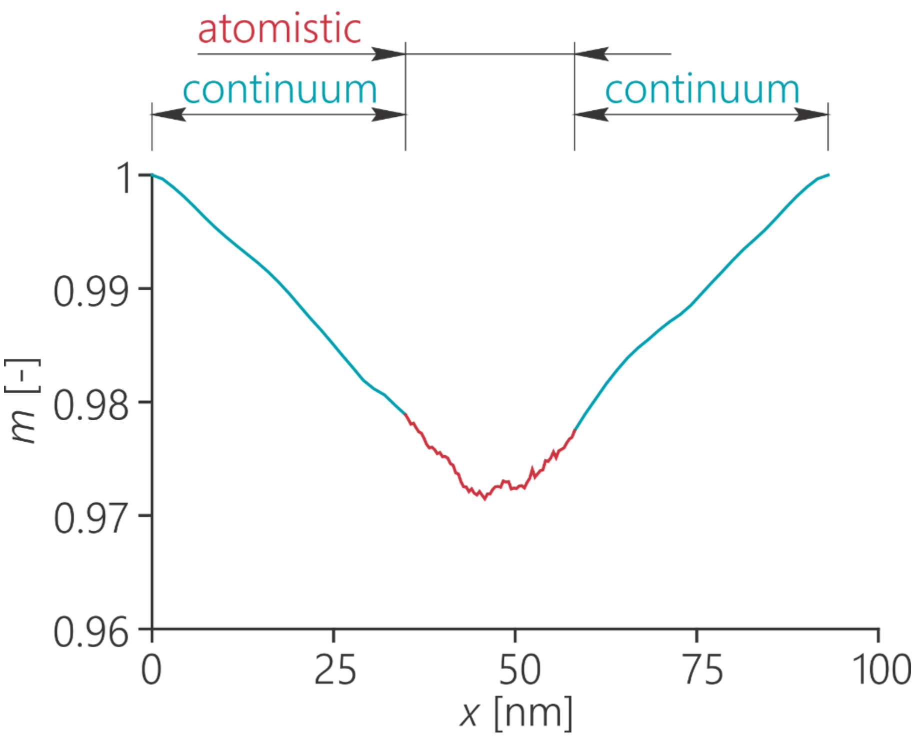
$$J \sin \frac{\theta}{N-1} = H \sin \frac{\phi - \theta}{2}$$



[Arjmand Poluektov Kreiss 2016 *In Preparation*]

Controlling magnetisation length

- unphysical wave propagation out of the atomistic region
  - damping band filters out waves which cannot be represented in the continuum region (by design)
  - ensemble averaging reduces $m(x)$
- continuum description relies on constant $m(x)$
- example: Dirichlet boundary conditions for the continuum



[Arjmand Poluektov Kreiss 2016 *In Preparation*]

Conclusions

- local/nonlocal mismatch at the atomistic-continuum interface
  - transition region with partly coarse-grained atoms
- damping zone at the interface eliminates wave reflections
  - finite width (depends on desired accuracy)
- severe limitations at finite temperatures

Open problems

- long-range (dipole) interaction
- PML-type damping zone
- eliminate the mismatch between continuum and atomistic descriptions
  - T=0
  - something similar to Cauchy-Born rule in mechanics
- HMM-type multiscale approach for finite-temperature spin dynamics
- deterministic continuum description for finite-temperature dynamics that avoids assumptions regarding magnetisation length (?)