Continuum Multiscale Modeling of Magnetic Composites for Engineering Applications

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Industry-academia day on computer simulations of material properties
May 16th 2018, Liège

Some background

- I am a professor at the University of Liège, where I lead a team of about 15 people at the intersection of applied mathematics, scientific computing and engineering physics
- Our research interests: modeling, analysis, algorithm development, and simulation for problems arising in various areas of engineering and science
- Currently: electromagnetics, biomedical problems, geophysics
- Innocent is a former PhD student, currently post-doc at Columbia University

Some background

- We write quite a lot of codes, mostly partial differential equation solvers
- Free and open source software:
  - Gmsh: mesh generator with built-in CAD engine and post-processor (http://gmsh.info)
  - GetDP: general finite element solver using mixed finite elements (http://getdp.info)
  - Combined through ONELAB (http://onelab.info): lightweight interface

Some background

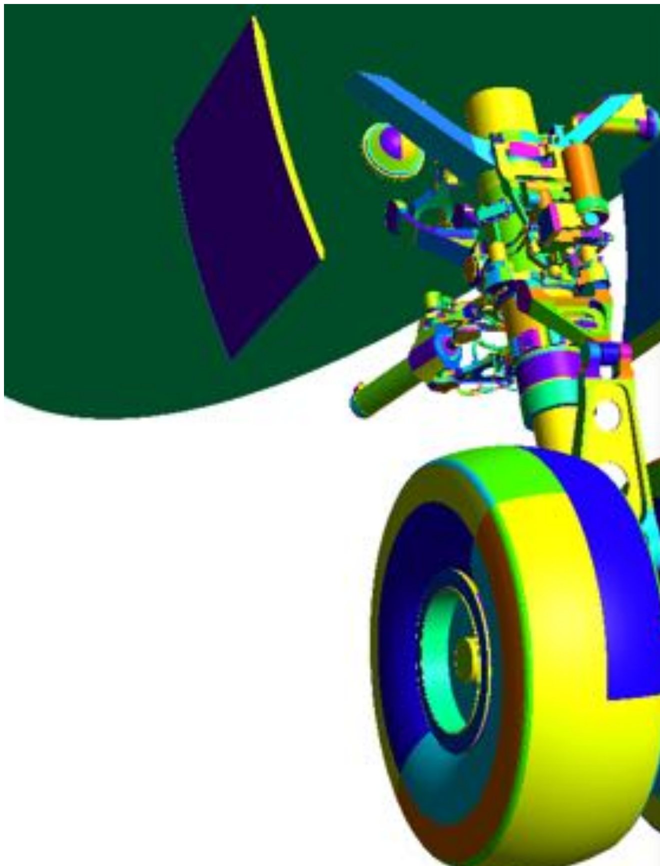
Today, Gmsh, GetDP and ONELAB represent

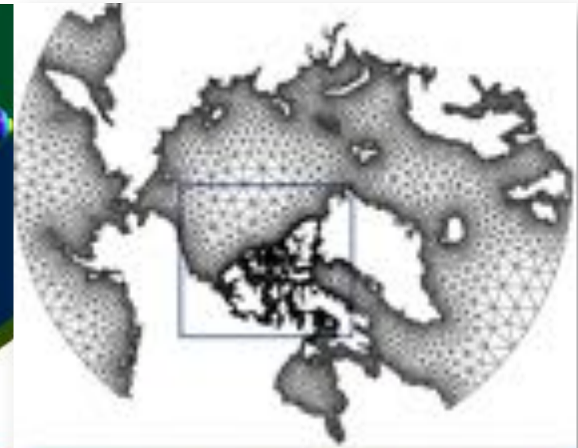
- about half a million lines of (mostly C++) code
- 3 core developers, about 100 with >= 1 commit
- about 1,000 people on mailing lists
- about 10,000 downloads per month
- About 500 citations per year – the Gmsh paper alone is cited about 3,000 times
- Gmsh probably one of the most popular open source finite element mesh generator in the world

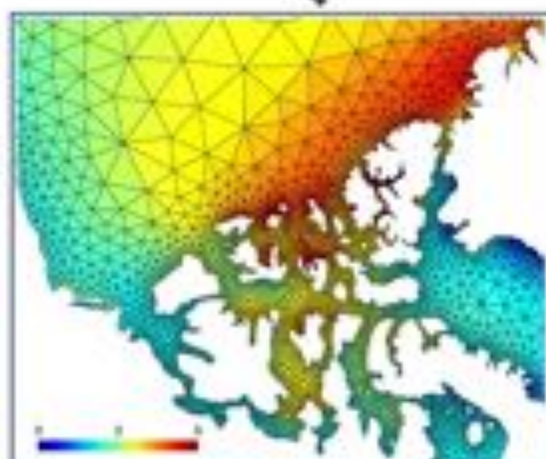
A flavour of our recent work on multiscale models and methods

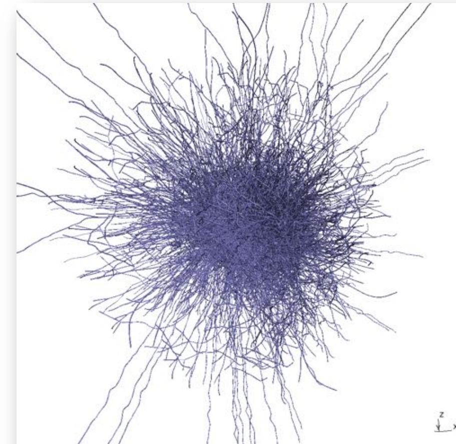
Brute-force discretization…

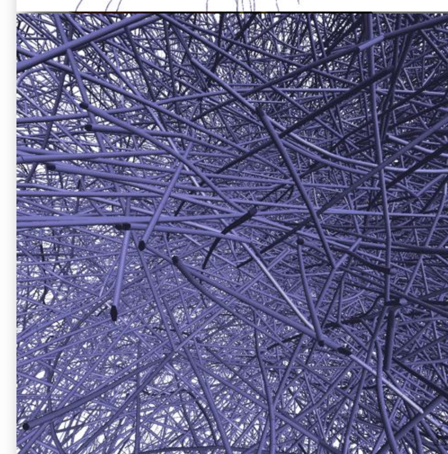
… of the underlying partial differential equations, in space and time



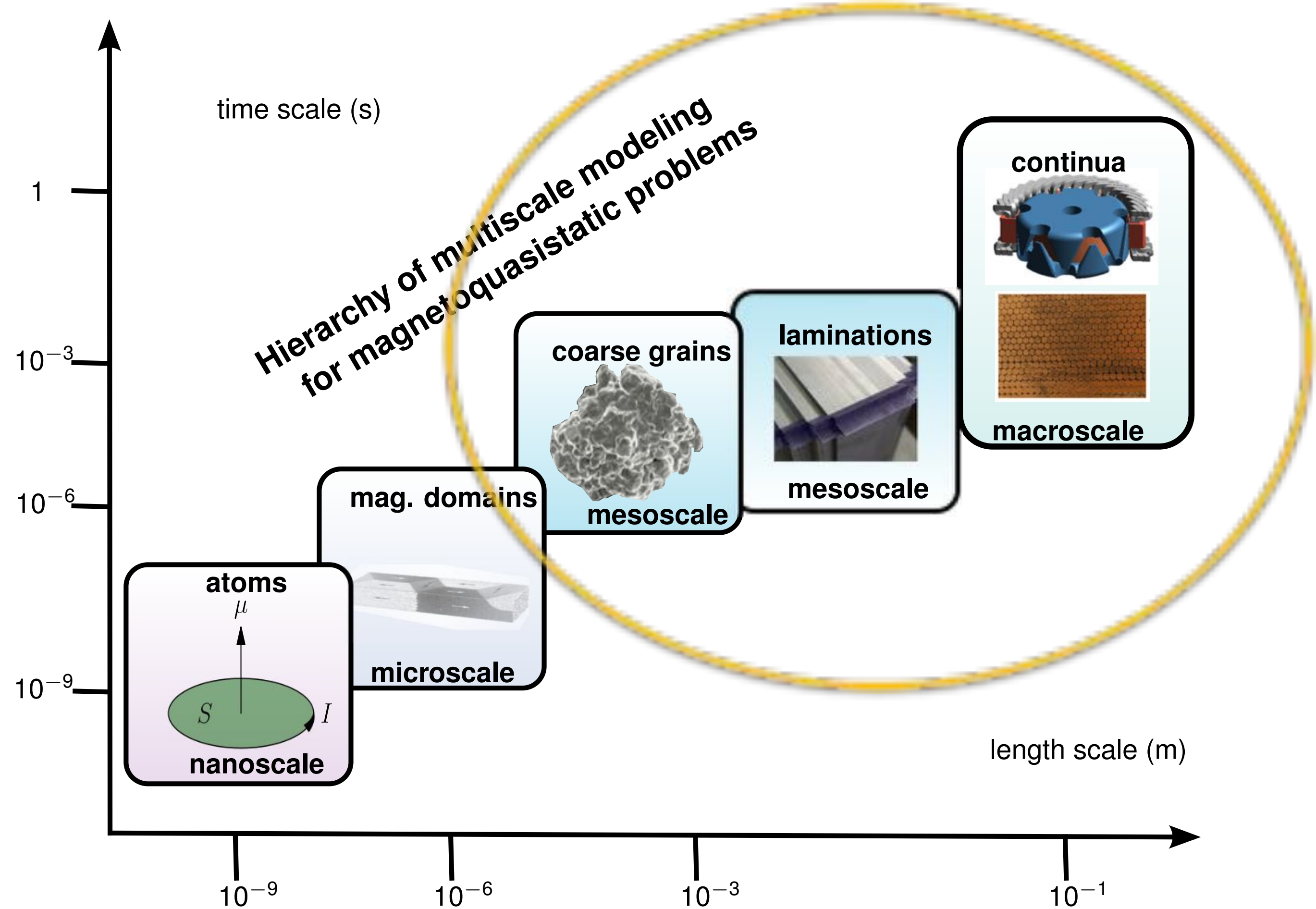








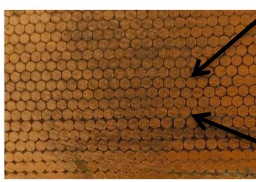
Focus today: multiscale magnetoquasistatics

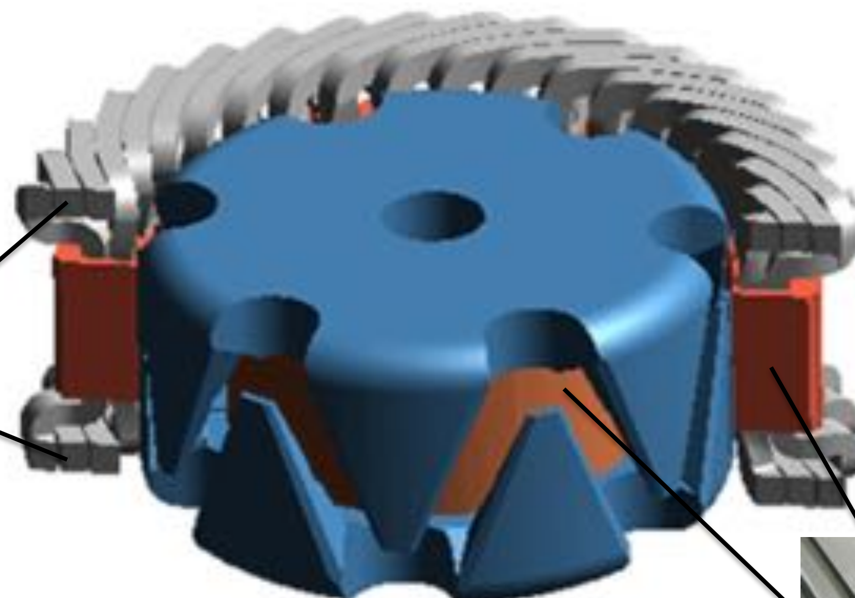


Typical engineering application

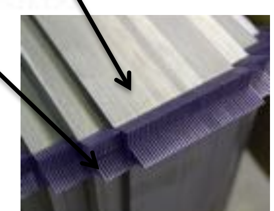
Dynamic modelling and optimization of industrial-complexity electromagnetic energy conversion system

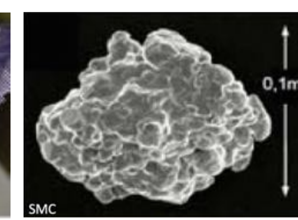
Coil windings





Steel lamination stacks or soft magnetic composites

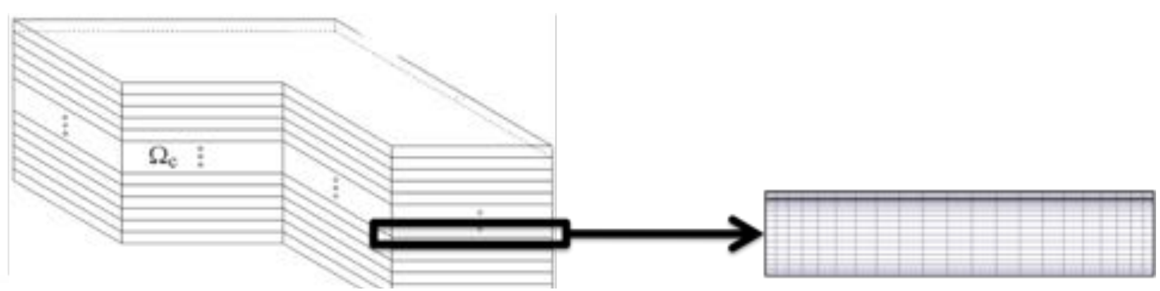




Goal

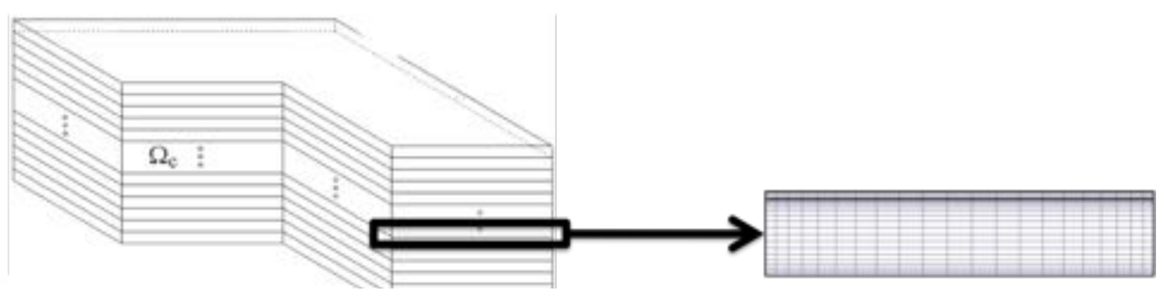
Improve performance/increase energy conversion efficiency

- Requires accurate, high-fidelity simulations
  - Current conversion efficiency is already around 90%
  - Improving by 5% is a tremendous challenge
- Brute-force simulation of a simple 300 sheet lamination stack
  - 25 discretization points per lamination (sheet + insulation)
  - 1000 x 1000 points in transverse direction
  - … leads to 7.5 billion DoF nonlinear, hysteretic system



Multiscale magnetoquasistatics

- Brute-force approach is computationally untractable for design or optimization
  - Simulation on a laptop ~ 1 million DoFs
  - Simulations on HPC clusters ~ 1 billion DoFs
- Reduce the cost with **two-scale computational homogenization**
  - Continuum models (magnetoquasistatics, i.e. Maxwell system without displacement currents) on both coarse and fine scales
  - Thermodynamic hysteresis model for anything below

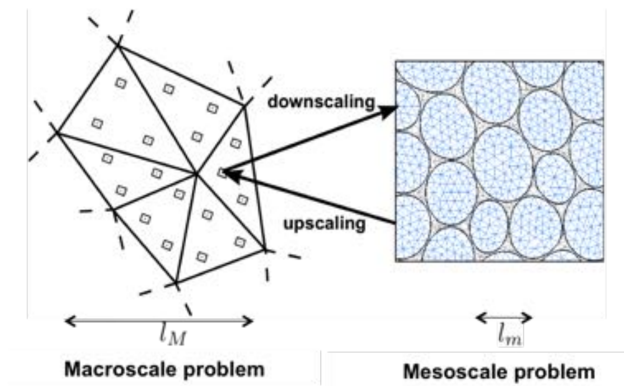


Wish list

- Homogenized problem that is easy to solve
- Macroscale solution that represents the average behavior
- Possibility to handle
  - Nonlinear, irreversible material behavior
  - Complex microstructures with stochastic distribution of heterogeneities
- Possibility to recover local fields around points of interest
- Accurate computation of global (engineering) quantities
  - Eddy current losses
  - Magnetic losses

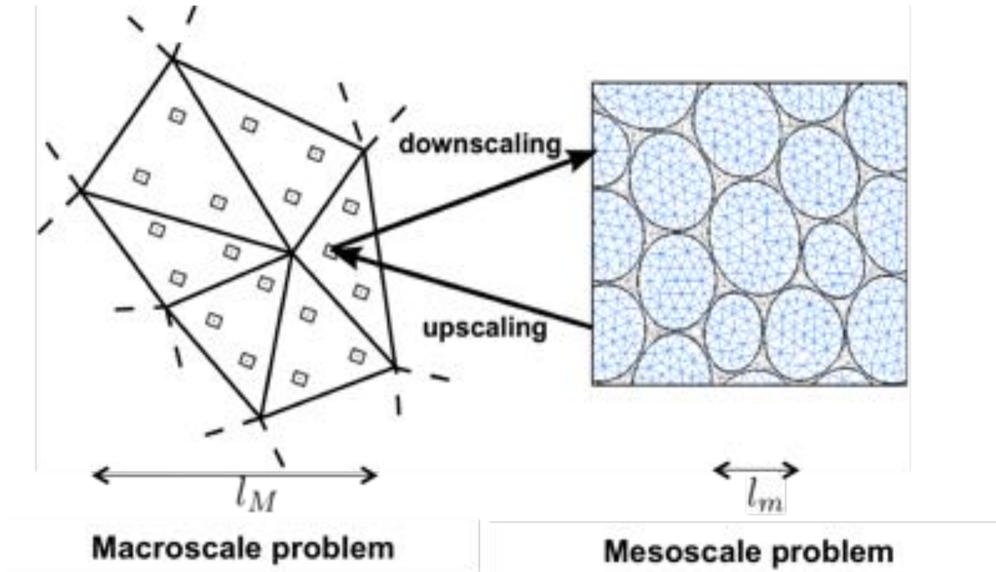
Multiscale modelling: a bit of history

- Homogenization theories
  - 1892: Classical mixing rules (Rayleigh - Maxwell - Garnett)
  - 1969: G-convergence (Spagnolo)
  - 1975: Γ-convergence (De Giorgio)
  - 1978: **Asymptotic expansion method (Bensoussan - Papanicolaou - Lions - Palencia)**
  - 1979: Stochastic homogenization (Kozlov - Papanicolaou - Varadhan)
  - 1984: H-convergence (Tartar)
  - 1989: **Two-scale convergence (Nguetseng - Allaire)**
  - 2002: **Periodic unfolding method (Cioranescu)**



- Multiscale methods
  - 1965: Mean-field homogenization – MFH (Hill)
  - 1994: FFT-based homogenization (Moulinec – Suquet)
  - 1997: Multiscale Finite Element Method – MsFEM (Hou)
  - 1998: Variational Multiscale Method – VMS (Hughes)
  - 2003: **Heterogeneous Multiscale Method – HMM (E)**

Heterogeneous Multiscale Method (HMM)



scale separation

$l_m \ll l_M$

1. **Derivation of the governing PDEs** using the homogenization theory
2. **Development of weak multiscale formulations** (**b**- and **h**-conforming formulations)
3. **Numerical resolution of the homogenized problem**

HMM: convergence of fields

Use classical and two-scale convergence theories to derive the homogenized problem $\rightarrow$ fields belong to appropriate function spaces

Convergence of electromagnetic fields:

$$\boldsymbol{h}^{\varepsilon} \underset{2}{\rightharpoonup} \boldsymbol{h}_m = \boldsymbol{h}_M + \textbf{grad}_y\, \phi_c \quad \text{in } \boldsymbol{L}^2(\mathbb{R}^3 \times \mathcal{Y}), \qquad \boldsymbol{h}^{\varepsilon} \rightharpoonup \boldsymbol{h}_M \quad \text{in } \boldsymbol{L}^2(\mathbb{R}^3),$$

$$\boldsymbol{b}^{\varepsilon} \underset{2}{\rightharpoonup} \boldsymbol{b}_m = \boldsymbol{b}_M + \textbf{curl}_y\, \boldsymbol{a}_c \quad \text{in } \boldsymbol{L}^2(\mathbb{R}^3 \times \mathcal{Y}), \qquad \boldsymbol{b}^{\varepsilon} \rightharpoonup \boldsymbol{b}_M \quad \text{in } \boldsymbol{L}^2(\mathbb{R}^3).$$

Convergence of fields involving differential operators:

$$\textbf{curl}\, \boldsymbol{h}^{\varepsilon} \underset{2}{\rightharpoonup} \textbf{curl}_x\, \boldsymbol{h}_M + \textbf{curl}_y\, \boldsymbol{h}_c \quad \text{in } \boldsymbol{L}^2(\mathbb{R}^3 \times \mathcal{Y}),$$

$$\text{div}\, \boldsymbol{b}^{\varepsilon} \underset{2}{\rightharpoonup} \text{div}_x\, \boldsymbol{b}_M + \text{div}_y\, \boldsymbol{b}_c \quad \text{in } \boldsymbol{L}^2(\mathbb{R}^3 \times \mathcal{Y}),$$

$$\textbf{curl}\, \boldsymbol{h}^{\varepsilon} \rightharpoonup \textbf{curl}_x\, \boldsymbol{h}_M \quad \text{in } \boldsymbol{L}^2(\mathbb{R}^3),$$

$$\text{div}\, \boldsymbol{b}^{\varepsilon} \rightharpoonup \text{div}_x\, \boldsymbol{b}_M \quad \text{in } \boldsymbol{L}^2(\mathbb{R}^3).$$

HMM: derivation of MQS equations

Multiscale problem

$$\textbf{curl}\, \boldsymbol{h}^{\varepsilon} = \boldsymbol{j}^{\varepsilon}, \qquad \boldsymbol{h}^{\varepsilon} = \mathcal{H}(\boldsymbol{b}^{\varepsilon}),$$
$$\textbf{curl}\, \boldsymbol{e}^{\varepsilon} = -\partial_t \boldsymbol{b}^{\varepsilon}, \qquad \boldsymbol{j}^{\varepsilon} = \sigma\, \boldsymbol{e}^{\varepsilon}.$$
$$\mathrm{div}\, \boldsymbol{b}^{\varepsilon} = 0,$$

Mesoscale problem derived using the two-scale convergence theory (macroscale sources)

$$\textbf{curl}\, \boldsymbol{h}_m = \boldsymbol{j}_m, \qquad \boldsymbol{h}_m = \mathcal{H}(\boldsymbol{b}_M + \boldsymbol{b}_c),$$
$$\textbf{curl}_x\, \boldsymbol{e}_M + \textbf{curl}_y\, \boldsymbol{e}_c = -\partial_t \boldsymbol{b}_m, \qquad \boldsymbol{j}_m = \sigma(\boldsymbol{e}_M + \boldsymbol{e}_c).$$
$$\mathrm{div}_x\, \boldsymbol{b}_M + \mathrm{div}_y\, \boldsymbol{b}_c = 0,$$

Macroscale problem derived using the classical convergence theory (upscaled material law)

$$\textbf{curl}\, \boldsymbol{h}_M = \boldsymbol{j}_M, \qquad \boldsymbol{h}_M = \mathcal{H}_M(\boldsymbol{b}_M + \boldsymbol{b}_c),$$
$$\textbf{curl}_x\, \boldsymbol{e}_M = -\partial_t \boldsymbol{b}_M, \qquad \boldsymbol{j}_M = \sigma_M \boldsymbol{e}_M.$$
$$\mathrm{div}_x\, \boldsymbol{b}_M = 0,$$

HMM: downscaling

Transfer of the macroscale sources terms $\boldsymbol{b}_M, \boldsymbol{e}_M$ and $\boldsymbol{j}_M$ to meso-problems.
Definition of boundary conditions for meso-problems:

- Mesoscale fields involve macroscal sources:

$$\mathbf{curl}_x\, \boldsymbol{e}_M + \mathbf{curl}_y\, \boldsymbol{e}_c = \mathbf{curl}_y \Big(\kappa(\mathbf{curl}_x\, \boldsymbol{e}_M \times \boldsymbol{y}) + \boldsymbol{e}_c \Big),$$

$$\boldsymbol{b}_m = \mathbf{curl}_y\, \boldsymbol{a}_c + \boldsymbol{b}_M,$$

- The two-scale convergence theory leads the periodic boundary conditions:

$$\frac{1}{|\Omega_m|} \int_{\Omega_m} \boldsymbol{b}_m \, \mathrm{d}\boldsymbol{y} = \boldsymbol{b}_M \qquad \text{fulfilled if} \qquad \oint_{\Gamma_m} \boldsymbol{n} \times \boldsymbol{a}_c \, \mathrm{d}\boldsymbol{y} = \mathbf{0}.$$

$$\frac{1}{|\Omega_m|} \int_{\Omega_m} \boldsymbol{j}_m \, \mathrm{d}\boldsymbol{y} = \boldsymbol{j}_M \qquad \Longleftrightarrow \int_{\Omega_m} \boldsymbol{j}_c \, \mathrm{d}y = \mathbf{0}.$$

HMM: upscaling

Computation of the missing macroscale constitutive laws from mesoscale fields:

The homogenized electric conductivity is derived using the asymptotic expansion:

$$(\sigma_M)_{ij} = \frac{1}{|\Omega_m|}\int_{\Omega_m}\Big((\sigma)_{ij} - (\sigma)_{ik}\frac{\partial \chi_j}{\partial y_k}\Big)\mathrm{d}y,$$

where χ_j is the solution of the cell problem

$$\int_{\Omega_m}\Big(\sigma(\mathbf{grad}_y\,\chi_j - \boldsymbol{e}_j)\cdot \mathbf{grad}_y\,\chi_j^{'}\Big)\mathrm{d}y = 0.$$

The homogenized magnetic constitutive law is derived using the two-scale convergence

$$\boldsymbol{\mathcal{H}}_M(\boldsymbol{b}_M + \boldsymbol{b}_c) = \frac{1}{|\Omega_m|}\int_{\Omega_m}\boldsymbol{\mathcal{H}}(\boldsymbol{b}_M + \boldsymbol{b}_c)\mathrm{d}y.$$

Computed using finite differences

Computation of the tangent

$$\frac{\partial \boldsymbol{\mathcal{H}}_M}{\partial \boldsymbol{b}_M} = \frac{1}{|\Omega_m|}\int_{\Omega_m}\Big(\frac{\partial \boldsymbol{\mathcal{H}}}{\partial \boldsymbol{b}_M} + \frac{\partial \boldsymbol{\mathcal{H}}}{\partial \boldsymbol{b}_c}\frac{\partial \boldsymbol{\mathcal{B}}_c}{\partial \boldsymbol{b}_M}\Big)\mathrm{d}y.$$

HMM: pseudo-code

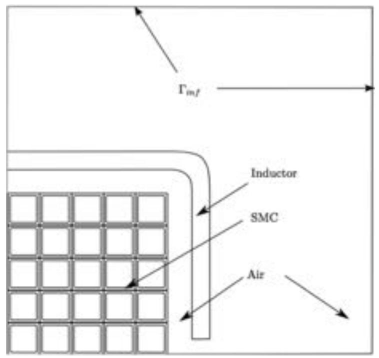
Algorithm 1 Pseudocode of the FE-HMM method for the MQS problem

begin
- $t \leftarrow t_0$, initialize the macroscale field $\boldsymbol{a}_{\mathrm{M}}|_{t_0} = \boldsymbol{a}_{\mathrm{M}0}$,
- *# begin the macroscale time loop (index k)*
- **for** $(k \leftarrow 1$ **to** $N_{TS})$ **do**
  - *# begin the macroscale NR loop (index j)*
  - **for** $(i \leftarrow 1$ **to** $N_{NR}^{\mathrm{M}})$ **do**
    - *# parallel resolution of mesoscale problems (index i)*
    - **for** $(i \leftarrow 1$ **to** $N_{GP})$ **do**
      - downscale the sources,
      - solve N_{meso} meso-problems per Gauß point on $[t, t + \Delta t_{\mathrm{M}}]$,
      - **compute the homogenized law** $\boldsymbol{\mathcal{H}}_{\mathrm{M}}^{(i)}$ **and** $\partial \boldsymbol{\mathcal{H}}_{\mathrm{M}}^{(i)} / \partial \boldsymbol{b}_{\mathrm{M}}^{(i)}$,
      - upscale the homogenized law $\boldsymbol{\mathcal{H}}_{\mathrm{M}}^{(i)}$ and $\partial \boldsymbol{\mathcal{H}}_{\mathrm{M}}^{(i)} / \partial \boldsymbol{b}_{\mathrm{M}}^{(i)}$,
    - **end**
    - assemble the matrix and the RHS and solve,
  - **end**
- **end**

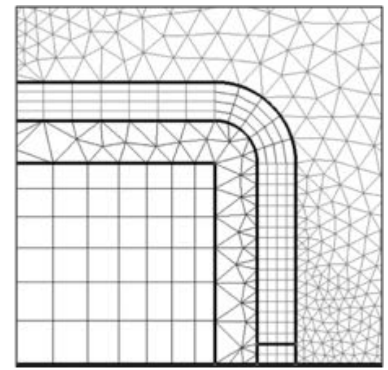
end

HMM: an example

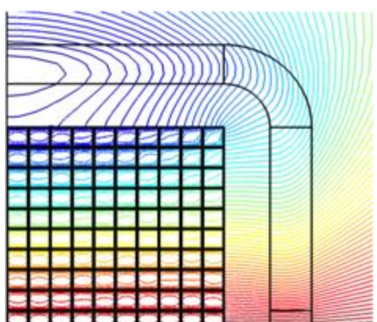
Macro-geometry (reference)



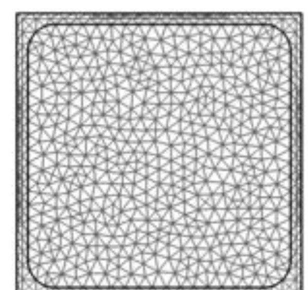
Macro-mesh (macroscale)



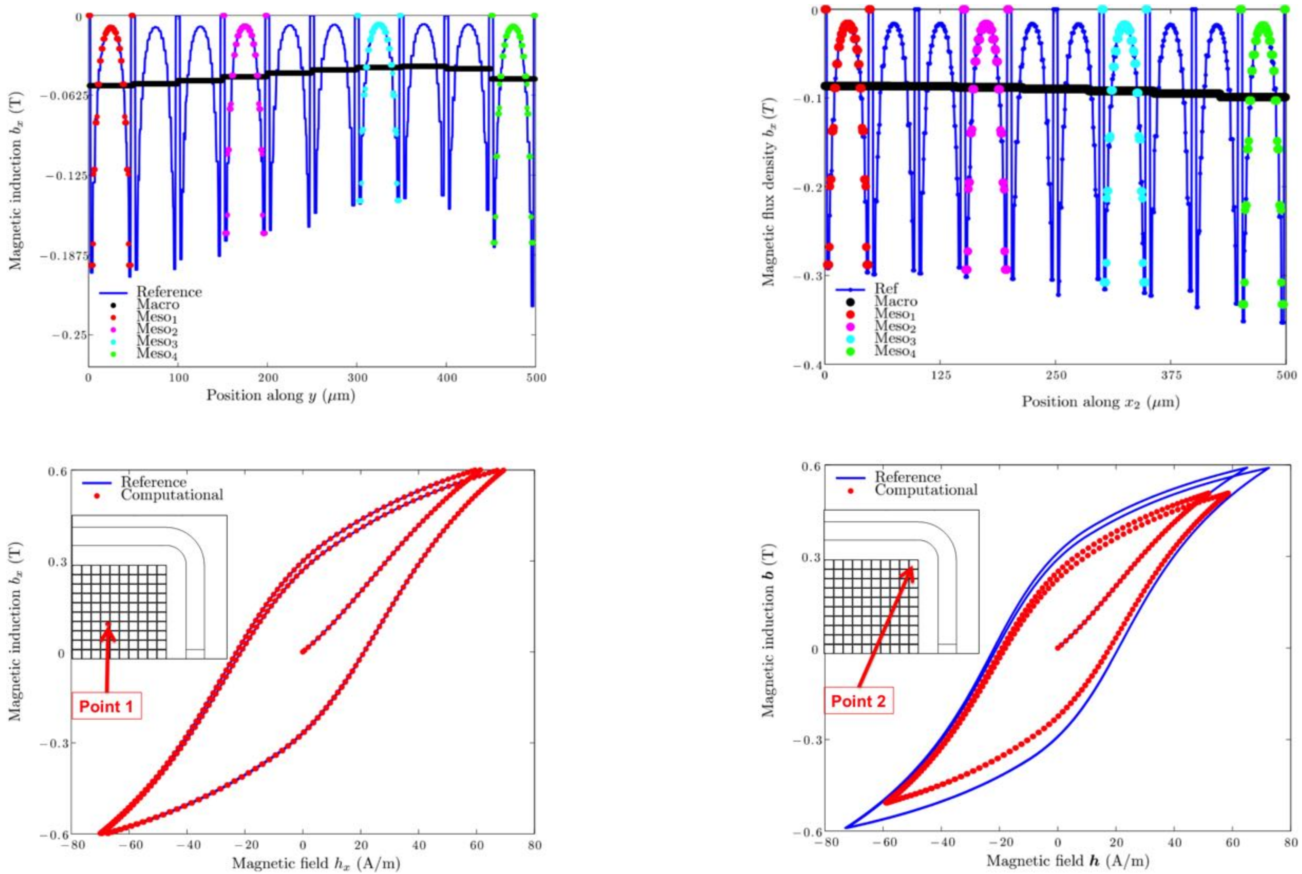
Field lines a_z



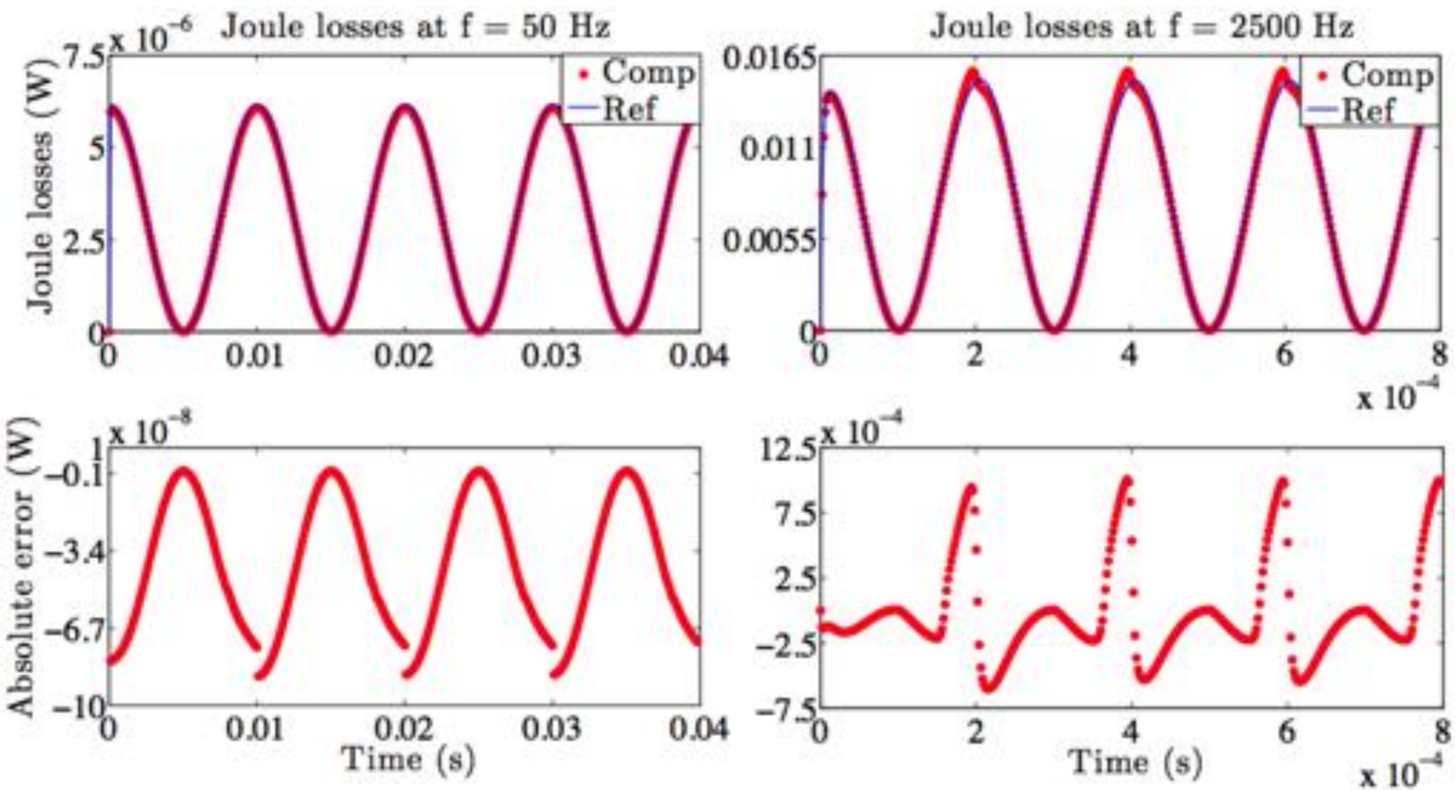
Mesoscale mesh



Recovery of local fields

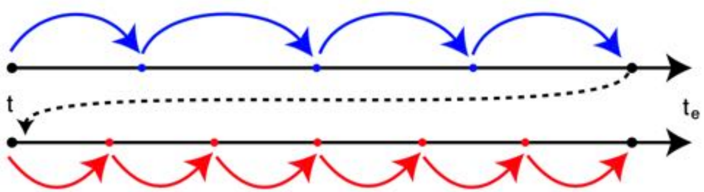


Recovery of global engineering quantities

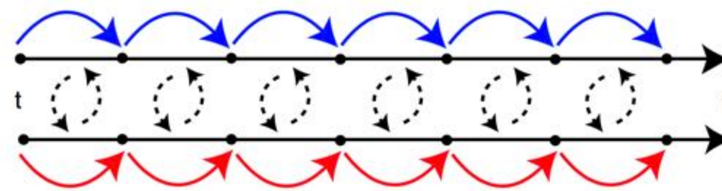


Similar ideas for multiple time scales

One-way coupling/parameter extraction

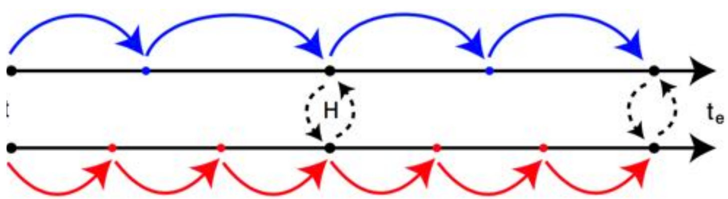


Strong coupling

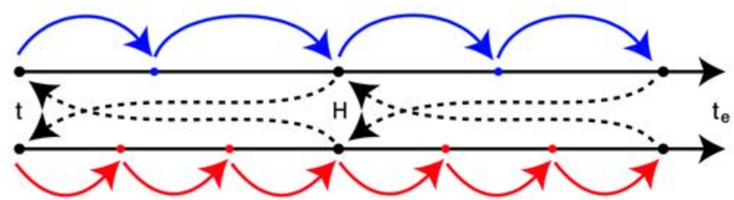


(synchronization in linear solve or during Newton iteration)

Weak coupling



Dynamic iteration/waveform relaxation



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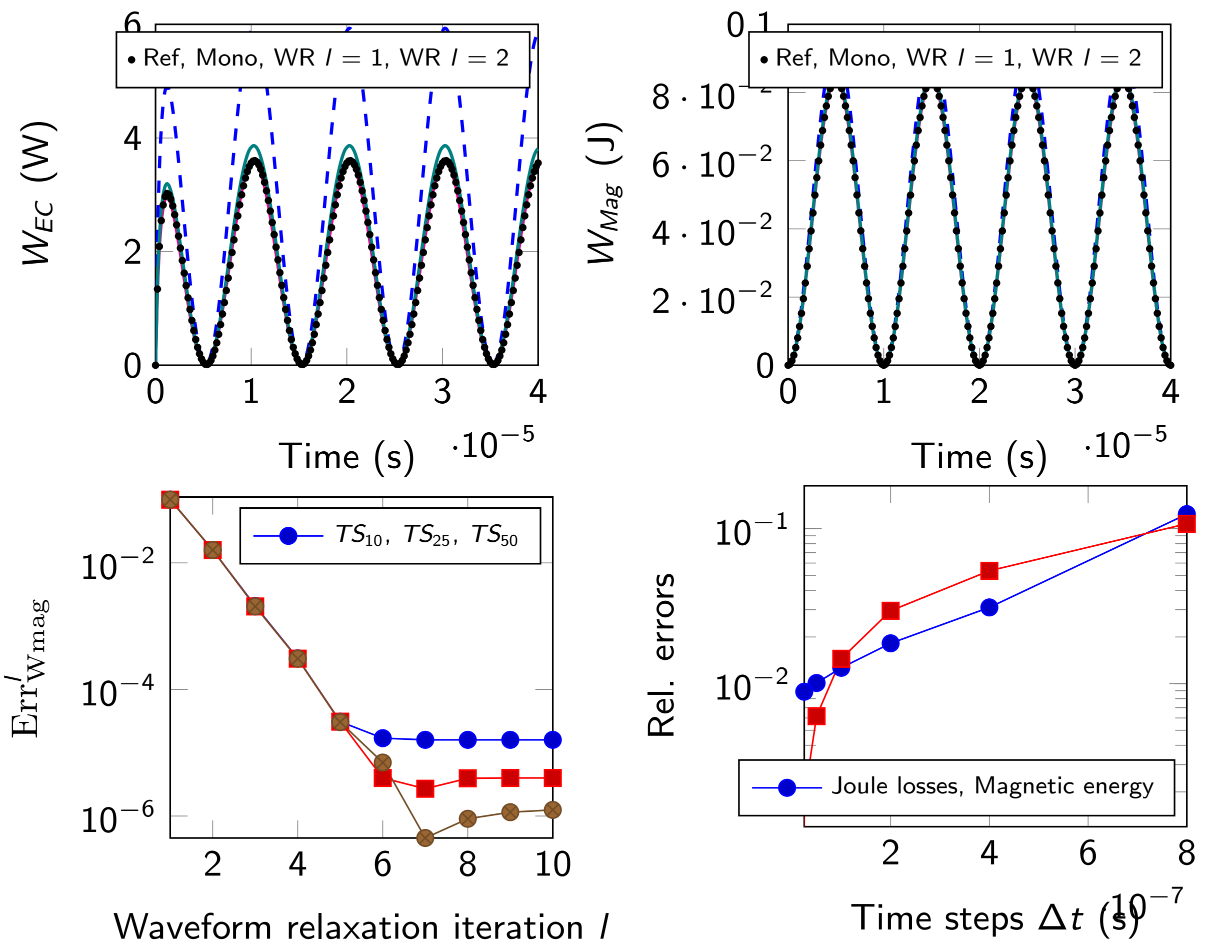

Conclusion

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- Engineering strategy for multiscale magnetoquasistatics
  - Solid mathematical foundation, even for strongly nonlinear problems
  - Embarrassingly parallel computations
  - But still continuum models at both scales

- **My main question for you today**: are there engineering electromagnetic problems where a strong coupling between atomic scales and meso/macro scales is useful?
  - In nano/micro systems? optics/imaging? bio?