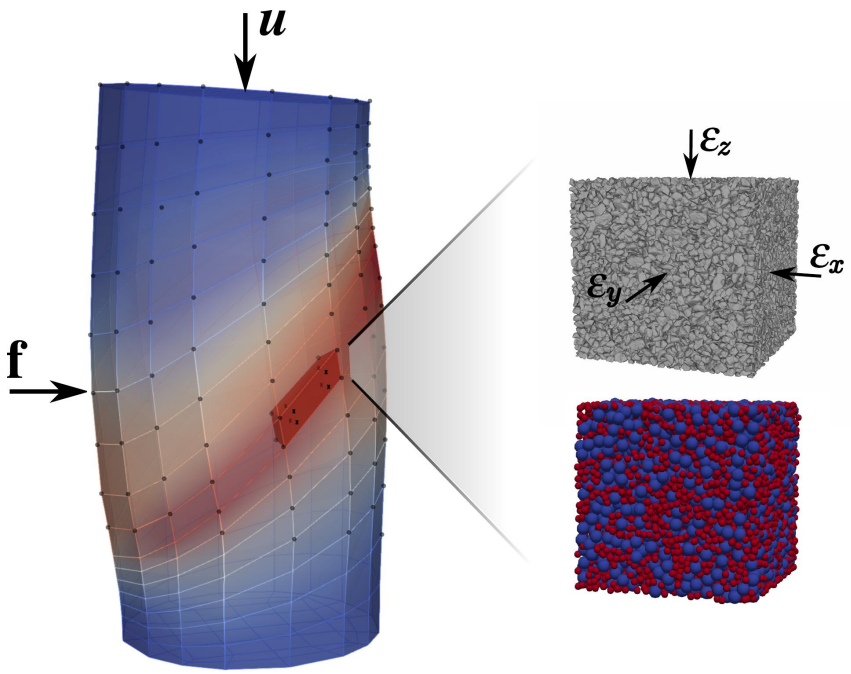

CIVIL-408 Multiscale Modeling in Mechanics

Prof. Kostas Karapiperis

Week 1

Course Organization

I. General Course Information

Instructor:	Prof. Kostas Karapiperis, konstantinos.karapiperis@epfl.ch
TAs:	Thomas Henzel, thomas.henzel@epfl.ch
	Hrishikesh Menon, hrishikesh.menon@epfl.ch
	Dr. Govinda Padmanabha, govinda.ananthapadmanabha@epfl.ch
Lectures:	Wednesdays 16:00-18:00 pm, DIA 003
Exercises:	Thursdays 09:00-11:00 am, DIA 005
Office hours:	By appointment.
Class material:	All course-related material can be found on Moodle.
	Slides uploaded each week.
Textbook:	No required textbook. Optional useful references:
	- Multiscale Modeling, D. M. Kochmann - ETH Zürich (2023)
	- Modeling Materials: Continuum, Atomistic and Multiscale Techniques, E. Tadmor - Cambridge (2011)
	- Particulate discrete element modelling: a geomechanics perspective, C. O'Sullivan - Spon Press (2011)
Exams:	Evaluation throughout the semester. No final exam.
Policy	Students are expected to attend all lectures and exercise sessions. Please bring your computers during exercise sessions of weeks 2,3,4,5,7,8,10. Collaboration during the exercise sessions is allowed and encouraged, yet everyone should ultimately produce their own Python implementation for each project. Late submissions of project reports will not be accepted. Final presentations of research papers will be 20 minutes long each. The dates assigned to each presentation will be uploaded to Moodle.
Grading	Project 1 (40%), Project 2 (40%), Final Presentation (20%)
Contents	The course introduces students to the fundamentals of multiscale modeling applied to mechanics problems. We cover principles and techniques for modeling materials across different spatial scales, from the level of atoms or grains to the continuum or structural scale. Emphasis is placed on hierarchical upscaling (homogenization), while asymptotic and concurrent techniques are also covered.
Prerequisites	Continuum Mechanics (e.g. CIVIL-225)
	Finite Elements (e.g. CIVIL-321)
	Numerical analysis (e.g. MATH-251a)

Course Organization

I. General Course Information

Instructor:	Prof. K
TAs:	Th
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Lectures:	W
Exercises:	T
Office hours:	B
Class material:	A
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Textbook:	N
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	Numerical analysis (e.g. MATH-251a)

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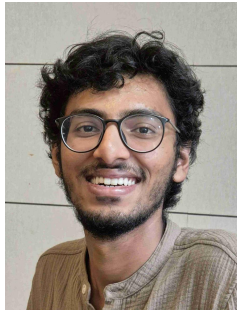
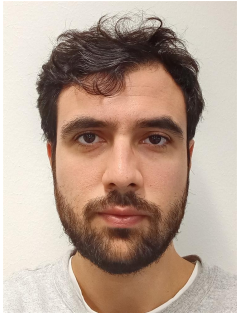
Office hours:	By appointment.

Govinda



Hrishikesh



Thomas

Course Organization

I. General Course Information

Instructor:	Prof. Kostas Karapiperis, konstantinos.karapiperis@epfl.ch
TAs:	Thomas Henzel, thomas.henzel@epfl.ch
	Hrishikesh Menon, hrishikesh.menon@epfl.ch
	Dr. Govinda Padmanabha, govinda.ananthapadmanabha@epfl.ch
Lectures:	Wed
Exercises:	T
Office hours:	B
Class material:	A
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Textbook:	N
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Contents

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Course Organization

II. Tentative syllabus

Week	Date	Topic	Type	Resp.	Room
1	10/09/2025	Introduction to multiscale modeling, Review of Continuum mechanics	Lecture	K.K.	DIA 003
	11/09/2025	No exercises during first week	-	-	-
2	17/09/2025	Periodic & random microstructures, RVEs, Averaging Theorems	Lecture	K.K.	DIA 003
	18/09/2025	Python - Fundamentals	Exercise	G.P.	DIA 005
3	24/09/2025	Continuum-to-continuum homogenization, Hill-Mandel condition	Lecture	K.K.	DIA 003
	25/09/2025	Python - Advanced topics	Exercise	G.P.	DIA 005
4	01/10/2025	RVE boundary conditions, Effective moduli, Bounds	Lecture	K.K.	DIA 003
	02/10/2025	Project 1 - Exercises	Exercise	T.H.	DIA 005
	02/10/2025	Project 1 Assigned			
5	08/10/2025	Analytical and asymptotic homogenization	Lecture	K.K.	DIA 003
	09/10/2025	Project 1 - Exercises	Exercise	T.H.	DIA 005
	15/10/2025	Discrete Element Method	Lecture	K.K.	DIA 003
6	16/10/2025	Project 1 - Office hours	Exercise	T.H.	DIA 005
-	22/10/2025	No lecture (Semester break)	-	-	-
	23/10/2025	No exercises (Semester break)	-	-	-
7	29/10/2025	Discrete Element Method, Discrete-to-continuum homogenization	Lecture	K.K.	DIA 003
	30/10/2025	Project 2 - Exercises	Exercise	H.M.	DIA 005
	30/10/2025	Project 1 Due, Project 2 Assigned			
8	05/11/2025	Molecular dynamics, Atomistic ensembles	Lecture	K.K.	DIA 003
	06/11/2025	Project 2 - Exercises	Exercise	H.M.	DIA 005
	12/11/2025	Concurrent multiscale modeling	Lecture	K.K.	DIA 003
9	13/11/2025	Project 2 - Office hours	Exercise	H.M.	DIA 005
	19/11/2025	Data-driven multiscale modeling	Lecture	K.K.	DIA 003
10	20/11/2025	Data-driven multiscale modeling	Exercise	K.K.	DIA 005
	27/11/2025	Project 2 Due			
	26/11/2025	Applications to various materials	Lecture	K.K.	DIA 003
11	27/11/2025	Final presentation discussion	Discussion	K.K.	DIA 005
	03/12/2025	Applications to various materials	Lecture	K.K.	DIA 003
12	04/12/2025	Final presentation discussion	Discussion	K.K.	DIA 005
	10/12/2025	Final presentations	Presentations	K.K.	DIA 003
13	11/12/2025	Final presentations	Presentations	K.K.	DIA 005
14	17/12/2025	Final presentations	Presentations	K.K.	DIA 003
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4	01/10/				
	02/10/				
	02/10/				
5	08/10/				
	09/10/				
6	15/10/				
	16/10/				
-	22/10/				
	23/10/				
7	29/10/				
	30/10/				
	30/10/20				
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10	19/11/2025	Data-driven multiscale modeling	Lecture	K.K.	DIA 003
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13	10/12/2025	Final presentations	Presentations	K.K.	DIA 003
	11/12/2025	Final presentations	Presentations	K.K.	DIA 005
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Introduction

Continuum-to-continuum

Course Organization

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	18/09/2025	Python - Fundamentals	Exercise	G.P.	DIA 005
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	25/09/2025	[illegible]	[illegible]	[illegible]	[illegible]
4	01/10/20[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	02/10/[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	02/10/[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
5	08/10/[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	09/10/[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
6	15/10/[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	16/10/[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
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	23/10/[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
7	29/10/[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	30/10/[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	30/10/[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
8	05/11/[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	06/11/202[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
9	12/11/2025	Concurrent multiscale modeling	Lecture	K.K.	DIA 003
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Discrete-to-continuum

Course Organization

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Data-driven

Applications

Student presentations

K.Karapiperis

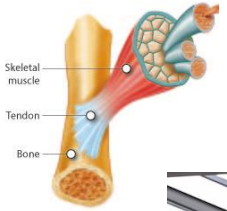
Welcome to Multiscale Modeling

The challenge of modeling materials

K.Karapiperis

Modeller's choice:

- **Linearized** vs **finite** kinematics
- **Isotropic** vs **anisotropic**
- **Elastic** vs **inelastic (plasticity, damage, ...)**
- **History-dependent** and/or **rate-dependent**
- **Coupled models:**
  - Thermomechanical coupling
  - Electro-magneto-chemical coupling



Materials models to be **determined/calibrated from experiments/lower-scale models** (tedious!)

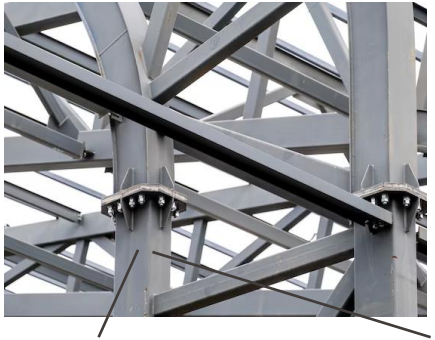
Hard to find suitable material model/parameters for the **full possible range of loading conditions/stress paths** during a simulation

Multiscale structure of materials

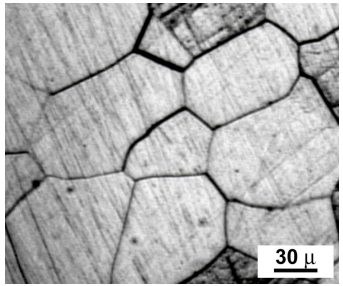
Metals

Composites

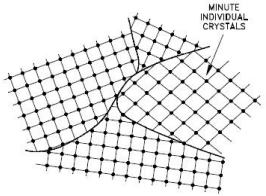
Macroscale

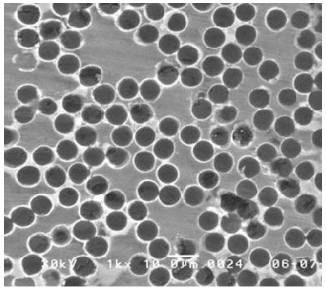


Microscale

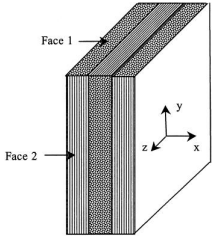


Polycrystalline structure





Fiber reinforced composite



Laminate

- Accurate material description requires resolution of the smaller scales

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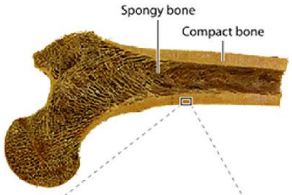
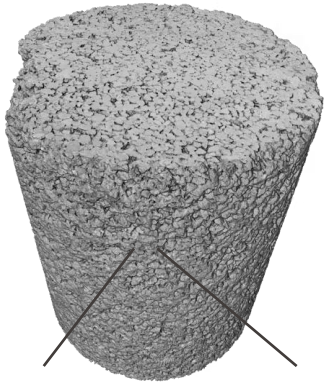
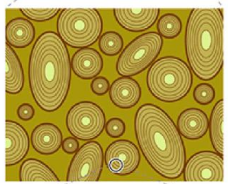
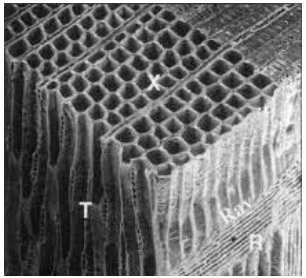
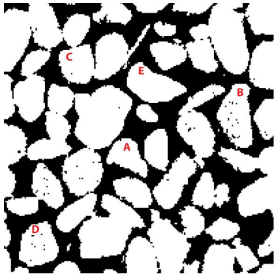
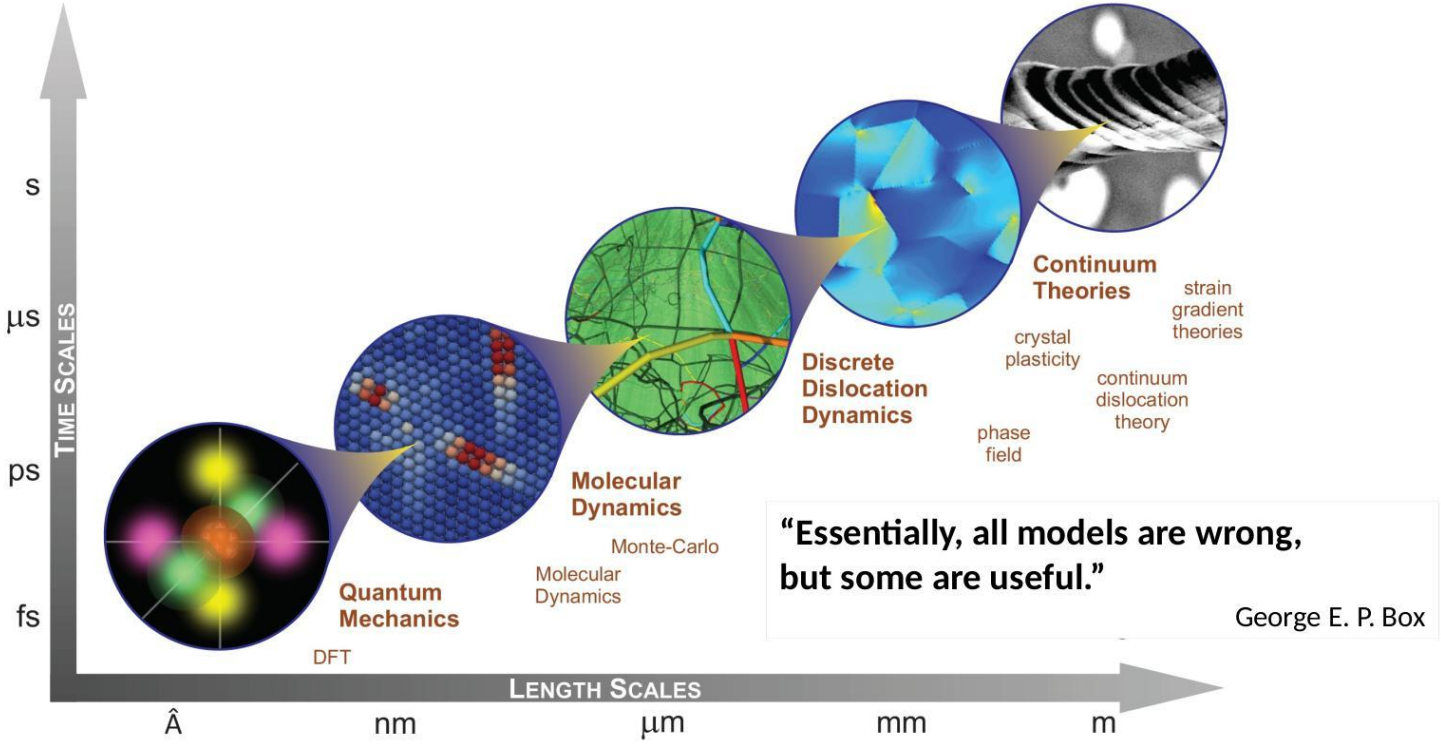
Multiscale structure of materials

	Biomaterials (Wood)	Biomaterials (Bone)	Geomaterials
Macroscale			
		Osteons (~100mm) 	
Microscale		Fiber patterns (~50mm) 	
	Cellular microstructure	Collagen fibrils (~1mm) 	Granular microstructure

- Accurate material description requires resolution of the smaller scales

Hierarchy of scales

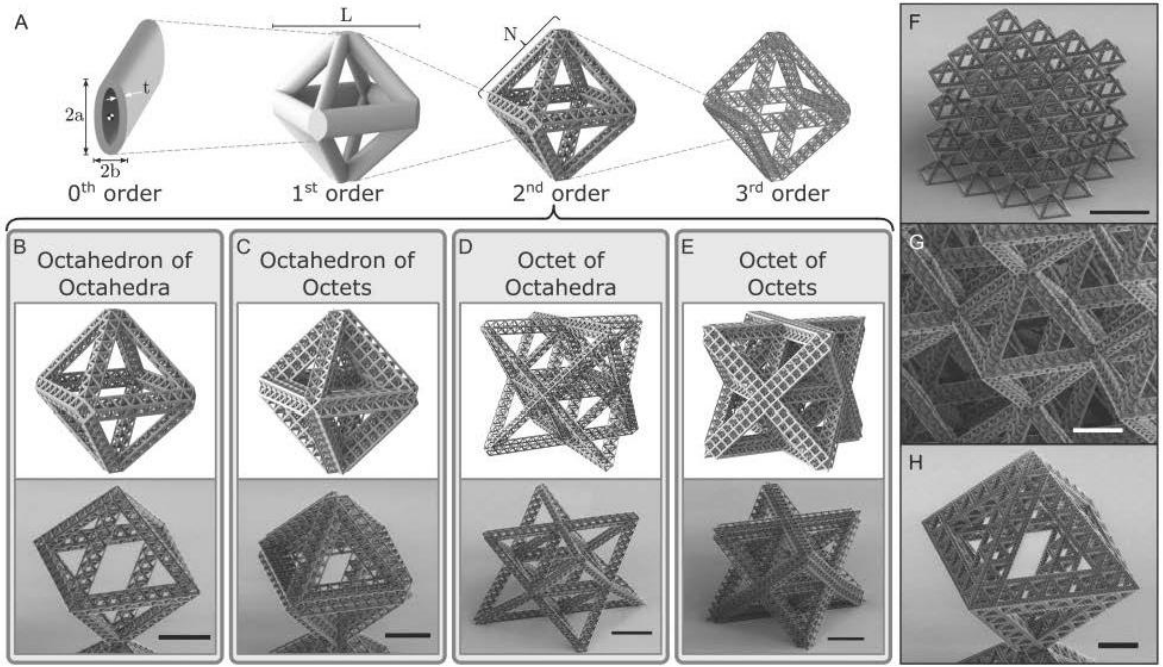


"Essentially, all models are wrong, but some are useful."

George E. P. Box

Hierarchy of scales

Architected materials (Metamaterials)



Meza et al., 2015

Computational & Continuum Mechanics Review

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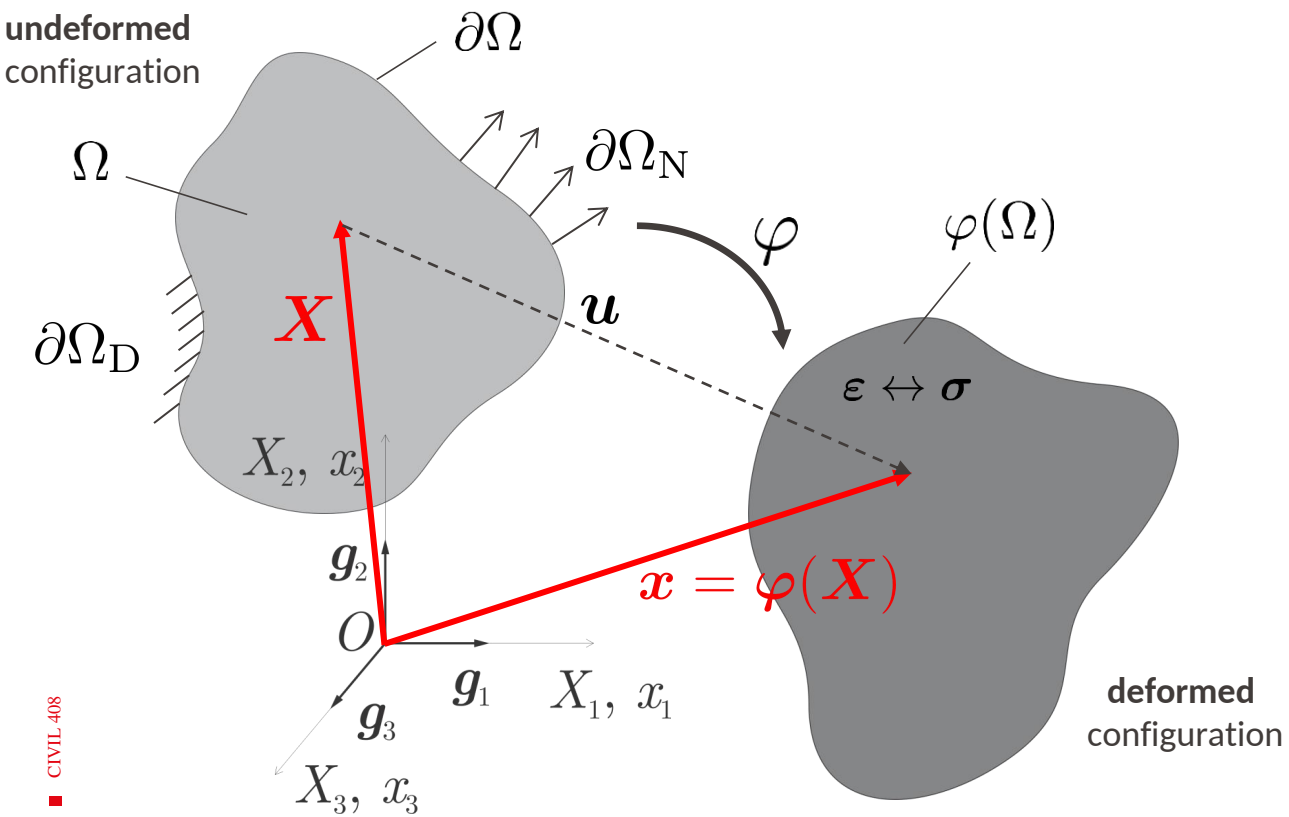


Model domain:

$$\boldsymbol{x} \in \Omega_h$$

Governing equations:

$$\operatorname{div} \boldsymbol{\sigma} + \rho\, \boldsymbol{b} = \rho\, \boldsymbol{a}$$

Boundary/initial conditions:

$$\boldsymbol{u} = \hat{\boldsymbol{u}} \text{ on } \partial\Omega_{\mathrm{D}}$$

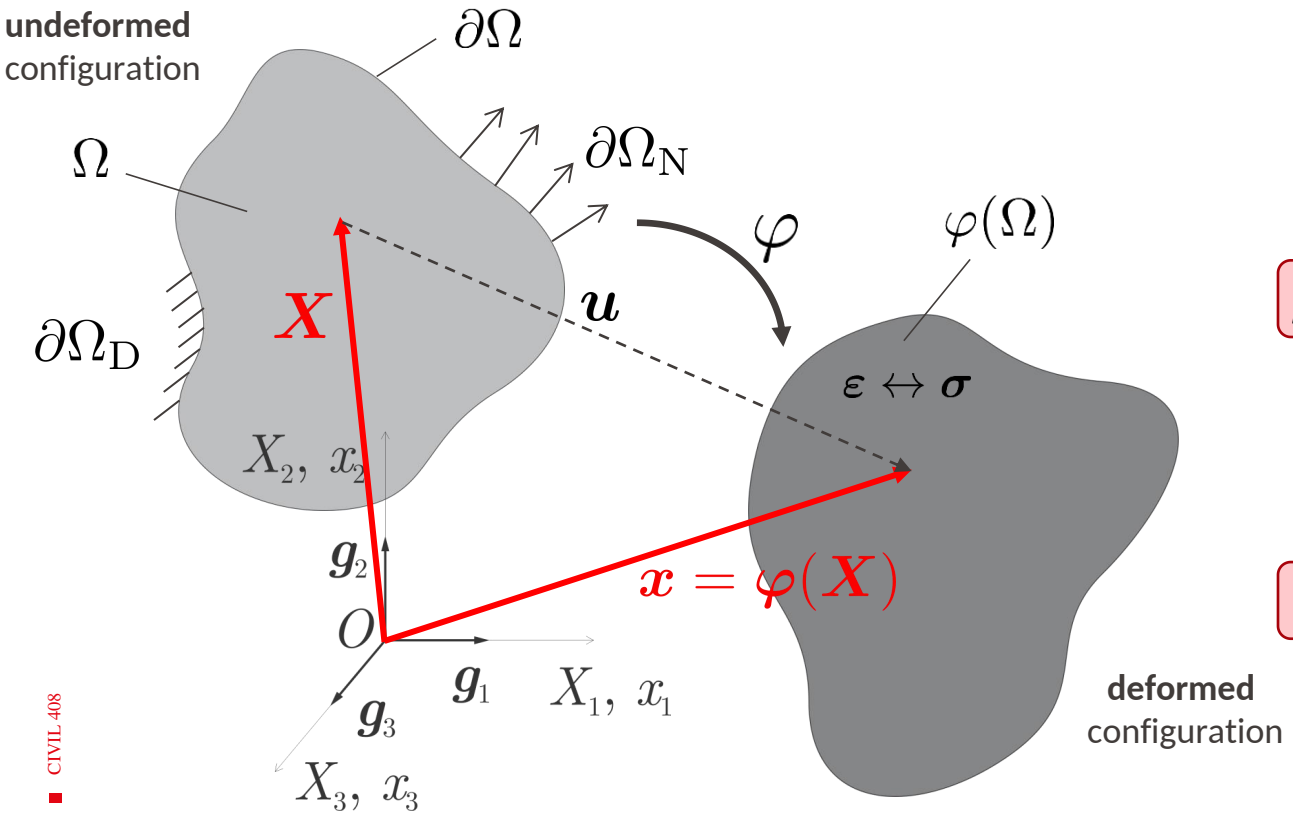
$$\boldsymbol{\sigma}\boldsymbol{n} = \hat{\boldsymbol{t}} \text{ on } \partial\Omega_{\mathrm{N}}$$

Material model:

$$\boldsymbol{\varepsilon} \leftrightarrow \boldsymbol{\sigma}$$

Computational & Continuum Mechanics Review

Extension to thermomechanics



Model domain:

$$\boldsymbol{x} \in \Omega_h$$

Governing equations:

$$\operatorname{div}\boldsymbol{\sigma} + \rho\,\boldsymbol{b} = \rho\,\boldsymbol{a}$$

$$\boxed{\rho c_V \dot{T} = -\operatorname{div}\boldsymbol{q} + \rho s}$$

Boundary/initial conditions:

$$\boldsymbol{u} = \hat{\boldsymbol{u}} \text{ on } \partial\Omega_{\mathrm{D}}$$

$$\boldsymbol{\sigma}\boldsymbol{n} = \hat{\boldsymbol{t}} \text{ on } \partial\Omega_{\mathrm{N}}$$

$$\boxed{T(\boldsymbol{X}, 0) = T_0(\boldsymbol{x})}$$

Material model:

$$\boldsymbol{\varepsilon} \leftrightarrow \boldsymbol{\sigma}$$

$$\boxed{q \leftrightarrow \nabla T}$$

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Computational & Continuum Mechanics Review

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Primary field:

Displacement field: $\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{X}, t) = \boldsymbol{x}(\boldsymbol{X}, t) - \boldsymbol{X}$

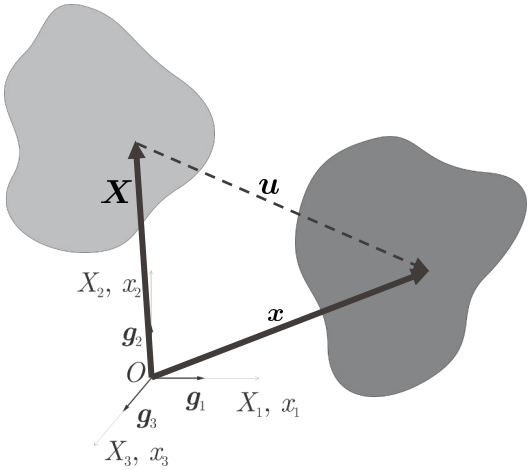
Kinematics:

Strain tensor: $\varepsilon_{ij} = \dfrac{1}{2}\left(u_{i,j} + u_{j,i}\right)$

Acceleration field: $\boldsymbol{a} = \dfrac{\partial^2 \boldsymbol{u}}{\partial t^2} = \ddot{\boldsymbol{u}}$

Constitutive relation:

Cauchy stress: $\boldsymbol{\sigma} = \dfrac{\partial W}{\partial \boldsymbol{\varepsilon}}$



Balance of linear momentum:

$$\operatorname{div} \boldsymbol{\sigma} + \rho\, \boldsymbol{b} = \rho\, \boldsymbol{a} \qquad \Leftrightarrow \qquad \sigma_{ij,j} + \rho\, b_i = \rho\, a_i$$

Computational & Continuum Mechanics Review

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Primary field:

Deformation mapping: $\boldsymbol{x} = \boldsymbol{\varphi}(\boldsymbol{X}, t)$

Kinematics:

Deformation gradient: $\boldsymbol{F} = \mathrm{Grad}\,\boldsymbol{\varphi} \quad \Leftrightarrow \quad F_{iJ} = \varphi_{i,J} = \dfrac{\partial x_i}{\partial X_J}$

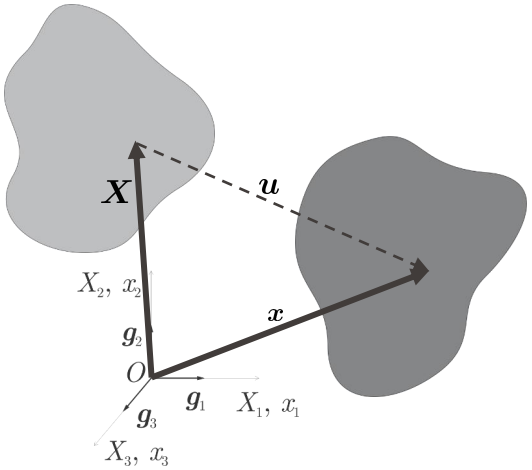
Acceleration field: $\boldsymbol{A} = \dfrac{\partial^2 \boldsymbol{\varphi}}{\partial t^2} = \dfrac{\partial \boldsymbol{V}}{\partial t}$

Constitutive relation:

1st Piola-Kirchhiff stress: $\boldsymbol{P} = \boldsymbol{P}(\boldsymbol{F}) = \dfrac{\partial W}{\partial \boldsymbol{F}}$

Balance of linear momentum:

$$\mathrm{Div}\,\boldsymbol{P} + R\boldsymbol{B} = R\boldsymbol{A} \quad \Leftrightarrow \quad P_{iJ,J} + RB_i = R\,A_i$$



Linear elasticity and Hyperelasticity

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Linear elasticity:

$$\sigma_{ij} = \mathbb{C}_{ijkl}\varepsilon_{kl}$$ where $\mathbb{C}_{ijkl}$ is a 4th-order tensor with 81 coefficients.

- Symmetry of stress tensor $\sigma_{ij} = \sigma_{ji} \rightarrow \mathbb{C}_{ijkl} = \mathbb{C}_{jikl}$
- Symmetry of strain tensor $\varepsilon_{kl} = \varepsilon_{lk} \rightarrow \mathbb{C}_{ijkl} = \mathbb{C}_{ijlk}$
- Strain energy $W(\boldsymbol{\varepsilon}) = \frac{1}{2}\varepsilon_{ij}\mathbb{C}_{ijkl}\varepsilon_{kl} \rightarrow \mathbb{C}_{ijkl} = \mathbb{C}_{klij}$

reduction to 21 coefficients

Hyperelasticity (NeoHookean):

- Strain energy $W(\boldsymbol{F}) = \frac{\mu}{2}(\bar{I}_1 - 3) + \frac{K}{4}((J-1)^2 + (\ln J)^2)$

where $\bar{I}_1 = J^{-2/3}I_1, J = \det \boldsymbol{F}$

$$P_{iJ} = \mu J^{-2/3}\left(F_{iJ} - \frac{1}{3}I_1 F^{-1}_{Ji}\right) + \frac{K}{2}J\left(J - 1 + \frac{1}{J}\ln J\right)F^{-1}_{Ji}$$

The Finite Element Method - Quasistatics

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Variational principle:

$$\mathcal{I}[\boldsymbol{u}] = \int_\Omega W(\boldsymbol{\varepsilon})\,\mathrm{d}V - \int_\Omega \rho \boldsymbol{b}\cdot\boldsymbol{u}\,\mathrm{d}V - \int_{\partial\Omega_N} \hat{\boldsymbol{t}}\cdot\boldsymbol{u}\,\mathrm{d}S \to \min$$

Weak form:

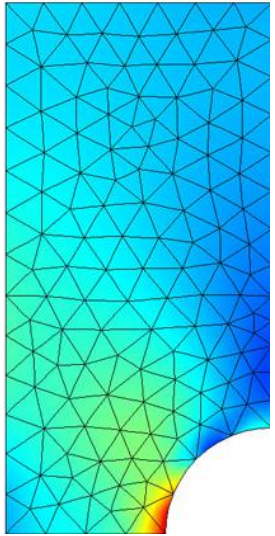
$$\mathcal{I}[\boldsymbol{u},\boldsymbol{v}] = \int_\Omega \sigma_{ij} v_{i,j}\,\mathrm{d}V - \int_\Omega \rho \boldsymbol{b}\cdot\boldsymbol{v}\,\mathrm{d}V - \int_{\partial\Omega_N} \hat{\boldsymbol{t}}\cdot\boldsymbol{v}\,\mathrm{d}S = 0 \qquad \forall\,\boldsymbol{v}\in\mathcal{U}_0$$

Discretization:

$$\boldsymbol{u} \approx \boldsymbol{u}^h = \sum_{a=1}^{n} \boldsymbol{u}^a N^a(\boldsymbol{x}), \qquad \boldsymbol{v} \approx \boldsymbol{v}^h = \sum_{a=1}^{n} \boldsymbol{v}^a N^a(\boldsymbol{x})$$

Finally:

$$\underbrace{\int_\Omega \sigma_{ij}(\boldsymbol{\varepsilon}^h) N^a_{,j}\,\mathrm{d}V}_{F^a_{\mathrm{int},i}} - \underbrace{\left[\int_\Omega \rho b_i N^a\,\mathrm{d}V + \int_{\partial\Omega_N} \hat{t}_i N^a\,\mathrm{d}S\right]}_{F^a_{\mathrm{ext},i}} = 0$$



The Finite Element Method - Dynamics

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Variational principle (Least action):

$$\mathcal{A}[\boldsymbol{u}] = \int_{t_1}^{t_2} \mathcal{L}[\boldsymbol{u}]dt \to \min \quad \text{with} \quad \mathcal{L}[\boldsymbol{u}] = T[\boldsymbol{u}] - I[\boldsymbol{u}] \qquad T[\boldsymbol{u}] = \int_\Omega \frac{\rho}{2}|\dot{\boldsymbol{u}}|^2 dV$$

Weak form:

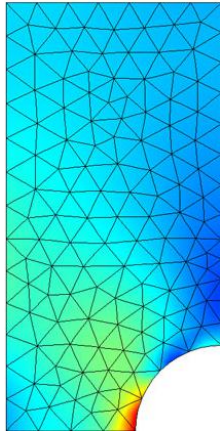
$$\mathcal{G}[\boldsymbol{u}, \boldsymbol{v}] = \int_{t_1}^{t_2} \left[\int_\Omega (\rho \dot{u}_i \dot{v}_i - \sigma_{ij} v_{i,j}) dV + \int_\Omega \rho b_i v_i dV + \int_{\partial\Omega_N} \hat{t}_i v_i dS \right] dt = 0 \qquad \forall \boldsymbol{v} \in \mathcal{U}_0$$

Discretization:

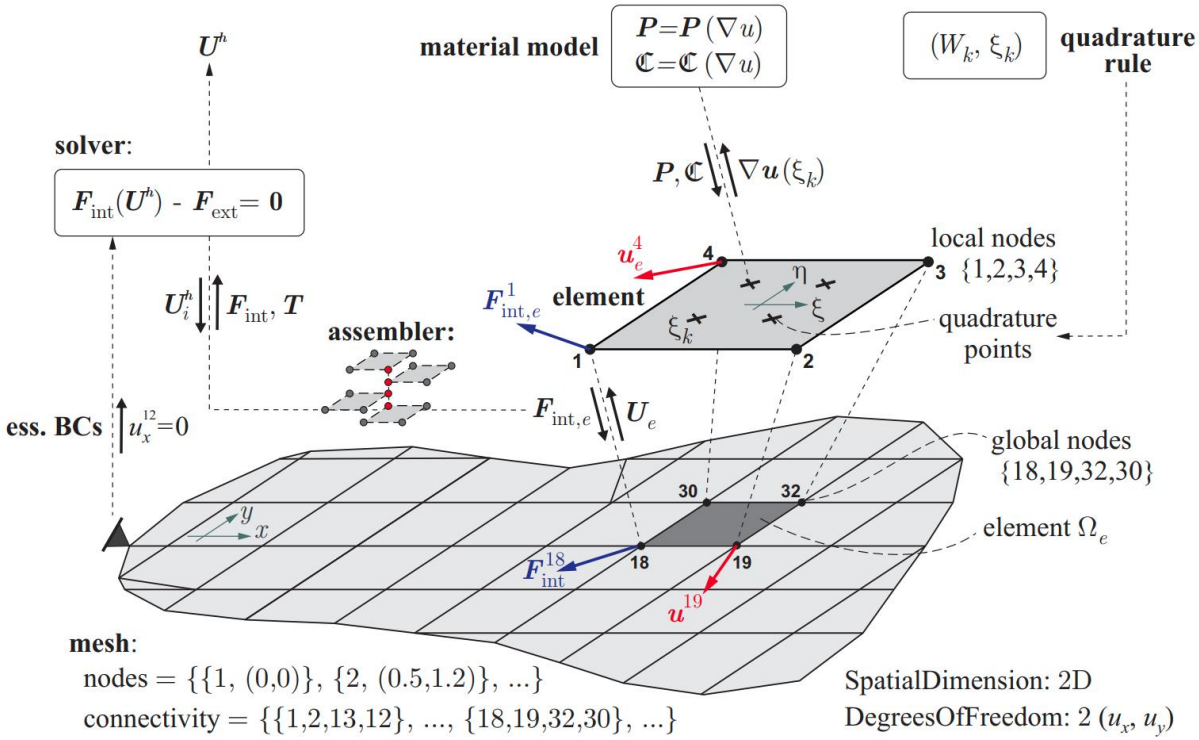
$$\boldsymbol{u} \approx \boldsymbol{u}^h = \sum_{a=1}^{n} \boldsymbol{u}^a N^a(\boldsymbol{x}), \qquad \boldsymbol{v} \approx \boldsymbol{v}^h = \sum_{a=1}^{n} \boldsymbol{v}^a N^a(\boldsymbol{x})$$

Finally:

$$\boldsymbol{M}\ddot{\boldsymbol{U}}_h + \boldsymbol{F}_{\text{int}}(\boldsymbol{U}_h) - \boldsymbol{F}_{\text{ext}}(t) = 0$$



Numerical implementation



Separation of scales

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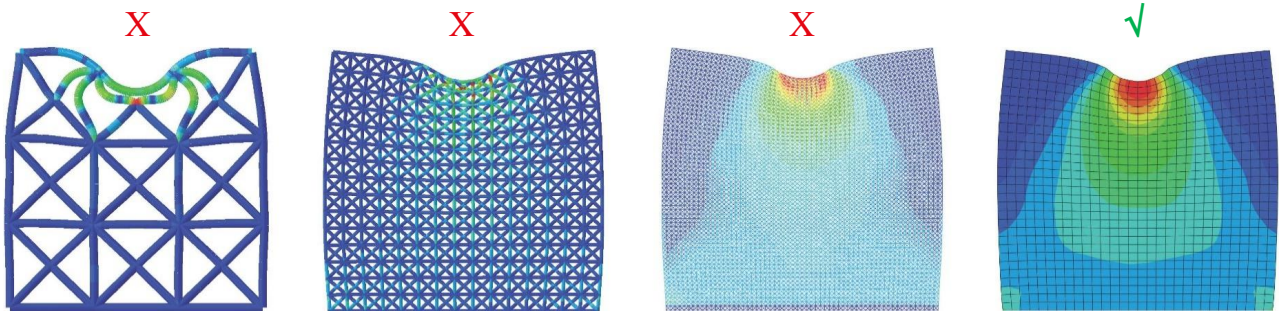
Scale separation:

Macroscopic field variables vary much more slowly than *microscopic* field variables, and characteristic dimensions on the macroscale are significantly larger than on the microscale:

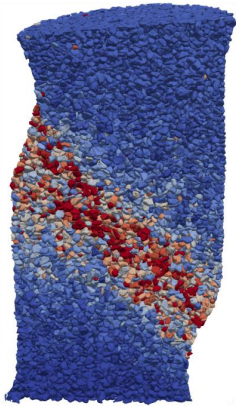
Examples where scale separation applies or not:



Separation of scales

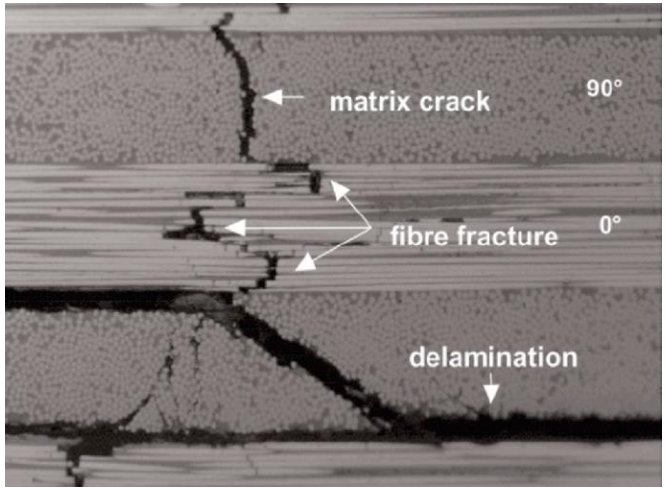
More examples where separation of scales fails:

Shear bands and faults



Desrues et al., 2002

Fracture in composites



Costa, 2019

Multiscale Modeling Methods

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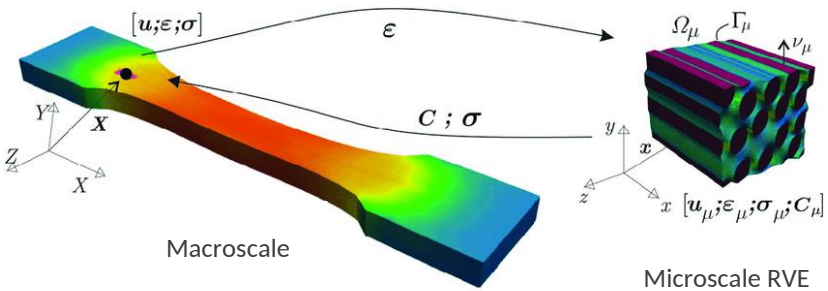
Hierarchical/Vertical scale-bridging

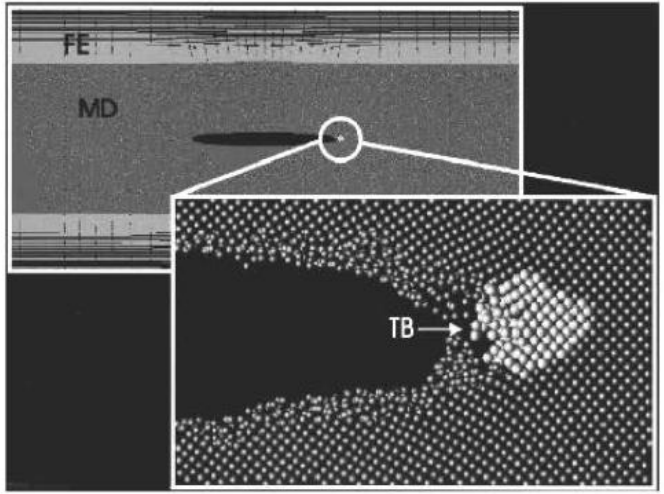
aka “computational homogenization”



Raschi et al., 2020

Concurrent/Horizontal scale bridging

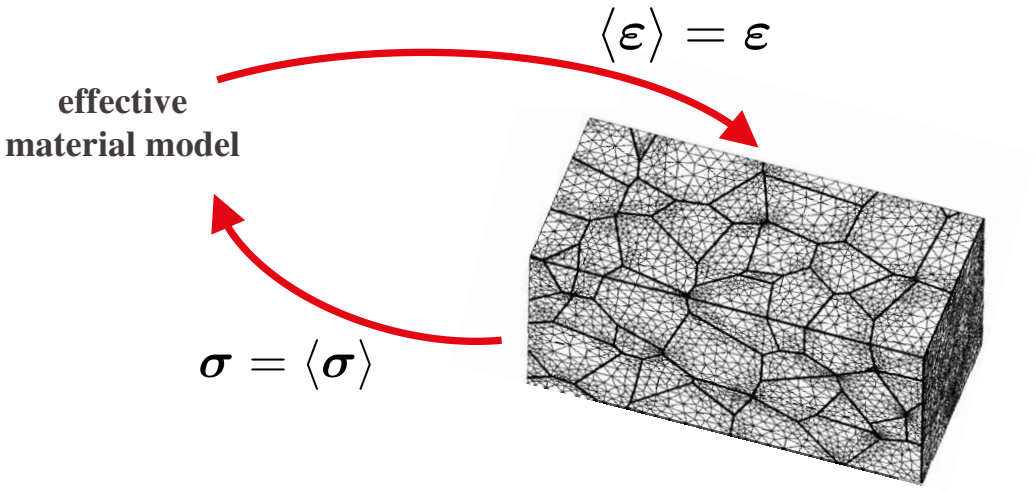
e.g. MAAD = macroscopic, atomistic, ab initio dynamics



Abraham et al., 1998

Hierarchical Modeling

Relies on **extracting the average or "effective" behavior** of the microscale.

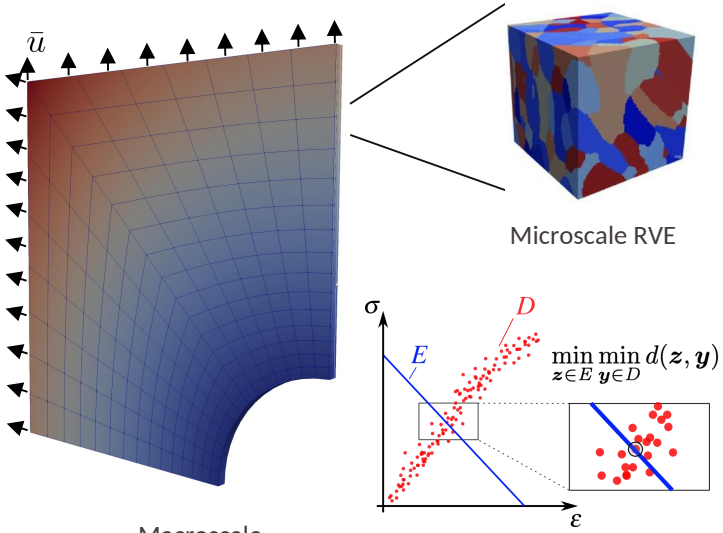


Questions:

- How do we impose an average strain?
- How do we calculate the ensuing average stress?

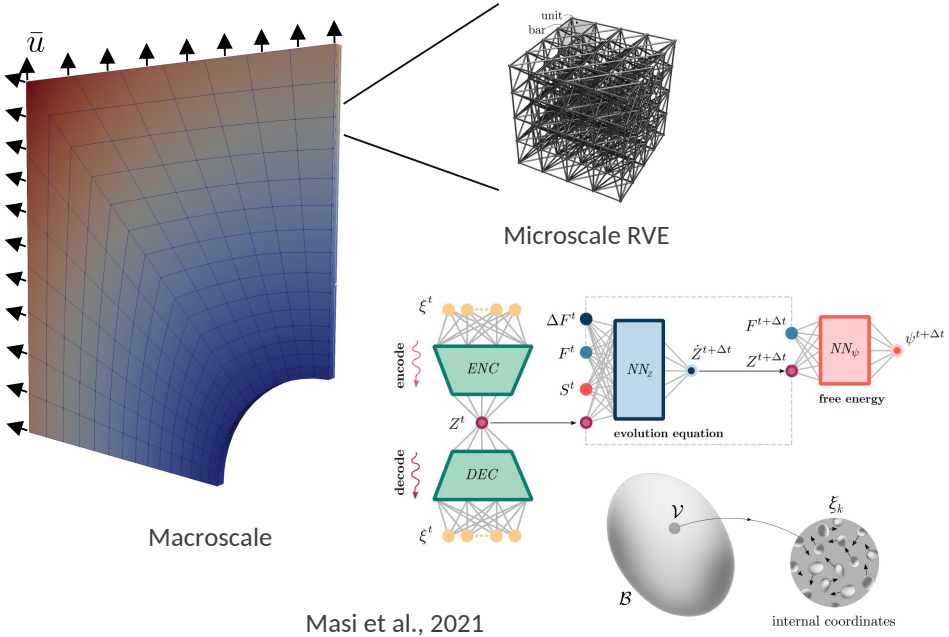
Data-Driven Hierarchical Modeling

Distance-minimizing scheme



Karapiperis et al., 2020

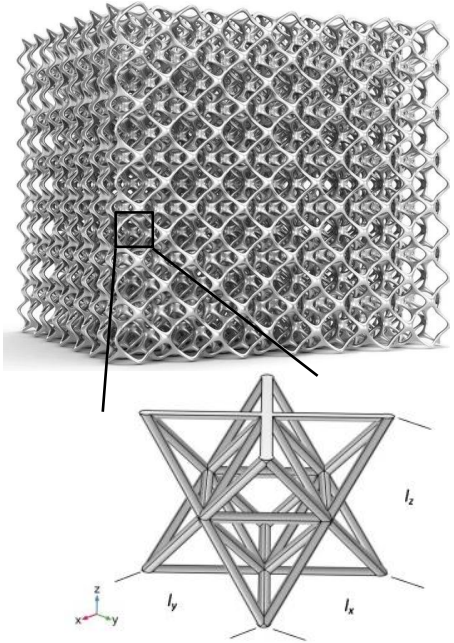
Machine learning



Masi et al., 2021

Periodic vs Non-periodic Microstructure

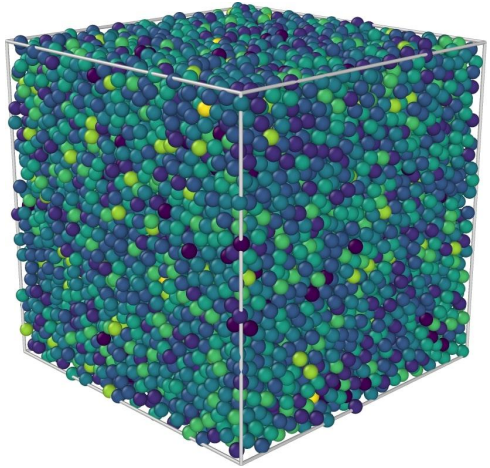
Periodic



Unit cell

(Smallest repeating unit whose periodic tiling tesselates the space)

Non-periodic



Representative Volume Element (RVE)

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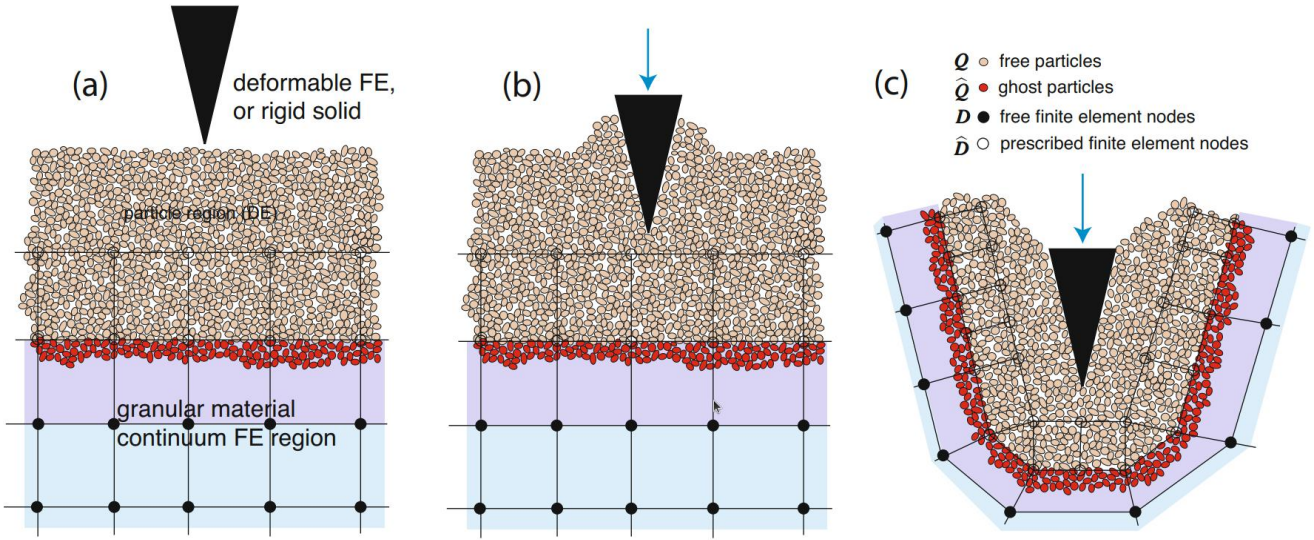
Concurrent Modeling

Relies on **spatially bridging** the microscale and the macroscale.



Regueiro et al., 2011

Questions:

- How do we ensure energetic consistency?
- How do we ensure smooth coupling of the two domains?

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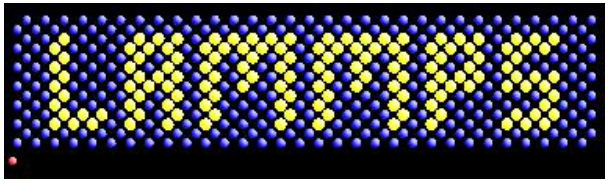
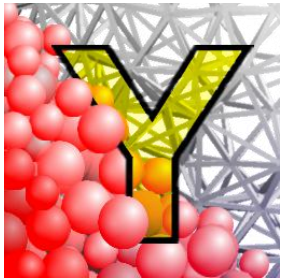
Why do we need this class?

Available software at different scales

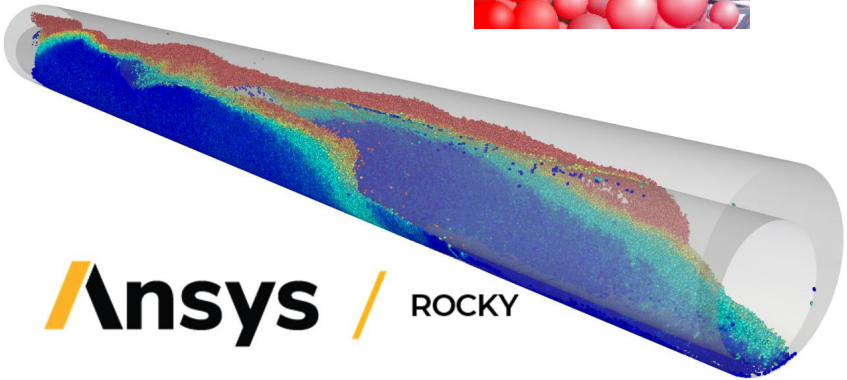


MOOSE

SIMULIA ABAQUS



FEAP



COMSOL MULTIPHYSICS®

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Course objectives

1. Understand theories and computational methods that bridge across scales (discrete-to-continuum, continuum-to-continuum)

2. Understand typical theories and models of individual scales (atomistic, mesoscale, continuum, ...)

3. Develop a code for computational multiscale analysis of a material (Python)

Outlook

Continuum-to-continuum

- Statistical homogeneity, RVEs
- Averaging theorems
- Hill-Mandel condition
- Computational homogenization
- Asymptotic methods
- Analytical methods (Cauchy-Born)

Discrete-to-continuum

- Discrete element method
- Atomistic simulation
- Mesoscale methods
- Hierarchical discrete-to-continuum scale bridging
- Concurrent discrete-to-continuum scale bridging
- Data-driven scale bridging

Applications

- Composites
- Metals
- Geomaterials
- Concrete
- Masonry
- Architected materials
- …

Reading for next class:

Multiscale Modeling, D.M. Kochmann

Chapters 1-3