Lab Talk #1

September 20, 2021

Ozgur Taylan Turan

New Machine Learning Strategies for Data Scarce Material Science Problems

Outline

- Introduction
- Modeling Composites
- Machine Learning in Mechanics
- My view
- Summary

Engineering Endeavours

- Limited world
- Performance
- Reliability

Material Behaviour

- Baby's understanding
- What do grown ups do?

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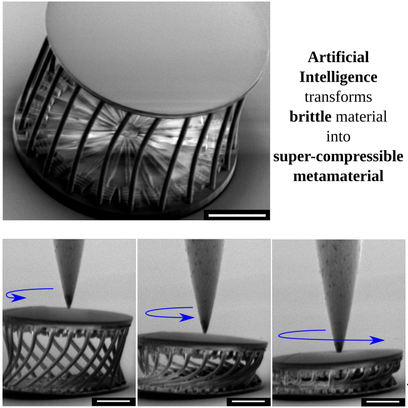


[1]

[1] M. A. Bessa, P. Glowacki, and M. Houlder (2019). "Bayesian Machine Learning in Metamaterial Design: Fragile Becomes Supercompressible". In: *Advanced Materials* 31.48. ISSN: 15214095. DOI: 10.1002/adma.201904845

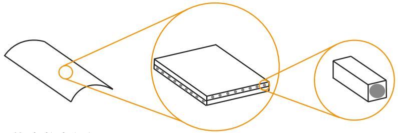
Composites

Experimental

- Time and money limitations

Numerical Analysis

- Multi-scale venture
- The Finite Element Method



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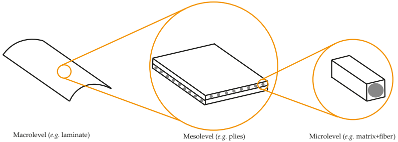

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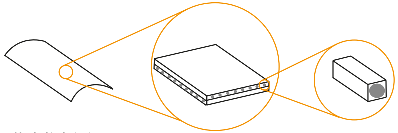

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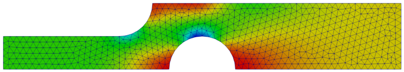
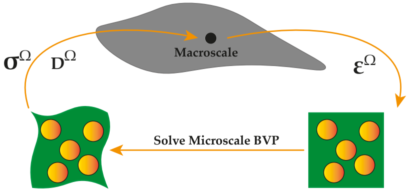


Numerical Modeling Composites

FE^2 (Concurrent FEM)[2]

- Couple scales [3]
- Average the response
- Is it enough?



[2] F. Feyel (2003). "A multilevel finite element method (FE2) to describe the response of highly non-linear structures using generalized continua". In: *Computer Methods in Applied Mechanics and Engineering* 192.28-30, pp. 3233–3244. ISSN: 00457825. DOI: 10.1016/S0045-7825(03)00348-7

[3] C. Miehe, J. Schotte, and M. Lambrecht (2002). "Homogenization of inelastic solid materials at finite strains based on incremental minimization principles. Application to the texture analysis of polycrystals". In: *Journal of the Mechanics and Physics of Solids* 50.10, pp. 2123–2167. ISSN: 00225096. DOI: 10.1016/S0022-5096(02)00016-9; C. Miehe, J. Schröder, and J. Schotte (1999). "Computational homogenization analysis in finite plasticity simulation of texture development in polycrystalline materials". In: *Computer Methods in Applied Mechanics and Engineering* 171.3-4, pp. 387–418. ISSN: 00457825. DOI: 10.1016/S0045-7825(98)00218-7

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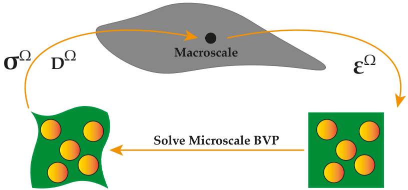

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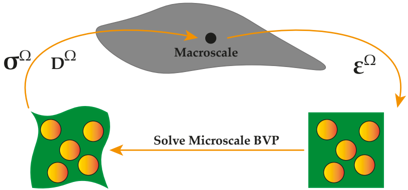

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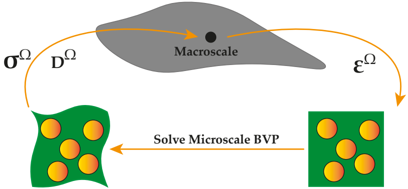

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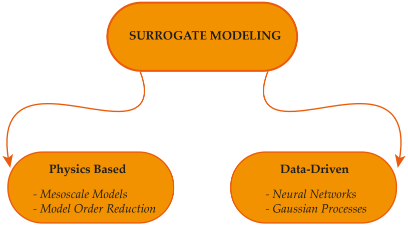
Numerical Modeling Composites

Surrogate Modeling

- Tackle computational burden
- Keep fidelity of FE^2



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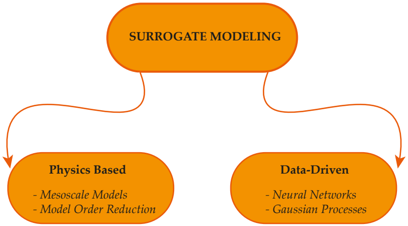

Constitutive Modeling

$\nabla \cdot \sigma = 0 \rightarrow$ Equilibrium Equation

Computationally Material

- Trying to learn $\sigma = \mathcal{C}(\varepsilon)$
- Any supervised learner

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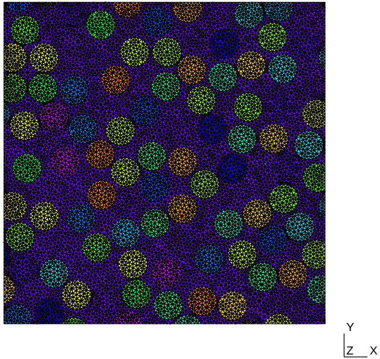
Assumptions

- Geometry
- Material Model



Constitutive Modeling

$$\nabla \cdot \sigma = 0 \rightarrow \text{Equilibrium Equation}$$

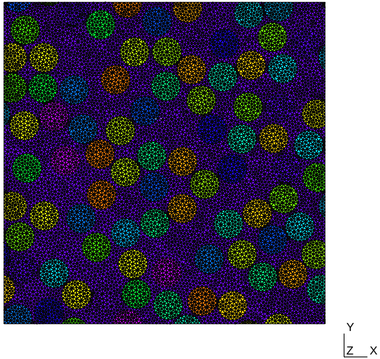
Assumptions

- Geometry
- Material Model

$$\Downarrow$$

Parametrizations Examples

- V_f, L
- E, ν



Current ML Approaches

- *Physics-informed* ML models (SCA [4], DMN [5], etc.)
- Brute force fitting to parameters of interest [6],[7]
- *Physics-driven* ML models (PINN[8])

[4] Z. Liu, M. A. Bessa, and W. K. Liu (2016). “Self-consistent clustering analysis: An efficient multi-scale scheme for inelastic heterogeneous materials”. In: *Computer Methods in Applied Mechanics and Engineering* 306, pp. 319–341. ISSN: 00457825. DOI: 10.1016/j.cma.2016.04.004

[5] Z. Liu, C. T. Wu, and M. Koishi (2019). “A deep material network for multiscale topology learning and accelerated nonlinear modeling of heterogeneous materials”. In: *Computer Methods in Applied Mechanics and Engineering* 345, pp. 1138–1168. ISSN: 00457825. DOI: 10.1016/j.cma.2018.09.020. arXiv: 1807.09829

[6] I. B. Rocha, P. Kerfriden, and F. P. van der Meer (2020). “Micromechanics-based surrogate models for the response of composites: A critical comparison between a classical mesoscale constitutive model, hyper-reduction and neural networks”. In: *European Journal of Mechanics, A/Solids* 82, p. 103995. ISSN: 09977538. DOI: 10.1016/j.euromechsol.2020.103995

[7] M. A. Bessa, R. Bostanabad, Z. Liu, A. Hu, D. W. Apley, C. Brinson, W. Chen, and W. K. Liu (2017). “A framework for data-driven analysis of materials under uncertainty: Countering the curse of dimensionality”. In: *Computer Methods in Applied Mechanics and Engineering* 320, pp. 633–667. ISSN: 00457825. DOI: 10.1016/j.cma.2017.03.037

[8] M. Raissi, P. Perdikaris, and G. E. Karniadakis (2017). “Physics Informed Deep Learning (Part II): Data-driven Discovery of Nonlinear Partial Differential Equations”. In: Part I, pp. 1–22. arXiv: 1711.10566

Starting Point

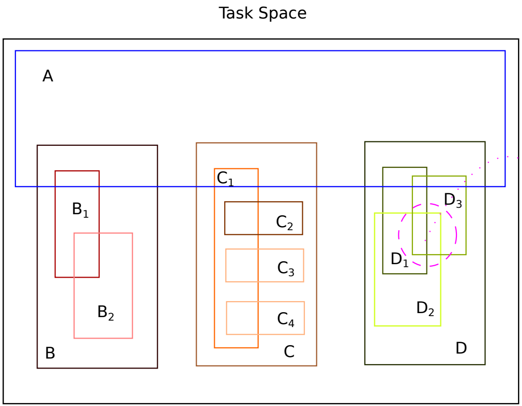
Transfer Learning for DNN Applications for Constitutive Modeling

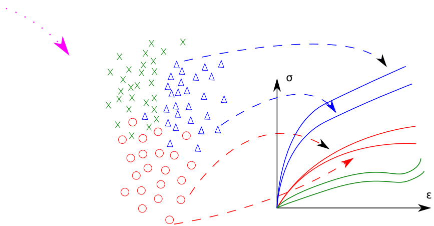
My View on Current ML Surrogate Models

Problems

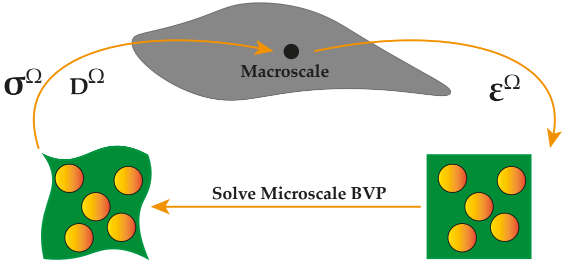
- Need of abundant data
- Problem specific applications
- Single parameter considerations

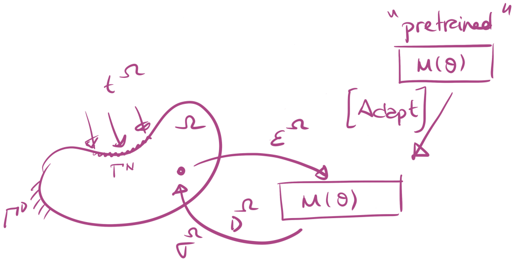
Holistic Problem





Overarching Goal





Possible Paths

Access

- A parameterized oracle model for $\sigma = \mathcal{C}(\varepsilon)$

Possible Paths

- Learning the tasks space $(\sigma = \mathcal{C}(\varepsilon))_{i=1}^{M}$
- Effect of continual task observation...
- Access to subspace of task as a whole
- Active sampling of tasks and data in a task

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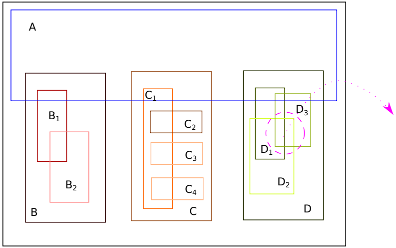
Task Space



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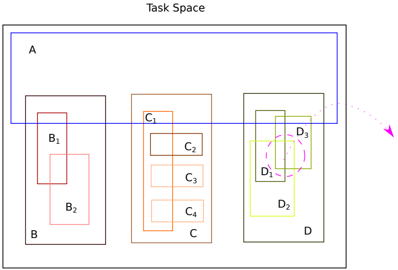

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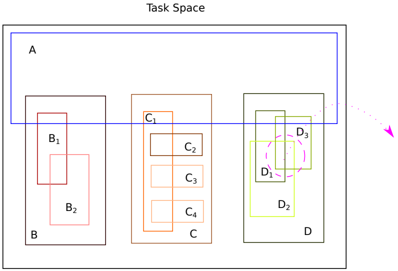

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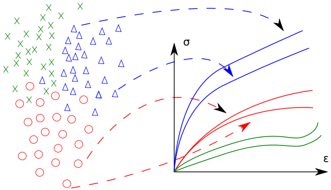

My work

Until now

- Data generation framework

Currently

- Model parameter based learning and knowledge transfer
- MAML in convex settings

Future

- Data related transfer of knowledge
- Domain adaptation and generalization if we consider the labels as full mappings?

Summary

- Accelerate conventional PDE solution techniques
- Learn $\sigma = \mathcal{C}(\varepsilon)$
- Data can originate from experiments too
- Either past data or actively sampling