New Machine Learning Strategies for Data Scarce Material Science Problems

November 15, 2021

Ozgur Taylan Turan

Go/No-go Meeting

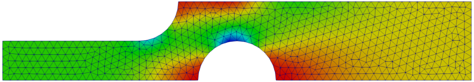
Outline

- Introduction
- Literature
- Aim
- Research Questions
- Planning
- Reflection

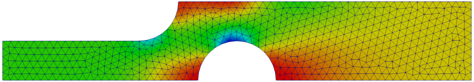
Computational Solid Mechanics

Solid Mechanics

- Relate deformation with internal force development
- $\nabla \cdot \mathbf{P} = 0$ with $\mathbf{P} = \mathcal{C}(\mathbf{F})$



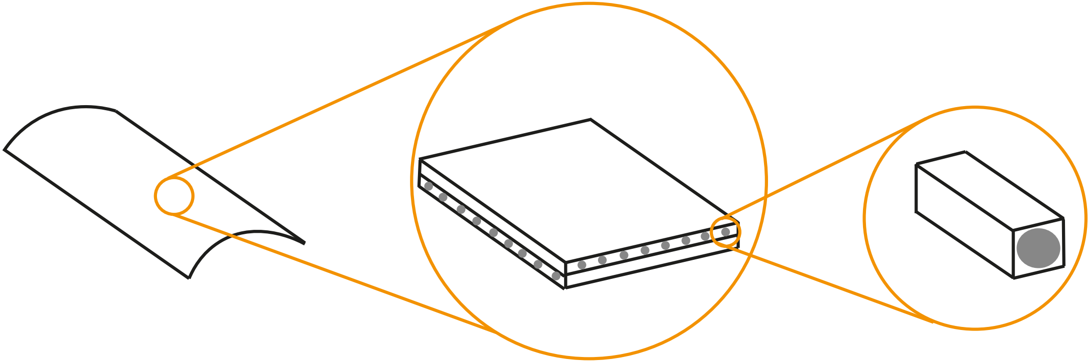
Computational Solid Mechanics



Finite Element Method

- General PDE solving method
- Discretize the domain
- Weakly satisfy the PDE at selected points

Composite Modeling



Macrolevel (*e.g.* laminate)

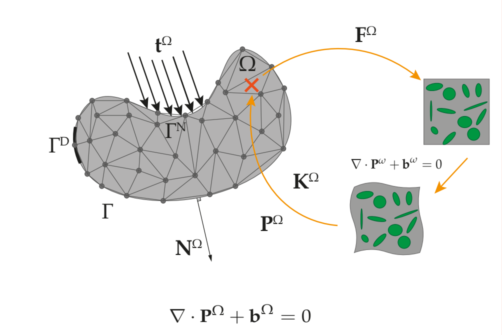
Mesolevel (*e.g.* plies)

Microlevel (*e.g.* matrix+fiber)

Composite Modeling

FE^2

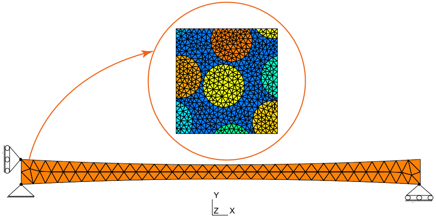
- Representative Volume Element (RVE)
- Solve for RVE and average the response
- Repeat for every selected point



Composite Modeling

FE^2-Bottleneck

- Micro-scale problem solution
- Repeating for every selected point
- Highly non-linear behaviour



Composite Modeling

FE^2-Bottleneck

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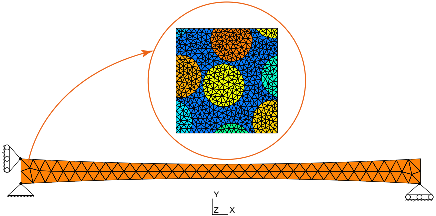
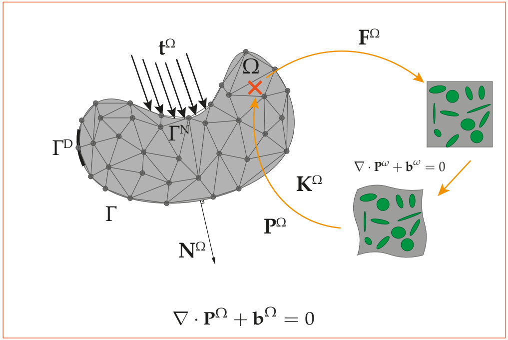
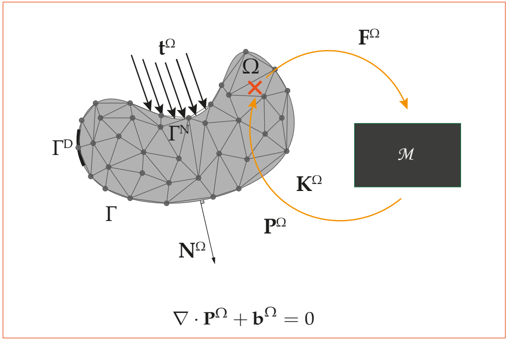


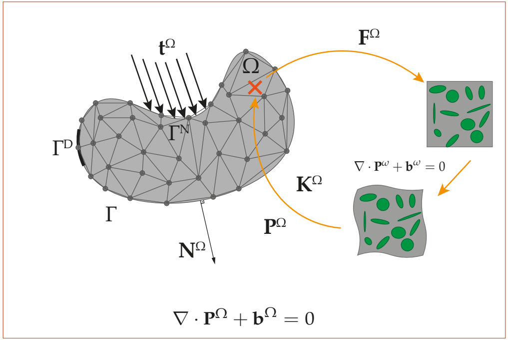
We need multiple of these simulations for real world applications!

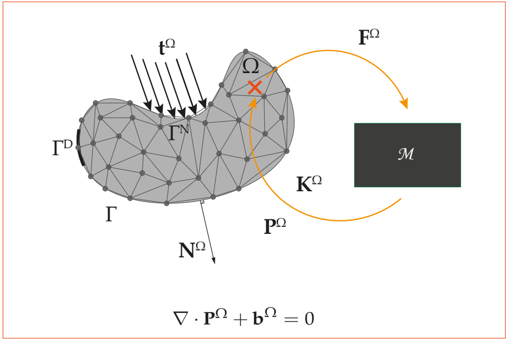
FE^2 via Machine Learning





FE^2 via Machine Learning



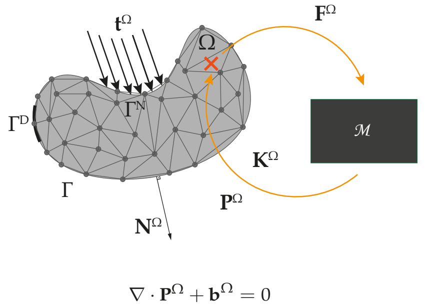


- Computationally a Material: $\mathbf{F} \to \mathbf{P}$

FE^2 via Machine Learning

Problems in Current State

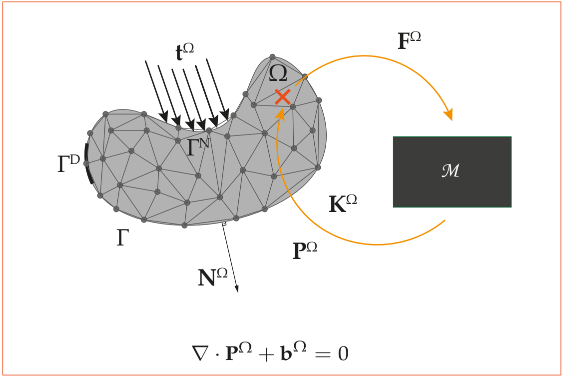
- Risky Extrapolation
- Data Scarcity
- Single Parameter Configuration
- General Applicability



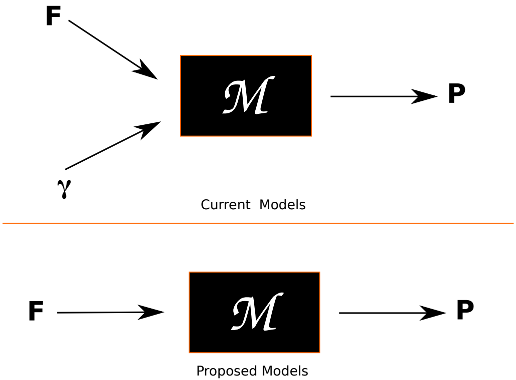
Hypothesis

- Most of the problems encountered can be tackled with more general use cases.
- The core problem is finding the mapping between a deformation measure and a force measure. ($\mathbf{P} = \mathcal{C}(\mathbf{F})$)
- Similarity between the problems can be exploited, without considering the different parameters that effect the model.

Aim-A

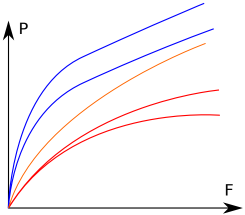


$\mathbf{t}^{\Omega}$
Ω
$\mathbf{F}^{\Omega}$
Γ^{D}
Γ^{N}
$\mathcal{M}$
$\mathbf{K}^{\Omega}$
Γ
$\mathbf{P}^{\Omega}$
$\mathbf{N}^{\Omega}$
$\nabla \cdot \mathbf{P}^{\Omega} + \mathbf{b}^{\Omega} = 0$

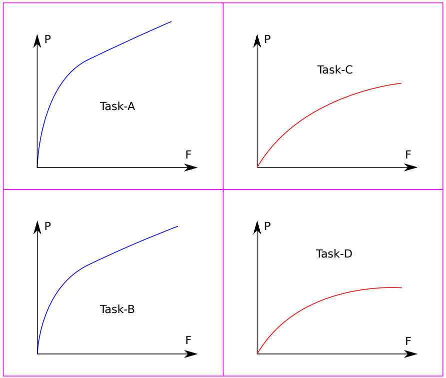


F
$\mathcal{M}$
P
γ
Current Models
F
$\mathcal{M}$
P
Proposed Models

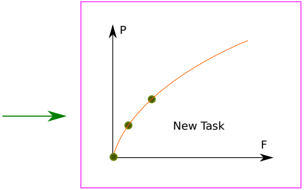
Aim-B



All Tasks



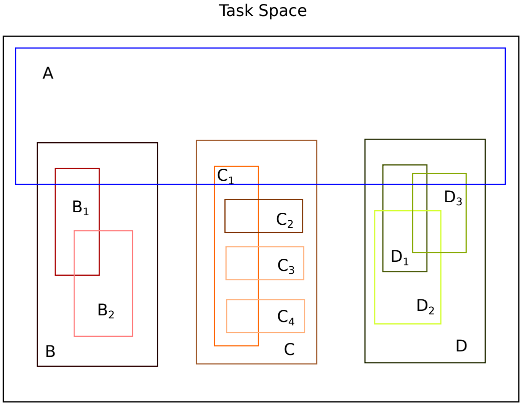
Batch of Previous Tasks



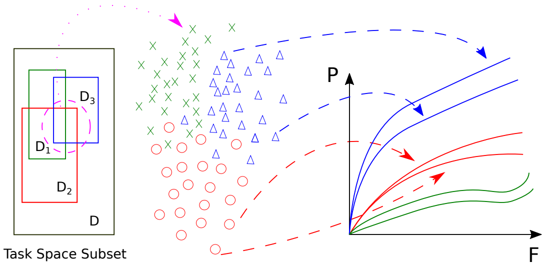
New and Unseen Task

Overall Learning Problem-A

Consider an arbitrary space that represents overall material behaviour, and the subsets of this space representing specific material types.



Overall Learning Problem-B



- Every label in this space becomes a full mapping! ($T_{D_1} := \{T_{D_{1i}} : \mathbf{F} \rightarrow \mathbf{P}_i\}_{i=1}^{M}$)

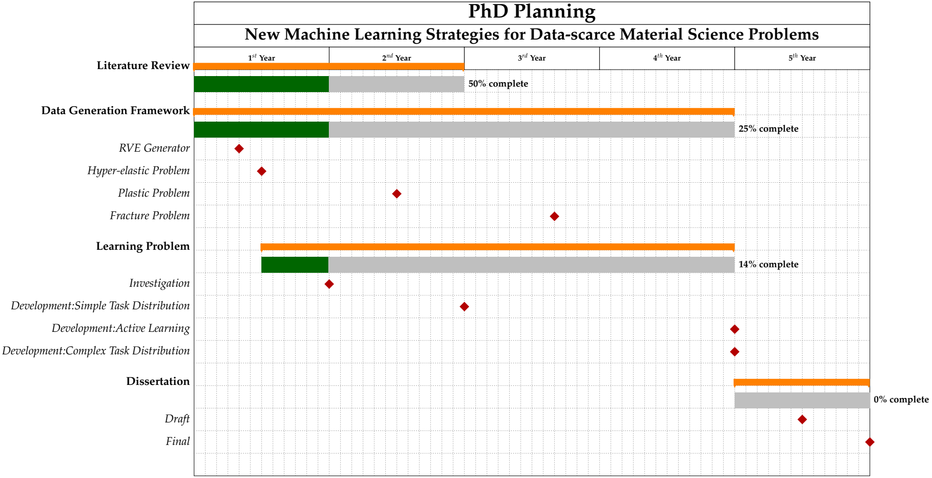
Research Questions

- To what extent this prediction is possible?
- Can we find a latent space where the tasks with different parameters live and exploit the similarities between these tasks?
- What information can we extract from the model trained with the batch of tasks at hand?
- Can we find an effective sampling strategy in the task space and in the feature space of the given task?

Related Paradigms in ML Literature

- Meta Learning (Learning-to-learn)
- Transfer Learning and Domain Adaptation
- Multi-task Learning

Project Planning



Collaborations

- Continuation of my MSc. Thesis Multi-fidelity Gaussian Process Regression
- Miguel Bessa and I in collaboration with Iuri Rocha and Frans van der Meer from Civil Engineering and Geosciences
- Data Generation

Doctoral Education Planning

Doctoral Education Planning				
Skills-Credit Balance	Course	Year	Credit	Status
Discipline Related-(10/16)	Machine Learning-1	1	5	✓
	Deep Learning	1	5	✓
	Linear Algebra and Optimisation for Machine Learning	2	6	✗
Research Related-(4/24)	Speaker at a national (or minor international) conference	1-5	1	✗
	Poster presentation conference/workshop	1-5	1	✗
	Internship of at least 1 month with another institute	1-5	2	✗
	Writing a research proposal	1-5	2	✗
	Writing a conference paper	1-5	1	✗
	Writing a journal article	1-5	3	✗
	Supervising a MSc. Student	1-2	4	**in-progress**
	Supervising a BSc. Student	1	4	✓
	Teaching assistance:laboratory course	2	2	**in-progress**
	Teaching assistance:providing material, correcting exams	2	2	**in-progress**
Transferable-(6/17)	PhD Startup Module (A-B-C)	1	2	✓
	Mental fitness Intervention Program	1	1	✓
	Standing up for yourself while keeping good relation	1	1	✓
	Analytical Storytelling	1	2	✓
	Work Smarter, stress less	2	3	**planned**
	Speedreading and Mindmapping	2	1.5	**planned**
	Time Management-Individual Crash Course	2	0.5	**planned**
	Research Design	2	3	**planned**
	Dutch for Foreigners	2	3	✗

Past Year with COVID19

Academic

- PRB
- Collaboration

Past Year with COVID19

Academic

- PRB
- Collaboration

Non-Academic

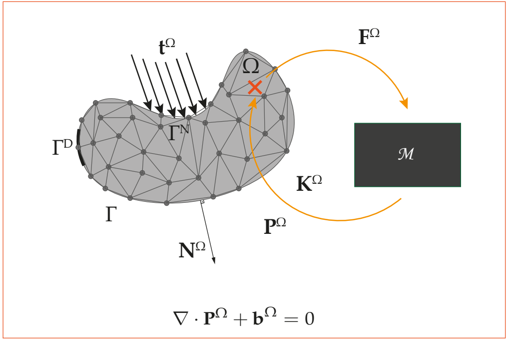
- Work-Life
- Well-being

Thanks for your attention!

Reformulate the Problem-A

$\mathbf{P} = \mathcal{C}(\mathbf{F})$

- Normally, $\mathbf{P} = f(\mathbf{F}, \gamma)$
- $\gamma := \{\gamma_i\}_{i=1}^{M}$ with $M \in \mathbb{Z}^+$
- $\mathbf{P} = \mathcal{M}(\mathbf{F}, \gamma)$
- Application specific models!



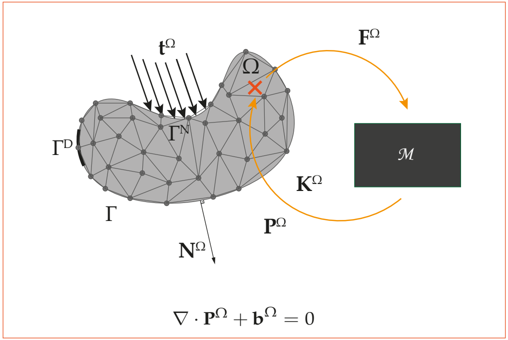
Reformulate the Problem-B

$\mathbf{P} = \mathcal{C}(\mathbf{F})$

- Let's stick to $\mathbf{P} = \mathcal{C}(\mathbf{F})$
- Then, $\mathbf{P} = \mathcal{M}(\mathbf{F})$

How to account for γ?

- Let's stick to $\{\mathbf{P}_i = \mathcal{C}_i(\mathbf{F})\}_{i=1}^{M}$ with $M \in \mathbb{Z}^+$
- $\mathbf{P} = \mathcal{M}(\mathbf{F})$
- Model input-output remains the same!



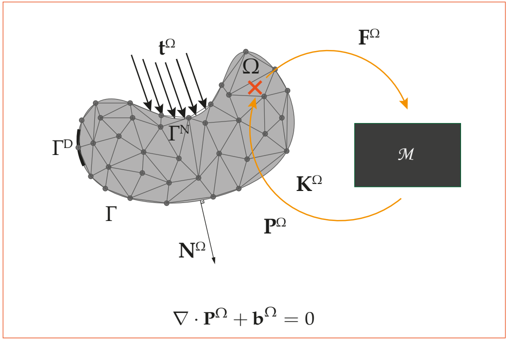
Reformulate the Problem-C

How do we end up with a parametrized relationships?

- Series of assumptions,
  $\mathcal{A} : \{a_n \subset a_{n-1} \subset ... \subset a_1\}$

Individual Learning Problem

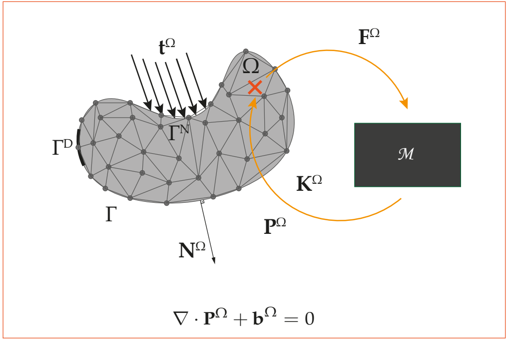
- If the aim is to learn $\mathbf{F} \rightarrow \mathbf{P}$
- Learning problem: $\mathcal{T}_{\mathcal{A}} : \mathbf{F} \rightarrow \mathbf{P}$



Reformulate the Problem-D

Overall Learning Problem

- Given $\{\mathbf{P}_i = \mathcal{C}_i(\mathbf{F})\}_{i=1}^{M}$ with $M \in \mathbb{Z}^+$
- Learning problem: $\{\mathcal{T}_{\mathcal{A}_i} : \mathbf{F} \to \mathbf{P}_i\}_{i=1}^{M}$



Single-Task Learning vs Bias Learning-A

Single-Task Learning

- Input Space $\mathbf{F}$ OutputSpace $\mathbf{P}$
- Probability Distribution p on $\mathbf{F} \times \mathbf{P}$
- Loss Function $l : \mathbf{P} \times \mathbf{P} \to \mathbb{R}$
- Hypothesis Space $\mathcal{H}$, a set of functions $h : \mathbf{F} \to \mathbf{P}$
- Minimize the expected loss to get $h \in \mathcal{H}$

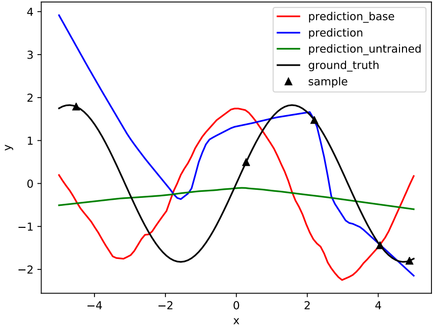
Single-Task Learning vs Bias Learning-B

Bias Learning

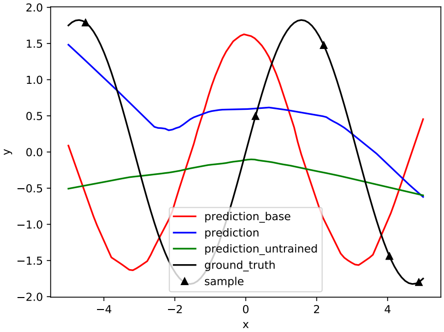
- Input Space $\mathbf{F}$ OutputSpace $\mathbf{P}$
- Probability Distribution p on $\mathbf{F} \times \mathbf{P}$
- Loss Function $l : \mathbf{P} \times \mathbf{P} \rightarrow \mathbb{R}$
- An environment $(\mathcal{Q}, \mathcal{P})$ where $\mathcal{P}$ is all possible distribution of p and $\mathcal{Q}$ is the distribution of $\mathcal{P}$
- Hypothesis Space Family $\mathbb{H} := \{\mathcal{H}\}$, where each $\mathcal{H}$ is a set of functions $h : \mathbf{F} \rightarrow \mathbf{P}$
- Minimize the expected future risk or transfer risk to find the appropriate Hypothesis Space $\mathcal{H}$

MAML vs Multi-task

- Problem: $y = a * \sin(x + p)$ for $x \in [0, 5]$ and $a \in [0.1, 5]$ & $a \in [0, \pi]$ for K $= 5$ and $\mathcal{B}(\mathcal{T})$ size 100



MAML



Multi-task

Small Investigation of MAML [1]

- $a \in \mathbb{R}^d \rightarrow p_a \sim \mathcal{N}(m\mathbf{1}, c\mathbf{I})$
- $x \in \mathbb{R}^d \rightarrow p_x \sim \mathcal{U}(\mathbf{0}, b\mathbf{1})$
- $\varepsilon \sim \mathcal{N}(0, \sigma^2)$
- $y = a^\mathsf{T} x + \varepsilon \quad \in \mathbb{R}$
- $Z := ((x_i, y_i))_{i=1}^N$
- $\hat{a}_N \rightarrow$ an estimator trained with N training points

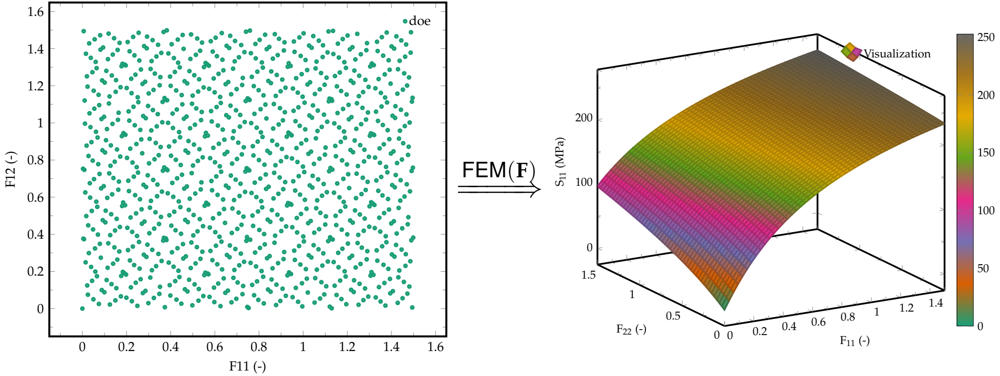
Expected Error over the whole task space,
$$\int \int \int (\hat{a}_N(Z)^\mathsf{T} x - y)^2 p(x,y)\, dx\, dy\, p_Z\, dZ\, p_a\, da$$

Investigating the performance of a future emprical risk minimizing algorithm for transfer risk.

[1] C. Finn, P. Abbeel, and S. Levine (2017). "Model-agnostic meta-learning for fast adaptation of deep networks". In: *34th International Conference on Machine Learning, ICML 2017* 3, pp. 1856–1868. arXiv: 1703.03400

F3DASM

- Design of Experiements
- Simulation or Machine Learning Module



Summer Schools & Conferences

Summer Schools

- Machine Learning Summer Schools (MLSS)
- Gaussian Process Summer School
- Nordic Probabilistic AI Summer School
- Oxford Machine Learning Summer School

Summer Schools & Conferences

Conferences on ML

- Conference on Computer Vision and Pattern Recognition (CVPR)
- International Conference on Learning Representations (ICLR)
- International Conference on Machine Learning (ICML)
- International Conference on Machine Learning and Pattern Recognition (ICMLPR)

Summer Schools & Conferences

Conferences on Mechanics

- FEniCS Conference
- International Conference on Mathematics and Computational Mechanics (ICMCM)
- International Conference on Computational Geomechanics and Material Response (ICCGMR)
- FEniCS Conference
- International Conference on Computational Continuum Mechanics and Dynamics (ICCCMD)
- International Conference on Computational Continuum and Continuum Mechanics (ICCCM)