Data Driven Surrogate Frameworks for Computational Mechanics: Bayesian and Geometric Deep Learning Approaches

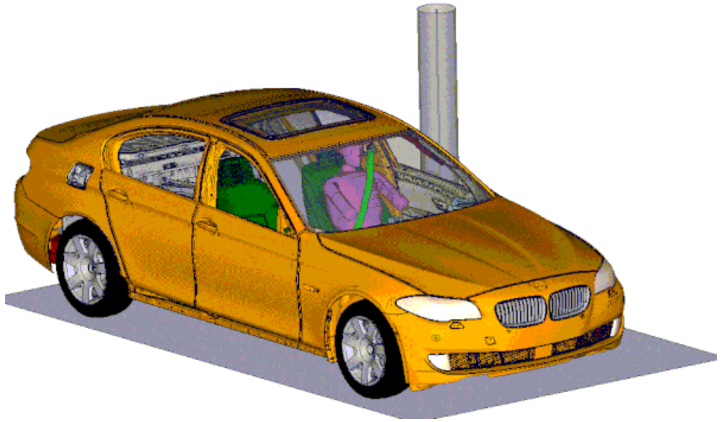
Saurabh Deshpande

PhD defense : 18th September 2023

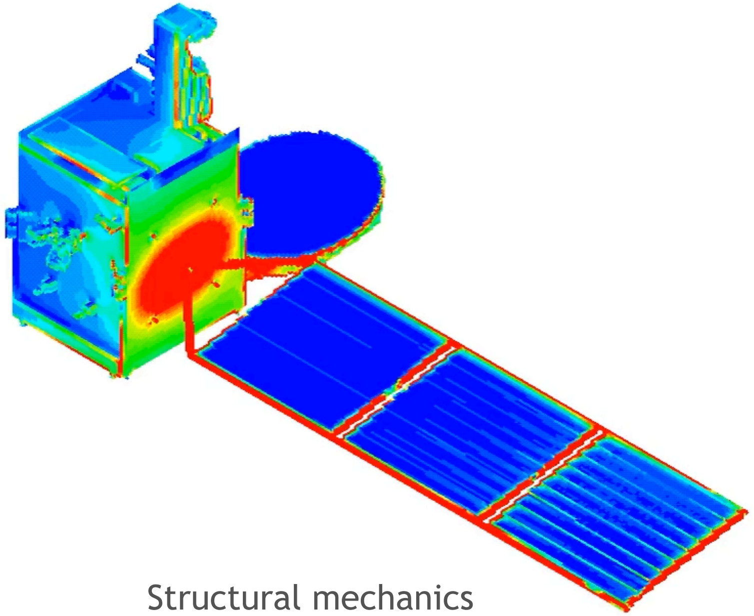
Defense committee

Prof. Stéphane Bordas	Prof. Andreas Zilian	Dr. Jakub Lengiewicz	Prof. Stéphane Cotin	Prof. Eleni Chatzi
(Supervisor)	(Chair)	(Co-chair)	(External)	(External)

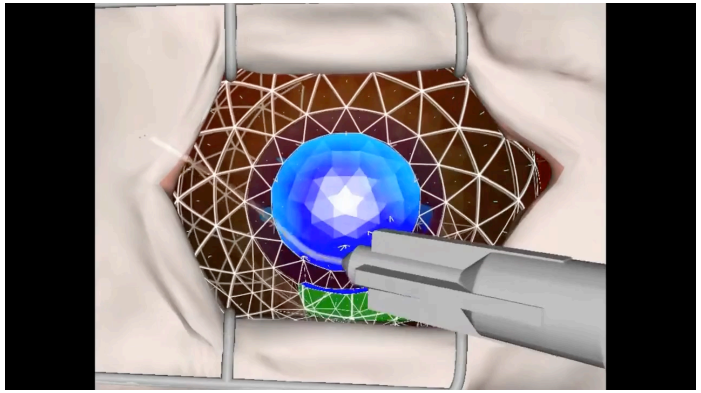
Motivation



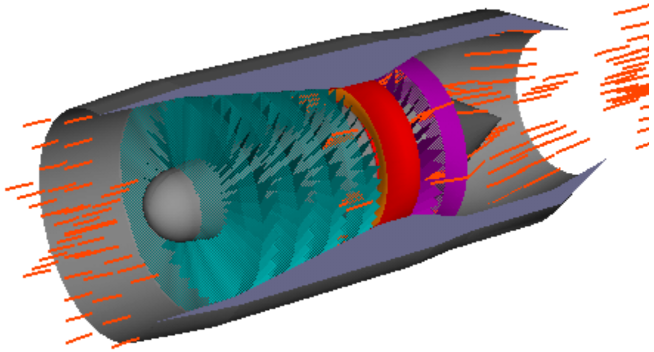
Impact simulations



Structural mechanics

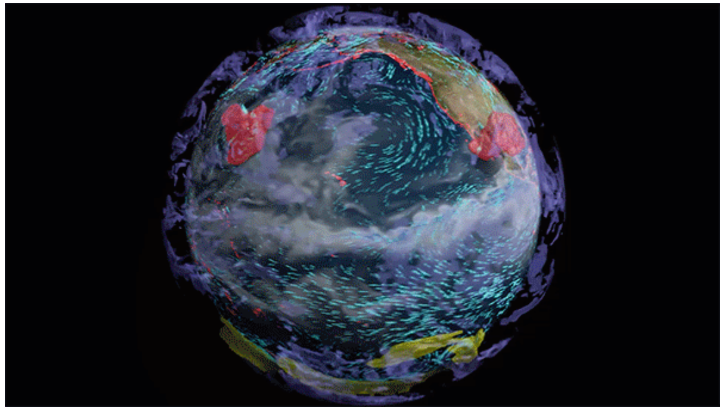


Surgical simulations



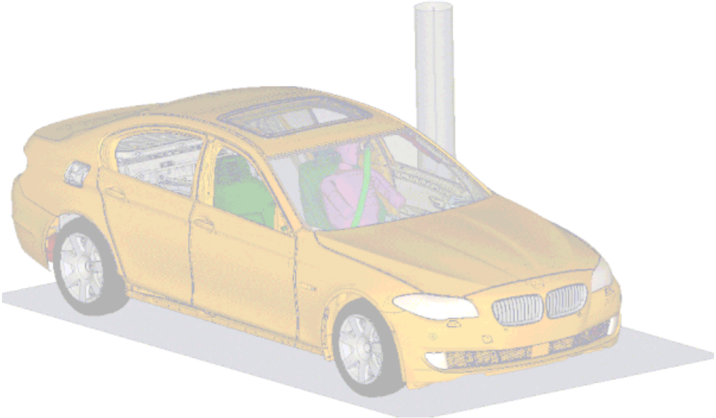
Airplane jet airflow

Drug discovery

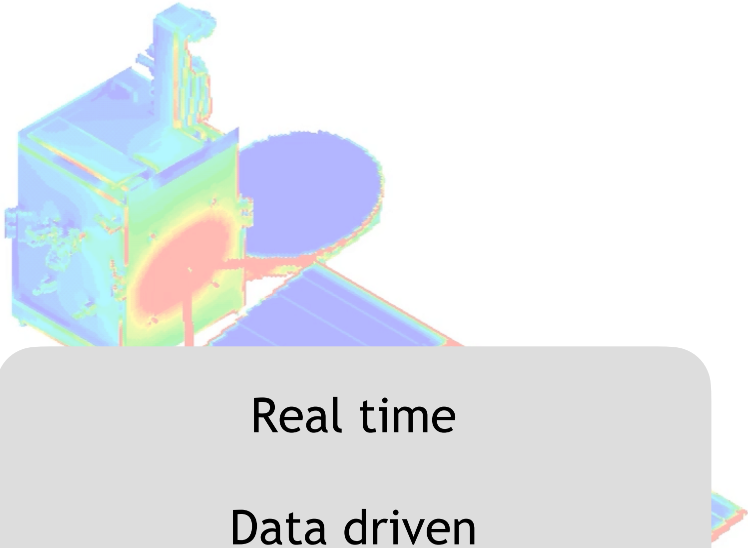


Weather forecast

Motivation



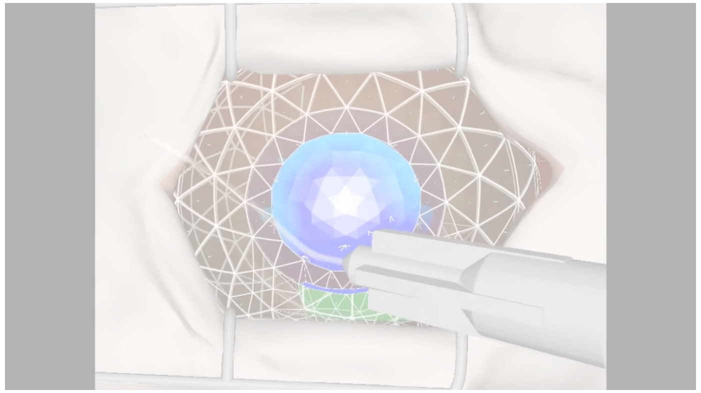
Impact simulations



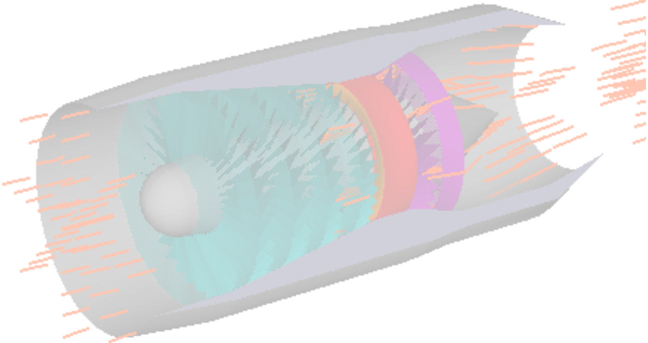
Real time

Data driven

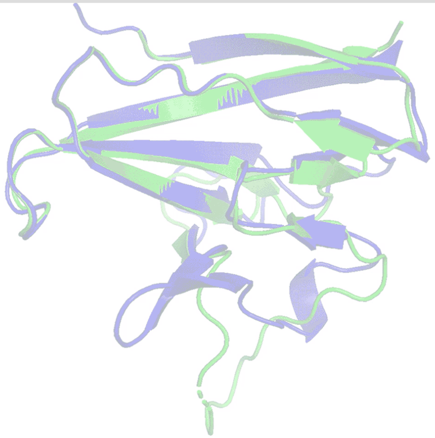
Uncertainty quantification



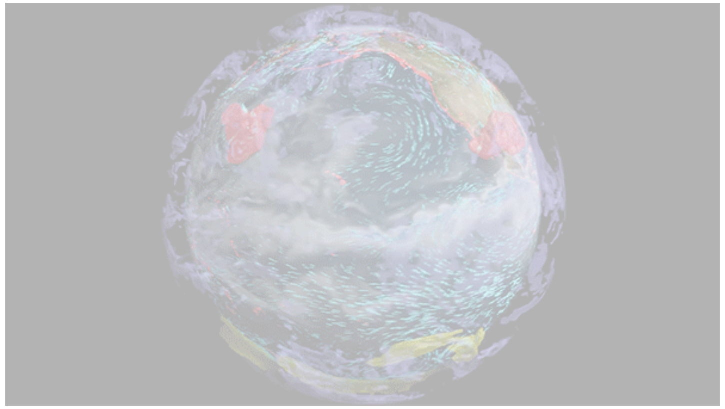
Surgical simulations



Airplane jet airflow



Drug discovery



Weather forecast

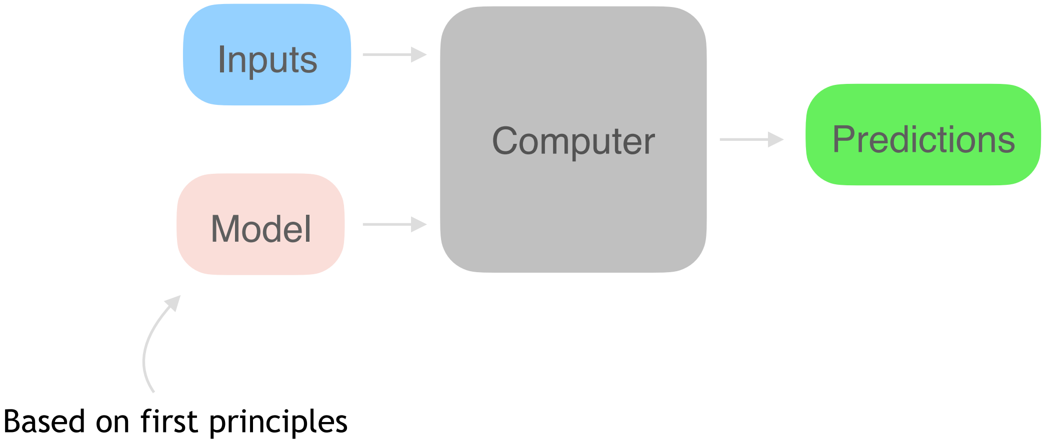
Outline

- **General introduction**
- Deterministic deep learning approaches
- Bayesian deep learning Approaches
- Conclusions

Hypothesis vs data driven models

Hypothesis driven approach

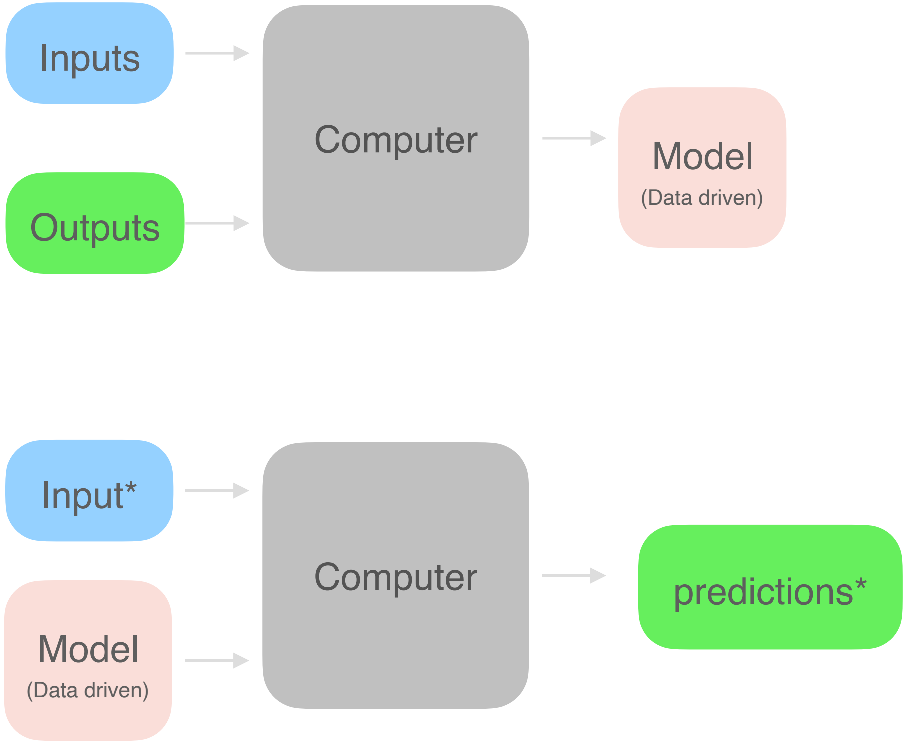
Observation -> intuition -> hypothesis -> theory/model



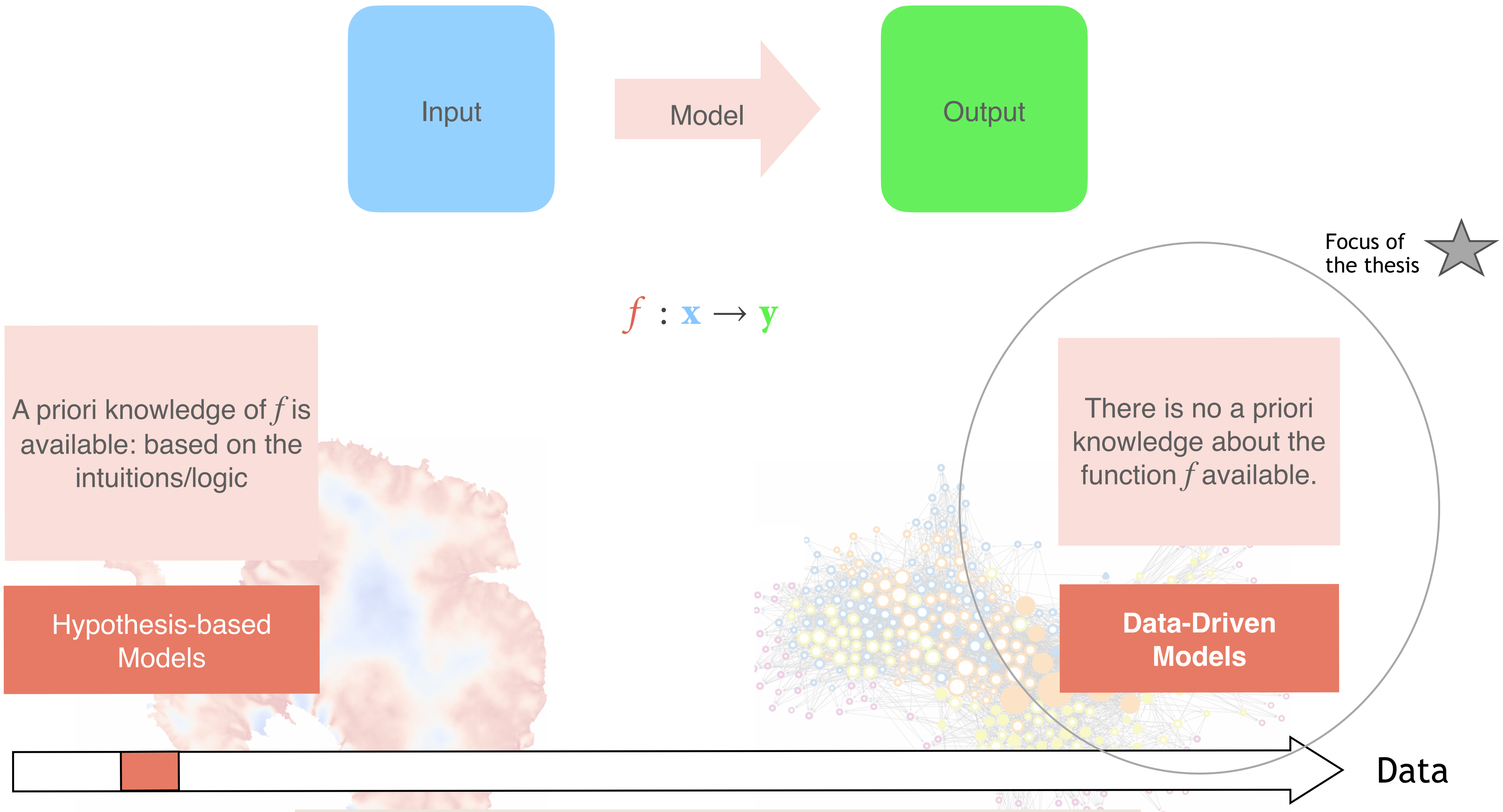
Hypothesis vs data driven models

Data driven approach

Underlying relationships through data directly

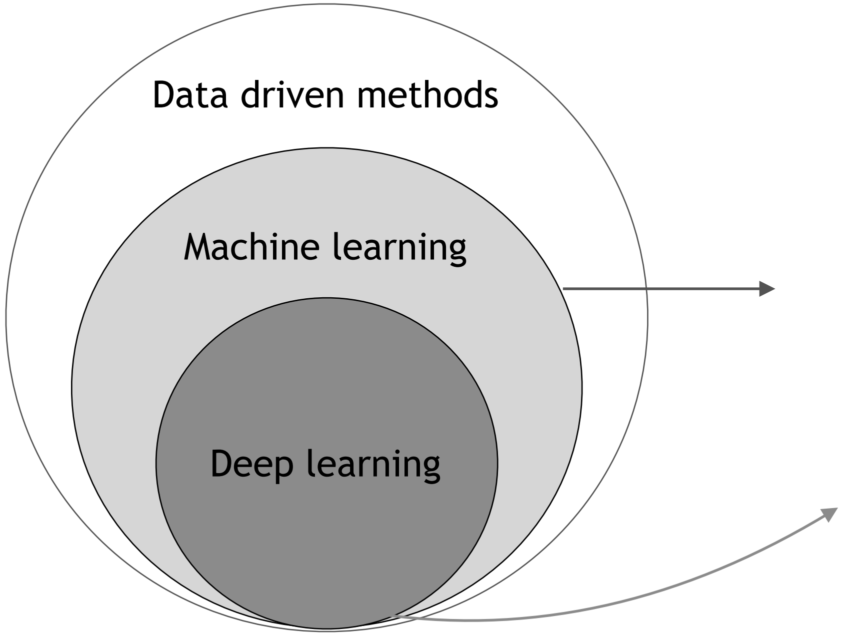


Hypothesis vs data driven models

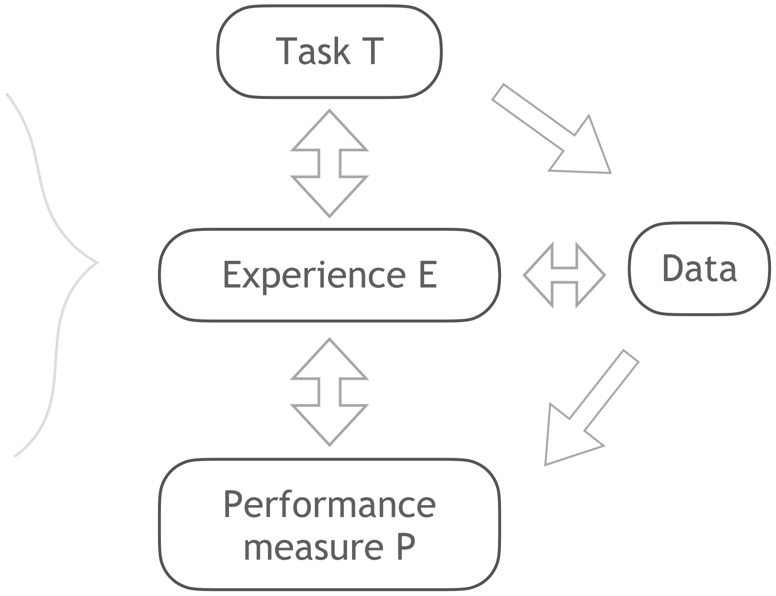


Conceptual shift from *"model through data abstraction"* to *"data is the model"*.

Machine learning methods



- Linear regression
- Logistic regression
- Decision trees
- Random forests
- Support vector machine
- Artificial neural networks



ML approaches in context of mechanics

- Model/constitutive law discovery
  - Efficient Unsupervised Constitutive Law Identification & Discover (EUCLID) [Flaschel et al. 2021]
  - Sparse identification of nonlinear dynamical systems (SINDY) [Brunton et al. 2016]

Inverse problems

- Parameter identification
  - Physics informed neural networks for inverse problems [Raissi et al. 2019]
  - Online parameter estimation with Kalman filters [Chatzi et al. 2010]

- Surrogate modelling
  - Physics informed neural networks for forward problems [Raissi et al. 2019]
  - Real time hyperelastic simulations of solids [Mendizabal et al. 2019]

Forward problems

- Unsupervised discovery of interpretable hyperelastic constitutive laws. Flaschel et al. CMAME 2021
- Discovering governing equations from data by sparse identification of nonlinear dynamical systems. Brunton et al. PNAS 2016
- Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Raissi et al. JCP 2019.
- Experimental application of on-line parametric identification for nonlinear hysteretic systems with model uncertainty. Chatzi et al. Structural Safety 2010.
- Simulation of hyperelastic materials in real-time using deep learning. Mendizabal et al. Medical Image Analysis 2019.

ML approaches in context of mechanics

- Model/constitutive law discovery
  - Efficient Unsupervised Constitutive Law Identification & Discover (EUCLID) [Flaschel et al. 2021]
  - Sparse identification of nonlinear dynamical systems (SINDY) [Brunton et al. 2016]

Inverse problems

- Parameter identification
  - Physics informed neural networks for inverse problems [Raissi et al. 2019]
  - Online parameter estimation with Kalman filters [Chatzi et al. 2010]

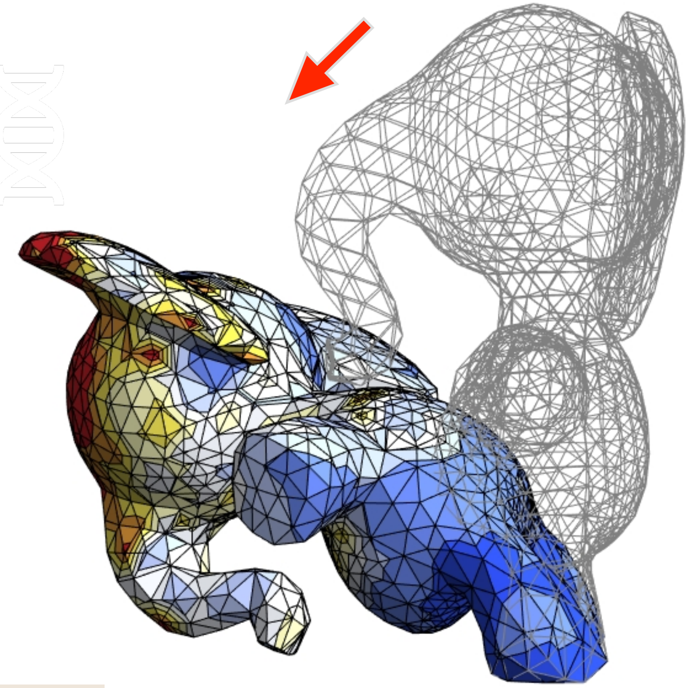
- Surrogate modelling
  - Physics informed neural networks for forward problems [Raissi et al. 2019]
  - Real time hyperelastic simulations of solids [Mendizabal et al. 2019]

Forward problems

- Unsupervised discovery of interpretable hyperelastic constitutive laws. Flaschel et al. CMAME 2021
- Discovering governing equations from data by sparse identification of nonlinear dynamical systems. Brunton et al. PNAS 2016
- Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Raissi et al. JCP 2019.
- Experimental application of on-line parametric identification for nonlinear hysteretic systems with model uncertainty. Chatzi et al. Structural Safety 2010.
- Simulation of hyperelastic materials in real-time using deep learning. Mendizabal et al. Medical Image Analysis 2019.

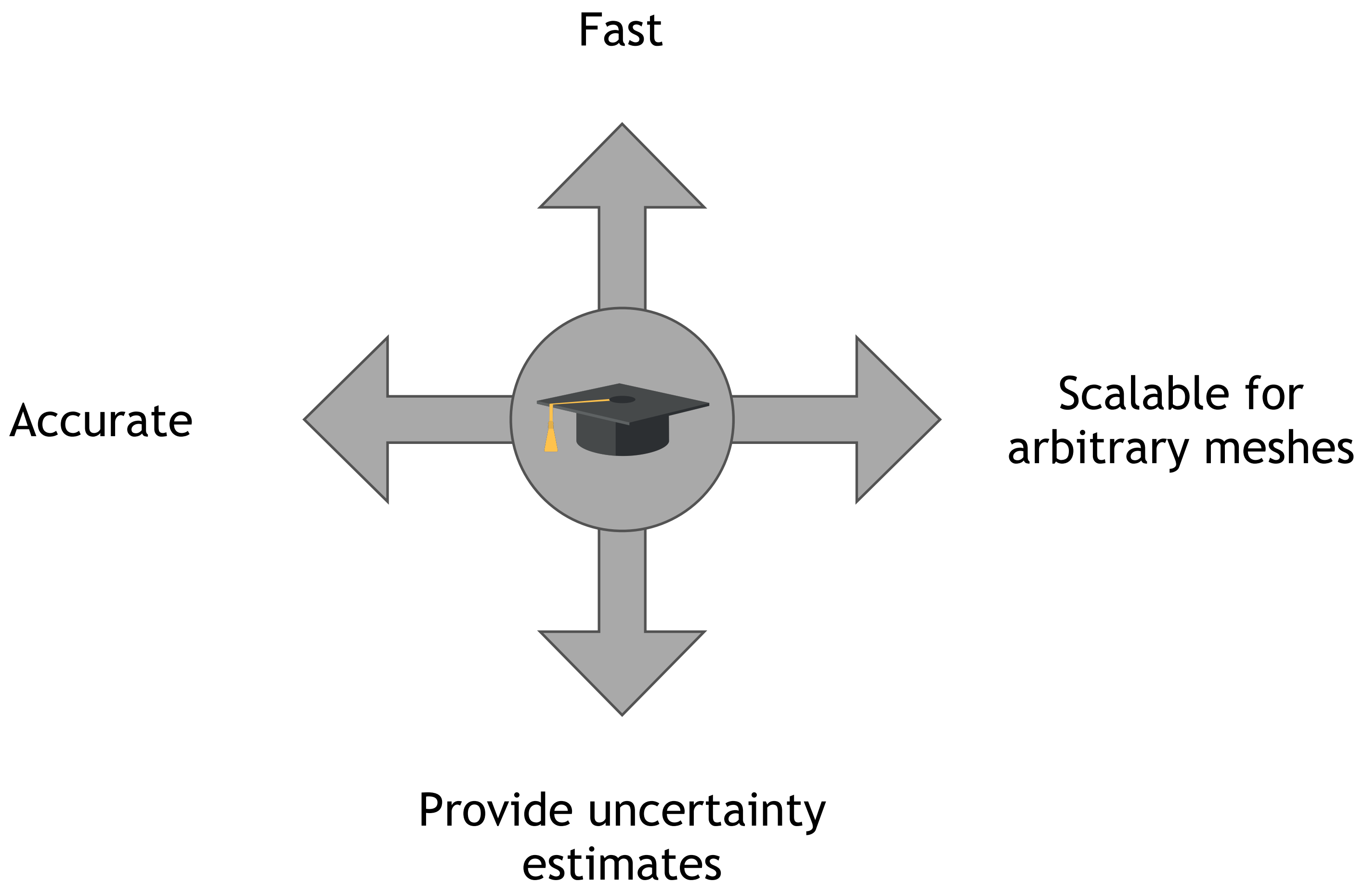
Surrogate models for non-linear deformations of solids

- Necessity of real time simulations in several applications
- Conventional solvers are computationally expensive



Goal: Deep learning surrogate model for simulating deformation of solids

Challenges in surrogate modelling

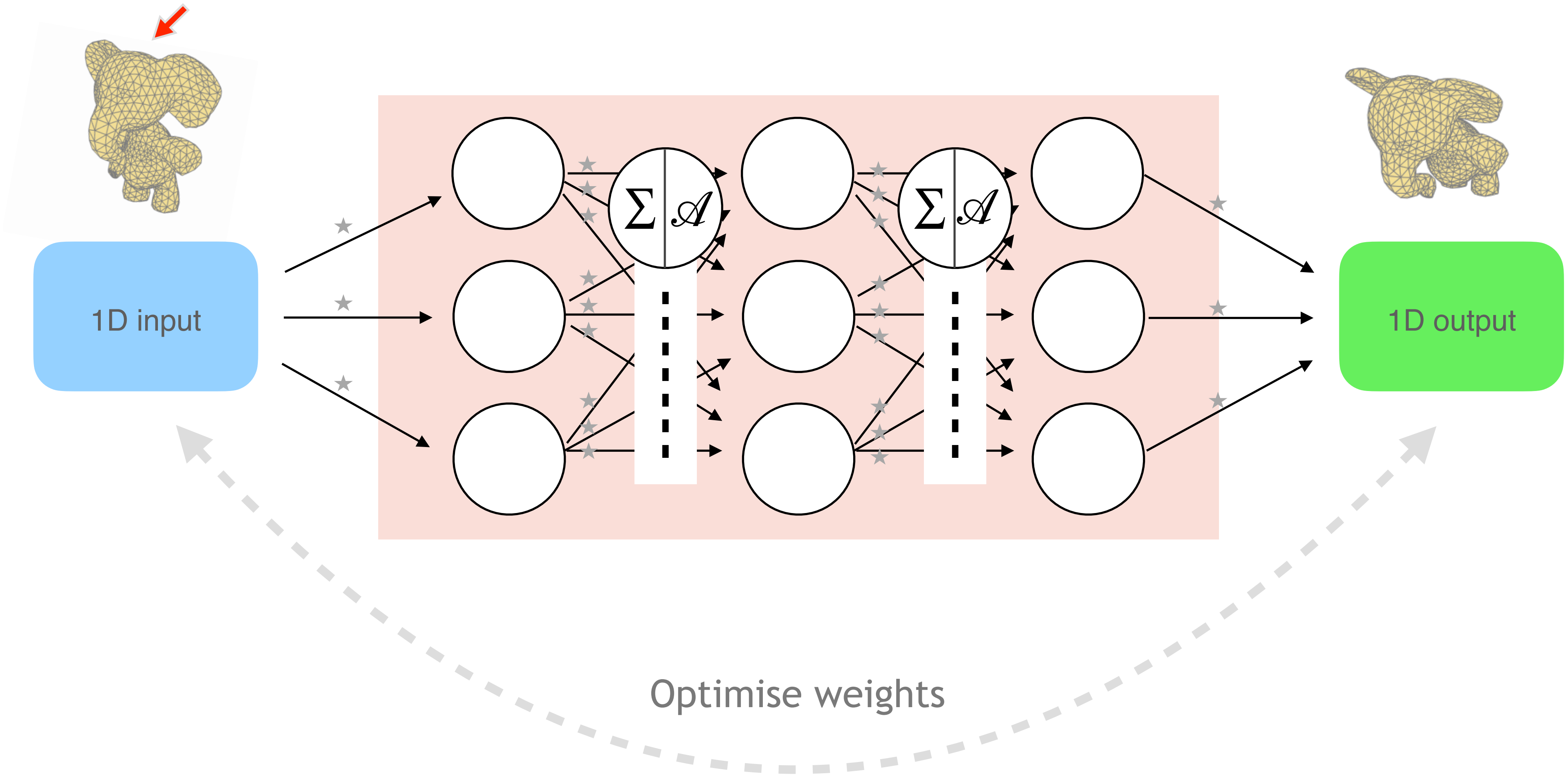


Outline

- General introduction
- **Deterministic deep learning approaches**
- Bayesian deep learning Approaches
- Conclusions

Artificial neural networks

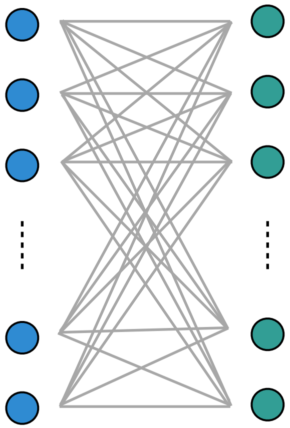
$$\text{output} = f(\text{input}, \theta) = \mathsf{T}^L(\mathsf{T}^{L-1}(\mathsf{T}^{L-2}(\ldots.); \theta^{L-1}); \theta^L)$$



Fully connected vs convolutional neural networks

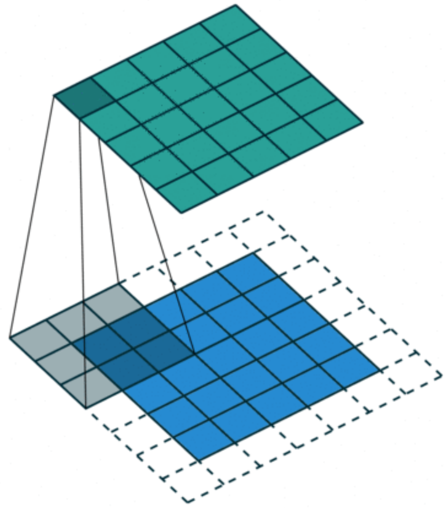
Input dimension = Output dimension = DOFs of the mesh

- Too many parameters :(



Fully connected

- Local operations and parameters sharing



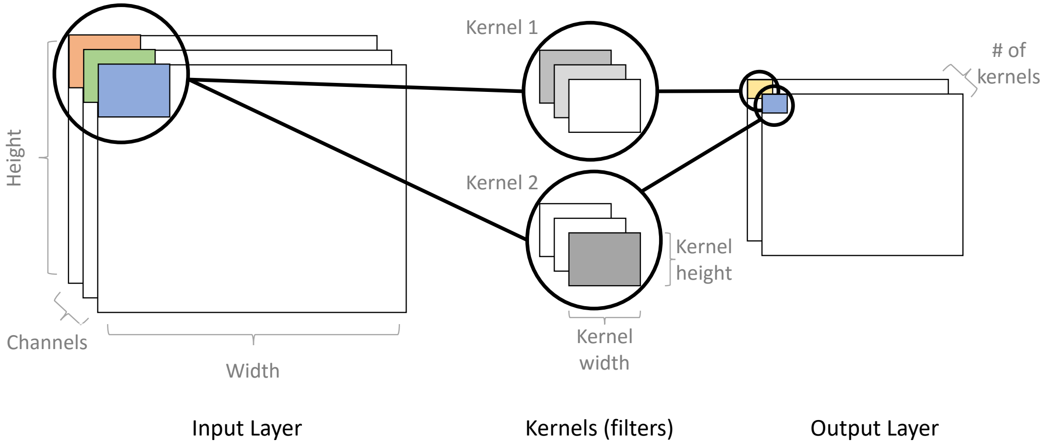
Locally connected (Covolutional Neural Networks)

Animation by Prof. Maucher

Types of convolutional network layers

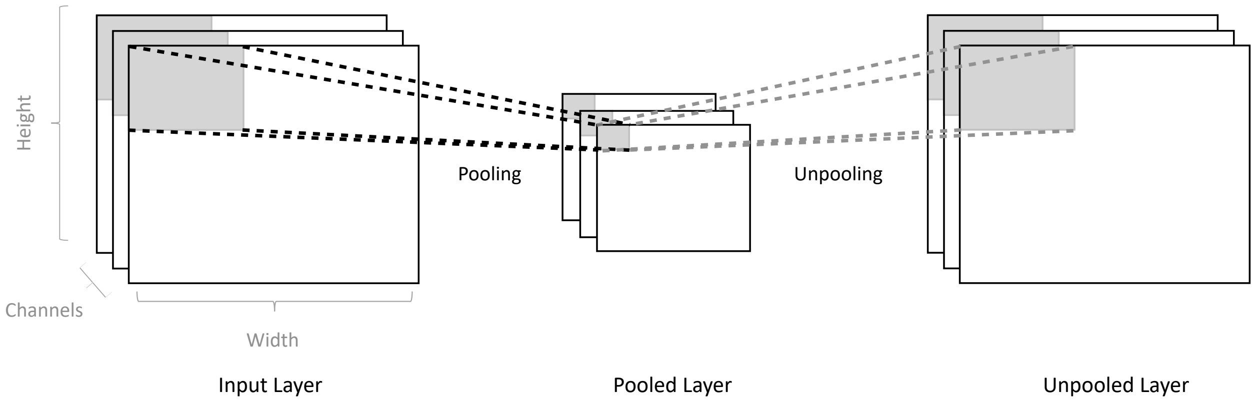
Convolution layer

- Non-linear mappings between input-output



Pooing layers

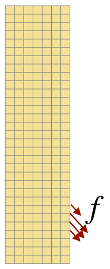
- Dimensionality reduction

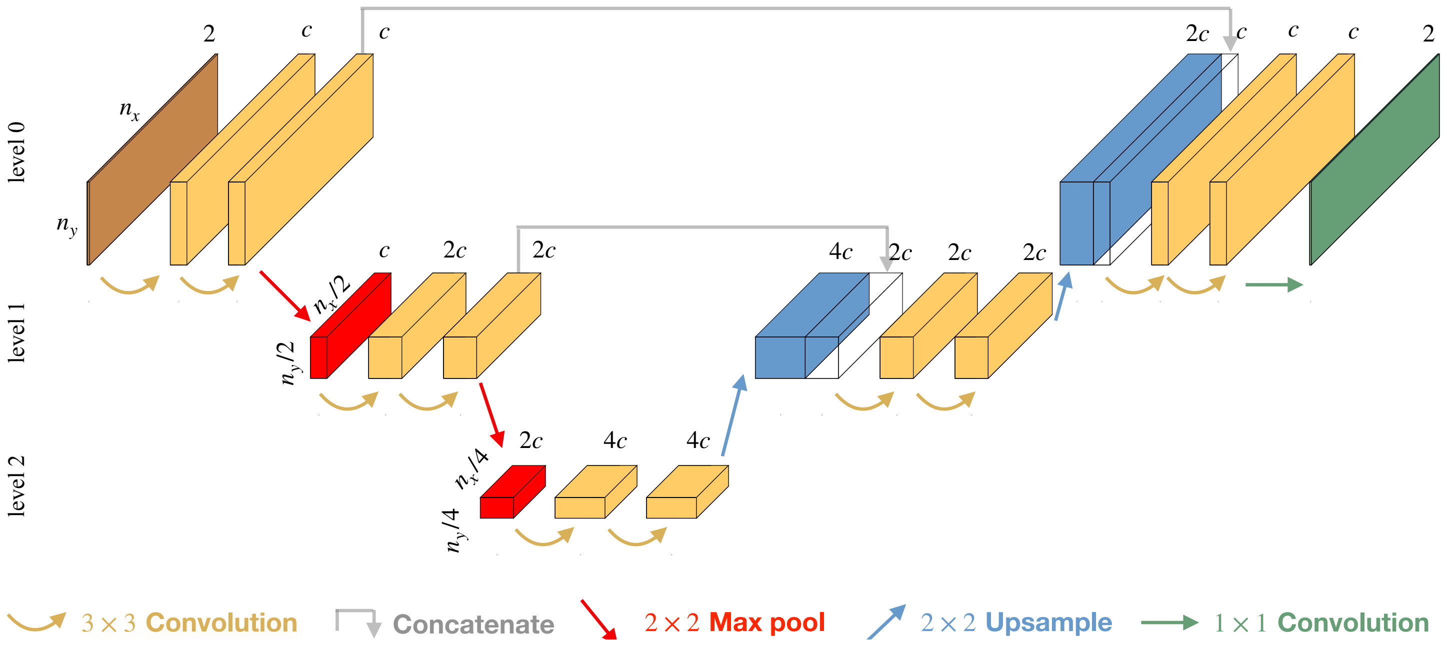


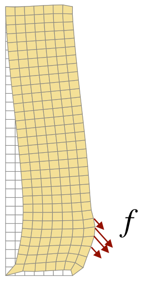
CNN U-Net surrogate model

Input: Force array of mesh

Output: Displacement array of mesh



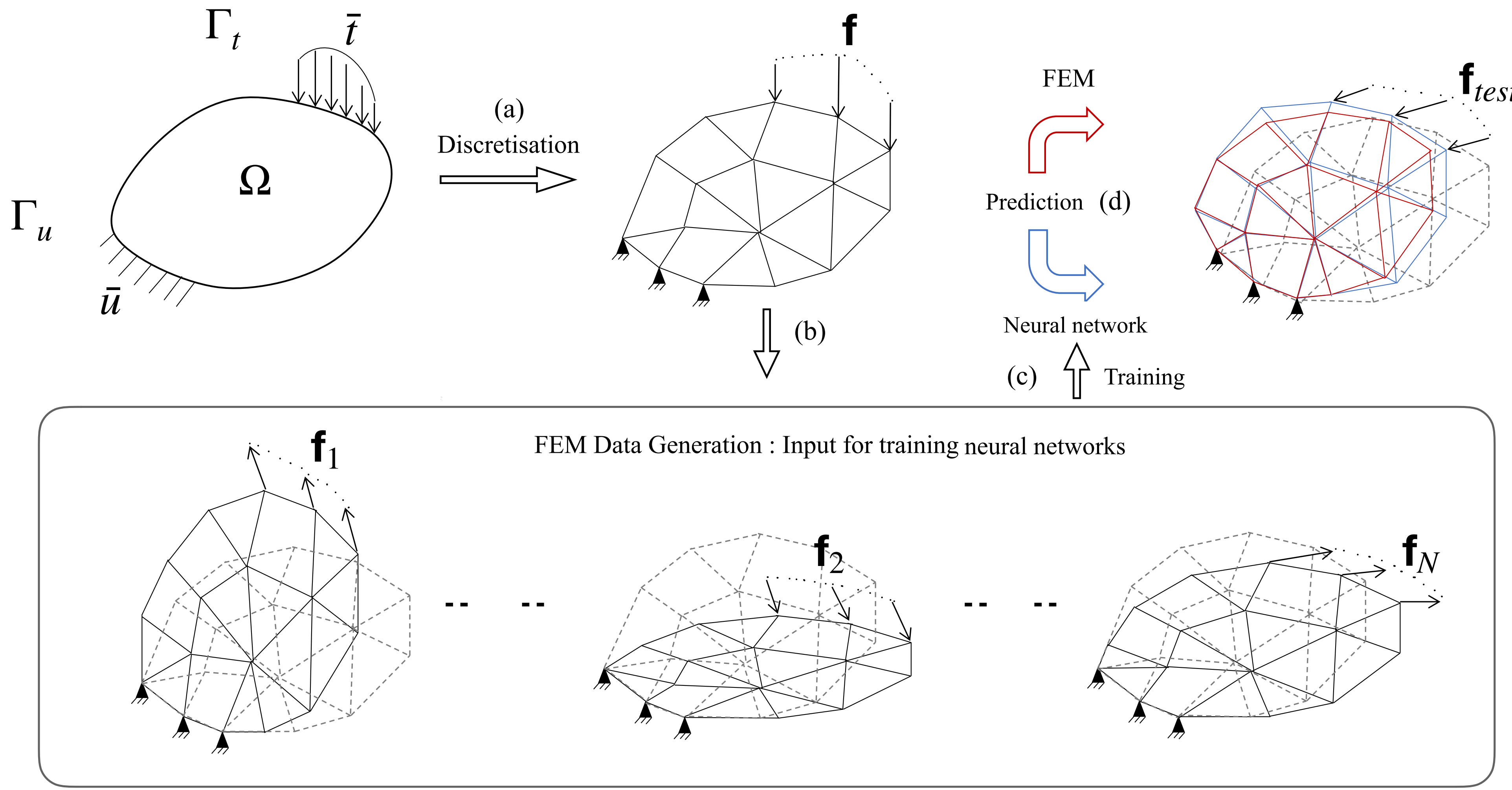




U-Net CNN architecture for 2D domains

[S. Deshpande and J. Lengiewicz and S. P. A. Bordas, Probabilistic deep learning for real-time large deformation simulations, Computer Methods in Applied Mechanics and Engineering (2022) 115307, https://doi.org/10.1016/j.cma.2022.115307]

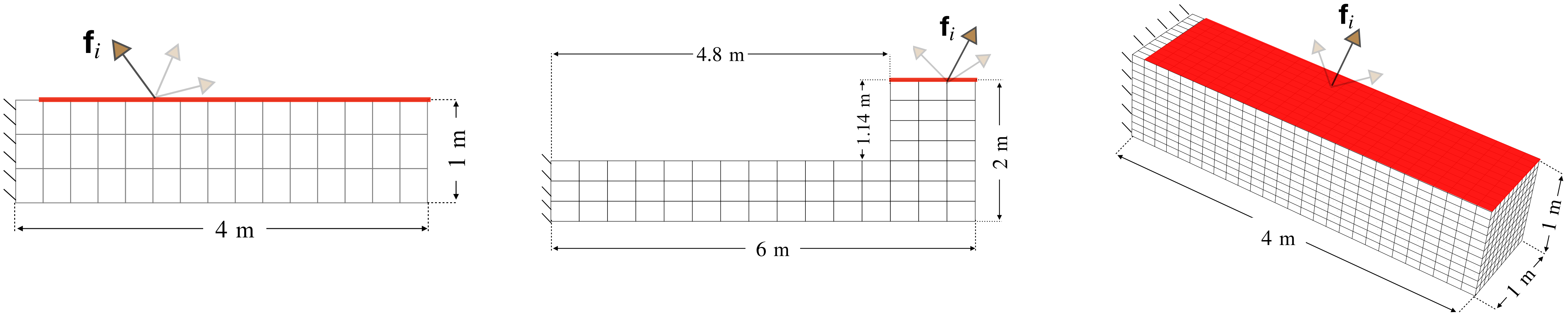
General framework



[S. Deshpande and J. Lengiewicz and S. P. A. Bordas, Probabilistic deep learning for real-time large deformation simulations, Computer Methods in Applied Mechanics and Engineering (2022) 115307, https://doi.org/10.1016/j.cma.2022.115307]

Finite Element Dataset generation

- Neo-Hookean hyper elasticity material law
- Random Point loads in the region of interest Γ_t
- Generation of synthetic dataset $D = \{(\mathbf{f}_1, \mathbf{u}_1), \ldots, (\mathbf{f}_i, \mathbf{u}_i), \ldots, (\mathbf{f}_N, \mathbf{u}_N)\}$



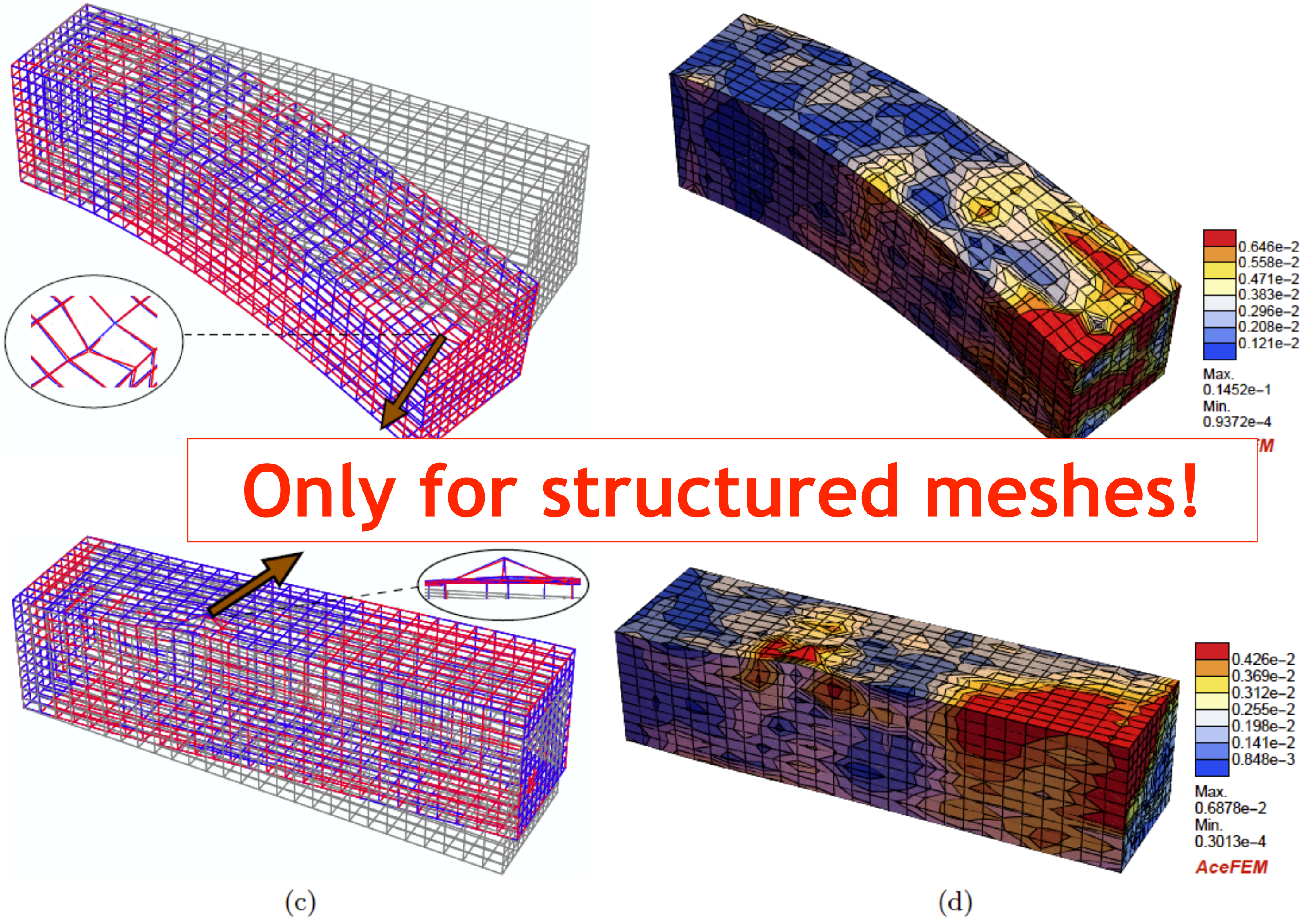
Data generation

Neo-hookean strain energy density ;

$$W = \frac{\mu}{2}(I_c - 3 - 2\ln J) + \frac{\lambda}{4}(J^2 - 1 - 2\ln J)$$

AceGen - http://symech.fgg.uni-lj.si

Visualisation for 3D cases



Only for structured meshes!

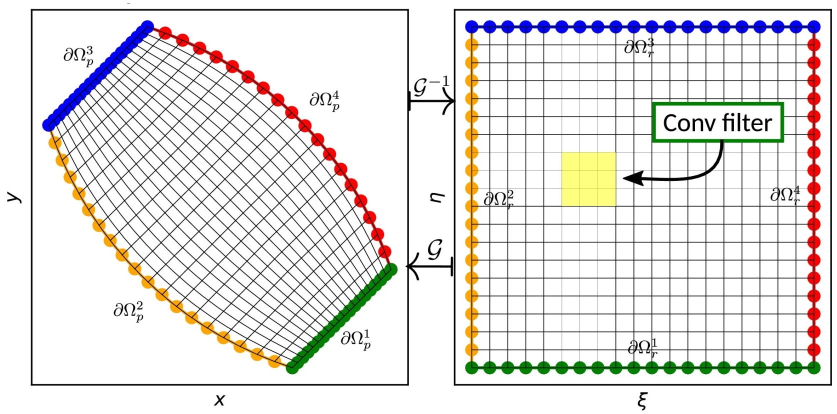
1.1 [m], 0.6%

0.26 [m], 1.6%

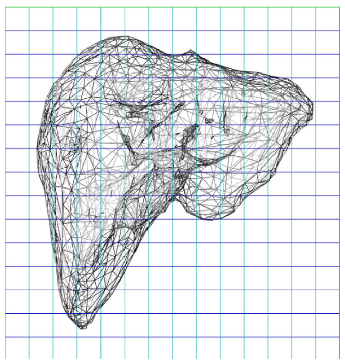
Deformed meshes

Error contours

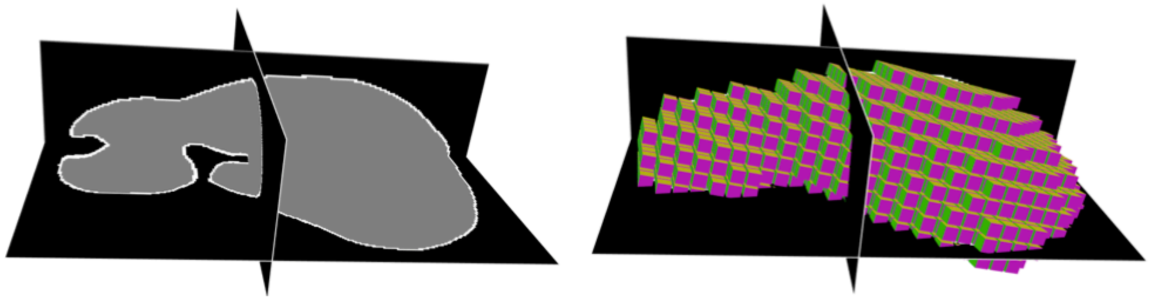
CNN U-Net for arbitrary meshes



(a) Parametric transformation
[Gao et al. 2021]



(b) Embed into hexahedron grid [Mendizabal et al. 2019]



(c) Immersed boundary method
[Brunet et al. 2019]

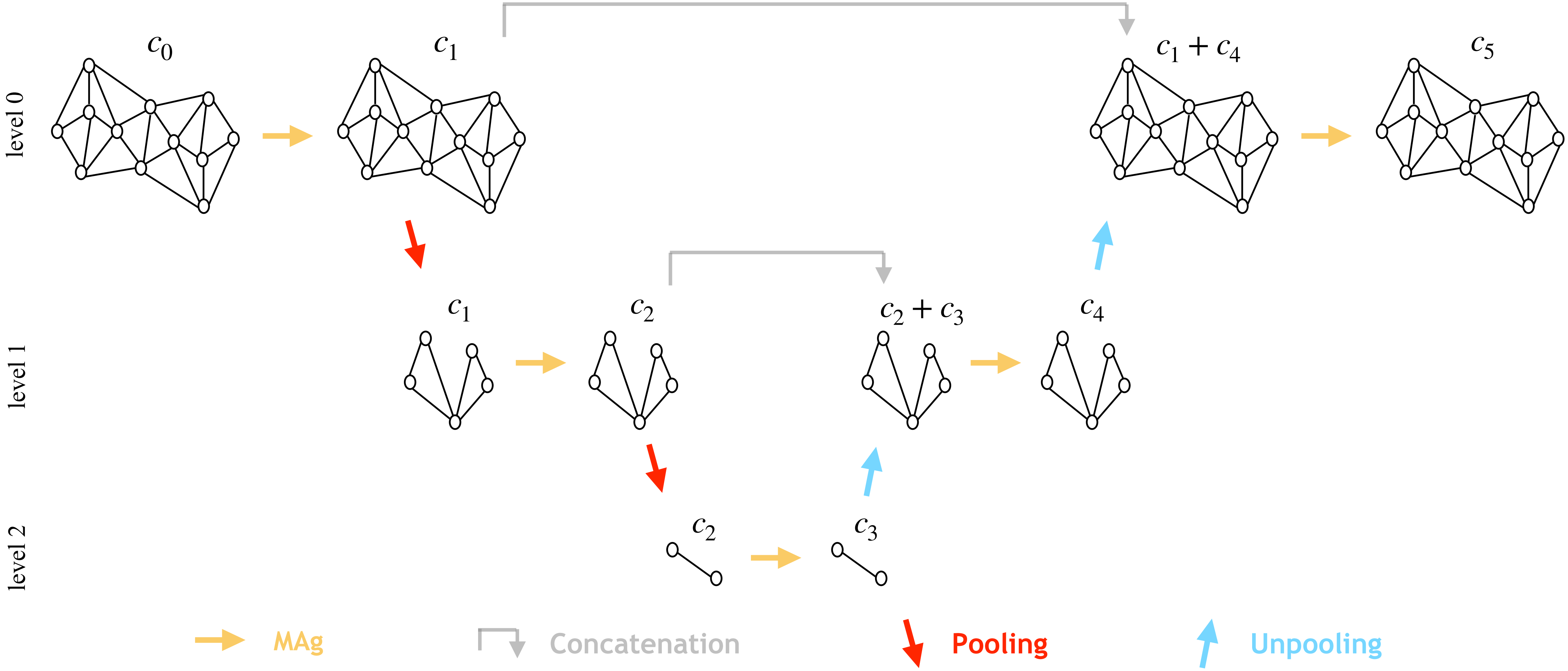
- **Associated preprocessing costs**
- **Inefficient for complex meshes**

- PhyGeoNet: Physics-informed geometry-adaptive convolutional neural networks for solving parameterized steady-state PDEs on irregular domain. Gao et al. JCP 2021
- Simulation of hyperelastic materials in real-time using deep learning. Mendizabal et al. Medical Image Analysis 2020.
- Physics-based deep neural network for augmented reality during liver surgery. Brunet et al 2019.

MAgNET: A graph U-Net architecture for mesh based simulations

[S. Deshpande, S. P. A. Bordas and J. Lengiewicz. MAgNET: A Graph U-Net Architecture for Mesh-Based Simulations (2023).
https://arxiv.org/abs/2211.00713 (under review at Engineering Applications of AI)]

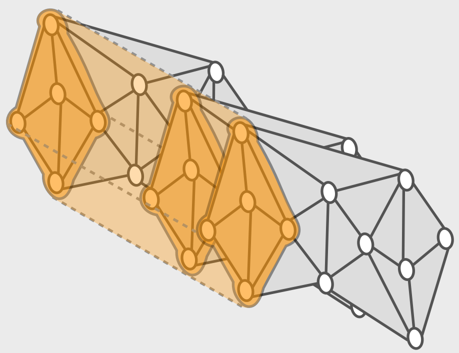
Multichannel Aggregation Network: MAgNET



[S. Deshpande, S. P. A. Bordas and J. Lengiewicz. MAgNET: A Graph U-Net Architecture for Mesh-Based Simulations (2023). https://arxiv.org/abs/2211.00713 (under review at EAAI)]

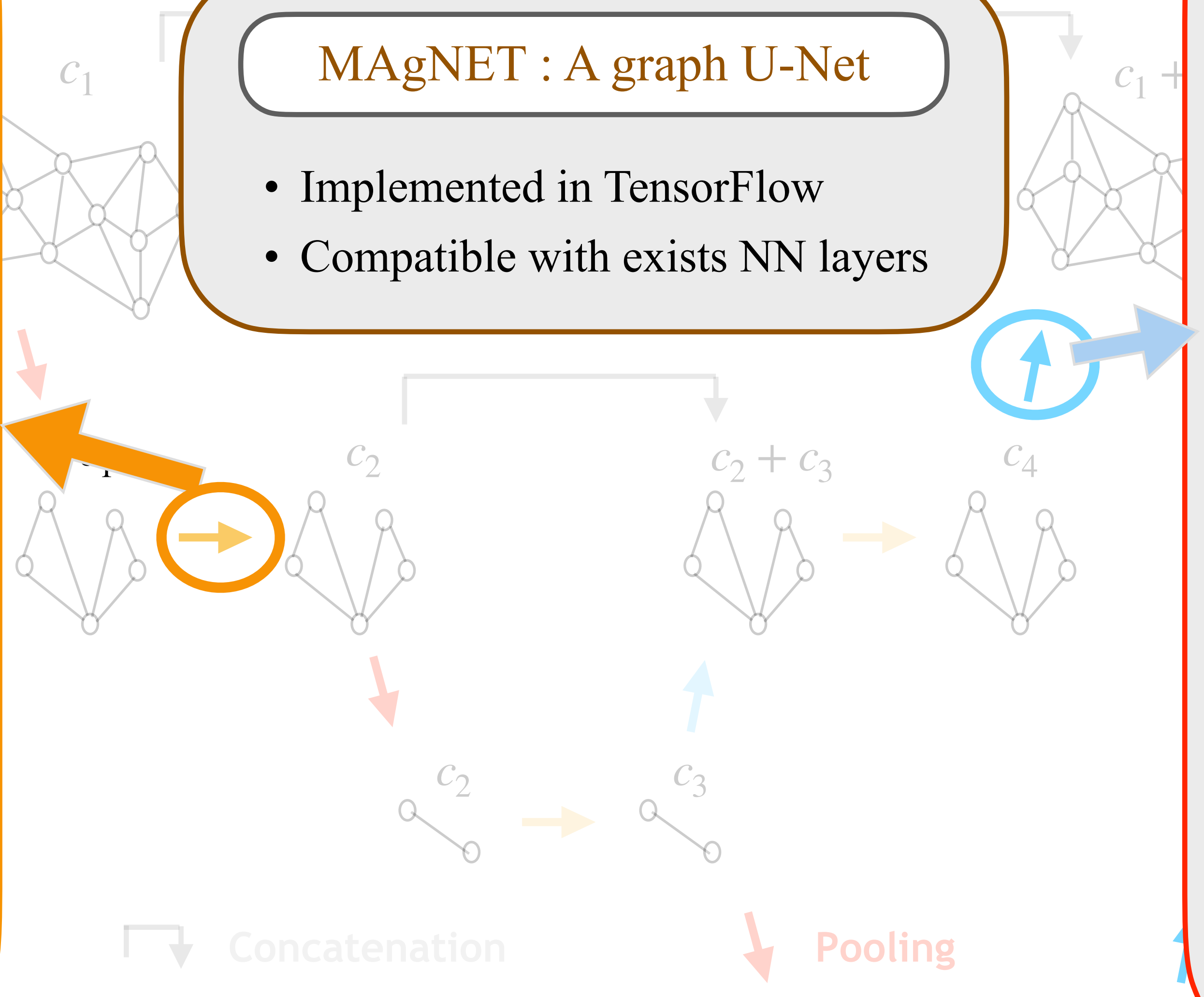
Multichannel Aggregation layer (MAg)

- For supervised learning on graph structured data.
- Extends the concepts of convolution operations to arbitrary graph inputs.



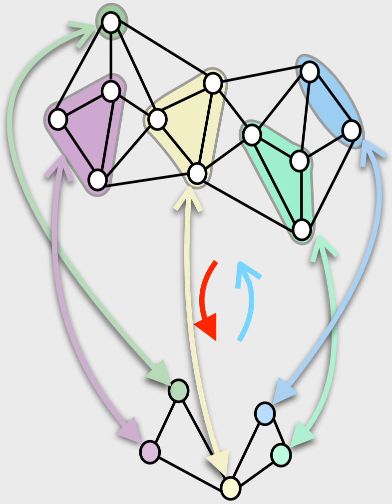
MAgNET : A graph U-Net

- Implemented in TensorFlow
- Compatible with exists NN layers



Pooling/Unpooling layers

- For efficient learning through reduced representations.
- Perform pooling on arbitrary graph inputs.

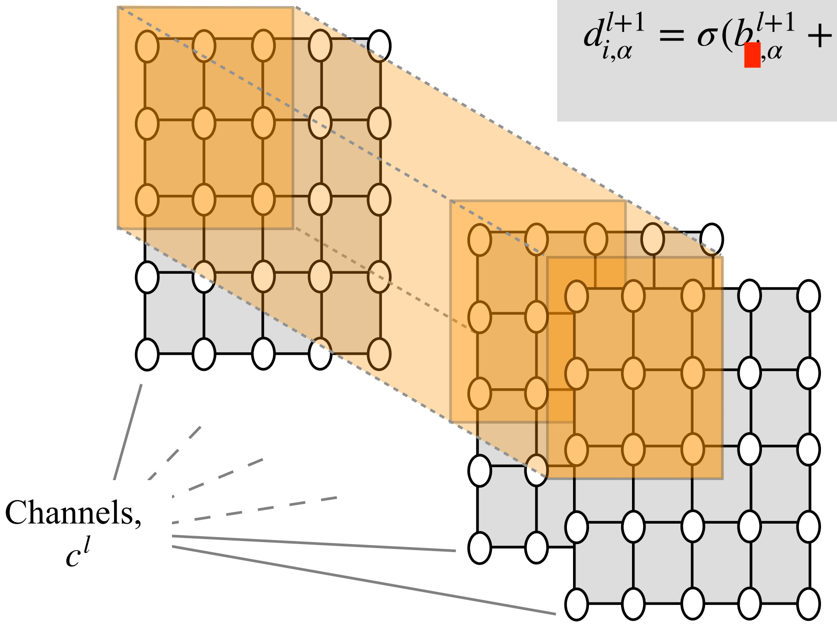


MAg : Multichannel Aggregation layer

- Extends the concept of localised operations in CNNs
- Learnable weighted aggregation (parameters are not shared)

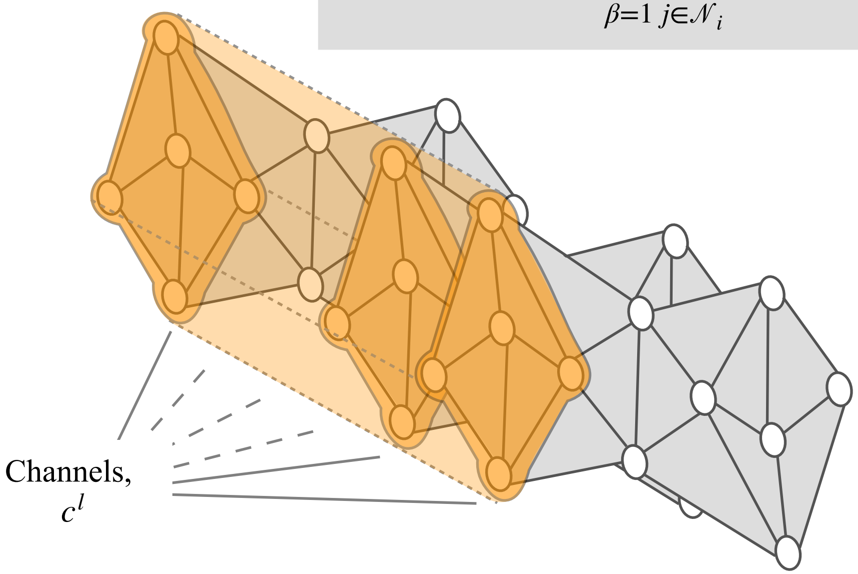
$$d_{i,\alpha}^{l+1} = \sigma(b_{{\color{red}\blacksquare},\alpha}^{l+1} + \sum_{\beta=1}^{c^l} \sum_{j \in \mathcal{N}_i} k_{{\color{red}\blacksquare},j,\alpha,\beta}^{l+1} d_{j,\beta}^{l})$$

Constant filter parameters



Convolution layer

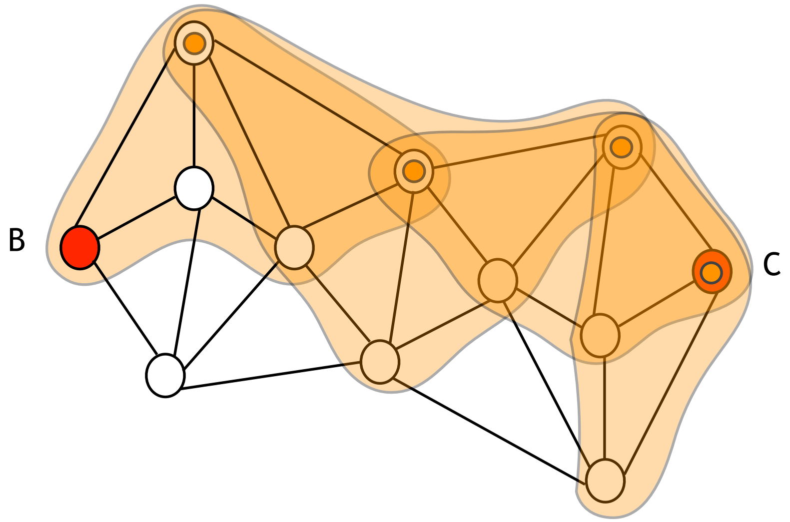
$$d_{i,\alpha}^{l+1} = \sigma(b_{i,\alpha}^{l+1} + \sum_{\beta=1}^{c^l} \sum_{j \in \mathcal{N}_i} k_{i,j,\alpha,\beta}^{l+1} d_{j,\beta}^{l})$$

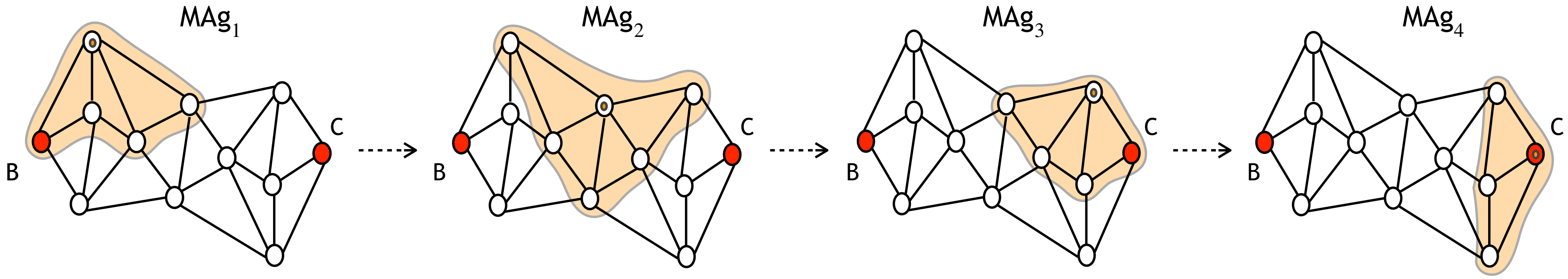


MAg layer

Message passing between topologically further nodes

- Complex topology demands multiple MAg operations
- Possible workaround - bigger aggregation window
- Computationally expensive procedure





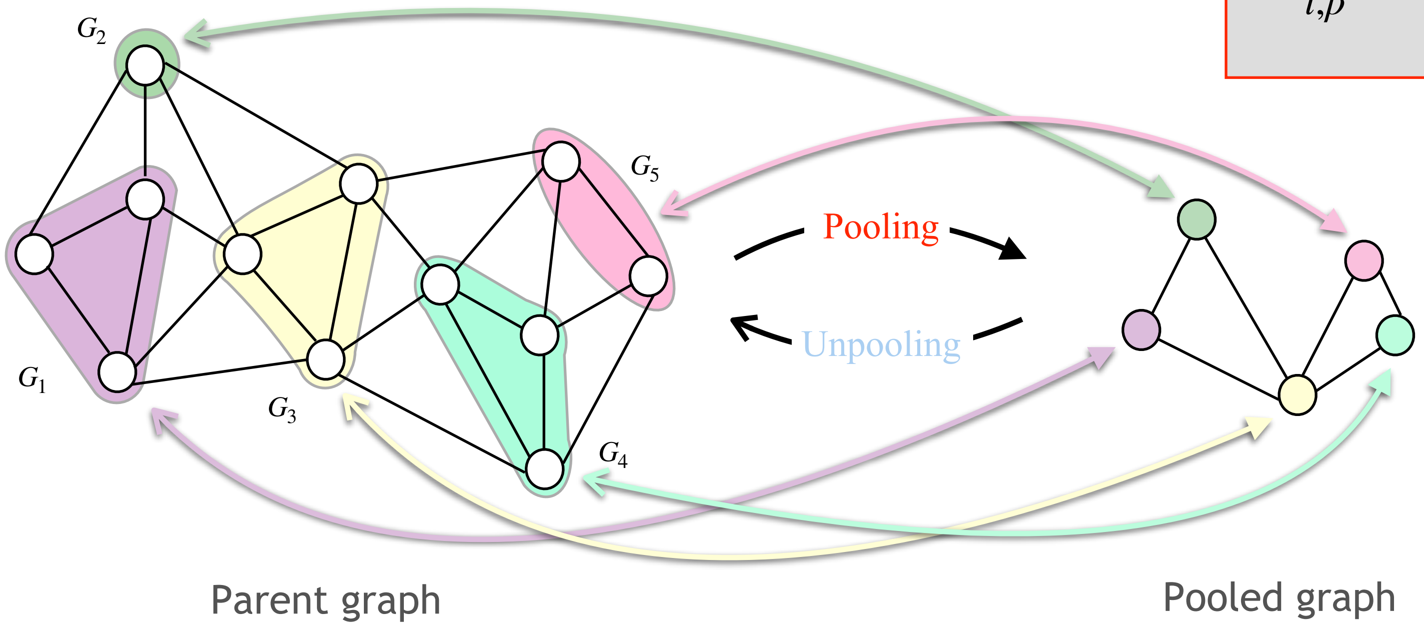
4 MAg local aggregation operations to propagate nodal feature information from B to C

Pooling/Unpooling layer

- Generate pooled graphs for arbitrary input graphs
- Algorithm to generate non-overlapping cliques (subgraphs)

max/min/avg

$$d_{i,\beta}^{l+1} = \underset{j \in \mathbf{S_i}}{\text{aggr}}\ d_{j,\beta}^{l}$$

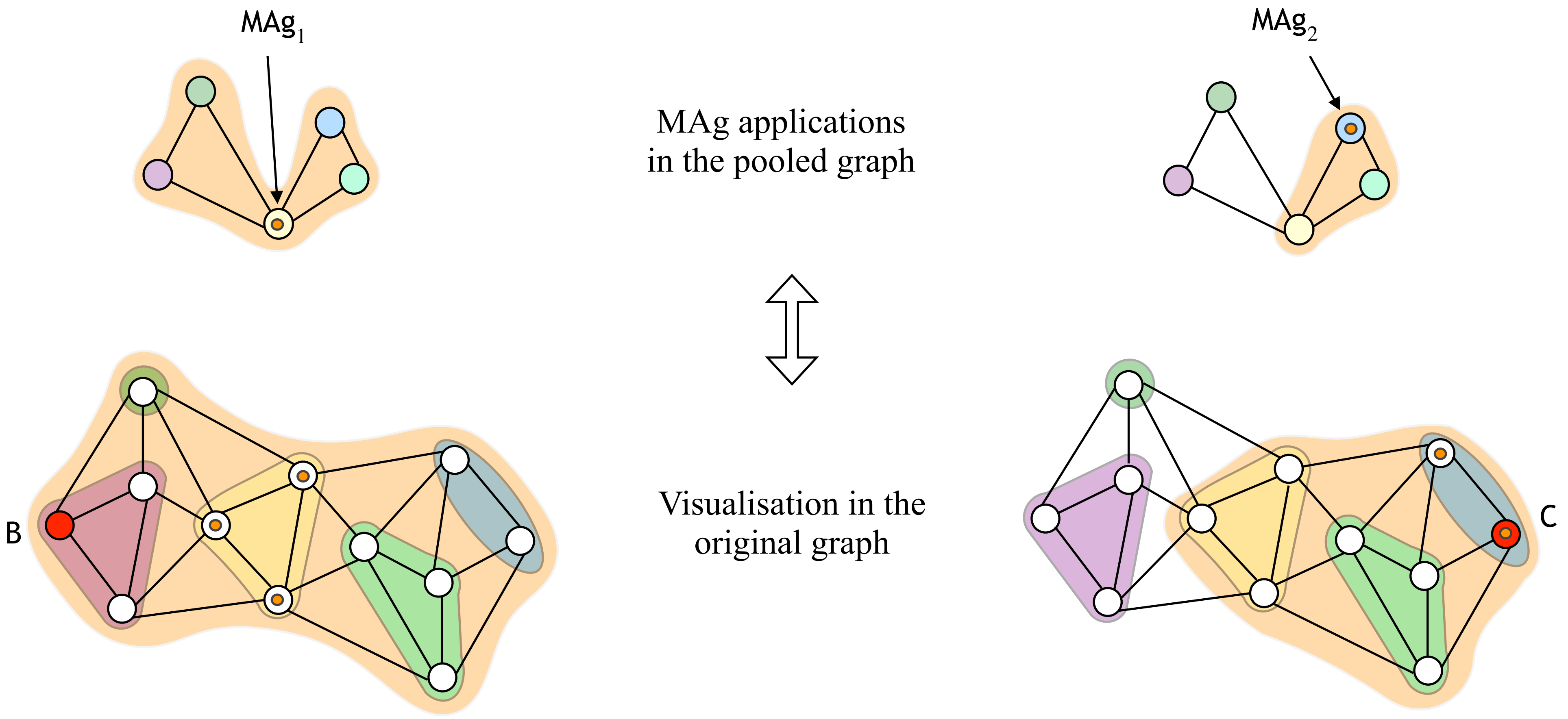


G_i is composed of node set S_i

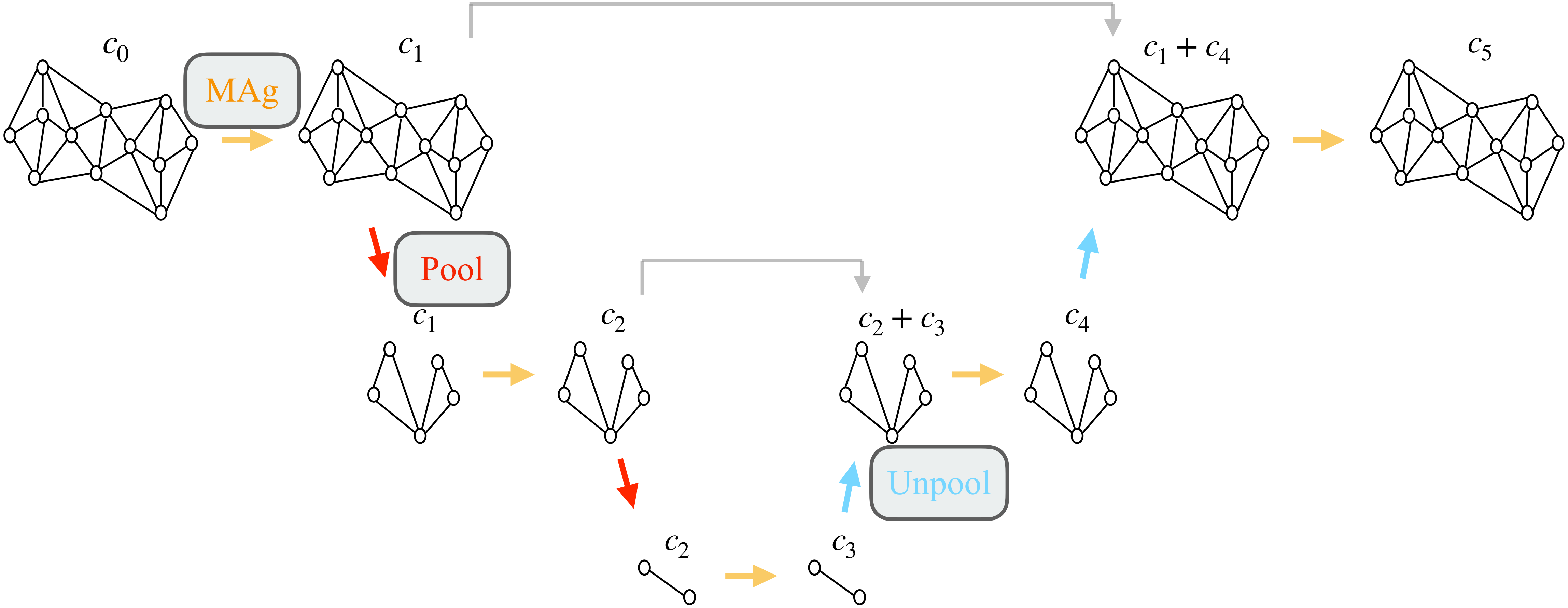
$$d_{i,\beta}^{l+1} = d_{j,\beta}^{l} \quad \text{for} \quad i \in \mathbf{S_j}$$

Visualisation of information exchange in the pooled graph

- Efficient learning through pooled representation

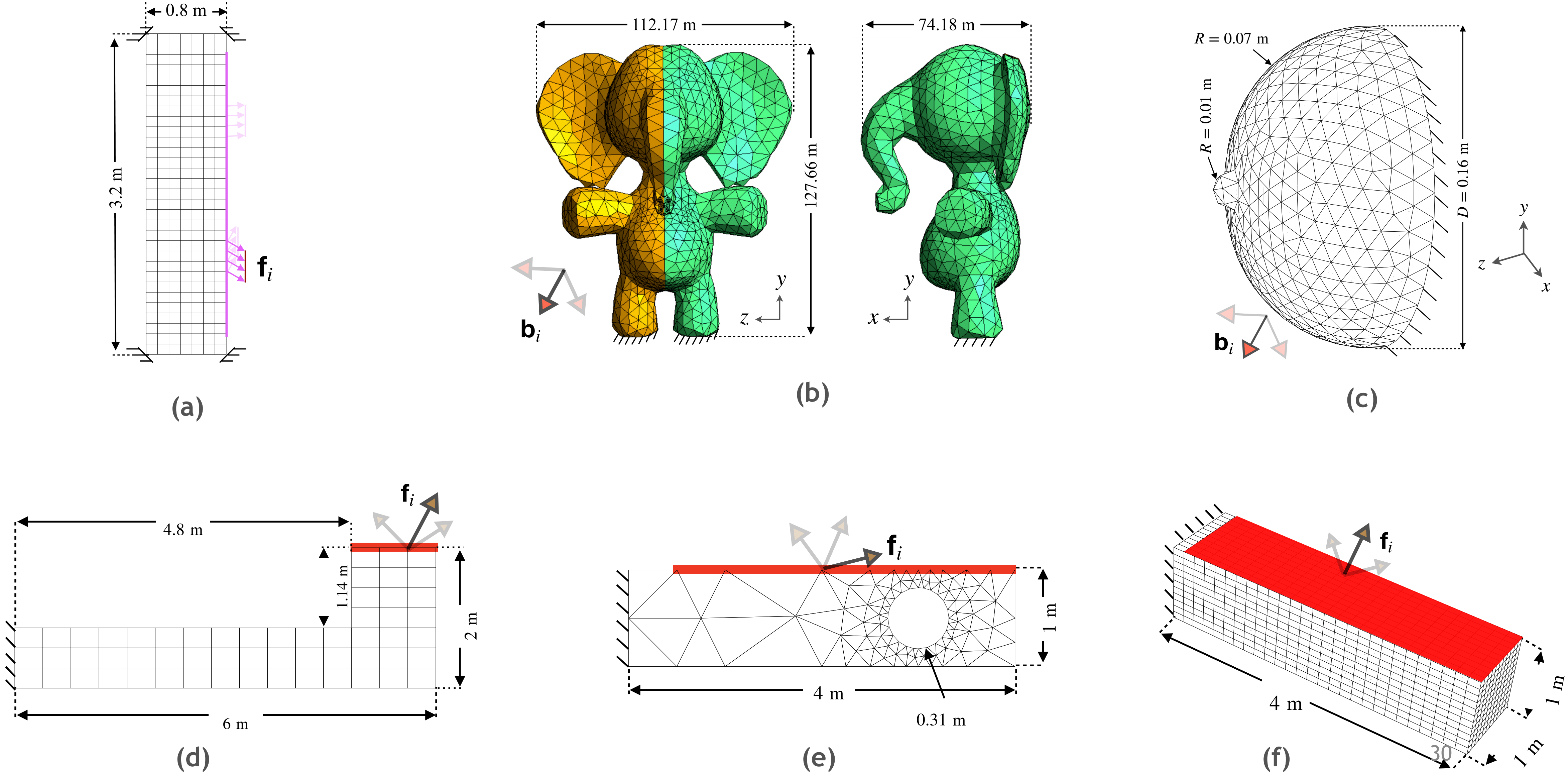


Multichannel Aggregation Network: MAgNET



This thesis advances neural network architectures : first type of such graph U-net

Non-linear FEM datasets $\{(\mathbf{f}_i, \mathbf{u}_i)\}$



Evaluation Metrics

Training Metric (Mean Squared Error)

$$\theta^* = \arg\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} ||\mathcal{U}(\mathbf{f}_i) - \mathbf{u}_i||_2^2$$

N - No of training examples

Testing Metric (Mean Absolute Error)

$$e(\mathcal{U}(\mathbf{f}_m), \mathbf{u}_m) = \frac{1}{\mathcal{F}} \sum_{i=1}^{\mathcal{F}} |\mathcal{U}(\mathbf{f}_m)^i - \mathbf{u}_m^i|$$

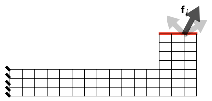
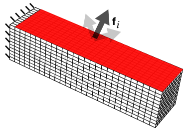
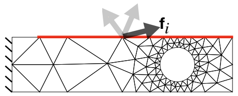
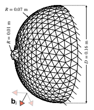
$$\bar{e} = \frac{1}{M} \sum_{i=1}^{M} e(\mathcal{U}(\mathbf{f}_m), \mathbf{u}_m)$$

$$\sigma(e) = \sqrt{\frac{1}{M-1} \sum_{m=1}^{M} [e(\mathcal{U}(\mathbf{f}_m), \mathbf{u}_m) - \bar{e}]^2}$$

$\mathcal{F}$ - No of Dofs

M - No testing examples

Prediction accuracy

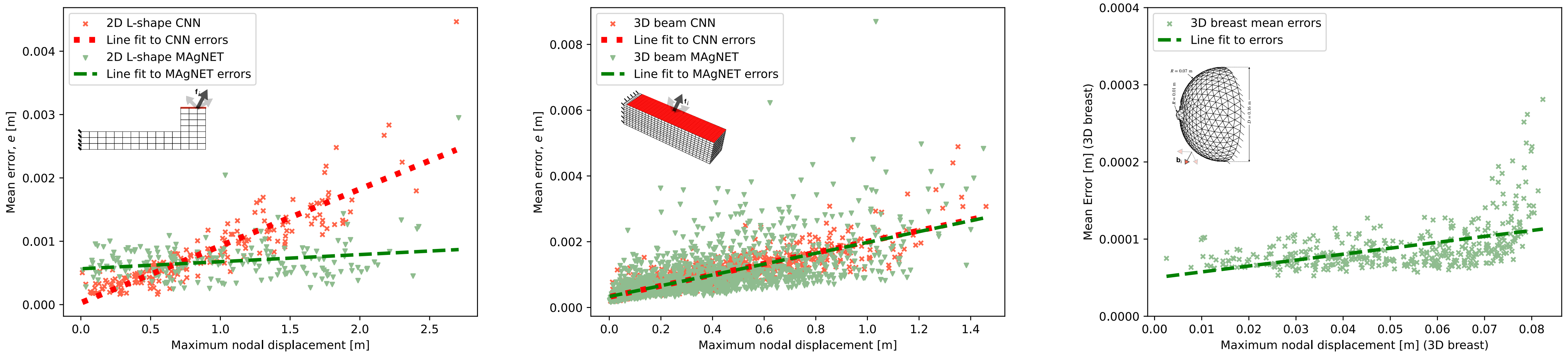





Example	NN type	N. tests	$\bar{e}$[m]	$\sigma(e)$[m]	Max nodal displacement [m]	e_{max}[m]
2D L-shape	CNN	200	0.7 e-3	0.6 e-4	2.7	1.8 e-2
	MAgNET		0.5 e-3	0.2 e-4		1.1 e-2
3D beam	CNN	1782	0.7 e-3	0.5 e-3	1.5	5.4 e-1
	MAgNET		0.8 e-3	0.7 e-3		7.7 e-1
2d beam (hole)	MAgNET	240	0.7 e-3	0.4 e-3	1.4	1.4 e-2
3D breast		400	8.9 e-5	3.1 e-5	0.7 e-1	5.1 e-3

Performance over test sets

Errors vs deformation magnitude

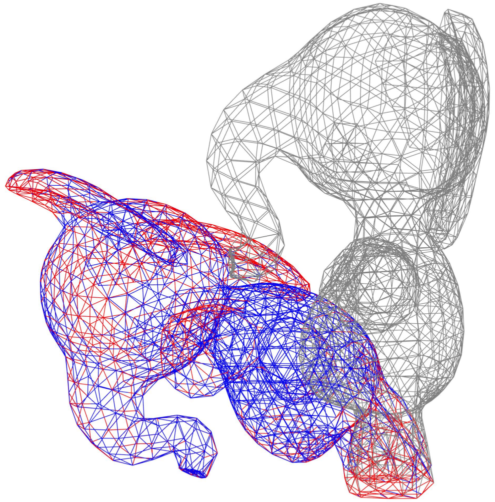
- Errors are less sensitive to maximum nodal deformation



Mean errors sorted as per maximum nodal displacements

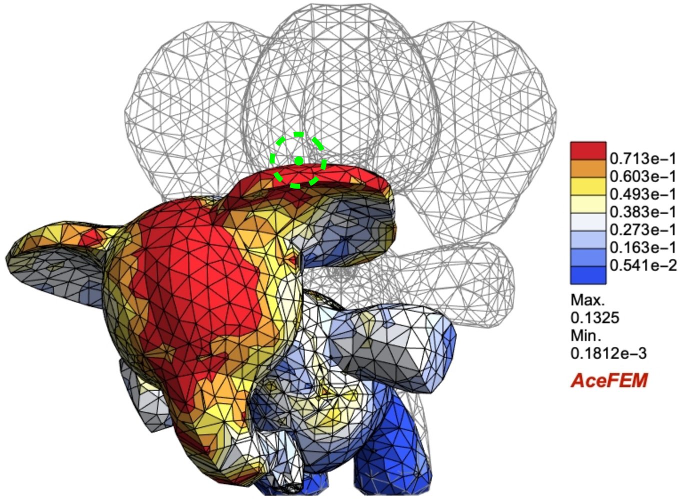
Error contours

- Max nodal displacement (green node) = 140.04 m
- 0.03%, 0.02% relative errors for MAgNET and perceiver IO (a transformer model) respectively

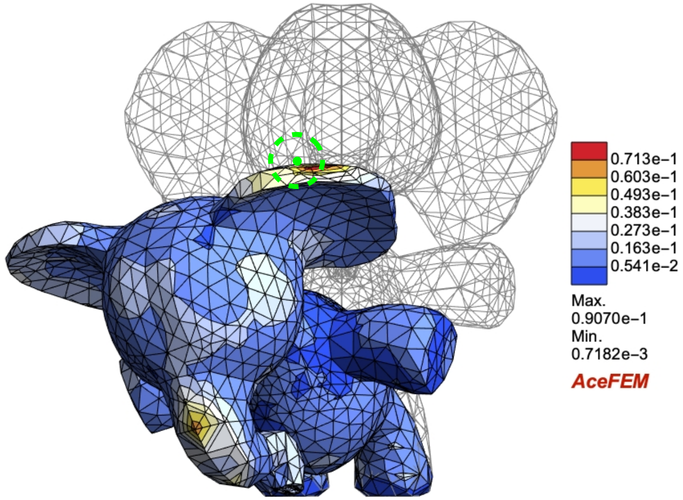


Deformed meshes

MAgNET



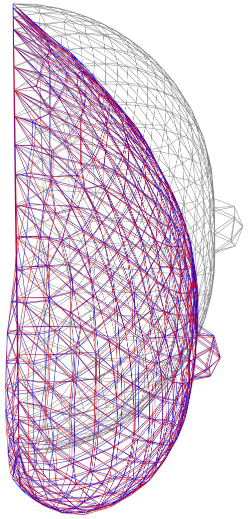
Perceiver IO



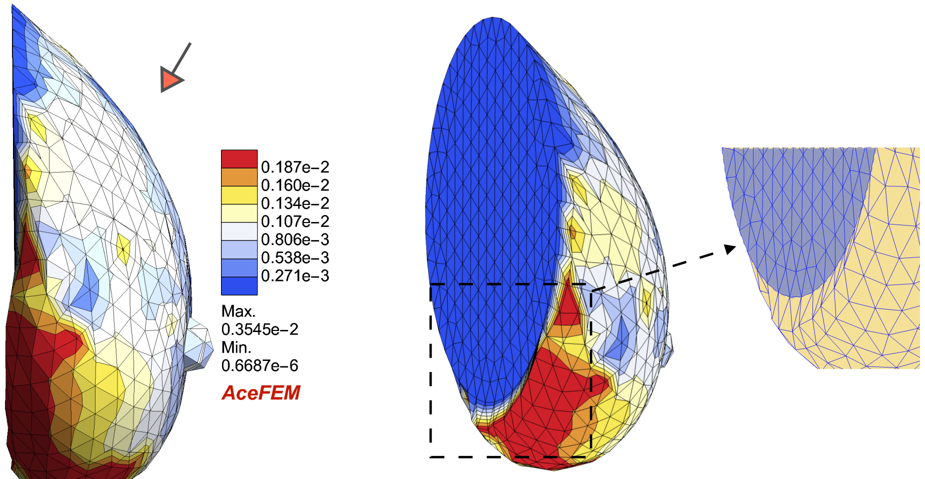
Nodal displacement error contours

S. Deshpande, R.I. Sosa, S.P.A. Bordas and J. Lengiewicz. Convolution, aggregation and attention based deep neural networks for accelerating simulations in mechanics. Frontiers in Materials (2023). 10:1128954. doi: 10.3389/fmats.2023.1128954

Retrieving boundary conditions



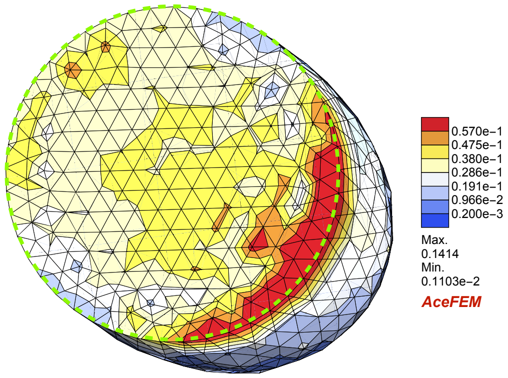
Deformed mesh



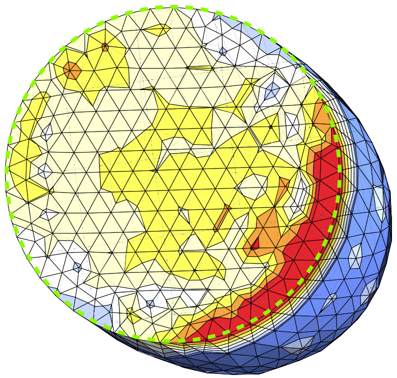
Nodal displacement error contours

- Maximum nodal displacement = 0.082 m

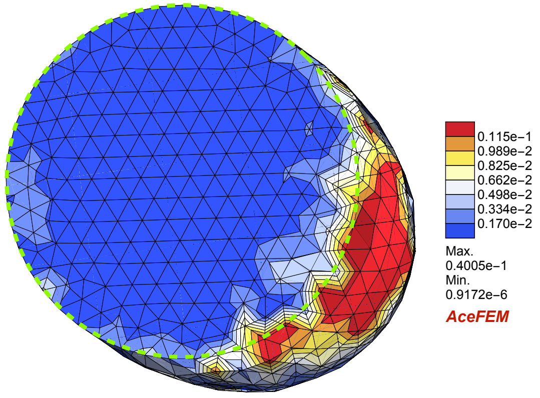
Reaction force at
the fixed boundary



MAgNET



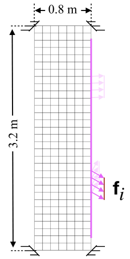
FEM

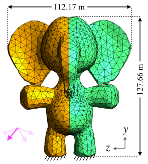


Error in retrieving
reaction force

- Easy extension to physics informed variant

Training and inference times



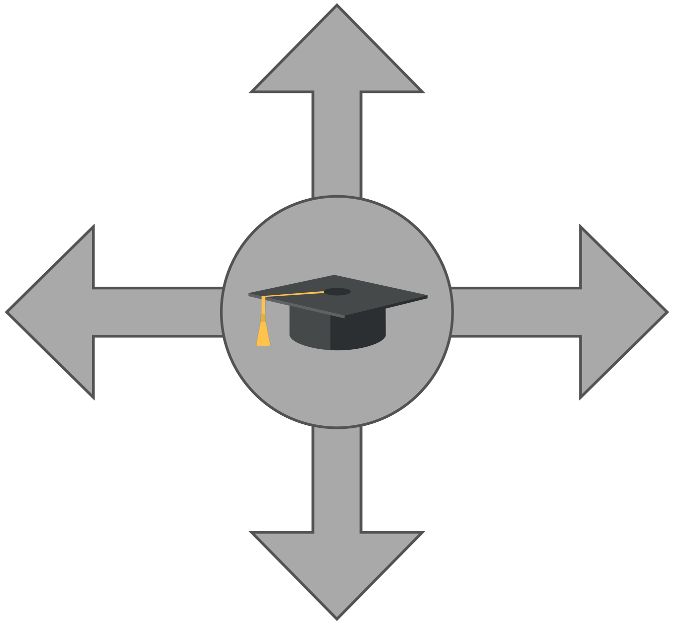


Example	NN type	N. Parameters (x E6)	Training time (hrs)	Inference time (s)	FEM solver time (s)
2D domain	CNN	4.8	18	0.021	0.6
	MAgNET	4.5	132	0.040	
	Perceiver IO	1.9	521	0.006	
3D elephant	MAgNET	33.9	161	0.217	2.5
	Perceiver IO	4.4	312	0.006	

Conclusion of the chapter 2

Fast ✓

✓ Accurate



Scalable for arbitrary meshes ✓

Provide uncertainty estimates ✗

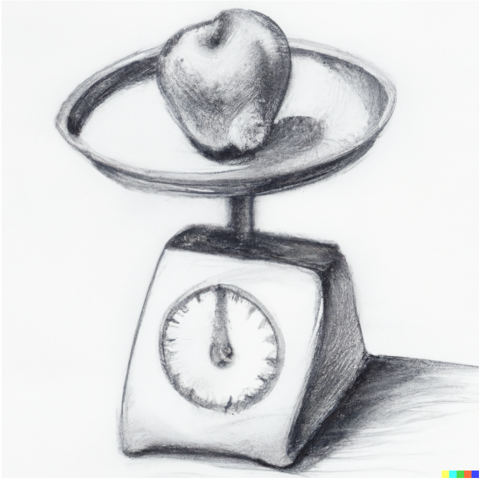
Outline

- General introduction
- Deterministic deep learning approaches
- **Bayesian deep learning Approaches**
- Conclusions

Uncertainty is inherent to real world

Aleatoric uncertainty

- Data uncertainty
- Can’t be reduced by adding data
- Describes confidence in the data



Epistemic uncertainty

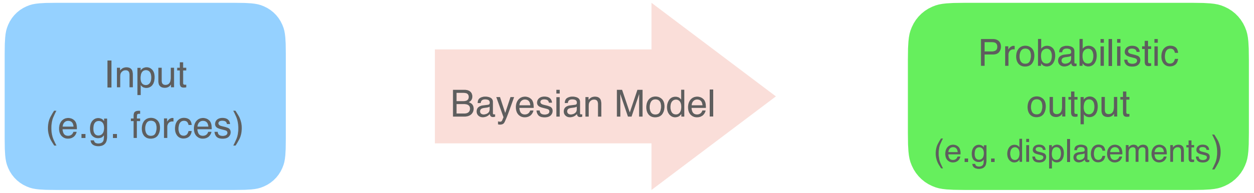
- Model uncertainty
- Can be reduced by adding more data
- Describes confidence of the prediction

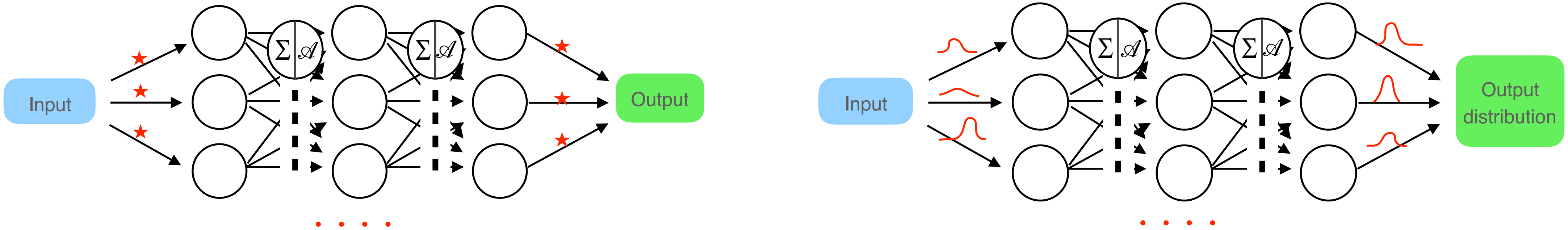
This thesis proposes two different Bayesian approaches

Probabilistic deep learning for real time large deformation simulations

[S. Deshpande and J. Lengiewicz and S. P. A. Bordas, Probabilistic deep learning for real-time large deformation simulations,
Computer Methods in Applied Mechanics and Engineering (2022) 115307, https://doi.org/10.1016/j.cma.2022.115307]

Bayesian neural networks



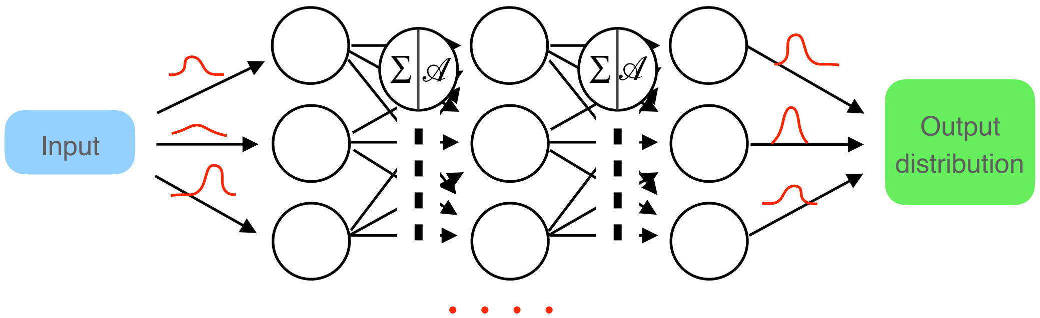


Deterministic vs bayesian neural networks

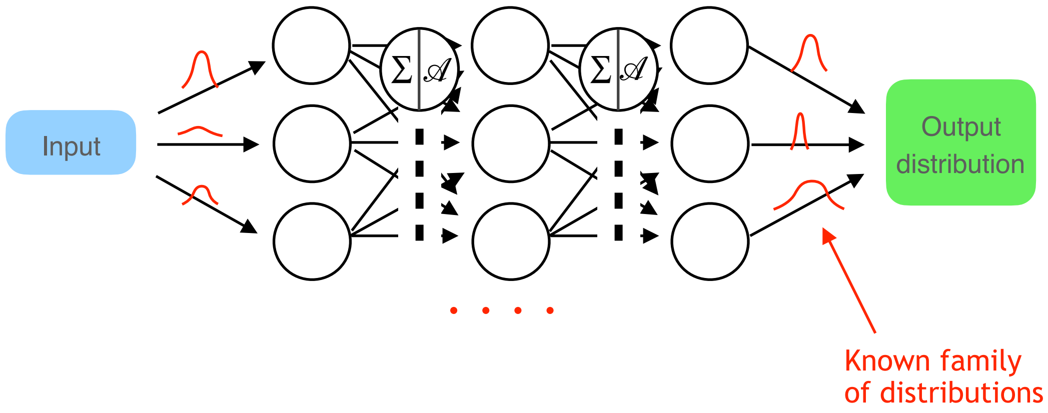
$$p(\mathbf{u}^* \mid \mathbf{f}^*, D) = \int p(\mathbf{u}^* \mid \mathbf{f}^*, \mathbf{w}) \cdot p(\mathbf{w} \mid D) d\mathbf{w}$$

Variational Inference formulation

True posteriors, $p(\mathbf{w} \,|\, D)$



Approximate posteriors, $q(\mathbf{w} \,|\, \boldsymbol{\theta})$



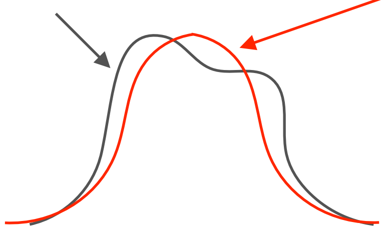
$$p(\mathbf{u}^* \,|\, \mathbf{f}^*, D) \approx \int p(\mathbf{u}^* \,|\, \mathbf{f}^*, \mathbf{w}) \cdot q(\mathbf{w} \,|\, \boldsymbol{\theta}) d\mathbf{w}$$

Training of Variational Bayes neural network

Replace all true with approximate ones

⇓

Find parameters of best fit approximate posteriors



$$\mathrm{KL}[q(x) \,||\, p(x)] = \int q(x) \log \frac{q(x)}{p(x)} dx$$

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \mathrm{KL}[q(\mathbf{w}|\boldsymbol{\theta}) \,||\, p(\mathbf{w}|D)]$$

$$\updownarrow$$

$$\arg\min_{\boldsymbol{\theta}} \underbrace{KL[q(\mathbf{w}|\boldsymbol{\theta})||p(\mathbf{w})]}_{\text{Model uncertainty}} - \underbrace{\int q(\mathbf{w}|\boldsymbol{\theta}) \log p(D|\mathbf{w}) d\mathbf{w}}_{\text{Data uncertainty}}$$

Loss Function

[Blundell et al.(2015) Weight Uncertainty in Neural Networks, *ICML*]

Empirical Bayes

- Gaussian distributions over parameters
- Inability to choose proper priors => Use of Empirical Bayes
- Prior deviation is fixed but prior mean is not fixed (is included in training procedure)

$$\underset{\boldsymbol{\mu},\boldsymbol{\rho},\boldsymbol{\mu}_p}{\arg\min}\ KL[q(\mathbf{w}\,|\,\boldsymbol{\mu},\boldsymbol{\rho})\,||\,p(\mathbf{w}\,|\,\boldsymbol{\mu}_{\boldsymbol{p}},\bar{\rho}_p)] - \mathbb{E}_{q(\mathbf{w}|\boldsymbol{\mu},\boldsymbol{\rho})}[\log p(D\,|\,\mathbf{w})]$$

Updated loss function

[S. Deshpande and J. Lengiewicz and S. P. A. Bordas, Probabilistic deep learning for real-time large deformation simulations, Computer Methods in Applied Mechanics and Engineering (2022) 115307, https://doi.org/10.1016/j.cma.2022.115307]

Prediction

- 'T' stochastic forward passes for the same input (T = 300 for our case)

$$p(\mathbf{u}^* \,|\, \mathbf{f}^*, D) \approx \int p(\mathbf{u}^* \,|\, \mathbf{f}^*, \mathbf{w}) \cdot q(\mathbf{w} \,|\, \boldsymbol{\theta}) d\mathbf{w}$$

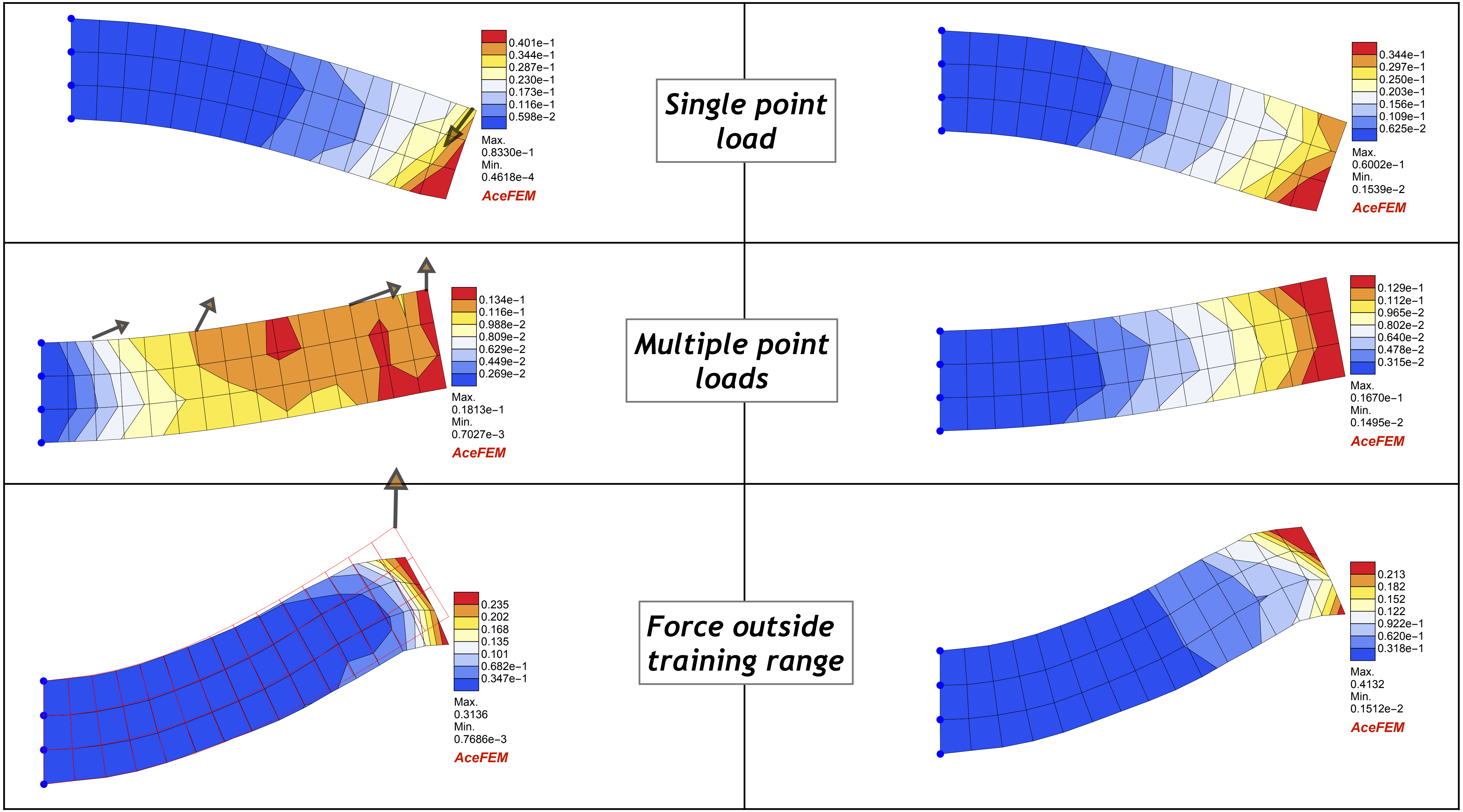
Predictive Distribution

↕

$$\mathcal{U}_\mu(\mathbf{f}^*, \mathbf{w}) \approx \frac{1}{T} \sum_{t=1}^{T} p(\mathbf{u}^* \,|\, \mathbf{f}^*, \widetilde{\mathbf{w}_t})$$

$$\mathcal{U}_\sigma^2(\mathbf{f}^*, \mathbf{w}) \approx \frac{1}{T} \sum_{t=1}^{T} p(\mathbf{u}^* \,|\, \mathbf{f}^*, \widetilde{\mathbf{w}_t})^T p(\mathbf{u}^* \,|\, \mathbf{f}^*, \widetilde{\mathbf{w}_t}) - \mathcal{U}_\mu(\mathbf{f}^*, \mathbf{w})^T \mathcal{U}_\mu(\mathbf{f}^*, \mathbf{w})$$

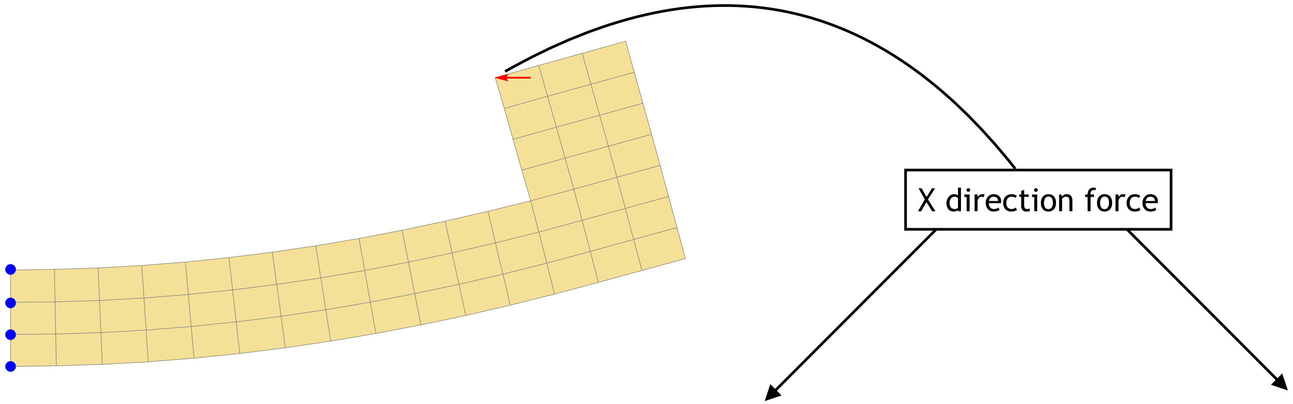
Output: Mean and uncertainty of prediction



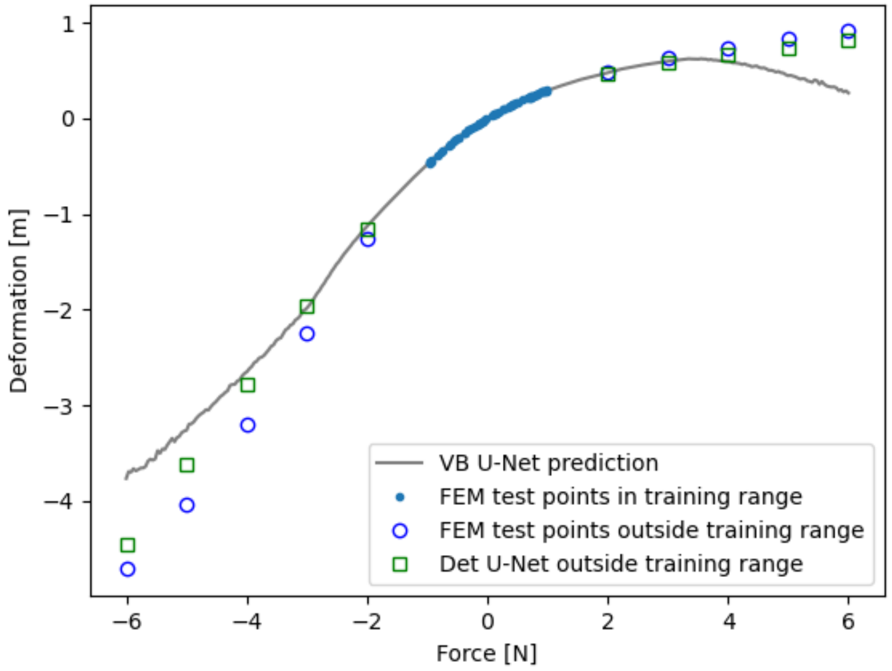
Errors for Bayesian CNN U-Net

Uncertainties for Bayesian CNN U-Net

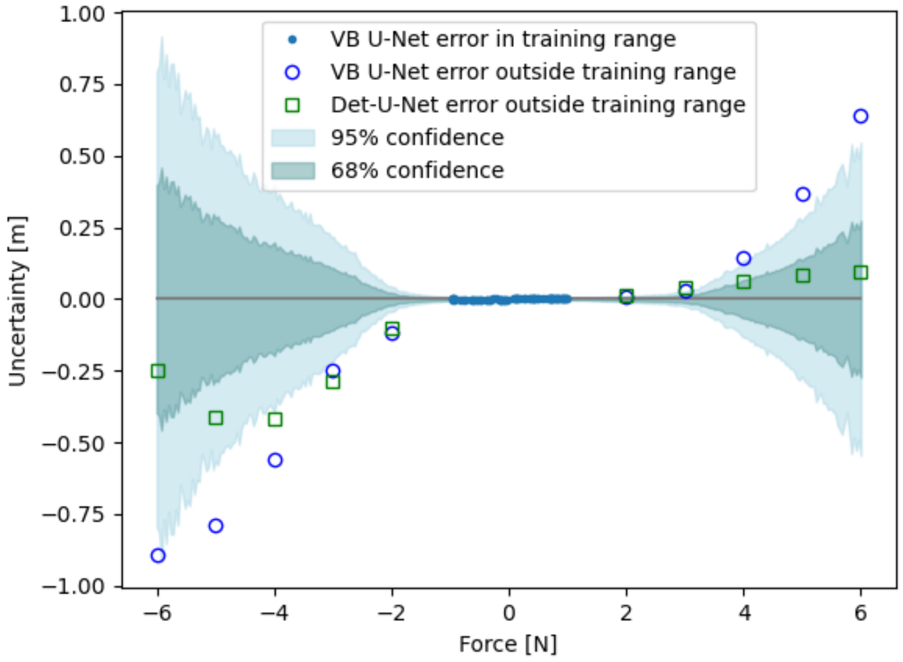
Deterministic vs Bayesian



$|F_{train}| < 1$ [N]



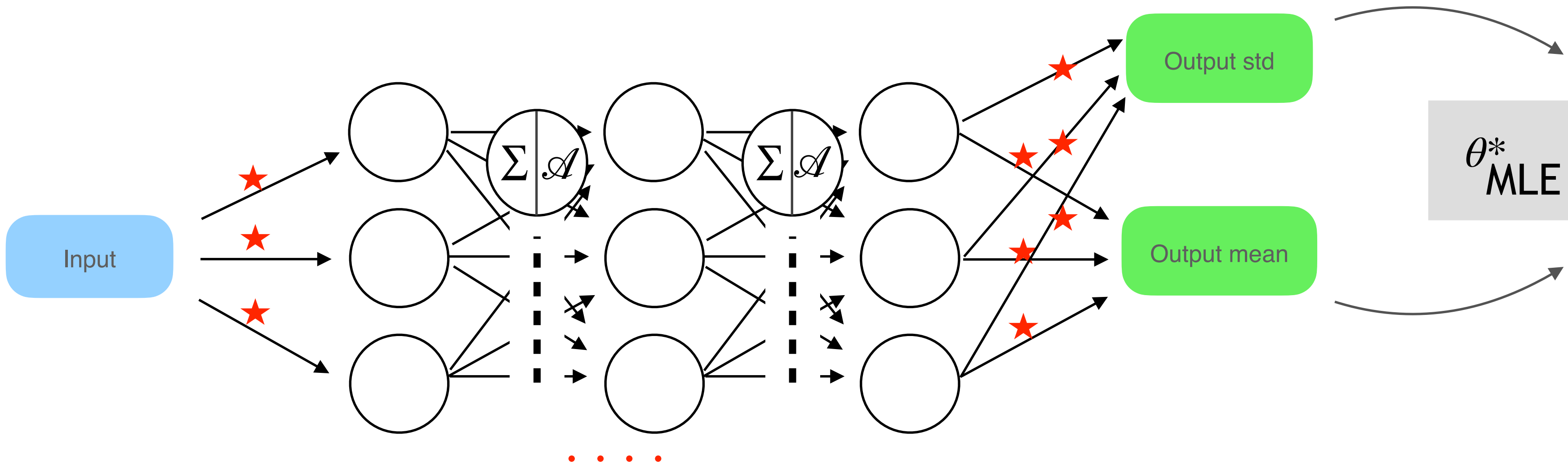
Deformation amplitude of X-dof



Uncertainty of prediction

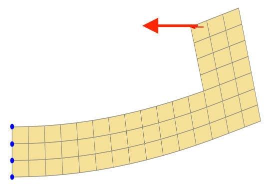
Capturing data noise only

- Maximum Likelihood Estimation (MLE) neural network

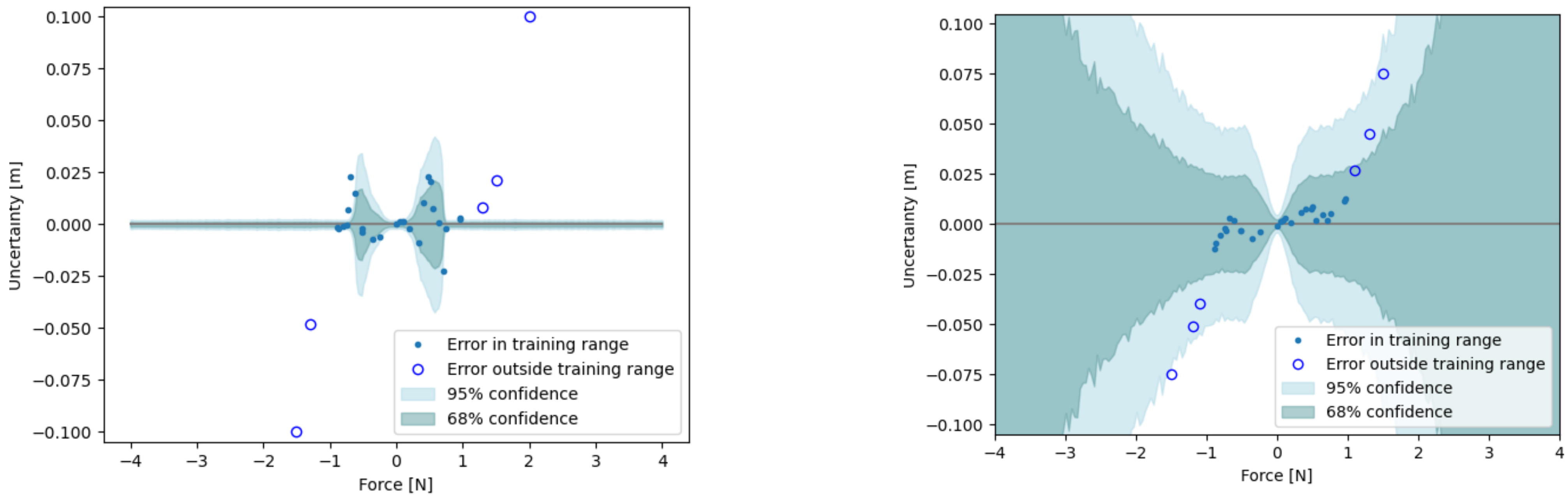


$$\theta^*_{\text{MLE}} = \arg\max_{\theta} \log p(D \,|\, \boldsymbol{\theta})$$

MLE VS Variational Bayes



- Artificial noise is added to the data while training
- MLE captures the data noise, fails to give uncertainties in extrapolated region



Uncertainty predictions for noisy data

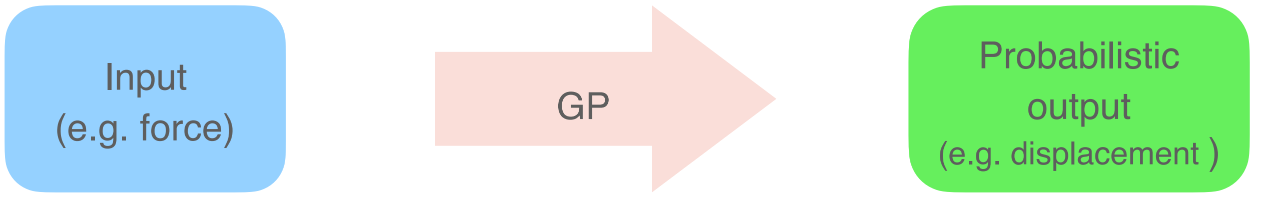
Take aways

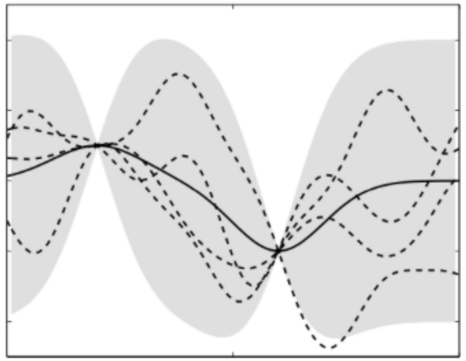
- We could capture both aleatoric and epistemic uncertainty
- Bayesian convolution neural network implementation => scalable
- Limited to structured meshes

A probabilistic reduced-order emulation framework for nonlinear solid

[**S. Deshpande**, H. Rappel, S. P. A. Bordas and J. Lengiewicz. A probabilistic reduced-order emulation framework for nonlinear solid mechanics.]

Gaussian process (GP)





Bayesian NN = distribution over parameters

$$\mathbf{u} = \mathscr{U}(\mathbf{f}, \boldsymbol{\theta}_{\text{BNN}}) + \epsilon$$

$$\boldsymbol{\theta}_{\text{BNN}} \sim \mathscr{N}(\boldsymbol{\mu}, \boldsymbol{\sigma})$$

GP = distribution over functions

$$\mathbf{u} = \omega(\mathbf{f}) + \epsilon \quad ; \quad \epsilon \sim \mathscr{N}(0, \sigma^2)$$

$$\omega \sim \mathscr{N}(\mu(\mathbf{f}), k(\mathbf{f}, \boldsymbol{\theta}_{\text{GP}}))$$

$$k_{\text{RBF}}(f_i, f) = exp(-\frac{||f_i - f_j||^2}{2l^2})$$

Predictive distribution

$$p(\mathbf{u}^* \mid \mathbf{f}^*, D) \sim \mathcal{N}(\mu_{\mathbf{p}}, \mathbf{\Sigma_p})$$

where,

$$\mu_{\mathbf{p}} = \mathbf{K}_*(\mathbf{K} + \sigma^2\mathbf{I})^{-1}\mathbf{u}$$

$$\mathbf{\Sigma}_p = \mathbf{K}_{**} - \mathbf{K}_*^T(\mathbf{K} + \sigma^2\mathbf{I})^{-1}\mathbf{K}_*$$

Predictive distribution

$$\mathbf{K} = k(f_i, f_j),\ \mathbf{K}_* = k(f_i, f_{j_*}),\ \mathbf{K}_{**} = k(f_{i*}, f_{j_*}) \quad ; \quad k_{\text{RBF}}(f_i, f) = exp(-\frac{||f_i - f_j||^2}{2l^2})$$

Train: Maximize the log-likelihood

$$p(\mathbf{y} \mid \mathbf{F}, \theta_{\text{GP}}, \sigma^2) = -\frac{1}{2}\mathbf{y}(\mathbf{K} + \sigma^2\mathbf{I}_n)^{-1}\mathbf{y} - \frac{1}{2}\log[\det(\mathbf{K} + \sigma^2\mathbf{I}_n)] - \frac{n}{2}\log(2\pi)$$

$$\mathbf{y} = [\mathbf{u}_i^l, \cdots, \mathbf{u}_N^l]$$

Poor scalability

$$p(\mathbf{u}^* \mid \mathbf{f}^*, D) \sim \mathcal{N}(\mu_{\mathbf{p}}, \Sigma_{\mathbf{p}})$$

where,

$$\mu_{\mathbf{p}} = \mathbf{K}_*(\mathbf{K} + \sigma^2\mathbf{I})^{-1}\mathbf{u}$$

$$\Sigma_p = \mathbf{K}_{**} - \mathbf{K}_*^T(\mathbf{K} + \sigma^2\mathbf{I})^{-1}\mathbf{K}_*$$

Predictive distribution

Issue: scales badly with the output dimension and number of data points

$$\mathbf{K} = k(f_i, f_j),\ \mathbf{K}_* = k(f_i, f_{j*}),\ \mathbf{K}_{**} = k(f_{i*}, f_{j*}) \quad ; \quad k_{\text{RBF}}(f_i, f) = exp(-\frac{||f_i - f_j||^2}{2l^2})$$

Train: Maximize the log-likelihood

$$p(\mathbf{y} \mid \mathbf{F}, \theta_{\text{GP}}, \sigma^2) = -\frac{1}{2}\mathbf{y}(\mathbf{K} + \sigma^2\mathbf{I}_n)^{-1}\mathbf{y} - \frac{1}{2}\log[\det(\mathbf{K} + \sigma^2\mathbf{I}_n)] - \frac{n}{2}\log(2\pi)$$

$$\mathbf{y} = [\mathbf{u}_i^l, \cdots, \mathbf{u}_N^l]$$

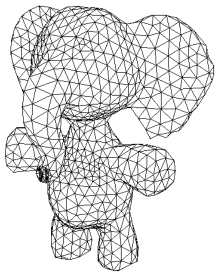
Poor scaling for high dimensional inputs

N. data points

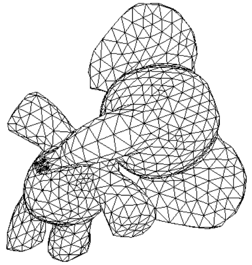
Dimension of full field output

$O(N^3 \cdot \mathscr{D}_f^3)$

Full field space



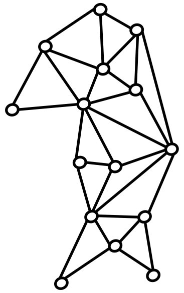
Gaussian process



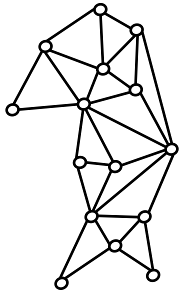
✗

Dimensionality reduction

Reduced space



Gaussian process



✓

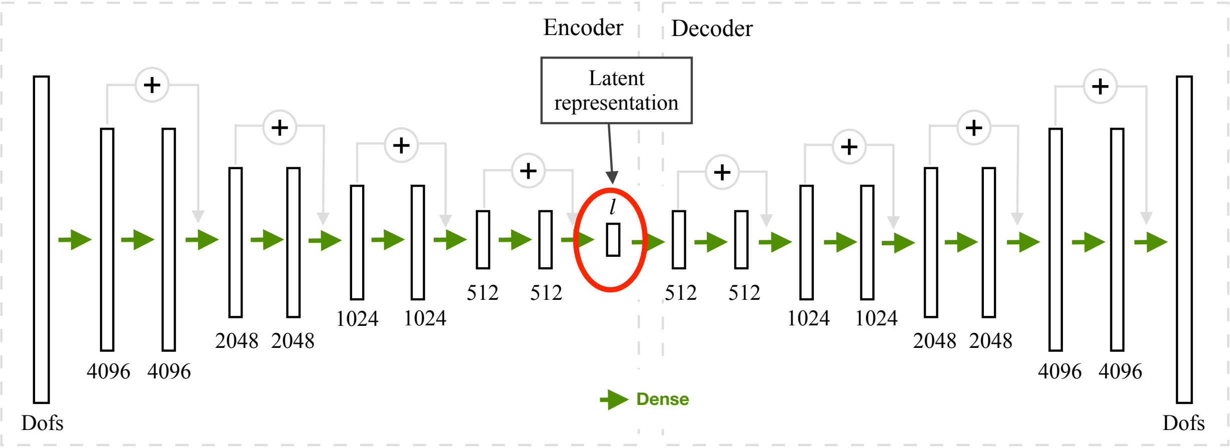
$O(N^3 \cdot \mathscr{D}_l^3)$

$\mathscr{D}_l << \mathscr{D}_f$

Dimension reduction using auto-encoder networks

- Powerful dimension reduction technique
- Enables non-linear compression

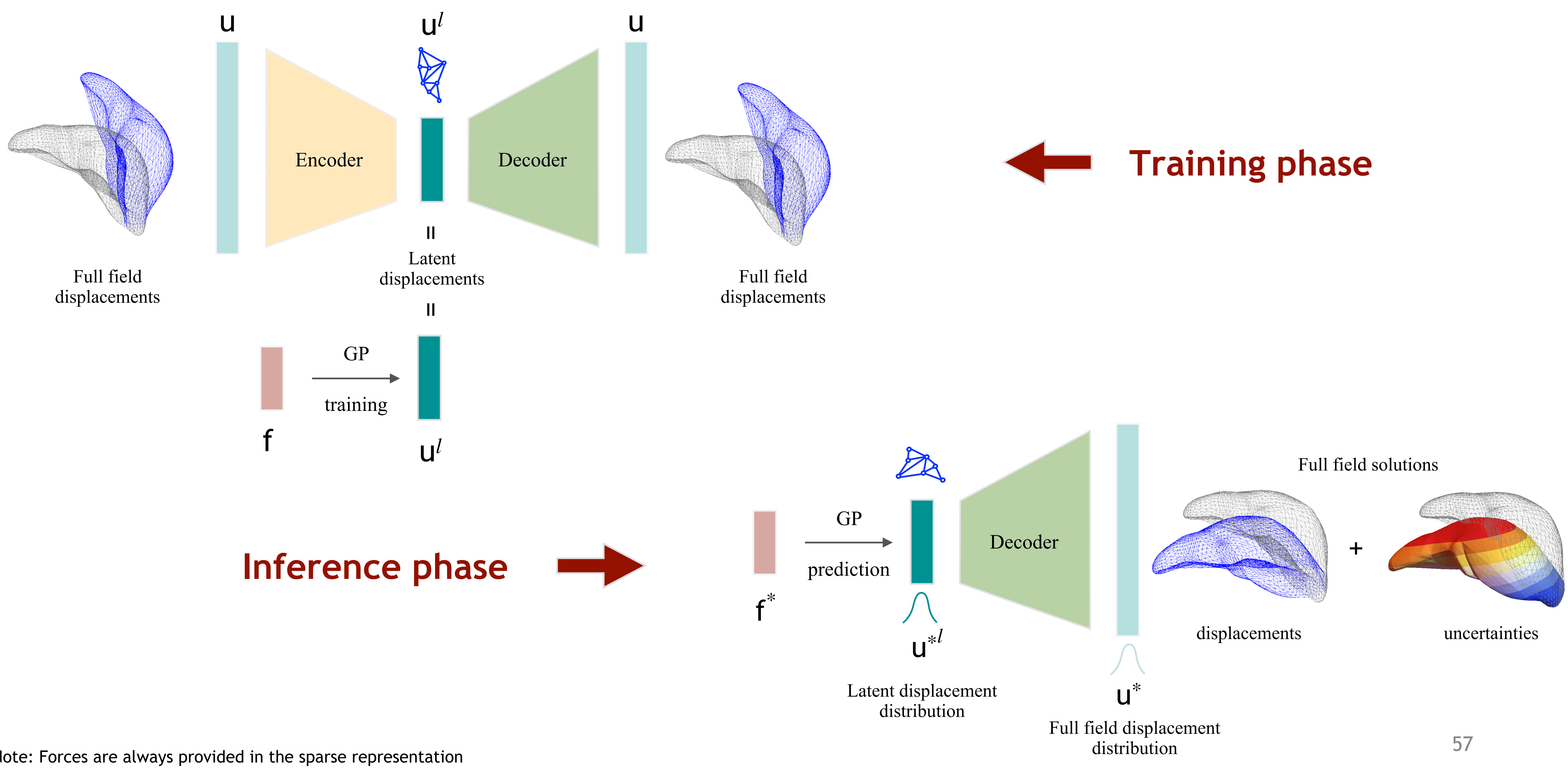
$$\theta^*_{\text{auto}} = \arg\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} || \mathscr{U}(\mathbf{u}_i, \theta_{\text{auto}}) - \mathbf{u}_i ||_2^2$$



$$\mathscr{U}(\mathbf{u}, \theta_{\text{auto}}) = \mathscr{U}_{\text{decoder}}(\mathscr{U}_{\text{encoder}}(\mathbf{u}))$$

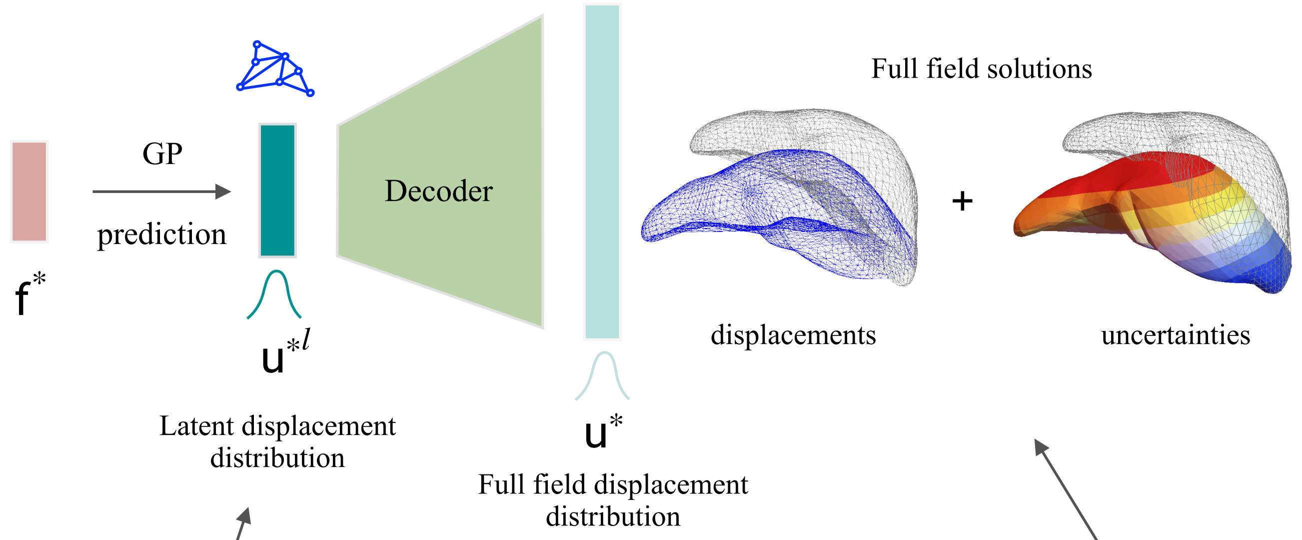
$$\mathbf{u}^l = \mathscr{U}_{\text{encoder}}(\mathbf{u}, \theta^*_{\text{auto}})$$

Autoencoder+GP framework



Note: Forces are always provided in the sparse representation

Prediction using GP + autoencoder



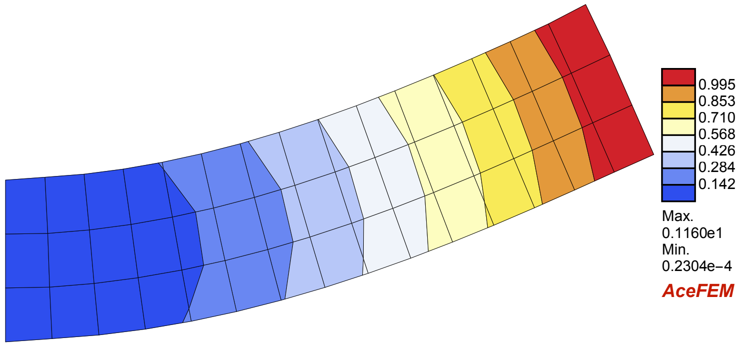
$$p(\mathbf{u}^{*l} \,|\, \mathbf{f}^{*}) = \mathcal{N}(\mu_{\mathbf{p}}, \boldsymbol{\Sigma}_{\mathbf{p}})$$

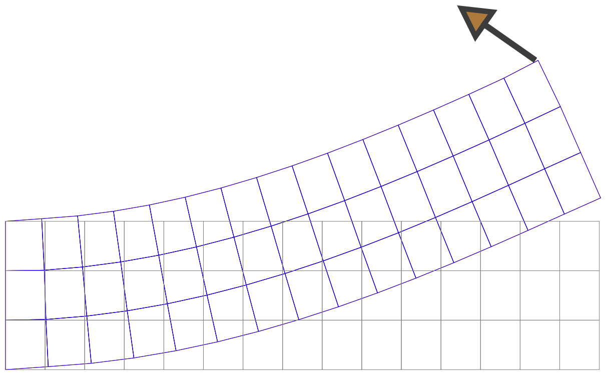
$$\mathbf{u}^{*}_{\mu} \approx \frac{1}{S} \sum_{s=1}^{S} \mathcal{U}_{\text{decoder}}(\mathbf{u}^{l}_{s}), \quad \text{where} \quad \mathbf{u}^{l}_{s} \sim p(\mathbf{u}^{*l} \,|\, \mathbf{f}^{*})$$

$$\mathbf{u}^{*2}_{\sigma} \approx \frac{1}{S} \sum_{s=1}^{S} \mathcal{U}_{\text{decoder}}(\mathbf{u}^{l}_{s})^{T} \mathcal{U}_{\text{decoder}}(\mathbf{u}^{l}_{s}) - \mathbf{u}^{*T}_{\mu} \mathbf{u}^{*}_{\mu}$$

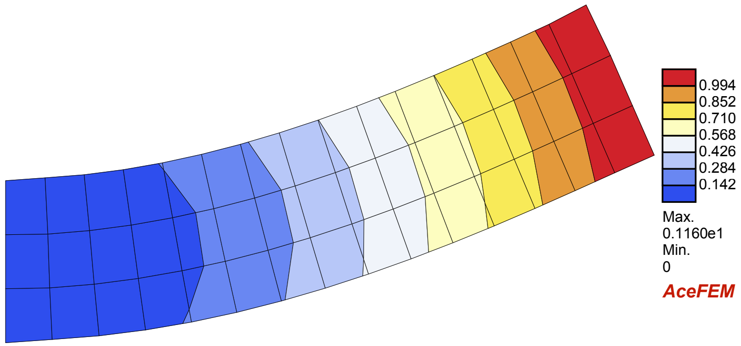
Prediction for the 2D beam

GP+NN prediction





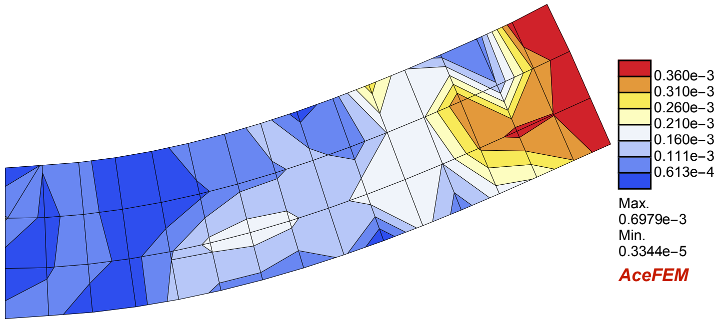
FEM solution



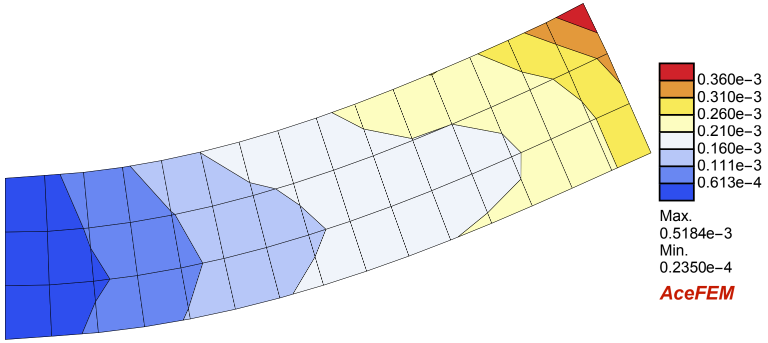
Max nodal disp = 1.16 m

0.05% relative error

GP+NN Nodal error

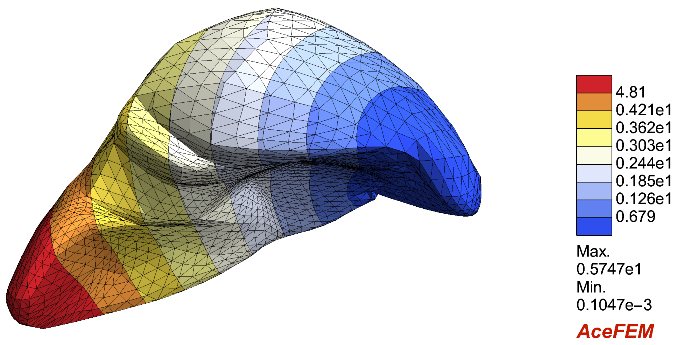


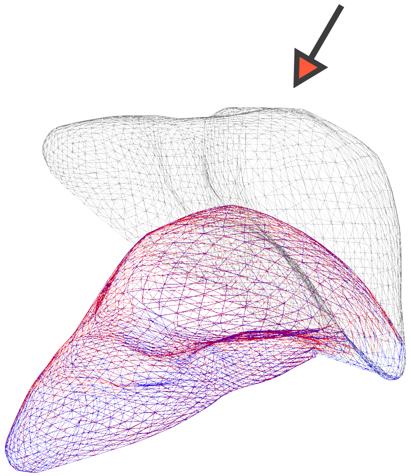
Uncertainty



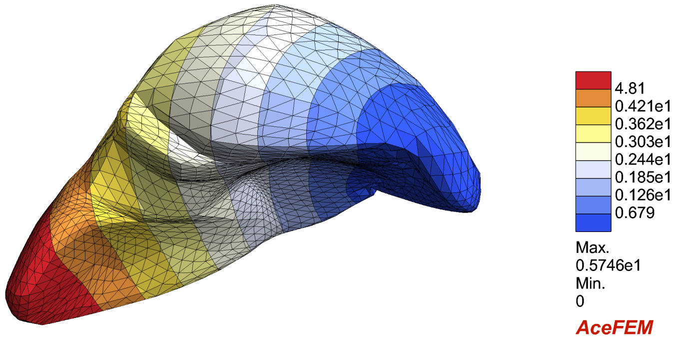
Prediction for the liver

GP+NN prediction

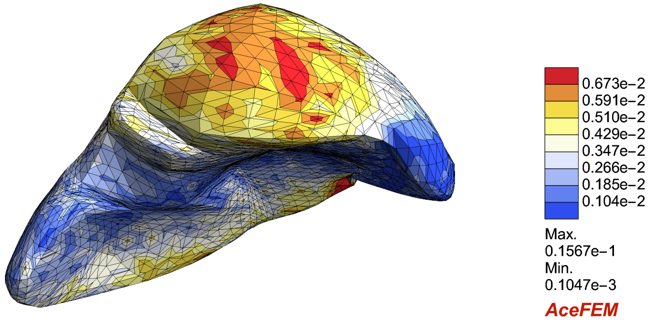




FEM solution



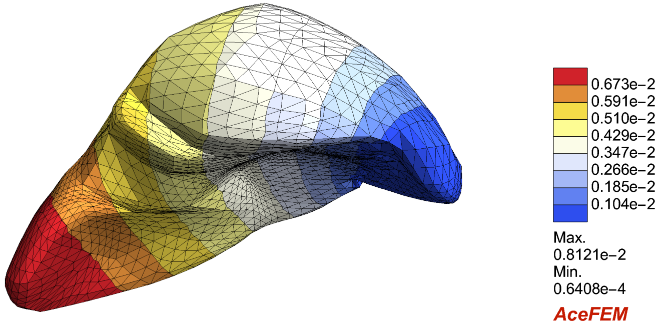
GP+NN Nodal error



Max nodal disp = 5.74 m

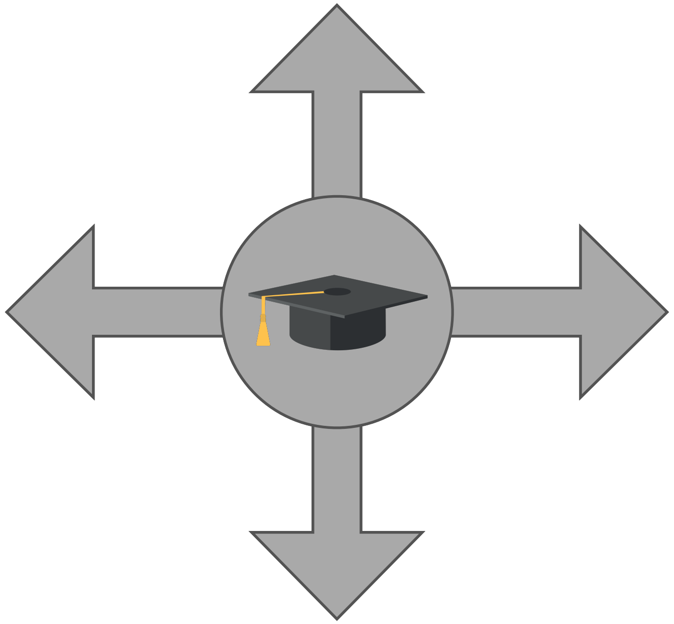
0.2% relative error

Uncertainty



Conclusion of the chapter 3

Fast ✓



✓ Accurate

Scalable for arbitrary meshes ✓

Provide uncertainty estimates ✓

Outline

- General introduction
- Deterministic deep learning approaches
- Bayesian deep learning Approaches
- **Conclusions**

General conclusions

Novel deep learning surrogate frameworks for solid mechanics simulations

- Accurate and fast simulations in solid mechanics.
- Robustness and efficient scaling with input dimensionality.

Versatility and Data Assimilation:

- Trained using synthetic data and adaptable to assimilate experimental data.

Advanced neural network architectures:

- Introduced MAgNET, a novel deep learning architecture for efficient supervised learning on graph-structured data.

Uncertainty Quantification:

- Data and model uncertainties using Variational Bayes and Gaussian process formulations.

Summary:

- Significant advancements in both deep learning and surrogate modelling in mechanics.

Future work

Integration of Physics into Learning:

- Easy extension of proposed frameworks to PINNs variants e.g. Physics Informed MAgNET.
- Modify the learning objective to incorporate physical quantities.

Extension to Path-Dependent Processes:

- Processes like elastoplasticity, dynamic simulations.

Enhancing Bayesian Deep Learning Approach:

- Variation Bayes MAgNET for probabilistic predictions for large scale arbitrary inputs.

Interdisciplinary research

- Proposed frameworks applicable to wide engineering applications.

Publications

Journal articles

1. **S. Deshpande** and J. Lengiewicz and S. P. A. Bordas, Probabilistic deep learning for real-time large deformation simulations. Computer Methods in Applied Mechanics and Engineering (2022). 115307, https://doi.org/10.1016/j.cma.2022.115307
2. **S. Deshpande**, R.I. Sosa, S.P.A. Bordas and J. Lengiewicz. Convolution, aggregation and attention based deep neural networks for accelerating simulations in mechanics. Frontiers in Materials (2023). 10:1128954. https://doi.org/10.3389/fmats.2023.1128954
3. **S. Deshpande**, S. P. A. Bordas and J. Lengiewicz. MAgNET: A Graph U-Net Architecture for Mesh-Based Simulations (2023). https://arxiv.org/abs/2211.00713
4. **S. Deshpande**, H. Rappel, S. P. A. Bordas and J. Lengiewicz. A probabilistic reduced-order emulation framework for nonlinear solid mechanics. (To be submitted)

In prep

1. S. Deshpande*, S. Urcun*, S.P.A. Bordas et al. 'Keloid nuclei counting with deep learning based object detection tools'.
2. C Suarez, S. Deshpande, S.P.A. Bordas et al. 'Surrogate models for estimating macroscopic thermoviscoelastic behavior of 3d printed composite polymers'.

Conferences

1. 14th World Congress on Computational Mechanics (WCCM), 2020
2. 18th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS), 2022.
3. 9th World Congress of Biomechanics (WCB), 2022.
4. The Platform for Advanced Scientific Computing (PASC), 2022.
5. 15th World Congress on Computational Mechanics (WCCM), 2022.
6. The Platform for Advanced Scientific Computing (PASC), 2023.
7. The The 14th International Conference of Computational Methods (ICCM), 2023

Seminars/ Outreach

1. Digital twinning for real-time simulation'. European Investment Bank (EIB) Tech fair, Luxembourg, 2019.
2. Machine Learning Seminars, Team Legato, University of Luxembourg. (presented in three seminars)
3. Team MEMESIS seminar, INRIA Strasbourg, 2022.

Publications

Software

https://github.com/saurabhdeshpande93/MAgNET

zenodo https://doi.org/10.5281/zenodo.7784804

https://github.com/saurabhdeshpande93/convolution-aggregation-attention

zenodo https://doi.org/10.5281/zenodo.7585319

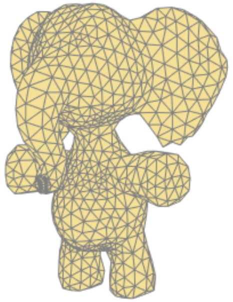
Student supervision

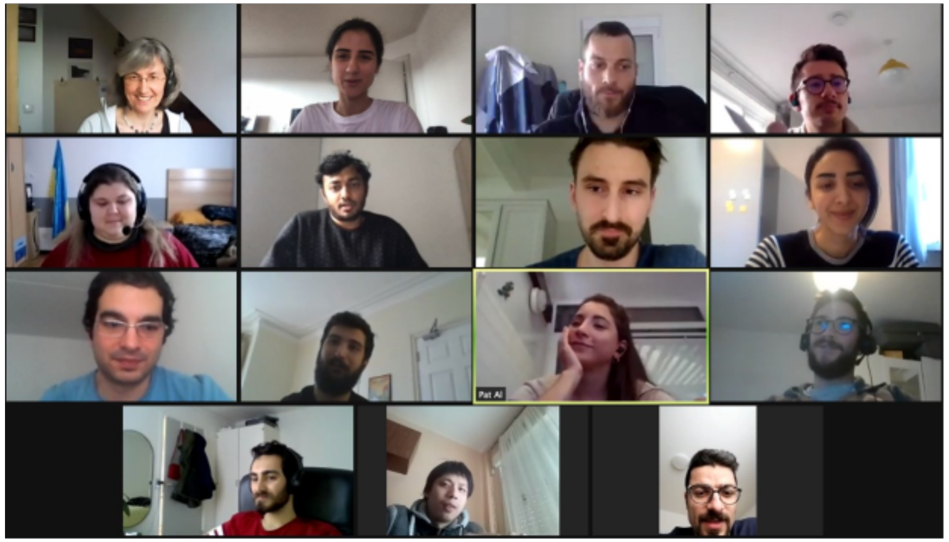
1. Siam Wang - Master's thesis, University of Southampton. "DL techniques for contact simulations of heterogenous materials".
2. Henri Donte - Bachelor Intern, EPFL. " Computer vision based object detection for counting keloid nuclei in microscopic images"
3. Jiajia Wang - First year PhD, University of Luxembourg. "An investigation of real-time interactive simulations for intuitive conceptual design"
4. Thomas Lavigne - Masters thesis, ENSAM/University of Luxembourg. "Surrogate Modeling of breast soft tissue deformation"

Positions of Responsibilities

1. Chair of Doctoral candidate council, Doctoral School of Science and Engineering.
2. Student representative, Doctoral Program in Computational Sciences.
3. Student representative, Marie Curie ITN RAINBOW network.

Thank you!





UNIVERSITÉ DU LUXEMBOURG

Inria

RAINBOW
Rapid Biomechanics Simulation for Personalized Clinical Design
A Marie Sklodowska-Curie European Training Network

MARIE CURIE ACTIONS