Multi-physical property prediction of fibre-reinforced composites using convolutional neural networks

Rajesh Nakka[1]
Phanendra Kumar A[1]
Dr. Sathiskumar A. Ponnusami[2]
Dr. Dineshkumar Harursampath[1]

1: NMCAD Lab, Department of Aerospace Engineering, Indian Institute of Science (IISc), Bangalore.

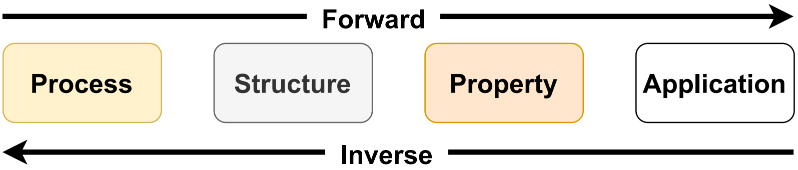
2: City, University of London, United Kingdom

The context

Motivation & Objectives

The context

Material Design



Multi-scale analysis: **Micro scale** - Meso scale - Macro scale
Inverse design is desirable but difficult to practice with

computationally demanding numerical tools.

Objective

With the aim of inverse modelling in the long run, the present aim is to **develop a deep learning model for the forward direction** that can

- **predict properties of composites with a wide range fibre volume fractions and property contrasts**
- **predict multi-physical properties to cater the multi-functional applications**

Approach

Broadly, the progress of machine learning domain depends on

1. Computing capabilities
2. Data
3. Efficient algorithms
4. Acceptance: interpretability and uncertainty-awareness

Approach

Plan for developing the surrogate model, $f(x) = y$

- **Data generation**
  - Sample microstructure images (V_f, E_f....etc)
  - Generate microstructure RVEs
  - Prepare binary images of desired resolution, x
  - Evaluate effective properties, y
    - Elastic Moduli, E_{22}, E_{33}, G_{23}
    - Thermal Expansion Coefficients, α_{22}, α_{33}
    - Thermal Conductivity K_{22}, K_{33}
- Model building and training, f
- Testing the model performance

Data Generation

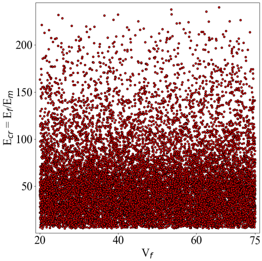
Data Generation

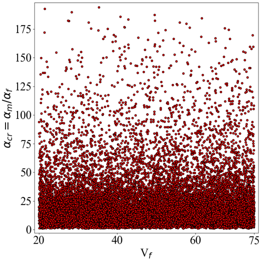
Microstructure sampling

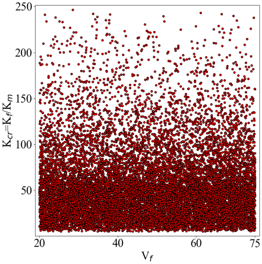
Parameters V_f, E_m, E_f, α_m, α_f, K_m, K_f sampled from,

	Fibre	Matrix	Contrast
V_f in %	[20, 75]	[25, 80]	-
E in GPa	[50, 500]	[2, 10]	$E_f/E_m \in$[5, 250]
α in $\times 10^{-6}/°C$	[1, 10]	[10, 200]	$\alpha_m/\alpha_f \in$[1, 200]
K in W/m.K	[50, 500]	[2, 10]	$K_f/K_m \in$ [5, 250]

Variation of property contrasts with V_f



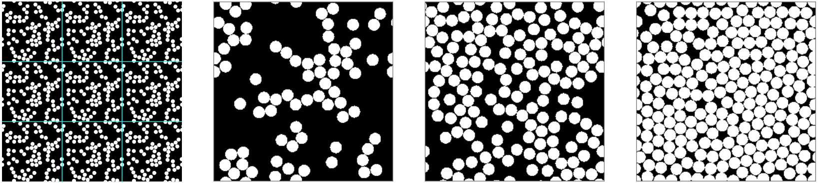




Microstructure RVE generation

Objective

Generating virtual **periodic** RVEs containing **high volume fractions** in a **computationally efficient** manner.



(a) $V_f = 28\%$ (b) $V_f = 25\%$ (c) $V_f = 50\%$ (d) $V_f = 75\%$

Microstructure RVE generation

1. **Draw the fiber radii from a distribution of choice.**
2. **Place fibre centres $\boldsymbol{x}$ randomly, allowing overlaps.**
3. **Minimise overlap magnitude, g**

$$g = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} C_{ij}^2 = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left[(\bar{d}_{ij} - d_{ij}) \boldsymbol{H} (\bar{d}_{ij} - d_{ij}) \right]^2$$

$$\text{subjected to } \boldsymbol{x} \in \Omega$$

Microstructure RVE generation

$$
\begin{aligned}
\bar{d}_{ij} &= r_i + r_j + d_{ss} \\
d_{ij} &= \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2} \\
\boldsymbol{H}(t) &= 1 \text{ if } t > 0 \\
&= 0 \text{ otherwise}
\end{aligned}
$$

Microstructure RVE generation

Gradient of g,

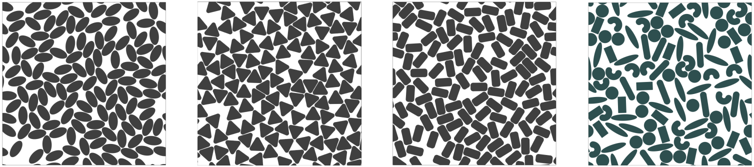
$$\frac{\partial g}{\partial x_i} = -2 \sum_{j=1(\neq i)}^{N} \frac{C_{ij}(x_i - x_j)}{d_{ij}}$$

$$\frac{\partial g}{\partial y_i} = -2 \sum_{j=1(\neq i)}^{N} \frac{C_{ij}(y_i - y_j)}{d_{ij}}$$

Microstructure RVE generation

- The algorithm is implemented using ***Julia*** language
- Generates about **300 RVEs** with $V_f \in [20\%, 75\%]$ of circular inclusions **per minute** on a computer with an Intel Xeon CPU 2.40 GHz processor and 64 GB RAM

Microstructure RVE generation

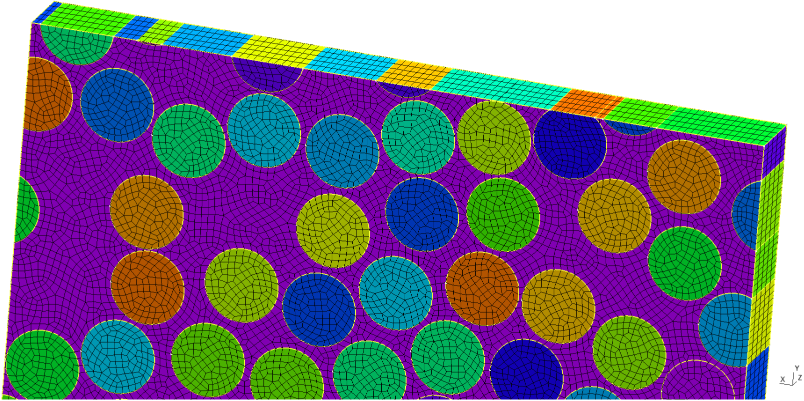


(e) $V_f = 28\%$ (f) $V_f = 25\%$ (g) $V_f = 50\%$ (h) $V_f = 75\%$

R. Nakka, D. Harursampath, M. Pathan, S. A. Ponnusami, A computationally efficient approach for generating rves of various inclusion/fiber shapes, Composite Structures (2022)

Target properties evaluation

RVEs are modelled and periodic mesh is generated in *gmsh* using Quad-dominated elements



Target properties evaluation

Homogenisation tool is developed in *Julia* based on Variational Asymptotic Method (VAM) based approach[1]

$$\overline{D} = \frac{1}{\Omega}[D_{pp} - D_{n_ap}^T D_{n_an_a}^{-T} D_{n_ap}]$$

$$D_{pp} = \int_{\Omega} D d\Omega$$

$$D_{n_ap} = \int_{\Omega} B^T D d\Omega$$

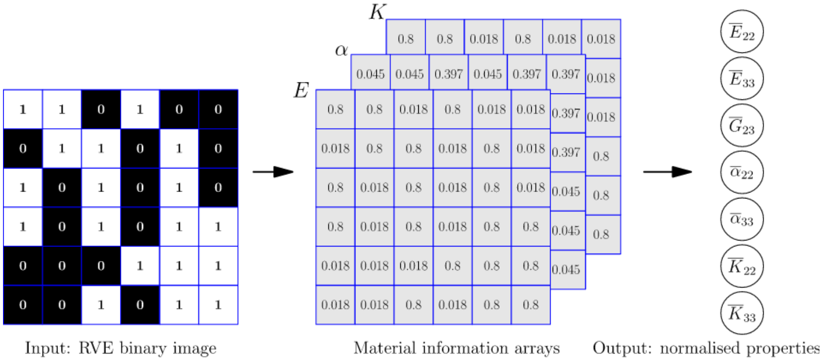
$$D_{n_an_a} = \int_{\Omega} B^T D B d\Omega$$

[1] Yu, W., & Tang, T. (2007). A variational asymptotic micromechanics model for predicting thermoelastic properties of heterogeneous materials. International Journal of Solids and Structures, 44(22-23), 7510-7525.

Target properties evaluation

On a computer with an Intel Xeon CPU 2.40 GHz processor and 64GB RAM, **two-dimensional homogenisation of 20 RVEs** using plane strain analysis took about **8.3 minutes with VAM** and about **32.5 minutes with the conventional FEA** approach with the same mesh and loading.

Material Property Encoding



R. Nakka, Dineshkumar Harursampath and Sathiskumar A Ponnusami, A generalised deep learning-based surrogate model for homogenisation utilising material property encoding and physics-based bounds, Scientific Reports(in press), 2023

Material Property Encoding

$$\mathbf{I}^{(\lambda)} = \frac{\lambda_{matrix} - \lambda_{min}}{\lambda_{max} - \lambda_{min}}\mathbf{J} + \frac{\lambda_{fibre} - \lambda_{matrix}}{\lambda_{max} - \lambda_{min}}\mathbf{I}^{(g)} \tag{1}$$

Example: Prepare information array of elastic modulus $\mathbf{I}^{(E)}$ with $E_{matrix} = 10$ GPa, $E_{fibre} = 400$ GPa,
$E_{min} = 1$ GPa, $E_{max} = 500$ GPa.

0	0	0	0	0
0	0	1	1	0
0	0	1	1	0
1	0	0	0	0
1	0	0	0	1

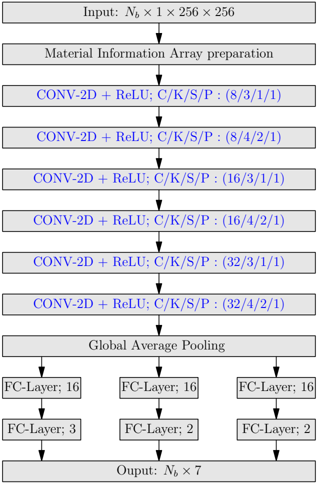
0.018	0.018	0.018	0.018	0.018
0.018	0.018	0.8	0.8	0.018
0.018	0.018	0.8	0.8	0.018
0.8	0.018	0.018	0.018	0.018
0.8	0.018	0.018	0.018	0.8

CNN model for property prediction [1]

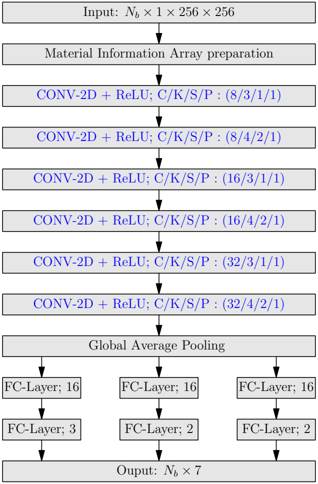
[1] R. Nakka, D. Harursampath, S. A. Ponnusami, (in press) Scientific Reports

- built in **PyTorch**
- # parameters: 29,375
- Dataset size
  - $\mathcal{X}_{tr} \in \mathbb{R}^{10000\times1\times256\times256}$
  - $\mathcal{Y}_{tr} \in \mathbb{R}^{10000\times7}$
  - $\mathcal{X}_{ts} \in \mathbb{R}^{4500\times1\times256\times256}$
  - $\mathcal{Y}_{ts} \in \mathbb{R}^{4500\times7}$
- Loss function: MSE

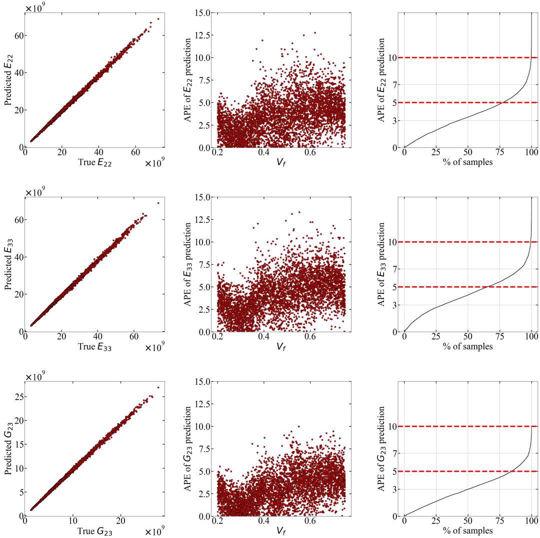
$$\mathcal{L} = \frac{1}{N_b}\sum_{i=1}^{N_b}\sum_{j=1}^{7}(y_{ij}^{(t)} - y_{ij}^{(p)})^2$$



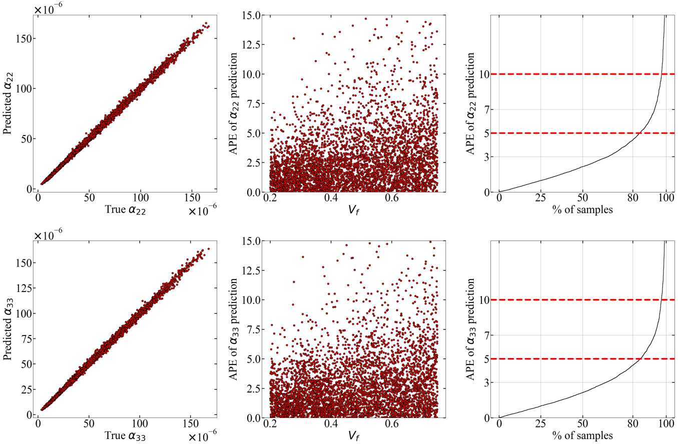
- Batch Size: 64
- Adam optimisation; learning rate $= 0.001$
- Number of epochs: 300
- Training time: 72 minutes
- inference time: < 1 second



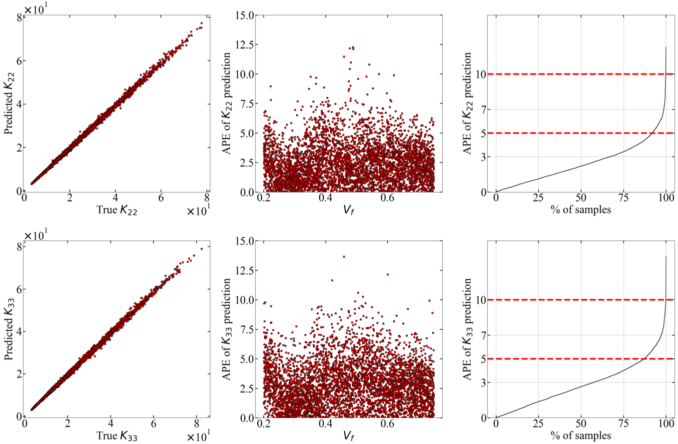
Test performance: Elastic properties



Test performance: Thermal expansion properties



Test performance: Thermal conduction properties



Thank you!