Data driven computational analysis of open foam RVEs

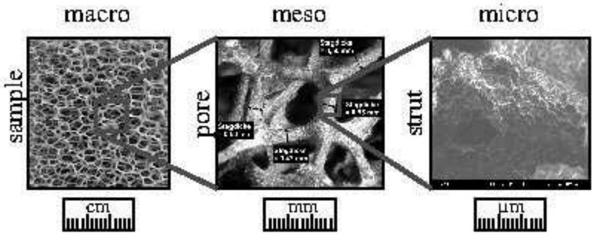
Nanda G. Kilingar[1][2]
K. Ehab Moustafa Kamel[2]
B. Sonon[2]
C. Leblanc[1]
L. Noëls[1]
T.J. Massart[2]
A. Jung[3]

Kilingar, N. G., et al, Computational generation of open-foam representational volume elements with morphological control using distance fields, *Under review*

[1] University of Liege, Aerospace and mechanics, Liege 4000, Belgium
[2] Université Libre de Bruxelles, Building, Architecture and Town planning Department, Brussels 1050, Belgium
[3] Saarland University, Applied Mechanics, Campus A4.2, Saarbrücken 66123, Germany

Open foam materials and numerical models

- Metallic open foams
  - Low density
  - Novel physical, mechanical and acoustic properties.
  - Offer potential for lightweight structures, with high stiffness and energy absorption capability.
  - With advancing manufacturing capabilities, they are becoming more affordable.
- Ability to model 3D foams based on actual foam samples
  - Helps in characterization
  - Stochastic approaches and multi-scale mechanics used to simulate the behavior

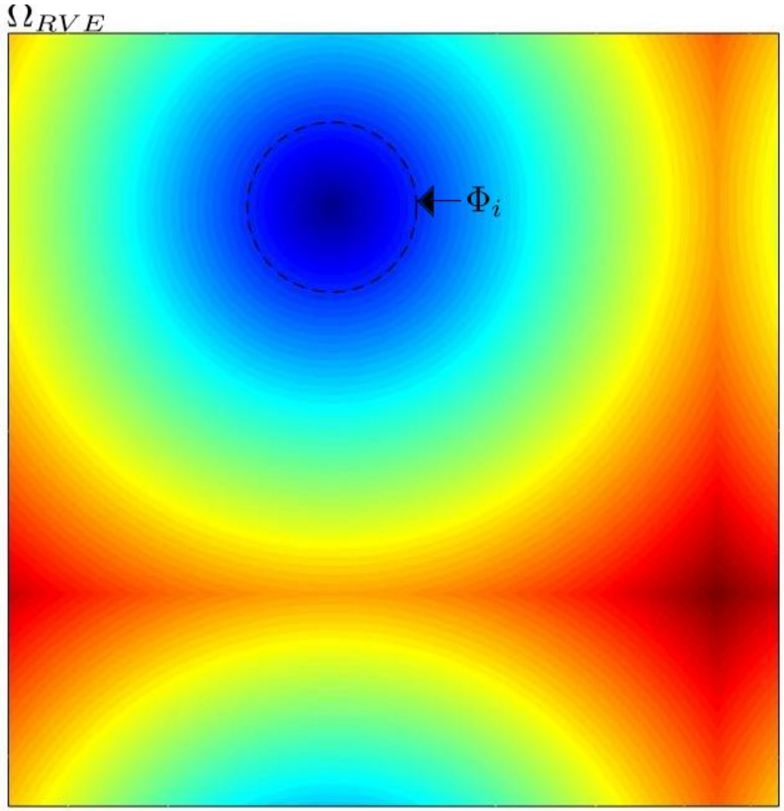


Jung & Diebels 2014

- Microstructure → Plateau's law (Sonon et al 2015)
  - Soap bubble → Plateau's law, Surface energy minimization
- Tessellations of sphere packing distribution – Laguerre tessellations
  - Sphere packing generation
  - Tessellation generated by methods like convex hull (QHull, Barer et al 1996)
  - Morphological parameters like face-by-cell count, edge-by-face count, interior angles match very well
- DN-RSA: Distance neighbor based random sequential packing algorithm for arbitrary shaped inclusions (Sonon et al 2012)
- Multiscale approaches → High cost, leads us to data driven solvers

DN-RSA Notation

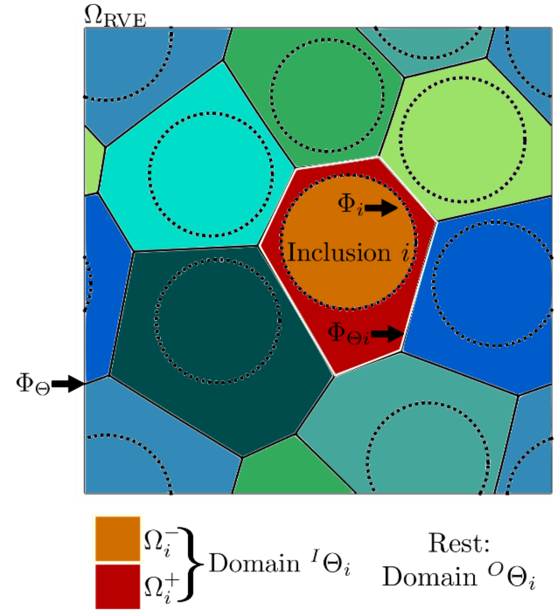
- Inclusions from desired distribution/shape are generated and placed in the domain.
  - Each grid point assigned a $DN_k(\boldsymbol{x})$ value, k - the kth nearest inclusion to the given point.
- $DN_k(\boldsymbol{x})$
  - negative inside the inclusion
  - positive outside.
- With addition of more inclusions, the $DN_k(\boldsymbol{x})$ value gets updated, depending on the k-th nearest inclusion and this inclusion mapping is stored as $NN_k(\boldsymbol{x})$.

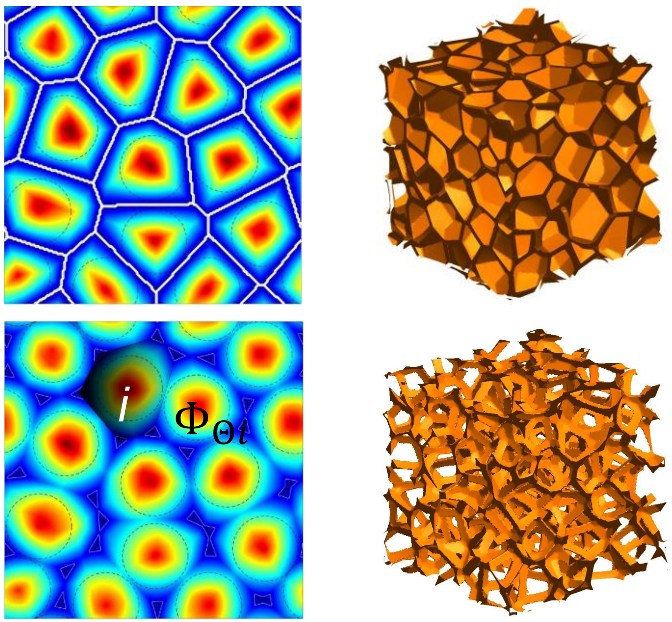


$DN_1(\boldsymbol{x})$ plot with only 1 inclusion

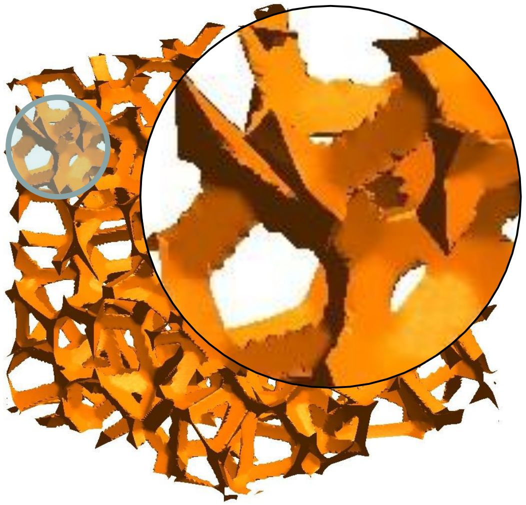
Open foam morphology

- Implicitly extracted in DN-RSA by "Voronoï" level set function:
  - $O_V(\boldsymbol{x}) = DN_2(\boldsymbol{x}) - DN_1(\boldsymbol{x})$
- A closed cell geometry can be extracted using a quasi-constant thickness, *t*:
  - $O_v(\boldsymbol{x}) - t = 0$
- "Plateau" Level set function
  - $O_P(\boldsymbol{x}) = \frac{DN_3(\boldsymbol{x})+DN_2(\boldsymbol{x})}{2} - DN_1(\boldsymbol{x})$
- Function consists of triangles with vertex lying on the tessellation cell boundaries.
- Thus, we can extract plateau border like geometry through
  - $O_P(\boldsymbol{x}) - t = 0$
  - Parameter t used to control thickness of extracted borders

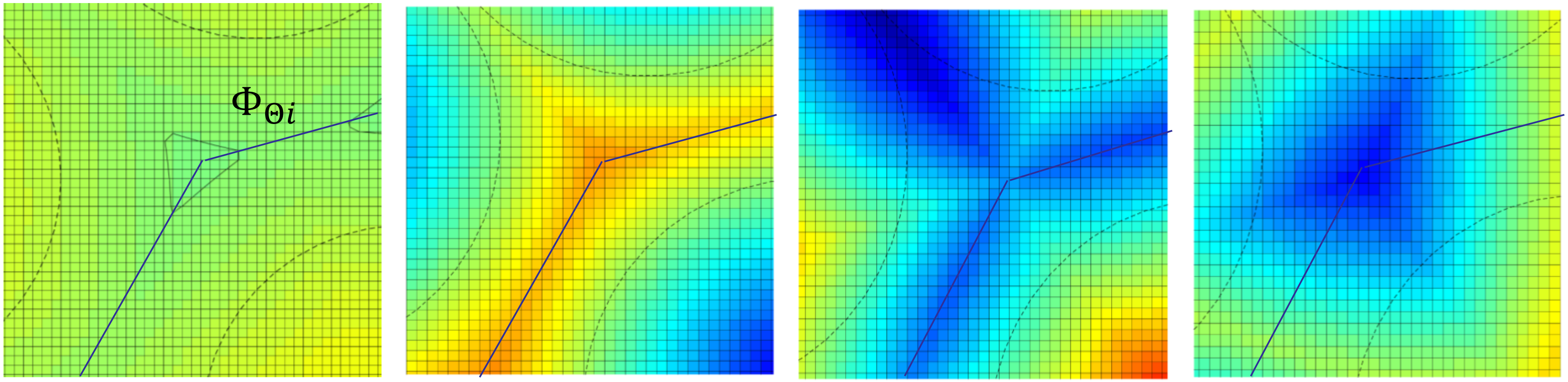




Sharp edge extraction

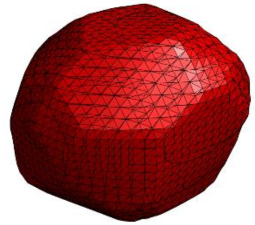


- Plateau borders present sharp edges due to their triangular prism shape
  - Origin is due to steep discontinuity of $DN_k(\boldsymbol{x})$ derivatives on Φ_Θ
- Single level set function can not represent this with discrete level set functions, and we need multiple level set function strategy
- Solved by extracting individual modified level sets for each inclusions

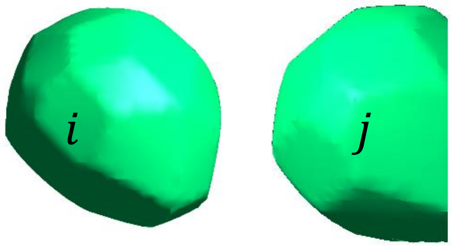


t Level Set $\quad DN_1(\boldsymbol{x}) \quad DN_2(\boldsymbol{x}) \quad DN_3(\boldsymbol{x})$

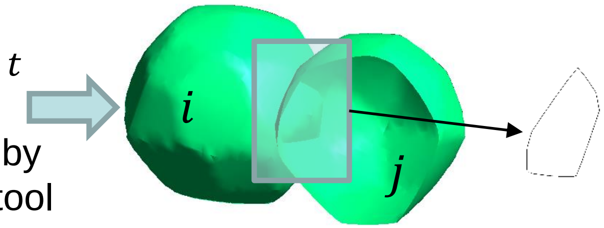
Clipping of the triangular section at grid positions and the presence of discontinuities in $DN_1(\boldsymbol{x})$ and $DN_2(\boldsymbol{x})$ across Φ_Θ. $DN_3(\boldsymbol{x})$ is continuous.



t level set of inclusion i extracted in MATLAB using $\boldsymbol{isosurface}$ function

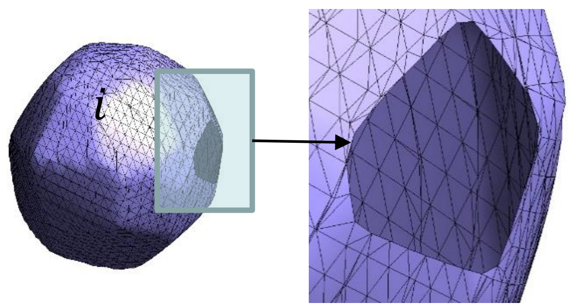


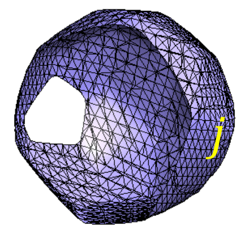
Intersection of t level sets of inclusion i and j by surface Boolean tool $Cork$



Extract, **re-mesh** and **fix** the line of intersection

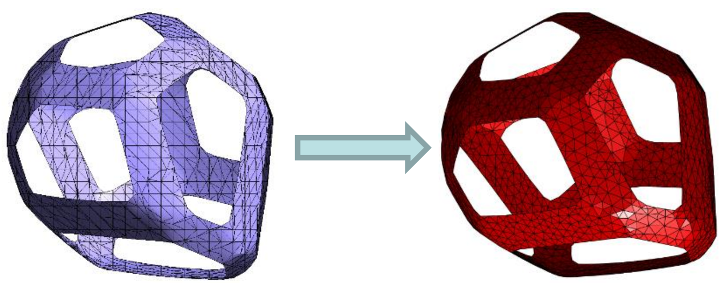
Slice-off the elements lying in the domain ${}^{I}O_{Pj}(\boldsymbol{x}) > 0, j \neq i$





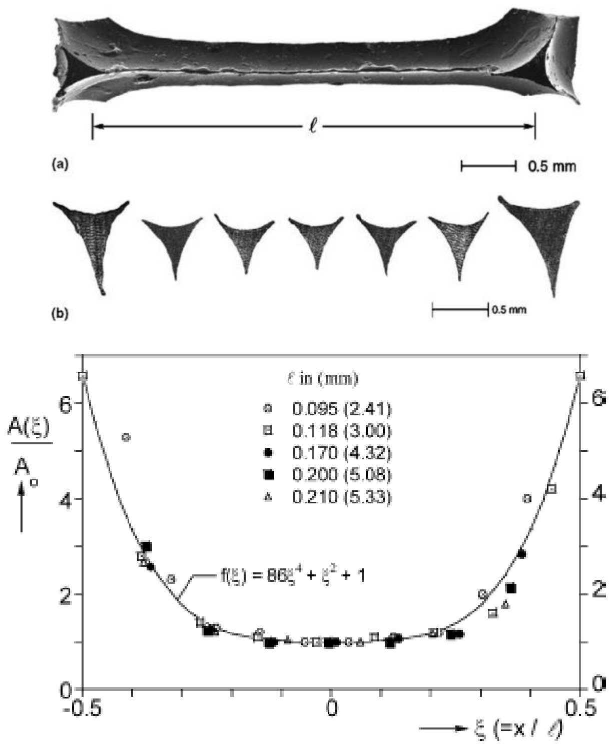
Similarly, **slice-off** the elements of t level set of inclusion j lying in the domain ${}^{I}O_{Pi}(\boldsymbol{x}) > 0, i \neq j$

Iteratively done, leaving only the plateau border part of the inclusion. Traditional *isosurface* operations result in ill-formed elements.

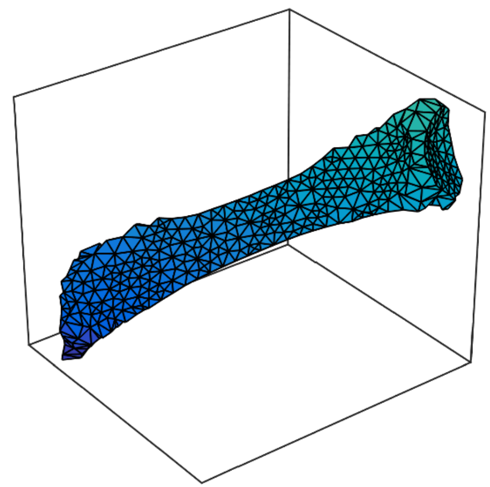


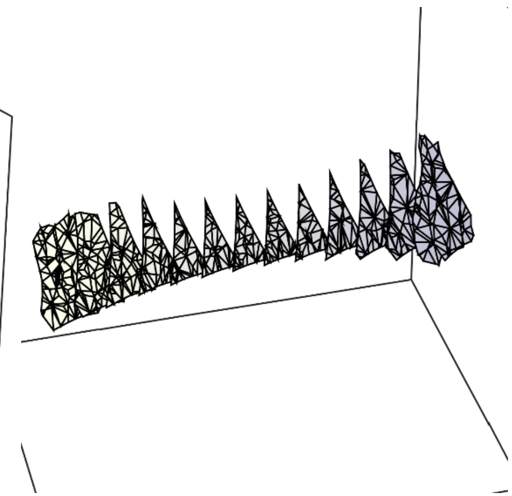
Inclusions are then refined by level set based mesh conforming approach designed by [Karim et al (under preparation)] using analogy of equilibrium of 3D truss system (Persson and Strang, 2004) before assembling. 3D mesh is generated using Tetgen (Hang Si 2015)

Strut cross section variation



Strut cross section variation and mid-span cross-sectional area of a polyurethane foam; Gong et al 2004





$$O_{S1}(\mathbf{x}) = DN_4(\mathbf{x}) - DN_3(\mathbf{x})$$

Value of the function increases from 0 at the intersection of struts to half the length of the strut at mid-span along the axis.

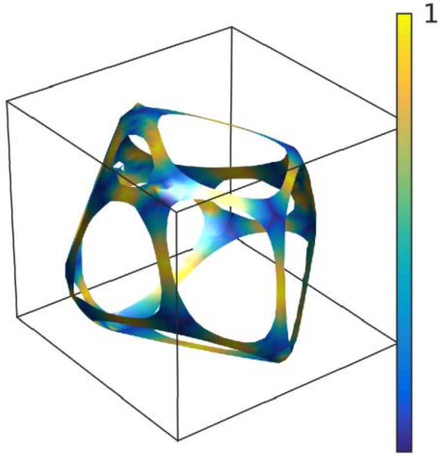
$$\Omega_{ijk} = (NN_1(\mathbf{x}) = i)\&(NN_2(\mathbf{x}) = j)\&(NN_3(\mathbf{x}) = k)$$

Tetrahedral domain joining the center of the inclusion *I*, center of the common face between *I* and *j*, and the two ends of the strut formed by *I*, *j*, and *k*

DN-RSA is able to incorporate these variations by modifying the "Plateau" function O_P according to the domain using DN_3 and DN_4.

Strut cross section variation

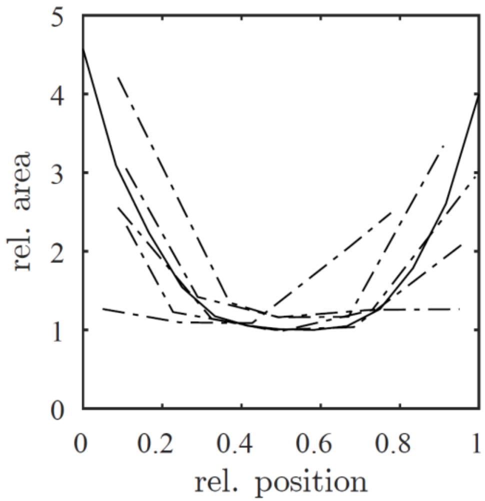
$$\xi' = \frac{O_{S1}(\Omega_{ijk})}{\max(O_{S1}(\Omega_{ijk}))}$$



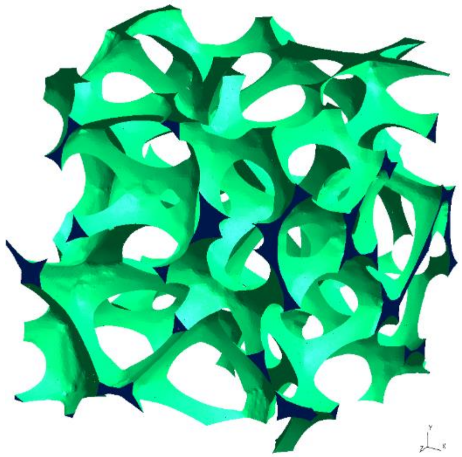
$$O_S(\mathbf{x}) = \sqrt{\frac{A(\xi')}{A_0}}$$

$$O_P(\mathbf{x}) - tO_S(\mathbf{x}) = 0$$

The final operator and the equation that enables to generate variation in strut cross-section



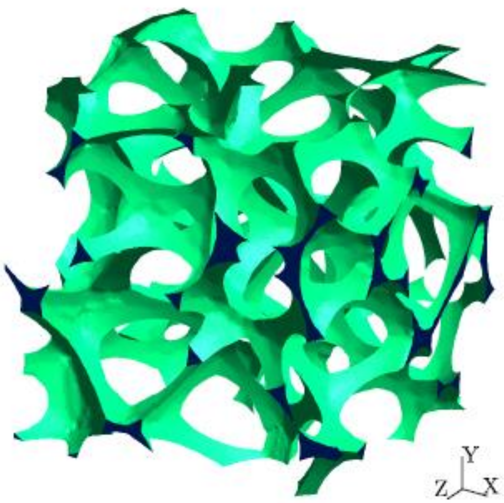
- Dotted line – strut cross section area data from 20ppi foam sample from Jung and Diebels 2017
- Bold line – data from a simulated 20ppi foam using DN-RSA

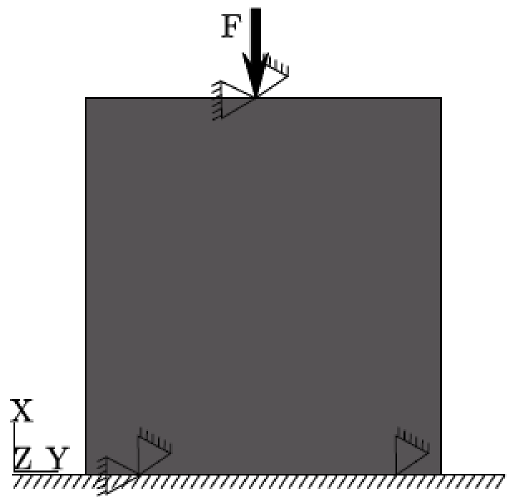


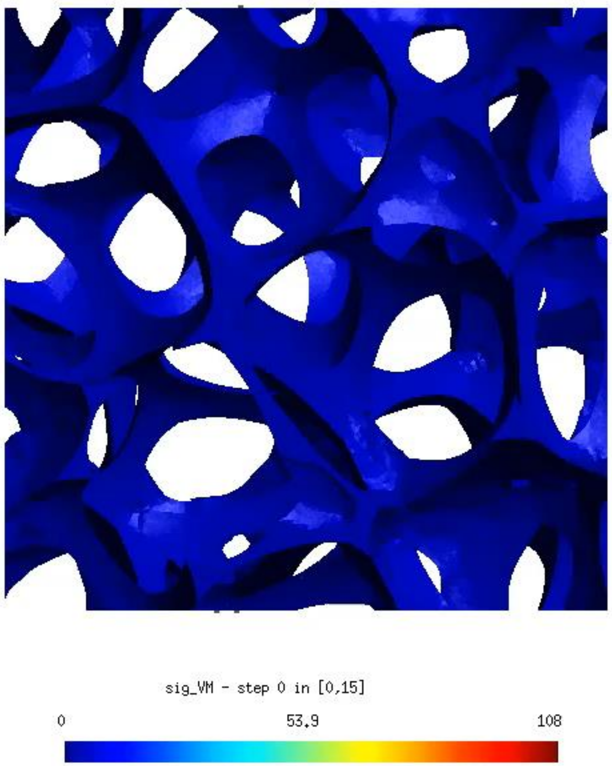
An RVE simulating a 20ppi foam with 25 inclusions

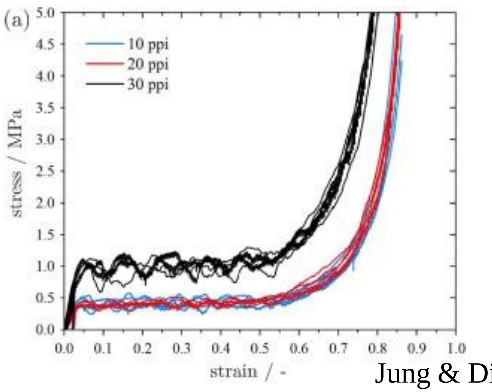
Numerical Simulation – RVE

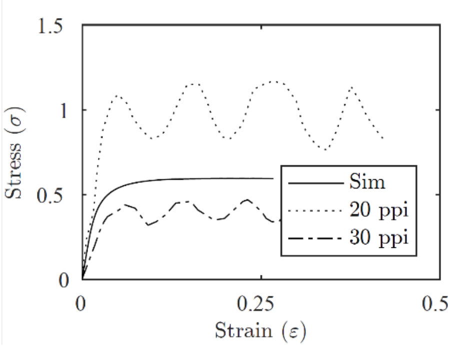
- Larger RVE with 25 inclusions completely inside the domain.
- Uniaxial compression test comparison with experimental values; contact criteria not implemented.







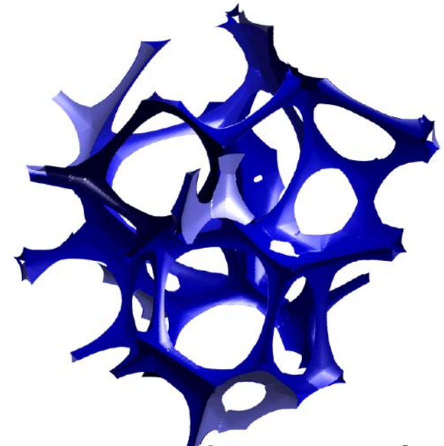




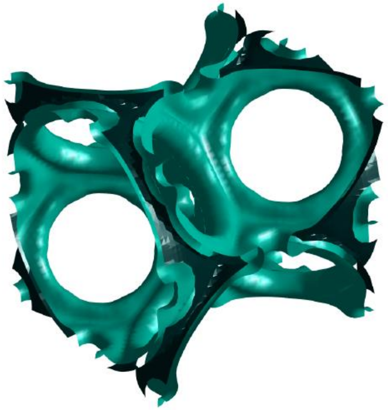
Jung & Diebels 2017

Further advantages of DN-RSA

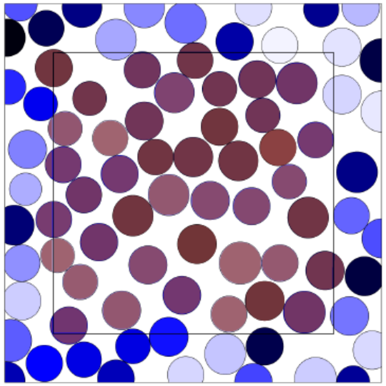
- Periodic RVEs and RVEs with free boundary
- Strut cross-section concavity and convexity using concavity operators based on distance function
- Generation of RVEs with layers of coatings with non-smooth coatings using distance functions



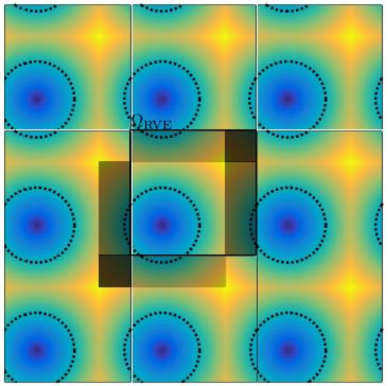
Concavity control



Layers of coatings



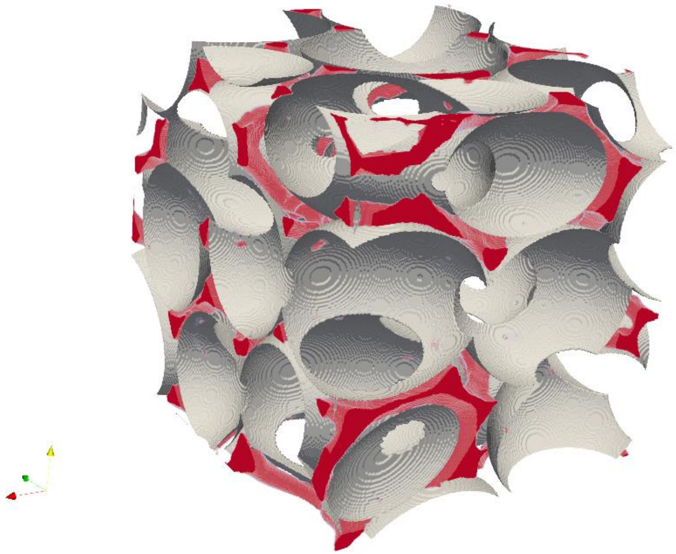
Free boundary RVE with minus sampling

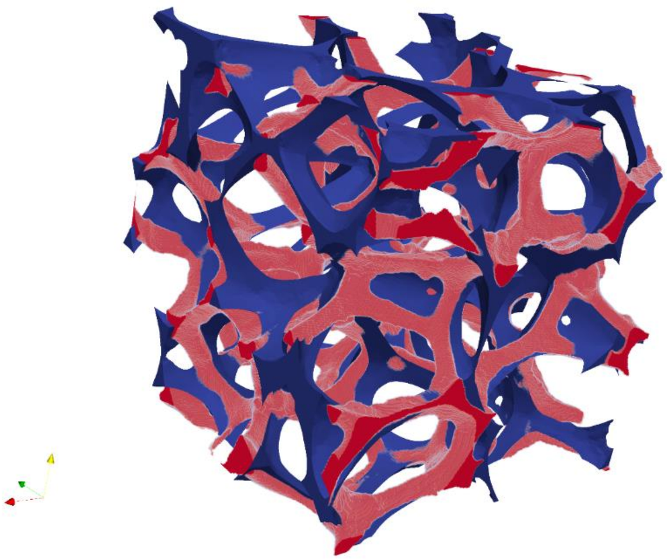


Periodicity in RVE

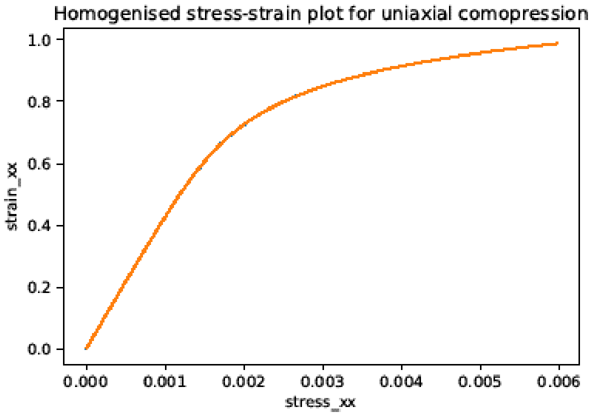
DN-RSA with ellipsoids

- Generate ellipsoids based on pores extracted from CT scans of physical foam samples (Leblanc et al, *under preparation*)
- Statistical validation for pore placement
- DN-RSA to extract foam morphologies using package made of ellipsoids – statistical validation of pore placement
- Sample made of 600 voxels in each dimension with each voxel = 24um





Relative Density
Voxel data 7%
DN-RSA 6.8%



Data driven models - Motivation

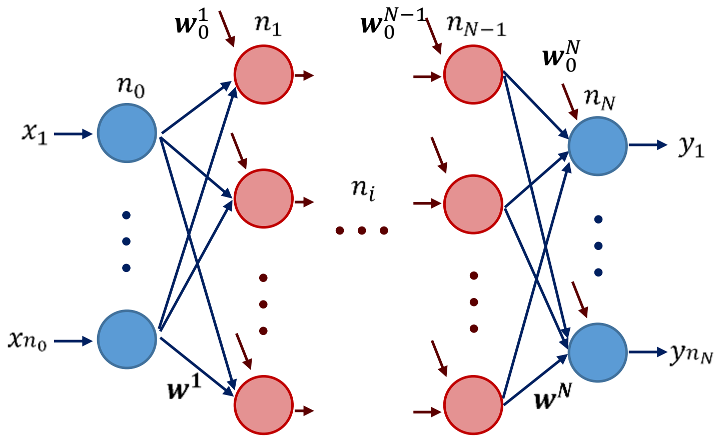
- Complexity in analysing open-foam materials by including all the relevant information in the extracted models
- Time consuming results – hierarchical coupling in classical multiscale methods
- Meso scale models not efficient in accounting for the complex loading conditions
- Non-uniformity of the microstructure
- High computational cost to run micro-mechanical simulations for full scale problems
- Difficulty to store, post-process and analyse large amount of data

Data driven models - Motivation

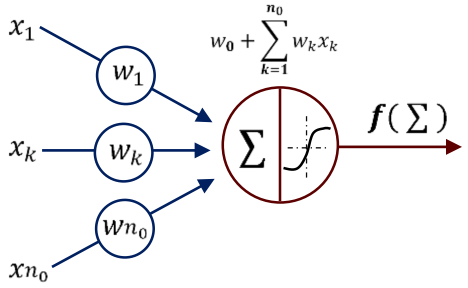
- Complexity in analysing open-foam materials by including all the relevant information in the extracted models
- Time consuming results – hierarchical coupling in classical multiscale methods
- Meso scale models not efficient in accounting for the complex loading conditions
- Non-uniformity of the microstructure
- High computational cost to run micro-mechanical simulations for full scale problems
- Difficulty to store, post-process and analyse large amount of data
- Neural networks – capability to directly incorporate the micro-mechanical data and direct numerical simulations on the microstructure
- Generation of datasets – offline implementation – significant reduction in computational cost

Data driven models using neural networks

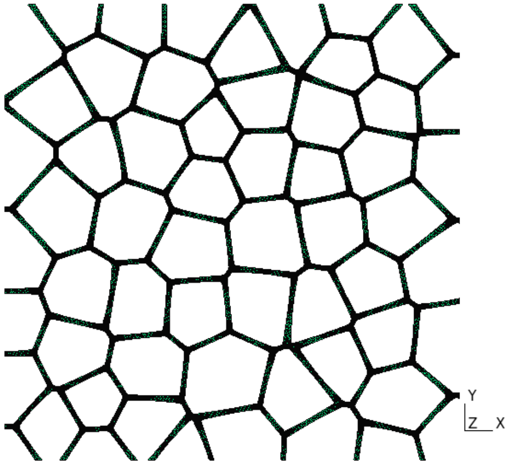
- Artificial neural network – inspired from biological counterpart
- Input layers -> Hidden layer(s) -> Output layer

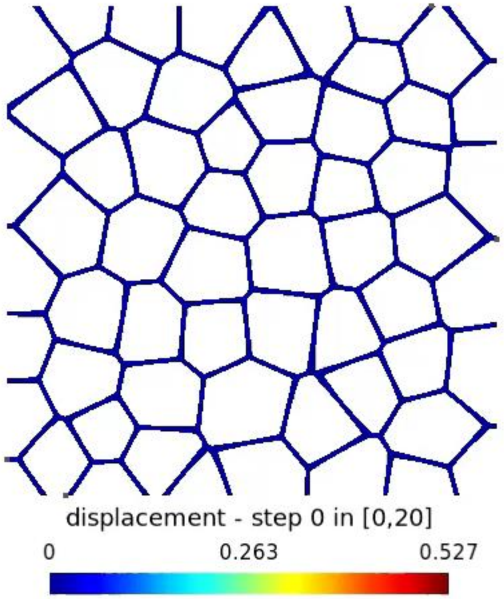


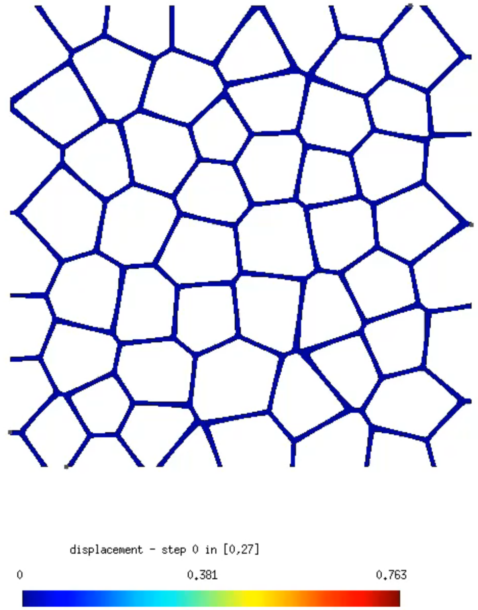
- Weights assigned to each artificial inner nodes
- Combination of input signals and activation functions used, neurons can activate, de-activate or change

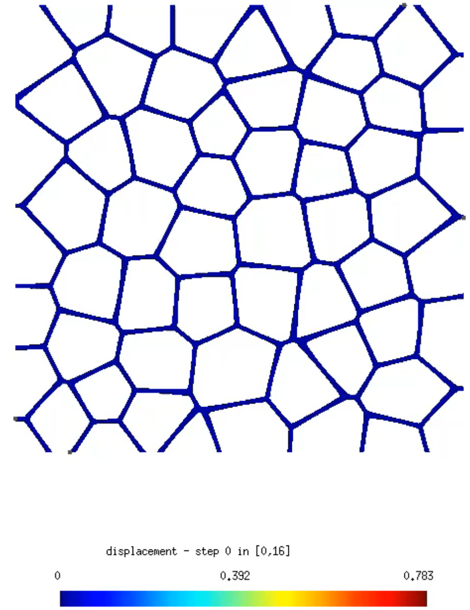


- 2D solution data preparation with around 400 sample simulations for training the neural network
- Modify deformation tensor while applying periodic boundary conditions
- Apply final values for $u_{xx}, u_{yy}, u_{xy}, u_{yx}$

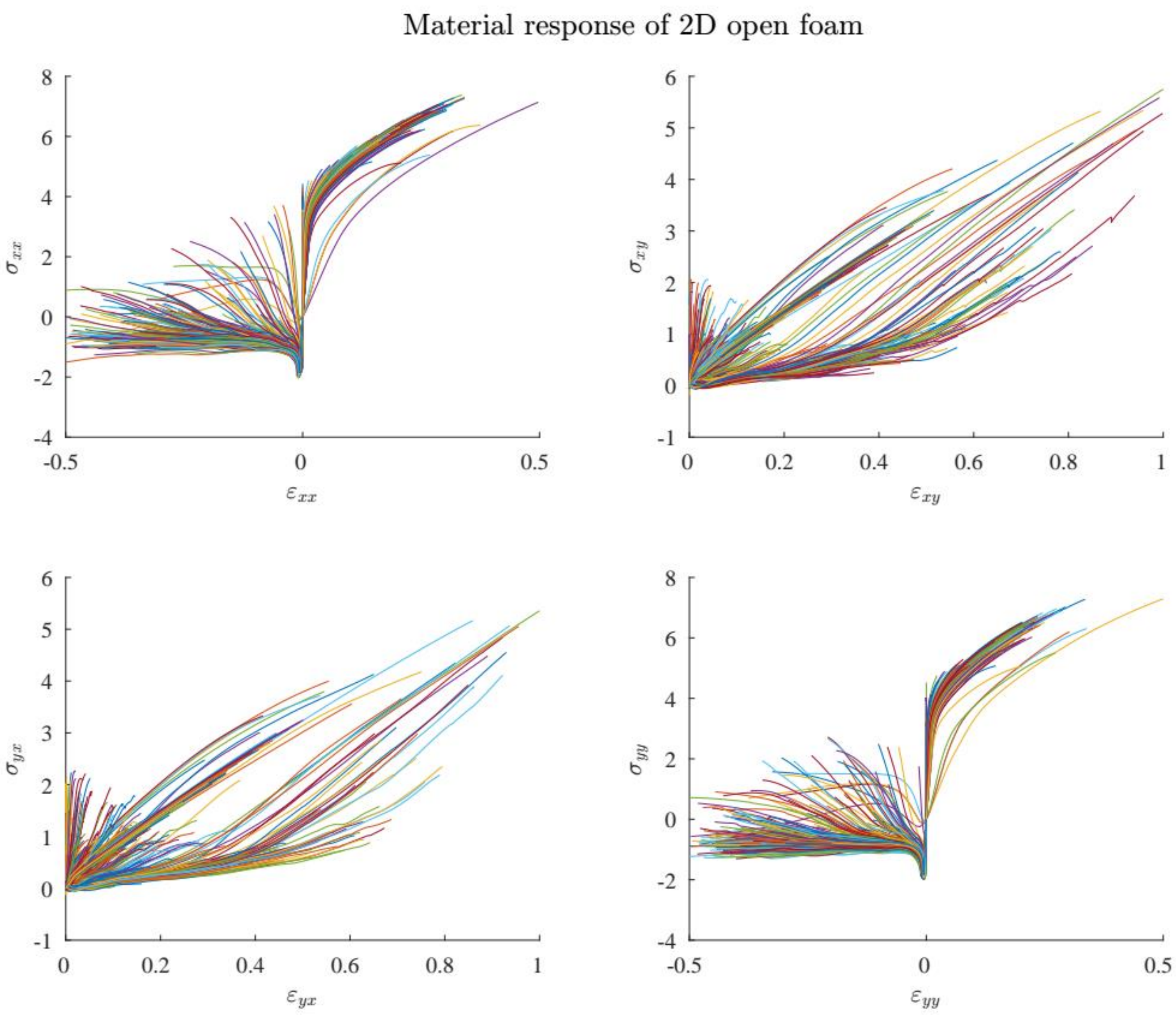






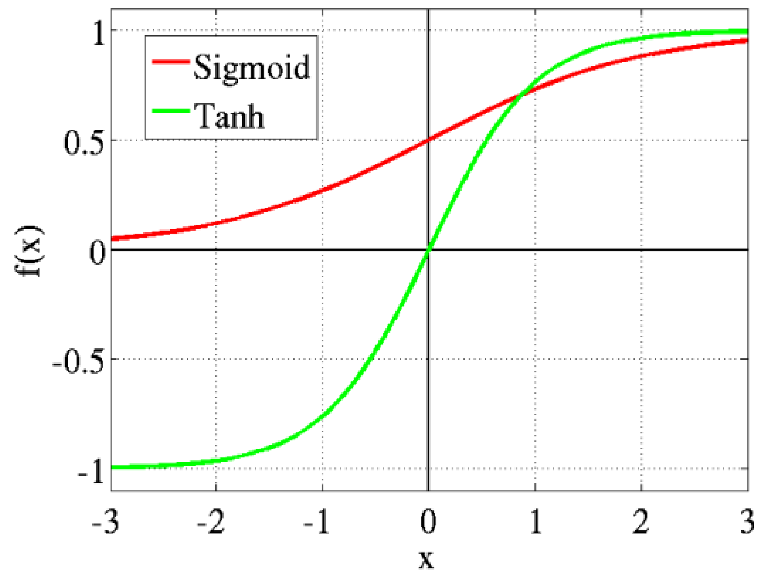


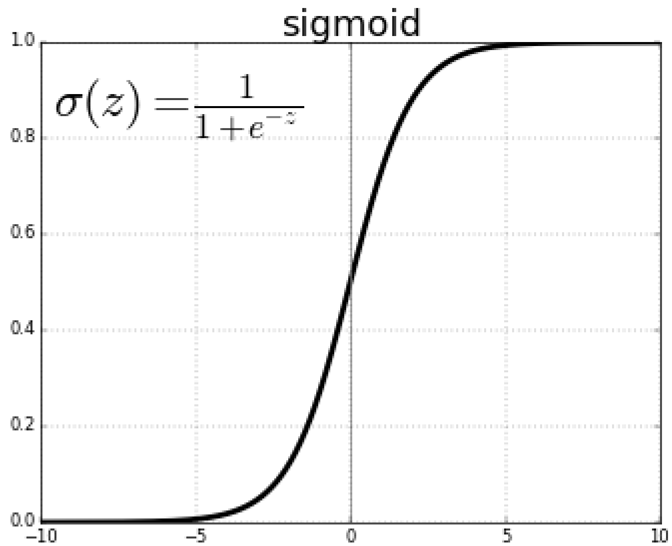
Data driven models using neural networks

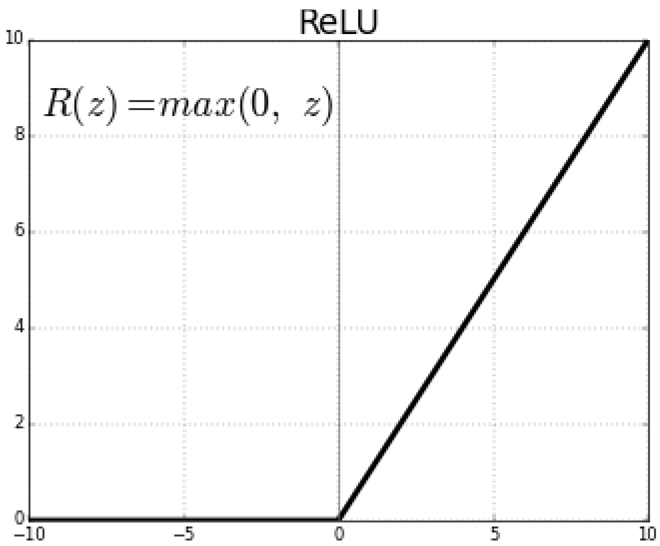


Activation functions for Neural Network

- Transfer function used to get output of node
- Used to determine the output of neural network and maps the resulting values
- Some examples of non linear activation functions
  - Sigmoid
  - Tanh ($= 2sigmoid(2x) - 1$)
  - Rectified Linear Unit (ReLU)



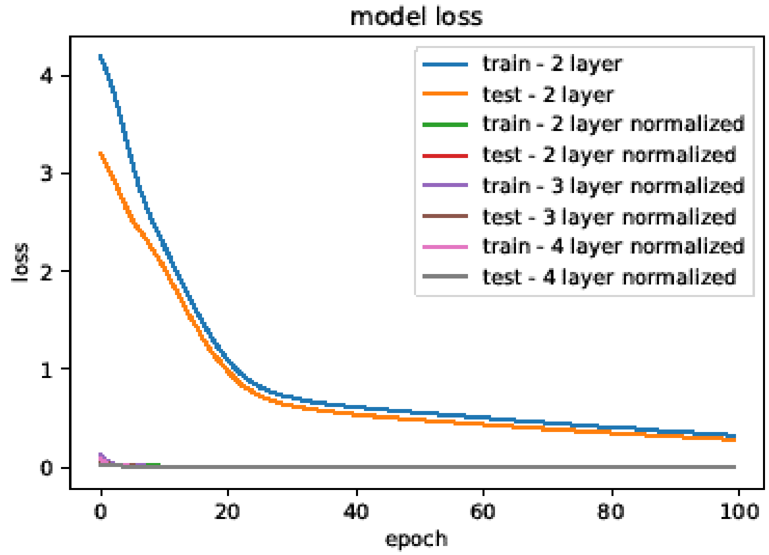


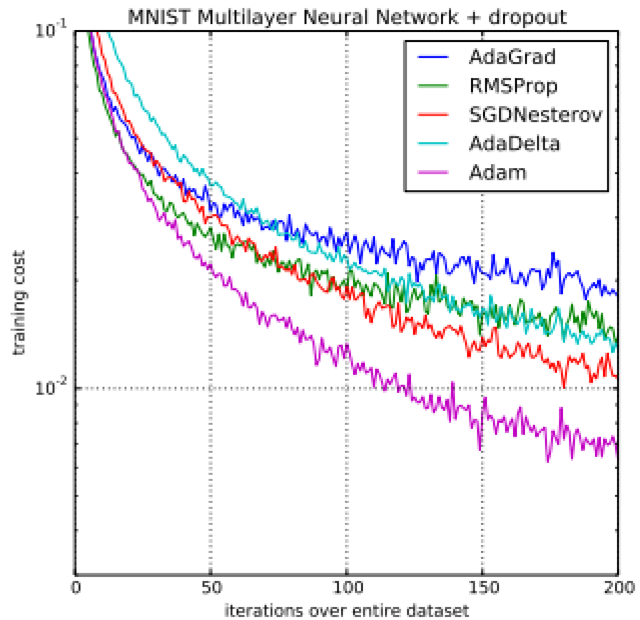


https://towardsdatascience.com/activation-functions-neural-networks-1cbd9f8d91d6

Layers for NN

- Use of feedforward nets to accurately classify sequential inputs
- Sequential layers are added piecewise
- More layers → deeper the model
- Epochs → Number of times the dataset is passed to the NN forward and backward
- Batch size → Number of training samples in a single batch
- Optimizers → Adaptive moment estimation (adam, combining adaptive gradient algorithm and root mean square propagation), stochastic gradient descent (SGD)

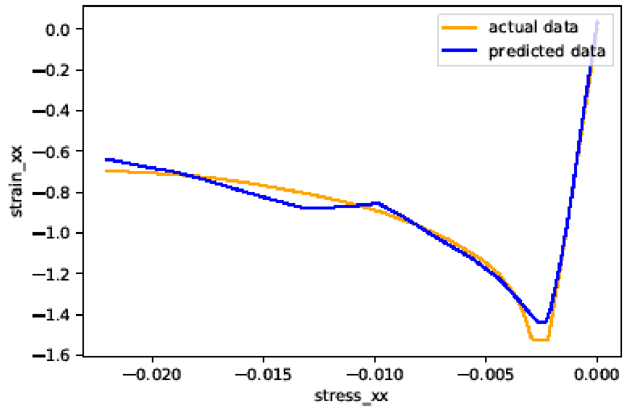


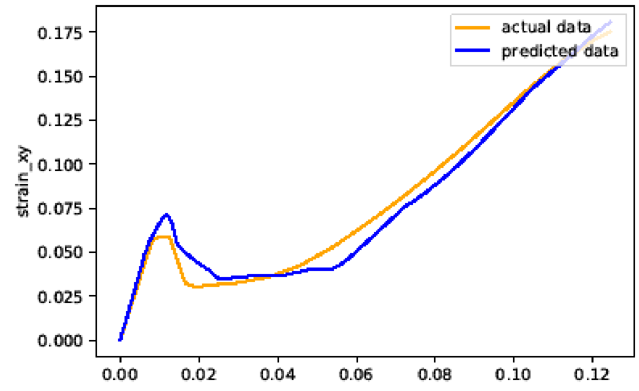


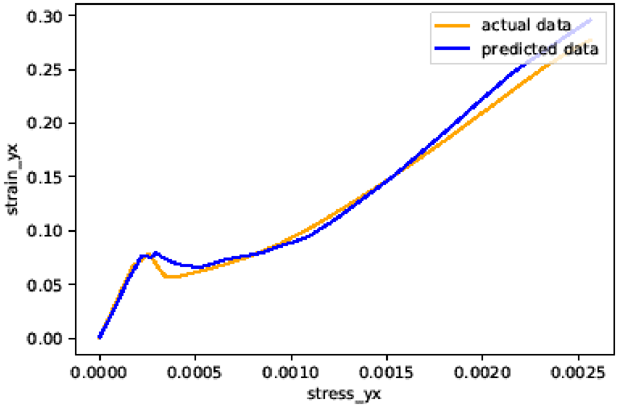
https://machinelearningmastery.com/adam-optimization-algorithm-for-deep-learning/

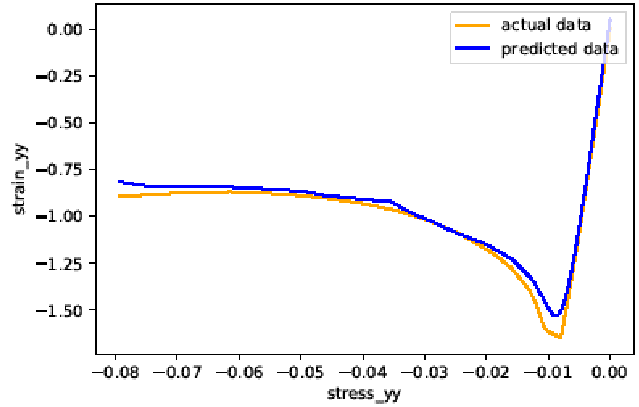
Data driven models using neural networks

- Solution
  - 400 training samples
  - 100 validation samples
  - 500 epochs
  - 1 sequential input layer with 200 nodes
  - 1 sequential hidden node with 100 nodes
  - 1 sequential hidden node with 20 nodes
  - 1 output node with 4 nodes
  - All layers activated with ReLU and optimized with adam
  - Prediction made on a new sample



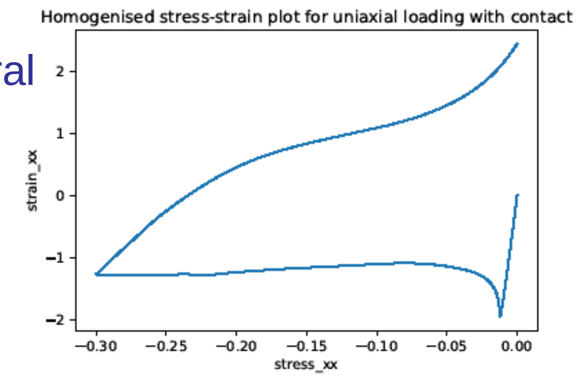


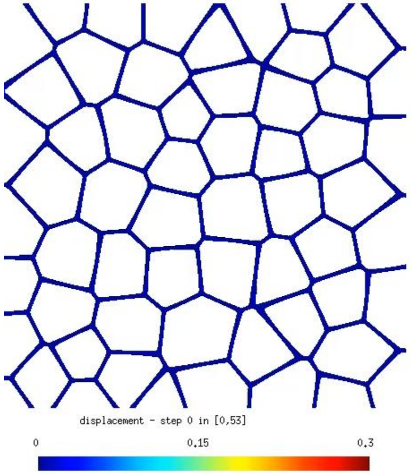


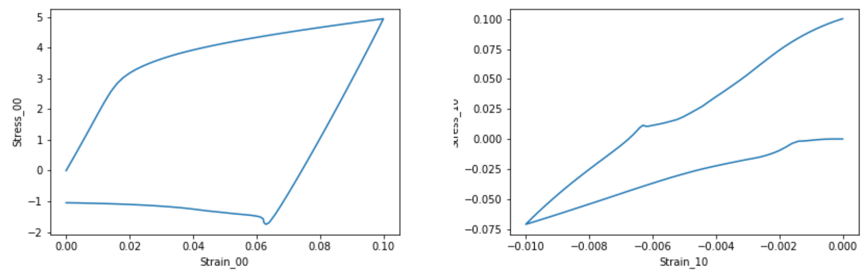


Towards the future with data science

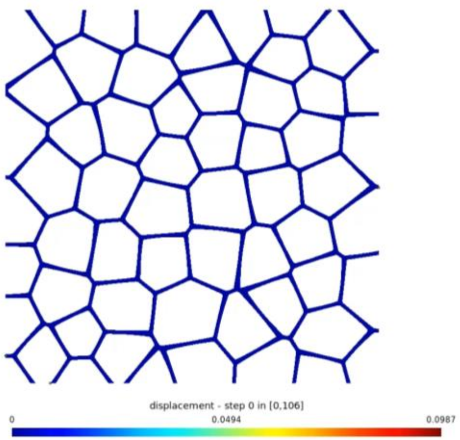
- Implementation of contact on all simulation series to be trained with neural networks
- Back propagation through time models and long short memory units models implementation to predict history dependant behaviour
- Develop models that take into account porosity and material behaviour parameters
- Use the NN models developed to train 3D material model for numerical simulations

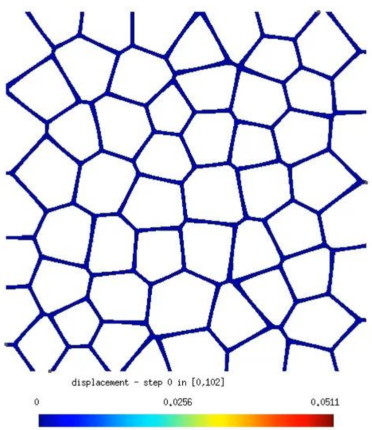






History dependant behaviour of 2D open foam





Thank you for your attention

Data driven computational analysis of open foam RVEs

Nanda G. Kilingar, K. Ehab Moustafa Kamel, B. Sonon, C. Leblanc, L. Noëls, T.J. Massart, A. Jung

Computational & Multiscale Mechanics of Materials – CM3
http://www.ltas-cm3.ulg.ac.be/
B52 - Quartier Polytech 1
Allée de la découverte 9, B4000 Liège
ngkilingar@uliege.be

Limitations and Advantages

- **Higher discretization** of the grid required to capture higher sphere packing
- Laguerre tessellations are known to have higher number of **small struts** and **triangular faces** that are skewed,
  - captured by DN-RSA in the limit of vanishing discretization size.
- Representation of foams with RVE having high dispersion rate of the inclusion size is difficult with this model due to the necessary discretization grid.

- Easy access to **the signed distance functions** allows us to implement variations in the morphology
  - strut cross-section variation at the mid-span and along the axis of the strut
  - combination of open-closed faces of tessellated cells
  - Coating of the RVE to represent realistic engineering applications
- A balance of discretization size allows us to model the foam without the issues of small/skewed faces as they are implicitly enveloped by the extracted t level set.
- Extracted mesh can be easily utilized for **a data-driven multi-scale study** and understand the effects of upscaling the model to study the elastic-plastic properties of such foams