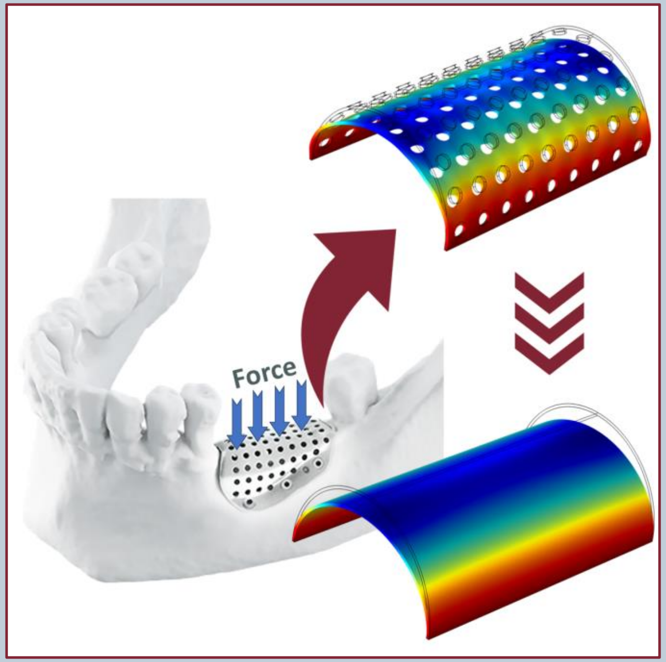

Developing 2D and 3D Micropolar FEM Models for Porous GBR Meshes in Dentistry Applications

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SAPIENZA
UNIVERSITÀ DI ROMA

AbdolMajid Rezaei

Dr. Razie Izadi

ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

Prof. N. Fantuzzi

Introduction

Guided Bone Regeneration (GBR) Mesh

- Using a mechanical barrier, such as a membrane, to separate and protect the area of bone loss from the surrounding tissue.

1 Exposing the Bone Defect: A small incision to access the area of defect.

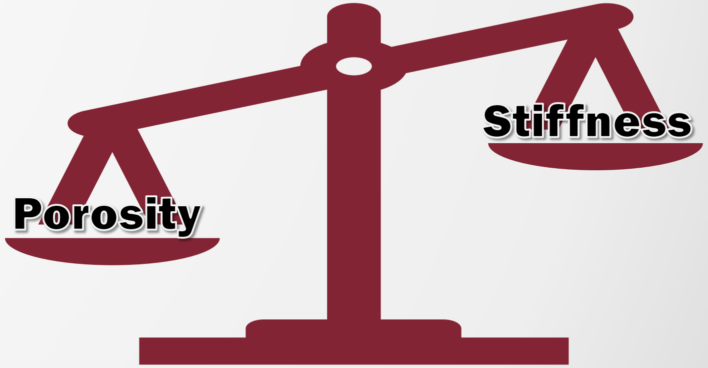
2 Bone Grafting: a cement that may contain bone, antimicrobial additives and stimulants that promotes new bone growth is placed under the membrane.

3 Preparing GBR Mesh: cut and formed by the surgeon

4 Placing and fixing the GBR Mesh

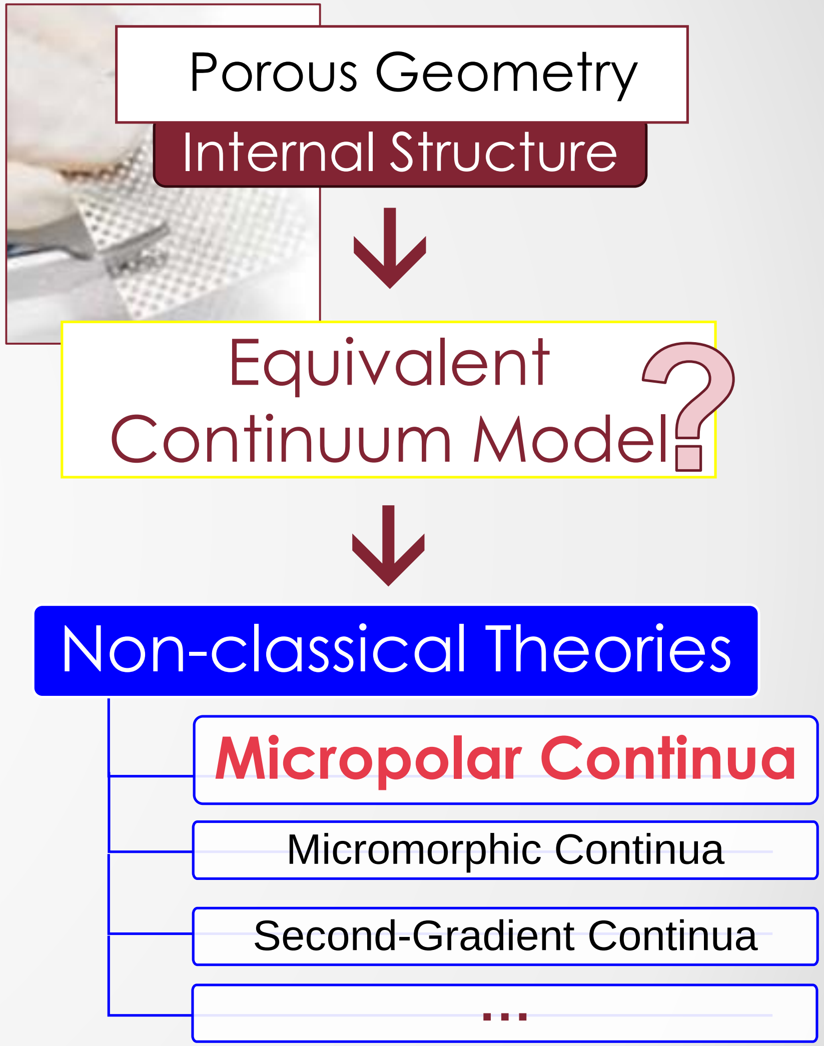
https://www.indigoortho.co.uk/gbr-systems

- New bone can grow in the designated area.
- Enough stiffness to create and maintain a suitable space for the intended bone regeneration.
- Enough porosity to facilitate the diffusion of fluids, oxygen, nutrients, and bioactive substances for cell growth.



Equivalent Homogenised Models for Porous Structures

- When the geometry includes pores, there is an internal structure.
- By using equivalent model and defining effective properties instead of the real microstructure, we can decrease computational expense of modelling and discretisation.
- Non-classical continuum theories can consider the internal structure without direct modelling of details.
- In the present work, non-classical micropolar theory as the homogenised equivalent model is implemented for the porous structures in 2D and 3D.



Introduction

Micropolar Theory

- Degrees of Freedom: **U**, Φ
- Kinematic Relations: $E_{ij} = U_{j,i} + e_{jik}\Phi_k$

$$K_{ij} = \Phi_{j,i}$$

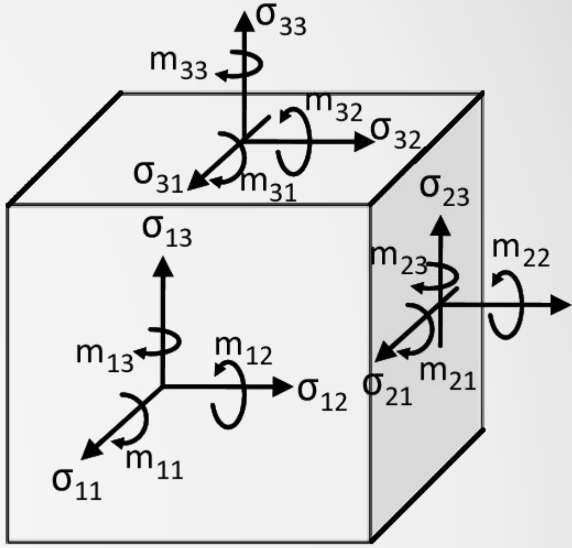
- Balance Equations: $\Sigma_{ij,i} + P_j = 0$

$$M_{ij,i} + e_{ijk}\Sigma_{jk} + Q_k = 0$$

- Constitutive Equations: $\Sigma_{ij} = A_{ijkl}E_{kl} + B_{ijkl}K_{kl}$
  (Linear Elastic)

$$M_{ij} = B_{ijkl}E_{kl} + D_{ijkl}K_{kl}$$

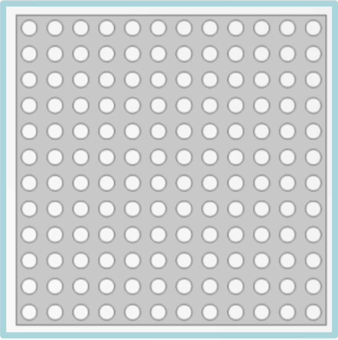
Φ	Micro-rotation
E	Nonsymmetric Strain
K	Curvature
Σ	Nonsymmetric Stress
M	Couple-stress
P	Body Force
Q	Body Couple

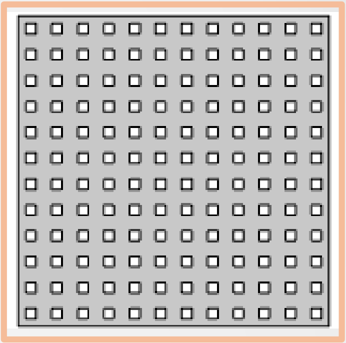


- New strain measure as **Curvature**.
- New stress measure as **Couple-stress**.

Methodology
2D Tetragonal Micropolar Model for Porous Plate

- General linear elastic constitutive equations in plane
- Ortho-tetragonal Material Symmetry
- Considering the linear elastic micropolar in 2D, for the geometries we study here, 5 independent material parameters are required to define the equivalent model.





$$
\begin{bmatrix} \Sigma_{11} \\ \Sigma_{22} \\ \Sigma_{12} \\ \Sigma_{21} \\ M_1 \\ M_2 \end{bmatrix}
=
\begin{bmatrix}
A_{1111} & A_{1122} & A_{1112} & A_{1121} & B_{111} & B_{112} \\
 & A_{2222} & A_{2212} & A_{2221} & B_{221} & B_{222} \\
 & & A_{1212} & A_{1221} & B_{121} & B_{122} \\
 & & & A_{2121} & B_{211} & B_{212} \\
 & & & & D_{11} & D_{12} \\
sym. & & & & & D_{22}
\end{bmatrix}
\begin{bmatrix} E_{11} \\ E_{22} \\ E_{12} \\ E_{21} \\ K_1 \\ K_2 \end{bmatrix}
$$

$$A_{1112} = A_{1121} = 0$$
$$A_{2212} = A_{2221} = 0$$
$$A_{1111} = A_{2222} \quad B_{ijk} = 0$$
$$A_{2121} = A_{1212}$$
$$D_{11} = D_{22}, D_{12} = 0$$

5 Independent Material Parameters

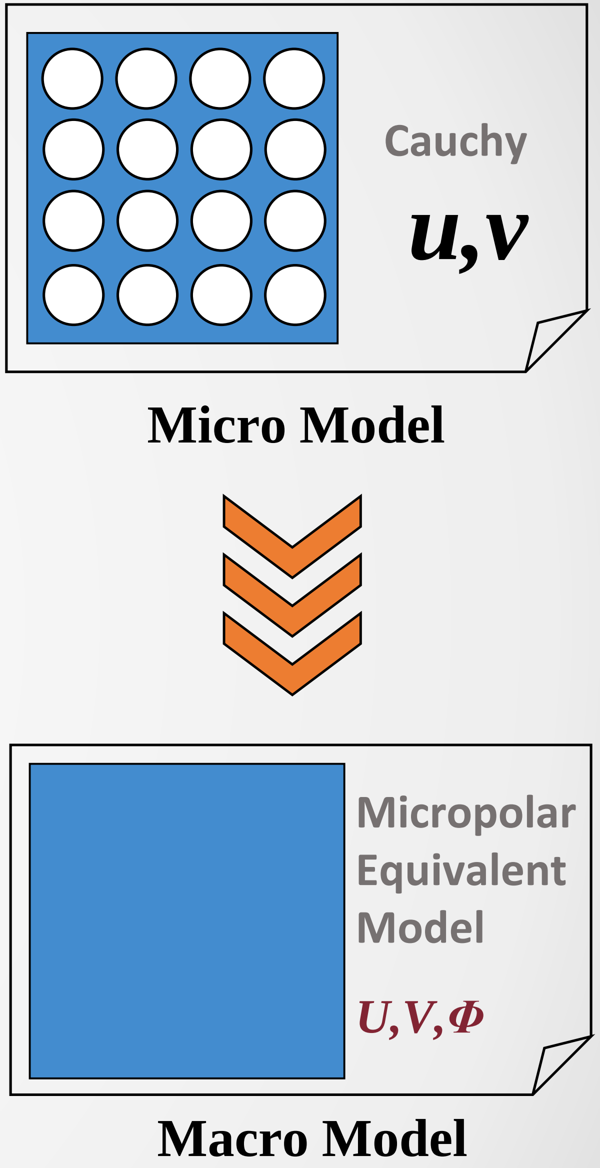
$$
\begin{bmatrix}
A_{1111} & A_{1122} & 0 & 0 & 0 & 0 \\
A_{1122} & A_{1111} & 0 & 0 & 0 & 0 \\
0 & 0 & A_{1212} & A_{1221} & 0 & 0 \\
0 & 0 & A_{1221} & A_{1212} & 0 & 0 \\
0 & 0 & 0 & 0 & D_{11} & 0 \\
0 & 0 & 0 & 0 & 0 & D_{11}
\end{bmatrix}
$$

Methodology
Homogenization of 2D Model

- The heterogeneous structure, is called **Micro Model** and is described by Cauchy continuum.
- Homogenised model is called **Macro Model** and is described by constitutive parameters of a micropolar continuum.
- Kinematic Map: Links the two levels of description
- Express the microscopic displacement field within the RVE as a function of the macroscopic strain measures at the material point on the macro-level.

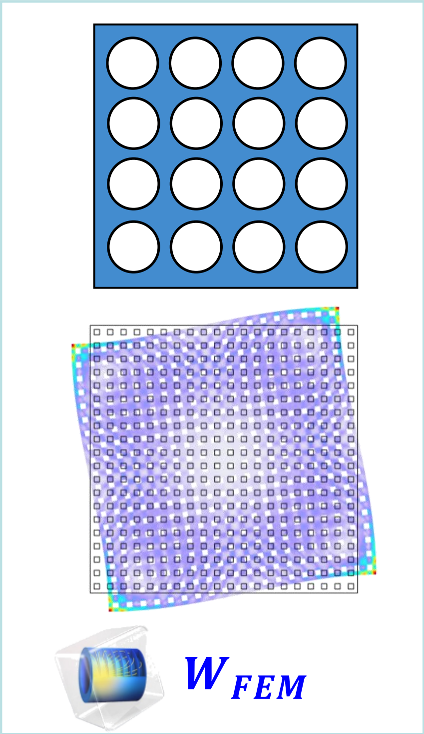
$$u^{\mathrm{hom}} = E_{11}\,x + E_{12}^{SYM}\,y - \frac{K_2}{2}\,y^2 - K_1\,xy - \frac{10}{L^2}\,\Theta(y^3 - 3yx^2)$$

$$v^{\mathrm{hom}} = E_{12}^{SYM}\,x + E_{22}\,y + \frac{K_1}{2}\,x^2 + K_2\,xy + \frac{10}{L^2}\,\Theta(x^3 - 3xy^2)$$



Methodology
Homogenization of 2D Model

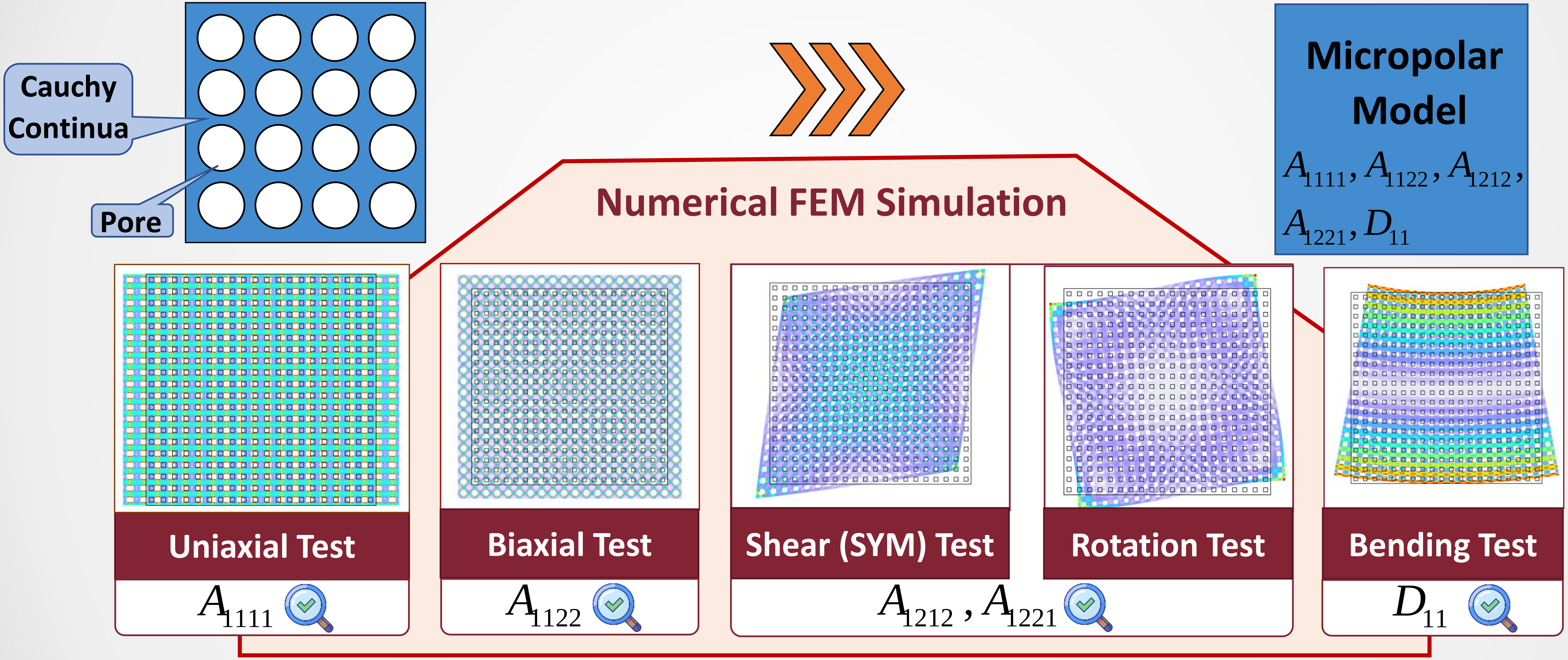
- Once the kinematic map is determined, we proceed to discover the micropolar material parameters.
- We use the finite element method (FEM) to compute the response of the porous structure under different loadings.
  - Extract the total elastic strain energy W_{FEM} stored in the RVE from COMSOL.
  - Equating to the energy of an equivalent micropolar continuum $W_{Micropolar}$ from analytical expression.
- For each scenario, the micropolar material parameters are determined in such a way that the homogenized model retains the same amount of strain energy when exposed to the same loading conditions.



$W_{Micropolar}$

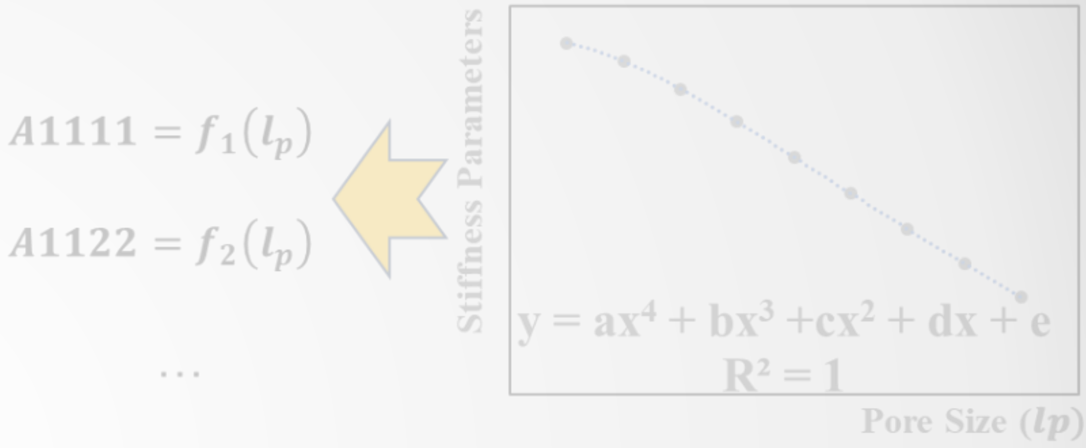
$$\frac{1}{2}\begin{bmatrix} \Sigma_{11}E_{11} + \\ \Sigma_{22}E_{22} + \\ \Sigma_{12}^{SYM}E_{12}^{SYM} + \\ \Sigma_{12}^{ASM}\Theta + \\ M_1K_1 + M_2K_2 \end{bmatrix}$$

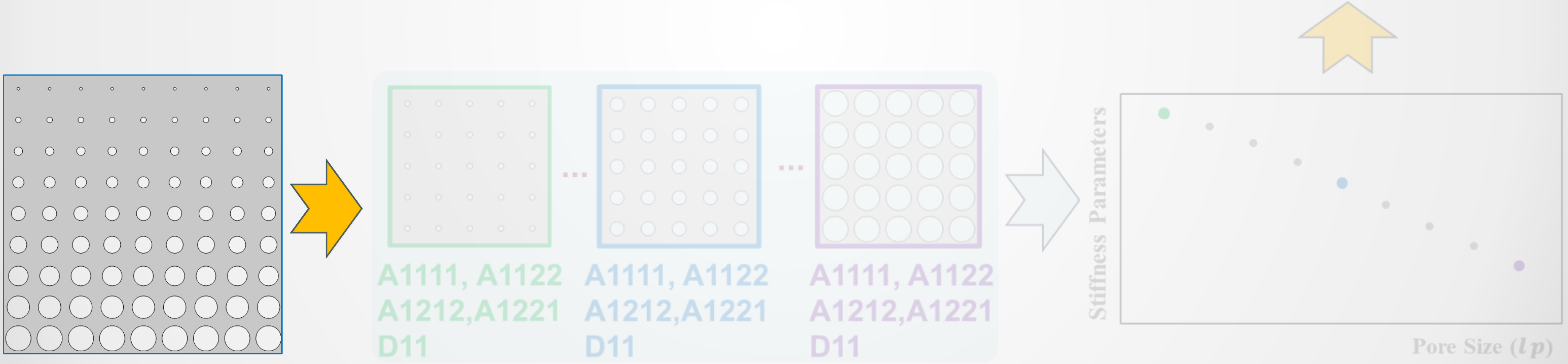
Methodology
Finding Effective Micropolar Material Parameters for 2D Model



Methodology
Extending the Homogenization Procedure for FG Porous Structures

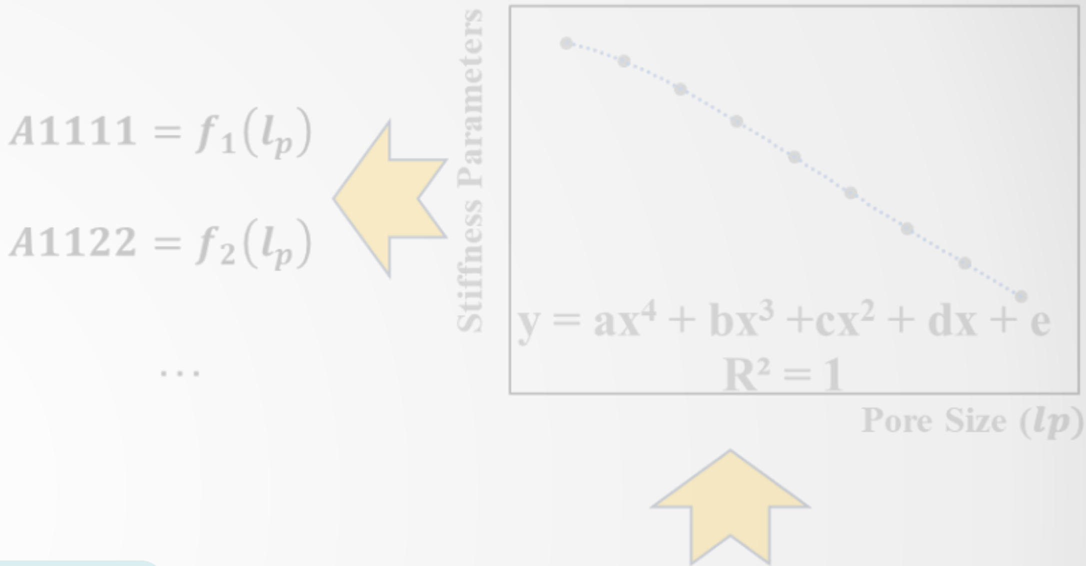
- Equivalent homogenized model for **F**unctionally **G**raded (**FG**) porous structure is derived by considering the homogenization procedure developed for homogenous porosities.

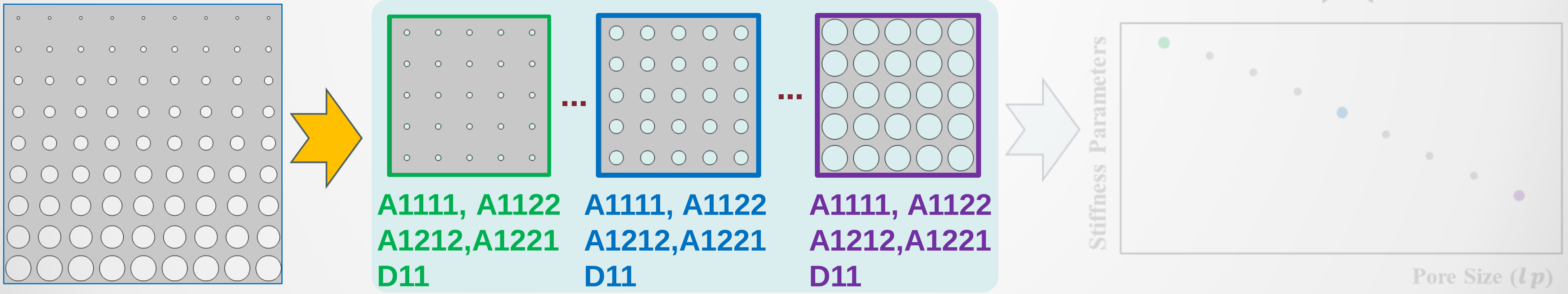




Methodology
Extending the Homogenization Procedure for FG Porous Structures

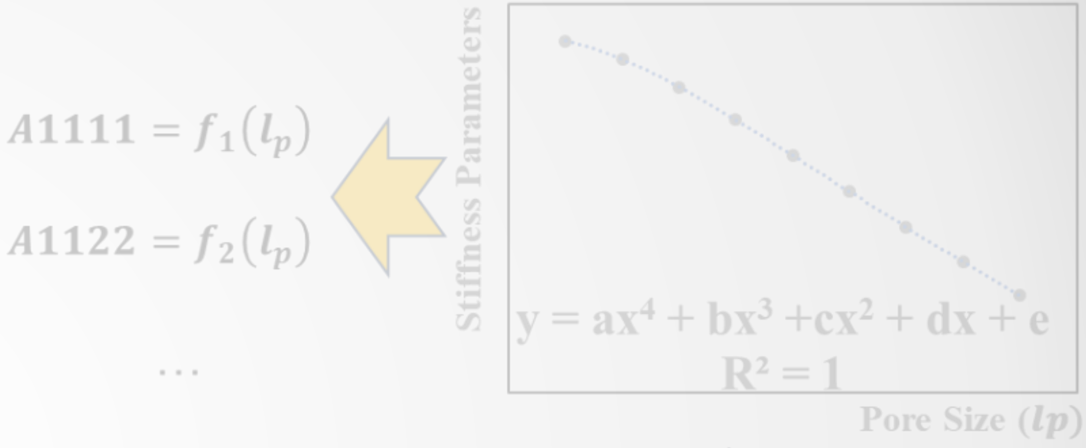
- First, a parametric study is conducted to find the equivalent parameters of uniform porous plates with various pore sizes.
- In this parametric study, the pore density (the number of pores per unit length) is kept constant.

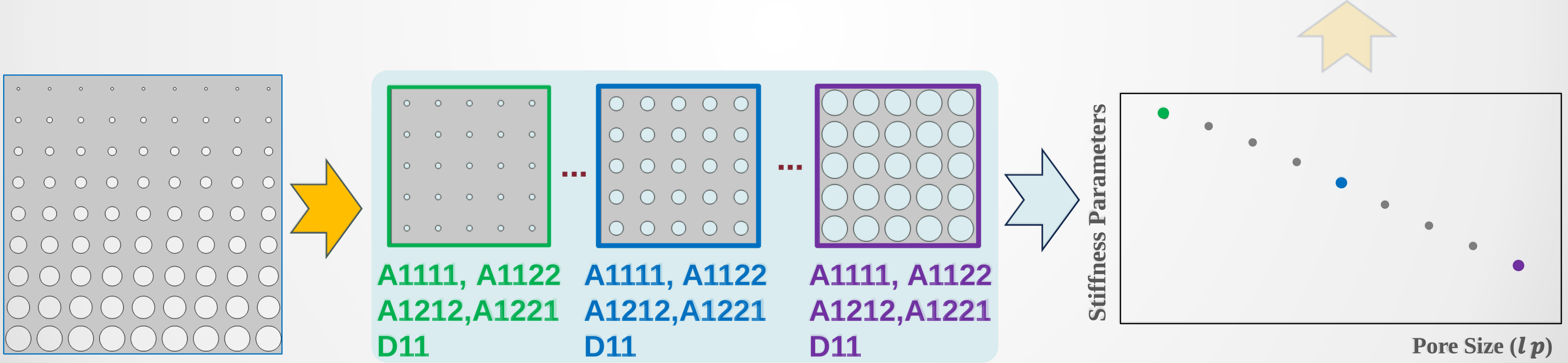




Methodology
Extending the Homogenization Procedure for FG Porous Structures

- Pore sizes are changed to find the required equivalent parameters for each section of the FG porous structure.





Methodology

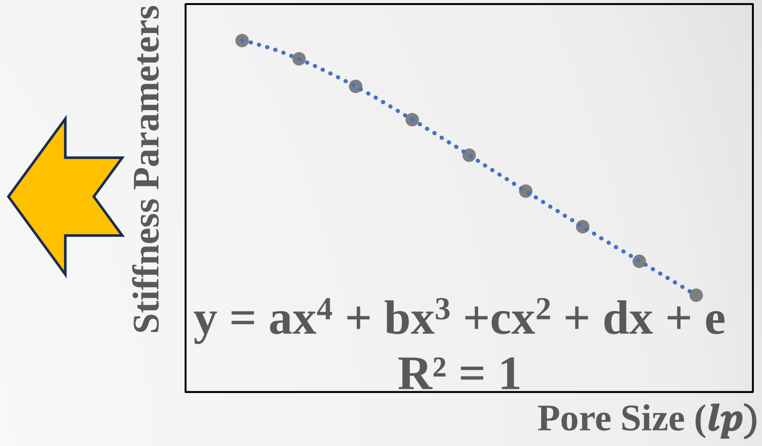
Extending the Homogenization Procedure for FG Porous Structures

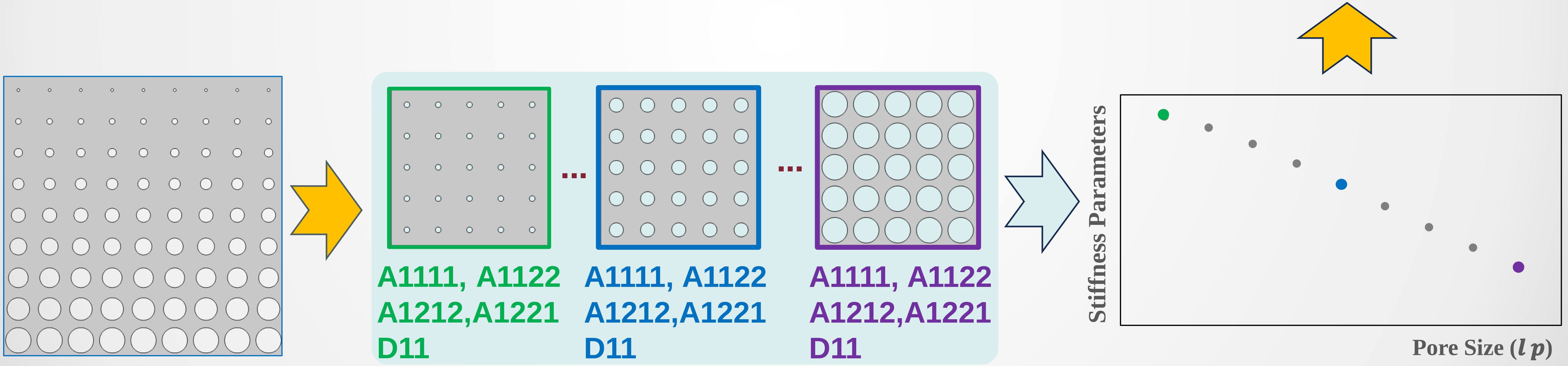
- These data are then utilised to find curve-fitted functions for each material parameter with respect to the pore size.

$$A1111 = f_1(l_p)$$

$$A1122 = f_2(l_p)$$

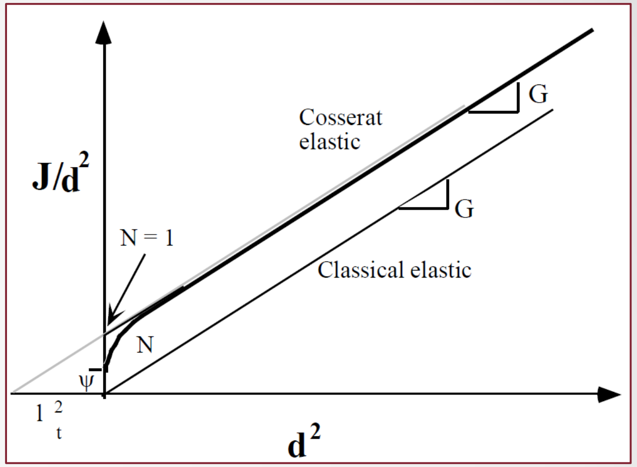
$$\cdots$$



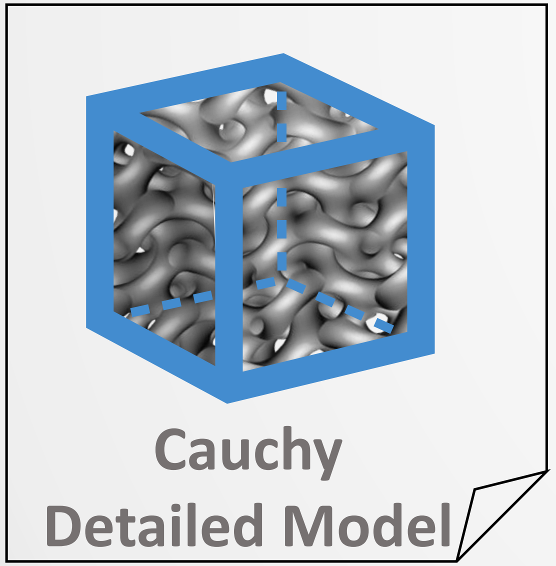


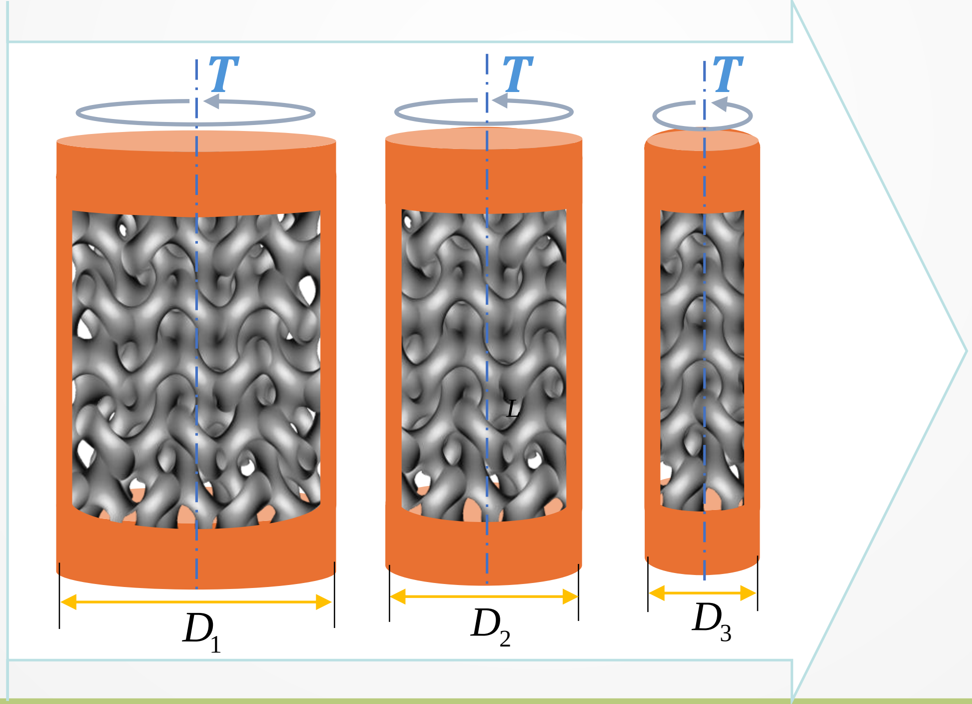
Methodology
Homogenization of 3D Model

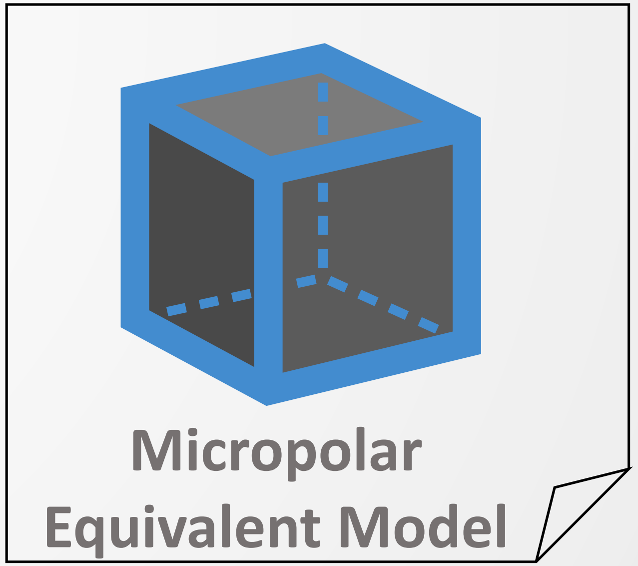
d: Diameter
J: Rigidity



- A size-effect is predicted by micropolar theory for the torsion of circular cylinders.
- It is possible to determine the micropolar parameters by measuring the torsional rigidity vs size.
- Specimens at different length scales, while keeping unit cell size constant.





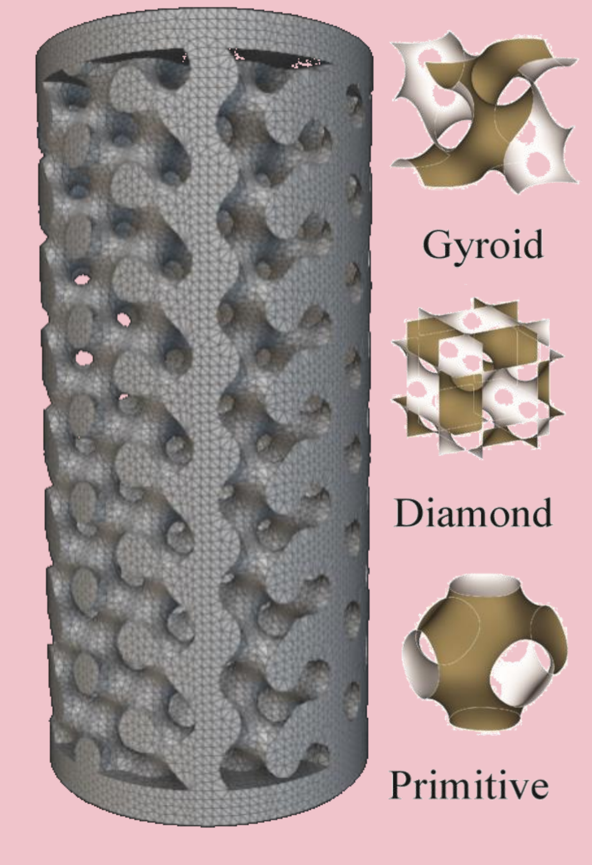


Methodology

Homogenization of 3D Model

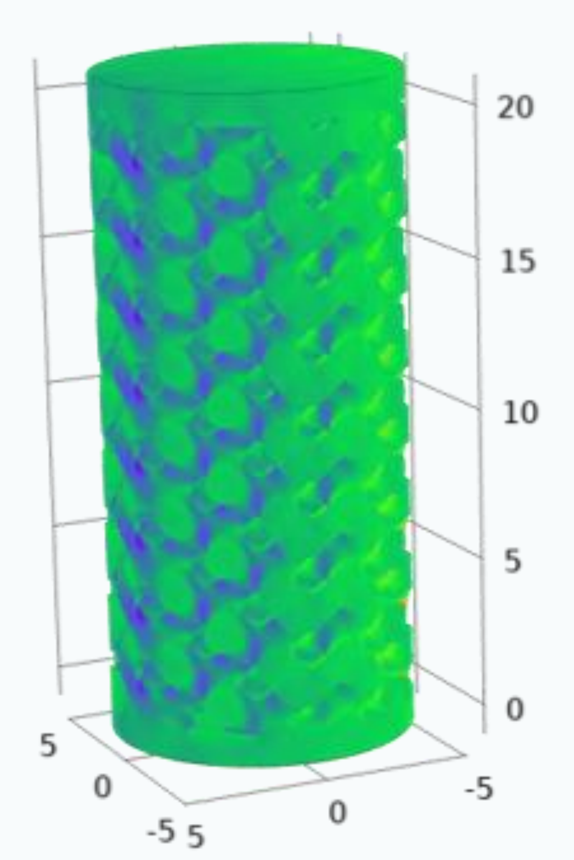
- Bio-inspired 3D microstructures such as gyroids and other Triply Periodic Minimal Surfaces (TPMS) can be employed for designing GBR bone scaffolds.
- Studying the impact of changes in microstructural architecture which reflects in the equivalent micropolar parameters.
- The unit cell design, porous structure and CAD model are developed using nTop software.
- Final 3D meshed part is imported in COMSOL for further FEM analyses.

nTop



CAD Model

COMSOL MULTIPHYSICS



FEM Tests

Methodology
FEM Micropolar Model in COMSOL Using PDE Weak Form

- Multiplying balance equations by the test functions, integrating over computational domain D

Balance Equations

Strong Form

$$\Sigma_{ij,i} + P_j = 0$$

$$M_{ij,i} - e_{ijk}\Sigma_{ik} + Q_j = 0$$

Weak Form

Test Function for **U**

$$\Rightarrow \int_D \Sigma_{ij,i} v_{U_j} + \int_D P_j v_{U_j} = 0$$

Test Function for ***Φ***

$$\Rightarrow \int_D M_{ij,i} v_{\Phi_j} - \int_D e_{ijk}\Sigma_{ik} v_{\Phi_j} + \int_D Q_j v_{\Phi_j} = 0$$

- Based on the product rule of derivatives:

$$\int_D \Sigma_{ij,i} v_{U_j} = \int_D \left(\Sigma_{ij} v_{U_j}\right)_{,i} - \int_D \left(\Sigma_{ij} v_{U_{j,i}}\right)$$

$$\int_D M_{ij,i} v_{\Phi_j} = \int_D \left(M_{ij} v_{\Phi_j}\right)_{,i} - \int_D \left(M_{ij} v_{\Phi_{j,i}}\right)$$

- And by using the divergence theorem:

$$-\int_D \Sigma_{ij} v_{U_{j,i}} + \int_B \Sigma_{ij} v_{U_j} n_i + \int_D P_j v_{U_j} = 0$$

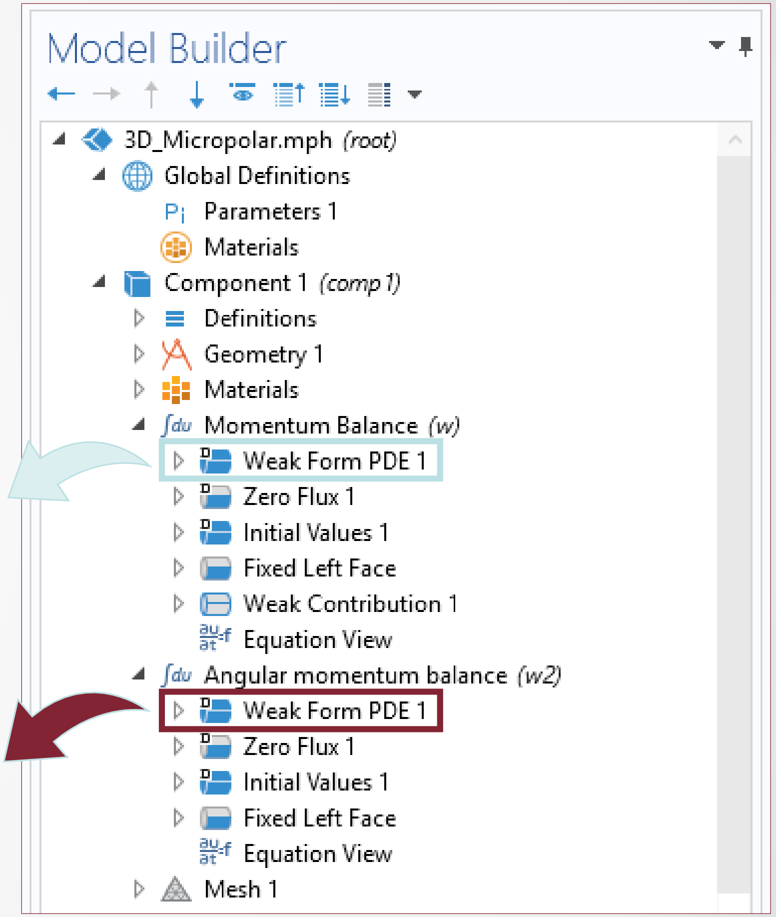
$$-\int_D M_{ij} v_{\Phi_{j,i}} + \int_B M_{ij} v_{\Phi_j} n_i - \int_D e_{ijk}\Sigma_{ik} v_{\Phi_j} + \int_D Q_j v_{\Phi_j} = 0$$

Methodology
FEM Micropolar Model in COMSOL Using PDE Weak Form

- By using partial differential equation (PDE) modelling in COMSOL instead of traditional FE modelling, no user subroutine is required.
- Various complex geometries, B.C., and loadings can be applied in a user-friendly graphical interface.
- Visualisation of the results is convenient.

```
-(s11*test(ux)+s12*test(uy)+s21*test(vx)+s22*test(vy)
+s23*test(vz)+s31*test(wx)+s32*test(wy)+s33*test(wz))
+ p1*test(u)+p2*test(v)+p3*test(w)
```

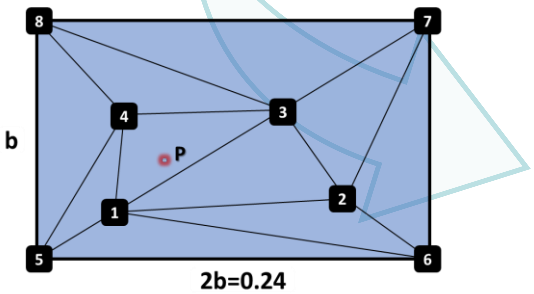
```
-(mu11*test(phi1x)+mu12*test(phi1y)+mu13*test(phi1z)
+mu21*test(phi2x)+mu22*test(phi2y)+mu23*test(phi2z)
+mu31*test(phi3x)+mu32*test(phi3y) + mu33*test(phi3z))
-((s12-s21)*test(phi3)+(s31-s13)*test(phi2)
+(s23-s32)*test(phi1))+q1*test(phi1)+q2*test(phi2)
+q3*test(phi3)
```

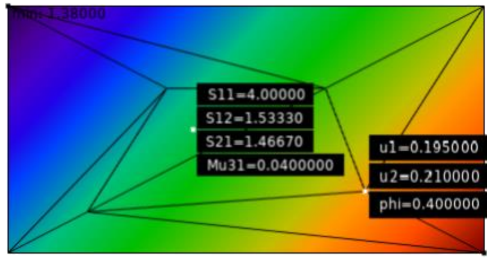


FEM Micropolar Model in COMSOL / Benchmarks for 2D Model

Patch Tests

- Test 1 (Cauchy)
- Test 2 (Micropolar, without Curvature)
- **Test 3** (Micropolar + Curvature)





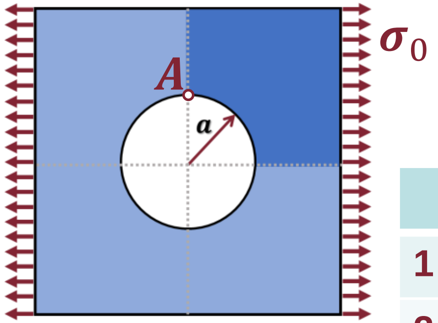
E. Providas, M.A. Kattis, 2002
DOI: 10.1016/S0045-7949(02)00262-6

	@	Benchmark	COMSOL
u1	P	0.1950	0.19500
u2	P	0.2100	0.21000
phi	P	0.0004	0.00040
S11	Node 2	4.0000	4.00000
S21	Node 2	1.4667	1.46670
Mu31	Node 2	0.0400	0.04000

Stress Concentration Factor

- Micropolar plate with a circular hole under uniform tension.
- Stress concentration factor (SCF) is compared with those of Reference.

M. Tuna et al., 2021
DOI: 10.1007/978-3-030-63050-8_11



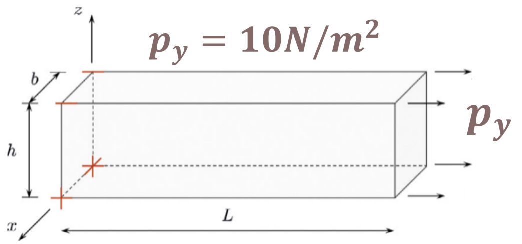
$$SCF = \frac{\sigma_{xx}@Point\ A}{\sigma_0}$$

	L / a	Element	Benchmark	COMSOL
1	3.0	4Node	2.49640	2.50110
2	3.0	9Node	2.42046	2.42128
3	10.0	4Node	2.28474	2.29980
4	10.0	9Node	2.22525	2.26834

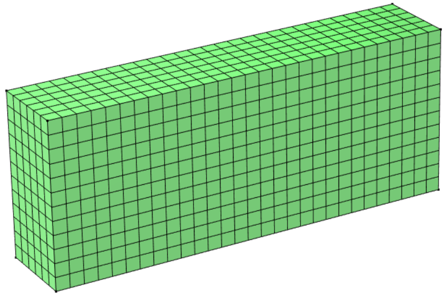
Methodology
FEM Micropolar Model in COMSOL / Benchmarks for 3D Model

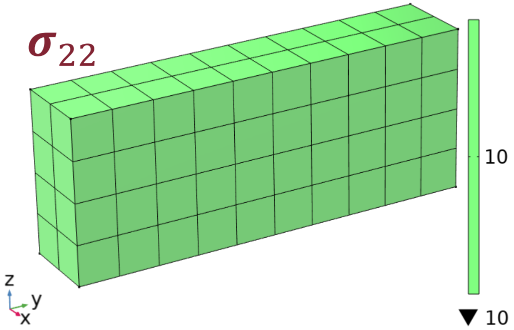
Force Patch Test

- Cantilever beam subject to pure tension
- Seeking the state of constant stress.
- For an arbitrary number of finite elements.



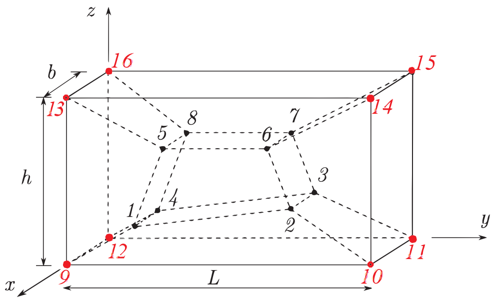
S. Grbčić et al., 2018
DOI:10.1016/j.compstruc.2018.04.005

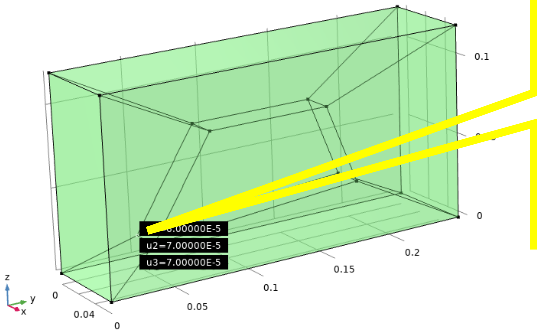




Displacement Patch Tests

- A generalization of 2D patch tests.
- Discretization with 7 arbitrarily distorted hexahedral finite elements.



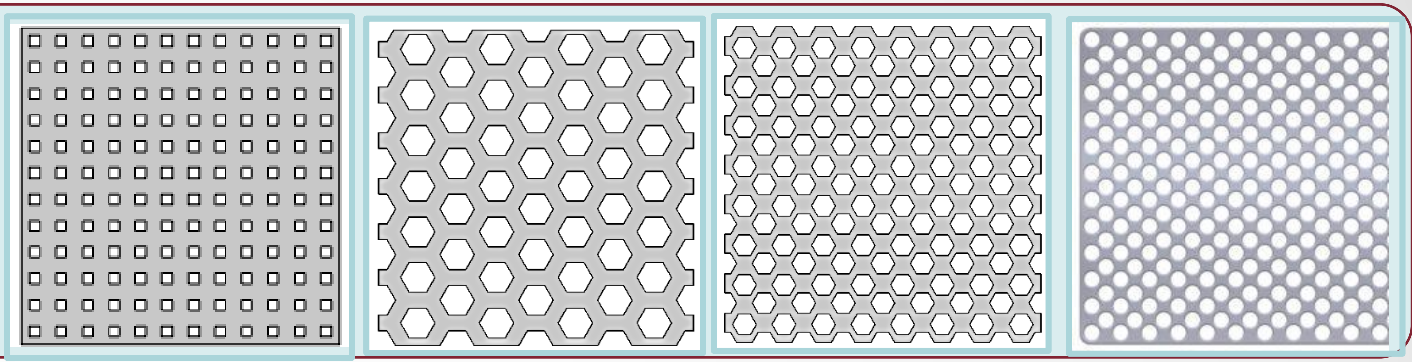


	Benchmark	COMSOL
u1($\times 10^{-4}$)	0.600	0.60000
u2($\times 10^{-4}$)	0.700	0.70000
u3($\times 10^{-4}$)	0.700	0.70000
phi1 ($\times 10^{-4}$)	2.100	2.10000
S11	5.000	5.00000
Mu11	0.020	0.02000
Mu12	-0.0400	-0.04000

Results
Parametric Study for Various Pore Patterns Using COMSOL

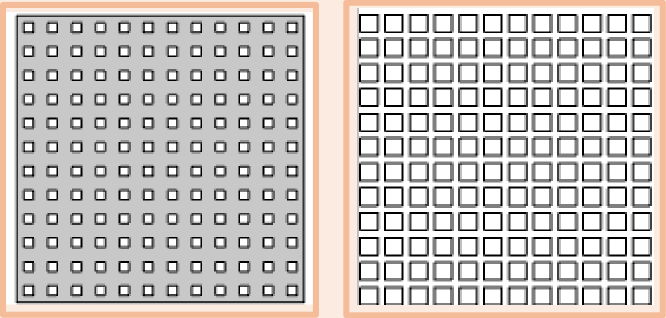
Pore Type & Pattern:

- Rectangular pores
- Honeycomb pattern
- Triangular pores, Honeycomb pattern



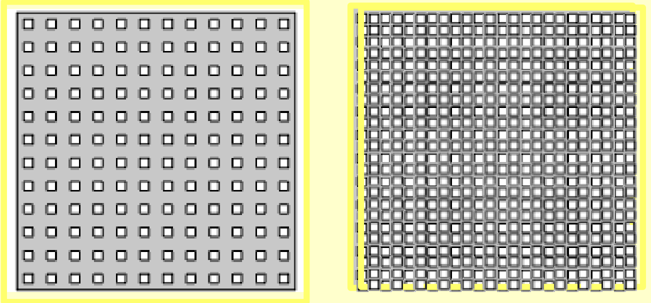
Pore Size:

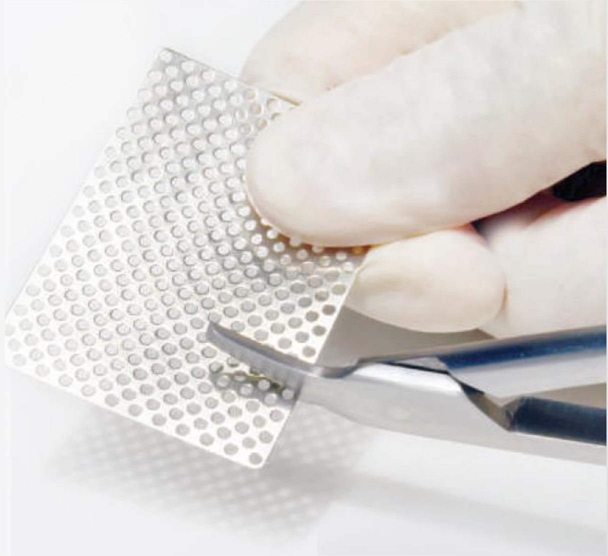
- Different length scale



Pore Density:

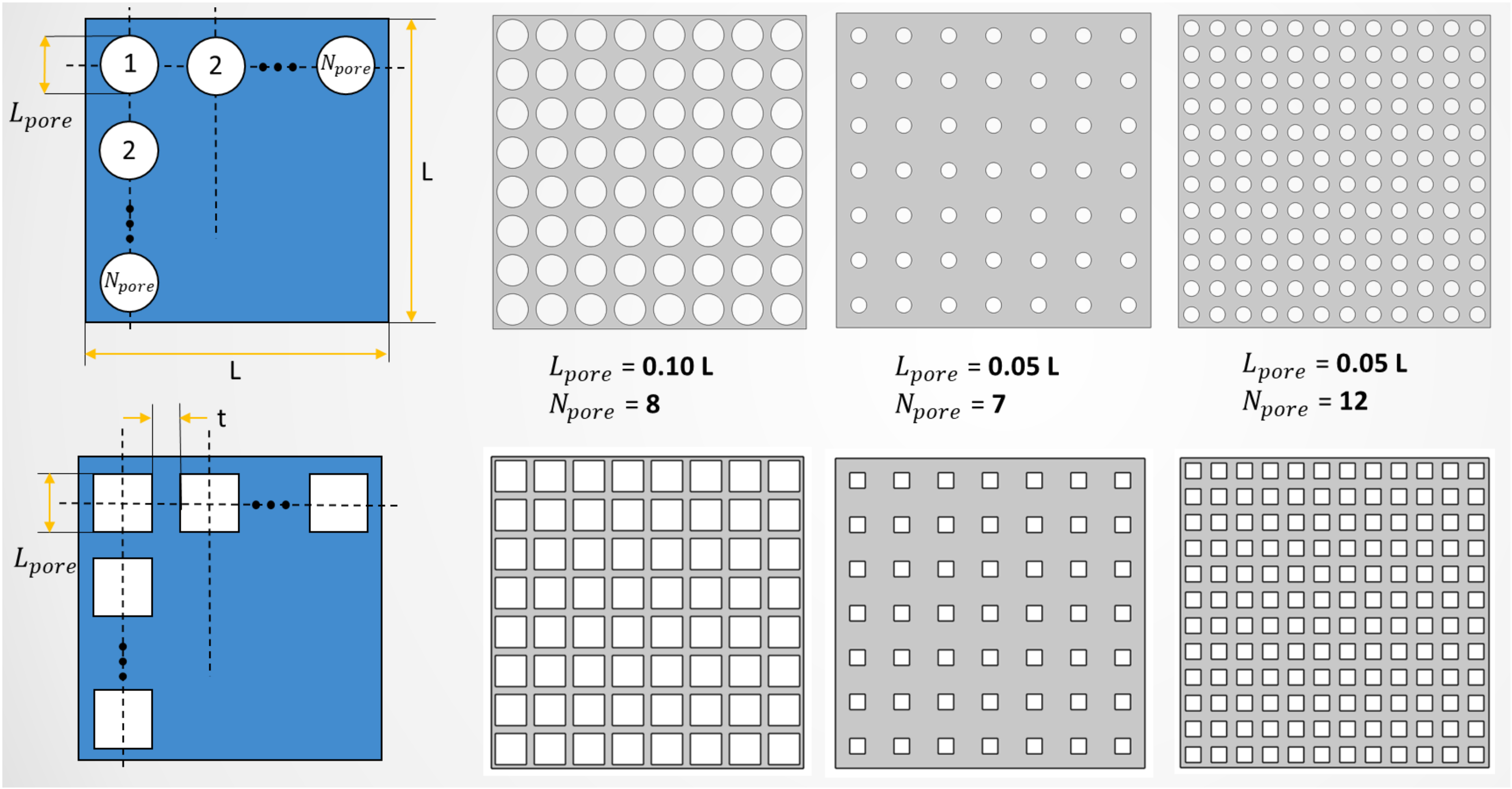
- Different No. of pores per length





Results

Parametric Study for Various Pore Patterns Using COMSOL / Parametrisation



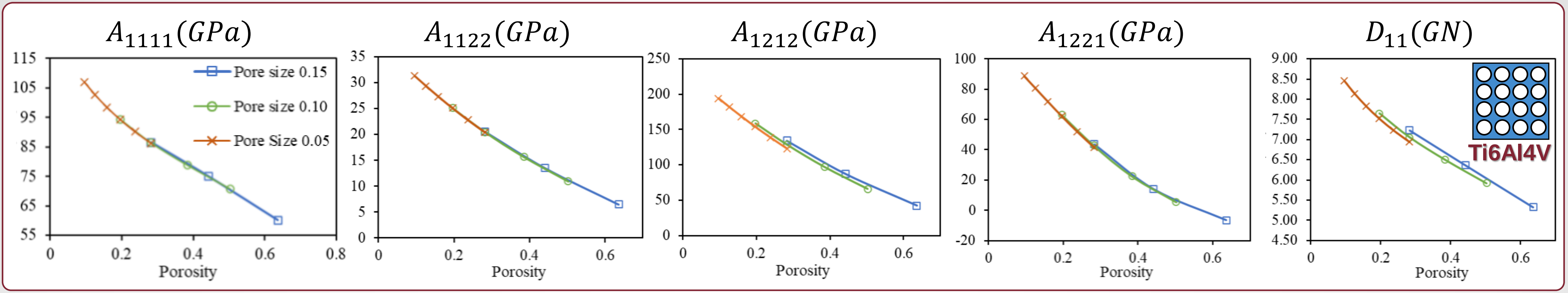
Titanium Alloy Ti6Al4V	Poly-Lactic Acid (PLA)
Young's Modulus, GPa	
114	1.03
Poisson Ratio	
0.30	0.32
Density, kg/m^3	
4500	1250

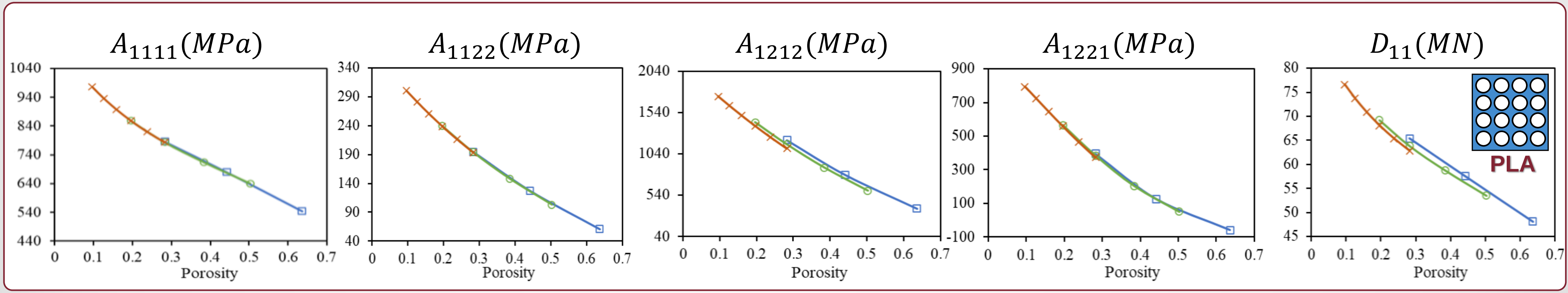
Mechanical Characterization of 3DPrinted Individualized Ti-Mesh for Alveolar Bone Defects L. Bai et al.

Physical and mechanical properties of PLA S. Farah et al.

Results

Parametric Study for Various Pore Patterns/Materials Using COMSOL



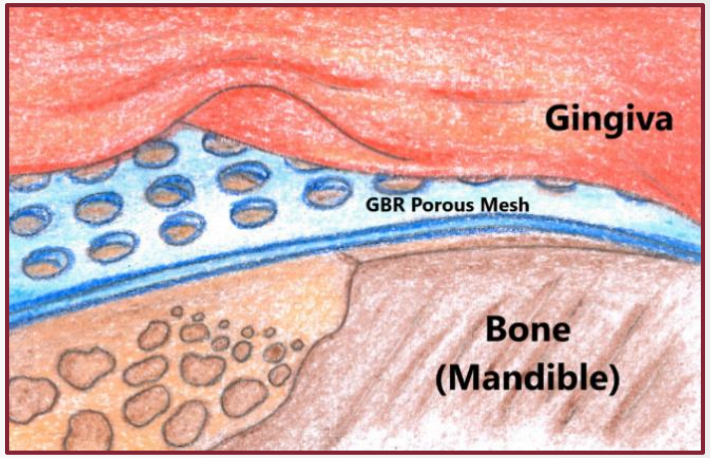


Discussion

Using the Equivalent Mechanical Parameters for Designing GBR Mesh

- Optimum Design for Porous GBR Meshes:
  Nearest mechanical properties to the bone.

- GBR mesh is in contact with the cortical (compact) bone.
- Try to make the material parameters of the GBR mesh consistent with its adjacent bone.
- Experimental estimate of the micropolar parameters of compact bone.
- Finding a configuration with the material parameters close to those reported for compact bone in the literature.



	Value	Unit
A_{1111}	12.00 ~ 43.43	GPa
A_{1122}	4.00	GPa
A_{1212}	21.10 ~ 36.77	GPa
A_{1221}	-13.05 ~ 2.67	GPa
D_{11}	3.24	kN

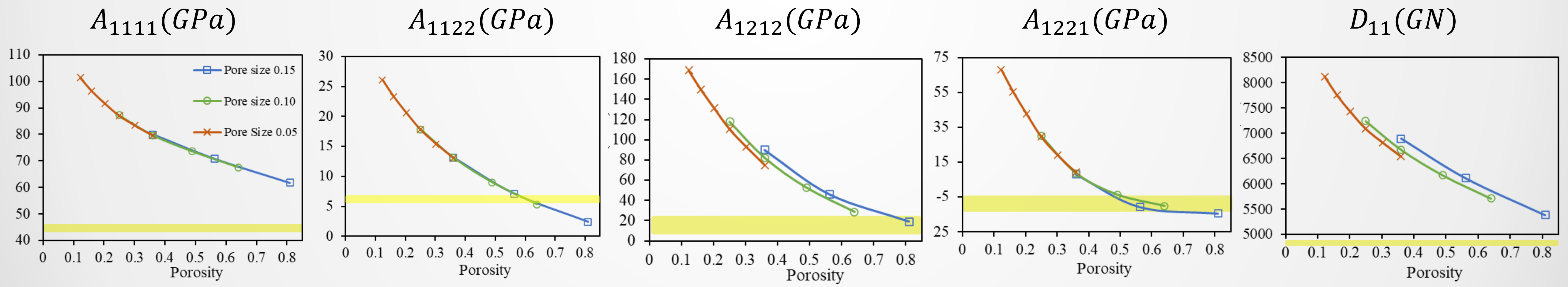
Experimental study of micropolar and couple stress elasticity in compact bone in bending J. Yang & R. Lakes

Discussion

Using the Equivalent Mechanical Parameters for Designing GBR Mesh

- Circular pores, Titanium Alloy
  → Parameters are beyond the required values.
- Rectangular pores, Titanium Alloy
  → Pore sizes of 0.13 L - 0.15 L and porosity about 0.7, a good agreement for A1122, A1212, A1221 can be achieved.

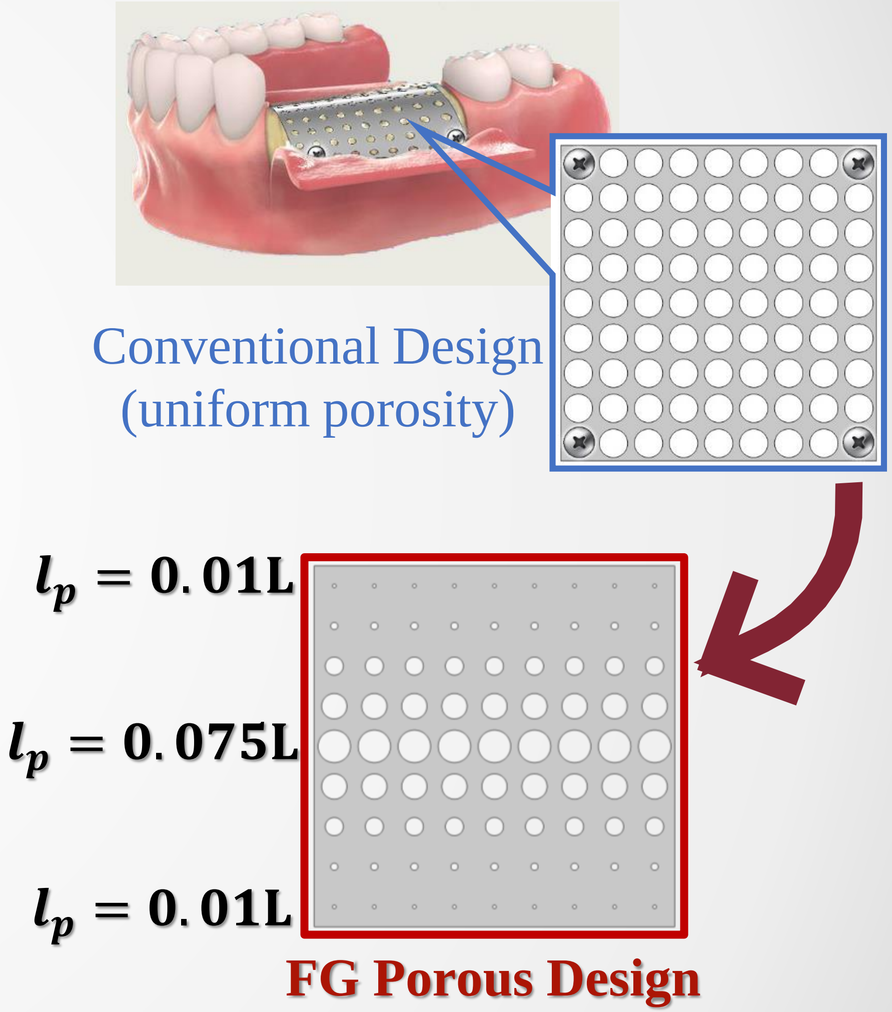
	Value	Unit
A_{1111}	12.00 ~ 43.43	GPa
A_{1122}	4.00	GPa
A_{1212}	21.10 ~ 36.77	GPa
A_{1221}	-13.05 ~ 2.67	GPa
D_{11}	3.24	kN



Discussion

Functionally Graded (FG) Porous Design for GBR Mesh

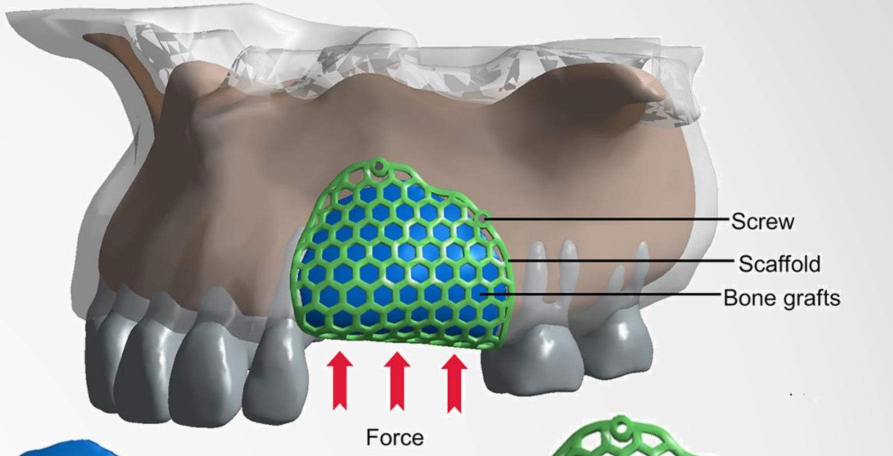
- GBR meshes are fixed to the mandible bone using biocompatible screws
- At these fixing locations higher stiffness is required. Therefore, smaller pore sizes are more desirable there.
- Mimicking natural FG structure of the bone
- FG structure of type O is suggested
- Central part → mechanical properties close to cancellous (trabecular) bone while providing a proper diffusion properties.
- Part near fixing areas → as near as possible to cortical (compact) bone to provide required load-bearing capacities.

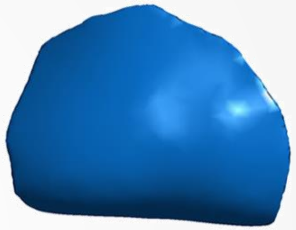


Discussion

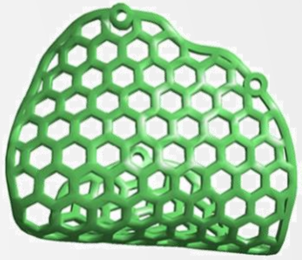
3D FG Design for Porous GBR Dental Scaffold

- Currently, metallic GBR sheets are used as a mechanical barrier and bone grafts are inserted into the space created by the barrier.
- After the healing period, it is necessary another surgery for removing the GBR mesh.
- To avoid a second surgery, a recent solution is to use biodegradable materials such as polylactic acid (PLA) instead of metallic meshes.
- However, suboptimal mechanical properties of biodegradable materials such as low stiffness and strength have limited their application.





Bone Grafts (Stimulating Bone Regeneration)



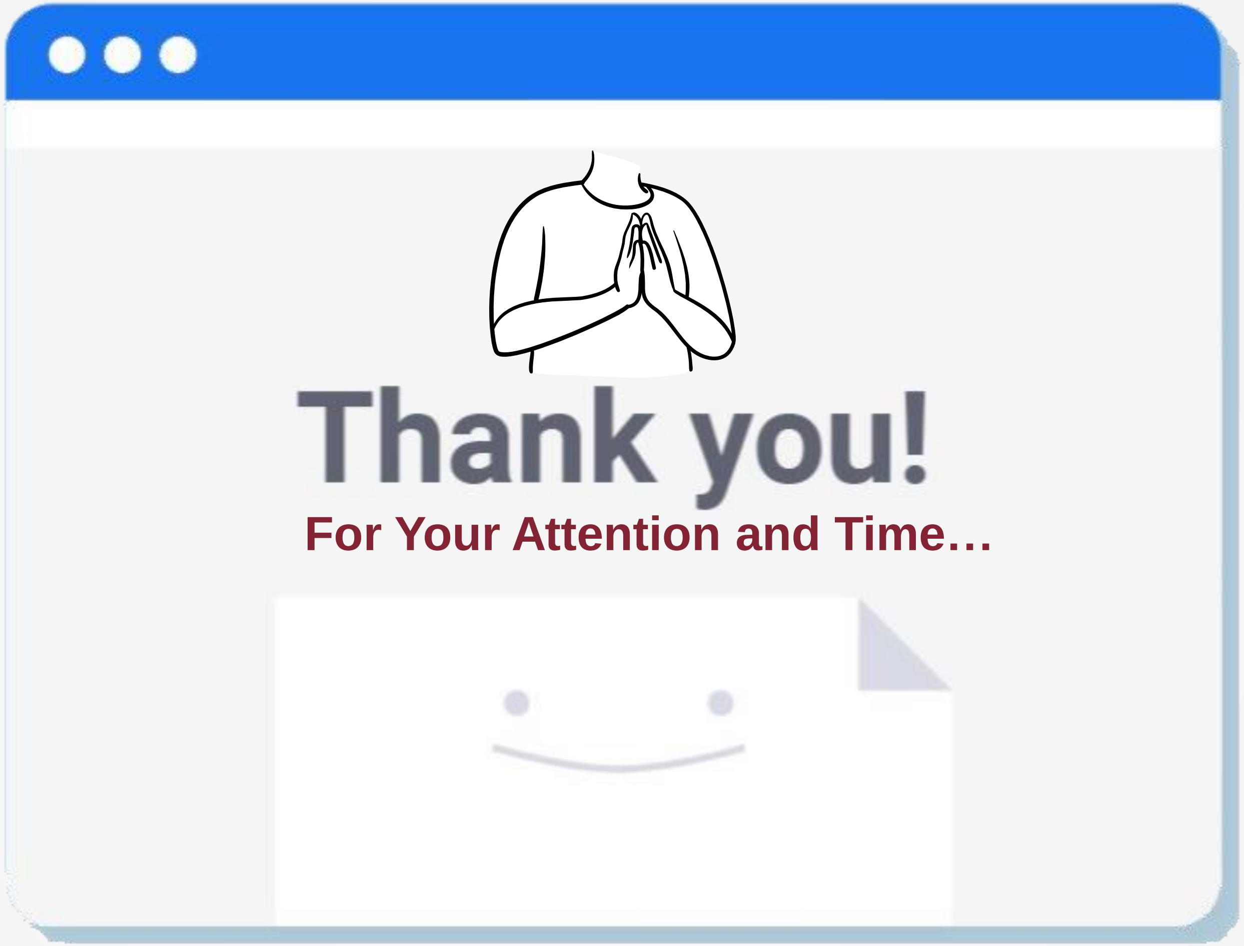
GBR Mesh (Space Maintaining)

3D GBR Dental Scaffold

Discussion
3D FG Design for Porous GBR Dental Scaffold

- With the developed framework, an innovative 3D design for GBR meshes is suggested.
- The microstructure evolves from the porous structure at the lower level to the compact structure at the top surface.
- The porous structure can host bio-active agents for stimulating bone regeneration
- While the upper compact surface should provide the required stiffness.
- By implementing our model, the distribution in both the internal structure and the material properties (for instance using bimodal material such as PLA+HA (Hydroxy appetite) or adding nano-reinforcements) can be customized.

3D Design
for
GBR Dental Scaffold



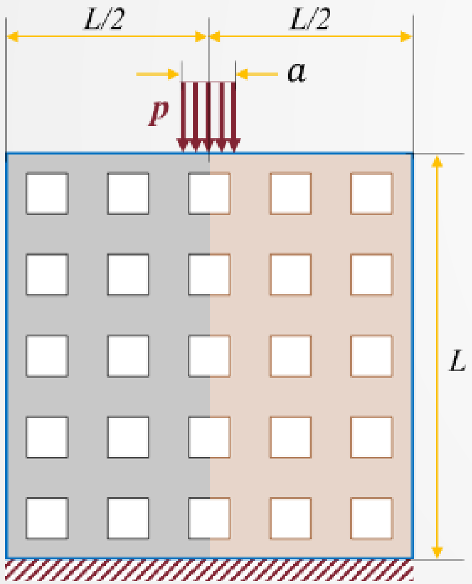
For Your Attention and Time…

Questions

Results

Effectiveness of Homogenized Micropolar Model

- Comparison of displacement magnitude contours for detailed and homogenized micropolar model.
- Indentation Test.
- Predicted values are close to those of the detailed model



$p = 10\,000$

$L = 1$

$a = L/10$

$l_p = 0.05$

$N_p = 12$