Elastic Wave Propagation and Heat Diffusion Studies in Polycrystalline Material

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Introduction

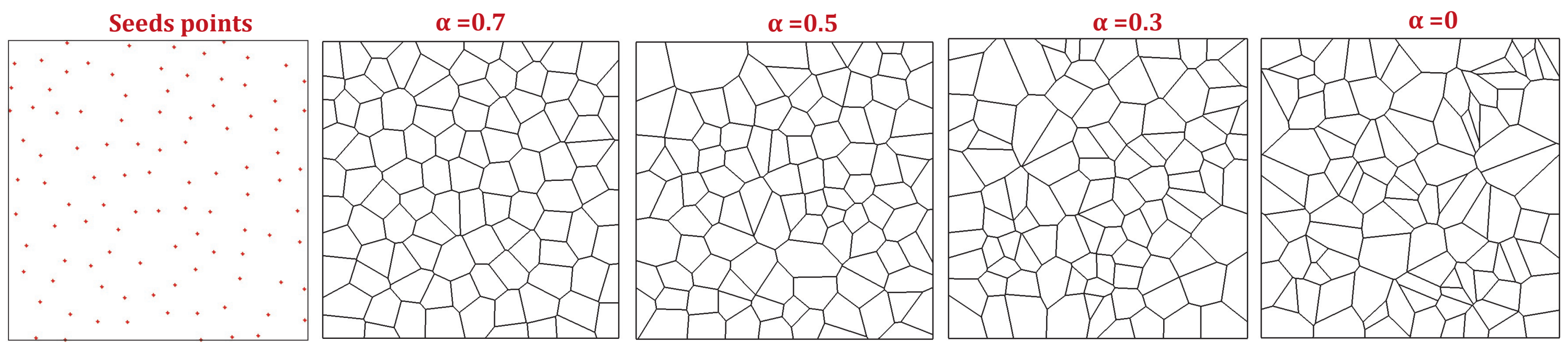
- The heterogeneous nature of materials at a certain scale has a significant impact on the macroscopic behaviour of multi-phase materials
- The physics and mechanics of the underlying microstructure are responsible for the various phenomena occurring in the macroscopic level
- Overall behaviour of micro-heterogeneous materials depends strongly on the size, shape, spatial distribution and properties of the microstructural constituents and their respective interfaces

Objective

- Develop a 2D model of the polycrystalline material explicitly using finite element method
- Implement methodologies for generating regularities in grains size and incorporating crystallographic orientation
- Study elastic wave propagation and heat diffusion phenomena through the polycrystalline material

Methodology

Microstructure Generation : Controlled Voronoi Tessellation[1]



⇒Distance d_0 between any two adjacent nuclei is a constant : $\boxed{do = \left(\frac{2Ao}{n3^{1/2}}\right)^{1/2}}$ *n = number of cells required*

⇒The parameter α used to quantify the regularity of a 2D Voronoi tessellation : $\boxed{\alpha = \frac{\delta}{do}}$

Modelling Orientational Disorder

Elastic Anisotropy

The transformation of stiffness constants for a cubic crystal by clockwise rotation of coordinates through an angle ξ about z-axis[2]

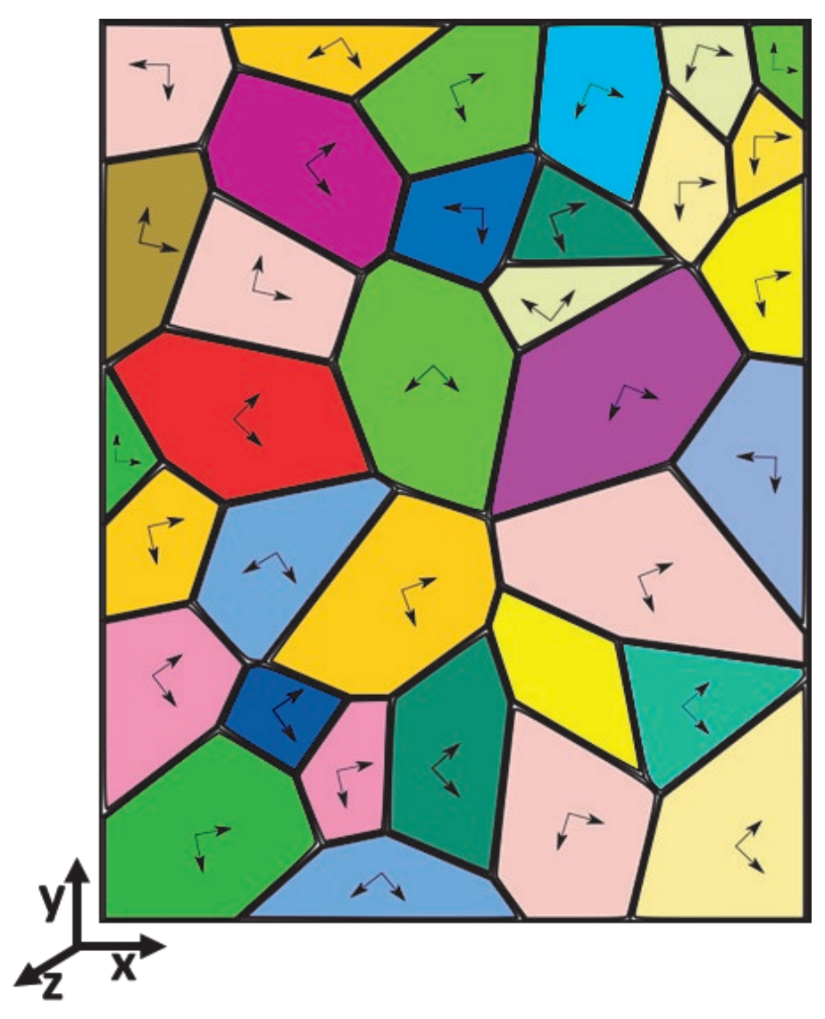
Stiffness Transformation Matrix $[c'] = [M][c][\overline{M}]$

Stiffness Matrix

$$[c]=\begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ 0 & C_{11} & C_{12} & 0 & 0 & 0 \\ 0 & 0 & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix}$$

Bond Transformation Matrix

$$[M]=\begin{bmatrix} \cos^2\xi & \sin^2\xi & 0 & 0 & 0 & \sin2\xi \\ \sin^2\xi & \cos^2\xi & 0 & 0 & 0 & -\sin2\xi \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \cos\xi & -\sin\xi & 0 \\ 0 & 0 & 0 & \sin\xi & \cos\xi & 0 \\ -\frac{\sin2\xi}{2} & \frac{\sin2\xi}{2} & 0 & 0 & 0 & \cos2\xi \end{bmatrix}$$



Thermal Anisotropy

A random field texture is considered, with grain orientation as variable. The property tensor calculation based on the global coordinate system

Global Thermal Conductivity Matrix $K_G = RK_LR^T$

Local Thermal Conductivity Matrix

$$[K_L]=\begin{bmatrix} K_{11} & 0 \\ 0 & K_{22} \end{bmatrix}$$

Transformation Matrix

$$[R]=\begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}$$

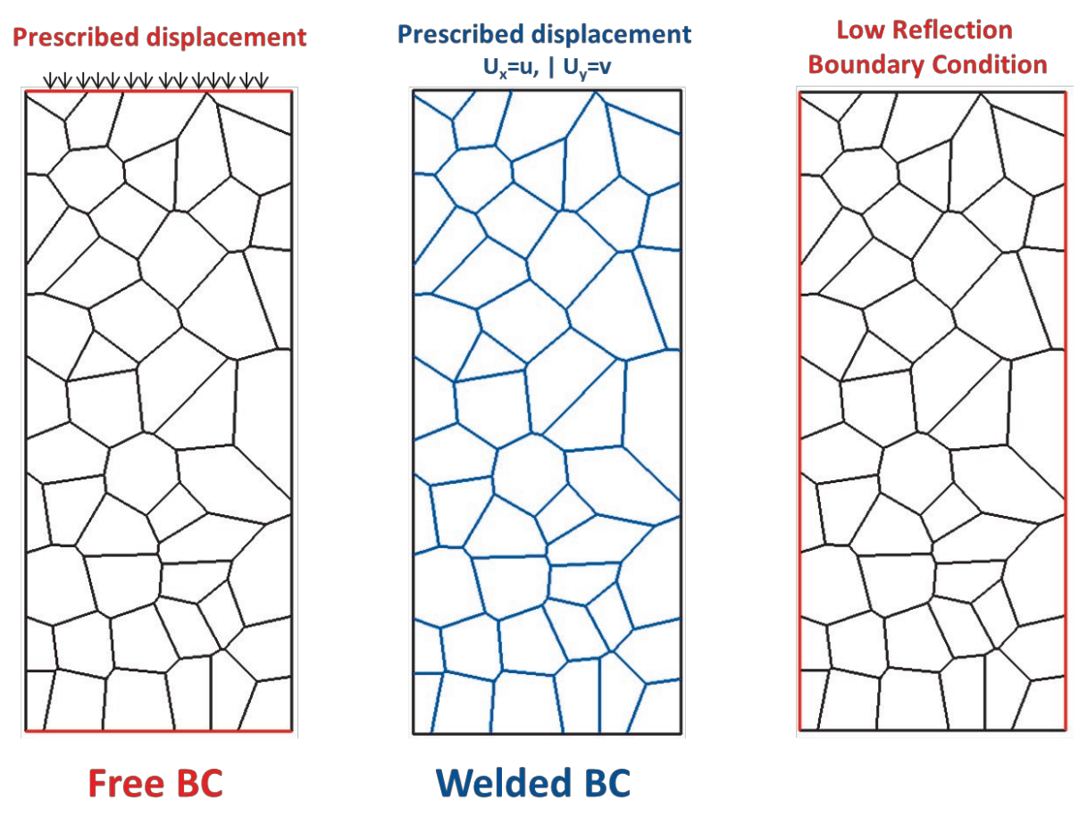
Modelling Elastic Wave propagation/Heat diffusion in anisotropic medium

Material property assignment

(i) Physics Node assignment Method : In this method, single domain material properties are assigned by invoking new physics node for each domain

(ii) Interpolation Method : Here, individual domain properties are described using a interpolation function and the material properties are invoked using concerned domain index number

Modelling Parameters : Elastic Wave Propagation[3]



Modelling Parameters

Products : COMSOL™ and Livelink™ for MATLAB™

Model Geometry : 12.5X30mm | Mesh Element: Triangular | Mesh Size : 2.33e^{-4}m (λ/10) | Step time : 1e^{-8} sec

Material Properties: Copper: Density : 8930 kg/m^3 | C_{11}=16.8e10 N/m^2 | C_{12}=12.1e10 N/m^2 | C_{44}=7.5e10 N/m^2

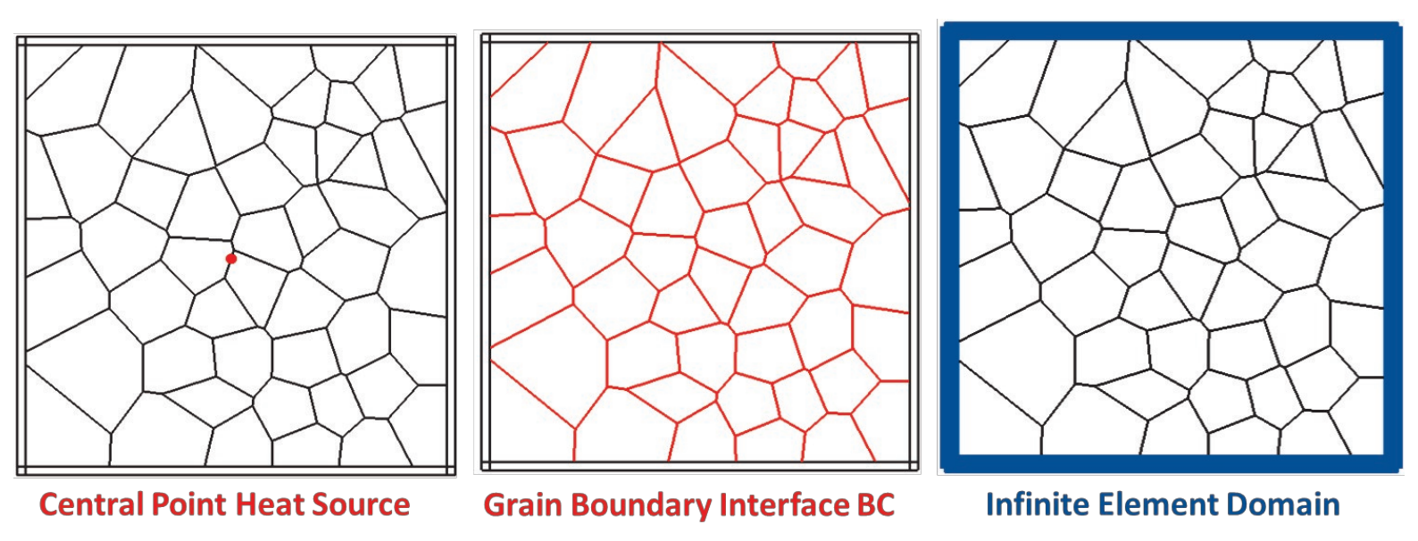
Physics : Structural Mechanics Module

Input Excitation : 1MHz,3 Cycle Hanning Pulse

Interface Boundary conditions : Displacement continuous BC (Welded BC)

Solver : MUMPS or PARADISO (for cluster)

Heat Diffusion[4]



Modelling Parameters

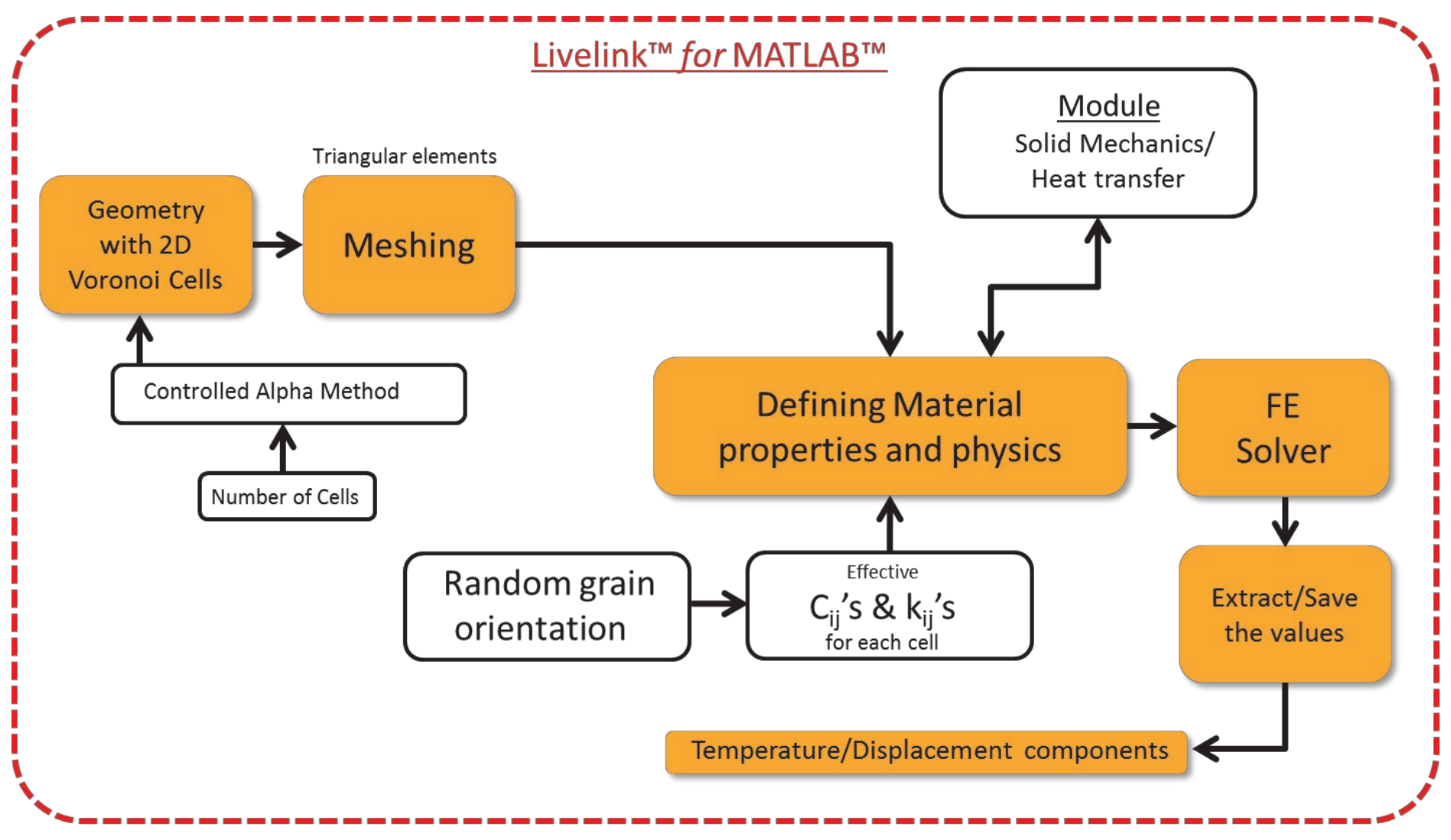
Products : COMSOL™ and Livelink™ for MATLAB™

Model Geometry : 50X50mm | Mesh Element: Triangular | Mesh Size : 10e^{-4}m | Step time : 0.01 sec

Material Properties: Alumina: Density : 3900 kg/m^3 | Specific Heat=775 J/kgK | Thermal Conductivity K_x=20.78 W/mK | K_y=16.77 W/mK

Interface Boundary conditions : (i) Heat flux continuity (ii) Thin thermally resistive layer (iii) Highly conductive layer

Physics : Heat transfer Module | Solver : PARADISO



Livelink™ *for* MATLAB™

Geometry with 2D Voronoi Cells → Meshing (Triangular elements)

Number of Cells → Controlled Alpha Method → Geometry with 2D Voronoi Cells

Meshing → Defining Material properties and physics

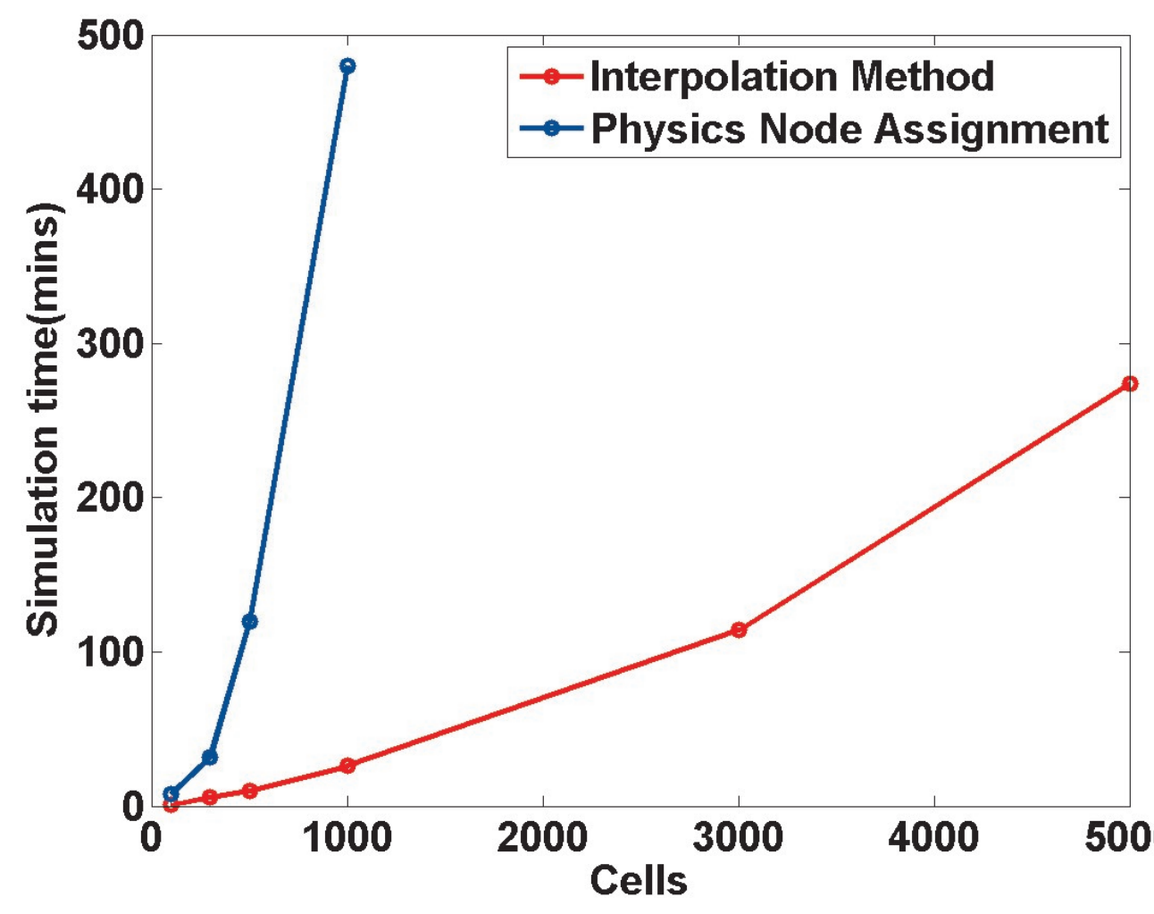
Module: Solid Mechanics/ Heat transfer ↔ Defining Material properties and physics

Random grain orientation → Effective C_{ij}'s & k_{ij}'s for each cell → Defining Material properties and physics

Defining Material properties and physics → FE Solver → Extract/Save the values → Temperature/Displacement components

Running in loop by varying the geometry and grain orientation

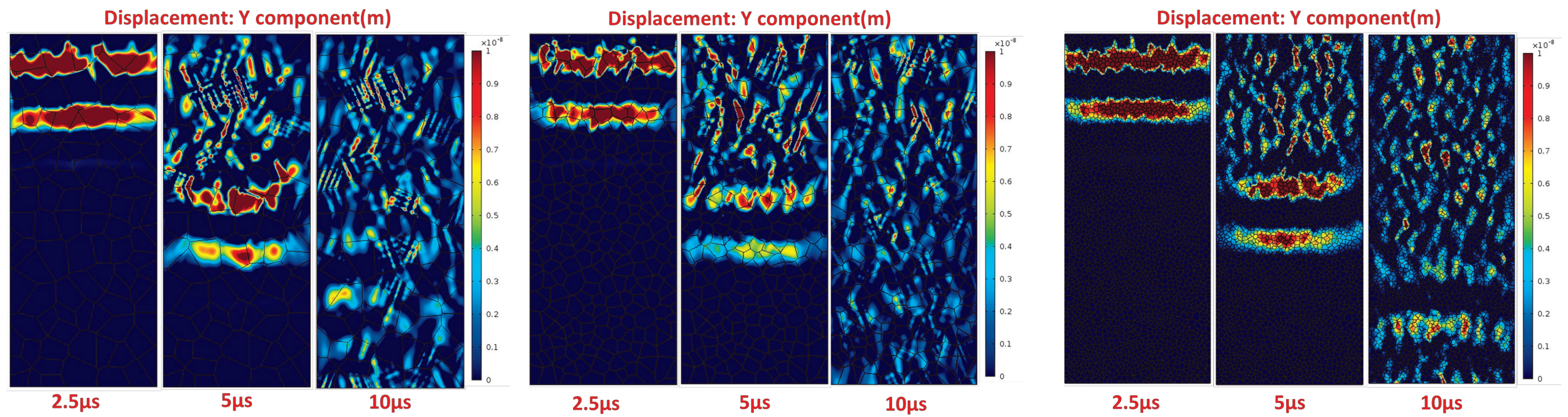
Modelling flowchart showing the sequence of operation implemented for wave propagation and heat diffusion studies in polycrystalline medium



Comparison of simulation time for Interpolation method and Physics node assignment with increasing cell number

Results:Visualization

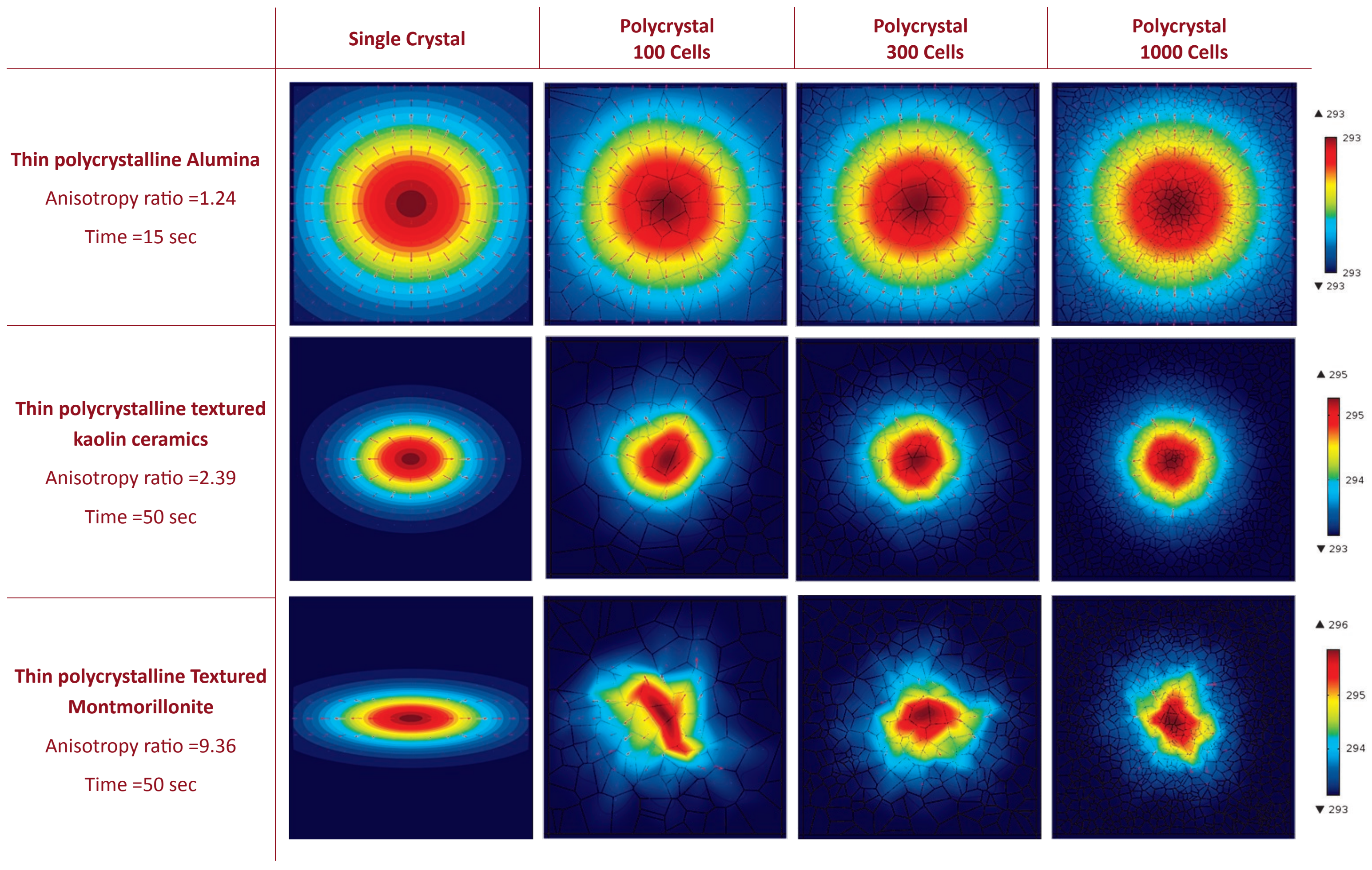
Elastic Wave Propagation



100 cells 300 cells 3000 cells

Visualization for elastic wave propagation through grains for increasing number of cells at various time steps

Heat diffusion



Summary and Future work

- A 2D finite element model based on Voronoi tessellation was developed for studying the transport phenomena through microstructural features.
- Implementation of Interpolation method for assigning material properties reduced the simulation time drastically and also permitting to achieve higher number of cells.
- The developed tool can be now extended for studying the effects of anisotropy, role of cell size distribution on elastic wave propagation and heat diffusion phenomena.
- Future work also involves, developing methodologies for generating realistic microstructure for numerical studies.
- Investigation of computational issues for extending the work towards three dimensional grains

References

[1]Zhu, H. X., S. M. Thorpe, and A. H. Windle. "The geometrical properties of irregular two-dimensional Voronoi tessellations." *Philosophical Magazine A*81.12 (2001): 2765-2783.

[2]B.A. Auld, *Acoustic Fields and Waves in Solids*,Wiley-Interscience,(1973)

[3]S Shivaprasad, Krishnan Balasubramaniam and CV Krishnamurthy, "Voronoi based microstructure modelling for Elastic wave propagation", Proceedings of the 41st Annual Review of Progress in Quantitative Non-destructive Evaluation,2015,Minneapolis,USA.

[4]Sreedhar Unnikrishnakurup, CV Krishnamurthy and Krishnan Balasubramaniam ,"Heat Diffusion in Polycrystalline Materials - A Microstructure based Material Model", Proceedings of the Quantitative Infrared Thermography- Asia,2015,Chennai,India.

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