Poly – Xtal Operations V9.04

A MATLAB based code base to generate Eulerian space partitioning

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Presentation to IP commercialization team requesting funding to support further development

FUNDING PROPOSAL REJECTED AS UNI DISINTERESTED IN NON-COMMERCIALIZEABLE PRODUCT

29 October 2020

About

- Free MATLAB codebase for researchers working on computational materials science, computational geology, dynamics of importance sampling Monte-Carlo schemes and graphenes, and kinetic spatiotemporal partitioning of Eulerian space.

- Make spatiotemporally gradient 2D grain structures and associate spatiotemporally gradient crystallographic texture to the grain structure

- Export ABAQUS input file for use in CPFEM

- Work with Ising model and Q-state Pott's model simulation on square lattices

Grain structures in real life and that obtained by Poly-XTAL operations

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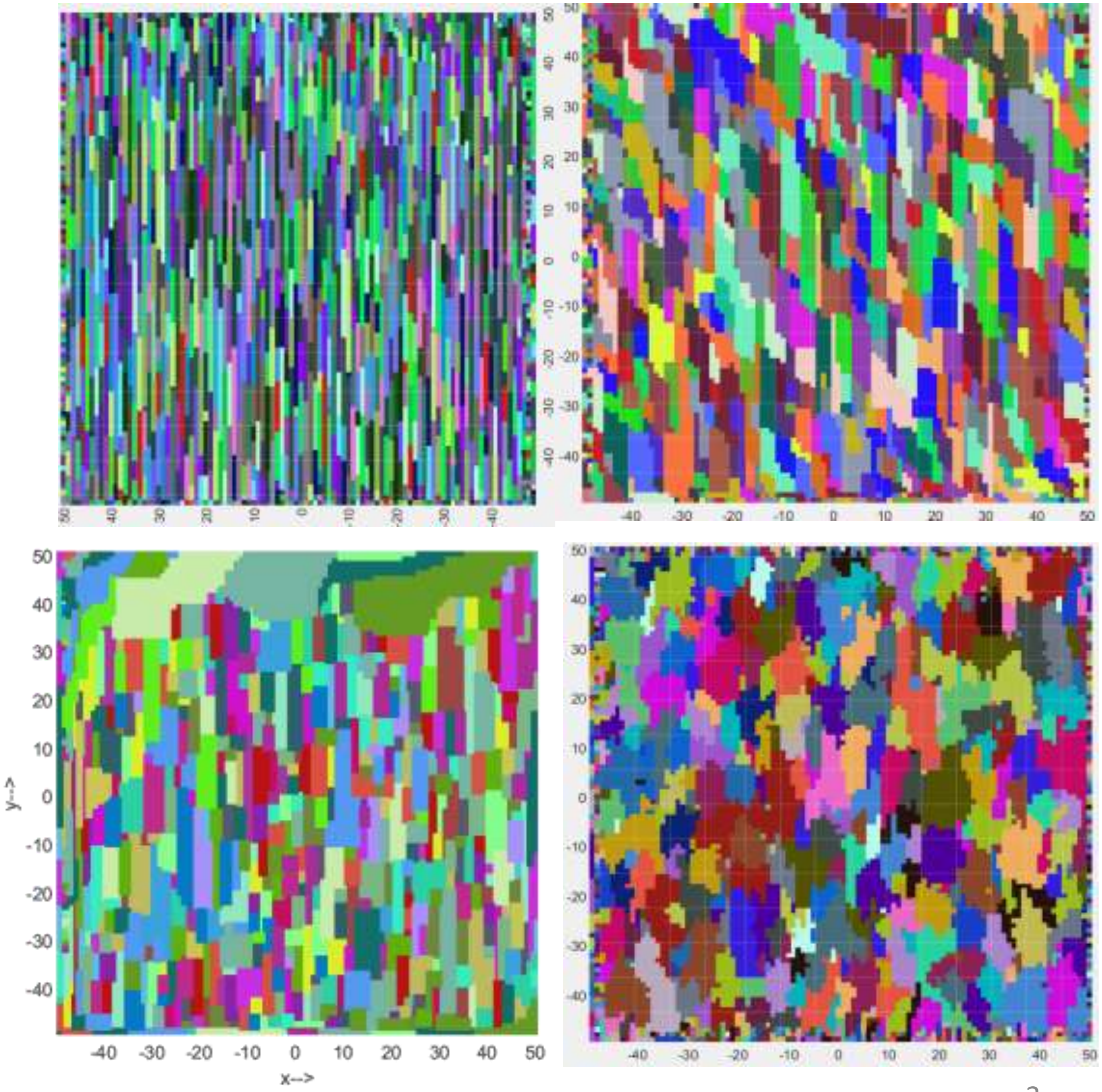


Development history

The 1st version to generate grain structures was written by me in 2010 in the department of mechanical engineering at PESIT, Bengaluru, India based on the basic explanations of Ising model and grain growth kinetics by Dr. Kishore T Kashyap when employed as Junior Research Fellow. Available online since 2012 at:

(1) https://www.mathworks.com/matlabcentral/fileexchange/34784-monte-carlo-simulation-of-two-dimensional-grain-growth-code-version-no-1-basic?s_tid=prof_contriblnk

(2) https://www.mathworks.com/matlabcentral/fileexchange/34985-monte-carlo-simulation-of-three-dimensional-grain-growth-code-version-no-1-basic?s_tid=prof_contriblnk. https://www.youtube.com/watch?v=FvlxVgXlbTI).

2nd to 7th version were written during 2013 – 2014 in the department of aerospace engineering at Indian Institute of Science for my master's project under the guidance of Dr. G Narayana Naik (IISc) and Dr. N G Subramania Udupa (NCET). Codes for finite element analysis were written here. 8th version was written during 2015 – 2016 in the department of mechanical engineering at PES University, with the technical inputs of Dr. Suneel Motru on grain boundary bridging.

Version 9 and above were written over the course of this PhD.

Universities/Institutions previously collaborated with

Dr. Suneel Motru (Ex-Colleague. Grain boundary bridging)

Associate professor, Department of Mechanical Engineering, PESIT, BSK-3rd stage, Bengaluru, India – 560085. 2016-2017

Poly-XTAL Operations versions 8.0

Dr. G Narayana Naik (Master's thesis guide, co-developed molecular mechanics-FEA framework for graphene implemented in Poly-XTAL Operations in 2008)

Principal Research Scientist, Department of Aerospace Engineering, Indian Institute of Science, Bengaluru, India – 560015. 2012-2017

Poly-XTAL Operations versions 2.0-8.0

Dr. N G Subramania Udupa (Master's thesis guide. Modelling metal matrix composites)

Professor & Head of post-graduate studies (Rtd.), Department of Mechanical Engineering, NCET, Mudugurki Village, Venkatagiri Kote Post, Devanahalli, Bengaluru, India – 562164. 2012-2017

Poly-XTAL Operations versions 2.0-8.0

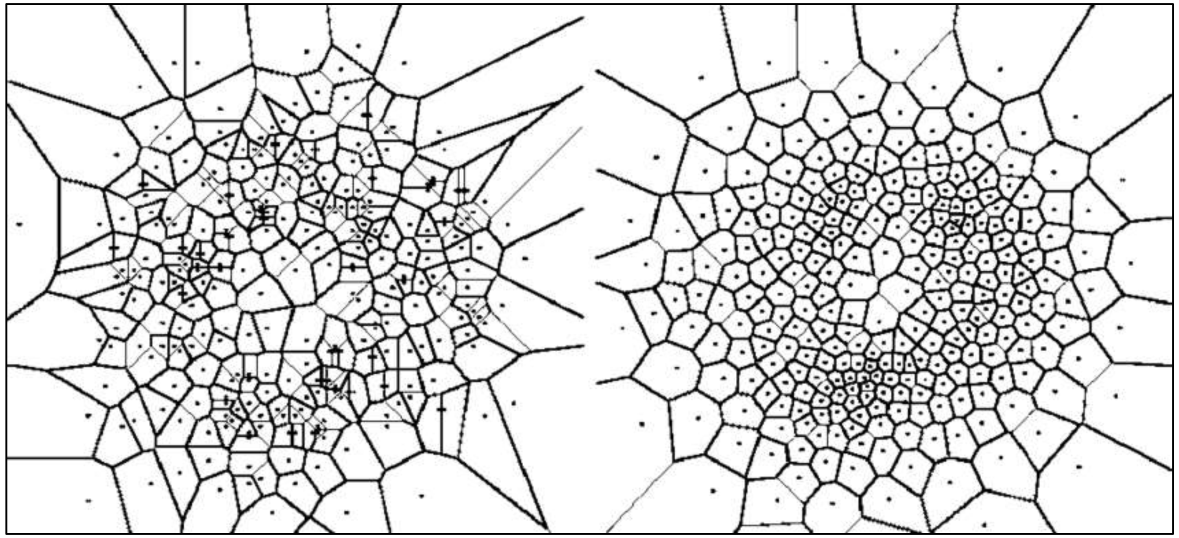
Dr. Kishore T Kashyap (Principal investigator and responsible for funding,)

Professor (Rtd.), Department of Mechanical Engineering, PESIT, BSK-3rd stage, Bengaluru, India – 560085. 2010

Poly-XTAL Operations versions 1.0

Applications: Mathematics

- Researchers are interested in the chaotic partitioning of a n-D bounded spatial domain and its spatiotemporal evolution under some governing rules.



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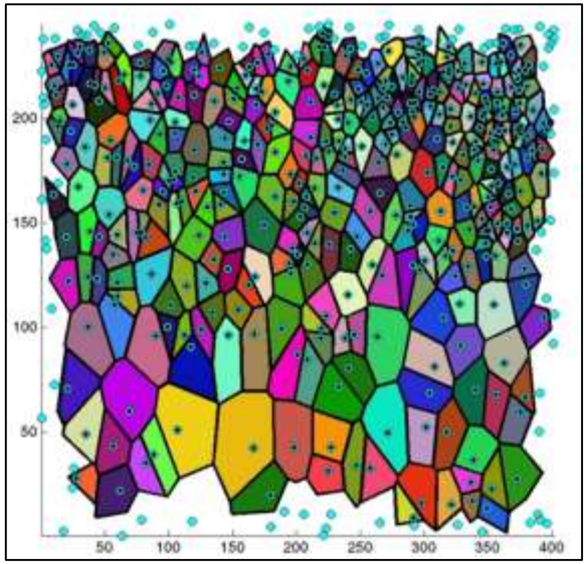

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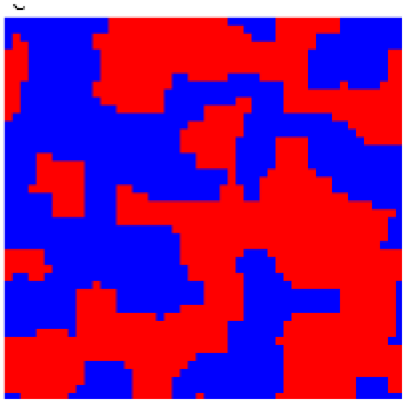
Applications: Statistical mechanics

- The 2nd example is from statistical mechanics, the very well-known Ising model of the importance sampling Monte-Carlo techniques studying the spatiotemporal evolution of the kinetics and thermodynamics of the distribution of two phases in a lattice.

- Exact solutions have been developed for such simple models involving 2 states, but for more complex models like the Q-state Pott's model, an exact model is impractical due to the vastness of the solution space.



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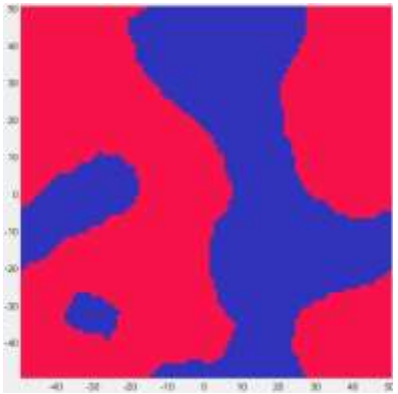

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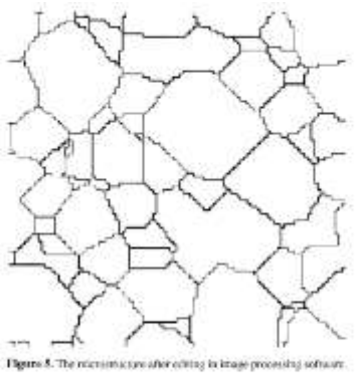
Applications: Fundamental materials science

- The 3rd example is from fundamental computational materials science where researchers are interested in grain growth, where the temporal evolution of the spatial and thermodynamical parameters of multi-phase grain structures is studies.
- A part of this research also touches upon understanding the kinematic and kinetic behaviour of insoluble 2nd phase particles in grain structures and how they interact with the grain boundaries.
- Some of these studies have tried to validate empirical models of grain structure geometry such as the Zener equation.
- As the shape of the particles influence the Zener drag working against grain boundary evolution during grain growth, and that nature presents irregularly shaped particles, computer models which can consider such particle shape and their spatial distribution becomes very essential.



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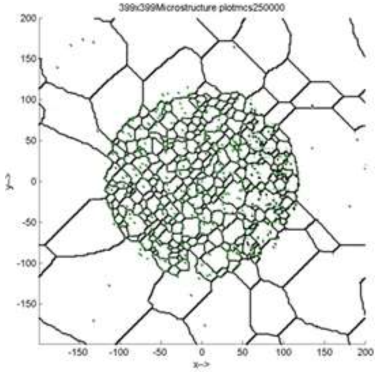

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Applications: Computational materials science

- The 4th example is from applied computational materials science where researchers need poly-crystalline grain structures to be used in techniques such as crystal plasticity based finite element analysis in order to study material’s phase-partitioned thermo-mechanical response and texture evolution under applied thermo-mechanical loads.

- Though Voronoi tessellated geometries of grain structures have been used before in crystal plasticity-based simulations, they are simplifications and do not accurately represent the geometric irregularities presented by nature.

Functionalities (V9.04)

1. Generate multi-phase 2D poly-crystalline grain structure. Ability to create:
    1. morphologically anisotropic grains
    2. spatially gradient grain morphologies in grain structure
2. Importance sampling Monte-Carlo on lattice to make realistic grains
    1. Ising model
    2. Q-state Potts model
3. Generate Voronoi equivalent of simulated and EBSD acquired grain structure
4. Consideration of following in grain growth simulation
    1. Artificial temperature gradients
    2. Spatiotemporal tracking of lattice energy
5. Grain identification and grain size statistics
6. Call MTEX libraries to:
    1. create spatial gradients in texture
    2. take advantage of its grain structure analysis routines native to MTEX
    3. carry out texture analysis
7. Export finite element mesh to ABAQUS input file for CPFEM studies using:
    1. in-built routines
    2. mtex2gmsh which uses gmsh

Capabilities

1. Store >10^7 temporal slices of grain structures on a 1000^2 square lattice

2. Study grain boundary pinning from point particles, fully packed and sparse particle clusters (regular), thin and thick whisker reinforcements and nanotubes

3. Achieve spatial gradients in 2D Voronoi grain structure

4. Domain reduction by sparsing and sub-domain extraction

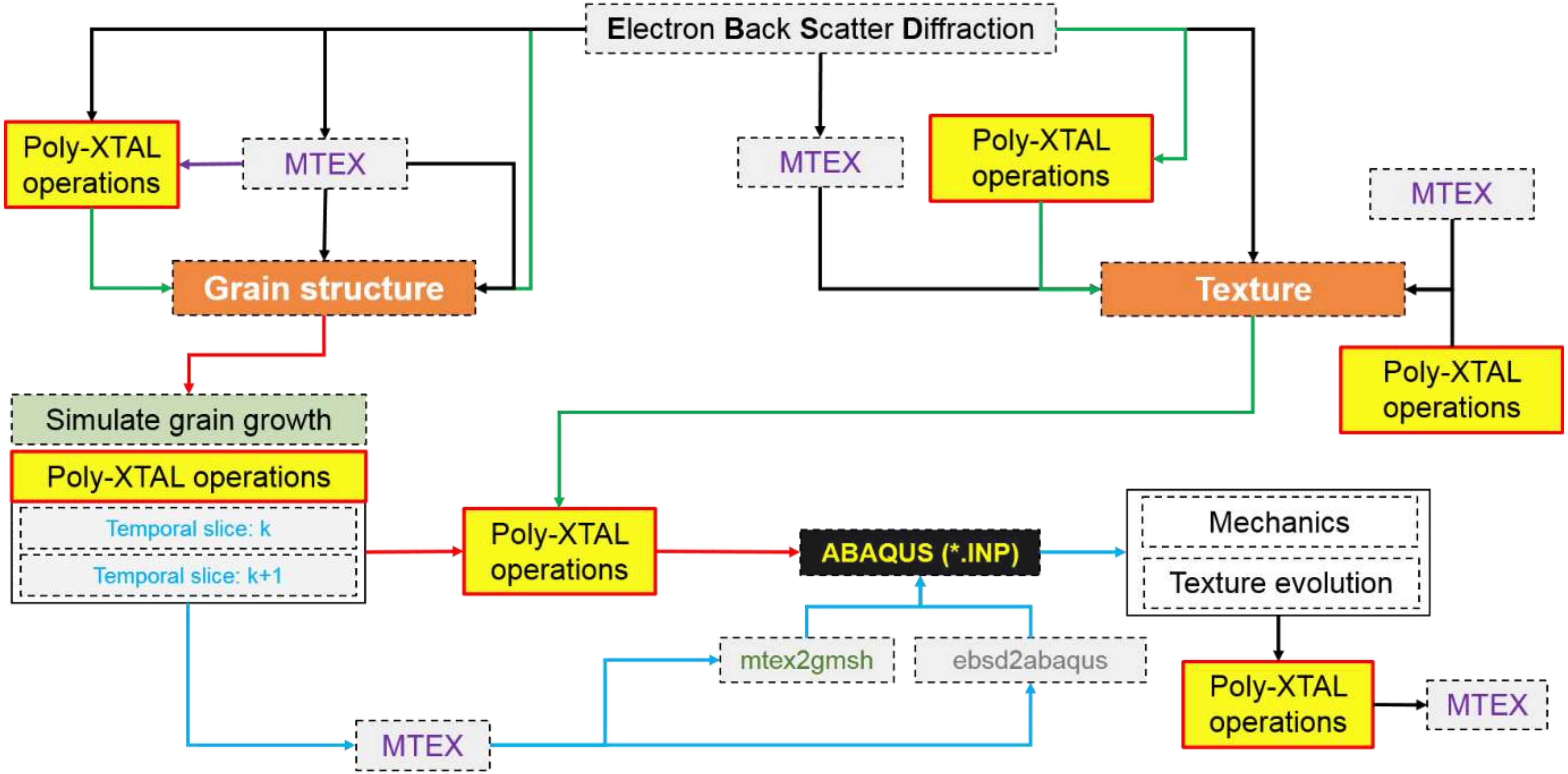
5. Open temporal slices of grain structures generated in Poly-Xtal operations in MTEX and take advantage of MTEX grain structure analysis tools

6. Track temporal evolution of grain structure statistics

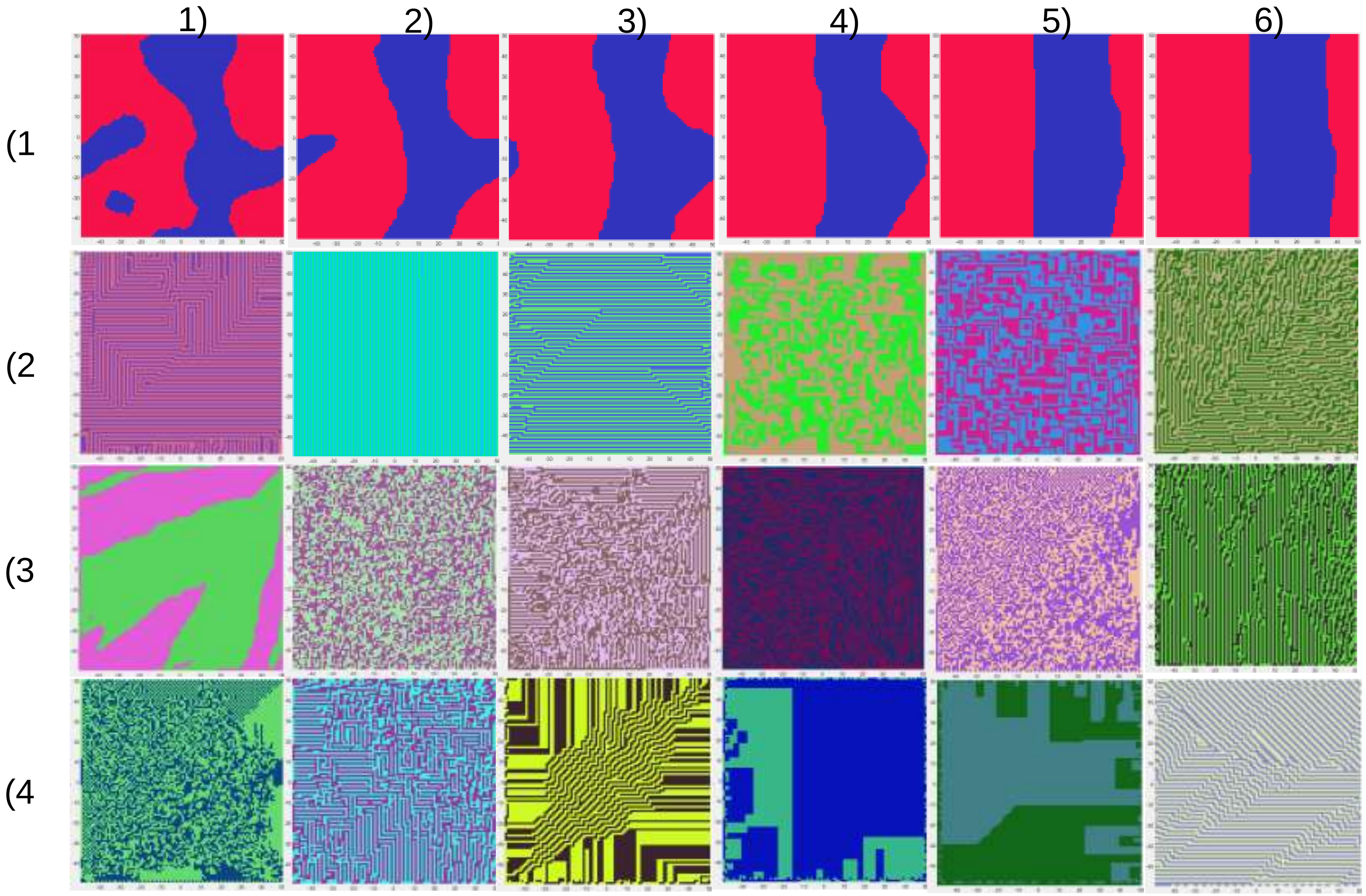
7. Track temporal change in total and phase partitioned Hamiltonian

8. Generate tensile testing specimen with grain structure in the test

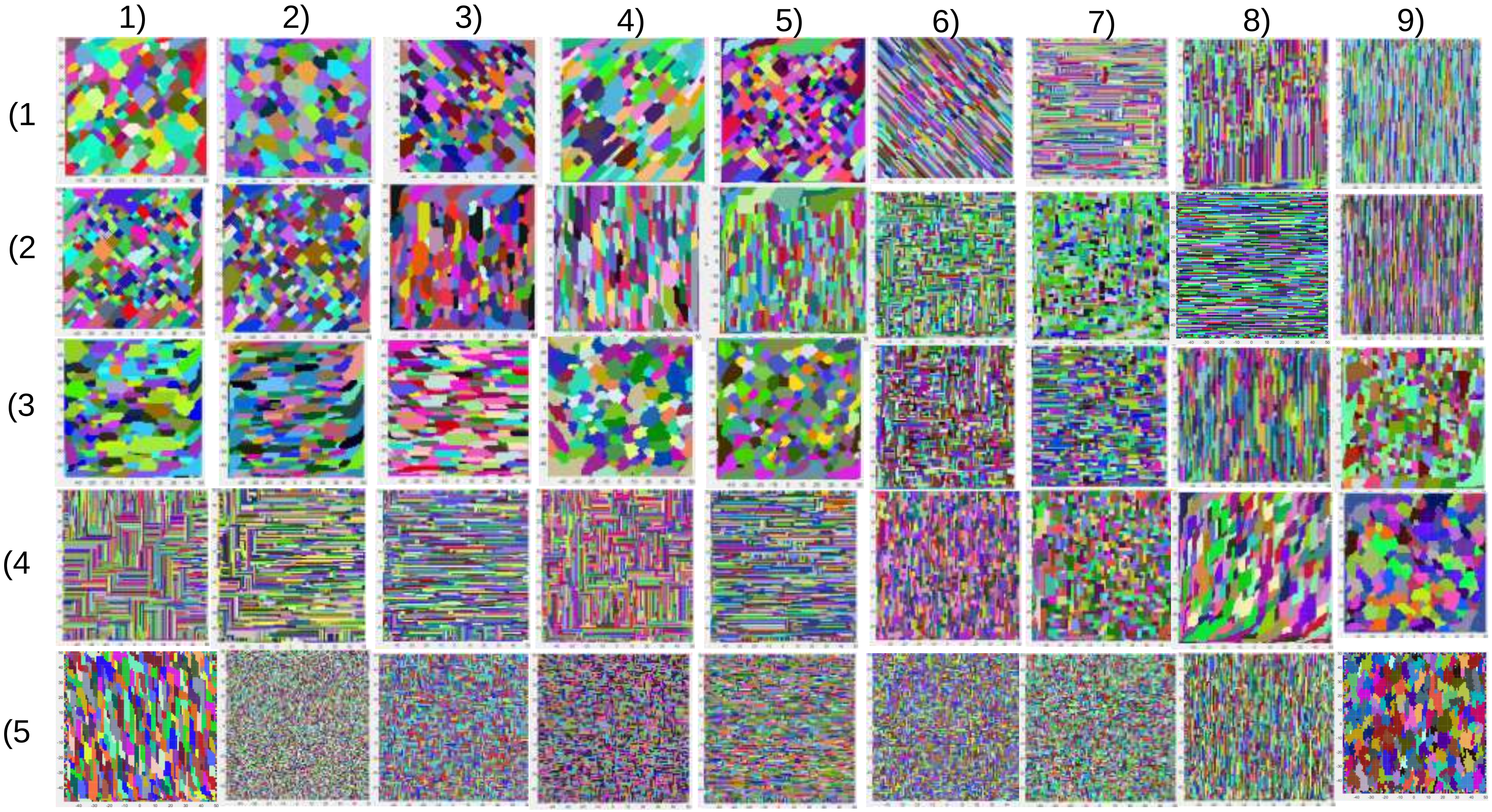
Available work flow paths

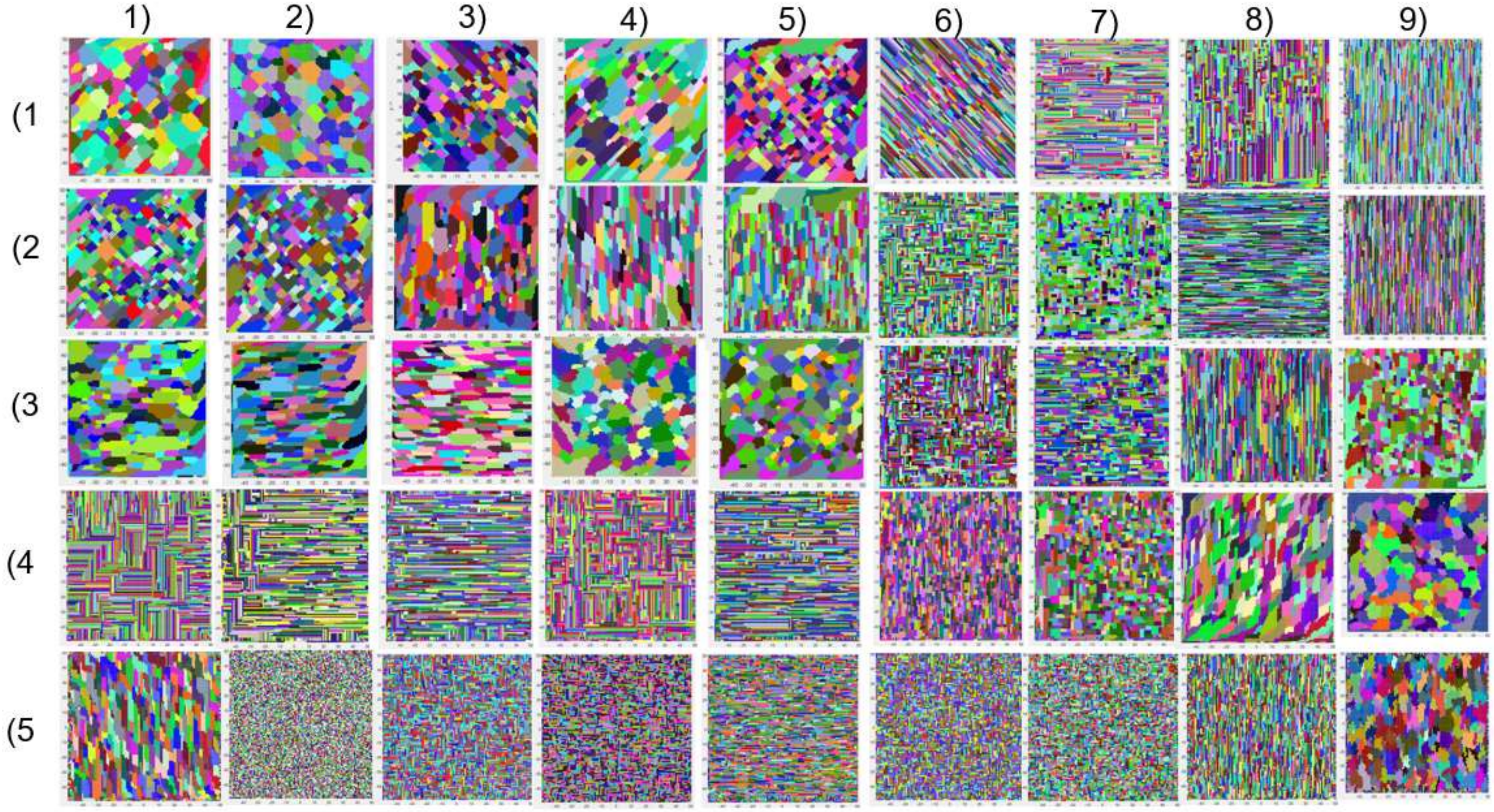


Weighted Ising model – 2D



Grain structure gradients

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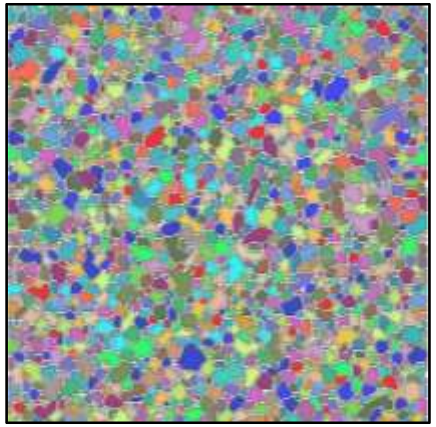
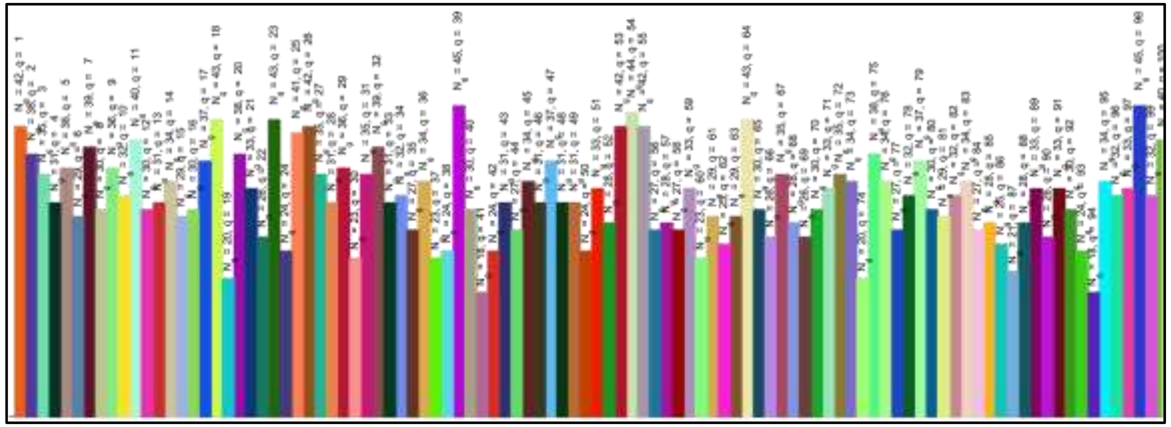
Grain structure characterization



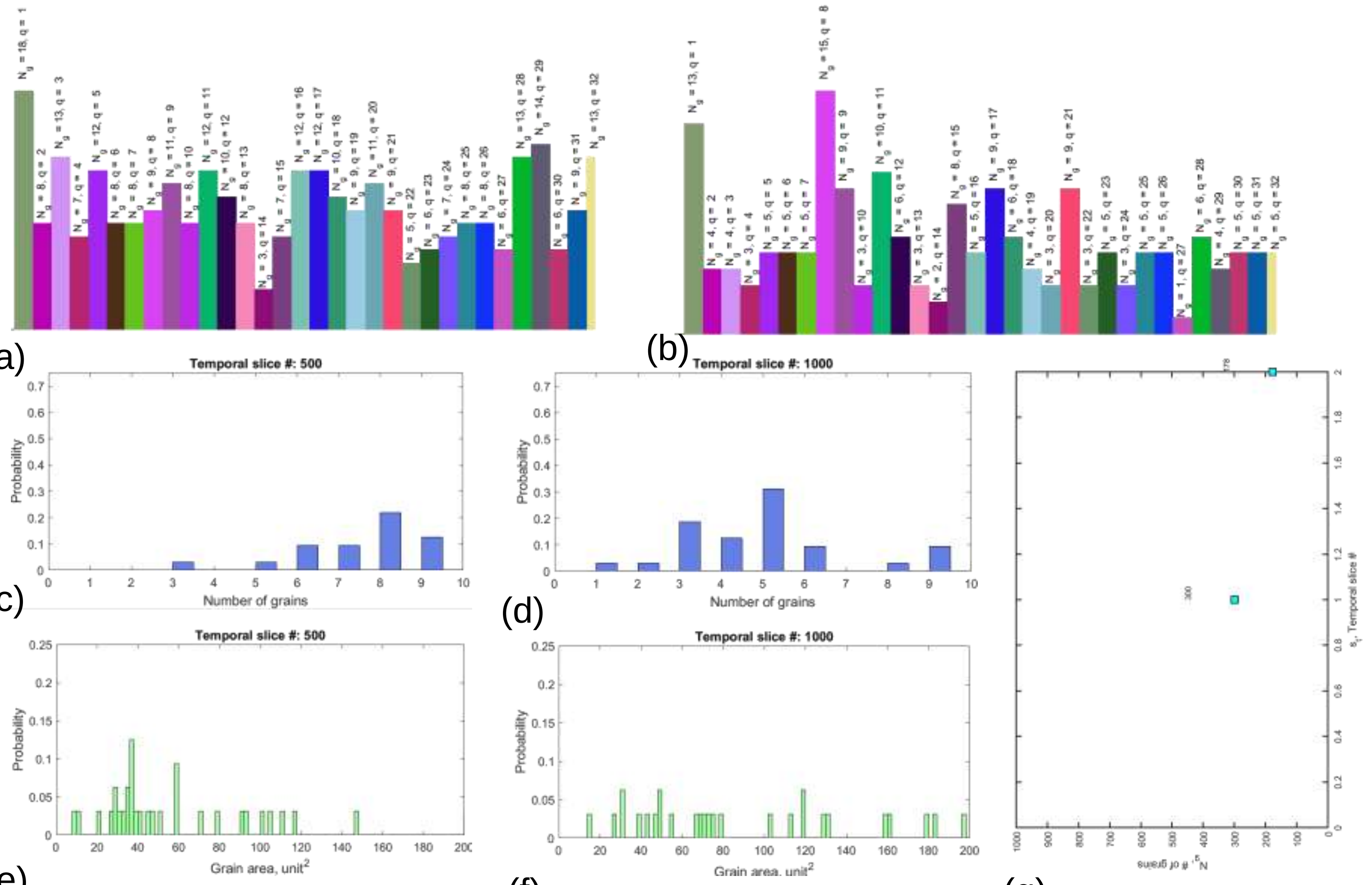
(a)



(b)

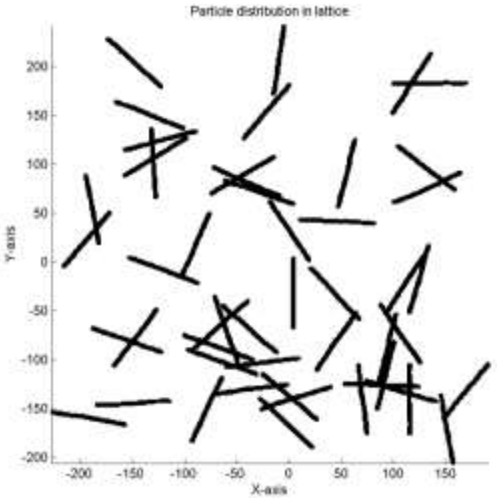
(c)

Grain structure characterization



(a) (b) (c) (d) (e) (f) (g)

Possibilities of second phase particles



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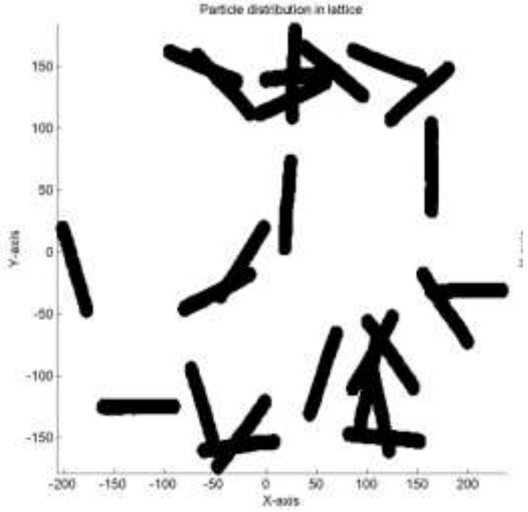

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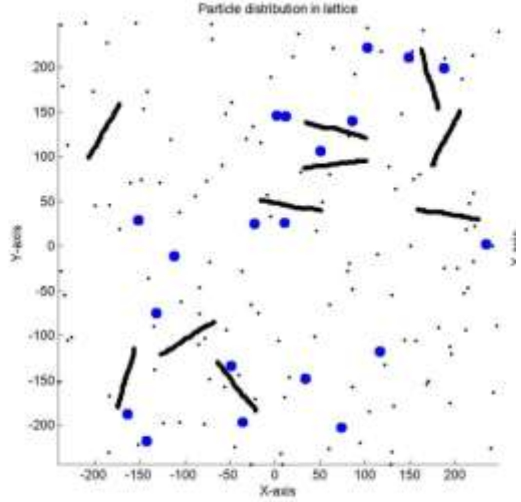

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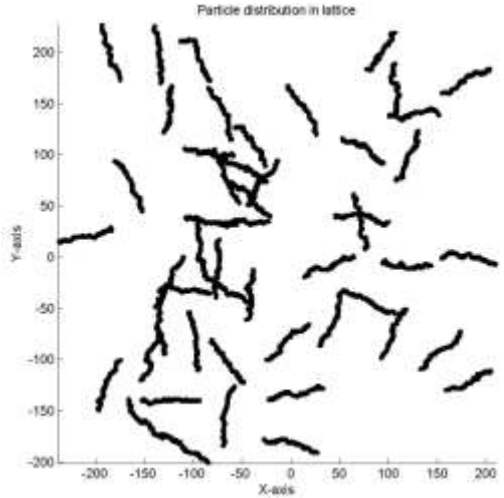

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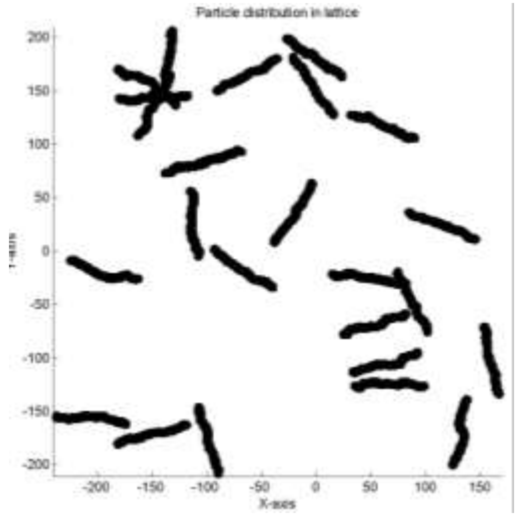

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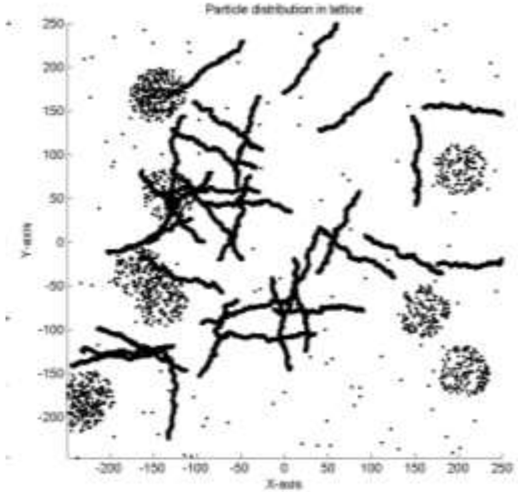

(f)

Carbon nanotube like particles

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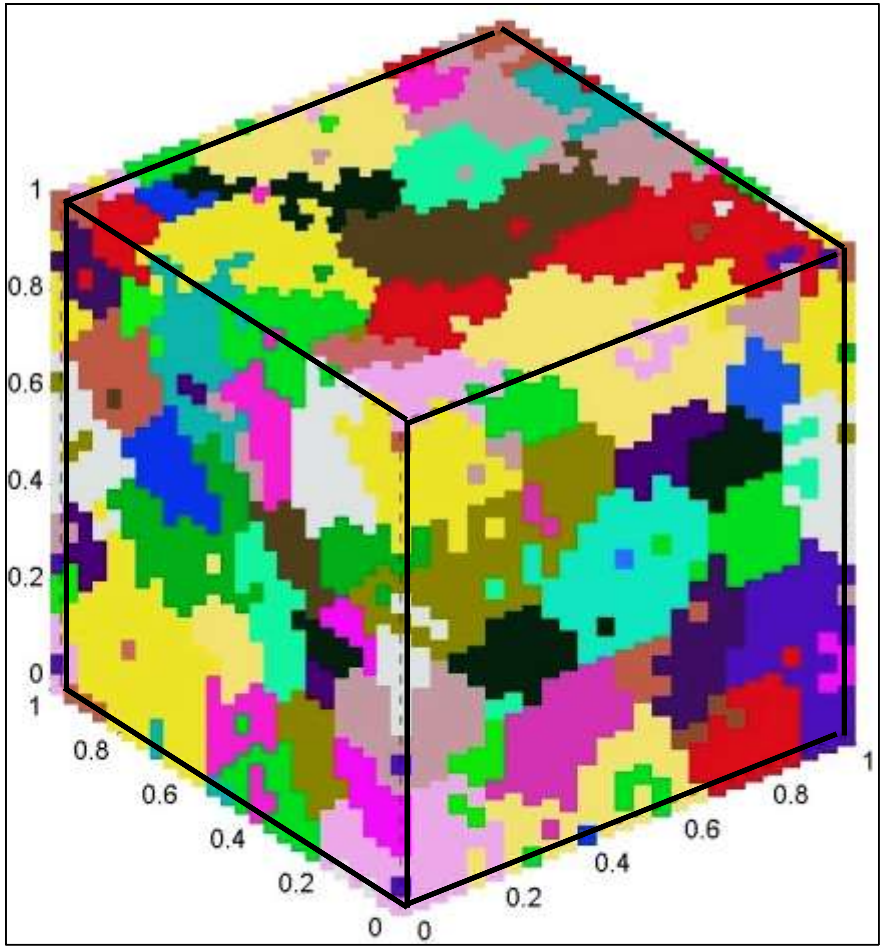
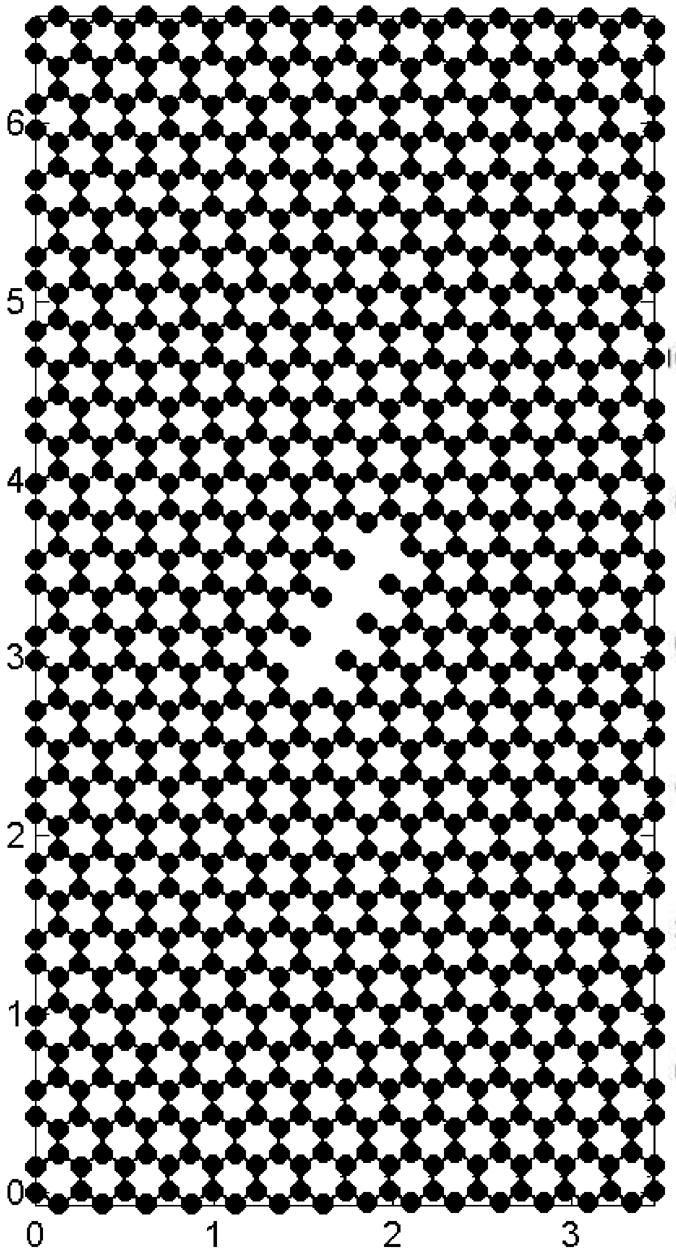
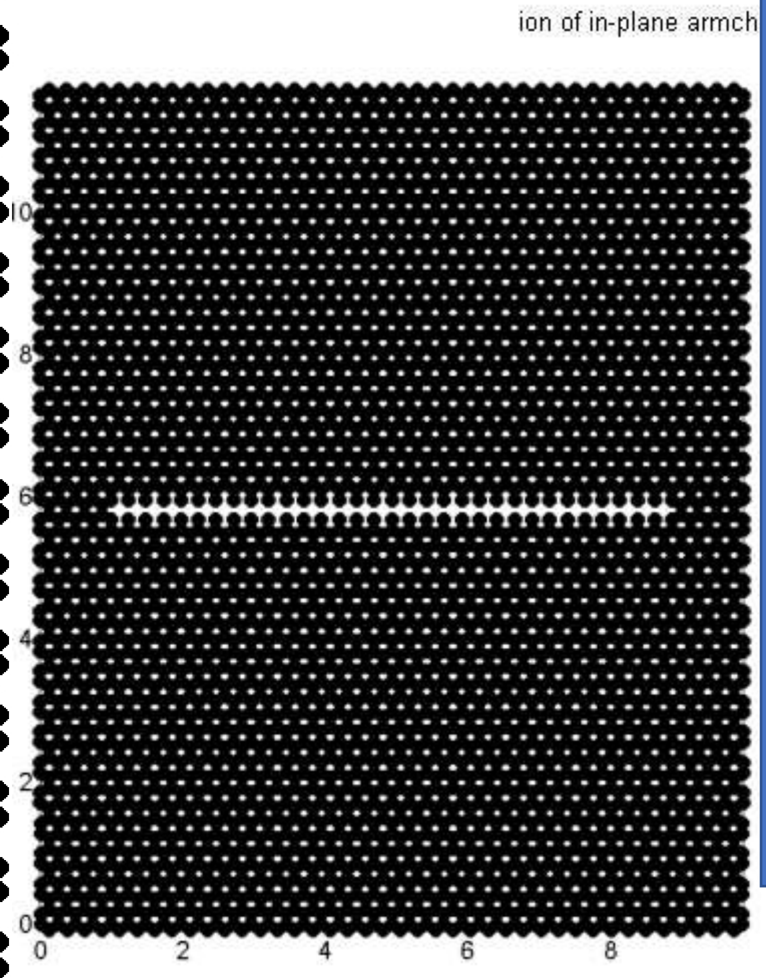
Further capabilities



A 3D poly-crystal

A graphene 2D crystal





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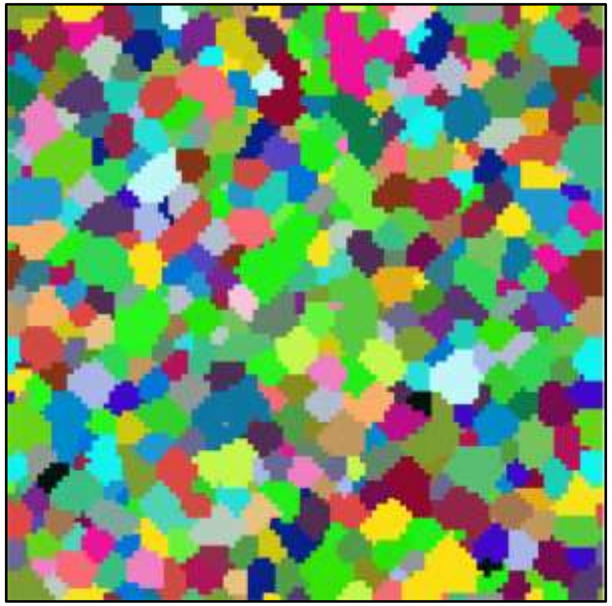
Linking 3rd party open source libraries: MTEX



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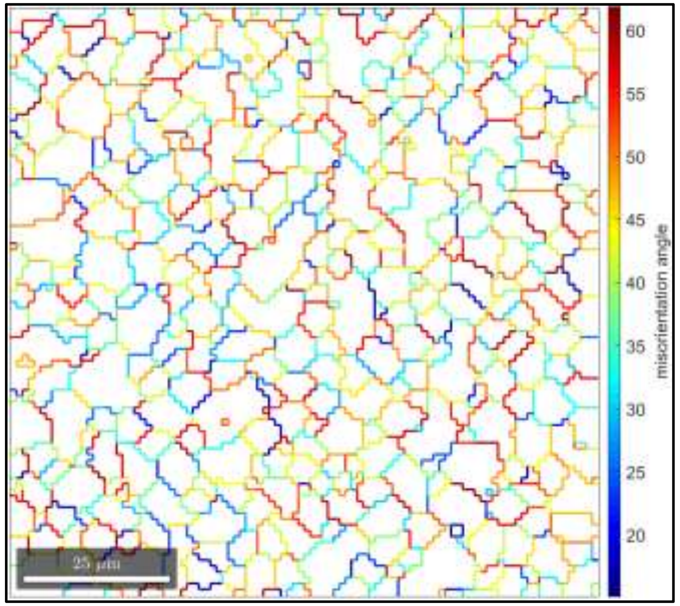

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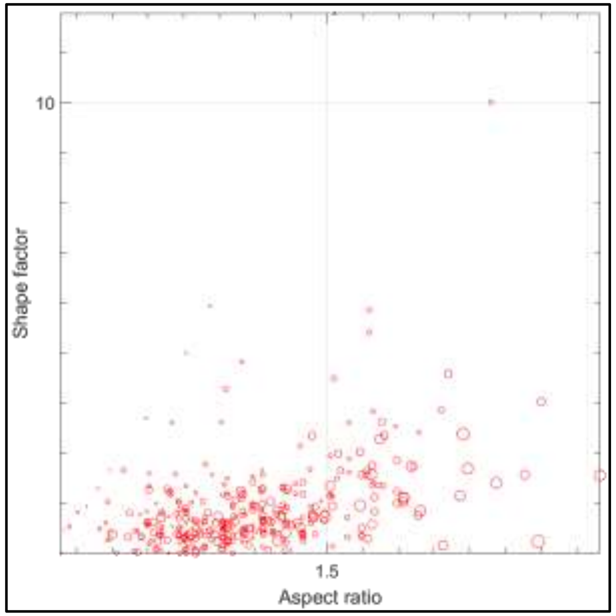
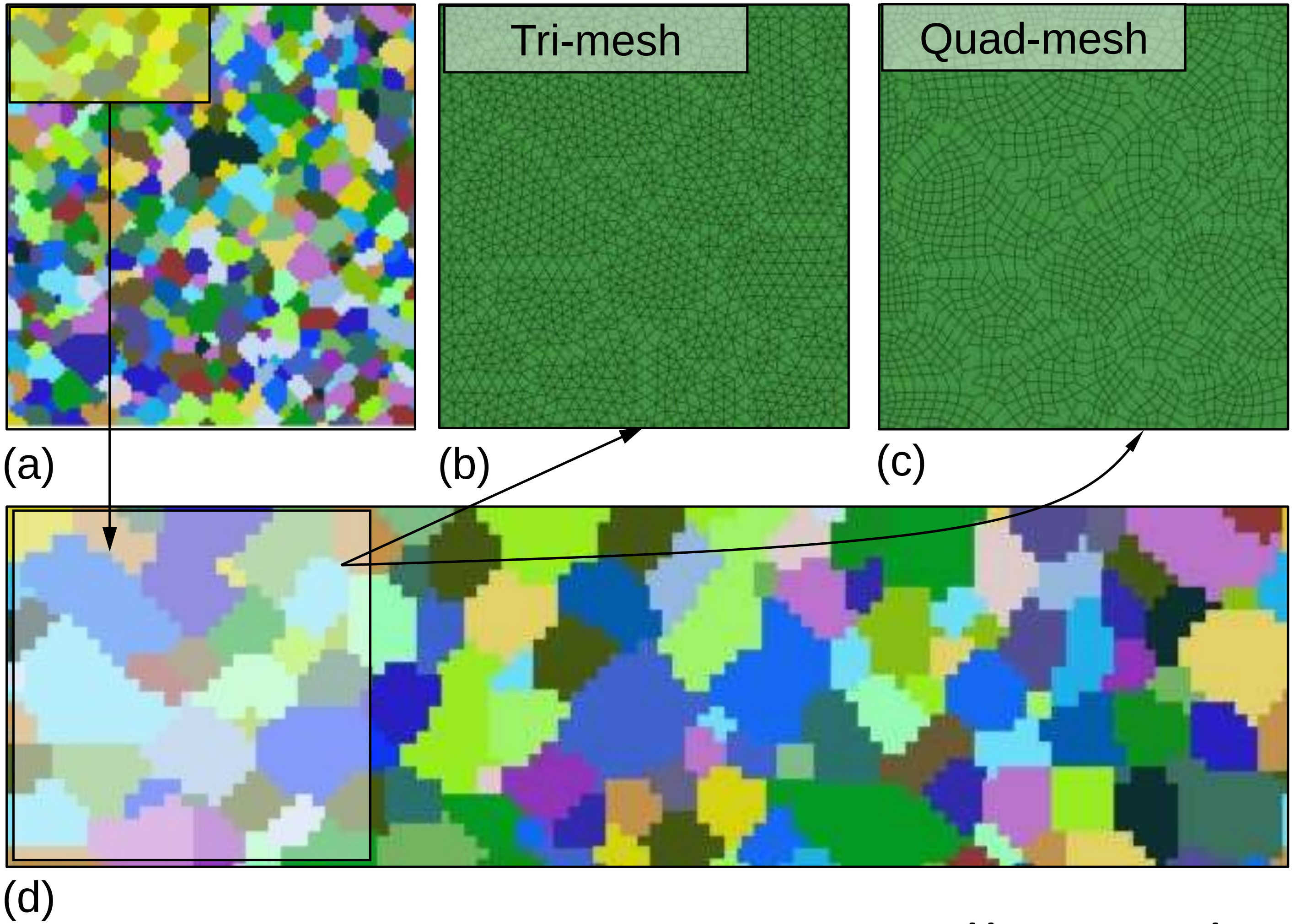


(c)

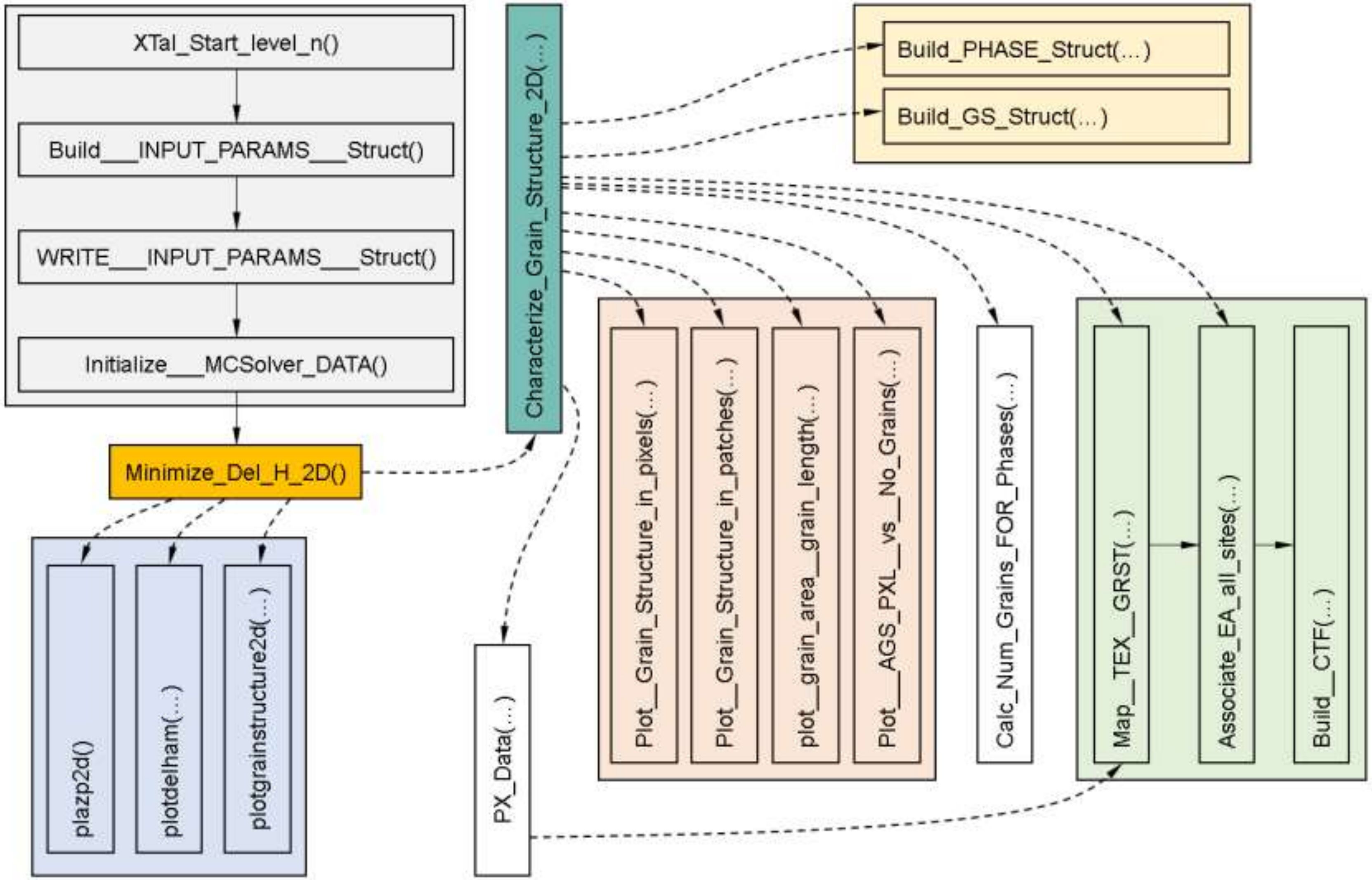
https://mtex-toolbox.github.io/

Linking 3rd party open source libraries: MTEX2gmsh



https://github.com/DorianDepriester/MTEX2Gmsh

High level structure



Future plans

- Extend all capabilities to 3D and generalize to nD
- GUI development
- Develop texture analysis routines
- Further development of the non-linear FE solver for molecular mechanics based FEA.
- Re-write in python with C assembly solver
- Develop into a self-contained software
- Commercialize the software

Licenses

- My requirement :

  - The license should allow developer to retain all development rights. The maintenance and distribution rights to be shared with Coventry University.

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Thank you

- Any questions?