---

title: 'PXO (Poly-XTAL Operations): Free MATLAB codebase to generate and analyse complex 2D grain structures'

tags:

- grain structure generation

- texture and grain structure

authors:

- name: Sunil Anandatheertha1

orcid: 0000-0001-6535-8191

affiliation: "1"

affiliations:

- name: Coventry University, Coventry, United Kingdom

index: 1

date: 23 January 2021

bibliography: paper.bib

---

# Summary

Computational materials scientists studying multi-scale thermo-mechanical and texture behaviour of poly-crystalline materials need parametric and realistically tessellated geometric morphologies of the constituent phases reflected in the virtual grain structure. They use such grain structures as an input to further studies such as crystal plasticity based finite element analysis. Though simplified and geometric grain structures have been used in the past, it is difficult to generate such parametric spatially gradient grain structures with multiple temporally low gradient slices as commonly observed in the real world. This work presents a MATLAB codebase which enables users to create and analyse such grain structures and associate them with either experimentally observed or mathematically modelled crystallographic texture. The tool is also useful for computational geologists, mathematicians interested in different ways of energy minimized n-D space partitioning and finally statistical mechanics understanding of the temporal evolution of Q-state Pott’s model. For material scientists, in addition to various in-built tools, ‘PXO’ can output the grain structure in a format which can be further opened in 3rd party open source libraries to tend to their specific requirements, and also simulate grain growth.

# Statement of need

Mathematicians, statistical mechanists and computational materials scientists are interested in studying the spatiotemporal evolutionary aspects of multi-phased partitioning of an n-dimensional space. We give four examples for this. The 1st example is from mathematics where researchers are interested in the chaotic partitioning of an n-D bounded spatial domain and its spatiotemporal evolution under some governing rules. 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 [1], 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. The 3rd example is from fundamental computational materials science where researchers are interested in grain growth [2], where the temporal evolution of the spatial and thermodynamical parameters of multi-phase grain structures [3,4] is studies. A part of this research also touches upon understanding the kinematic and kinetic behaviour of insoluble 2nd phase particles in grain structures [5] 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 [6]. As the shape of the particles influence the Zener drag working against grain boundary evolution during grain growth [7], and that nature presents irregularly shaped particles, computer models which can consider such particle shape and their spatial distribution becomes very essential. 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 [8]. 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. All these applications can be seen under single roof and the present work presents the free MATLAB codebase to enable such functionalities under one single platform.

# Citations

Citations to entries in paper.bib should be in

[rMarkdown](http://rmarkdown.rstudio.com/authoring\_bibliographies\_and\_citations.html)

format.

If you want to cite a software repository URL (e.g. something on GitHub without a preferred

citation) then you can do it with the example BibTeX entry below for @fidgit.

For a quick reference, the following citation commands can be used:

- `@author:2001` -> "Author et al. (2001)"

- `[@author:2001]` -> "(Author et al., 2001)"

- `[@author1:2001; @author2:2001]` -> "(Author1 et al., 2001; Author2 et al., 2002)"

# Acknowledgements

The author acknowledges the computational support offered by the institutions PES Institute of Technology in 2010, Indian Institute of Science during 2013-2014, PES University during 2014-2017 and Coventry University during 2017-2021. The author also acknowledges Dr. Kishore T Kashyap @ PESIT for his theoretical inputs on general grain growth and its simulation in 2010 and Dr. G Narayana Naik and Dr. N G Subramania Udupa for their supervising the author’s master’s project.

# References

Bibliography file: “paper.bib”

**@article**{Pearson:2017,

url = {http://adsabs.harvard.edu/abs/2017arXiv170304627P},

Archiveprefix = {arXiv},

Author = {{Pearson}, S. **and** {Price-Whelan}, A.~M. **and** {Johnston}, K.~V.},

Eprint = {1703.04627},

Journal = {ArXiv e-prints},

Keywords = {Astrophysics - Astrophysics of Galaxies},

Month = mar,

Title = {{Gaps **in** Globular Cluster Streams: Pal 5 **and** the Galactic Bar}},

Year = 2017

}

**@book**{Binney:2008,

url = {http://adsabs.harvard.edu/abs/2008gady.book.....B},

Author = {{Binney}, J. **and** {Tremaine}, S.},

Booktitle = {Galactic Dynamics: Second Edition, by James Binney **and** Scott Tremaine.~ISBN 978-0-691-13026-2 (HB).~Published by Princeton University Press, Princeton, NJ USA, 2008.},

Publisher = {Princeton University Press},

Title = {{Galactic Dynamics: Second Edition}},

Year = 2008

}

**@article**{gaia,

author = {{Gaia Collaboration}},

title = "{The Gaia mission}",

journal = {Astronomy **and** Astrophysics},

archivePrefix = "arXiv",

eprint = {1609.04153},

primaryClass = "astro-ph.IM",

keywords = {space vehicles: instruments, Galaxy: structure, astrometry, parallaxes, proper motions, telescopes},

year = 2016,

month = nov,

volume = 595,

doi = {10.1051/0004-6361/201629272},

url = {http://adsabs.harvard.edu/abs/2016A%26A...595A...1G},

}

**@article**{astropy,

author = {{Astropy Collaboration}},

title = "{Astropy: A community Python package for astronomy}",

journal = {Astronomy **and** Astrophysics},

archivePrefix = "arXiv",

eprint = {1307.6212},

primaryClass = "astro-ph.IM",

keywords = {methods: data analysis, methods: miscellaneous, virtual observatory tools},

year = 2013,

month = oct,

volume = 558,

doi = {10.1051/0004-6361/201322068},

url = {http://adsabs.harvard.edu/abs/2013A%26A...558A..33A}

}

**@misc**{fidgit,

author = {A. Smith},

title = {Fidgit: An ungodly union of GitHub **and** Figshare},

year = {2020},

publisher = {GitHub},

journal = {GitHub repository},

url = {https://github.com/arfon/fidgit}

}