ASME Hackathon 2023 Problem #2
Exascale Materials Design with Sandia/SPPARKS

Anh Tran (anhtran@sandia.gov), Dehao Liu (dehaoliu@binghamton.edu), Theron Rodgers (SNL), John Mitchell (SNL)

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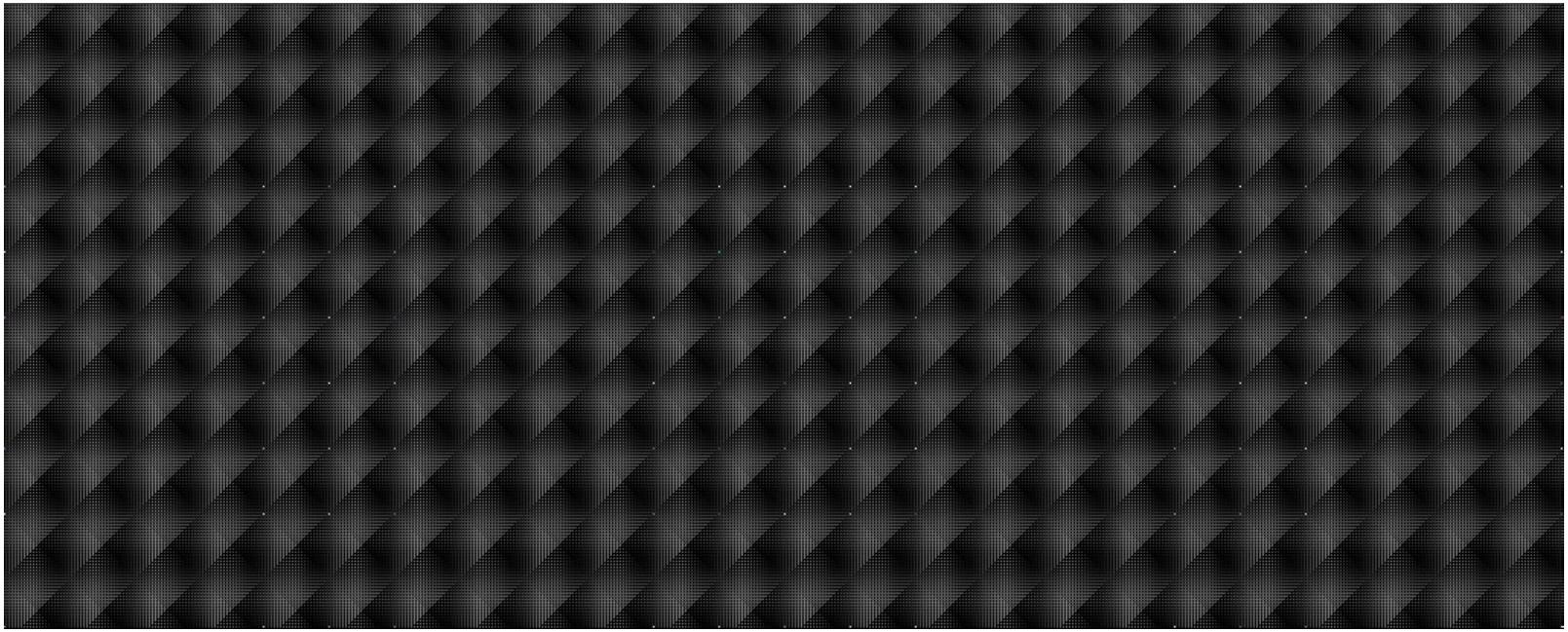
Introduction to SPPARKS

- acronym for **S**tochastic **P**arallel **PAR**ticle **K**inetic **S**imulator
- Sandia implementation of kinetic Monte Carlo model
- written in C++, supported by MPI+OpenMPI for massively parallelism
- publicly available at https://spparks.github.io/ or https://spparks.sandia.gov/
- open source code https://github.com/spparks/spparks
- usually used to simulate **process-structure** relationship in computational materials science
- example: normal grain growth, additive manufacturing, abnormal grain growth (pinning particulate, gradient temperature, etc.)

Additive manufacturing with SPPARKS



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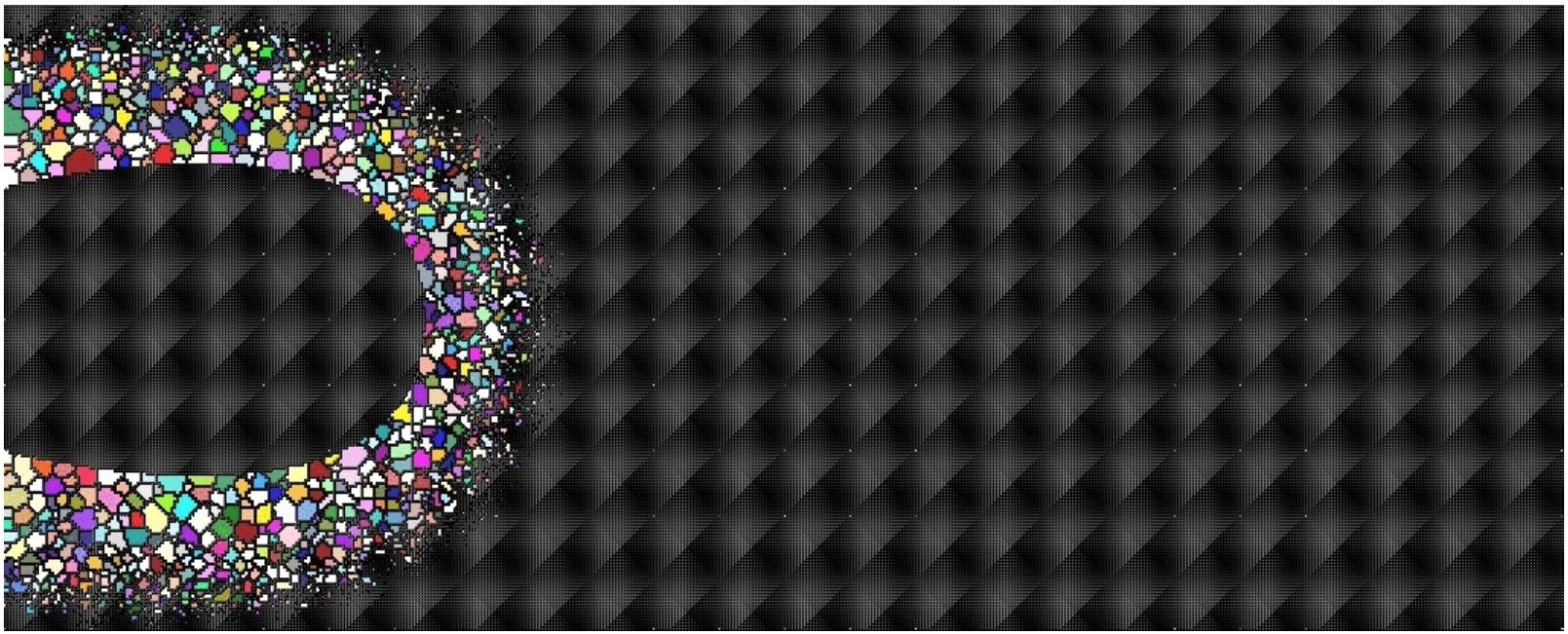

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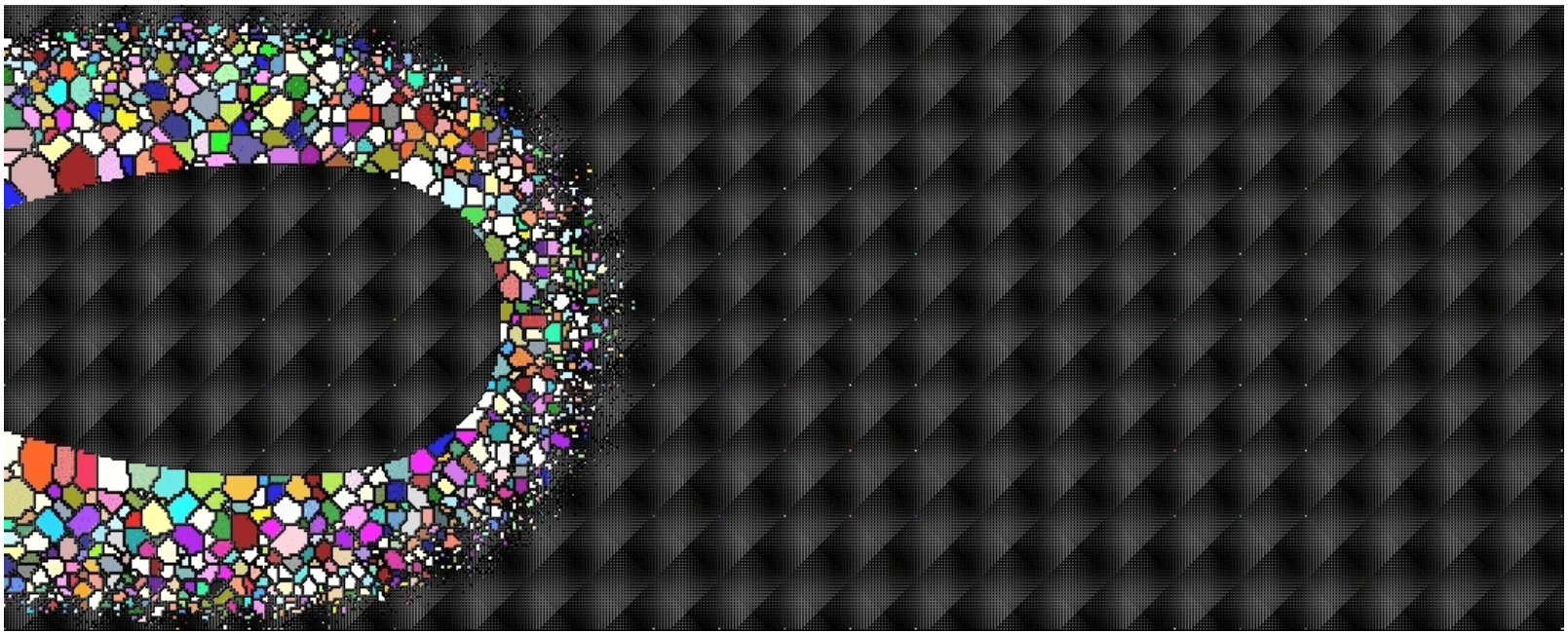

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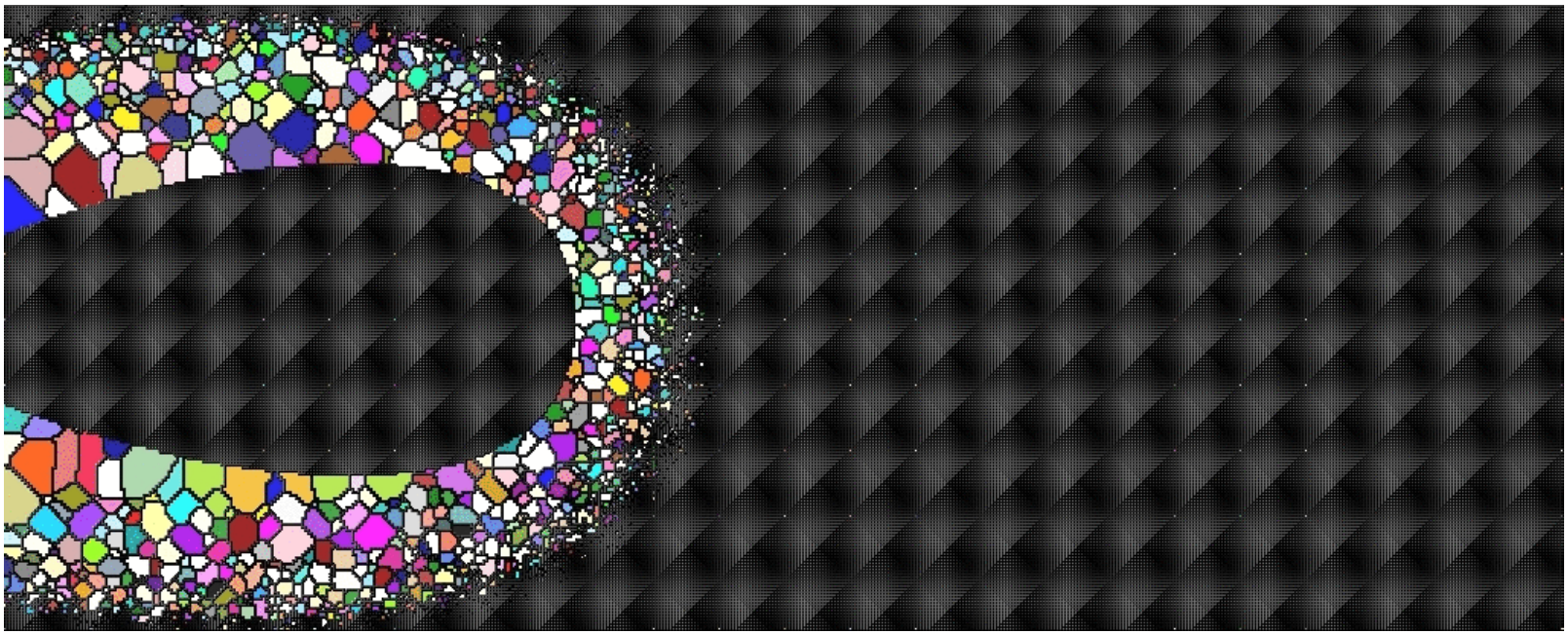

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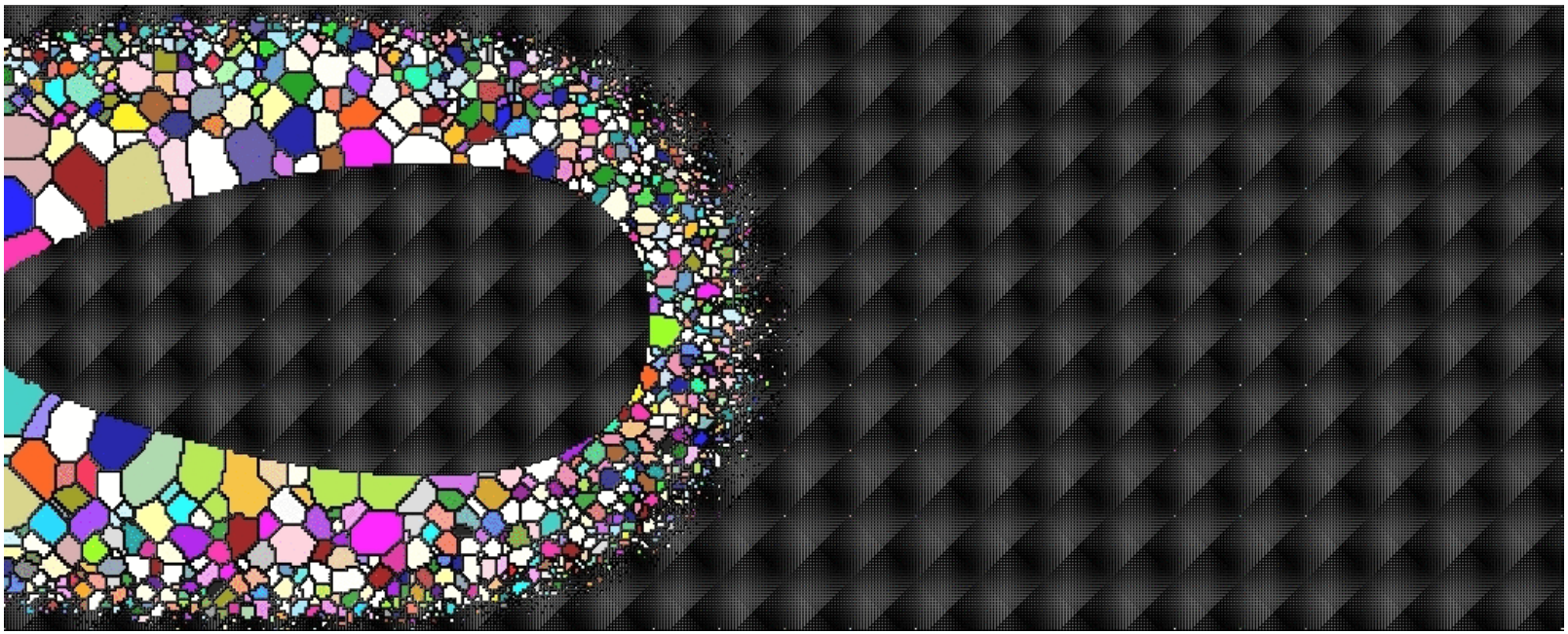

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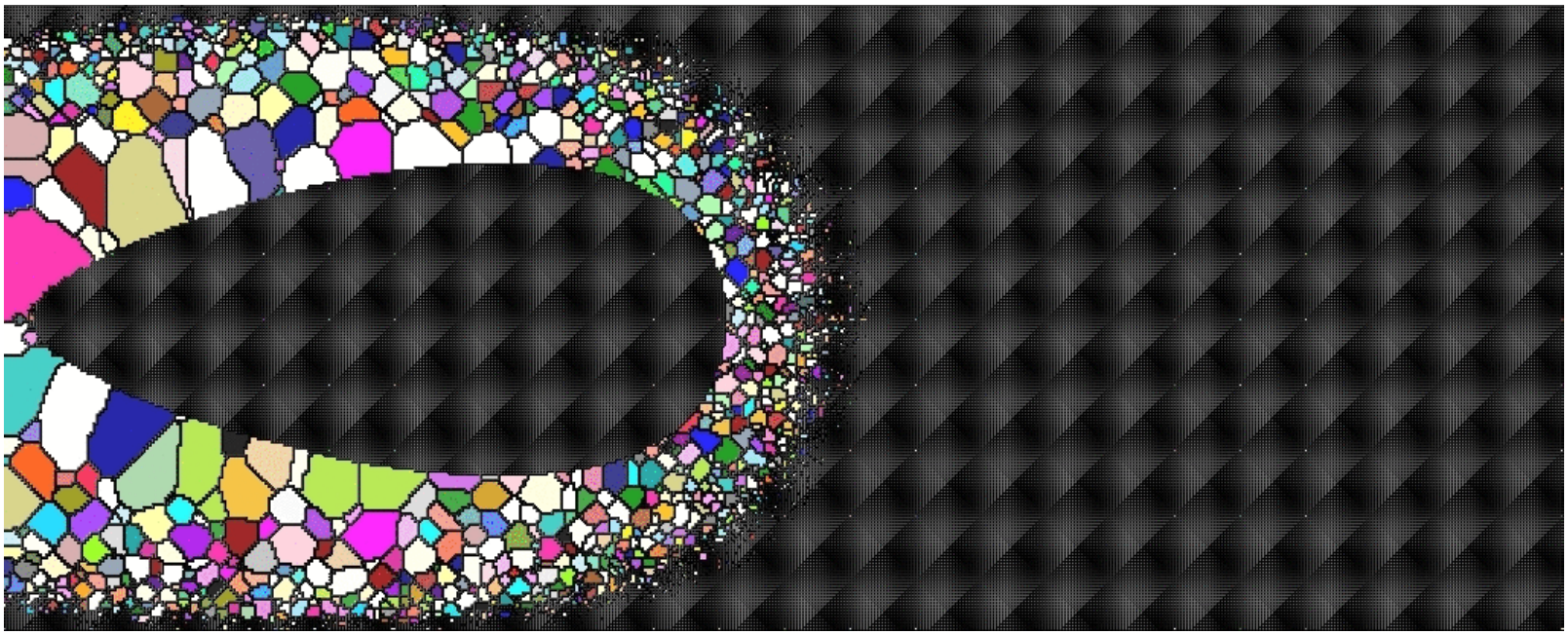

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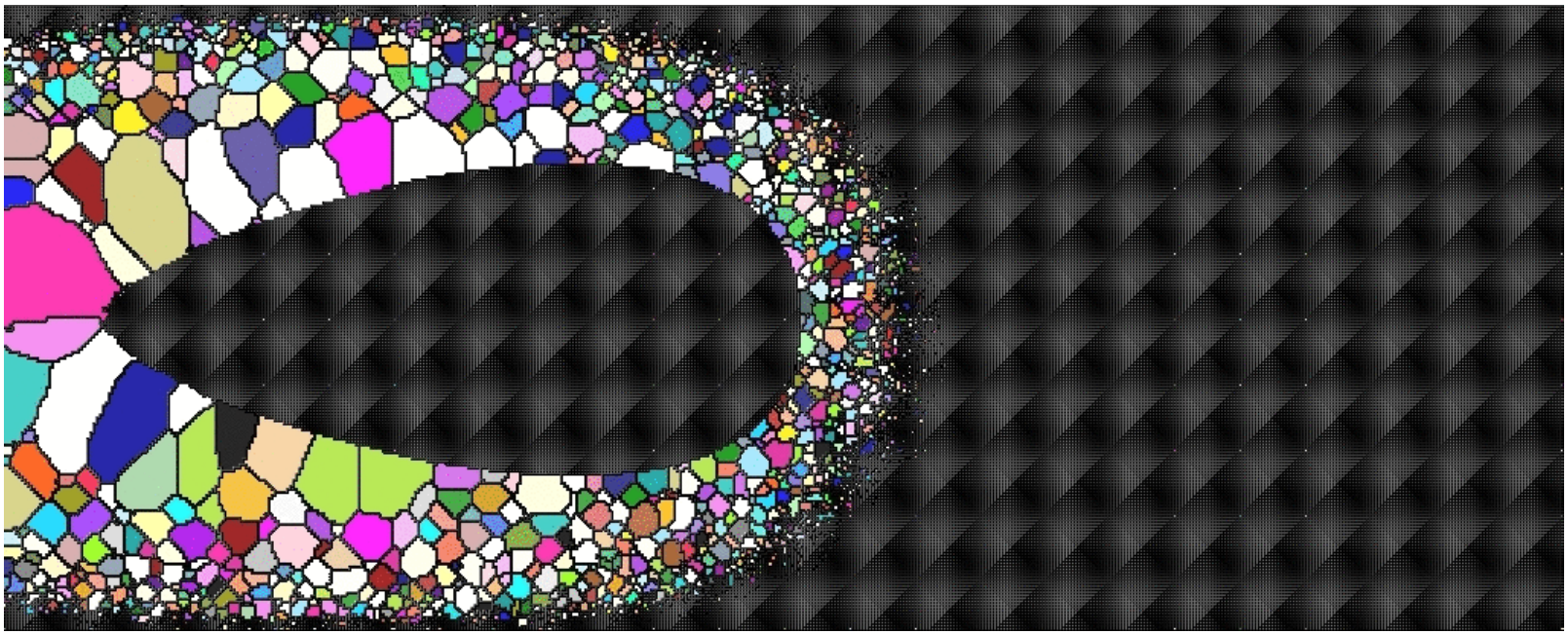

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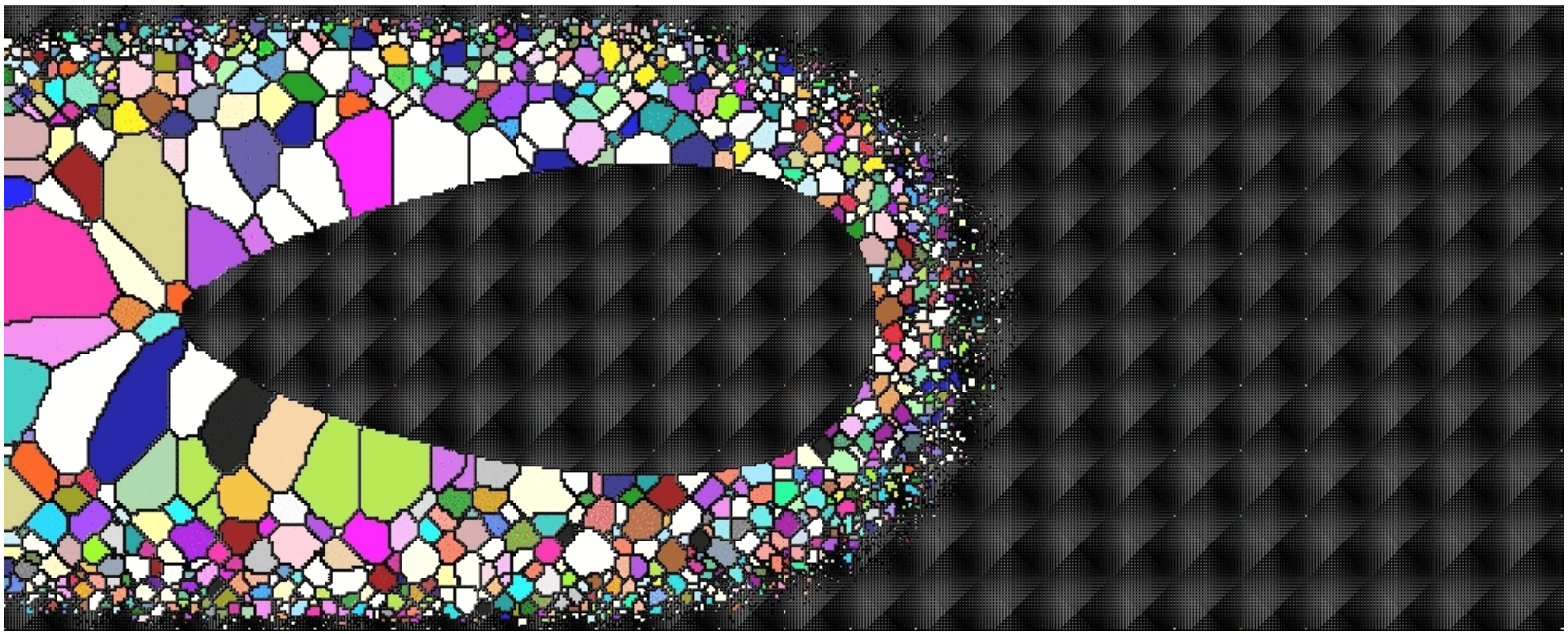

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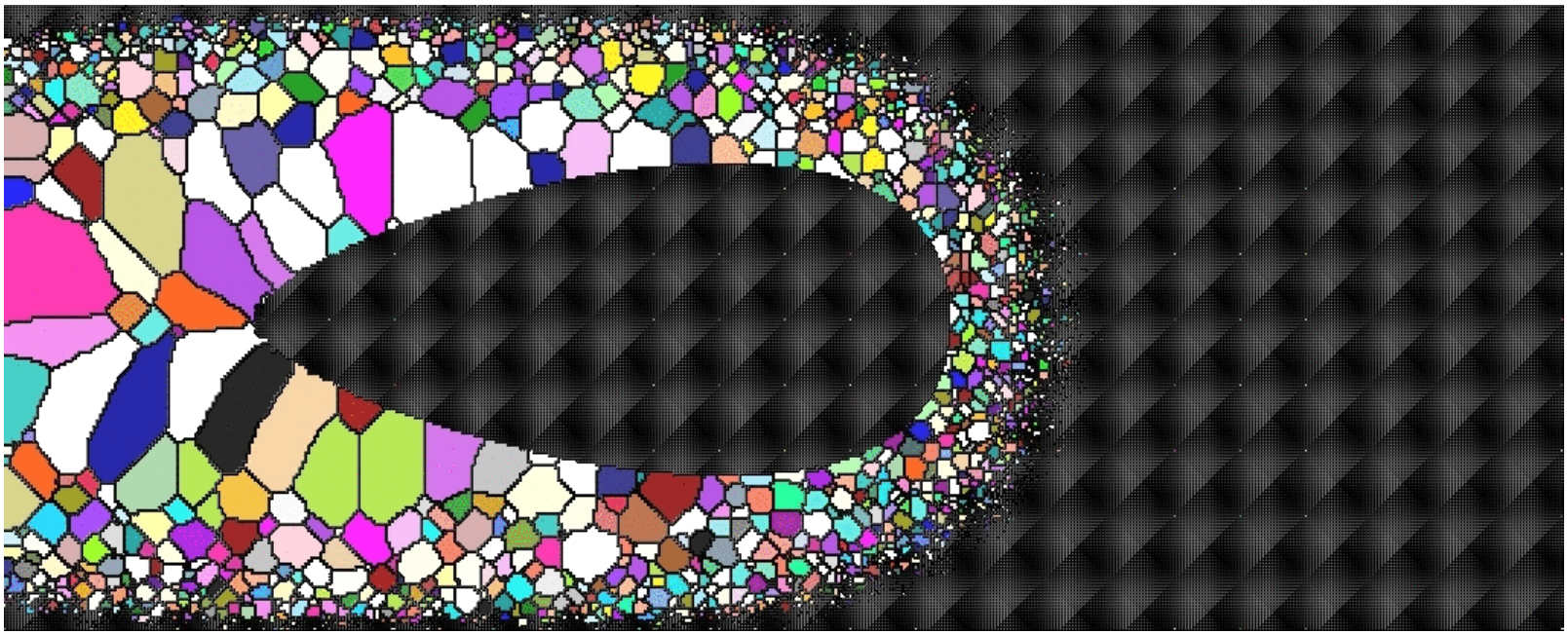

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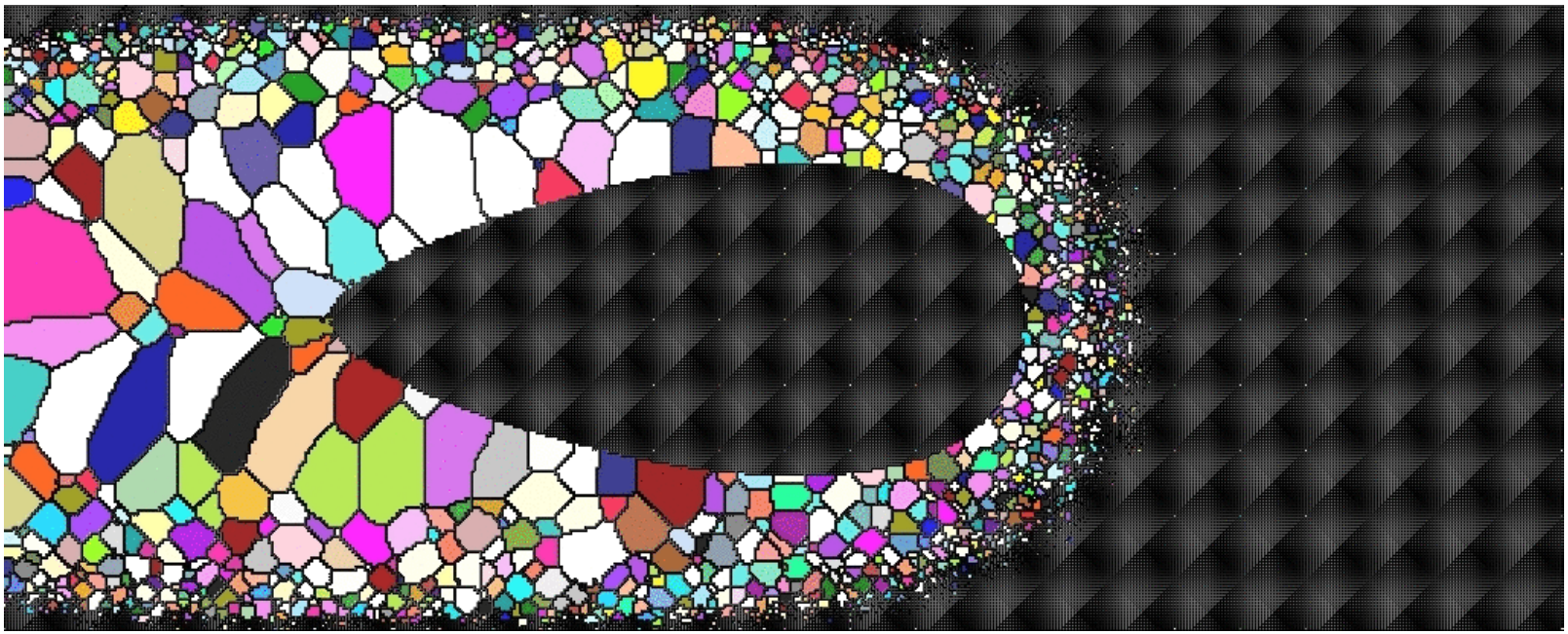

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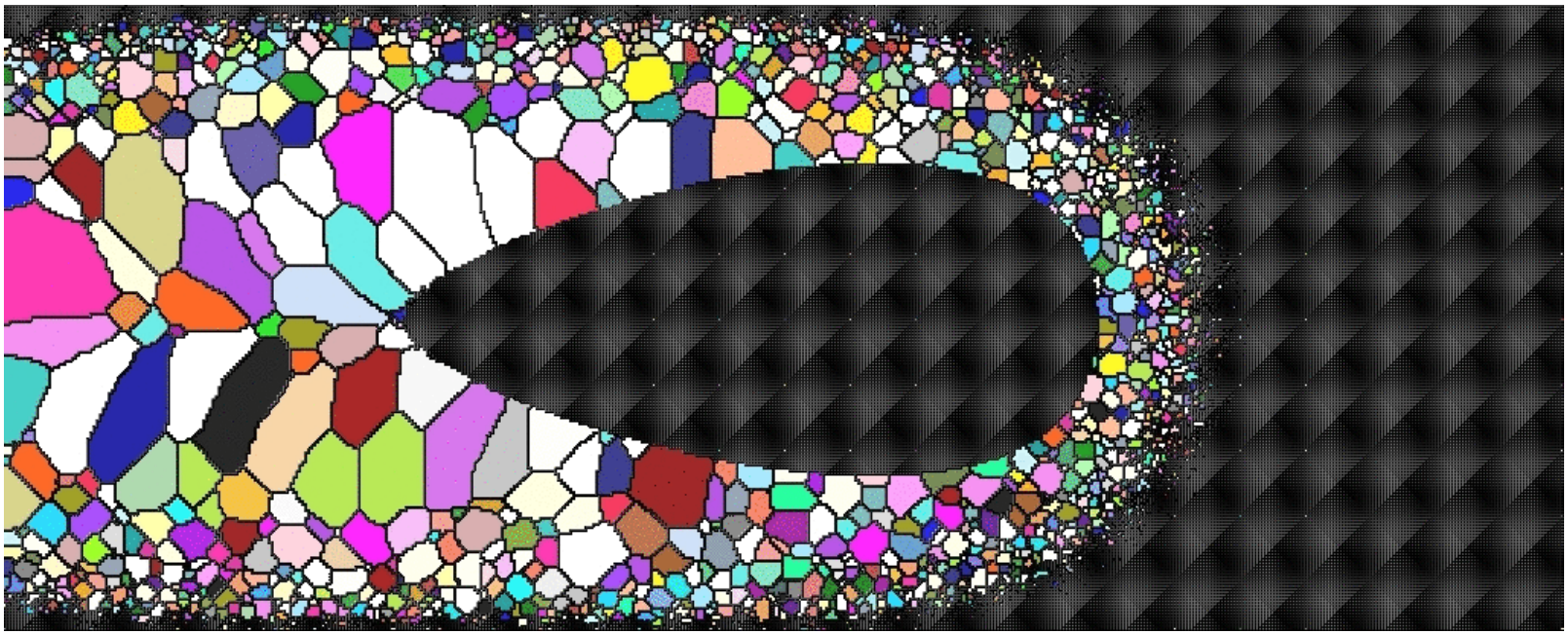

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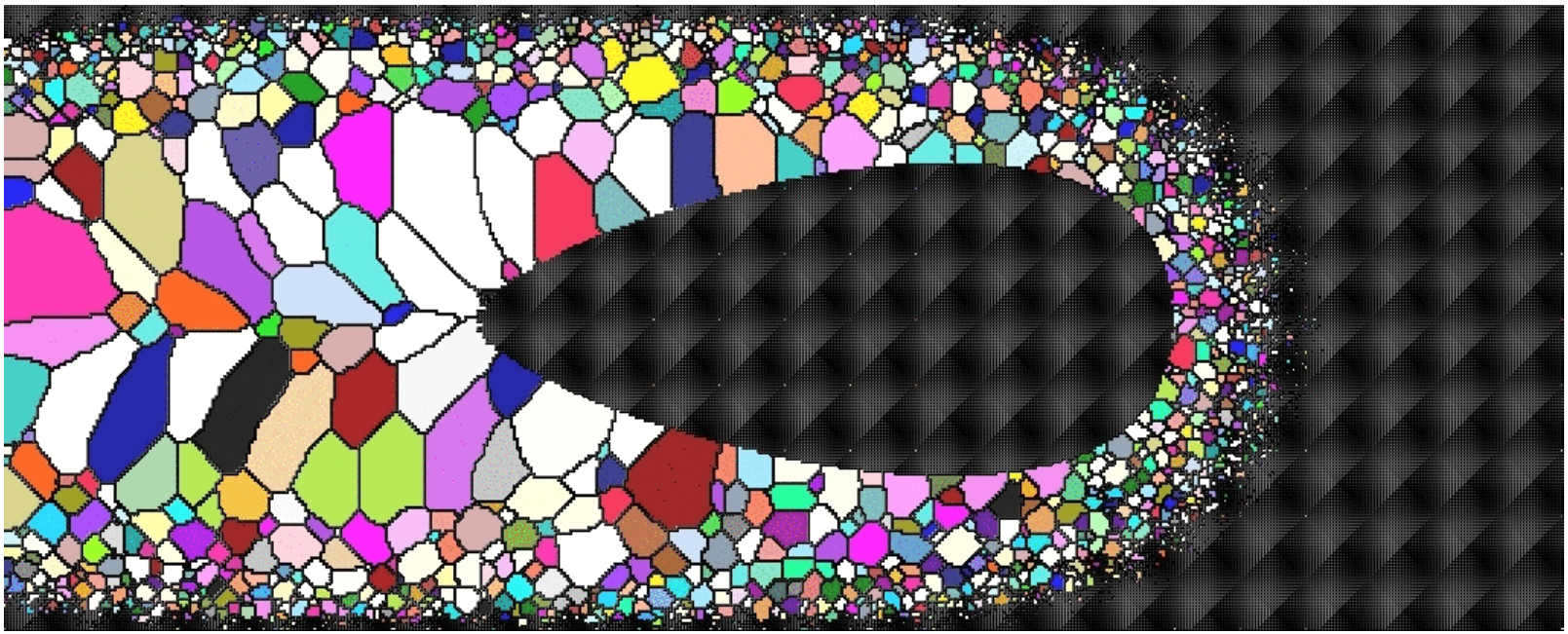

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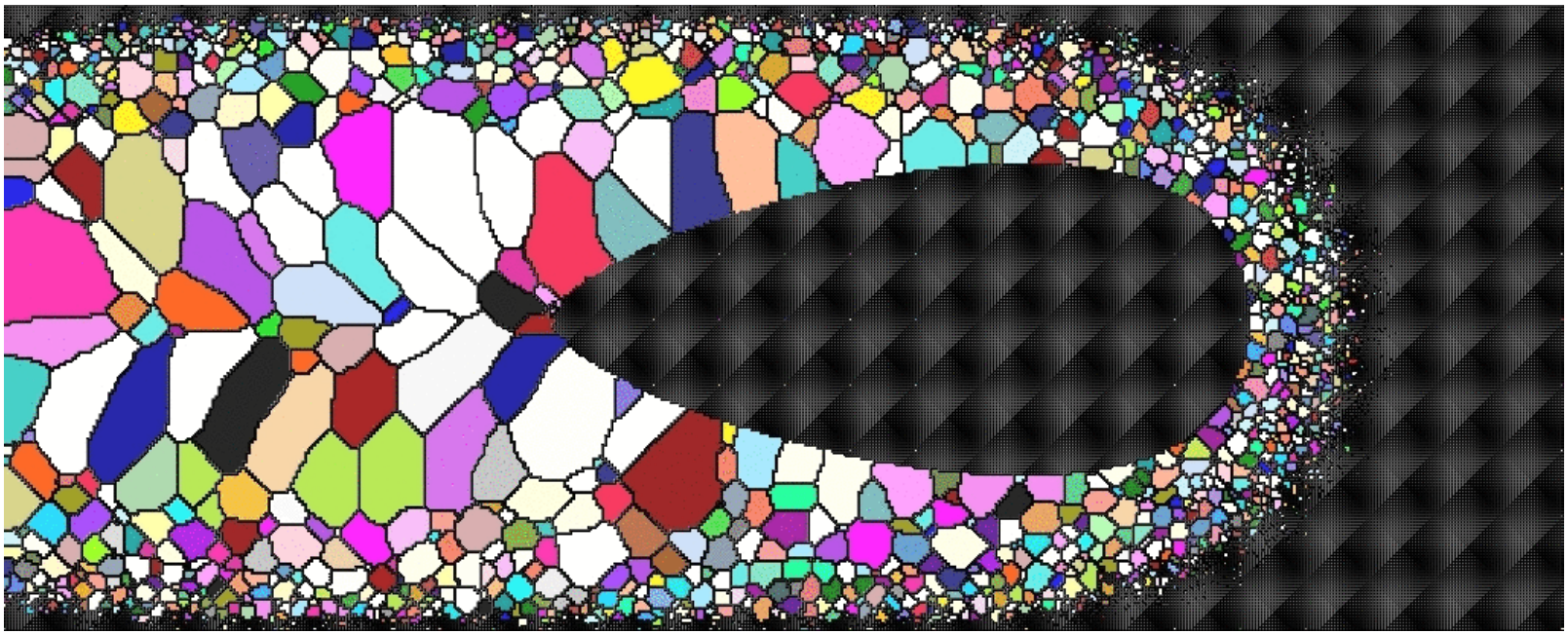

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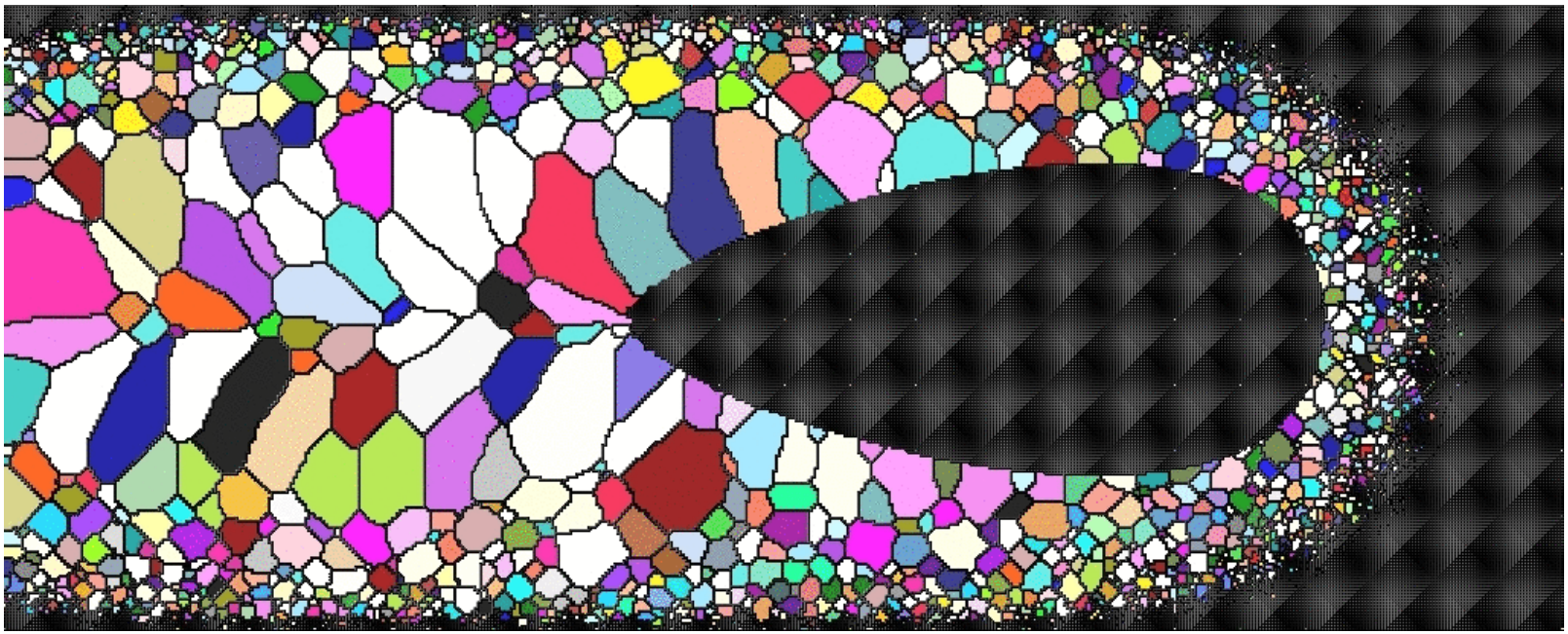

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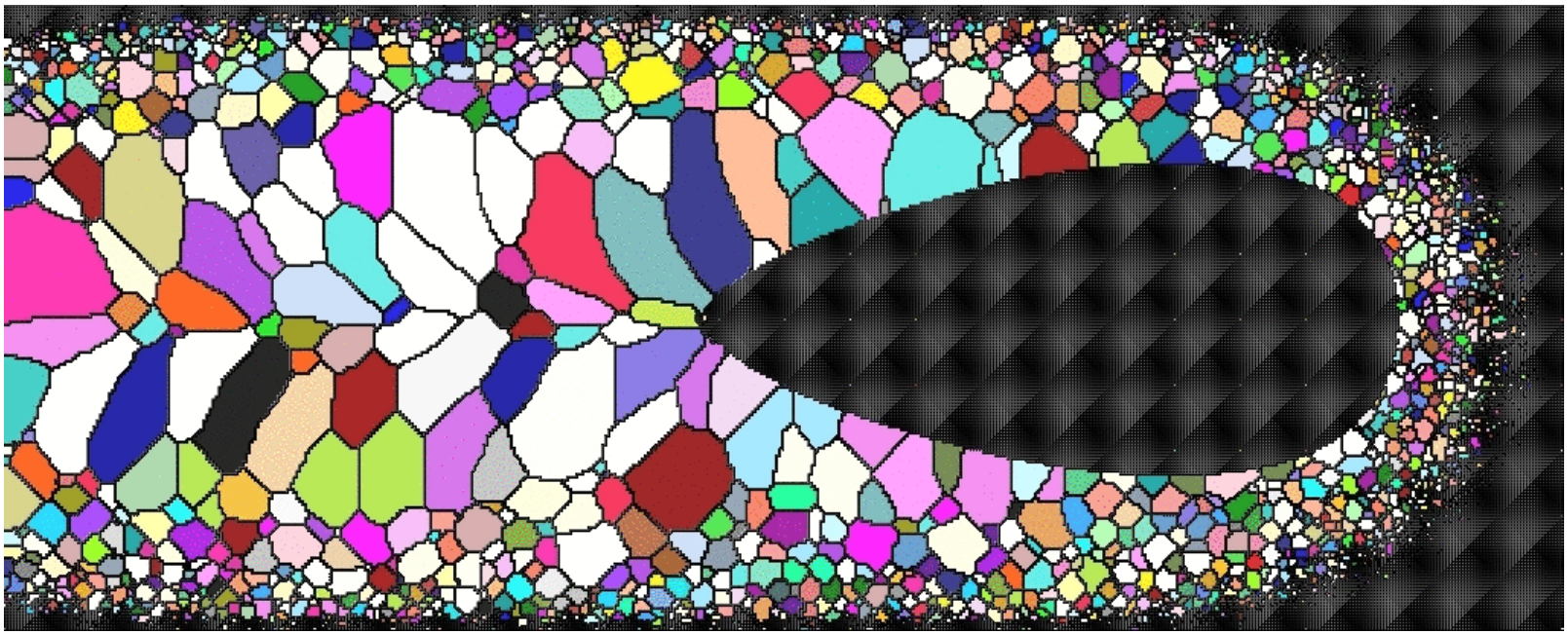

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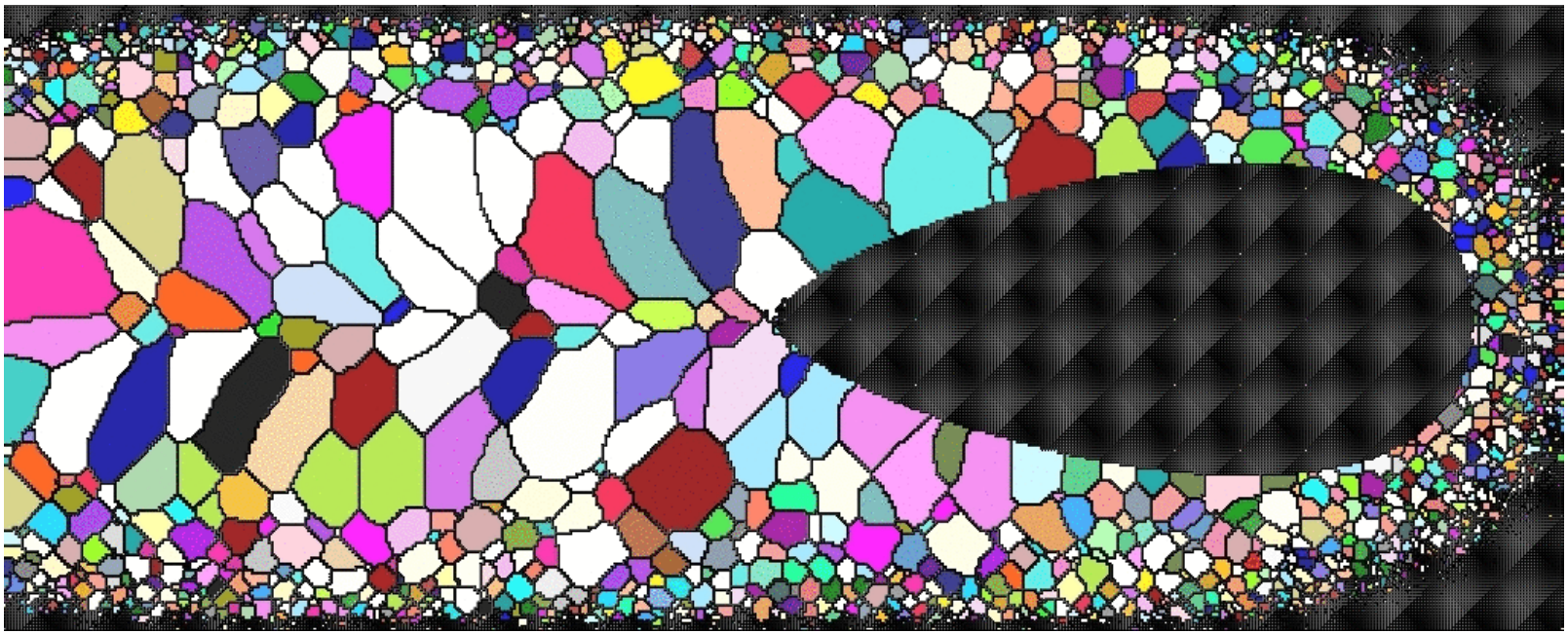

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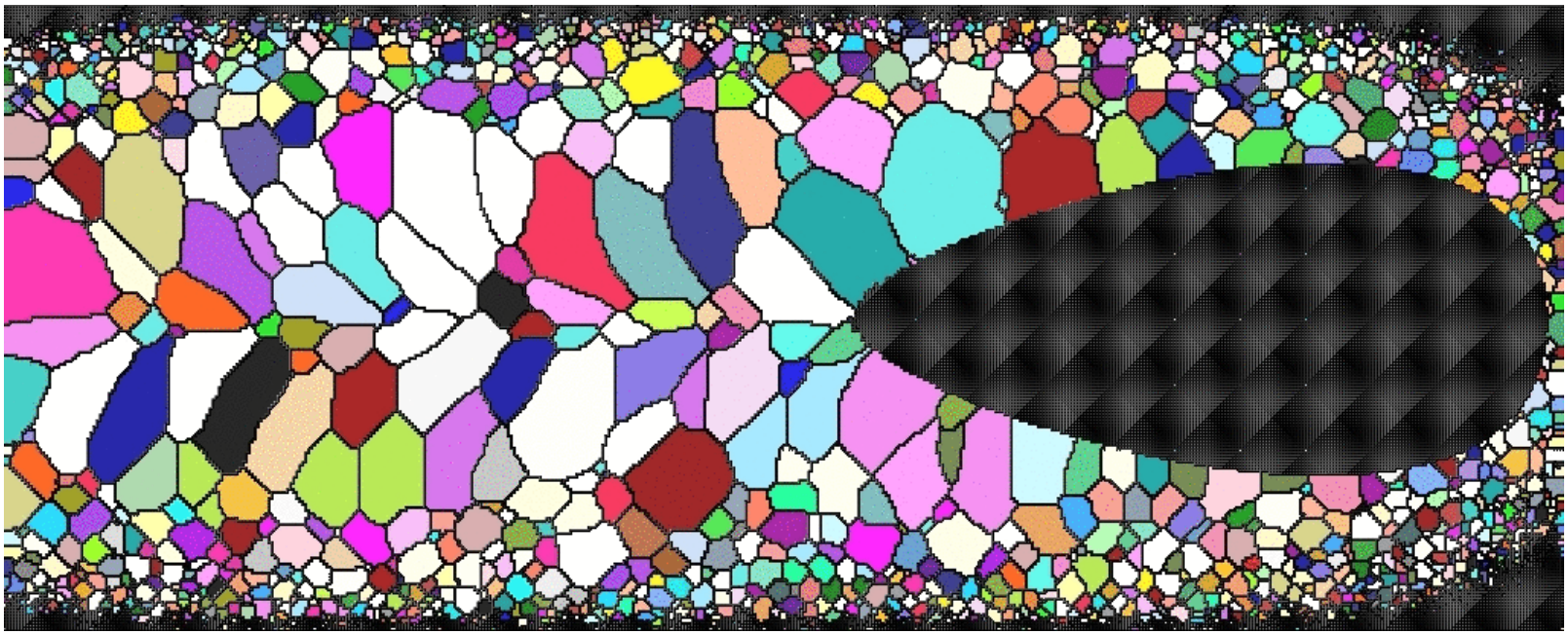

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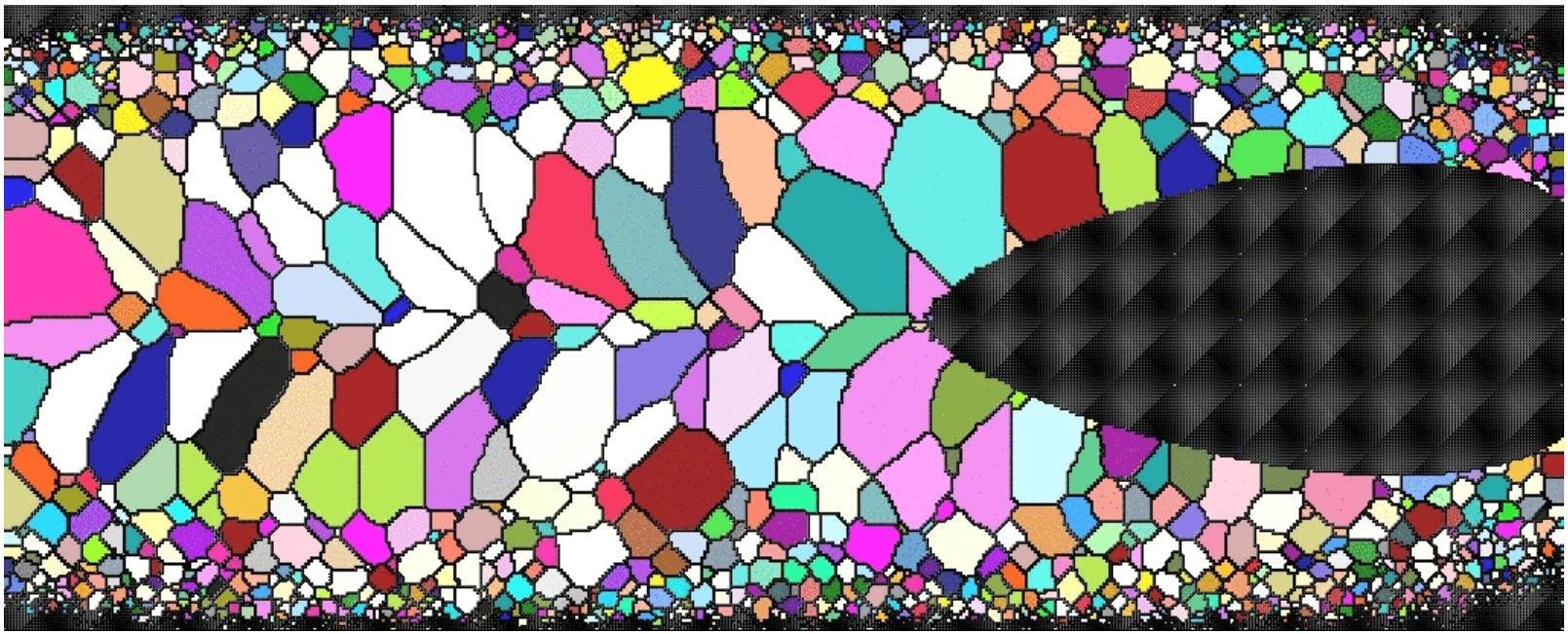

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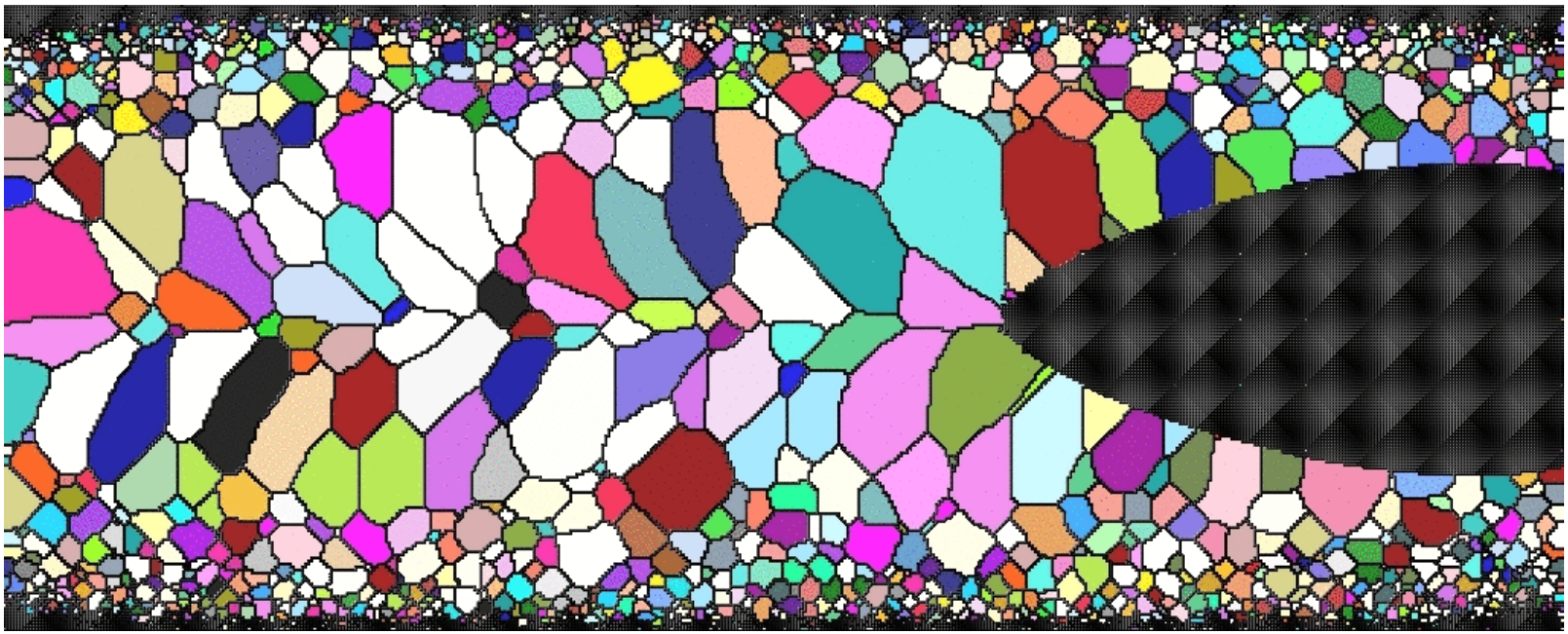

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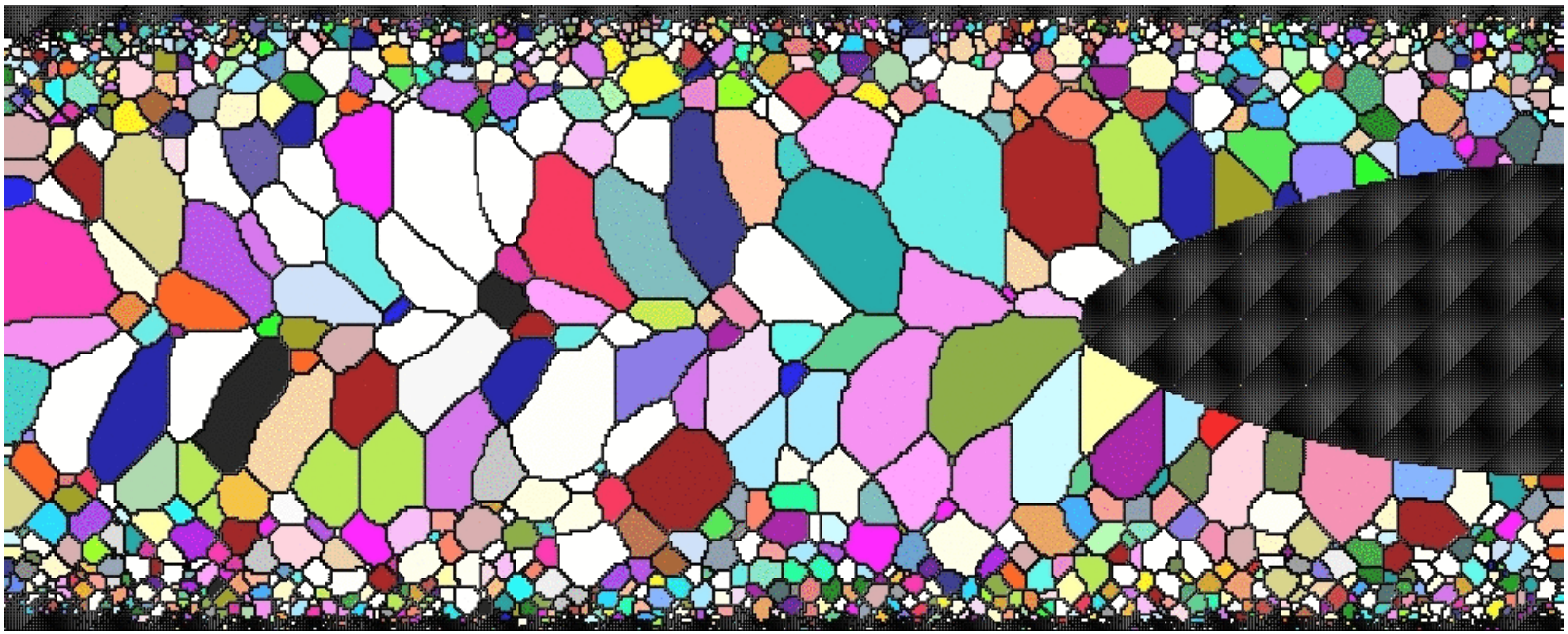

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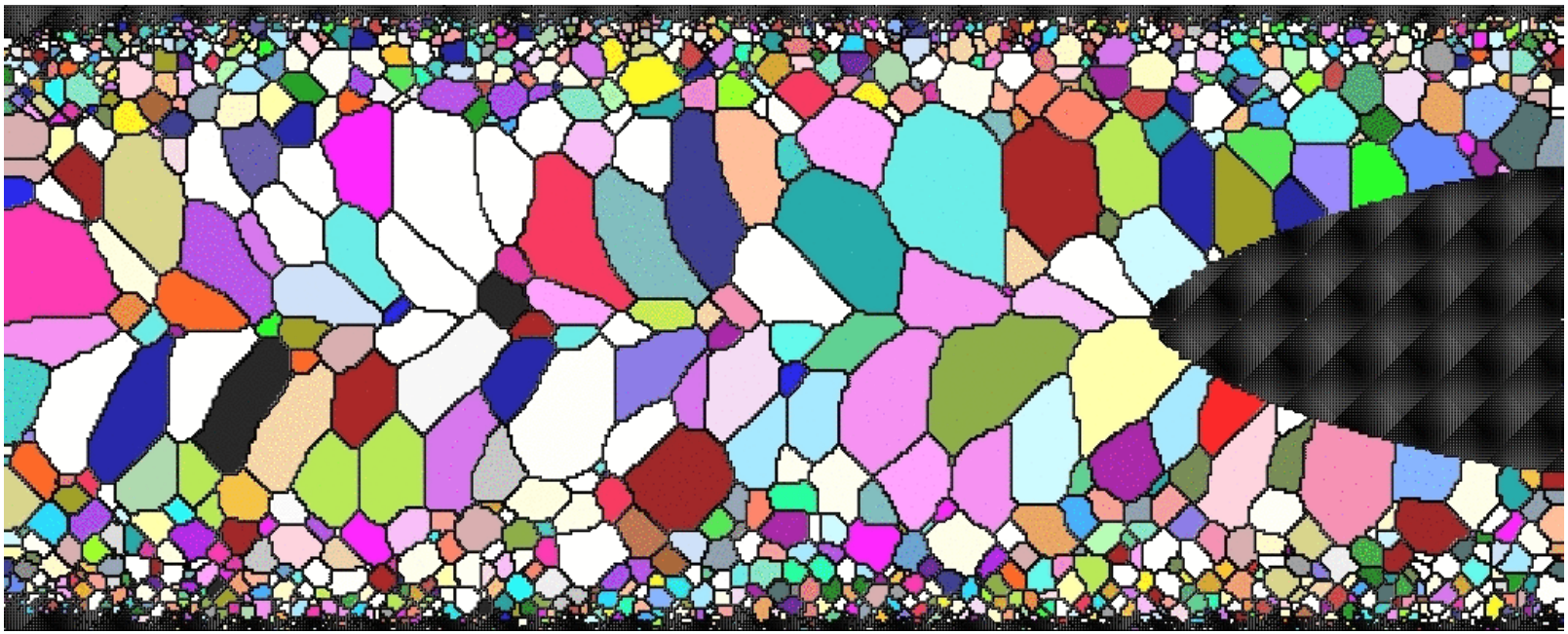

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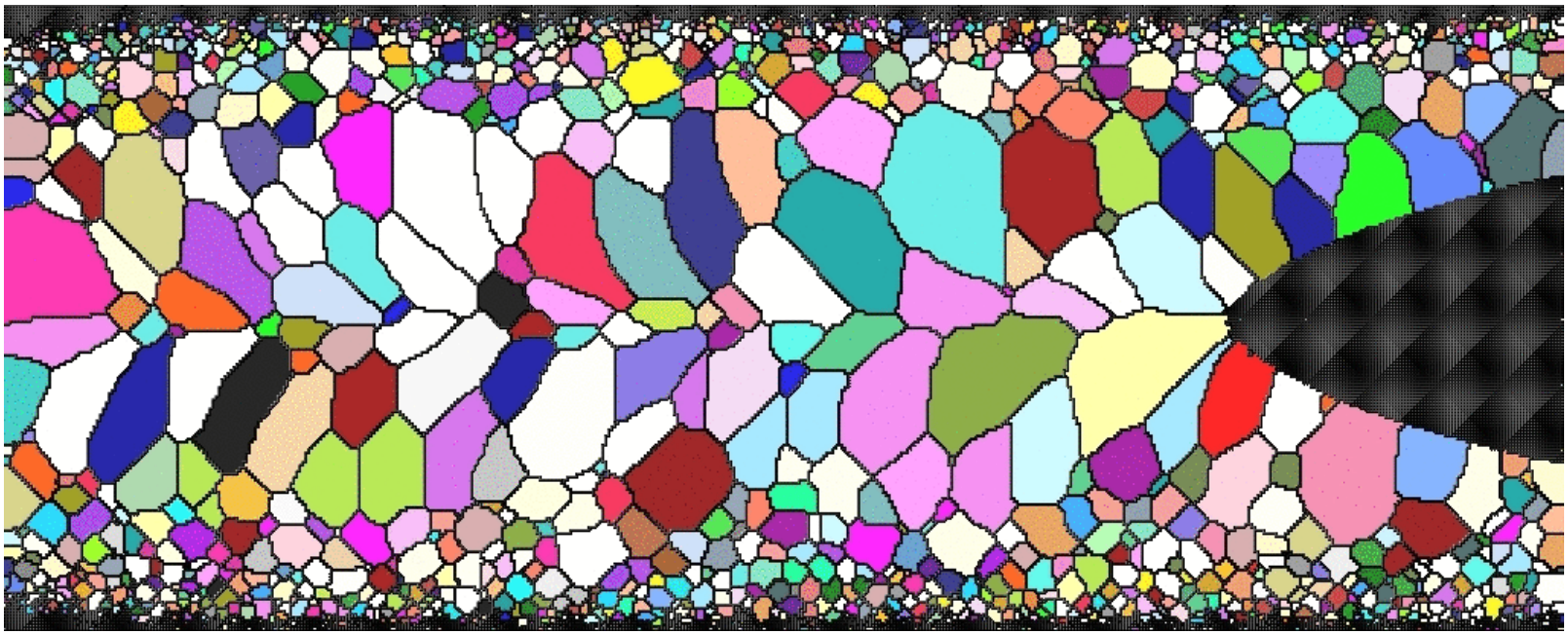

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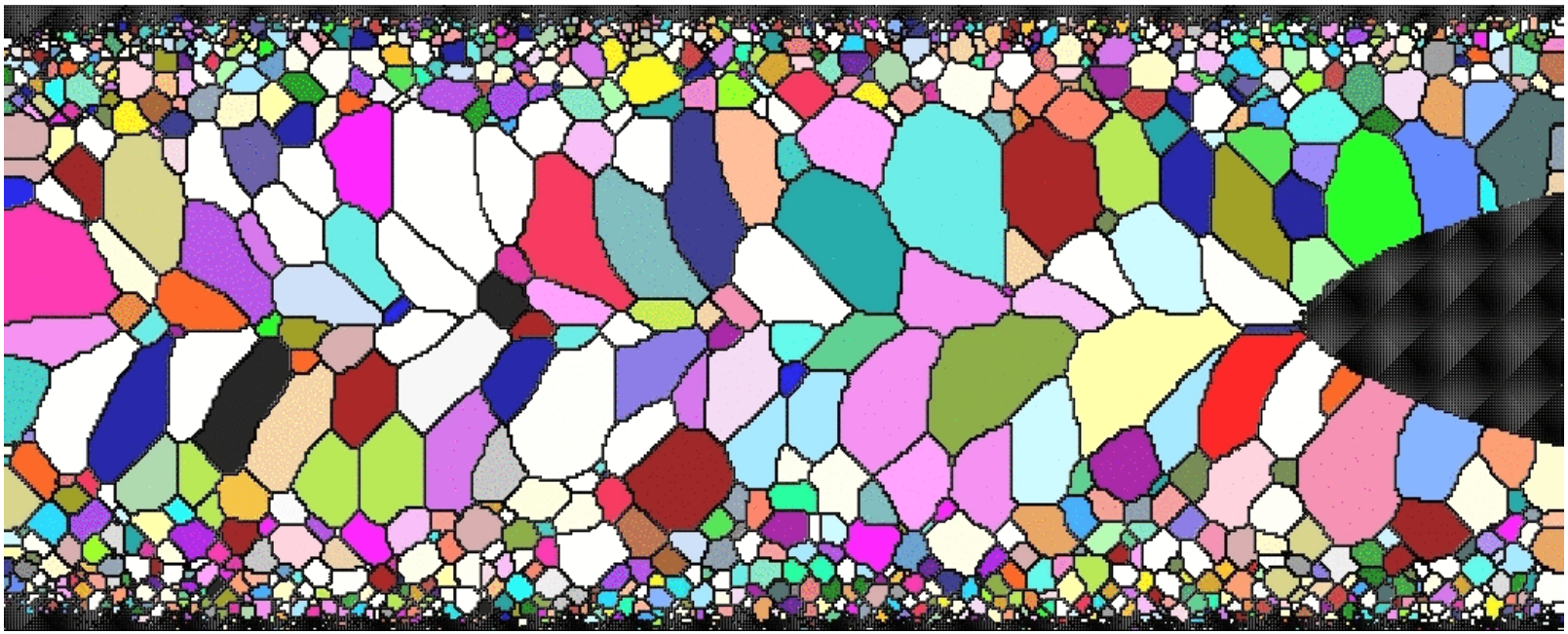

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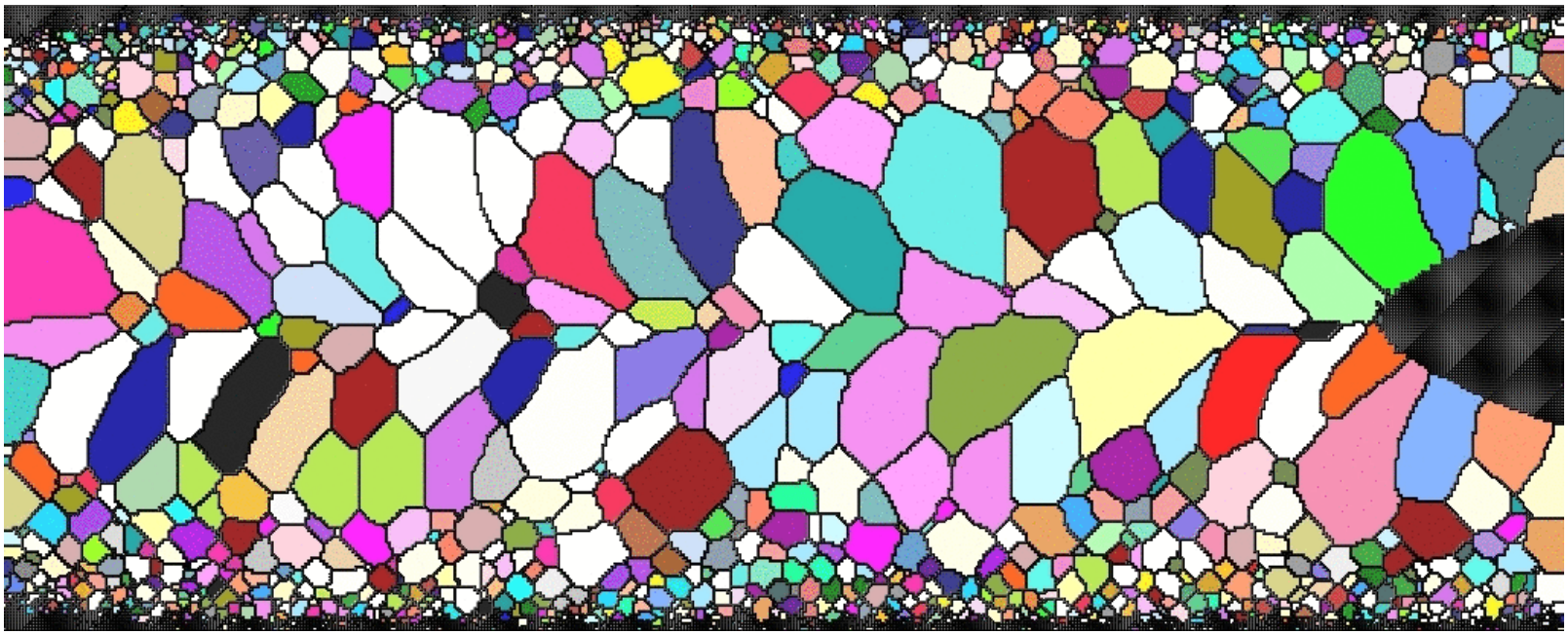

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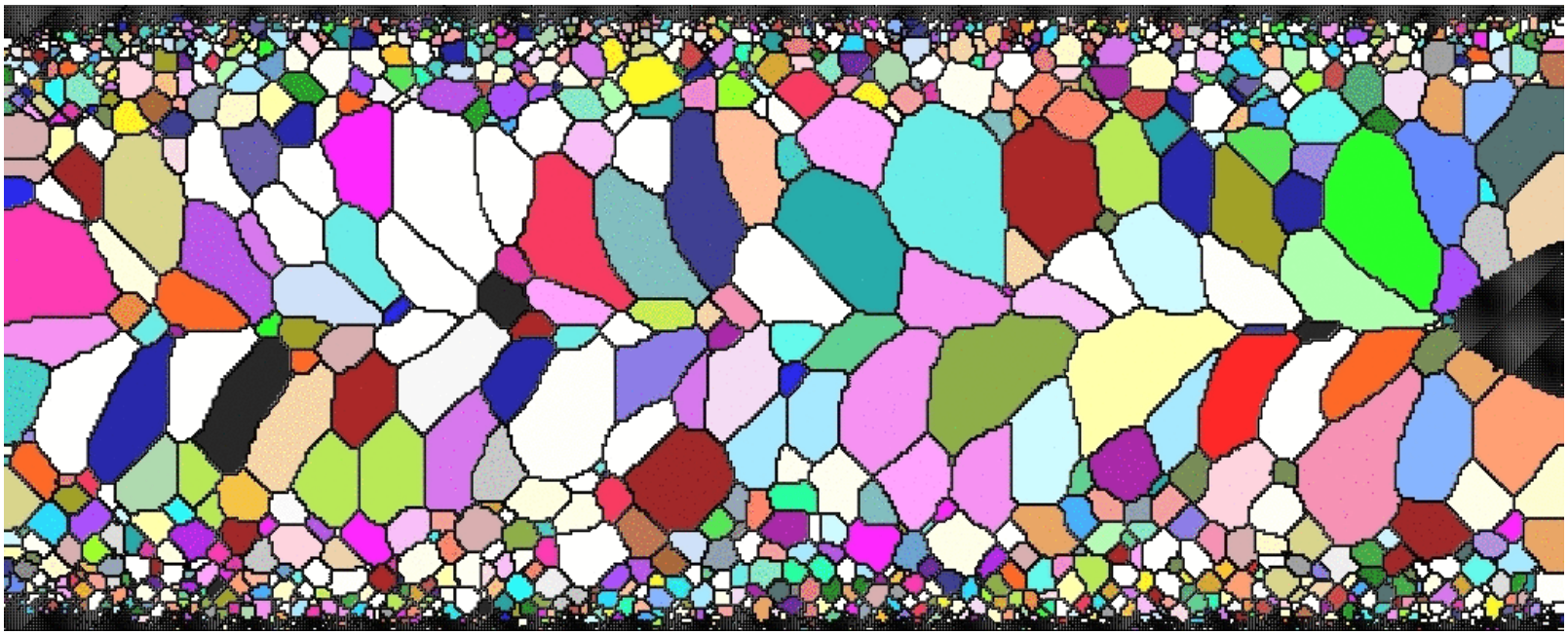

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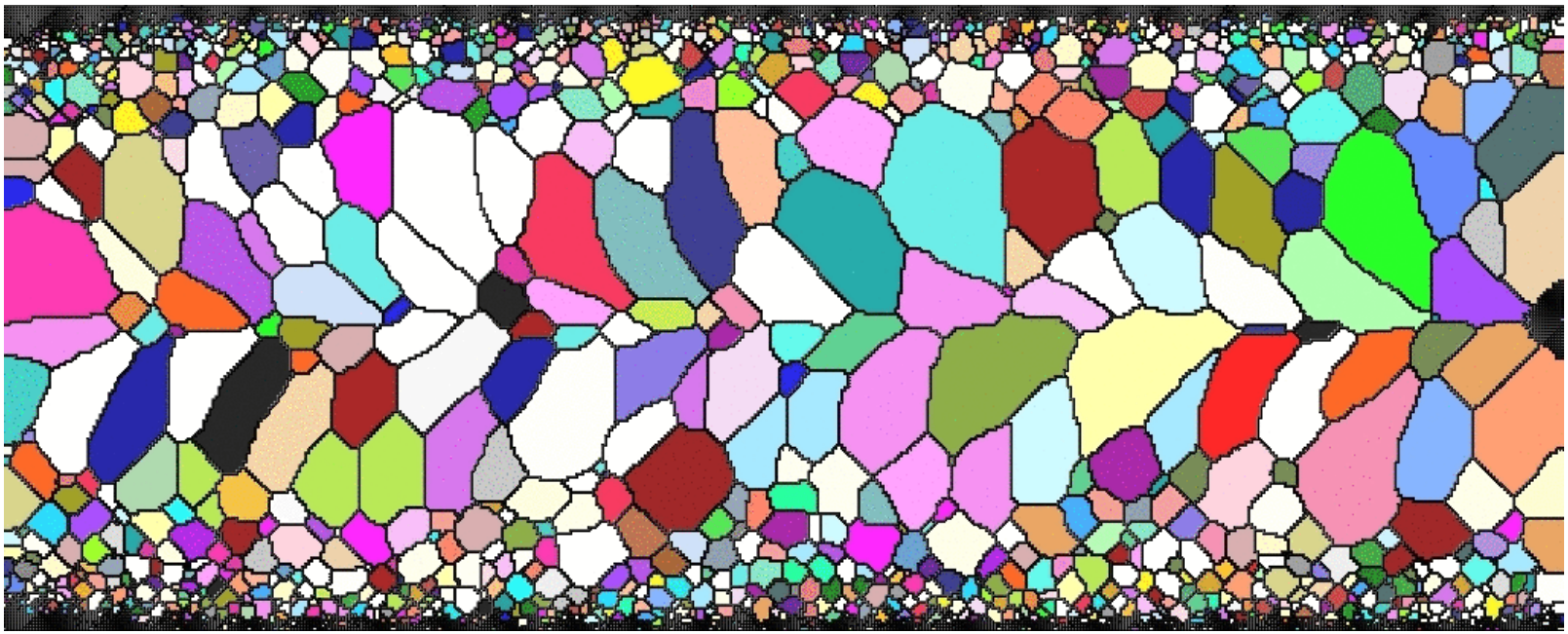

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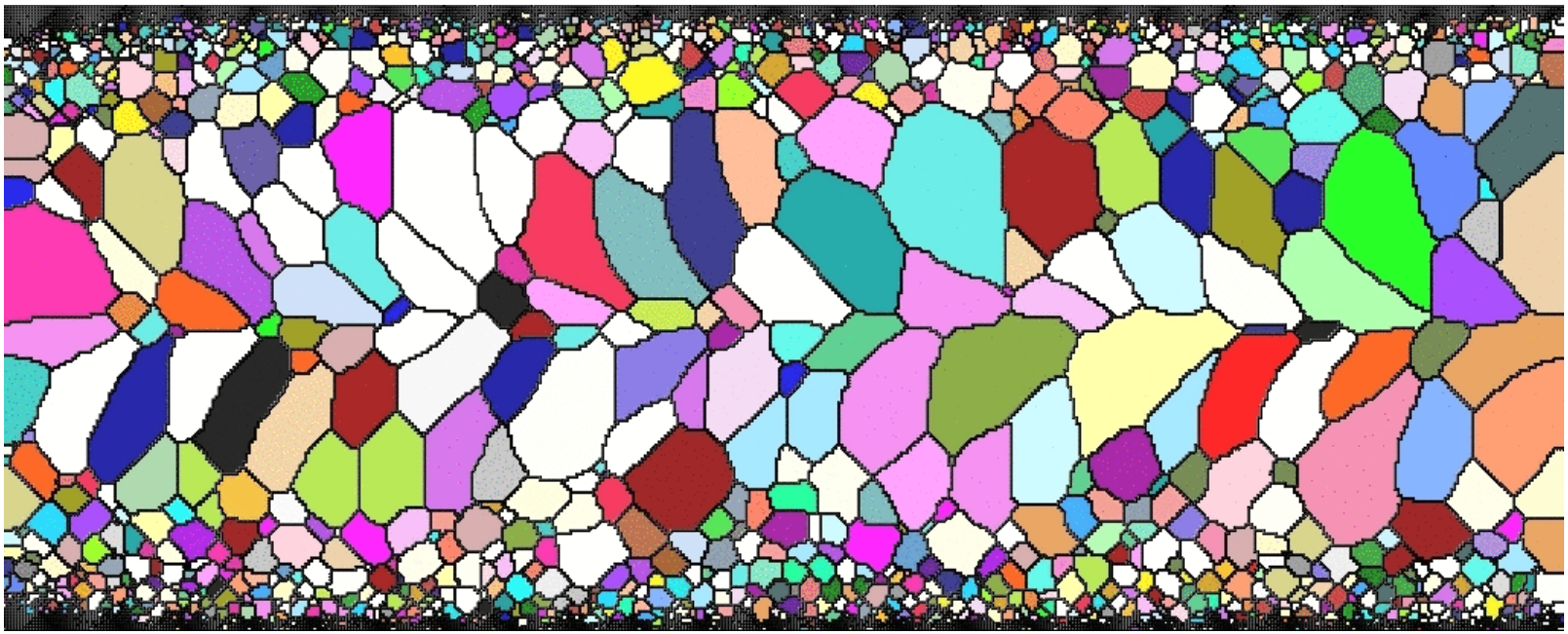


FAQs

- Is the simulation deterministic? No, the microstructure is random, so you should expect some randomness. It is computationally reproducible via the random seed, but once the seed changes, the results change.
- Can I run SPPARKS? Yes, and you are definitely encouraged to try it out.
- Do I need to run SPPARKS? You can, but it is not entirely necessary. We provide the dataset, but it is entirely up to you if you want to run more.
- Is there a SPPARKS tutorial? https://spparks.github.io/tutorial/html/index.html
- Can SPPARKS run on Windows? Unfortunately, no. You will need a Mac-based or Linux-based machine to run SPPARKS. If you use Windows, you can consider installing a virtual machine (e.g. VMware).
- How to compile and run SPPARKS? Please connect with us. We can help you compile and run SPPARKS on your machine. You need a C++ compiler, perhaps supported by OpenMPI or MPICH. After compiling, you can run the SPPARKS executable.

Introduction

General ideas:

- every big metallic object has its own unique microstructure, but it is too big
- SPPARKS can generate microstructure, but it is pretty small
- given a microstructure dataset, we ask you to generate/synthesize microstructure for some given CAD objects (in STL format)
- points vary on difficulty levels (beginner: 10 pts, intermediate: 30 pts, hard: 50 pts)
- pick three CAD objects (depending on their difficulty) from the problem statement (located in `cad/` folder)

Dataset

- download from https://zenodo.org/record/8241535
- 1000 folders `seed-{001-1000}`
- each folder contains a snapshot of a normal grain growth simulation size $100 \times 100 \times 100$ voxels: `dump.50.out` and `potts_3d.50.vti`
- resolution: 1 voxel $= 10\mu$m; volume $= 1$ mm^3
- grain ID as a function of (x, y, z)
- two types of files to pay attention to
  - `dump.*.out`
  - `potts_3d.*.vti`
  - `*` denotes SPPARKS time-stamp
  - `Spin` or `id` means grain ID
  - can be visualized through `ParaView` (https://www.paraview.org/) or `Ovito` (https://www.ovito.org/)

Tasks

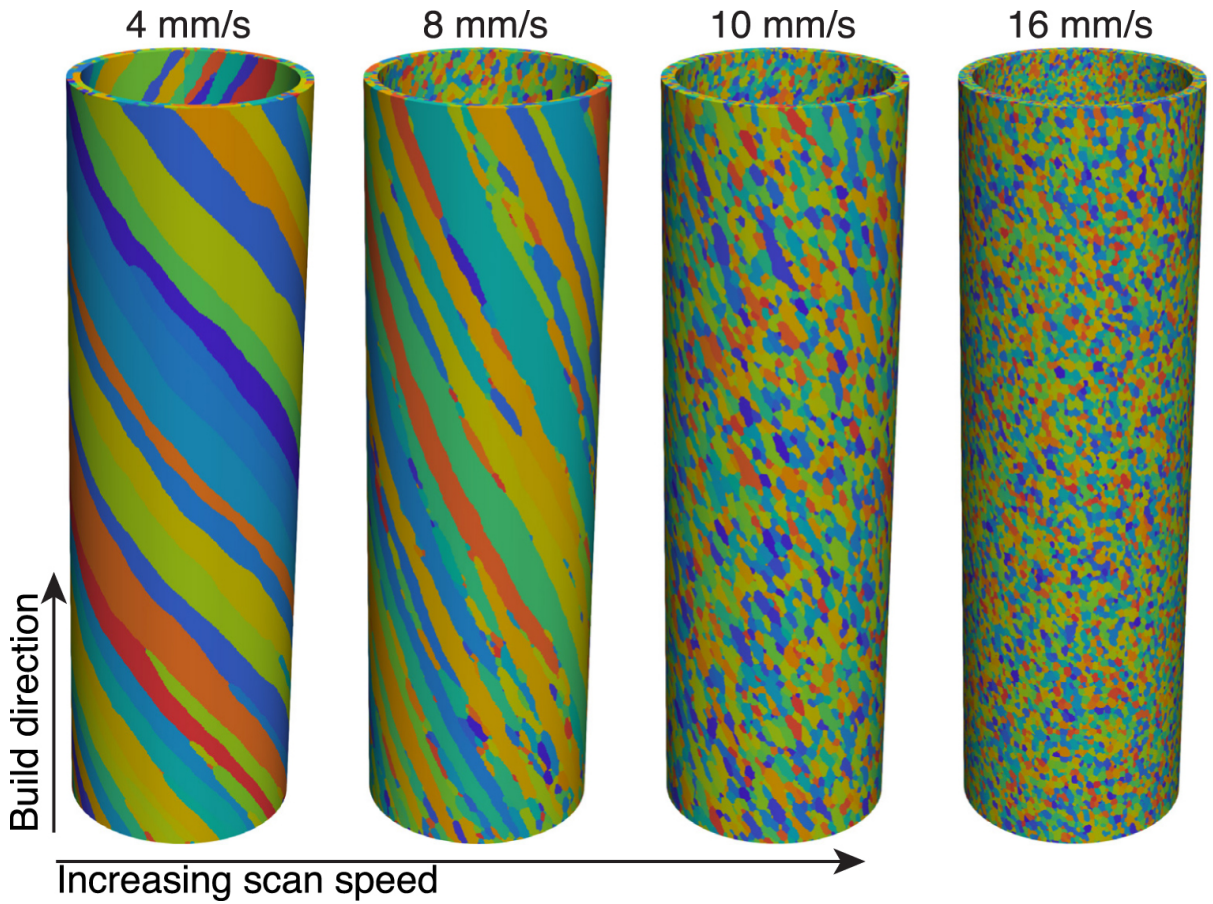
Tasks:

- use the provided dataset or generate your own SPPARKS dataset to generate microstructure for CAD objects.
- bonus point: generate multiple microstructures for the same CAD object.
- visualize the results via `ParaView` or `Ovito`

Difficulty levels depend on the geometric complexity of the CAD object. Pick any 3 that fits your taste.

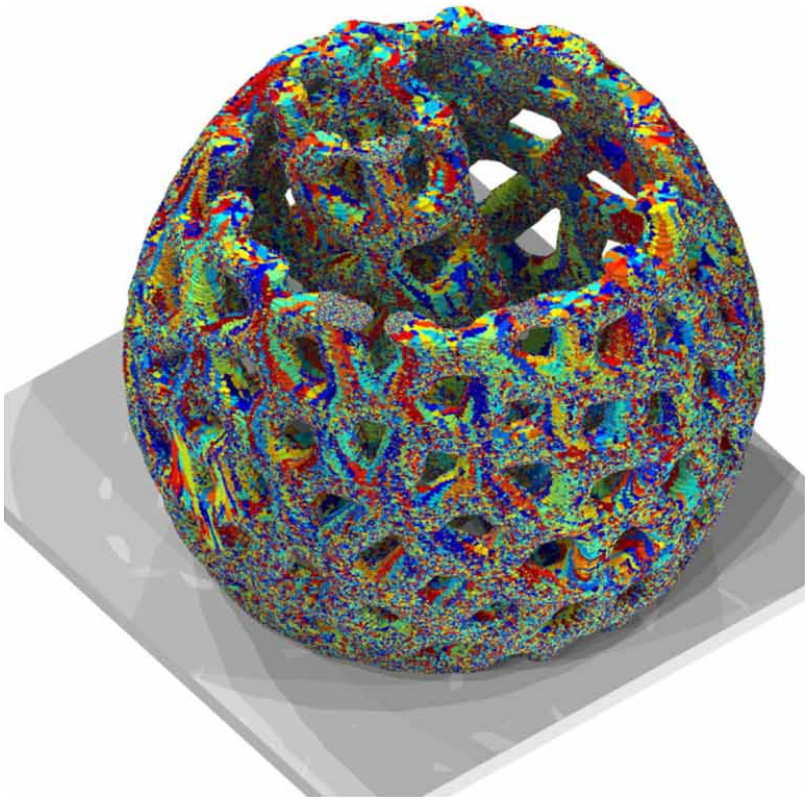
- beginner: 10 pts,
- intermediate: 30 pts,
- hard: 50 pts.

Example 1



A hollow tube by Rodgers, Bishop, and Madison.
https://iopscience.iop.org/article/10.1088/1361-651X/aac616/meta.

Example 2



An open lattice structure from John A Mitchell et al

2023 Modelling Simul. Mater. Sci. Eng. 31 055001.
https://iopscience.iop.org/article/10.1088/1361-651X/accc4b.

GitHub repository

Please check https://github.com/anhvt2/spparks-hackathon/ for the most update:

1. problem statement,
2. link to the SPPARKS dataset,
3. CAD objects in STL format.

Dataset: https://zenodo.org/record/8241535

Submissions

Submissions:

- upload the generated microstructure somewhere, e.g. Zenodo.org or directly to GitHub (if less than 100MB)
- visualize, capture and submit screenshots

Must include

1. the generated microstructure file in the same given format (`dump.*.out` or `*.vti`) that can be visualized by `ParaView` or `Ovito`
2. the screenshots that capture the visualization
3. the presentation that describes the approach

Q&A

Thanks and Good luck!

Remarks:

- SPPARKS tutorial upon request
- question via Slack channel or virtual office hour or virtual appointment (Zoom meeting upon request)
- participants are not obligated to use the provided dataset if fluent in SPPARKS. Indeed, the input script to generate the dataset is included within the dataset, so please feel free to go in any direction that you deem best.