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MATBOX, an Open-Source Microstructure Analysis Toolbox for Meshing, Generation, Segmentation, and Characterization of 3D Heterogenous Volumes

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InterPore2021 Online, 13th Annual Meeting, 31 May – 4 June 2021

Resources

Journal article: F. L. E. Usseglio-Viretta et al., *MATBOX: An Open-source Microstructure Analysis Toolbox for microstructure generation, segmentation, characterization, visualization, correlation, and meshing*, SoftwareX, submitted

Software repository and documentation:
https://github.com/NREL/MATBOX_Microstructure_analysis_toolbox

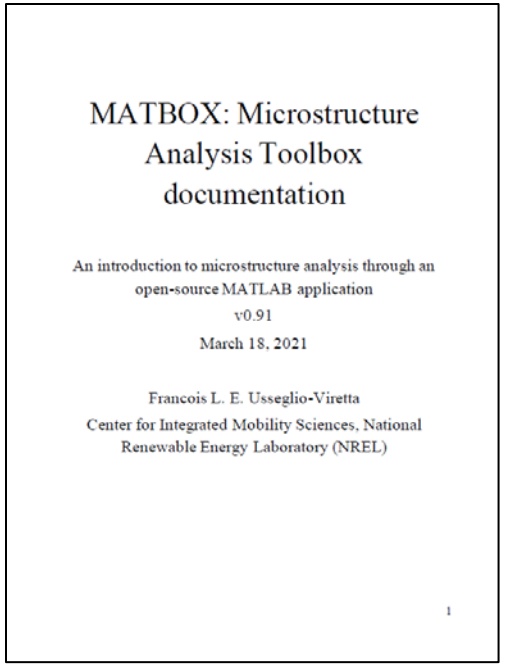
Requirements: MATLAB 2020a + Image Processing toolbox

Current version: v1.0 - May 2020

License: BSD license. NREL Software Record number SWR-20-76

Third-party algorithms/software: *TauFactor*[1] (UCL, S. Cooper), *Iso2mesh*[2] (Northeastern Univ., Q. Fang), *additive generation*[3] (Purdue University, A. Mistry, P. P. Mukherjee)

+ other codes from MATLAB file exchange (full list in documentation)


MATBOX: Microstructure Analysis Toolbox documentation

An introduction to microstructure analysis through an open-source MATLAB application

v0.91

March 18, 2021

Francois L. E. Usseglio-Viretta

Center for Integrated Mobility Sciences, National Renewable Energy Laboratory (NREL)

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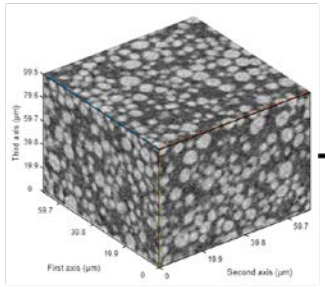
Exhaustive documentation (~190 pages)

[1] S.J. Cooper et al., Softwarex. 5 (2016) 203–210, https://doi.org/10.1016/j.softx.2016.09.002.
[2] Q. Fang et al., IEEE (2009) 1142–1145, https://doi.org/10.1109/isbi.2009.5193259.
[3] A. Mistry et al., ACS Applied Materials & Interfaces. (2018), https://doi.org/10.1021/acsami.7b17771.

What is MATBOX / what for ?

MATBOX is a MATLAB application for performing various microstructure-related tasks including **microstructure numerical generation**, **image filtering** and **microstructure segmentation**, **microstructure characterization**, **three-dimensional visualization**, **result correlation**, and **microstructure meshing**. MATBOX was originally developed to **analyze electrode microstructures for lithium-ion batteries**; however, the algorithms provided by the toolbox are widely applicable to other heterogeneous materials.



A lithium-ion battery cathode
3D volume obtained from nanoscale imaging
(computed tomography or FIB-SEM)

Application 1:
Macrostructure scale battery modeling.
MATBOX calculates microstructure parameters (particle size, effective diffusion coefficient, etc.) useful for battery macroscale models such as Pseudo-2D.

Application 2:
Microstructure scale battery modeling.
MATBOX produces meshes of full cells useful for battery microscale model (direct numerical simulation).

+ generation module allows you to investigate large design space for both applications, for optimization or microstructure-parameter sensitivity calculations.

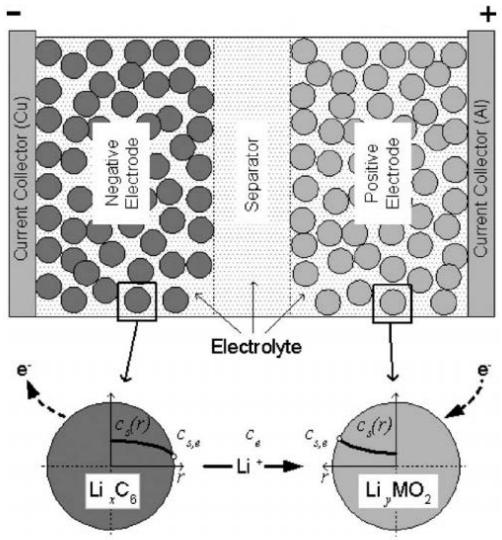
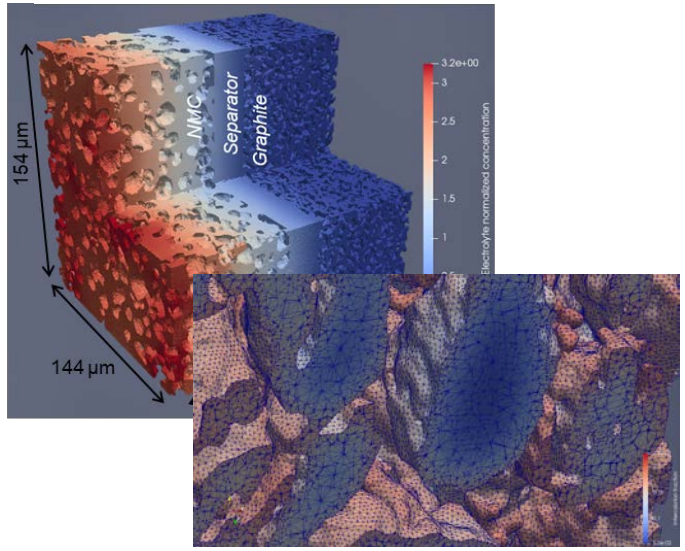
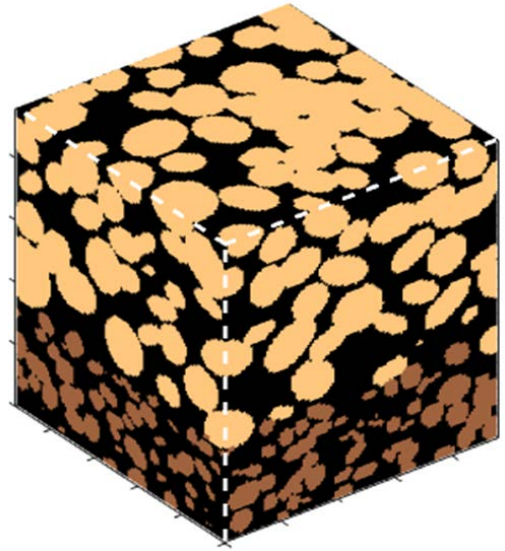


Fig. 1. Schematic of 1D (*x*-direction) electrochemical cell model with coupled 1D microscopic (*r*-direction) solid diffusion model.

Microstructure parameters for macroscale LIB model*



Full cell meshing**



Design space analysis***

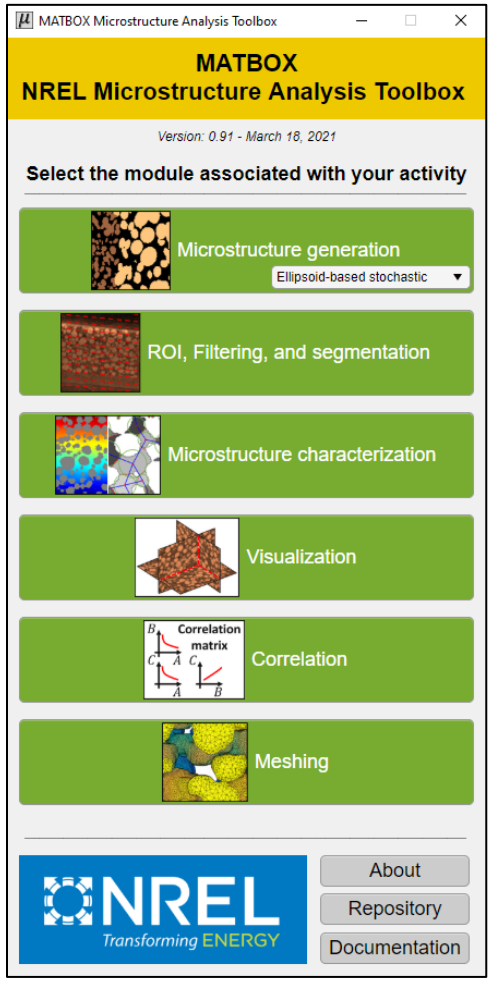
* F. Usseglio*viretta et al., JES. (2020), https://doi.org/10.1149/1945-7111/ab913b
* F. Usseglio-Viretta et al., JES. 165 (2018), https://doi.org/10.1149/2.0731814jes
* F. Usseglio-Viretta et al., ECS Transactions. 77 (2017), https://doi.org/10.1149/07711.1095ecst

** J. Allen et al., J Sci Comput. 86 (2021), https://doi.org/10.1007/s10915-021-01410-5

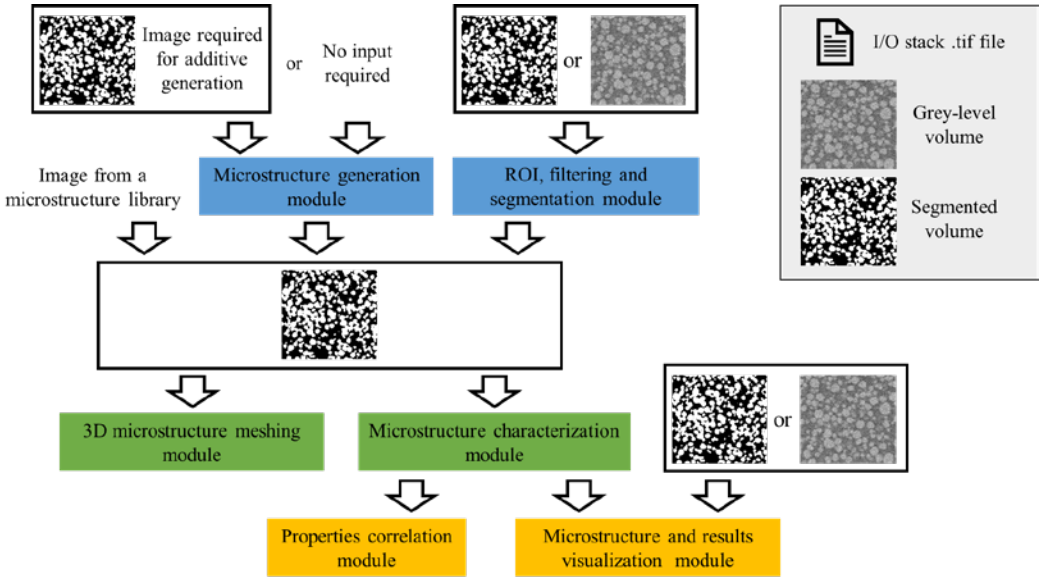
*** ANL, INL, NREL, SLAC, LBNL, XCEL, extreme fast charge cell evaluation of Lithium-ion batteries, 2019. https://blogs.anl.gov/access/wp-content/uploads/sites/53/2019/09/Q3FY19-XCEL-Report.pdf (pp 10-11)

How to use MATBOX ?

Divided into modules

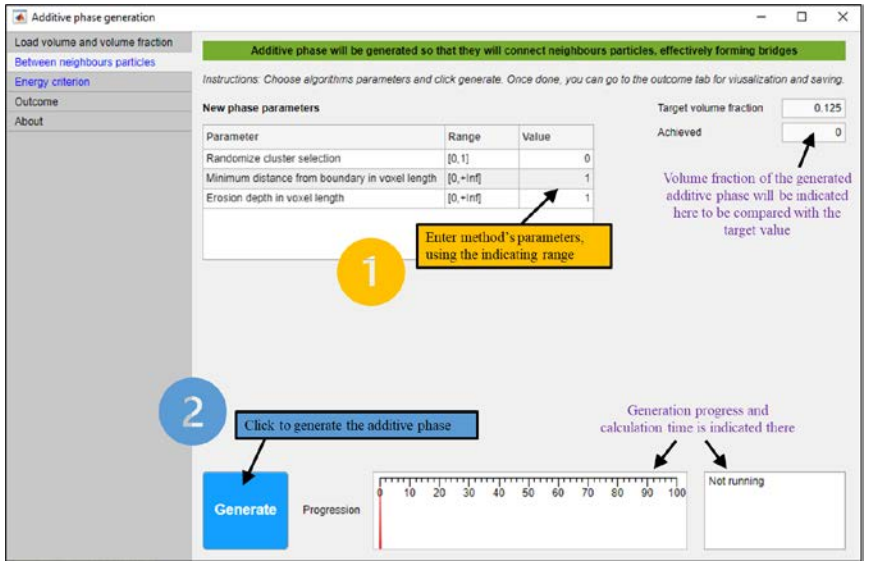


Modules I/O



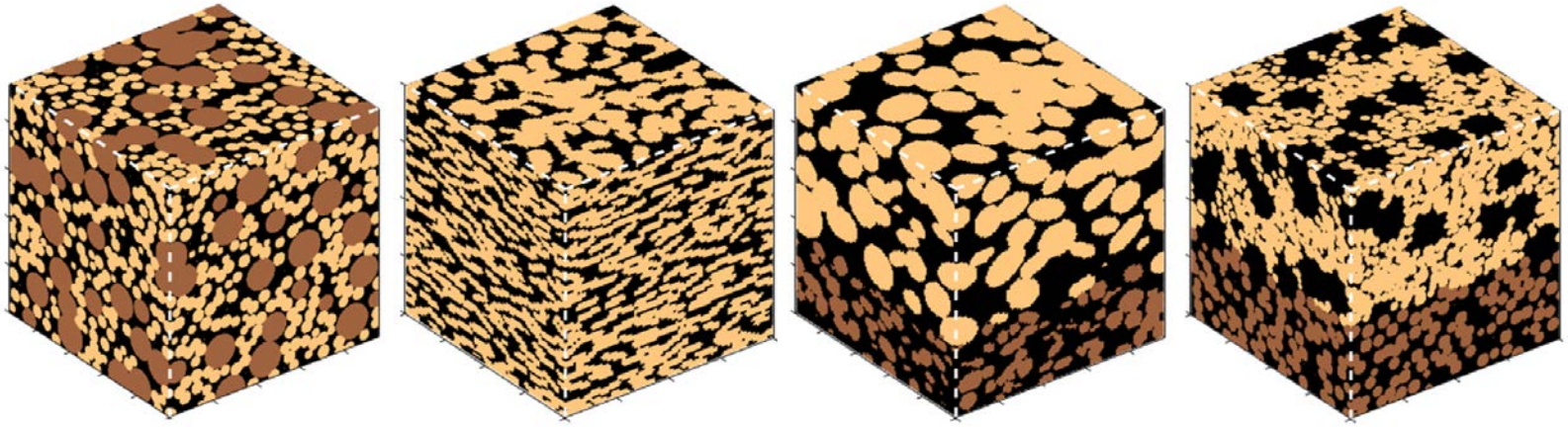
➢ Module connectivity

GUI for each module



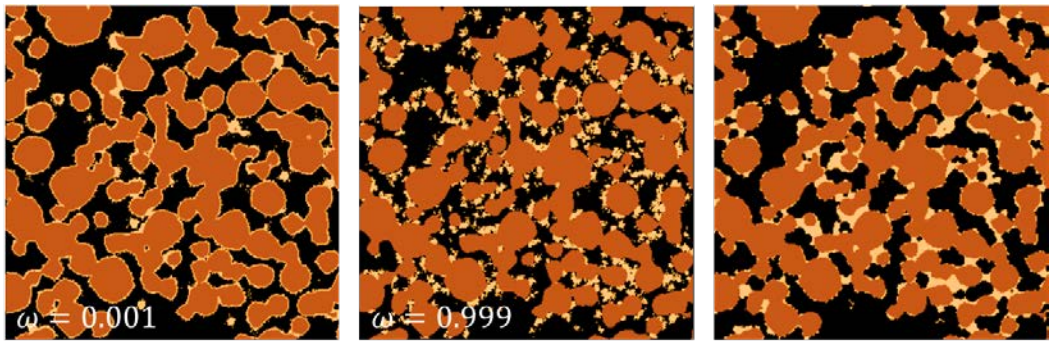
➢ User friendly interface

Microstructure generation



In-house stochastic generation algorithm

- n-phases microstructure
- Ellipsoid-based, with particle overlapping control
- Control of volume fractions, particle size, elongation and orientation distributions all along the thickness
- Generation order control



In-house distance-based additive generation algorithm and third-party energy-based additive generation algorithm

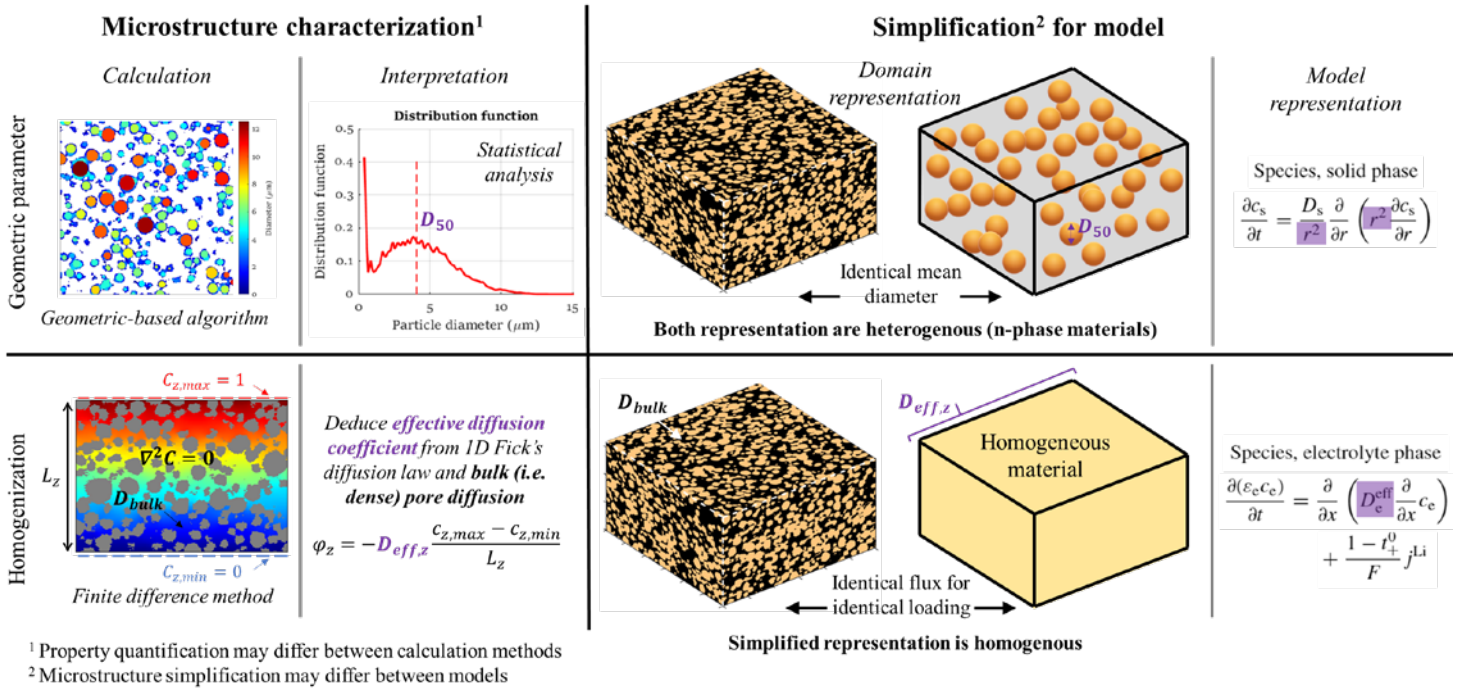
- Preferential location between neighbored particles (bridge).
- Preferential deposition toward active material (thin surface layer, w=0.001) or additive phase (dendritic-like phase, w=0.999).

Investigate 'what if' microstructures and complement imaging limitations

- Provide **effective parameters for macroscale electrochemical model**
- Provide **geometries for microscale electrochemical model**

Pre-screening tool to down-select few architectures worth manufacturing/testing from large design space

Microstructure characterization and homogenization



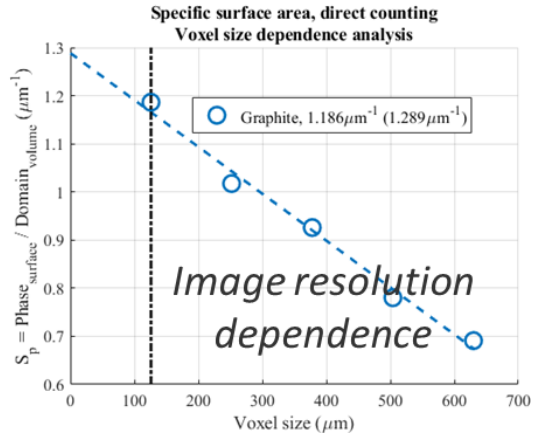
[1] Property quantification may differ between calculation methods
[2] Microstructure simplification may differ between models

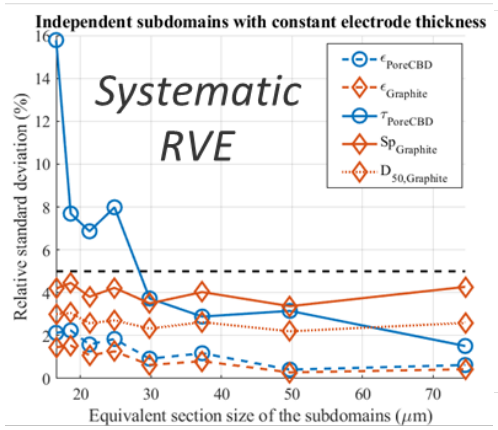
Microstructure characterization and homogenization for macroscale models

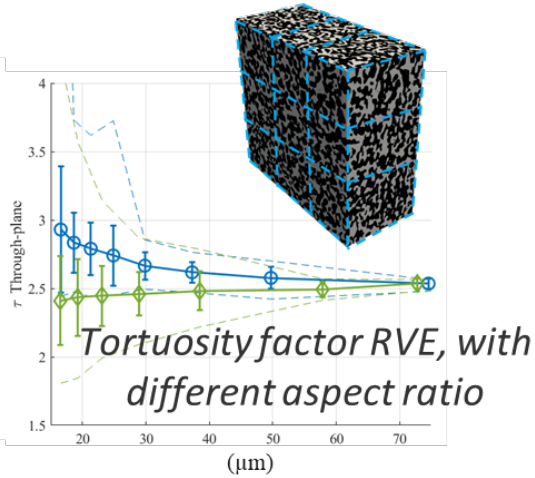
- volume fractions, connectivity (both isotropic and directional), tortuosity factor, geometric tortuosity
- specific surface area, particle size, particle identification and morphology.

Error evaluation / time saving

- Automated voxel size dependence analysis (evaluate microstructure parameter error induced by limited image resolution)
- Automated representative volume element (RVE) analysis (evaluate microstructure parameter error induced by limited field of view) → **hundreds of calculations automated**
- batch calculations to characterize multiple volumes in a row.
- Results organized in subfolders (.png, .fig, .xlsx)



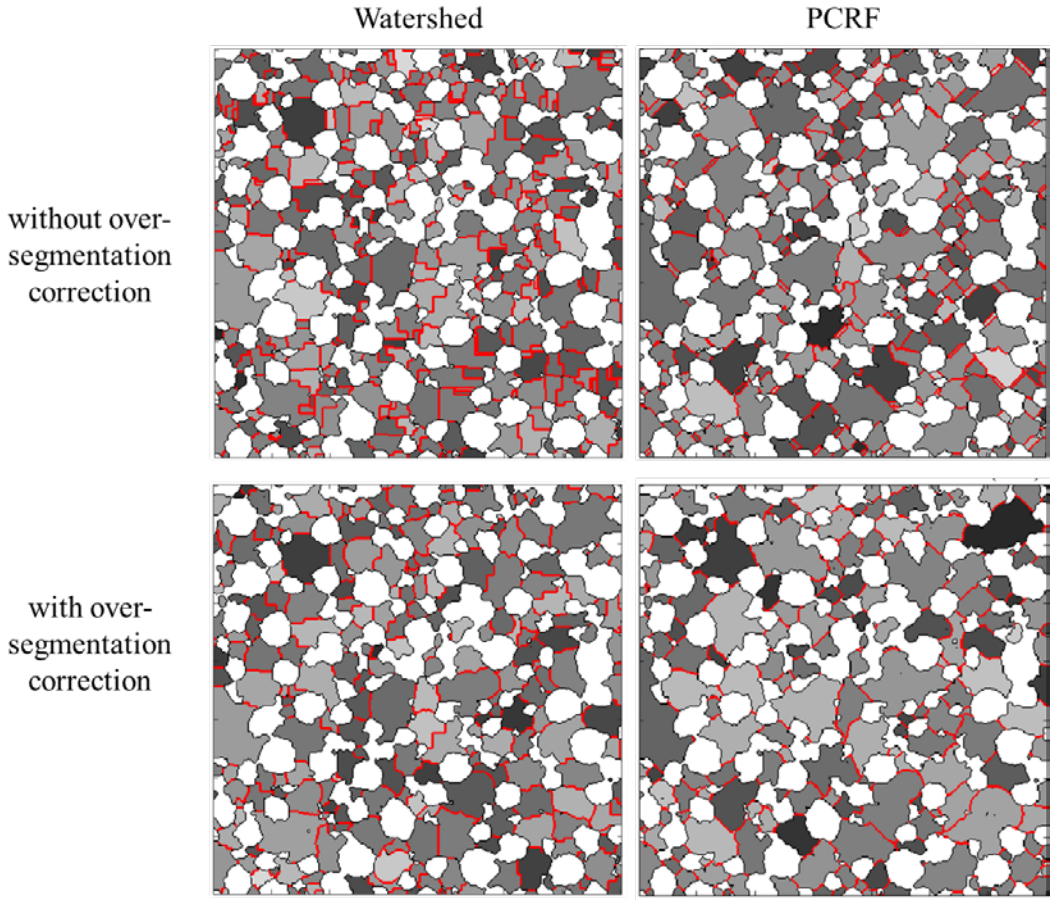


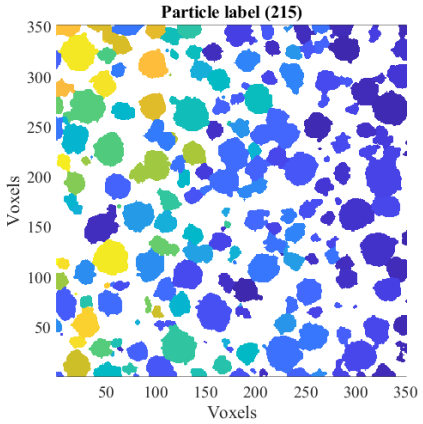


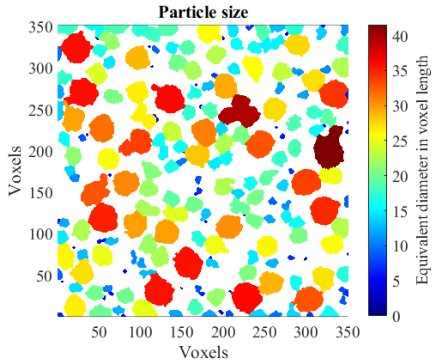
Microstructure characterization: particle analysis

X-ray Computed tomography typically provides a near fully connected active material phase.

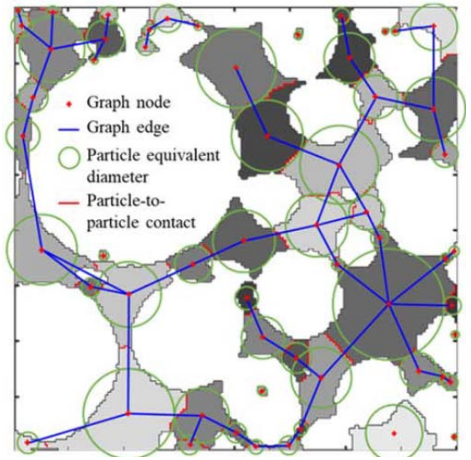
- There is not a unique definition of what is a particle in a connected cluster.
- There is a large choice of numerical methods in the literature consequently, with a wide range of diameter between methods.
- Module provides **continuum particle size distribution (c-PSD)**, in-house **Euclidean distance map fitting (EDMF)**, **Watershed algorithm with** in-house **over segmentation correction**, and in-house **particle identification algorithm** (PCRF, F. Usseglio-Viretta et al., JES. (2020), https://doi.org/10.1149/1945-7111/ab913b)







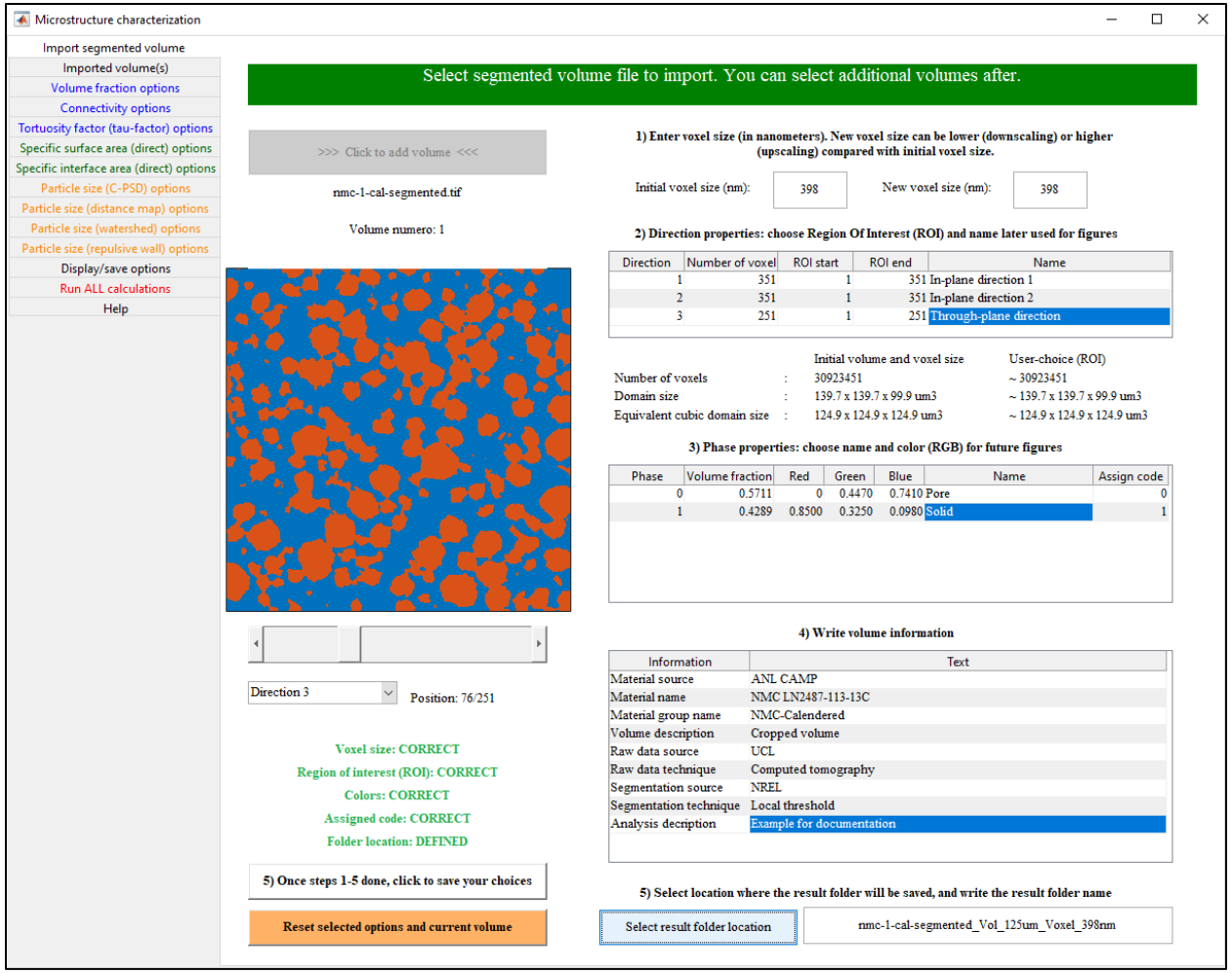
Better estimation of particle size compared with oversimplified spherical assumption (+ sphericity and elongation calculation)



- Particle (or pore segment) identification is used to calculate **geometric tortuosity**
- Contact area variation is used to calculate **constriction factor**

$$\frac{D_{eff,i}}{D_{bulk}} = \frac{\varepsilon}{\tau_i} \approx \frac{\varepsilon\delta_i}{\tau_{geo,i}}$$

Microstructure characterization: how to use



Select microstructures to analyze and properties to investigate using GUI

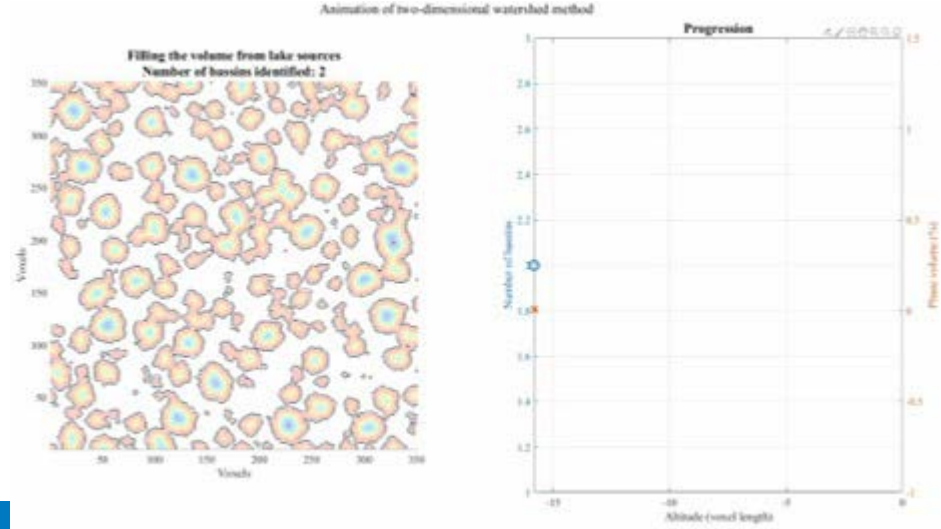
Functions have two syntax: one for the GUI (no command line required), one to be used as standalone

```
function [] = Function_particle_size_CPSD(Phase_microstructure, PROPERTY, OPTIONS, INFO)
%Calculate Particle size with a spherical assumption (C-PSD)
% Function_particle_size_CPSD(array, PROPERTY, OPTIONS, INFO) - when use with the toolbox
% or
% Function_particle_size_CPSD(array, voxelsize) - when use as a standalone function
```

Look for *_algorithm.m for the core function (i.e., w/o any post-processing and figures). Allow you to easily modify code w/o touching the GUI.

```
M=function_load_tif('C:\Users\fussegli\Desktop\nmc-1-cal-segmented.tif');
solid_phase_id = 1;
binary_phase = zeros(size(M));
binary_phase(M==solid_phase_id)=1;
[Particle_size] = Function_particle_size_CPSD_Algorithm(binary_phase);
```

Some complex functions have a step-by-step visualization optional arguments for education/understanding (see documentation)

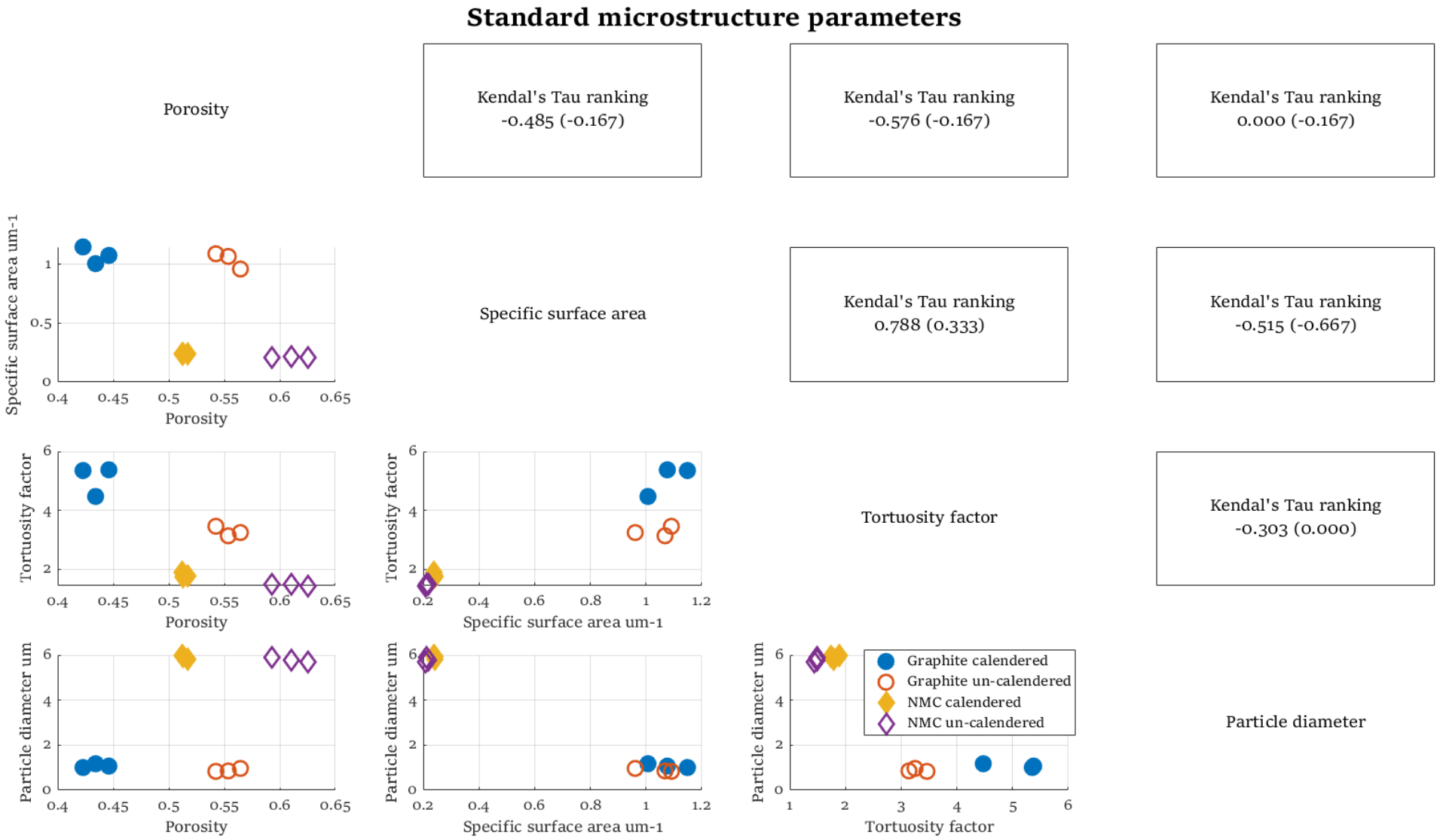


Microstructure correlation

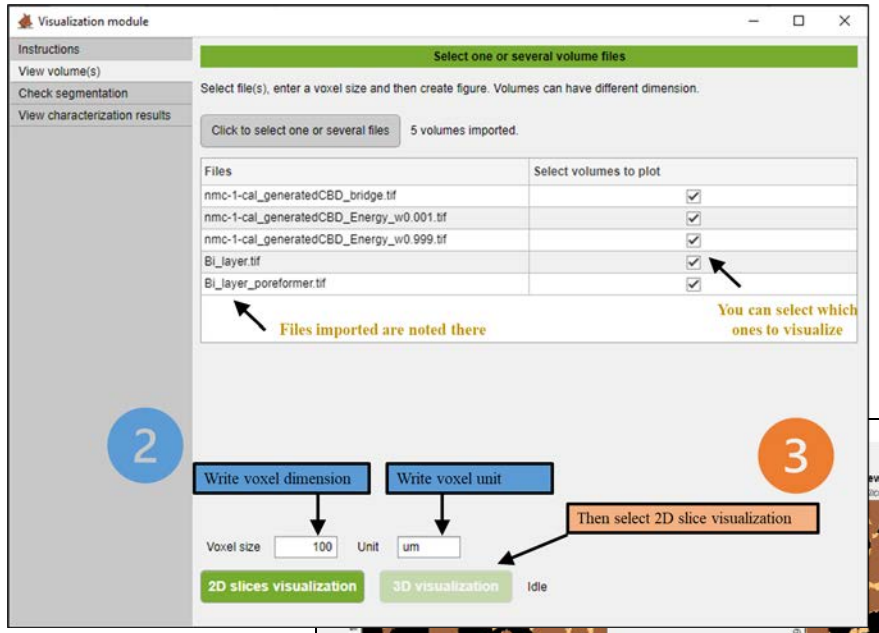
Microstructure parameter correlation:

- Load results from the characterization module.
- Choose what parameters to correlate. A lot of parameters are available, not only basic results (e.g., RVE size, std(d50) etc.).
- User can easily add custom parameters (see documentation).
- Generate correlation-matrix-type graph and table and export it.
- Plot each result with its own legend, or group them (cf. right illustration).
- All done within a GUI.

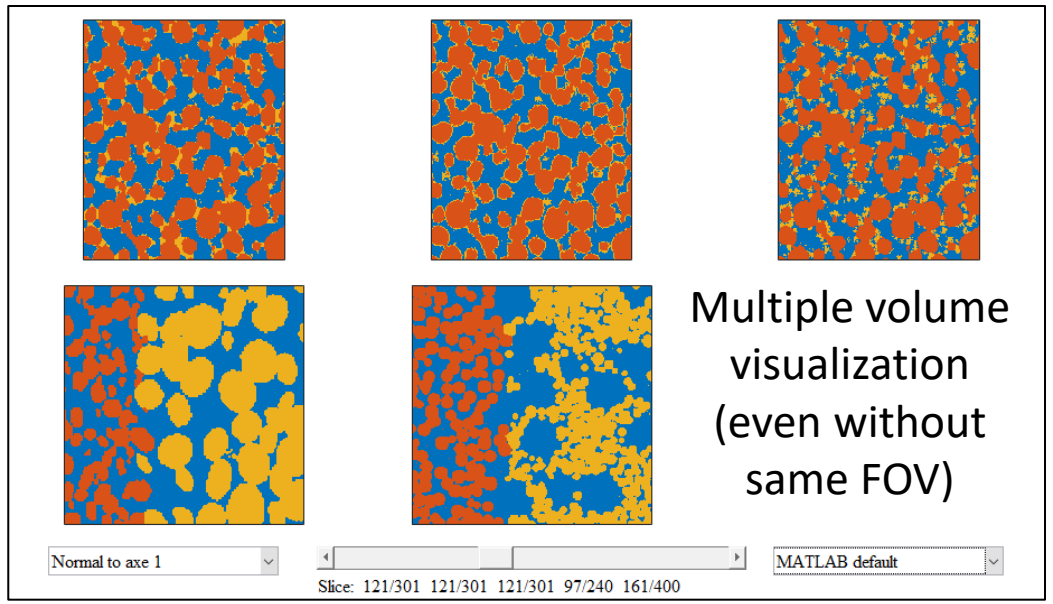
➢ Useful to reveal unsuspected correlations.



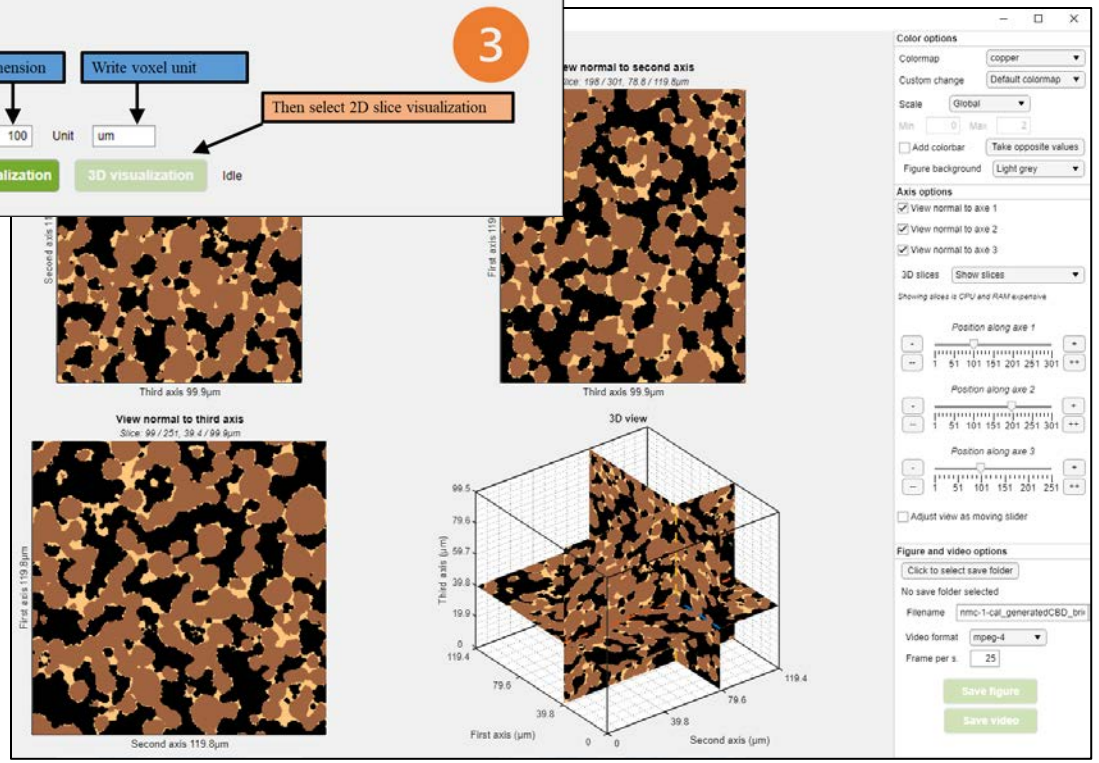
Microstructure visualization: 1/3 simple visualization



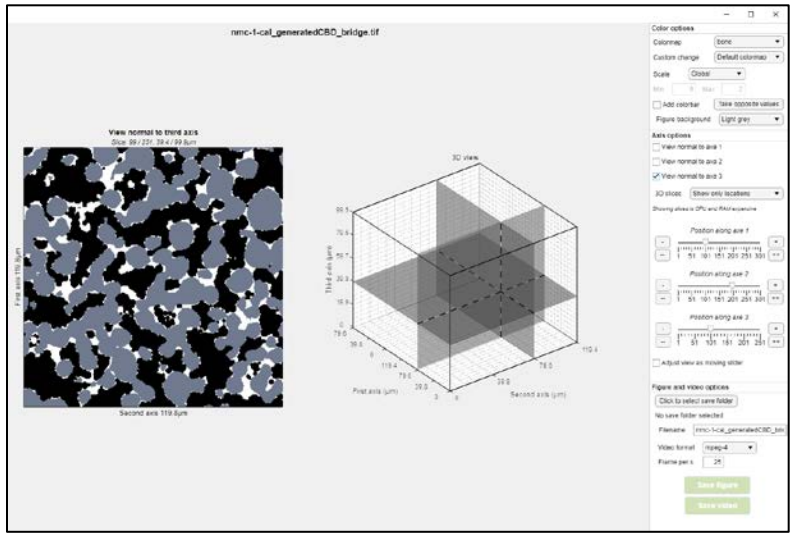
Select volumes



Multiple volume visualization (even without same FOV)

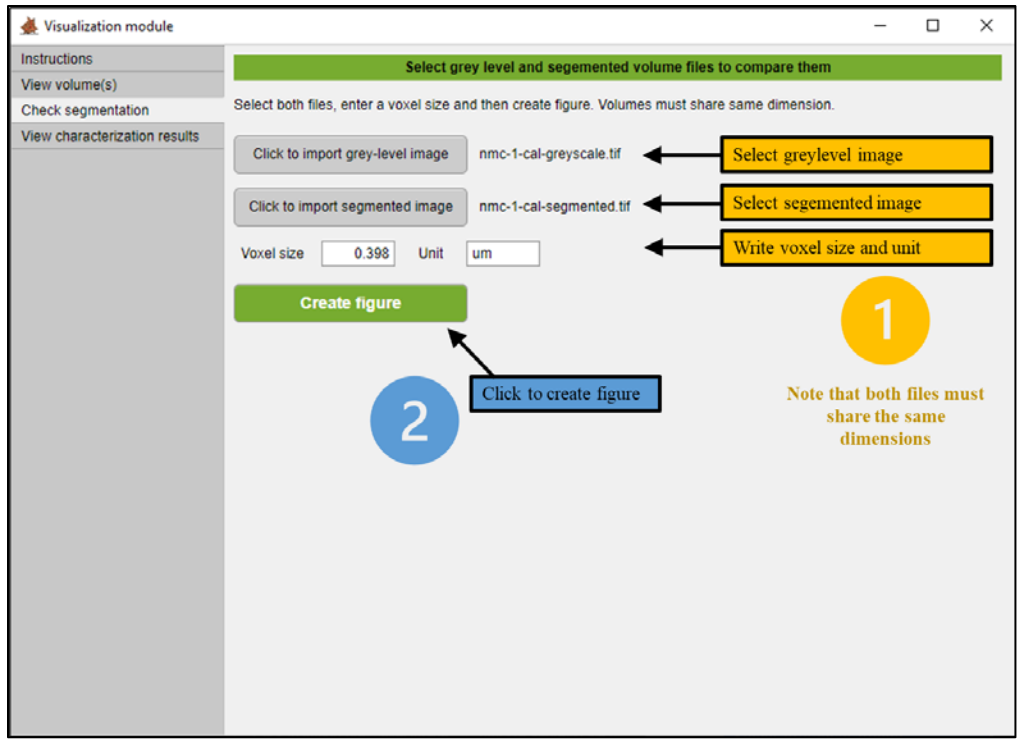


Multi-axis visualization. Export still images or videos

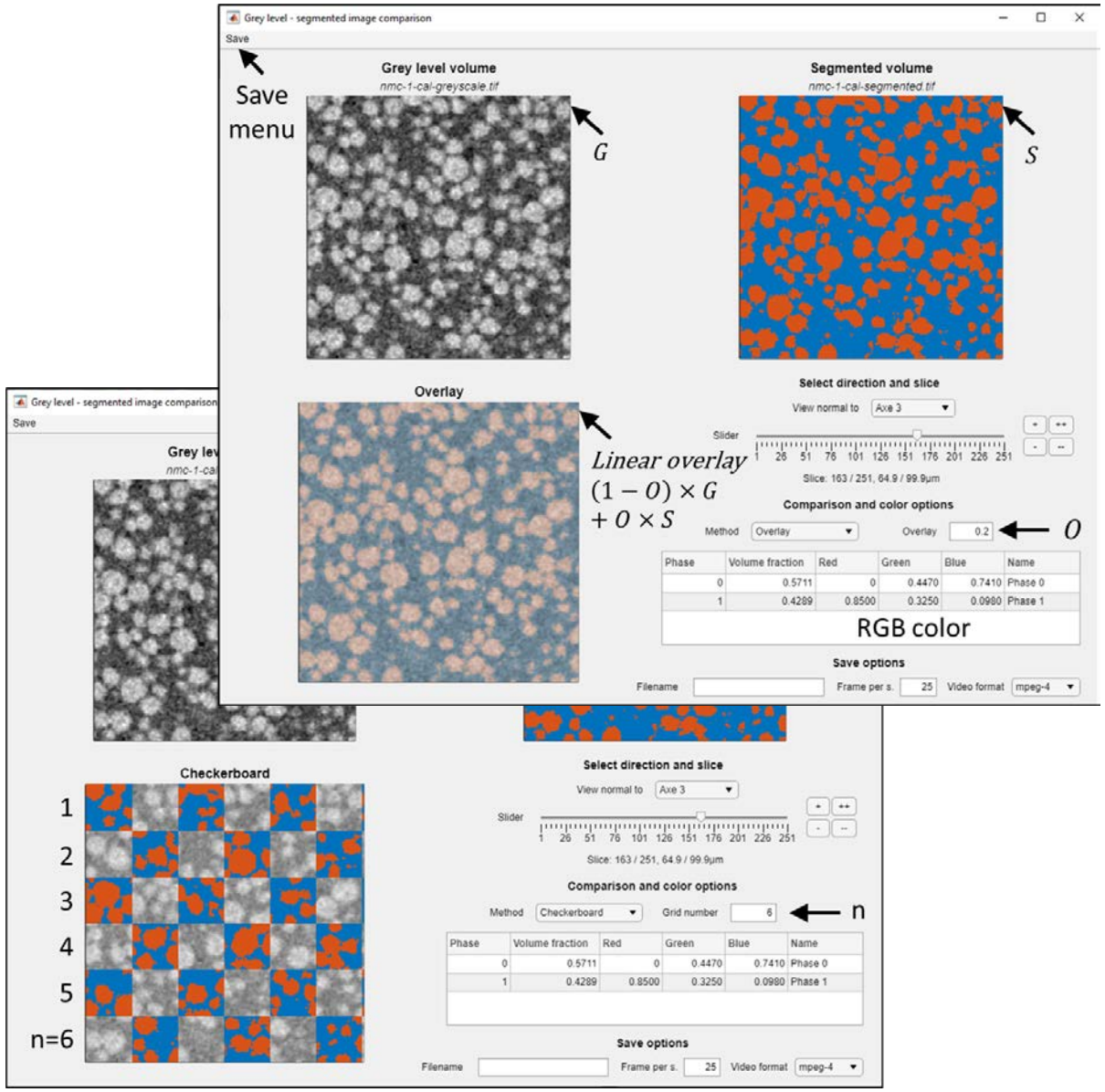


Dynamic layout

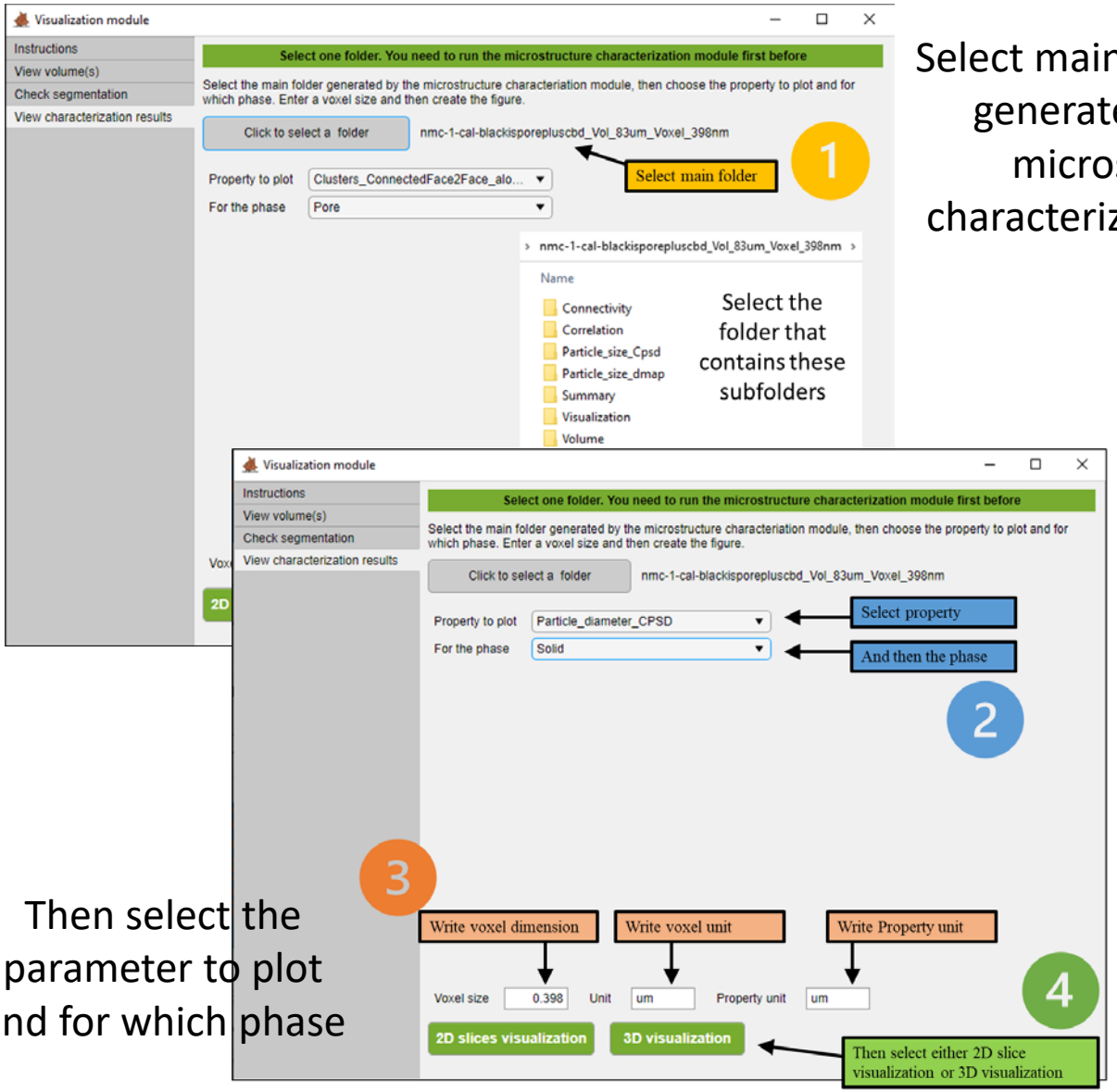
Microstructure visualization: 2/3 segmentation



Select gray-level segmented volumes and visually compare them

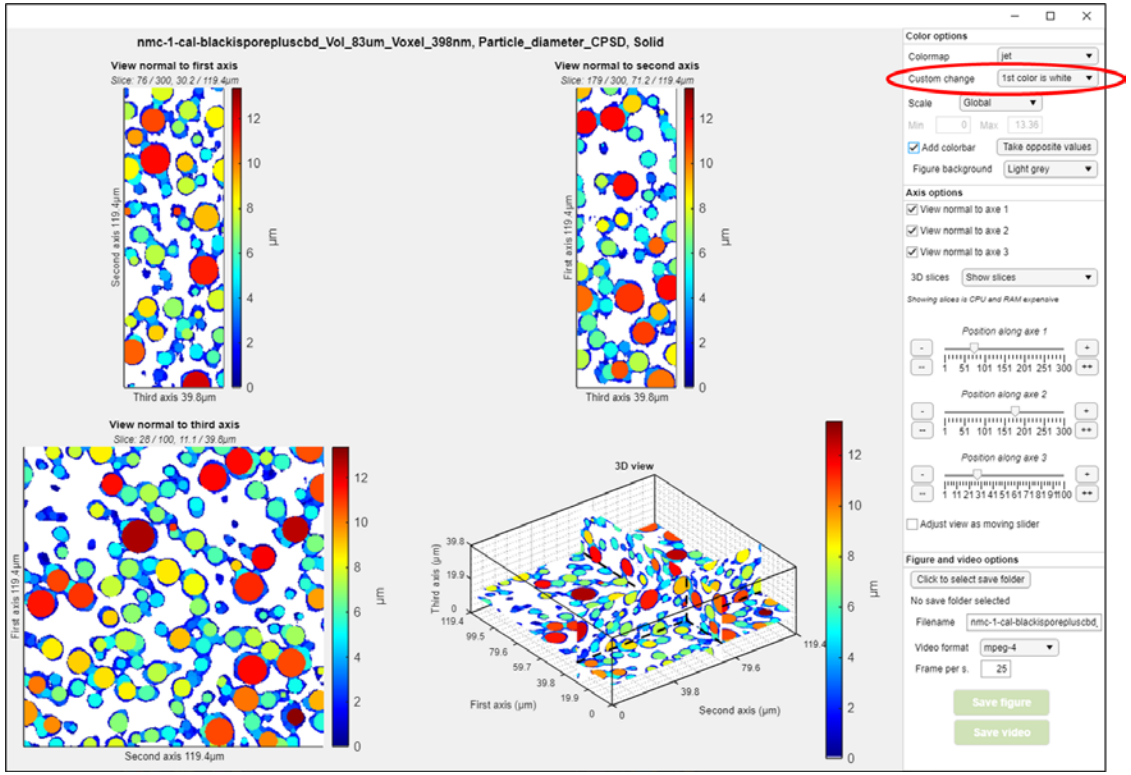


Microstructure visualization: 3/3 microstructure results



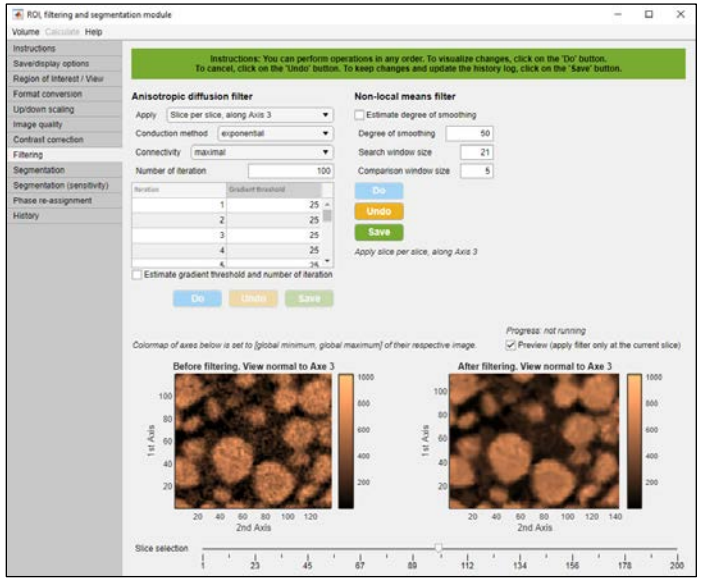
Select main output folder generated with the microstructure characterization module

Then select the parameter to plot and for which phase



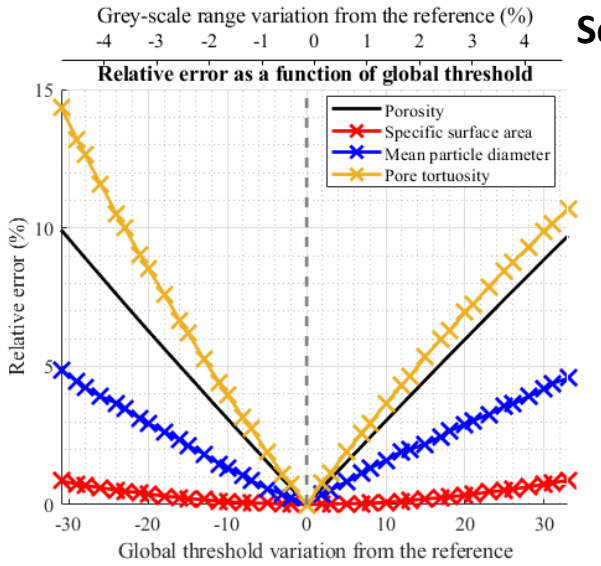
Visualize voxel/pixel-wise parameters

Microstructure filtering and segmentation



Filtering and contrast correction

(**QOL**: preview, do/undo/save)

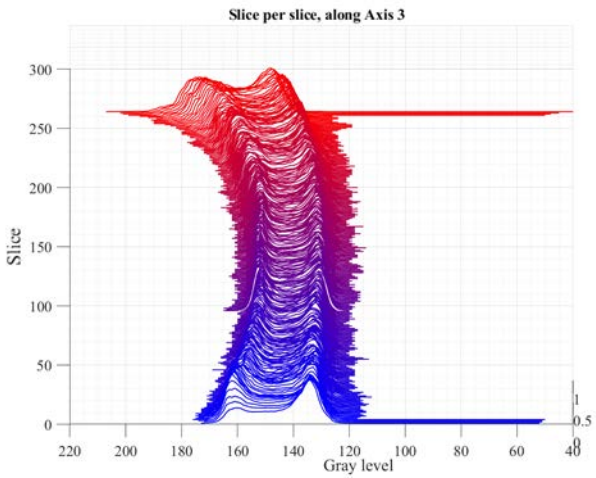


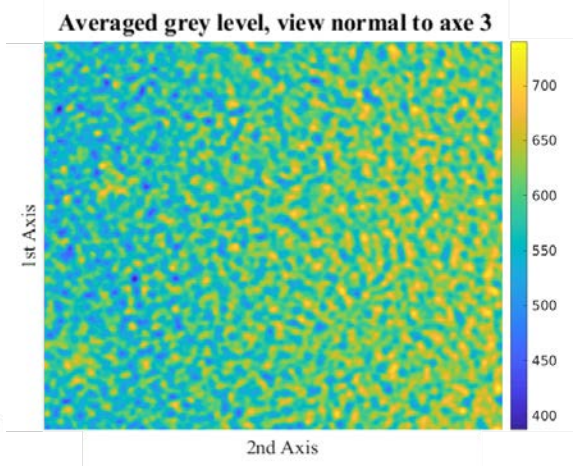
Segmentation error propagation to microstructure parameters

(Segmentation is threshold-based, local or global)

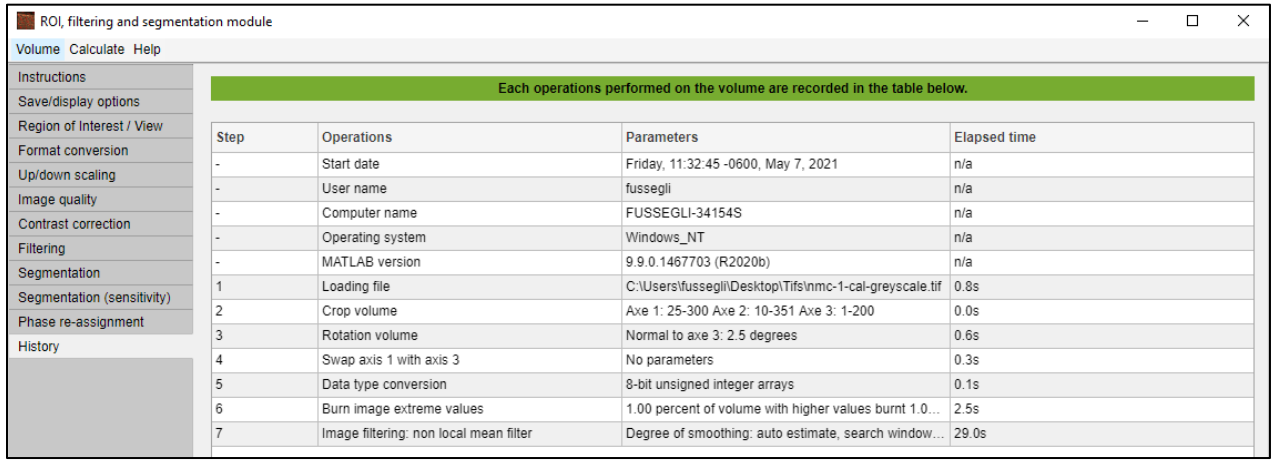
- **Module uses quite simple methods.**
- **Focus is on user-friendliness and reproducibility**
- If filtering and contrast correction followed by threshold-based segmentation is usually enough for your application the tool is relevant.

Image quality (gray level deviation has been spotted)



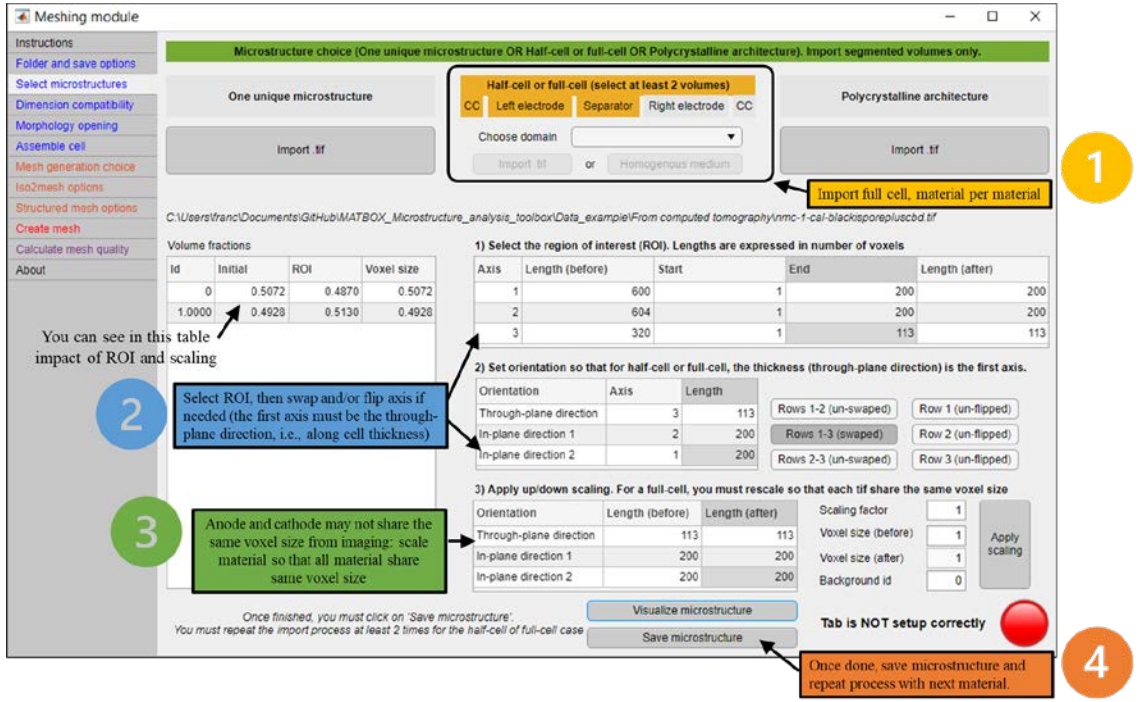


History log (keep tracks of all changes, useful to enforce a systematic segmentation method)



Step	Operations	Parameters	Elapsed time
-	Start date	Friday, 11:32:45 -0600, May 7, 2021	n/a
-	User name	fussegli	n/a
-	Computer name	FUSSEGLI-34154S	n/a
-	Operating system	Windows_NT	n/a
-	MATLAB version	9.9.0.1467703 (R2020b)	n/a
1	Loading file	C:\Users\fussegli\Desktop\Tifs\nmc-1-cal-greyscale.tif	0.8s
2	Crop volume	Axe 1: 25-300 Axe 2: 10-351 Axe 3: 1-200	0.0s
3	Rotation volume	Normal to axe 3: 2.5 degrees	0.6s
4	Swap axis 1 with axis 3	No parameters	0.3s
5	Data type conversion	8-bit unsigned integer arrays	0.1s
6	Burn image extreme values	1.00 percent of volume with higher values burnt 1.0…	2.5s
7	Image filtering: non local mean filter	Degree of smoothing: auto estimate, search window…	29.0s

Microstructure meshing



Mesh for a unique volume or a combination of several to create full cell mesh (**inputs are segmented 3D tiff**)

Meshing process divided into subtasks:

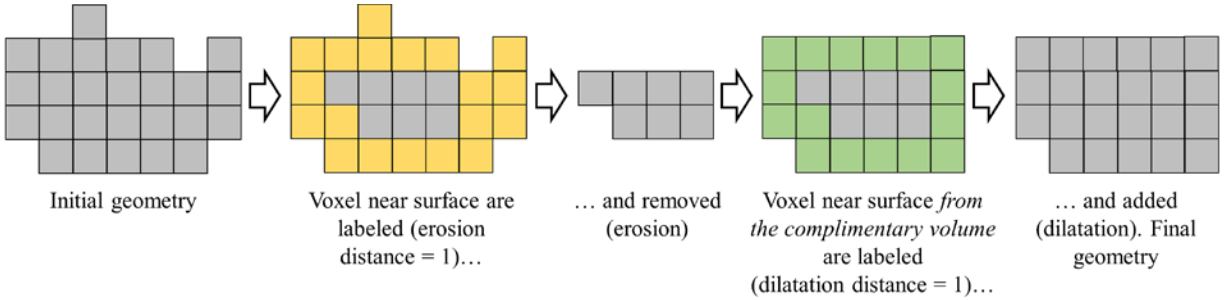
1) 3D array pre-processing: Import / dimension compatibility / morphology opening

2) Mesh options: Unstructured of structured

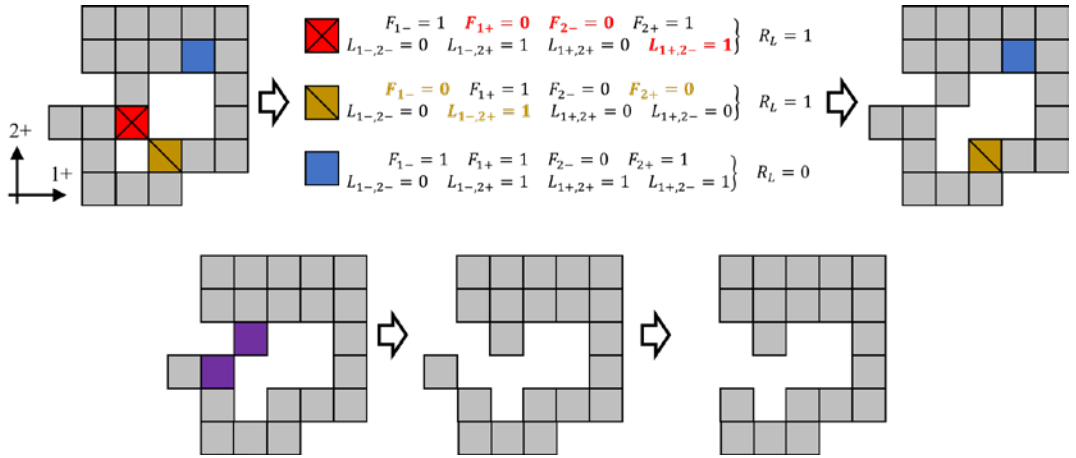
3) Meshing

Morphology opening to reduce surface roughness and remove ill-defined voxel connectivity to ease mesh generation process and improve model numerical convergence.

Erosion + dilatation



Voxel connectivity (in-house algorithm)



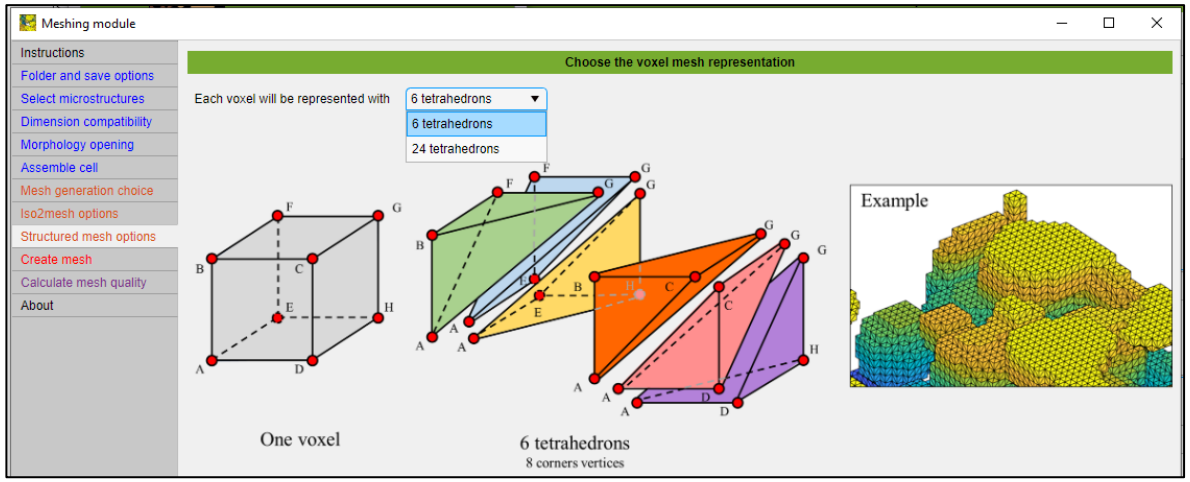
Microstructure meshing (tetrahedron-based)

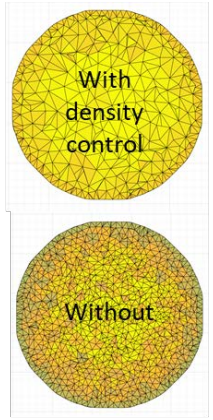
Unstructured mesh

(with Iso2mesh. Q. Fang et al., IEEE (2009) 1142–1145, https://doi.org/10.1109/isbi.2009.5193259.)

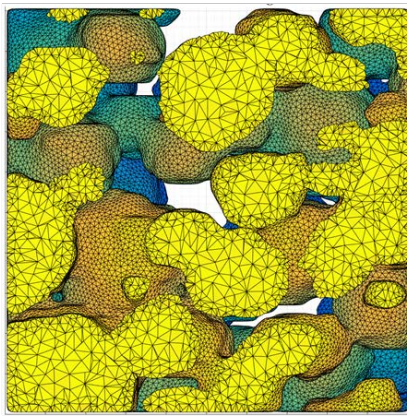
- Surface mesh extraction: **surface simplification** or **constrained Delaunay tetrahedralization (CGAL)**
- Surface mesh smoothing: **Laplacian**, **Laplacian-HC**, **Low-pass filters**
- Volumetric mesh generation and adaptative resolution: **Tetgen**

Structured mesh (voxel divided into 6 or 24 tetrahedrons)

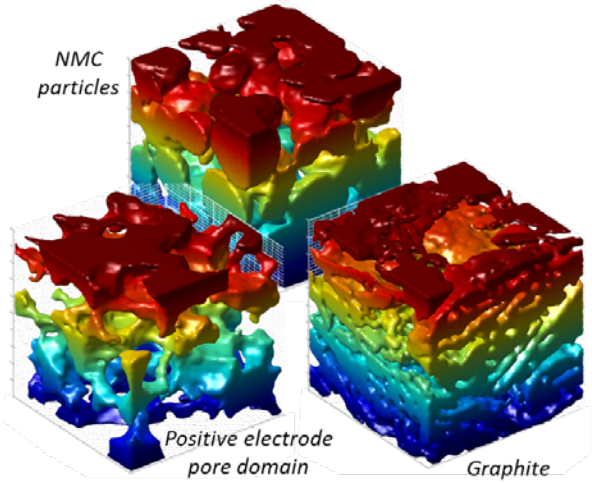


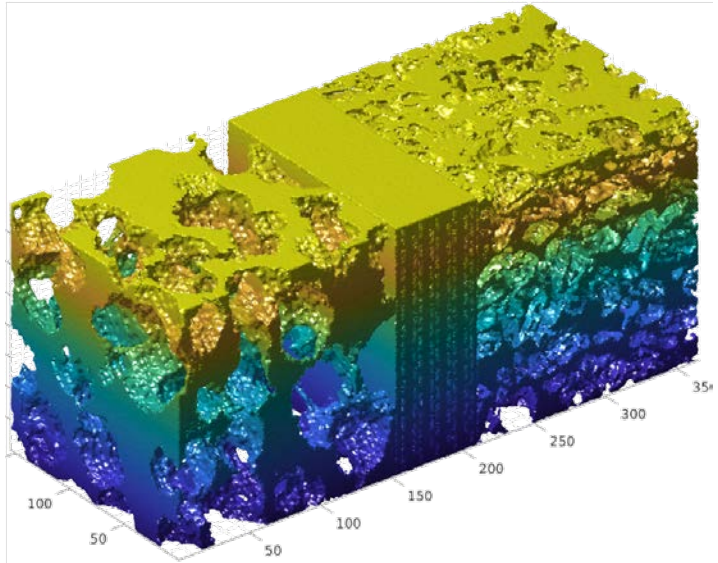


Slice within a sphere



Slice within an NMC mesh





Create one mesh for whole volume (monolithic model) and/or meshes per phase or group of phase (segregated domain model)

+ mesh quality calculations, export in .mat, .csv, .msh, .inp, .stl

Acknowledgments

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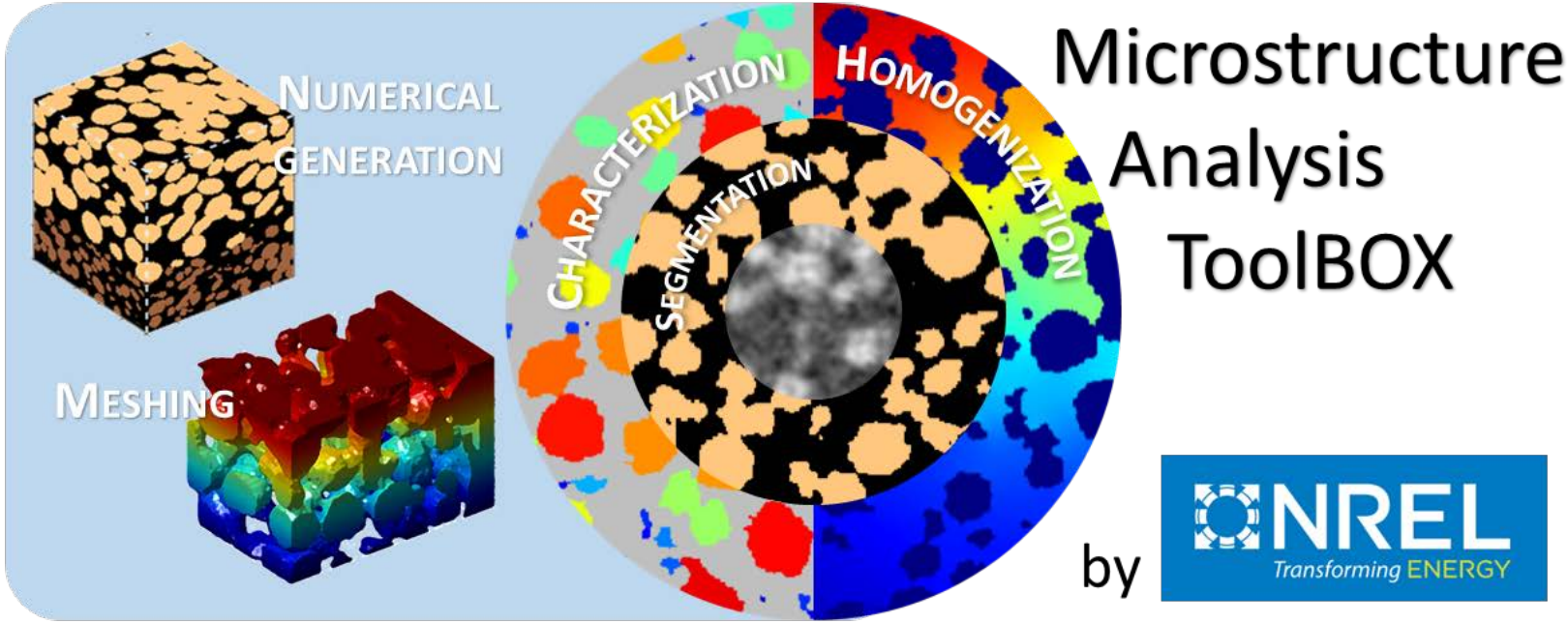

F. L. E. Usseglio-Viretta et al., MATBOX: An Open-source Microstructure Analysis Toolbox for microstructure generation, segmentation, characterization, visualization, correlation, and meshing, SoftwareX, submitted

https://github.com/NREL/MATBOX_Microstructure_analysis_toolbox

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