



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

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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

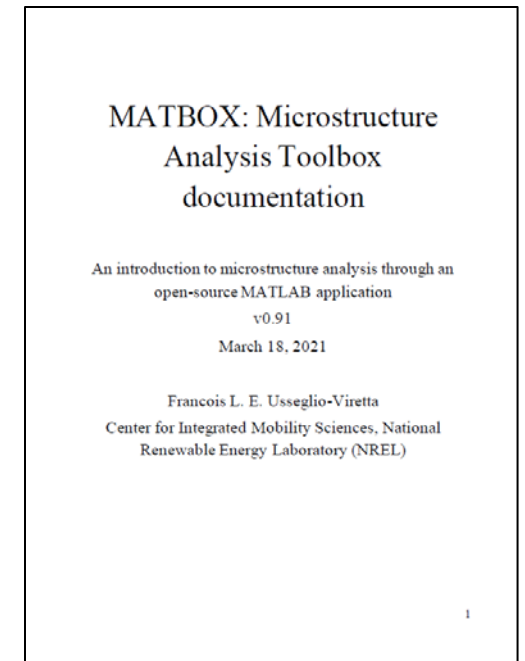
Third-party algorithms/software: *TauFactor*¹ (UCL, S. Cooper), *Iso2mesh*² (Northeastern Univ., Q. Fang), *additive generation*³ (Purdue University, A. Mistry, P. P. Mukherjee)

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

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>.

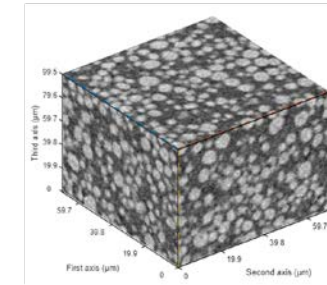
³ A. Mistry et al., ACS Applied Materials & Interfaces. (2018), <https://doi.org/10.1021/acsami.7b17771>.



*Exhaustive documentation
(~190 pages)*

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.

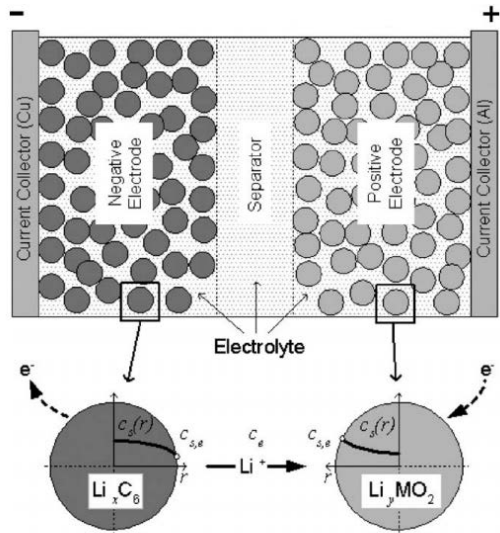
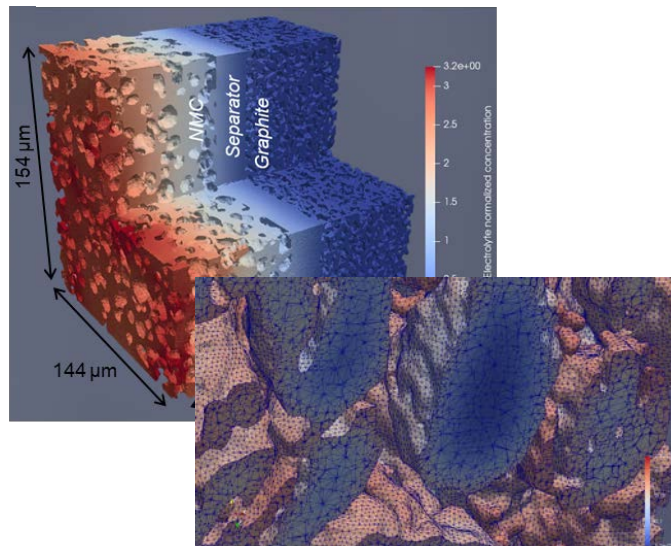
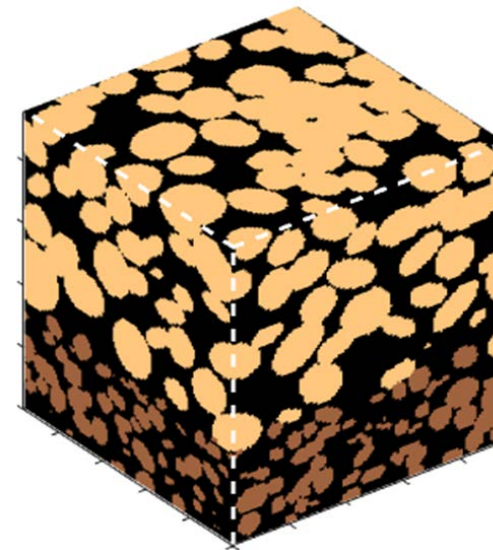


Fig. 1. Schematic of 1D (x -direction) electrochemical cell model with coupled 1D microscopic (r -direction) solid diffusion model.



Full cell meshing**

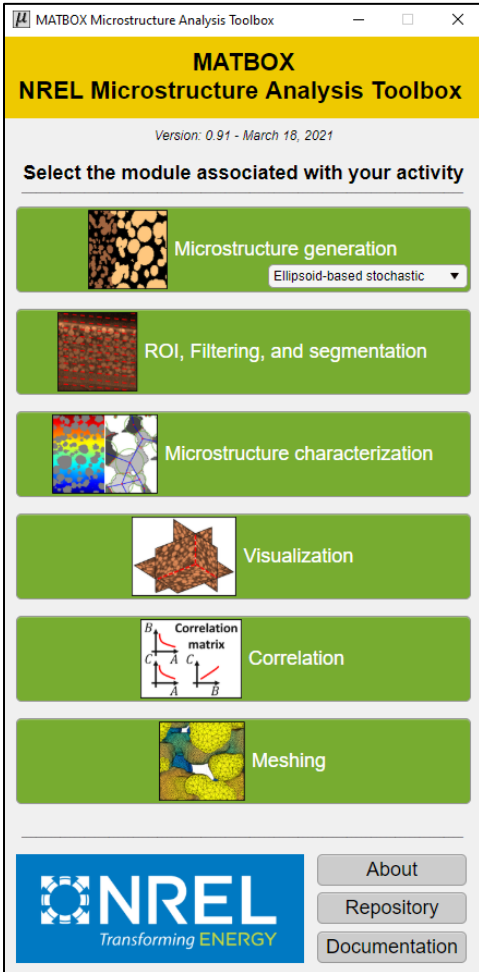


Design space analysis***

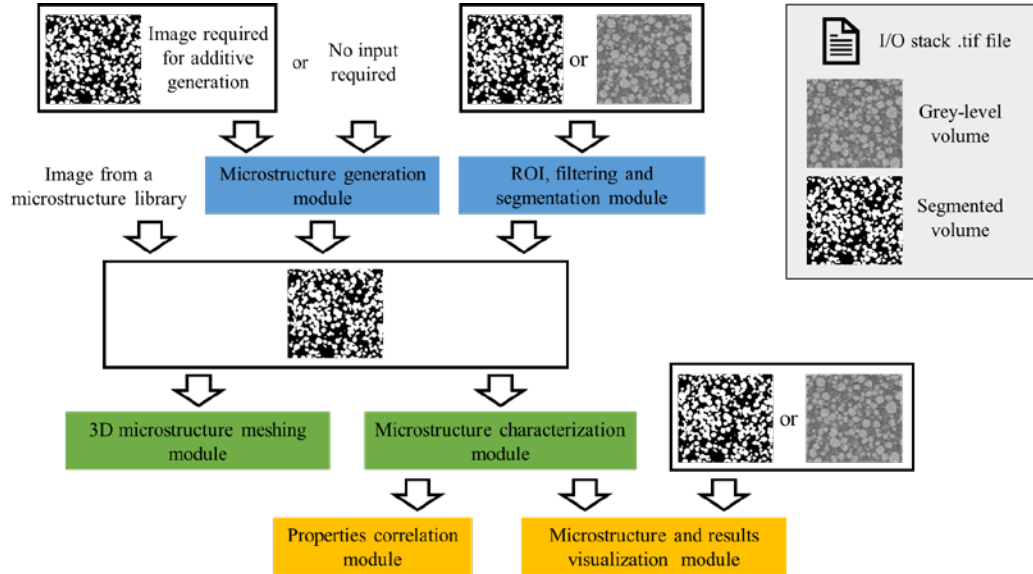
* F. Usseglio-Viretta et al., JES. (2020), <https://doi.org/10.1149/1945-7111/ab913b>
 * F. Usseglio-Viretta et al., JES. 165 (2018), <https://doi.org/10.1149/2.0731814jes>
 * F. Usseglio-Viretta et al., ECS Transactions. 77 (2017), <https://doi.org/10.1149/07711.1095ecst>
 ** J. Allen et al., J Sci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

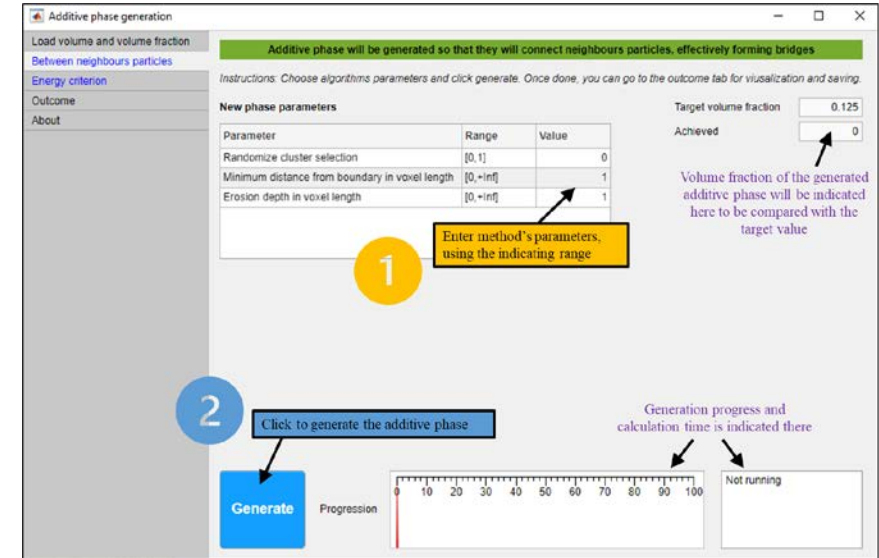


Modules I/O



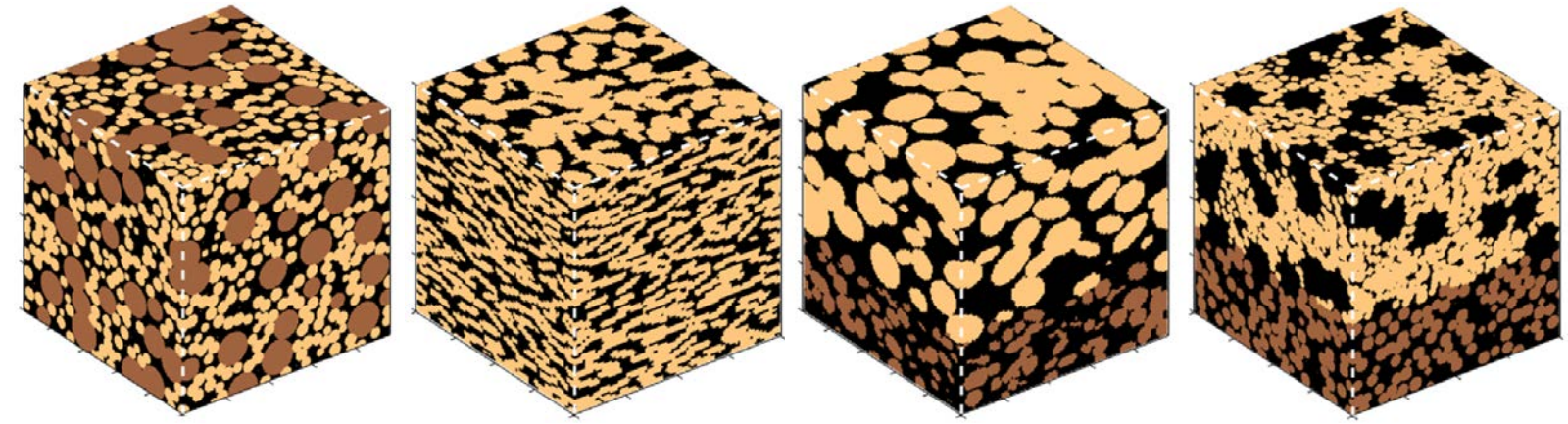
➤ Module connectivity

GUI for each module

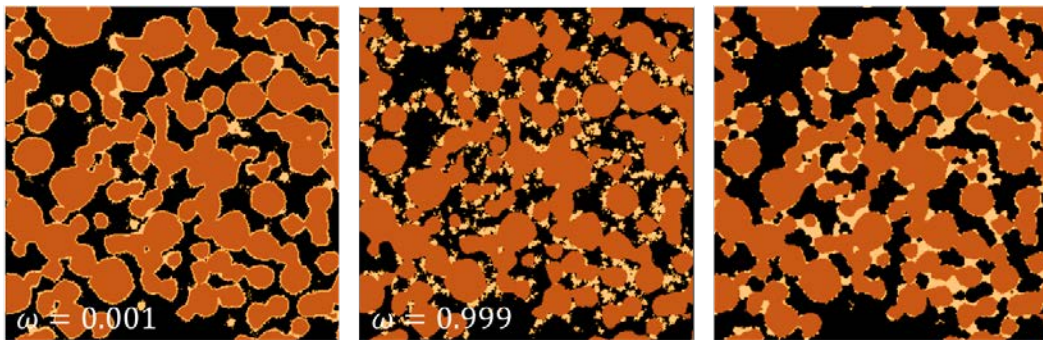
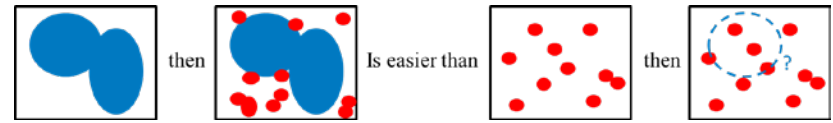


➤ User friendly interface

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



Pore
 Active material
 Additives

Energy criterion approach Bridge approach

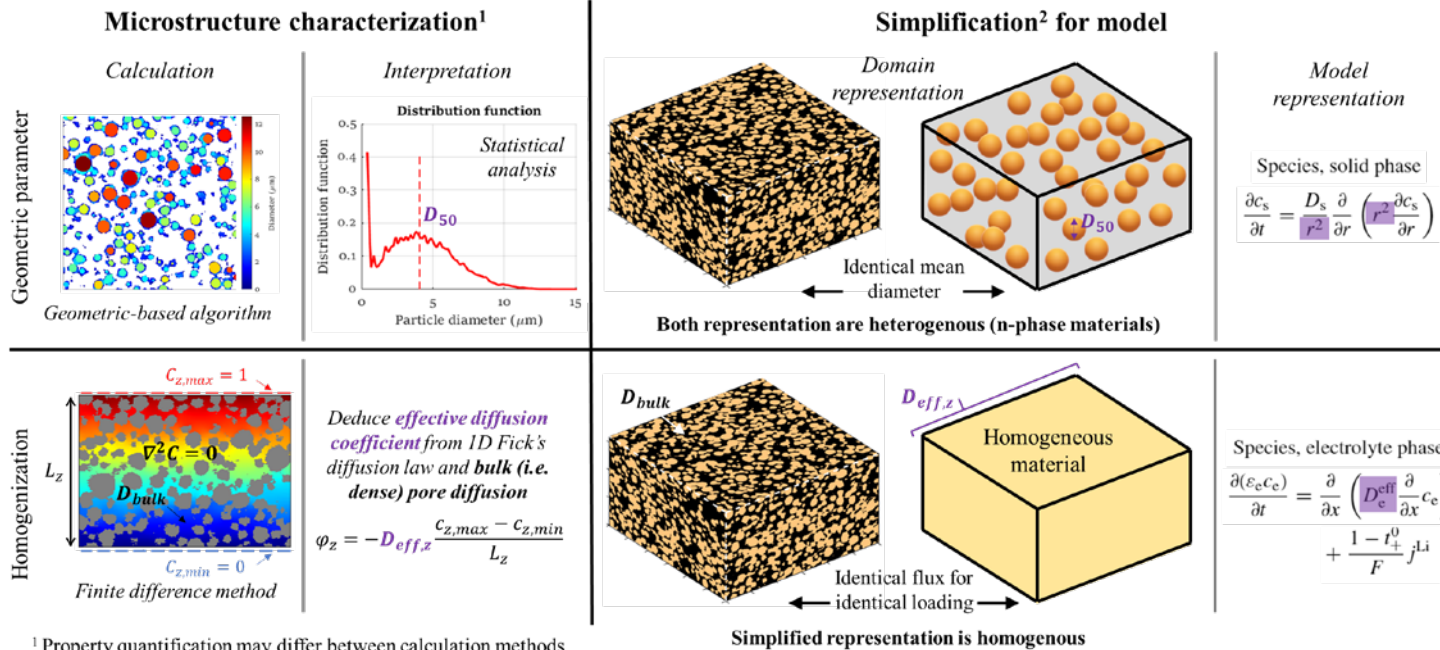
- In-house distance-based additive generation algorithm and third-party energy-based additive generation algorithm**
- Preferential location between neighbored particles (bridge).
 - Preferential deposition toward active material (thin surface layer, $w=0.001$) or additive phase (dendritic-like phase, $w=0.999$).

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

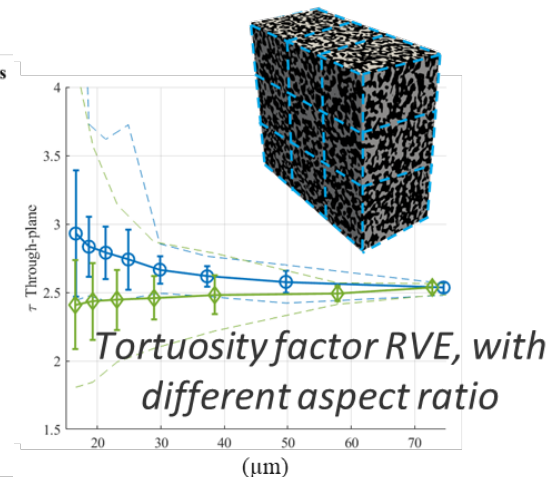
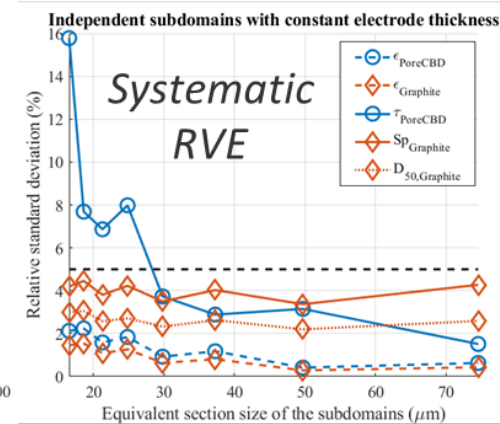
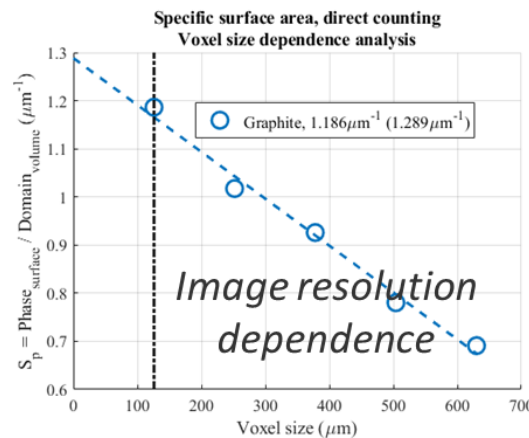
² Microstructure simplification may differ between models

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

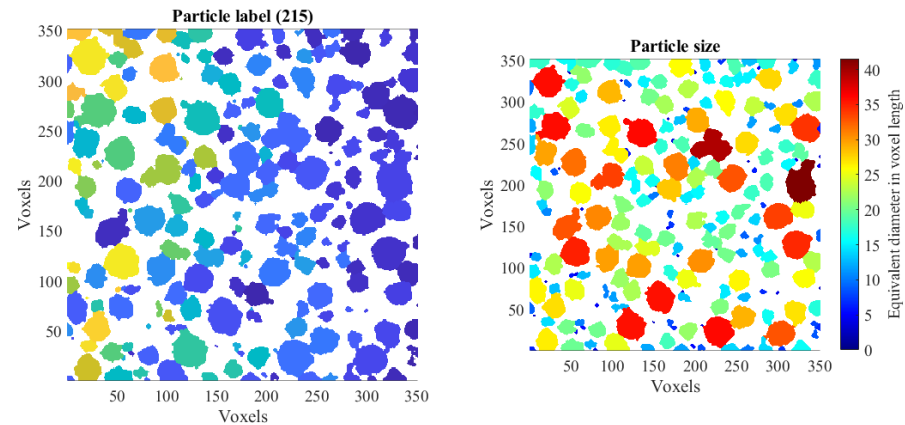
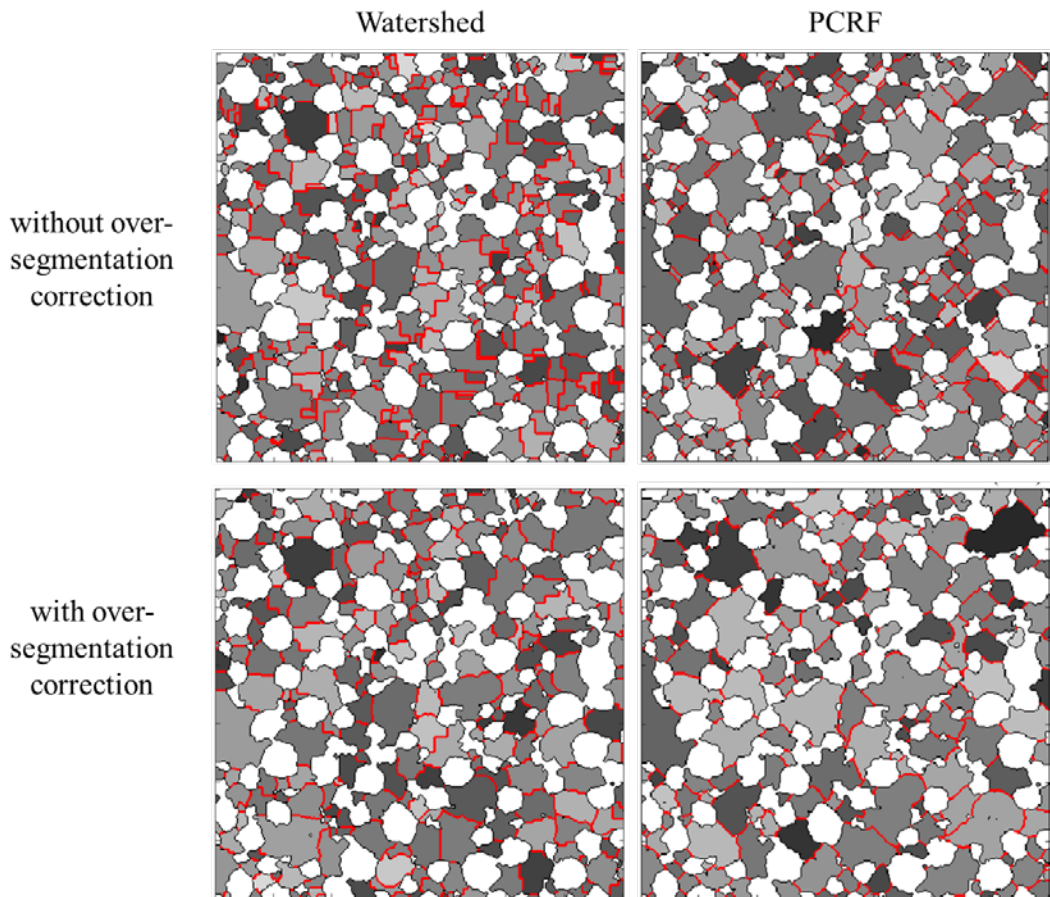
- Automated voxel size dependence analysis (evaluate microstructure parameter error induced by limited image resolution)
- Automated representative volume element (RVE) analysis (evaluate microstructure parameter error induced by limited field of view) → **hundreds of calculations automated**
- batch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



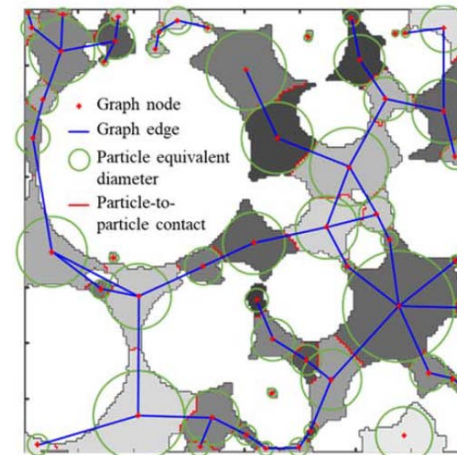
Microstructure characterization: particle analysis

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

Microstructure characterization

Import segmented volume

Imported volume(s)

Volume fraction options

Connectivity options

Tortuosity factor (tau-factor) options

Specific surface area (direct) options

Specific interface area (direct) options

Particle size (C-PSD) options

Particle size (distance map) options

Particle size (watershed) options

Particle size (repulsive wall) options

Display/save options

Run ALL calculations

Help

Select segmented volume file to import. You can select additional volumes after.

>>> Click to add volume <<<

nmc-1-cal-segmented.tif

Volume numero: 1

1) Enter voxel size (in nanometers). New voxel size can be lower (downscaling) or higher (upscaling) compared with initial voxel size.

Initial voxel size (nm): 398 New voxel size (nm): 398

2) Direction properties: choose Region Of Interest (ROI) and name later used for figures

Direction	Number of voxel	ROI start	ROI end	Name
1	351	1	351	In-plane direction 1
2	351	1	351	In-plane direction 2
3	251	1	251	Through-plane direction

Initial volume and voxel size User-choice (ROI)

Number of voxels : 30923451 ~ 30923451

Domain size : 139.7 x 139.7 x 99.9 um3 ~ 139.7 x 139.7 x 99.9 um3

Equivalent cubic domain size : 124.9 x 124.9 x 124.9 um3 ~ 124.9 x 124.9 x 124.9 um3

3) Phase properties: choose name and color (RGB) for future figures

Phase	Volume fraction	Red	Green	Blue	Name	Assign code
0	0.5711	0	0.4470	0.7410	Pore	0
1	0.4289	0.8500	0.3250	0.0980	Solid	1

4) Write volume information

Information	Text
Material source	ANL CAMP
Material name	NMC LN2487-113-13C
Material group name	NMC-Calendered
Volume description	Cropped volume
Raw data source	UCL
Raw data technique	Computed tomography
Segmentation source	NREL
Segmentation technique	Local threshold
Analysis description	Example for documentation

5) Once steps 1-5 done, click to save your choices

Reset selected options and current volume

Select result folder location nmc-1-cal-segmented_Vol_125um_Voxel_398nm

5) Select location where the result folder will be saved, and write the result folder name

Direction 3 Position: 76/251

Voxel size: CORRECT

Region of interest (ROI): CORRECT

Colors: CORRECT

Assigned code: CORRECT

Folder location: DEFINED

Select microstructures to analyze and properties to investigate using GUI

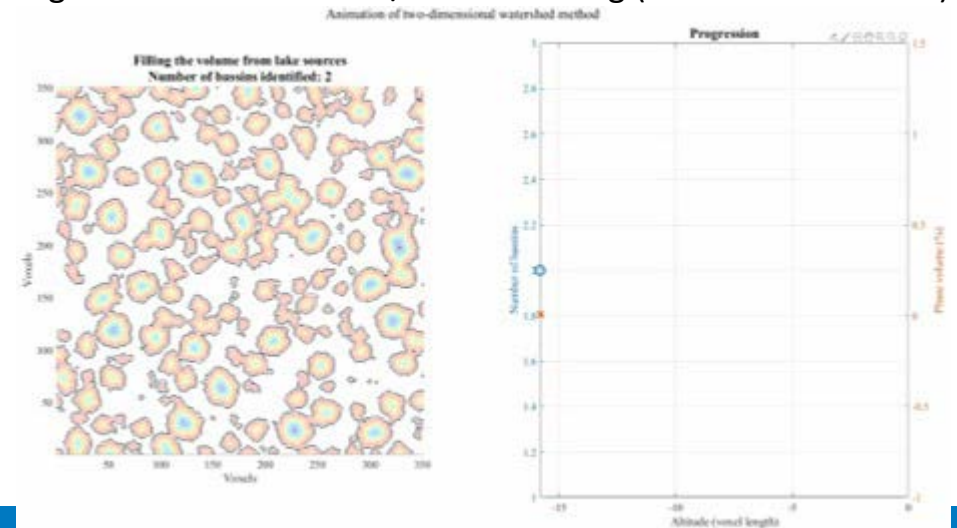
Functions have two syntax: one for the GUI (no command line required), one to be used as standalone

```
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)

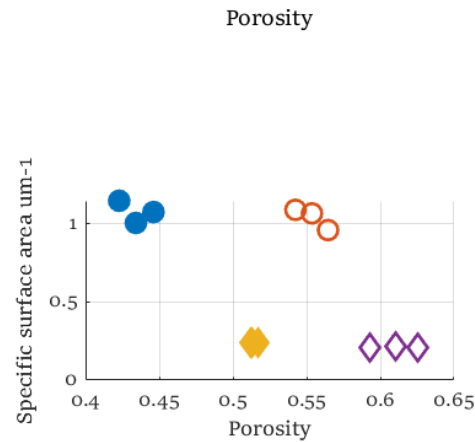


Microstructure correlation

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.

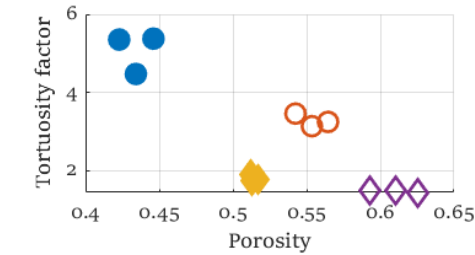
Standard microstructure parameters



Kendal's Tau ranking
-0.485 (-0.167)

Kendal's Tau ranking
-0.576 (-0.167)

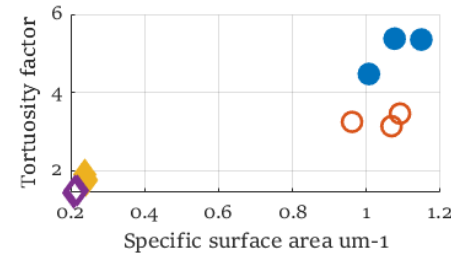
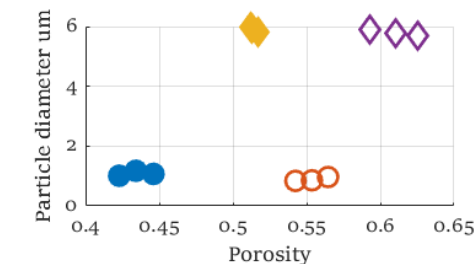
Kendal's Tau ranking
0.000 (-0.167)



Specific surface area

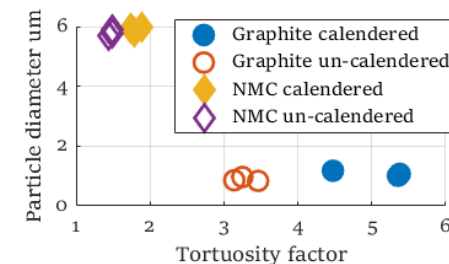
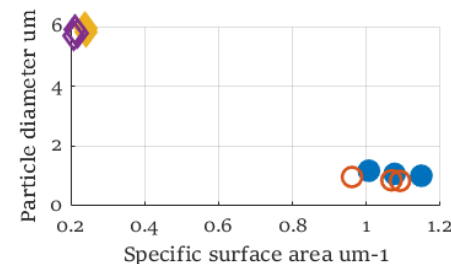
Kendal's Tau ranking
0.788 (0.333)

Kendal's Tau ranking
-0.515 (-0.667)



Tortuosity factor

Kendal's Tau ranking
-0.303 (0.000)



Particle diameter

Microstructure visualization: 1/3 simple visualization

Visualization module

Instructions

Select one or several volume files

View volume(s)

Check segmentation

View characterization results

Select file(s), enter a voxel size and then create figure. Volumes can have different dimension.

Click to select one or several files 5 volumes imported.

Files	Select volumes to plot
nmc-1-cal_generatedCBD_bridge.tif	<input checked="" type="checkbox"/>
nmc-1-cal_generatedCBD_Energy_w0.001.tif	<input checked="" type="checkbox"/>
nmc-1-cal_generatedCBD_Energy_w0.999.tif	<input checked="" type="checkbox"/>
BI_layer.tif	<input checked="" type="checkbox"/>
BI_layer_poreformer.tif	<input checked="" type="checkbox"/>

Files imported are noted there

You can select which ones to visualize

2 Write voxel dimension Write voxel unit

Voxel size 100 Unit um

3 Then select 2D slice visualization

2D slices visualization 3D visualization Idle

Select volumes

Multiple volume visualization (even without same FOV)

Normal to axe 1

Slice: 121/301 121/301 121/301 97/240 161/400

MATLAB default

View normal to second axis

View normal to third axis

3D view

Color options

Colormap: copper

Scale: Global

Axis options

View normal to axe 1

View normal to axe 2

View normal to axe 3

3D slices: Show slices

Figure and video options

Save figure Save video

Multi-axis visualization. Export still images or videos

nmc-1-cal_generatedCBD_bridge.tif

Color options

Colormap: bone

Scale: Global

Axis options

View normal to axe 1

View normal to axe 2

View normal to axe 3

3D slices: Show only locations

Figure and video options

Save figure Save video

Dynamic layout

Microstructure visualization: 2/3 segmentation

Visualization module

Instructions

Select grey level and segmented volume files to compare them

Select both files, enter a voxel size and then create figure. Volumes must share same dimension.

Click to import grey-level image nmc-1-cal-greyscale.tif **Select greylevel image**

Click to import segmented image nmc-1-cal-segmented.tif **Select segmented image**

Voxel size 0.398 Unit um **Write voxel size and unit**

Create figure

2 Click to create figure

1 Note that both files must share the same dimensions

Select gray-level segmented volumes and visually compare them

Grey level - segmented image comparison

Save menu

Grey level volume nmc-1-cal-greyscale.tif **G**

Segmented volume nmc-1-cal-segmented.tif **S**

Overlay

Linear overlay
 $(1 - O) \times G + O \times S$

Comparison and color options

Phase	Volume fraction	Red	Green	Blue	Name
0	0.5711	0	0.4470	0.7410	Phase 0
1	0.4289	0.8500	0.3250	0.0990	Phase 1

RGB color

Save options

Filename Frame per s. 25 Video format mpeg-4

Checkerboard

1

2

3

4

5

n=6

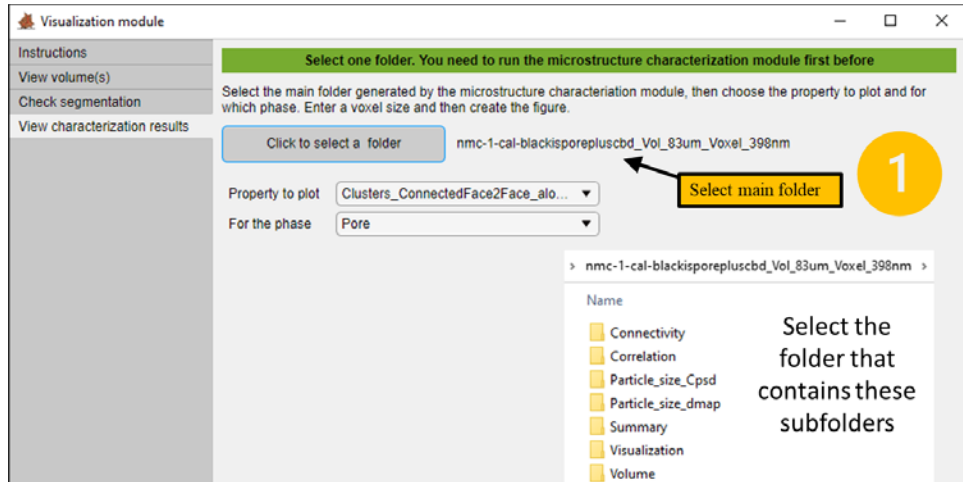
Comparison and color options

Method Checkerboard Grid number 8 **n**

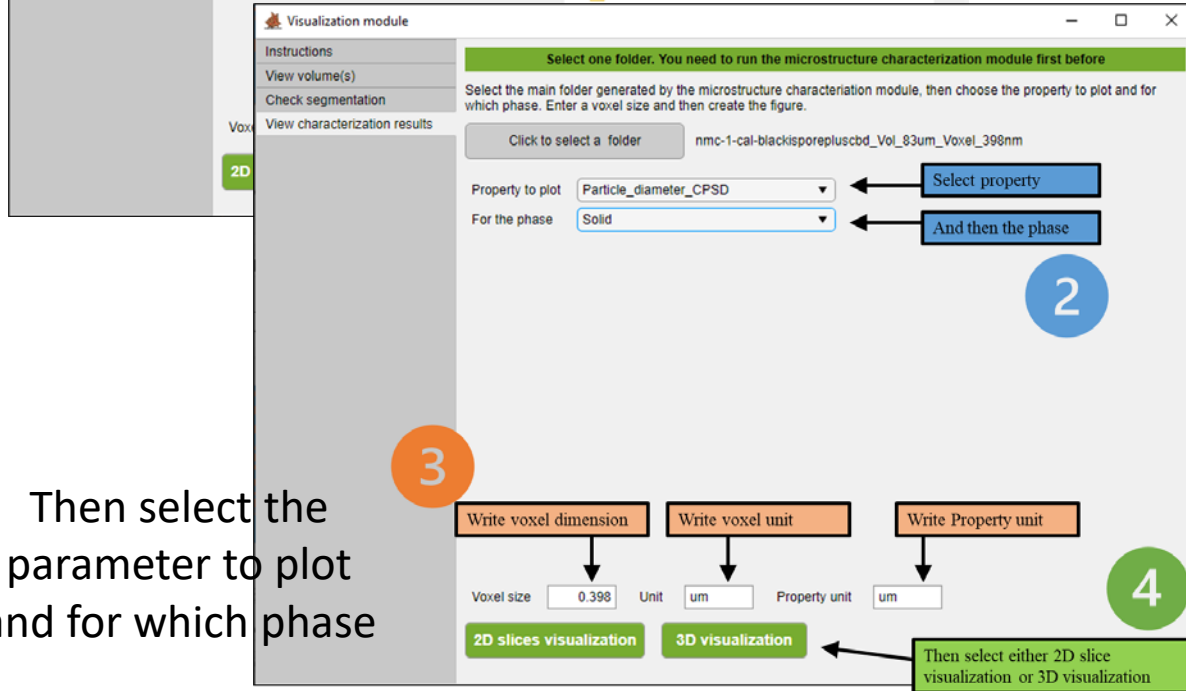
Save options

Filename Frame per s. 25 Video format mpeg-4

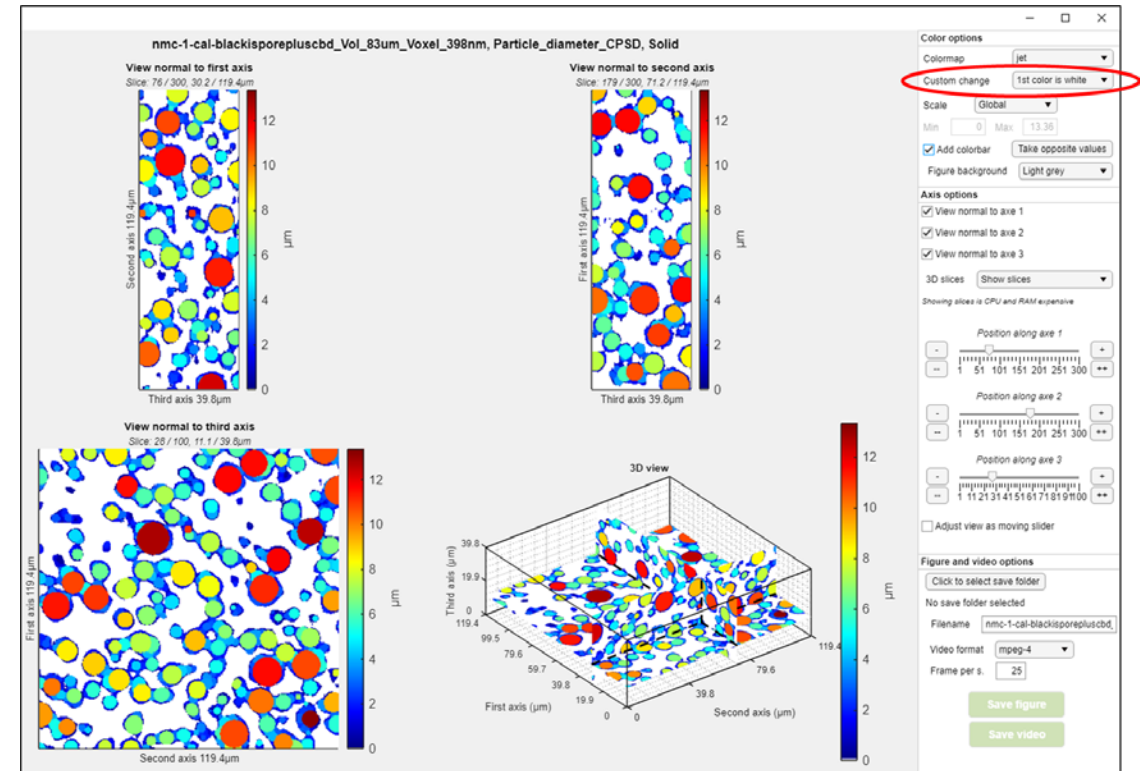
Microstructure visualization: 3/3 microstructure results



Select main output folder generated with the microstructure characterization module

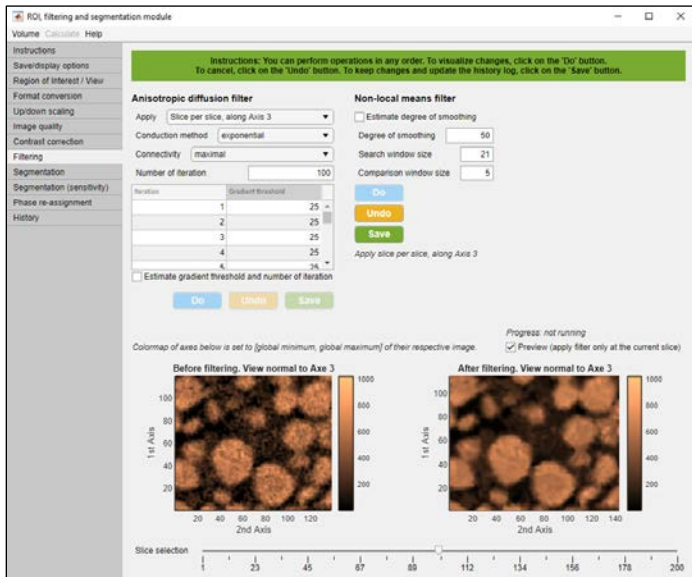


Then select the parameter to plot and for which phase

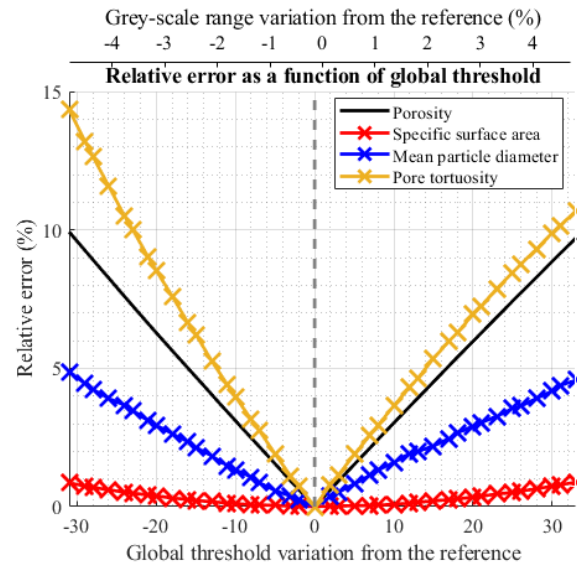


Visualize voxel/pixel-wise parameters

Microstructure filtering and segmentation



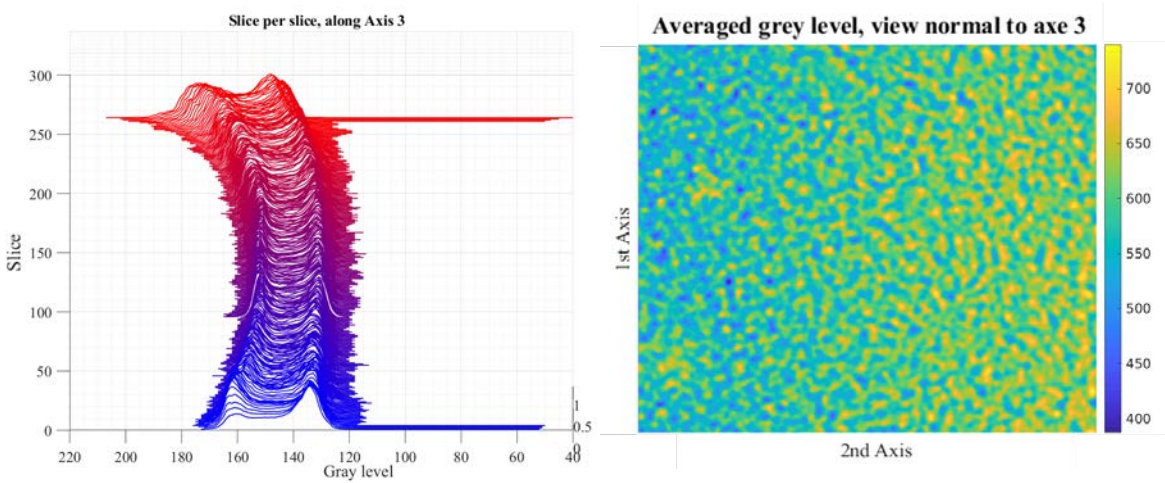
Filtering and contrast correction
(QOL: preview, do/undo/save)



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\mnc-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

1 Half cell or full cell (select at least 2 volumes)
 CC Left electrode Separator Right electrode CC
 Choose domain: [Dropdown]
 Import .tif or Homogenous medium

2 Select ROI, then swap and/or flip axis if needed (the first axis must be the through-plane direction, i.e., along cell thickness)

3 Anode and cathode may not share the same voxel size from imaging: scale material so that all material share same voxel size

4 Once done, save microstructure and repeat process with next material.

Volume fractions table:

Id	Initial	ROI	Voxel size
0	0.5072	0.4870	0.5072
1.0000	0.4928	0.5130	0.4928

1) Select the region of interest (ROI). Lengths are expressed in number of voxels

Axis	Length (before)	Start	End	Length (after)
1	600	1	200	200
2	604	1	200	200
3	320	1	113	113

2) Set orientation so that for half-cell or full-cell, the thickness (through-plane direction) is the first axis.

Orientation	Axis	Length
Through-plane direction	3	113
In-plane direction 1	2	200
In-plane direction 2	1	200

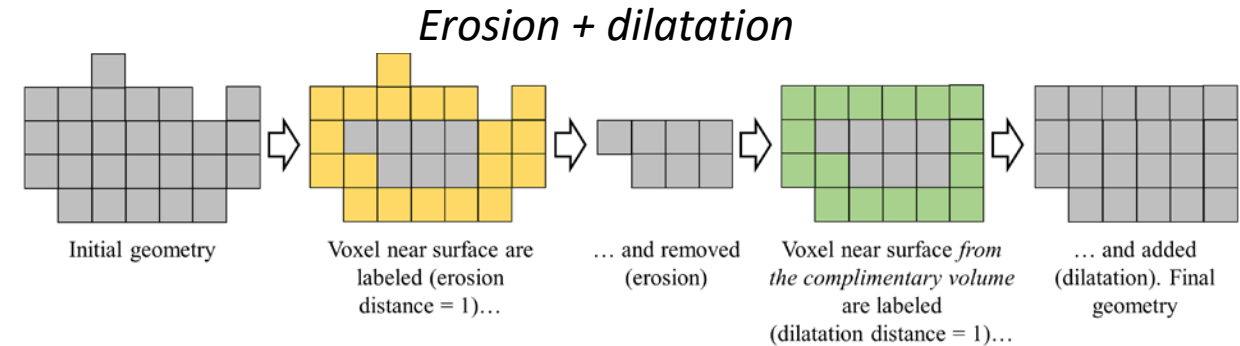
3) Apply up/down scaling. For a full-cell, you must rescale so that each tif share the same voxel size

Orientation	Length (before)	Length (after)	Scaling factor
Through-plane direction	113	113	1
In-plane direction 1	200	200	1
In-plane direction 2	200	200	1

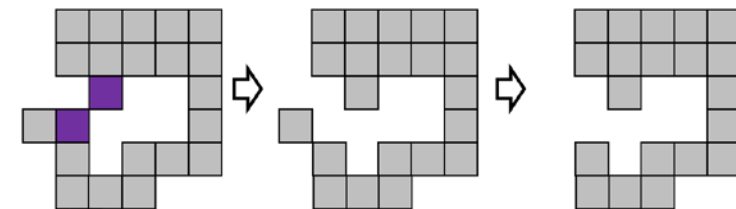
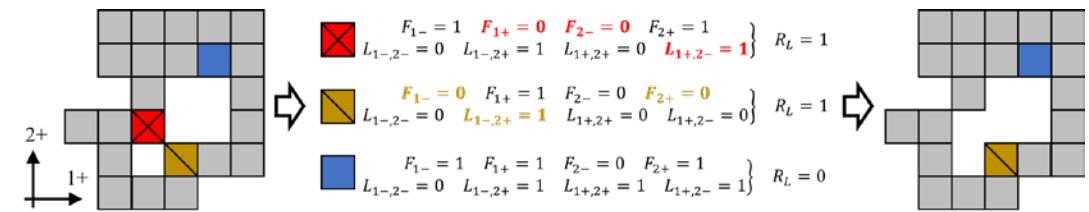
Buttons: Visualize microstructure, Save microstructure

Warning: Tab is NOT setup correctly

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



Voxel connectivity (in-house algorithm)



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:

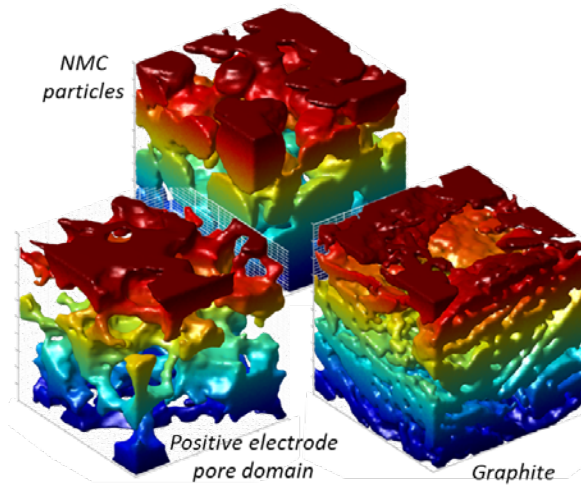
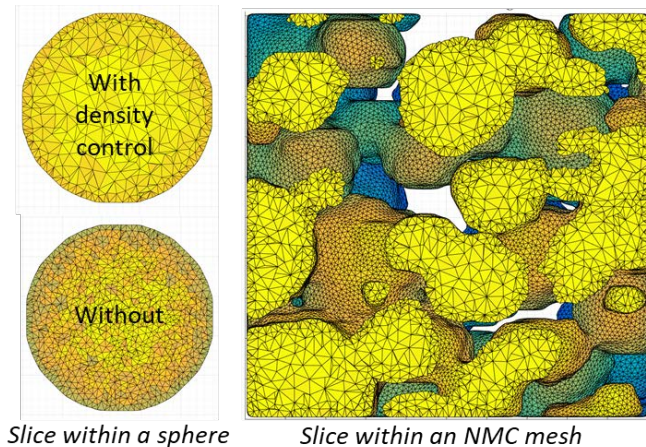
- 1) 3D array pre-processing: Import / dimension compatibility / morphology opening
- 2) Mesh options: Unstructured or structured
- 3) Meshing

Microstructure meshing (tetrahedron-based)

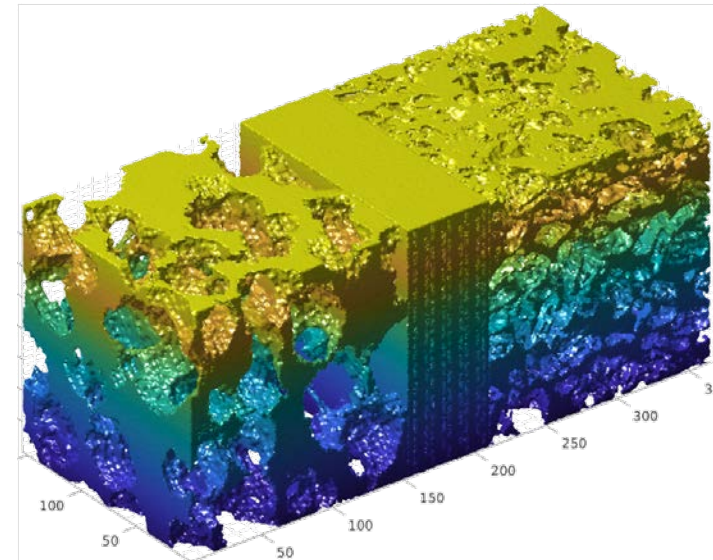
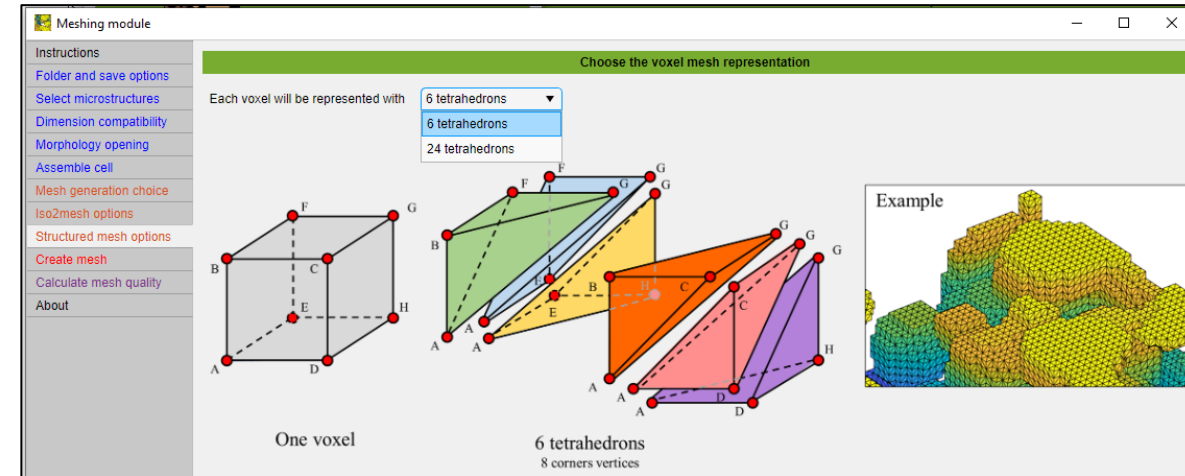
Unstructured mesh

(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 adaptive resolution: **Tetgen**



Structured mesh (voxel divided into 6 or 24 tetrahedrons)

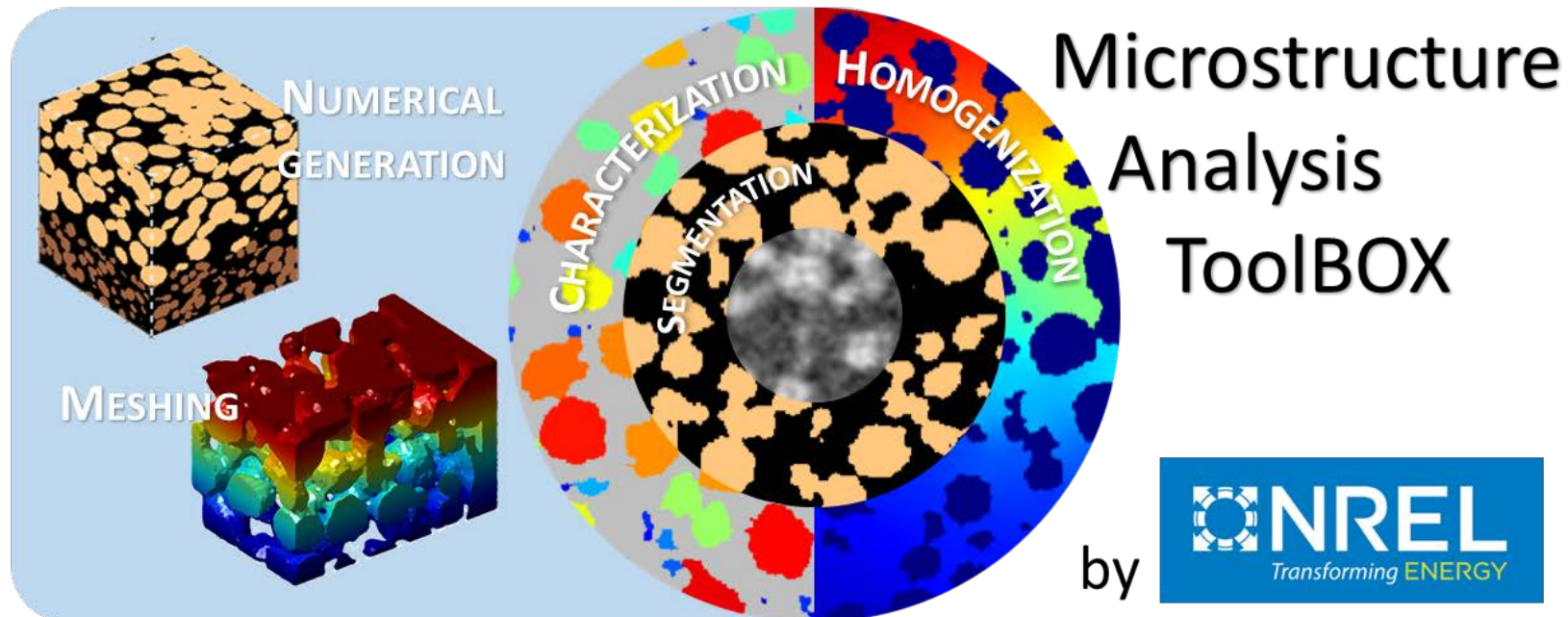


Create one mesh for whole volume (monolithic model) and/or meshes per phase or group of phase (segregated domain model)

+ 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

www.nrel.gov



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