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# Study of the impact of microstructure on electrical properties in lithium-ion batteries; simulations on actual microstructures and generation of numerical architectures

François Cadiou, François Willot, Bernard Lestriez, Jérôme Adrien, Thierry Douillard, Éric Maire

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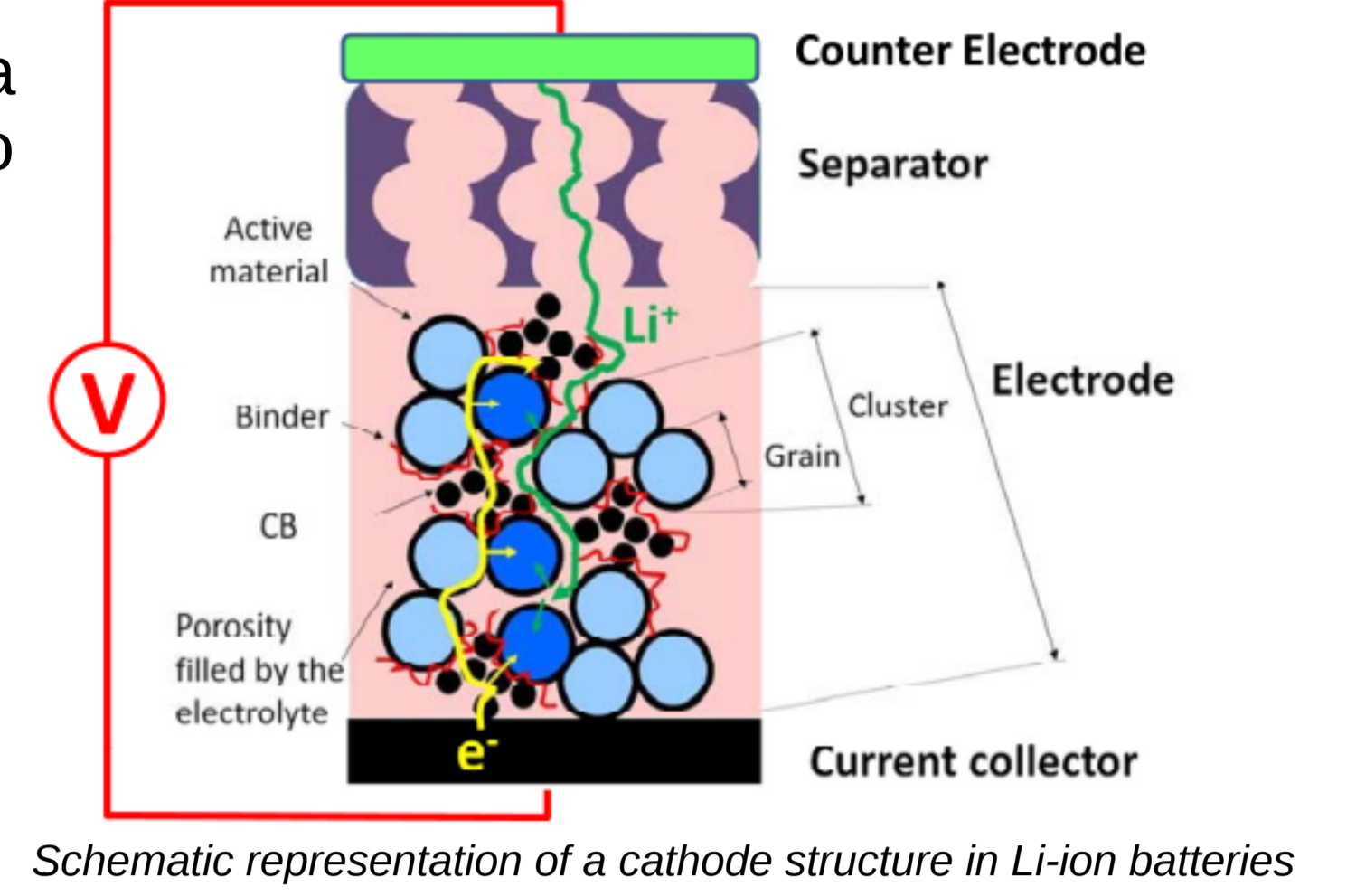
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Li-ion batteries are interesting for multiple applications because of their **power and energy densities**. However there is still a **gap to be bridged between theoretical models like Newman's and experiments**. One of the reasons for that is the difficulties to understand the **links between microstructure and effective properties within the positive electrodes** also named cathodes.

### Cathode composition:

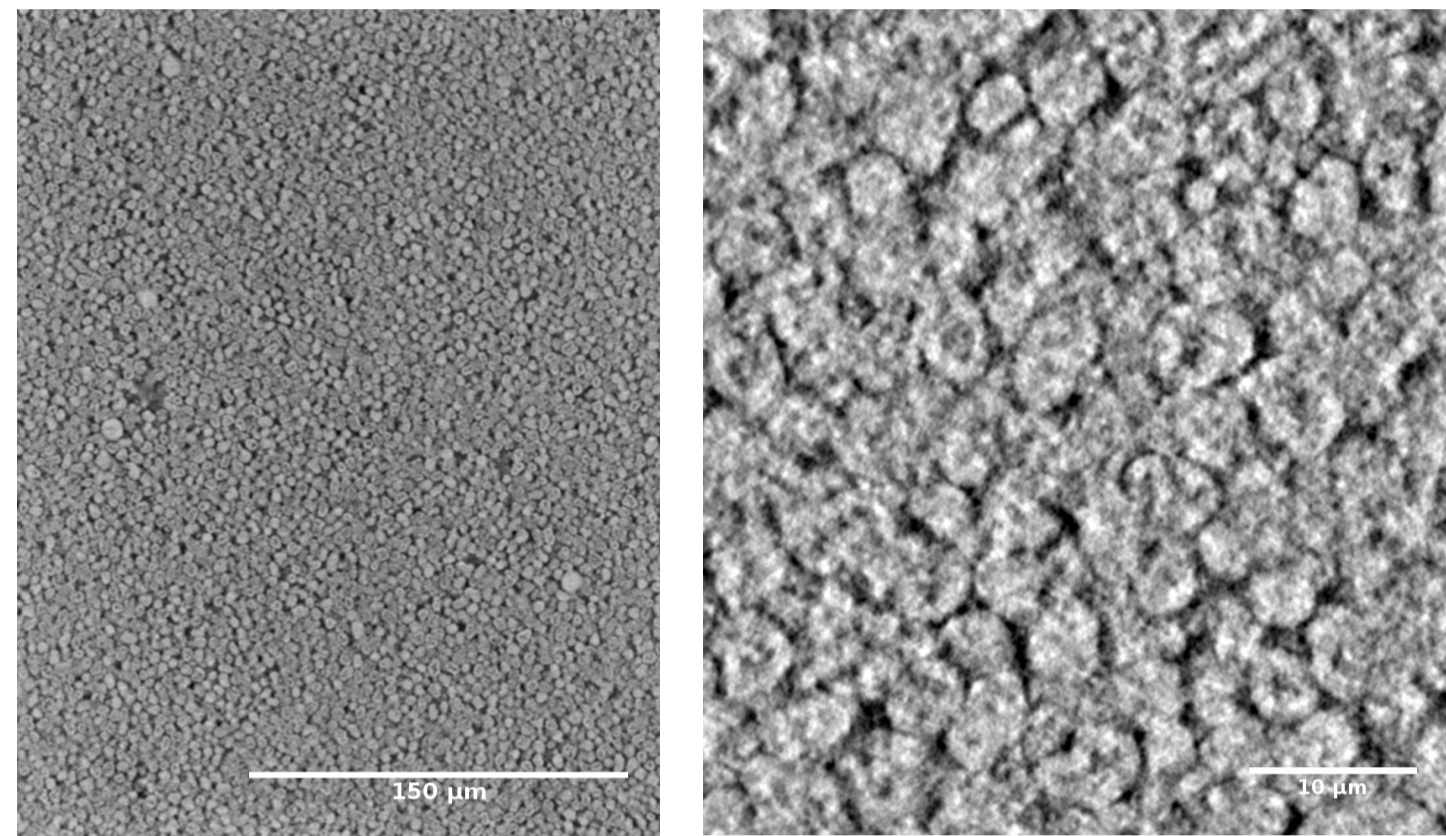
- clusters of **active material (AM)**, energy storage;
  - **blend of polymer with conductive additive** (mechanical coherence and main electronic conduction)
  - **porosity/electrolyte** (ionic conduction)
- => complex multiphase composite that have a **huge impact on effective properties** like conduction.

The aim of this work is to **investigate this microstructure in 3D** and use this data to conduct simulations for effective properties.



### Volume acquisition X-ray tomography

- **Non destructive** technique
- Lab tomography at **0.3µm resolution**
- Synchrotron tomography at **0.05µm resolution**
- **Polymeric phase non visible**

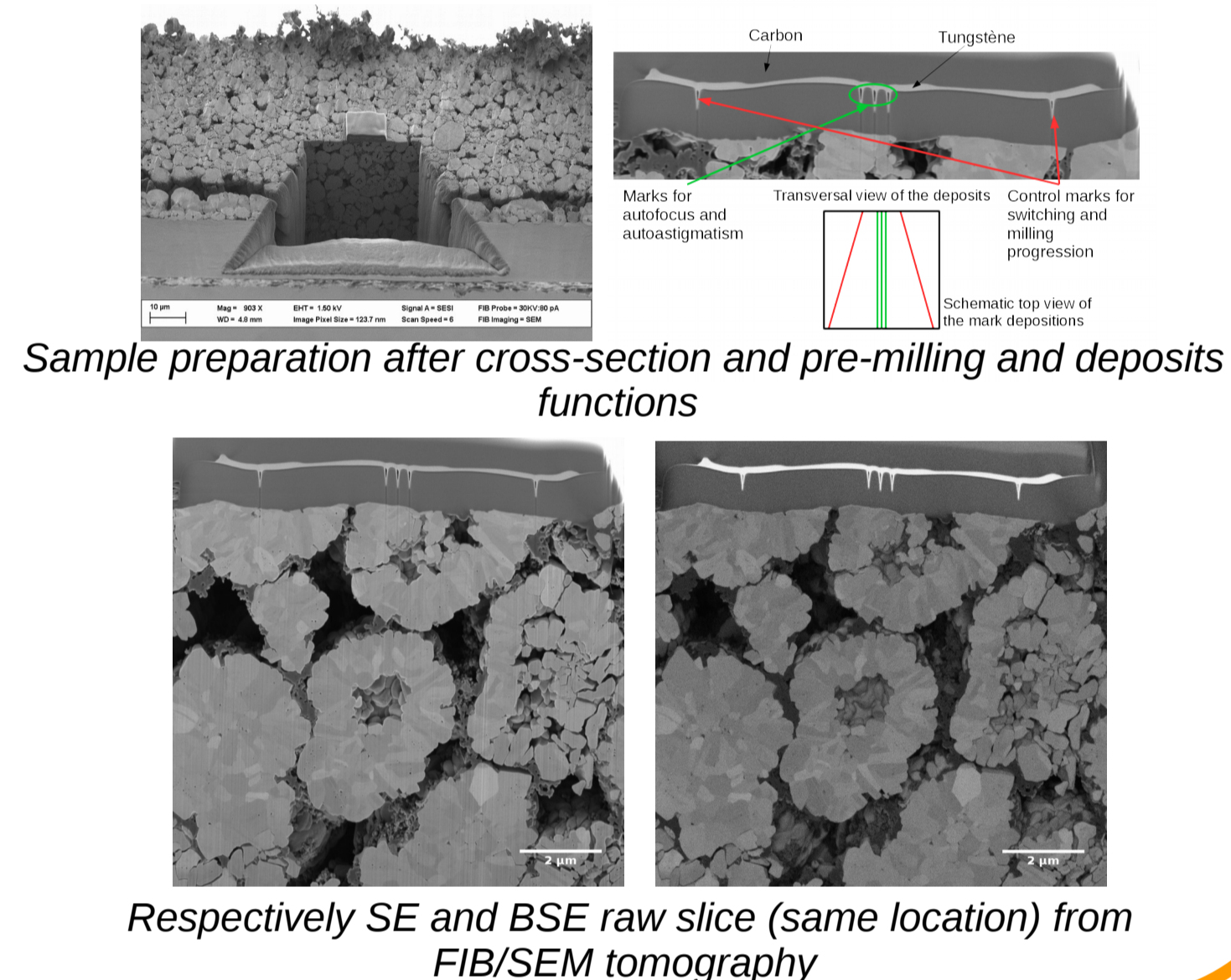


Respectively lab and synchrotron tomography results on samples from the same cathode

Ideal for wide range views but of limited interest for simulation (resolution and phase visibility).

### FIB/SEM tomography

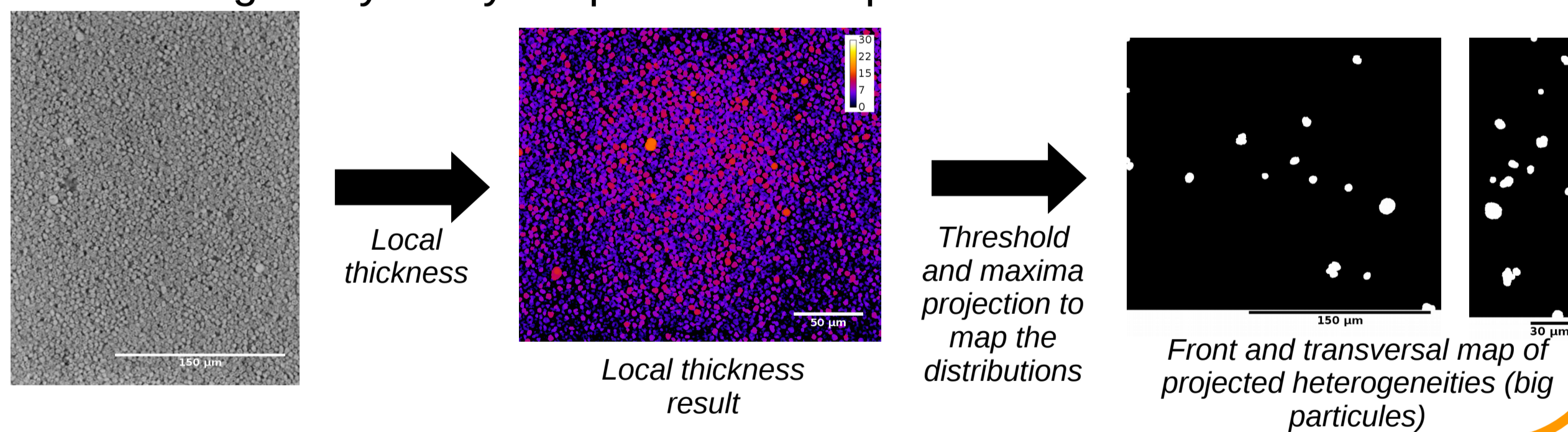
- **Destructive** technique
- **10nm resolution**
- **10x10x10µm³ volume maximum**
- **Special preparation**
- **All phases visible**
- **Zeiss Nvision 40 and Fibics software**



Very good description of the microstructure except for ROI size (representativity), setup complexity and time consuming.

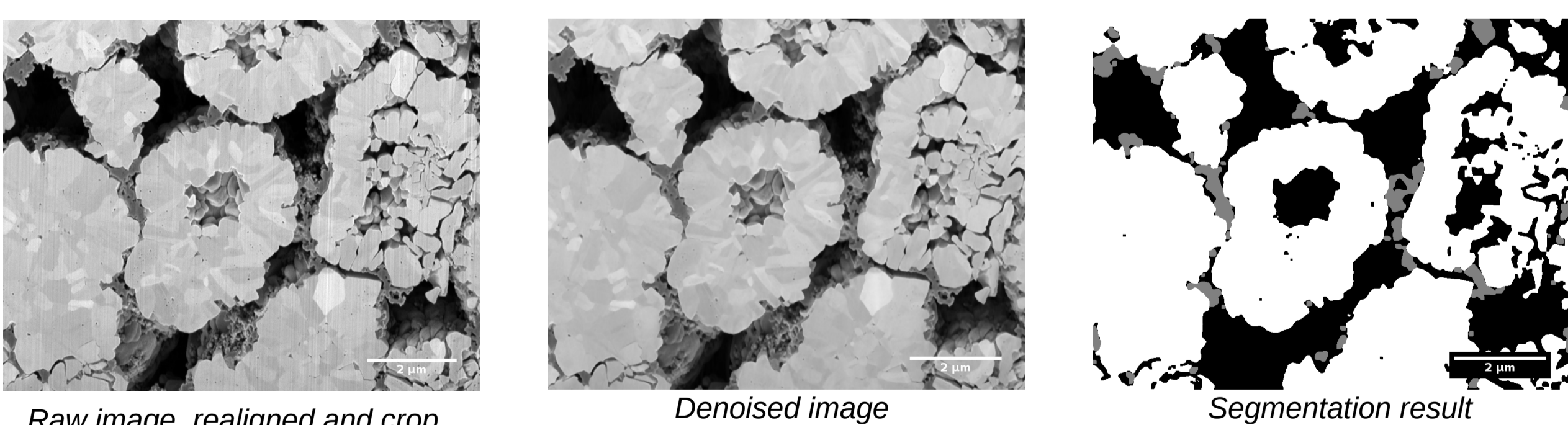
### Image post-treatment Image analysis from XR tomography

- Mean radius determination
- Heterogeneity analysis: particles and pores



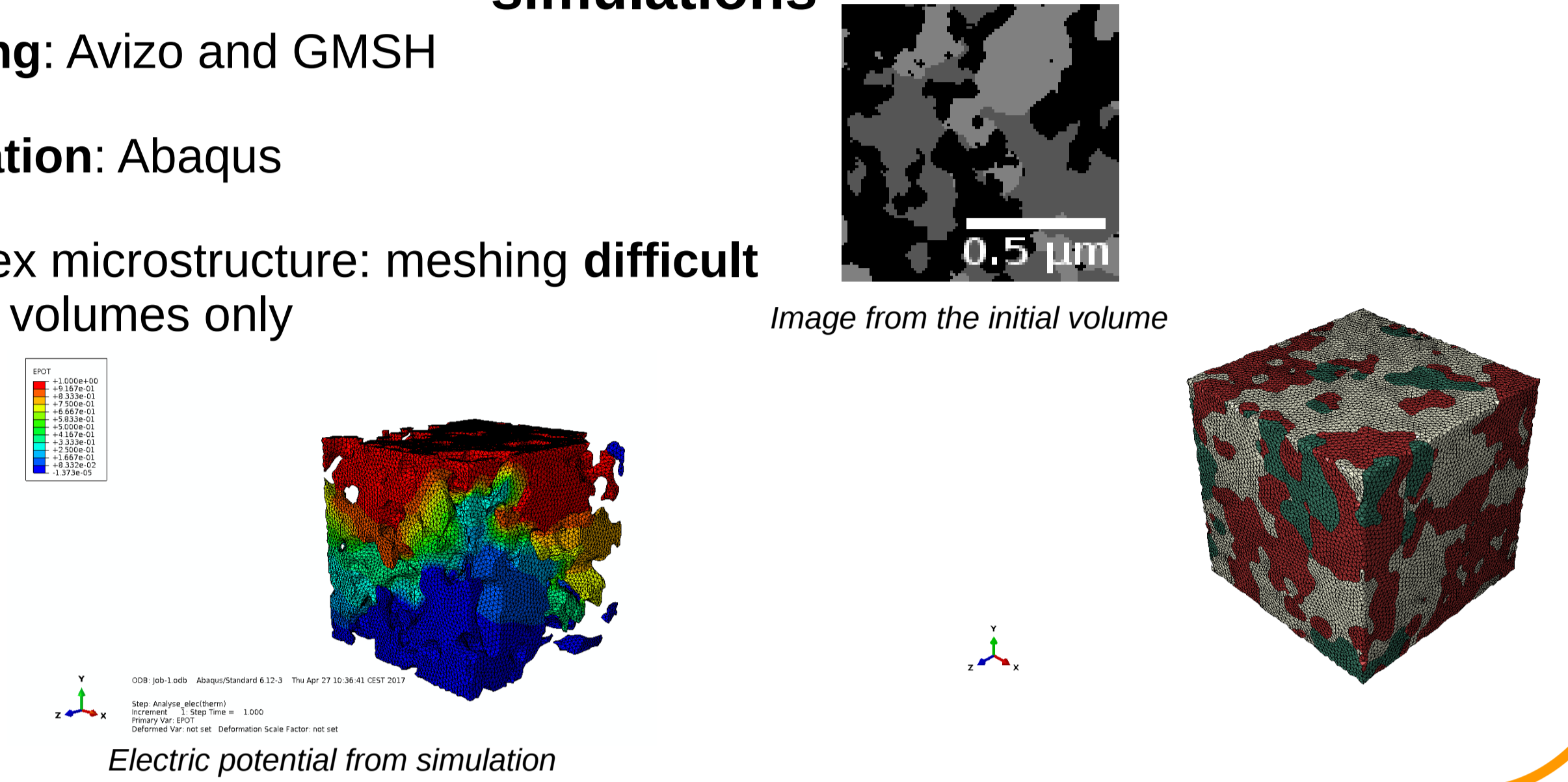
### FIB/SEM tomography volume segmentation

- Process:**
- Image **realignment**: Fiji MultiStackReg plugin
  - Crop to **ROI**
  - Remove **draped effect**: Fiji VSNR\_V2 plugin
  - **Segmentation**: Fiji Macro (shine through artifact) (T. Prill and A. Etienne)



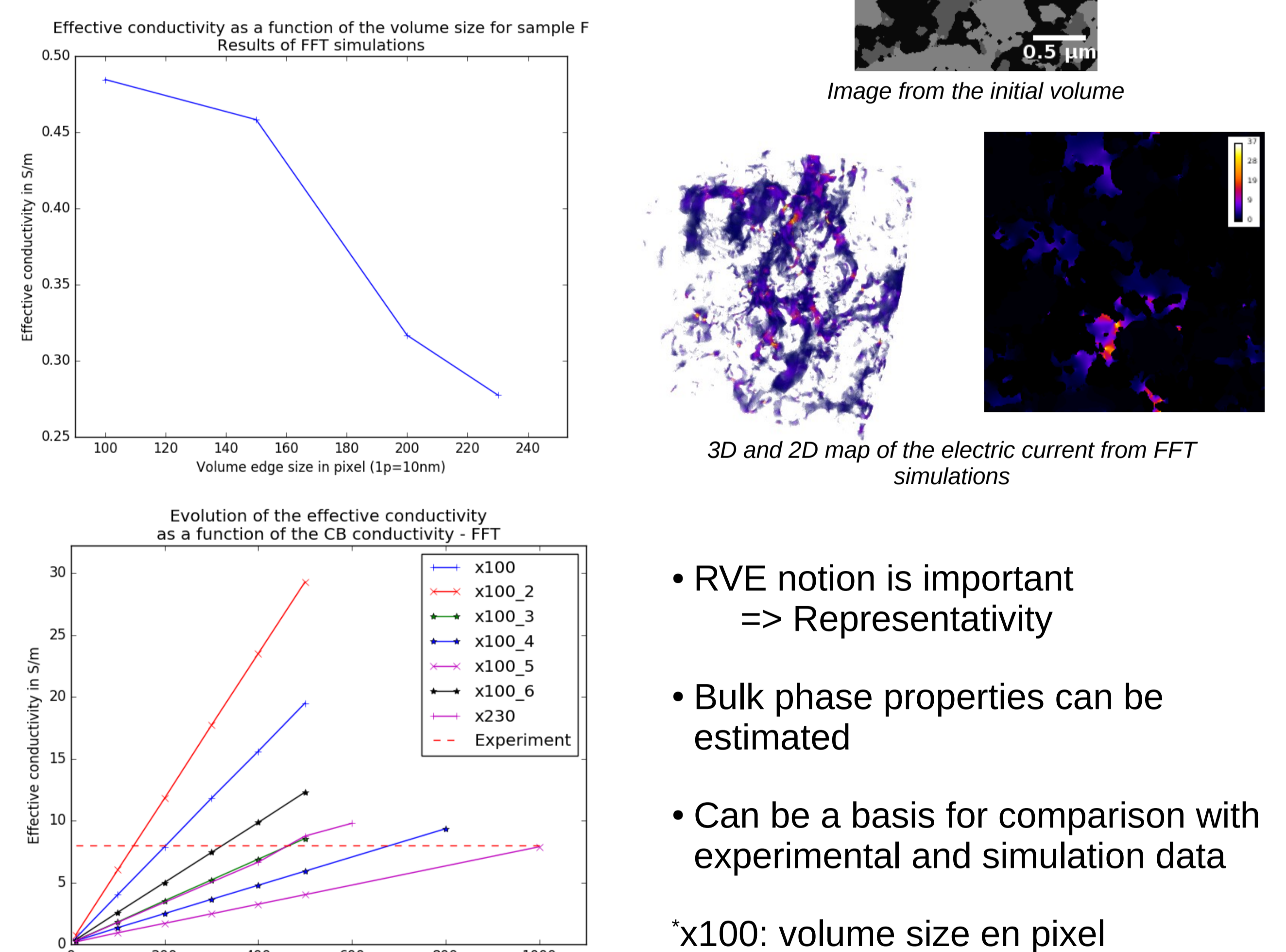
### Numerical simulations Finite elements simulations

- **Meshing**: Avizo and GMSH
- **Simulation**: Abaqus
- **Complex microstructure: meshing difficult**
- **Small volumes only**



### FFT simulations

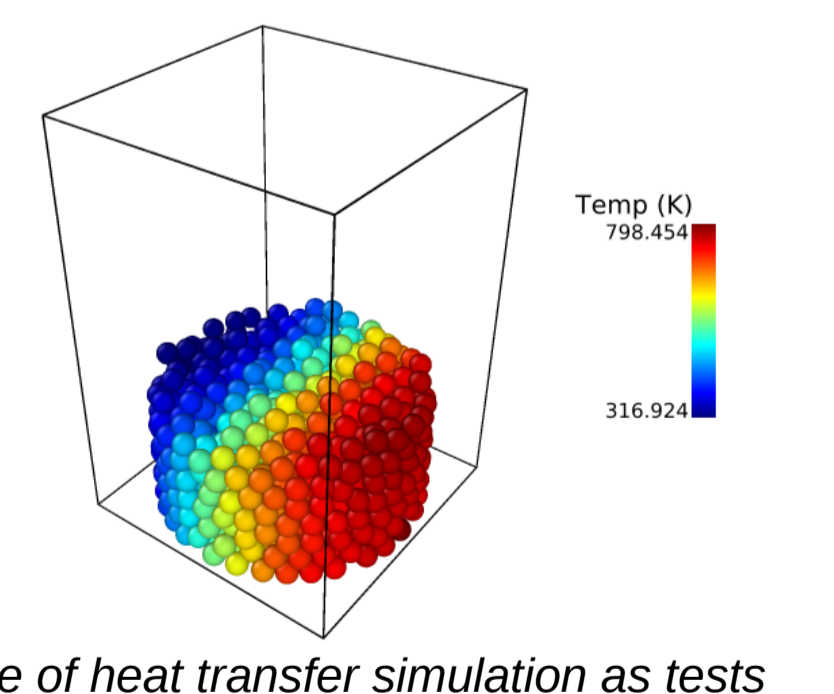
- **Morphomm software** from F. Willot
- Useful for test campaigns and property determinations



- RVE notion is important => Representativity
- Bulk phase properties can be estimated
- Can be a basis for comparison with experimental and simulation data

### Discrete elements simulations

- **LIGGGHTS software**
- Collaboration with SIMAP laboratory and C.L. Martin
- Very **versatile** and promising tool
- Heat transfer feasible then electric conduction too
- **2 ways** for simulations:
  - Classic: 1 numerical particle = 1 physical particle => works, have been done
  - 1 physical particles = multiple numerical particles with global simulation laws => possibilities for complex behaviour
- **Work in progress**
- Models to be developed



### Conclusion:

- **2 imaging technologies** and **3 simulation ways** investigated
- **XR tomography** shows some **limitations** (resolution and phase description) which reduce its interest for simulation while **FIB/SEM tomography** allows a **precise description** of the microstructure. However it is time consuming and more difficult to setup and post-process.
- **FEM** simulation seems particularly unadapted due to the **difficulties** to perform the meshing. On the contrary **FFT** simulation is an easier way to perform calculation as long as a segmented volume is available. The **DEM** simulation gathers good possibilities and should be a good way to conduct complex behaviour simulations.

### Prospects:

- There is mostly two major leads for the short time works:
- **Develop the DEM** models and simulations
  - **Improve the segmentation** method