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A versatile and efficient voxelization-based meshing algorithm of multiple phases

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Voxelization, Mesh, Computational chemistry, Modeling

This paper presents a new algorithm (INNOV) capable of generating a mesh of three-dimensional objects containing multiple phases. This mesh can later be imported into commercial or open-source software to perform multiphysics-based simulations based on partial differential equations. While the range of application is large, this algorithm is designed as a post-processing tool of electrode mesostructures predicted from Coarse Grained Molecular Dynamics (CGMD) simulations of the electrode fabrication process carried out in LAMMPS software. With INNOV
it becomes possible to import the predicted multi-particle electrode mesostructures into COMSOL Multiphysics in order to simulate electrochemistry and transport in discharging lithium ion batteries.

1. Introduction

Despite of the rapid success of lithium ion batteries (LIBs), most of the progresses reached during the last years have arisen from trial-and-error approaches without deep theoretical understanding of the detailed operation mechanisms behind. Nonetheless, in order to reduce the fabrication costs and to further optimize batteries in regards of their integration in the transportation section, the development of predictive mechanistic models is critically needed.\textsuperscript{1–3} Among the most used mechanistic modeling approach, the so-called pseudo-2D (P2D) model dominated during several years the theoretical studies of LIBs since its introduction by Newman and co-workers.\textsuperscript{4,5} However, 2D or P2D models cannot capture the impact the fully resolved 3D mesostructure will have on the LIB cell behavior. In battery modeling, the mesostructure is of importance because the geometry of the pore network and of the CBD will drive the electrochemical performances of the cell. Only a 3D model accounting for the mesostructure of the system can lead to an accurate representation (see Figure S1.). This constrain is shared by many scientific fields where effective or average values assumed because of the complexity of the geometry cannot model faithfully the real behavior of the system.

In the last 10 years there has been a sharp rise of 3D-resolved electrochemical models in the scientific community on multiple chemistries.\textsuperscript{6–9} Used electrode mesostructures are either computer-generated by using random location algorithms (e.g. GeoDict software) or obtained by
computer-tomography. However, reported 3D-resolved models rely on oversimplifications, such as an implicit representation of the carbon-binder domains (CBD) through the use of effective parameters for porosity and tortuosity\textsuperscript{10,11} or by merging CBD with the Active Material (AM) as a single solid phase.\textsuperscript{12}

Meshing an explicit representation of carbon, binder and AM would be like trying to paint with the same paintbrush a rock and a mountain next to each other. Either the paintbrush is too wide and the rock will be deformed but the time to paint the mountain will be short. Either the paintbrush is too fine and the rock will retain its geometry but it will take an impossible amount of time to paint the mountain.

In the case of an adaptive mesh, the complexity relies on assembling a coarser and a finer mesh together. The surface area mesh of the AM in contact with the carbon should have the same size as the one of the carbon. This task is challenging to do at each interface.

This work reports a computational efficient and versatile algorithm capable of meshing multiple phases by using voxelization. The algorithm has been named INfinite Number Of phases meshing through Voxelization (INNOV). This algorithm is capable of importing a multi-phased volumetric mesh into COMSOL Multiphysics benefitting from the native format improvement in the latest update at this date (COMSOL 5.4,\textsuperscript{13} January 2019).

In this paper, INNOV will be illustrated through its application to LIB composite electrodes predicted by using CGMD in LAMMPS. Such composite electrodes are made of AM particles with multiple sizes (radius 1.4-9.4 µm) and CBD particles (radius 0.65 µm). This is useful in order to implement multiscale modeling workflows able to predict the impact of the manufacturing process on the battery performance, as carried out in the scope of the ARTISTIC project.\textsuperscript{14} However, the algorithm can be applied to a wider spectrum of scientific fields.
2. Methods

The algorithm INNOV embeds as its segmentation method the mathematical approach of Nielson and Franke\textsuperscript{15} and a function of the open source program Iso2Mesh\textsuperscript{16} to remove duplicated nodes. This segmentation method has been translated and optimized for MATLAB language and modified to suit the COMSOL Multiphysics meshing importation process. For instance, this new algorithm could lead to considering explicitly the CBD particles in an electrode, which has not yet been reported in the battery field to the knowledge of the authors. Application of this algorithm to a composite electrode will be presented later in this work.

\textbf{Figure 1.} Algorithmic workflow of INNOV with the inputs of each step.

\textit{Inputs of INNOV}

The algorithm takes as input binary stack of images. Such a stack of images can result from different processes.

Firstly, it can be generated from a various selection of imaging tools, such as the segmentation of tomography data. Secondly, binary images can be obtained through the slicing of 3D object
files. The last origin of binary images can be a file with the coordinates of particles center and radius.

This algorithm has been designed to this end in the scope of the ARTISTIC project,\textsuperscript{14} where the coordinates arose from CGMD simulations of the LIB electrode fabrication process. A specific function converts this input into binary images to feed the algorithm with and to reconstruct the electrodes (see Figure S2.).

\textit{Node generation}

In the voxelization technique, each node is related to a pixel in the segmented images so each node is coded with a particle type depending its phase (AM, CBD, electrolyte, separator, etc…). The node generation is the computational-time limiting step for the next to come simulation due to the number of faces and elements increasing with the number of nodes. Since the number of nodes equals the number of pixels, aiming for high-resolution images can be a double edge sword. To address this specific issue, the function embeds an anisotropic downsizing tool in the form of the parameter “precision”. This can be a scalar (isotropic) or a vector (anisotropic) indicating the downsizing factor along each axis i.e. one node out of how many will be saved for the node generation. While slightly losing in precision, the gain in time can be tremendous. Taking a given electrode structure with 3 phases (AM, CBD, Electrolyte) with input stack of images (201×200×179 pixels), the computation time for the generation of the mesh is 177.20 s without downsizing, and 4.48 s with a precision = [4 4 3].

Going further, a more relevant observation would be that the simulation time (which can be up to several days in some cases) of the downsized mesh will also decrease compared to the original one. Indeed, the downsized mesh has more than 1.5 million elements when the mesh without
downsizing has more than 48 million elements. An example of the impact of downsizing can be found Error! Reference source not found.2.

Further in this communication we present INNOV calculated observables to account for the integrity of the structure geometry after the meshing.

Finally, a scale factor parameter (ratio m/pixel) ensures the exact dimensions of the structure.

Figure 2. Slices of a mesh without downsizing (precision = 1) on the left and with downsizing (precision = 5) on the right. In green AM, in yellow CBD and in purple void.

Element Generation

The voxelization divides the space into voxels based on 4 pixels of an image and the 4 pixels associated on the next slide. Which means that a cubic element is generated from 4 nodes of a layer and the 4 nodes associated on the next layer (see Figure S3). In a 3D mesh, elements can be of different shape; in the algorithm they are tetrahedrons which are a classical choice due to their efficiency (4 nodes/elements). The cubic elements need to be divided into tetrahedrons, the function offers two different decompositions: into 5 or 6 tetrahedrons. On the one hand, the decomposition into 6 is more precise and easier to implement since the decomposition into 5 asks
for some additional operations as discussed in the original paper of Nielson and Franke. On the other hand, the computational cost will be higher as it will result in more elements.

**Algorithm**

The voxelization addresses the issues at the interface by meshing every phase all at once. In that way, the surface mesh at the interfaces are by design the same across a given interface between two different phases. To do so, it has to distinguish between four different cases depending on the phases of the nodes of a given element. A trivial one is when all nodes belong to the same phase, no decomposition is needed and the element is retained. The three others occur when the nodes belong to different phases and demand for a decomposition into several more tetrahedrons and creation of triangular faces to effectively separates the phases. Which means the more intricate the phases are, the more surface area there is between them, the more the number of elements and faces will be high.

**Importation**

A non-trivial step in the modeling process is the importation of importing a mesh into an outside software. Whether due to the formalism of the format or its lack of documentation, one must tread carefully when converting a mesh. The algorithm presented here performs a successful importation of the mesh in the native format mphtxt of COMSOL Multiphysics software.

INNOV takes full advantage of the new “Selections” feature in COMSOL 5.4\(^\text{13}\) which allows the user to create automatically selections of faces and elements in the text file. In this case, manual selections would have been prohibitory since they are thousands of domains and boundaries in the imported mesh in COMSOL. Selections provide access to every domains or boundary of interest to apply equations into COMSOL, which is the trickiest part of the importation.
3. Results and Discussion

In this section we discuss the results of INNOV applied to a three-phased LiNiMnCo electrode (AM + CBD + Void) generated from CGMD calculations using LAMMPS software, as explained in the article of Ngandjong et al.\textsuperscript{10} In this case, the input is a text file with the coordinates of the centers and the radius of each of the particles (see Figure S3.).

Meshing

Once the binary stacks of images are generated, a precision of [4 4 3] is set to decrease the computation time. Time-efficient meshing is achieved thanks to the simplicity of the operations and to an optimization through a matrix formalism in MATLAB. The meshes represented in Error! Reference source not found.3 both have 339 067 nodes, 371 213 faces and 1 737 665 elements. The unsmoothed mesh has been generated in 4.48 s on a desktop computer (32 Go RAM).

The voxelization technique is known for its staircase shape so the algorithm embeds a smoothing option, which relies on Kroon’s function.\textsuperscript{17,18} It is noteworthy that the smoothing algorithm tends to shriek the volume of the elements, resulting in a slight increase of the porosity (for the example here, 49.69 % before and 50.07 % after smoothing).

Observables

The core of this work is to increase the current level of precision of the modeling of batteries by separating active and inactive materials. In doing so, one must not sacrifice the integrity of the
mesostructure geometry. To ensure this, INNOV provides a number of observables, which can be compared to experimental numbers (e.g. arising from tomography characterizations).

Among them, two distinct values of porosity are displayed by INNOV, the porosity of the mesh and the porosity of the stack of images. In the example of this communication, the porosity of the stack is 50.1 % and the porosity of the resulting mesh is 49.7 %. Furthermore, the volume ratio of each phase in the mesh is compared to its value in the stack of images in Table 1. This can render proof of the overall volume conservation of each phase; however, these are average values and cannot highlight local deformations within the mesh. Here, the meshing step introduces an error below to 2% on the volume of each phase, which is considered satisfactory in our study. Another useful insight is the surface coverage between different phases. For example, the surface area of the interfaces between Active Material and CBD (36.2 %) or the Active Material and Electrolyte (63.8 %) are provided once the mesh is done.

Figure 3. Mesh of a NMC electrode generated without smoothing (a) and with smoothing (b). The spherical active material particles are in red and the carbon binder domains are in yellow.
Table 1. Observables provided by INNOV after the meshing of the electrode in Figure 3a.

|                  | Volume percentage | Volume conservation |
|------------------|-------------------|---------------------|
| Void             | 49.7 %            | 99.2 %              |
| AM               | 30.5 %            | 101.6 %             |
| CBD              | 19.8 %            | 99.7 %              |
| AM with CBD      |                   |                     |
| Coverage percentage | 36.2 %          | 63.8 %              |

4. Conclusions

This communication reports a flexible MATLAB-based algorithm (INNOV) to tackle the meshing process and importation of multiphase objects in computational frameworks for multiphysics simulations based on sets of partial differential equations. From a selection of input format, INNOV generates a volumetric mesh able to contain an unlimited number of phases. This mesh can then be converted into the desired format to suit a variety of commercial and open-source software. INNOV embeds a set of observables to ensure the geometric integrity of the structure after the meshing step. While designed for the battery field, this algorithm can be applied to a wide spectrum of scientific fields. It offers a time-efficient tool to perform meshing without requiring substantial computational resources.

ASSOCIATED CONTENT
**Supporting Information.** The following file is available free of charge. It presents figures mentioned in this communication, explicating the complexity of LIBs geometry and the process of voxelization (PDF).

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**Notes**

The authors declare no conflict of interests.

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**ABBREVIATIONS**

AM, active material; CBD, carbon binder domain; CGMD, coarse grained molecular dynamics; INNOV, infinite number of phase meshing through voxelization; LIB, Lithium-ion battery; P2D, Pseudo-2D.

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