Supporting Information

A novel multi-physics coupled heterogeneous single-cell numerical model for solid oxide fuel cell based on 3D microstructure reconstructions

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As shown in Fig. S1, all simulation steps were integrated into the MATLAB main function, including the following steps: 1) converting multi-phase volume data based on 3D reconstruction; 2) calling ISO2MESH to generate tetrahedral meshes; 3) automate identifying features, defining equations, adding boundary conditions and batch post-processing of data. Each phase in the 3D reconstruction was identified and labeled to generate a matrix. The generation of tetrahedral meshes was accomplished based on the *v2m* function script in ISO2MESH, and the method '*cgalmesh*' was chosen to generate meshes according to its robustness in multi-phase mesh generation. At the same time, we also developed a script to refine the mesh at TPBs to increase computational accuracy. The nodes and elements of meshes were sorted so that the index nodes and elements are closer to each order (this may reduce cache misses in computations) using the *sortmesh* function, the nodes in tetrahedral meshes were reordered to ensure that all elements are in the appropriate directions using the *meshreorient* function. Then the meshes were imported into COMSOL via the LiveLink with MATLAB interface. The main commands include *mesh.data.setVertex*(vertex, array), *mesh.data.setElem*('tet', elem.array), *mesh.data.ElemEntity*('tet', phase array) and *mesh.data.createMesh*. Besides, the *mphmeshstats* function was utilized to obtain meshes information imported into COMSOL, and then TPBs and DPBs were automatically identified through custom script. Governing equations and boundary conditions were automatically applied in COMSOL through custom scripts. Finally, the multi-physics coupling problems were solved and the computational results were processed in batch automatically.
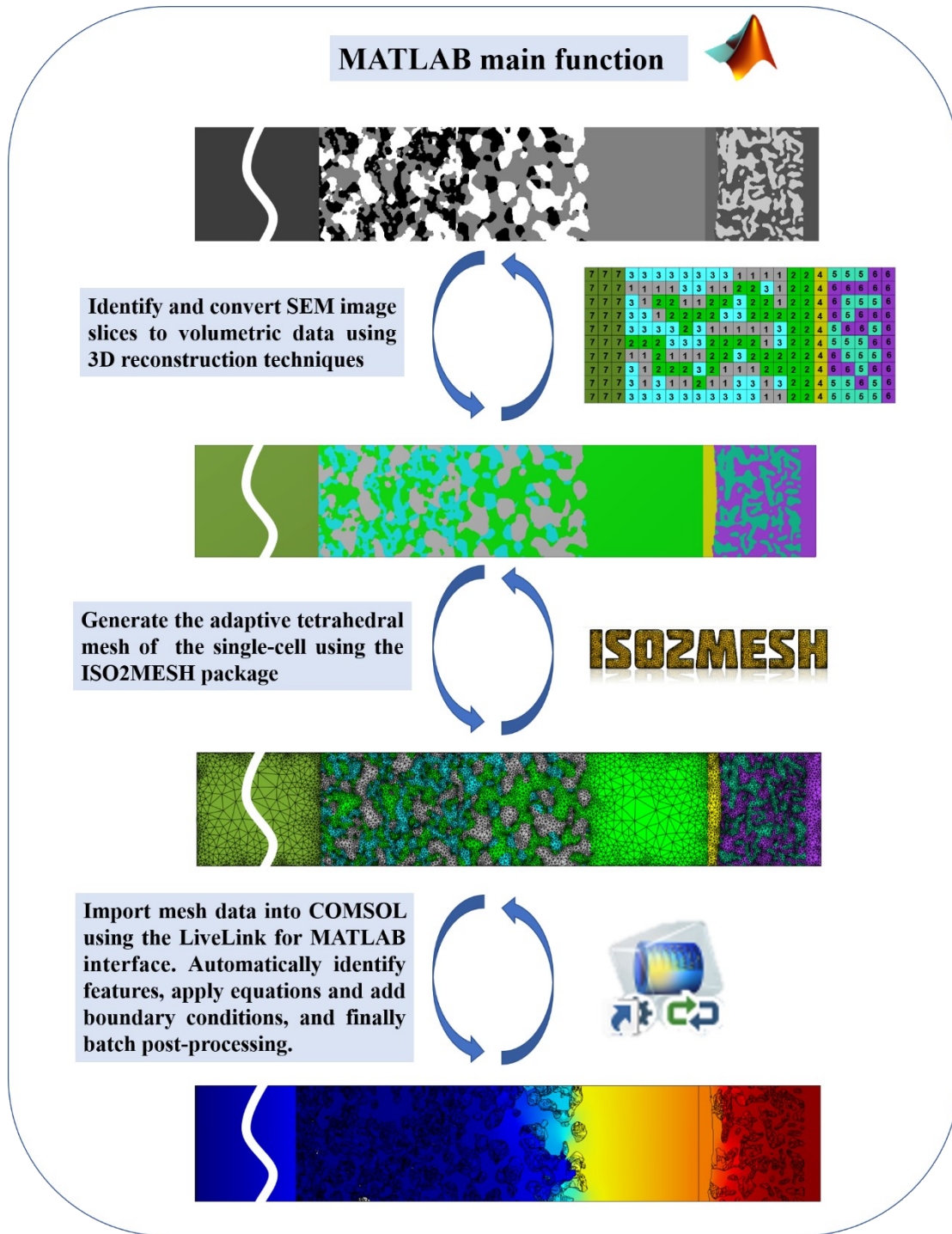
Figure S1. Automated processes for 2D image segmentation, 3D microstructure reconstruction, meshing, FEM solution and post-processing.