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Dynamic Coupling of a Finite Element Solver to Large-Scale Atomistic Simulations

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We propose a method for efficiently coupling the finite element method with atomistic simulations like molecular dynamics or kinetic Monte Carlo. It is a continuation of our earlier attempt to develop a tool to perform multiscale-multiphysics simulations about evolution of nanostructures under high electric field. Our method enables to dynamically build an unstructured mesh with optimized density that follows the geometry defined by atomistic data. On this mesh, multiphysics problems can be solved to obtain distributions of physical quantities of interest, which can be fed back to the atomistic system. The simulation flow is optimized to maximize computational efficiency while maintaining good accuracy.

On the first stage of development, the code solved dynamically the Laplace's equation in 3D domain and used the solution to obtain electron emission currents, charges and electrostatic forces for surface atoms. By taking into account Joule and Nottingham heating and solving 1D heat equation, we obtained also atomistic velocity perturbation.

Over the last year we have extended and improved the capabilities to the code. By incorporating particle-in-cell technique, we obtained the possibility to include space charge in electric field calculation. Replacing 1D heat equation solver with a 3D one increased the overall accuracy and extended the spectrum of possible applications of the code. Several improvements in the algorithm base have significantly improved the tolerance against the geometry under scope.

The tests have shown remarkable overlapping with an analytical solution and proved the code to be efficient and robust enough to simulate large-scale thermal runaway processes.

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