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# Atomistic modeling of metal surfaces under high electric fields: direct coupling of electric fields to the atomistic simulations

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In 2011 the hybrid electrodynamics –molecular dynamics code HELMOD was developed to study the effect of electric field to the stability of metal surface. That code has been successfully used in several projects. However, to cope with the forthcoming challenges, the efficiency of the software must be enhanced. This will be done by transferring the electric field solver from the finite difference basis into the finite element framework and by adding parallel computations capability. The code will be entirely open-source and will be shared with all the interested colleagues.

The code has the tools to generate the finite element mesh around the atomistic simulation domain, solves multi-physics problems in 3D domain and accommodates the communication layer with atomistic simulations. On the first stage of development, the code will dynamically solve the Laplace's equation in 3D domain to obtain electron emission currents, charges and electrostatic forces for surface atoms. The results of those calculations are coupled to classical molecular dynamics and kinetic Monte Carlo code in order to model the dynamic evolution of an atomistic system under high electric field.

The tests with the code have shown significant increase in computational efficiency for large systems and remarkable tolerance against system geometry.

## Type of contribution

Oral

## session

Modelling and Simulations

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