A model for the multiscale simulation of thermo-chemo-mechanical problems

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ABSTRACT

Modeling mechanical problems at the atomistic level is always complex, but when, in addition, thermal and mass transport phenomena play an important role, even the most advanced simulation methods face enormous difficulties to produce solutions at useful space and time scales. For example, molecular dynamics simulations are commonly employed for solving processes lasting picoseconds, but problems of segregation, and corrosion can require solution times of the order of hours, days or even months.

In this talk we will present a recently proposed model [1, 2] which allows to upscale in time the atomic oscillations in thermal problems and the stoichiometric hops due to mass diffusion. The idea of this work is to use Jaynes' principle of maximum entropy [3, 4] to derive a statistical mechanics model that averages those oscillations in an optimal fashion, effectively eliminating them from the governing equations. The variational nature of the approach makes it simple to couple it with Quasicontinuum approximations [5], thus leading to a space and time multiscale method.

In the talk we will summarize the ideas leading to the method and illustrate its predictive capabilities by showcasing equilibrium and out-of-equilibrium simulations.

References

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