Virtual DCMIC Seminar Series 2021

Seminar #2.2
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Coarse grained kinetic simulations of chemo-mechanical processes at the nano-to-micro mesoscale

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The formation and degradation of materials at the mesoscale, between the nano and the micro metre, are driven by coupled chemo-mechanical processes. Existing simulation techniques, such as molecular dynamics, Phase Field, and Kinetic Monte Carlo, are either limited in length/time scales or rely on assumption that break down at this mesoscale.
This talk presents a new method that combines (off-lattice) Kinetic Monte Carlo with a coarse-grained particle-based description of the material. Per-particle rates of dissolution and precipitation are derived from Transitions State Theory, featuring also the contribution from mechanical interaction. Simulation results on dissolution at dislocations and precipitation involving particle aggregation, show that the emerging mesoscale morphologies are indeed controlled by both mechanical interactions and chemical potentials.
The simulator, called MASKE, can be used for various material chemistries, is massively parallelized, and will soon be available for download on GitHub.

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