Design of an Optimal Overlap Algorithm for Dynamically Coupling Continuum and Noncontinuum Codes in Multiscale Simulation

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Different simulation methods are most effective at different length scales, which motivate efforts to simulate overall multi-scale systems by linking multiple simulation codes created by experts at each scale. There are numerous examples where length and time scales are coupled in a serial fashion, where the results from a simulation code are used in another simulation code [1-7]. For example, it is common to use quantum mechanics to compute force fields that are used in a molecular dynamics code. For quasi-static problems, the quasi-continuum method [8,9] couples the atomistic and continuum scales by using a system-wide finite element mesh that is refined to the atomic dimensions where needed. Unlike conventional finite elements, the energy of each cell is computed from the underlying atomistic Hamiltonian. Many other papers propose iterative algorithms to converge codes at multiple length scales to a steady-state or quasi-steady-state solution [10-13].

The need to simulate *dynamic* systems where a wide range of time and length scales are tightly coupled have motivated recent efforts to address the more challenging problem of *concurrent* multiscale simulation [14]. The FE/MD/TB hybrid approach [15] spatially divides the system into continuum, atomistic, and overlap regions and appropriate boundary conditions are shared among the various regions to obtain a self-consistent solution. An approach applicable to some reacting systems is the use of an effective reactivity to atomic and continuum scales [16,17]. In the coarse-grained molecular dynamics (CGMD) approach [18], the constitutive relations are derived directly from the interatomic potential by means of a statistical coarse graining procedure [19]. Thus, the average thermodynamic effect of the atomic-scale quantities is retained in the coarse-scale motion. A coarse-grained Monte Carlo simulation approach was recently derived that can represent mesoscopic length scales while correctly capturing atomistic information on intermolecular forces [20].

The direct numerical simulation approach involves running the simulation codes at each length scale simultaneously, with each code continually passing updated boundary conditions to the other codes [21-23] (e.g., see Figure 1). A weakness of the direct numerical simulation approach is that it can induce numerical instabilities at the interface between simulation codes (e.g., see Figure 2). A modified approach uses internal iterations to force convergence of the information passed between simulation codes [24,25]. Another modification updates the continuum codes more slowly than the atomistic codes, in accord with their different time scales [26,27]. Yet another modification introduces a dynamic coupling filter to improve numerical accuracy and enhance numerical stability [28]. A systematic design procedure for these filters has been developed using control systems theory [29,30].

Although the overlap algorithms like the FE/MD/TB hybrid approach [15] have significant promise, due to their ability to reduce the impact of fluctuations from the stochastic simulation codes (e.g., kinetic Monte Carlo simulation) on the deterministic simulation codes (e.g., finite differences), there is no systematical approach to the design of such algorithms.

This presentation shows how control theory can be used to systematically design overlap algorithms for multiscale simulation. The approach is applied to the multiscale simulation of the electrodeposition of copper, which is the primary method used to manufacture on-chip interconnects in electronic devices. The product quality is a function of deposit shape and morphology. The evolution of shape and morphology is determined by nucleation phenomena and the macroscopic transport of ion species in the bulk onto a substrate, which includes adsorption of species, desorption of species, and surface diffusion. A hybrid model that incorporates continuum and kinetic Monte Carlo (KMC) descriptions have been developed in our group [28] to simulate this process for the range of time and length scales of interest. For a copper deposition formed using a rotating disk electrode, the thickness of the boundary phase forming on the substrate is ~50 microns, while the dimension of a cube lattice simulated in the KMC code is 12.5 nm. Similarly, the time scale of the process varies from 1 ns, which is the average time step of KMC code to several milliseconds, which is the time constant for depletion of copper at the interface under high potential.

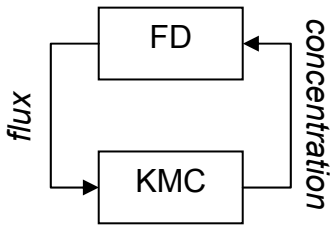

Figure 1. The direct dynamic coupling of a finite difference and a kinetic Monte Carlo code to simulate copper electrodeposition into a submicron trench. A finite difference code simulates the continuum model that describes the transport of ions from the bulk to the surface and a kinetic Monte Carlo code simulates the surface evolution and morphology.

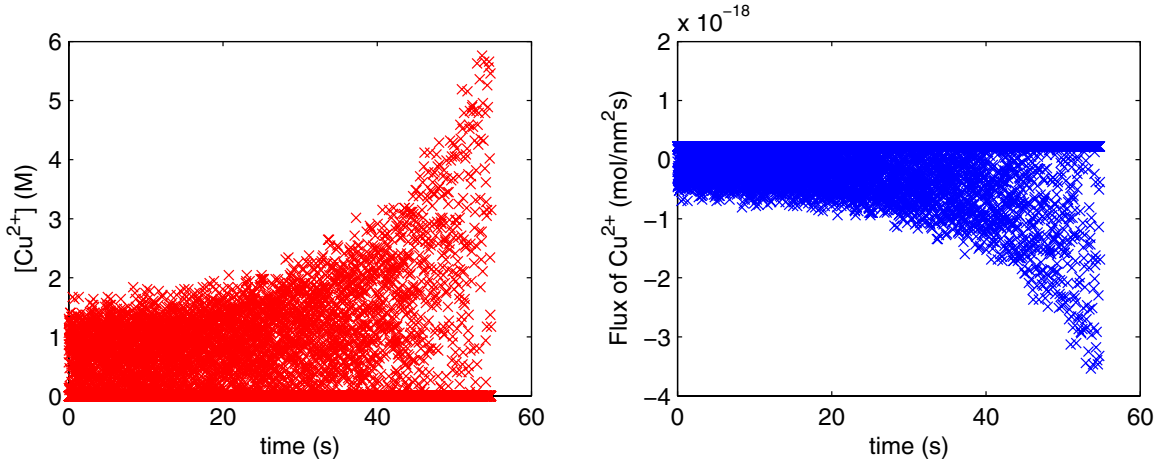

Figure 2. The concentration and flux of cupric ions at the interface between the domains of a directly coupled finite difference and kinetic Monte Carlo (FD-KMC) code obtained from a simulation of copper electrodeposition into trench feature in the absence of additives. Both signals shown are highly noise-corrupted and growing exponentially with time.

The main component of the overlap algorithm is a minimum variance KMC output estimator [31] constructed based on a continuum model that captures the adsorption-diffusion processes simulated in the Monte Carlo domain (see Figure 3). At every time step, the KMC code computes the average concentration for each species at the interface and passes that information to the continuum code. The continuum code then integrates the continuum model over the same time step and passes the flux information to the KMC code. The coupling algorithm, which is a recursive output estimator, uses the flux information passed from the continuum code and the stochastic KMC output calculated over the same period to estimate the concentration for each species at the interface, which is then passed to the continuum code for the next computation iteration. The description of the continuum model in the Monte Carlo domain is constantly updated at each time step to track the moving boundary condition determined by the deposit surface simulated in the KMC code. This continuum model is then solved by finite differences to obtain a linear discrete time varying system upon which the minimum variance estimator algorithm can be applied. The state of the resulting system is the concentration field inside the Monte Carlo domain (see Figure 3). The linear time varying system is a stochastic system with additive Gaussian white noises. The output of the system is a realization of a Poisson event, which models the output distribution of the KMC code.

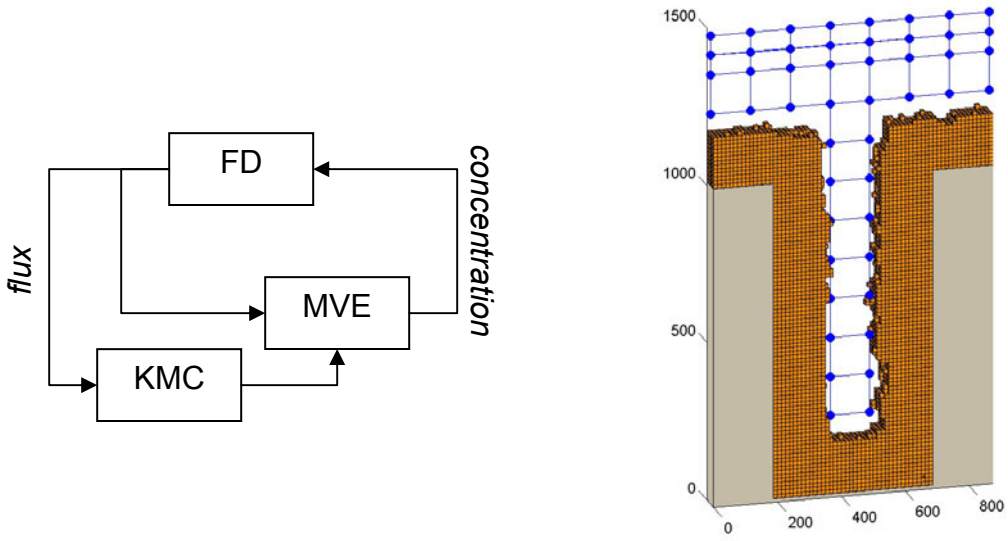

Figure 3. The minimum variance estimator (MVE) estimates the concentrations at each grid node in the overlapped region within the kinetic Monte Carlo domain based on cumulative information feed from FD and KMC codes. The estimates at the interface (shown here at the top) are then passed to the finite difference code.

The simulation results show that the estimator not only numerically stabilizes the linkage between the continuum and the KMC codes, but also it gives more physically consistent simulation results as the noise of the concentrations and fluxes along the boundary is significantly reduced (see Figure 4). The results of the coupled continuum and KMC code were evaluated for consistency using the test proposed by Drews et al. [28].

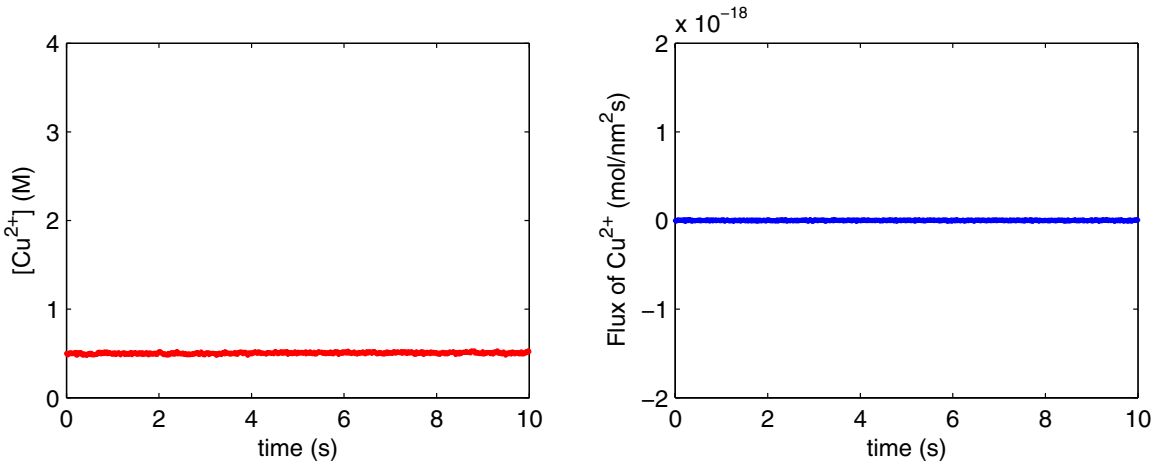

Figure 4. The concentration and flux of cupric ions at the interface between the domains of the coupled finite difference and kinetic Monte Carlo (FD-KMC) codes that incorporate a minimum variance estimator with the overlapped algorithm. The results were obtained from copper electrodeposition with identical conditions as in Figure 2. The system reaches steady-state rapidly and displays no numerical instability.

Acknowledgments

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