Simulating extended time and length scales using parallel kinetic Monte Carlo and accelerated dynamics

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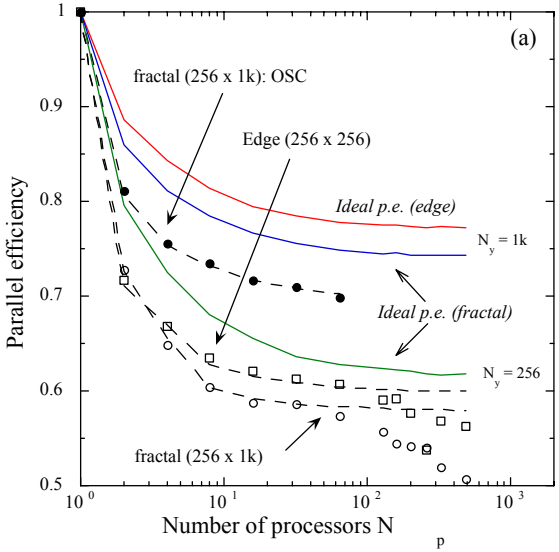
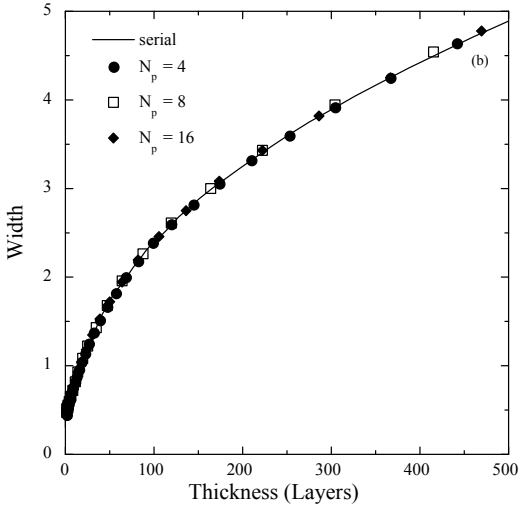
To model non-equilibrium processes, simulations over a wide range of time- and length-scales are needed. For example, in thin-film growth the elementary atomic-scale processes may take place over microseconds while simulation times of minutes or longer are required. To address this problem, we are developing and applying algorithms for parallel kinetic Monte Carlo (KMC) and accelerated dynamics simulations. Fig. 1(a) shows measured and ideal parallel efficiencies (p.e.) obtained in parallel KMC simulations of thin-film growth using our recently developed ***synchronous sublattice algorithm***. Using this algorithm, p.e.'s greater than 50% may be obtained in simulations with 1000 processors or more. Surface morphology (inset) and comparison with serial simulations are shown in Fig. 1(b).





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Education:
This work is being carried out in collaboration with a postdoctoral research associate, Dr. Yunsic Shim, as well as three Ph.D. graduate students (Giridhar Nandipati, Feng Shi, and Valery Borovikov) at the University of Toledo who are being trained in kinetic Monte Carlo and parallel computing. An undergraduate Summer student (Travis Smith) also contributed to this work.

Outreach:
We have recently begun a collaboration with a computer scientist (Prof. Hassan Rajaei) and an undergraduate student (Mark Randles) at Bowling Green State University to enhance the performance of our parallel KMC simulations. We have also started a collaboration on parallel accelerated dynamics with Dr. Arthur Voter of Los Alamos National Laboratory. A preliminary account of this work was presented at the Ohio Supercomputer Center in April 2003 and more recently at the American Physical Society meeting in March 2004.