Crossing the Mesoscale No-Man's Land: Parallel Kinetic Monte Carlo Simulation

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Sandia National Laboratories

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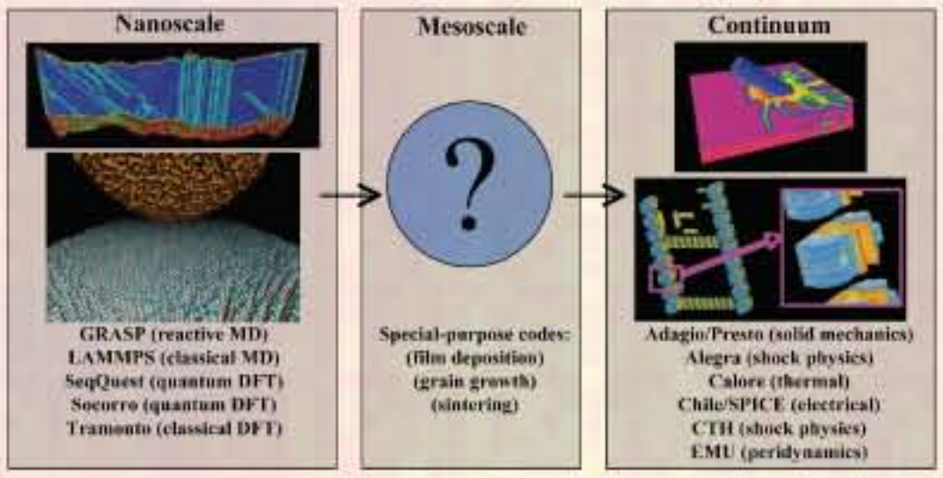
The Challenge

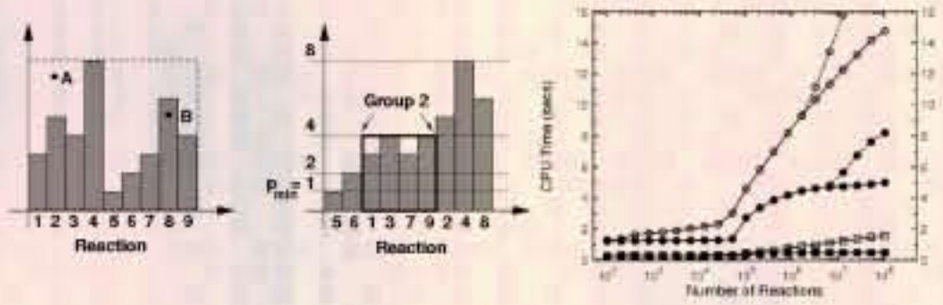
- Kinetic Monte Carlo can address mesoscale (one event per timestep)



- But ... fundamental KMC algorithm is not inherently parallel need general purpose code for new models (tend to be specialized)

Approach

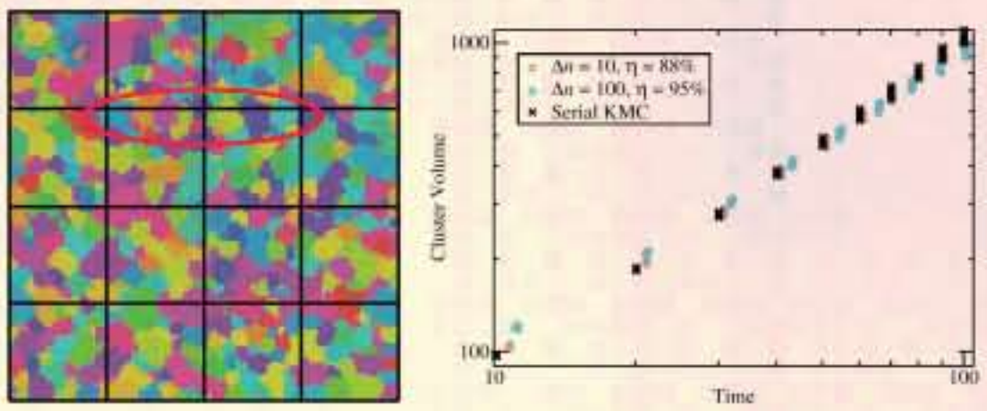
O(1) KMC Algorithm for Event Selection



- Traditional KMC algorithms are O(N) or O(logN) in number of events
- Grouping/rejection algorithm is O(1), independent of number of events
- From random variate generation literature, we applied to KMC
- Enables efficient implementation of very large KMC models
- Useful for large biology networks or large-scale materials models
- Slepoy, Thompson, Plimpton, J Chem Phys, **128**, 205101 (2008)

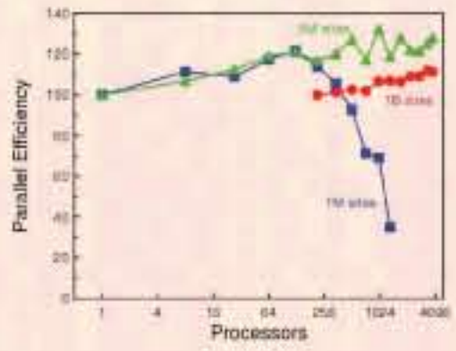
Results

Approximate Parallel KMC Algorithm



- Spatial decomposition of physical domain to processors
- Sub-cycle on 4 (2d) or 8 (3d) sectors per proc to avoid event collisions
- Inaccurate "shish-kebab" effect across frozen domain boundaries
- Solution: adaptively vary Δt as simulation runs
- If adapted properly, approximate algorithm → exact solution
- Maintains high parallel efficiency (η)

Parallel Scalability

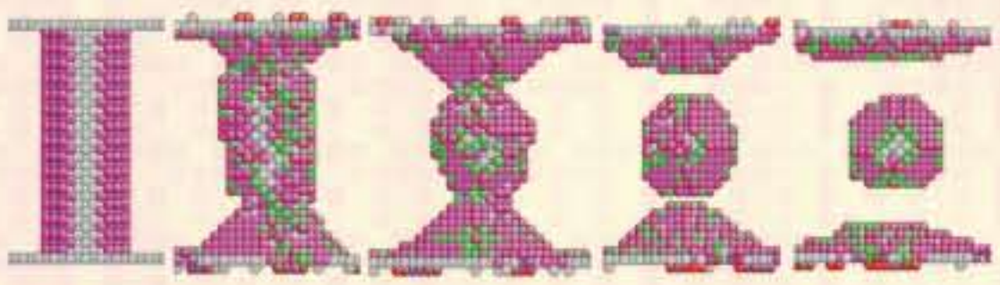


- 3d grain growth model: 100^3, 200^3, 1000^3 lattice sites
- 1 to 3840 processors of Sandia's Red Storm machine (Cray XT3)
- Efficiency increases due to smaller problem for NlogN KMC solver
- Efficiency decreases due to communication costs (surface-to-volume)

Grain Growth Application

- 3d Potts model for grain growth
- Boundary curvature drives growth
- Hamiltonian can describe constraint conditions on growth (impurities, pinning, strain, etc) leading to variety of grain morphologies
- Can now address very large sample sizes

Stability of Nanoporous Palladium



- Greg Wagner (8700), Hydrogen/Tritium storage in Pd
- Nanoporosity may alleviate Helium bubble formation issues
- How long are pores stable to surface diffusion effects ?
- Compare to expt and to molecular dynamics (small samples, high T)
- Parallel will enable large-scale nanoporous geometries

Significance

- SPPARKS KMC code (Stochastic Parallel PARticle Kinetic Simulator)
- SPPARKS = KMC algorithms with applications in parallel framework
- Easy to add new applications: define events and their probabilities
- Current apps are mostly on-lattice KMC, off-lattice is next
- Just approved for open-source release (WWW site soon)

- Materials science at the mesoscale has a variety of KMC needs:
  film growth, grain growth, surface chemistry, transport
  CVD, electrodeposition, flame spray, sintering, annealing, aging

- Final year LDRD focus is on developing new SPPARKS applications

- Nice KMC overview: C Battaile, Computer Methods in Applied Mechanics & Engineering, 197, 3386-98 (2008)

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