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SPPARKS Modeling for Gordon Research Conference 2017

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Sandia National Laboratories

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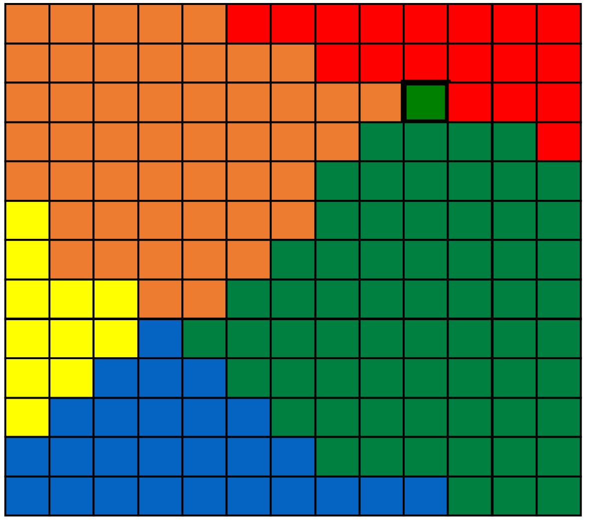
SPPARKS Framework

- Stochastic Parallel PARticle Kinetic Simulator
  - Developed at Sandia National Laboratory
  - Monte Carlo as well as PDE Solvers
- Rejection Kinetic Monte Carlo (rKMC) algorithm for selection and simulation of events on regular lattice
  - Rate is defined as energy required to overcome an energy barrier
- Time is easily associated with this algorithm by comparison with experimental results
- Potts model uses the Monte Carlo portion of SPPARKS
- Diffusion of $Si(OH)_4(g)$ uses PDE solvers for Fick's Second Law

Representation of Microstructure and Composition rKMC

- Potts rKMC digitizes space into discrete 'bits' of material
  - Each color represents a membership in a phase and / or feature (i.e. grain)
  - Each color can also represent composition, but true gradients in composition would require huge simulations



- Suppose rKMC occurs at boxed green site with initial energy 5 with three possible outcomes
  - Flip to red color – final energy of 4
  - Flip to orange color – final energy of 7
  - Stay green – energy of 5
  - Coarsening of red color minimizes energy and is accepted

Kinetics of Evolution
Potts rKMC

- Ensemble is statistically manipulated to mimic atomistic diffusive processes
- Boltzmann statistics used for evolution
  - P is probability of an event occurring

$$P = \begin{cases} 1 & for \quad E \leq 0 \\ \exp\left(\dfrac{-\Delta E}{kT}\right) & for \quad E > 0 \end{cases}$$

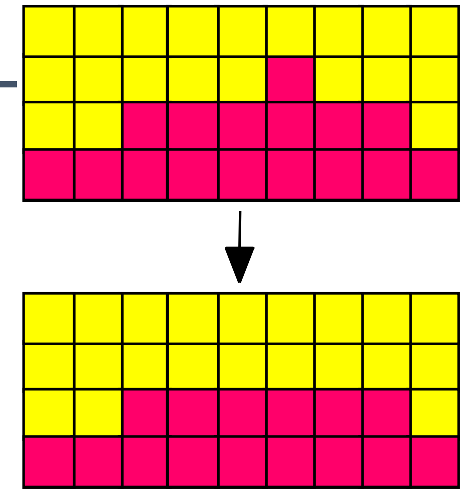
Tested against a randomly generated integer. Exponential must be less than this for acceptance of event.

Evolution of the ensemble

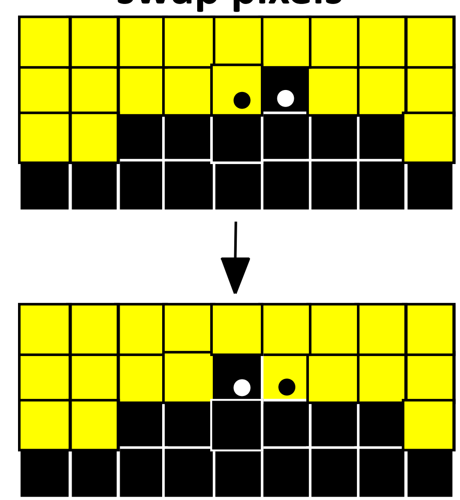
Minimization of Total Free Energy

Kinetics of Microstructural Evolution

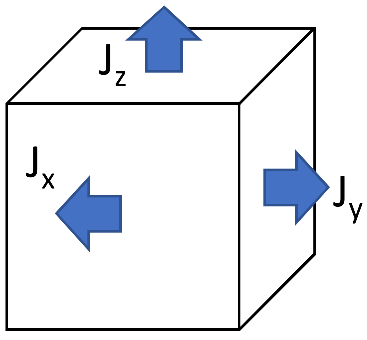
grain growth
change pixel color



surface diffusion
swap pixels



Kinetics of Evolution
Diffusion PDE



Fluxes of $Si(OH)_4(g)$ in and out of the element, considering up to second nearest neighbor. Summed to create second derivate term.

$$\frac{\delta^2 c}{\delta x^2} = J_x + J_y + J_z$$

$$\frac{\delta c}{\delta t} = D * \frac{\delta^2 c}{\delta x^2}$$

Fick's Second Law

Sum fluxes into and out of element → Numerically Solve Fick's Second Law → Kinetics of Diffusion

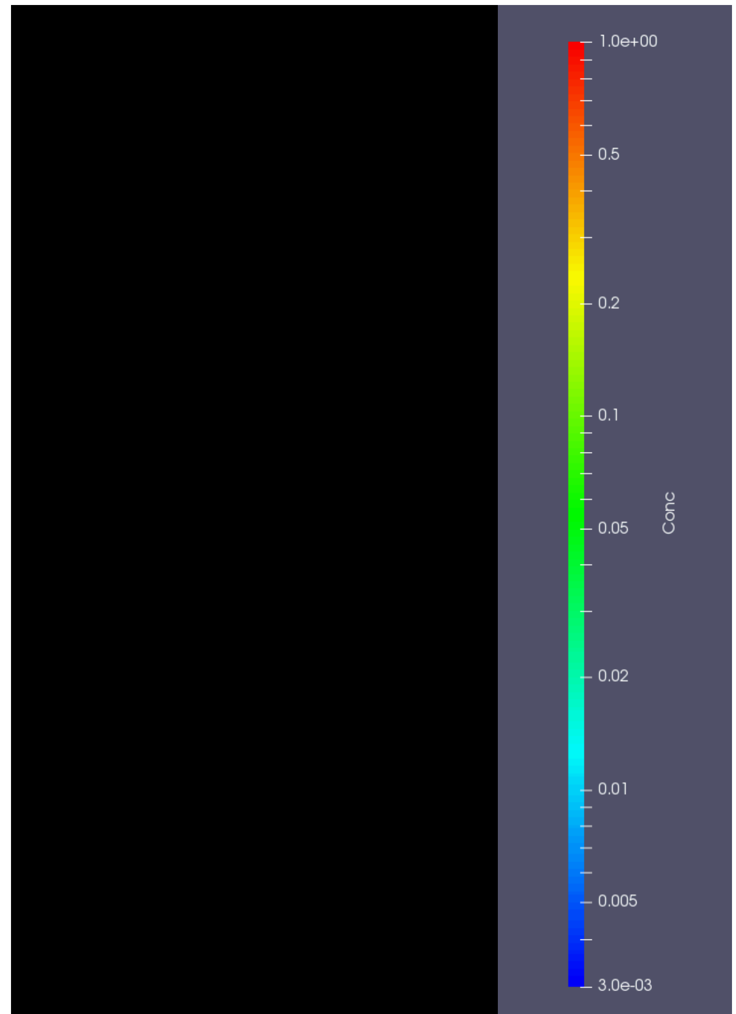
Combination Potts/Diffusion Model Processes

- Gas site
  - Surface diffusion/pore coalescence via swap with neighbor solid site
- REDS Site
  - Are there two neighbor gas sites? Then react
  - If not, coarsen
- REMS Site
  - Coarsening

- Only occurs on gas sites
  - Sum up fluxes into and out of site
  - Solve Fick's second law
  - Raster to next site in order
  - Update lattice with new concentration values

Animation of Potts/Diffusion Model

- Solid phases are grayscale
  - Difference in shade only identifies different grains
  - Black is YDS
- Scale bar colors are for concentration of $Si(OH)_4$ in the gas phase
- Reaction of YDS to YMS forms $Si(OH)_4$ with concentration of 1 then diffusion occurs upward
- YMS grains start extremely fine and sinter
- Physical scale and time will be applied to the system from comparison with micrographs and measurements of depletion depth



Future Prospects

- Implement gas phase transport mechanisms for observed parabolic diffusion kinetics from experiments
- Physical scale and time will be applied to the system from comparison with micrographs and measurements of depletion depth
- Use model for prediction of lifetime depletion