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Modeling Solidification Microstructures

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CPSD

ITR/AP: Multiscale Models for Microstructure Simulation and Process Design
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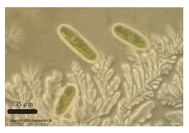
Cryopreservation

Cryopreservation is an important process for the long term storage and maintenance of cells and organs. The freezing process can cause damage to the biological materials by several mechanisms, including intracellular ice formation, forming lethal concentrations in the environment around the cells, or mechanical interactions. In this project, we use advanced computational methods to model the interaction of the freezing solid (ice) with cells in a directional solidification cell. These studies complement a series of experiments studying the same problem.

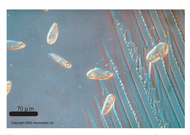
The model includes computation of the movement of an irregular ice interface, and its interaction with the cells. Our goal is to find the process paramters that lead to satisfactory capture of the cells in the ice structure. This is a difficult computational problem because there is a moving boundary whose location is a priori unknown, and because the interaction of the solid front with the cells requires complex physical models. We have benefited from the interaction with computer scientists in order to parallelize the computations, as described below.

1. Cryopreservation Procedure

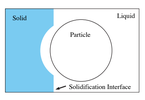
- Typical cryopreservation procedure
  - § Cool from $0^{\circ}C^{+}$ to $\mathcal{O}$(-15°C)
    - Formation of extracellular ice
    - Express H_2O from cell
  - § Cool to -196°C (LN_2)
- Major issues for consideration
  - § Lethal solute concentrations
  - § Intracellular ice formation (ICF)
  - § Mechanical deformation of cell



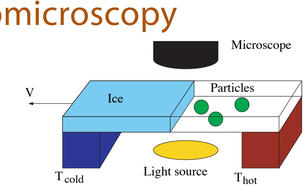
Freezing algae (Asymptote Ltd.)



Freezing protozoa (Asymptote Ltd.)

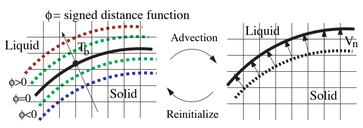


2. Cryomicroscopy



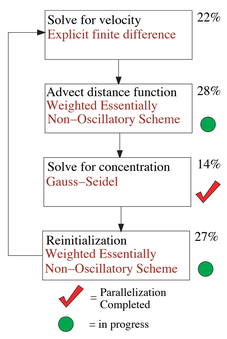
- Standard method to examine cell interaction with freezing interface
- Slide moves at constant velocity, V
- Interface morphology depends on thermal gradient
- Difficult to determine cellular environment during experiment
  - § Calculations adjunct to experiments at University of Minnesota

3. Level set method



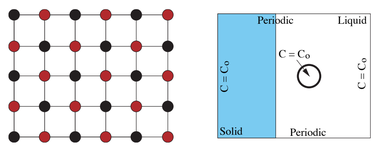
- Solve for interface velocity using interface solute balance:
  $$-D_\ell \partial_z C_\ell = V_n(1-k_\circ)C_\ell$$
- Advect ϕ:
  $$\partial_t \phi + V_n \mathbf{n}\cdot\nabla\phi = 0$$
- Solve for concentration with Gibbs-Thompson equation at interface:
  $$T_i = T_m - m_\ell C_\ell + \Gamma\kappa$$
- Reinitialize distance function:
  $$\partial_\tau \phi + S(\phi_\circ)(|\nabla\phi| - 1) = 0$$

4. Path to parallelization



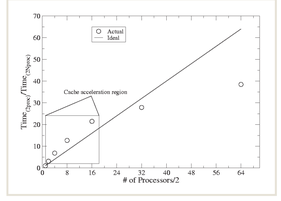
- Explicit velocity solution can be easily parallelized
- Weighted Essentiall Non-Oscillatory (WENO)
  - § Method is essentially explicit
  - § Only necessaryto obtain solution around interface
  - § Dynamic load balancing required as interface moves
- Solving for concentration field
  - § Completed implementationof red black Gauss-Seidel

5. Parallel red black Gauss-Seidel



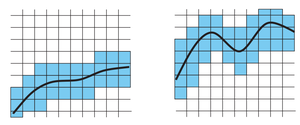
- Gauss-Seidel used to solve for concentration field
- No data dependency between points of similar color
  - § Update red nodes with black values
  - § Update black nodes with new red values
- Highly parallelizable
- Easily applied to higher dimensions by adding more colors

6. Parallelization results: Gauss-Seidel



- Uniform square grid: 250000 nodes
- Scaled to 2 processors (cache behavior)
- Gauss-Seidel routine only
- Timing obtained using Lemieux - Pittsburgh Supercomputing Center
  - § 750 Compaq Alphaserver ES45 nodes (4 1-Ghz processors per node)

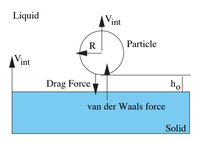
7. Weighted Essentially Non-Oscillatory method



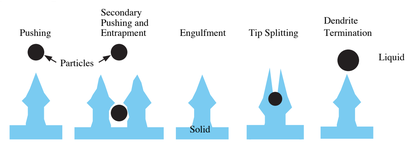
= Active computational nodes

- High order shock capture scheme
- Necessary for stability of level set method
- Parallelization in Charm++ framework offers many advantages
  - § Dynamic load balancing necessary for evolving computational domain
  - § Allow further growth to more advanced computation methods
    - Multigrid methods for solving pressure Poisson equation
    - Adaptive grid methods for computational efficiency

8. Particle pushing

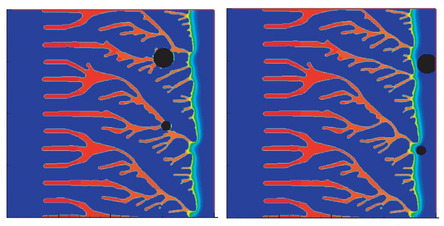


- Force balance on particles
  - § van der Waals repulsion
  - § Drag force from flow between solid and particle
- Analytical solution exists for flat interface interaction
  - § Dendritic interface interaction is significantly more complex
- Several types of particle interaction can occur



9. Capture vs. pushing: Hamaker constant

- Set principal anisotropy at 45° to growth direction
- Capture depends on placement, size, parameters...



(a) Capture: Ha = 5×10^3 (b) Pushing: Ha = 5×10^7

10. Summary

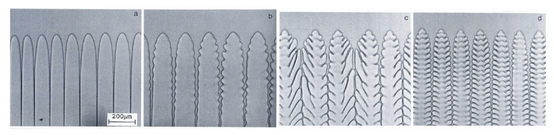
- Analysis of cellular interaction with a solidifying interface
  - § Particles can alter the morphology of the interface
  - § Further examine cell environment during solidification
    - Understand contribution of various cell damage mechanisms
    - Faster development of useful cryopreservation procedures
  - § Simulation of larger systems required for realistic analysis
- Parallelization of level set method
  - § Substantial improvement with red black Gauss-Seidel
  - § Future work includes:
    - Integration of code into Charm ++ framework
    - Parallelization of WENO scheme
    - Development and parallelization of drag force model

Constrained Growth

Many experimental studies of dendritic growth morphologies use a directional soldification apparatus, as shown at the left. There are discrepancies in the observed microstructures when these experiments are performed using slide separations that vary from one investigator to the next. In this project, we use computational models to examine the development of microstructure in such apparatus. The complex, 3-D moving boundary problem requires the advanced computational techniques developed under this grant.

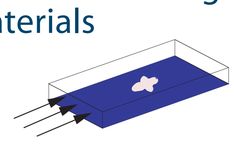
1. Spatial constraint

- Alloy solidification: SCN-Salol experiments (Liu and Kirkaldy, JCG, 1994)
  - § L_z = 55 μm, G = 4.5 K/mm, V = 4.2, 5.7, 7.6, 10.8 μ/s

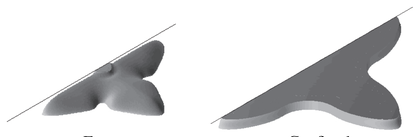


- Observe 2-D to 3-D transition for different V
- Get different growth morphology as L_z varies (Liu et al., TMS, 2004)
- Models assume free 3-D growth
- Presence of boundaries can affect results

2. Spatially constrained growth: pure materials



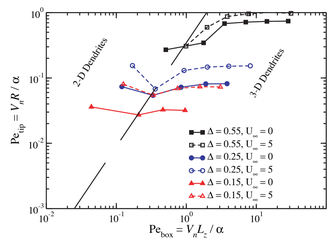
- Example: $\Delta = 0.55$, $U_\infty = 0$, $L_z = 16,\ 4$, $\epsilon_4 = 0.05$
- Find 3D - to 2-D transition for small enough slide spacing



Free Confined

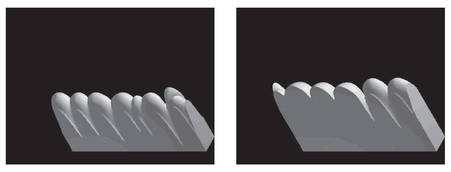
3. 3-D to 2-D transition

- Find 3-D to 2-D transition as box height decreases
- Correlation for transition
$$\rho_{tip}(L_z)^{-8/5}\left(\frac{V_{tip}}{\alpha}\right)^{-3/5}\begin{cases}\leq 0.345 & 3-\mathrm{D}\\ \geq 0.345 & 2-\mathrm{D}\end{cases}$$



4. 3D alloy directional solidification

- Follow phase-field model by Karma for different D_S and D_L (Karma, PRE, 2002)
- Use "Frozen temperature" approximation



- Find 3-D to 2-D transition
- Determine correlation for transition
- Comparison with experiments by Trivedi, Kirkaldy

5. Conclusion and future work

- 2D models not representative of 3D conditions
- Confinement effects can contaminate experimental observations
- Evidence of critical spacing causing 3D to 2D growth transition
- Need to quantify this phenomenon in context of directional solidification