Characterization and Modeling of Interfaces and Interphases in Polymeric Systems

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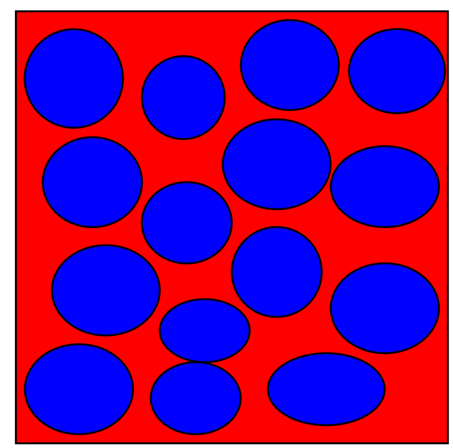
Consortium Update

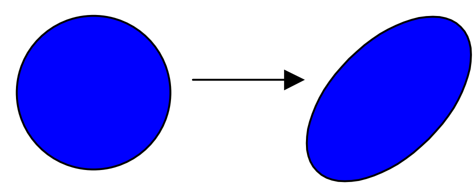
Modeling of Interfaces and Interphases in Polymeric Systems

- **REVIEW**
  - » **Objectives**
  - » **Approach**
  - » **Initial Results**
- **MESOSCALE FLOW MODELING**
  - » **Scope**
  - » **Results (to date)**
- **SUMMARY & FUTURE WORK**

Modeling of Interfaces and Interphases in Polymeric Systems

- **OBJECTIVE**
  - » **Computer simulation for modeling interface and interphase morphology in polymer blends during processing operations.**
- **INITIAL PROBLEM**
  - » **Injection molding of two-phase systems**
  - » **Predict injection molding filling**
  - » **Predict drop size distribution/morphology**
- **POLYMERS**
  - » **Polyisoprene/Polybutadiene**
  - » **Polyolefins**

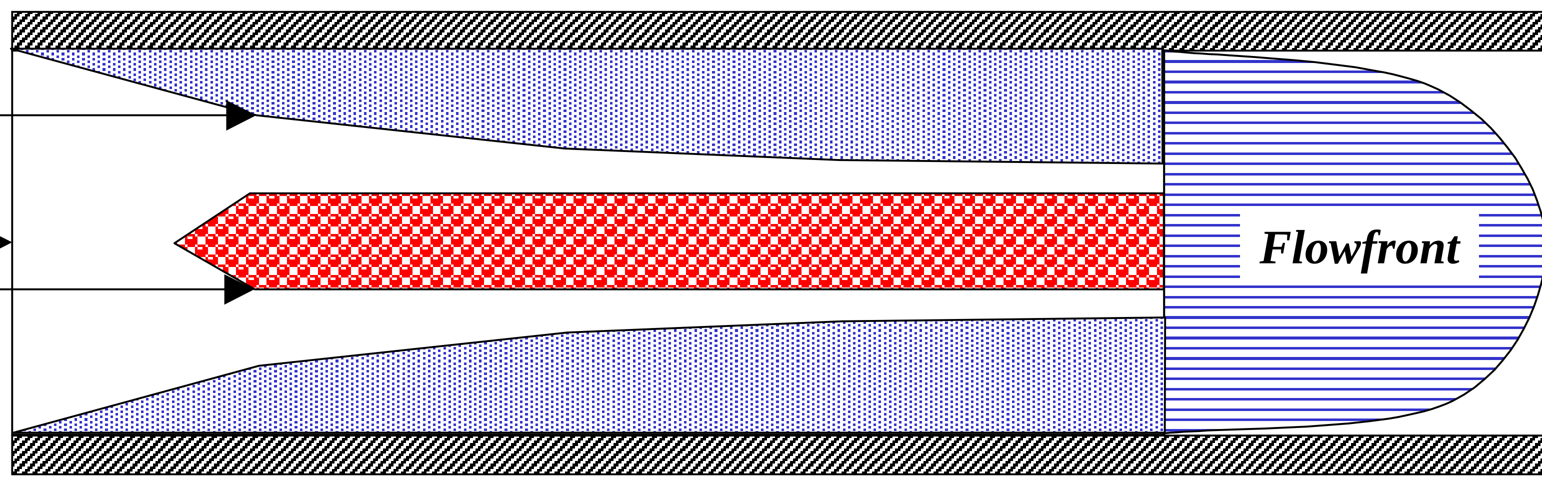




Polymer Blend Injection Molding

Inflow -- Well mixed extrudate

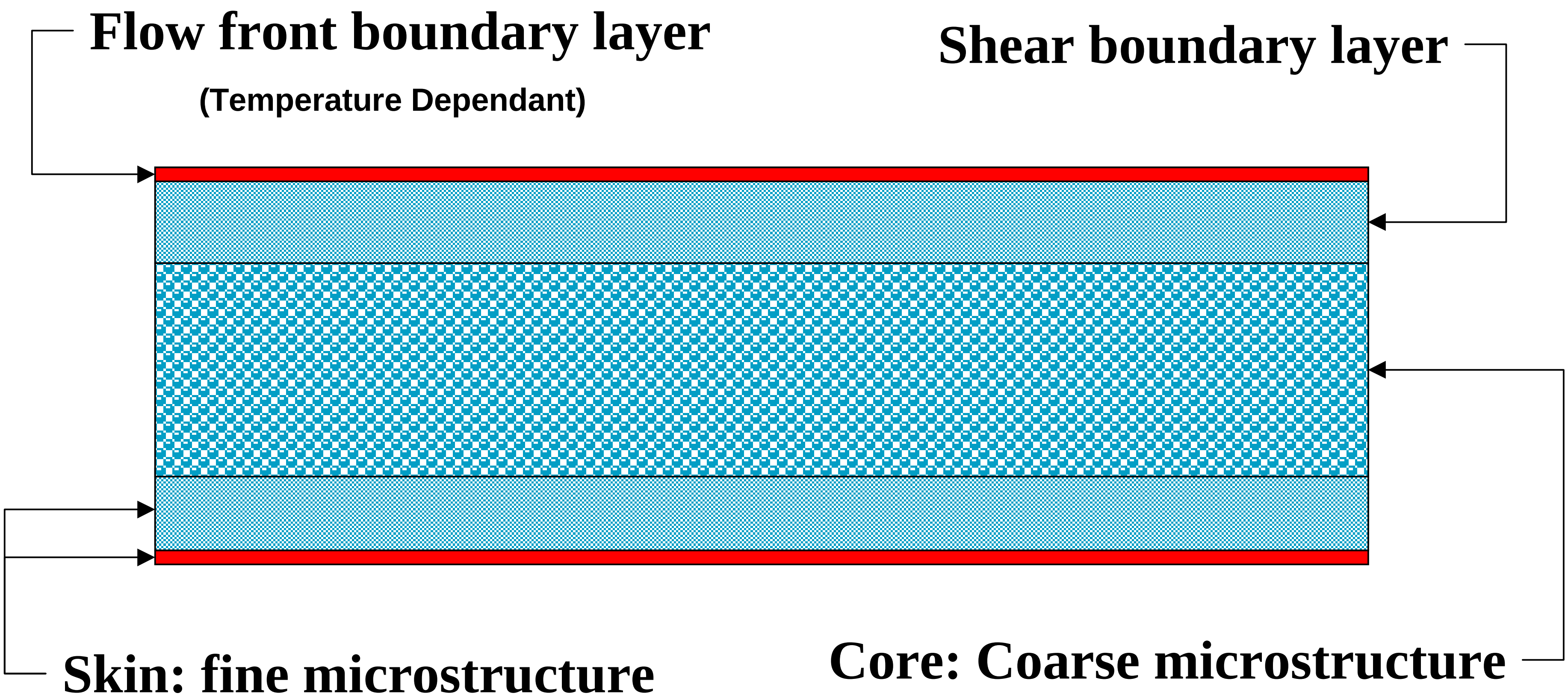
Wall Region -- High Shear, Stretching and Breakup, Small Drops



Center -- Low Shear, Coarsening, Larger Drops

Flowfront -- Extensional Flow, “Front to wall flow”

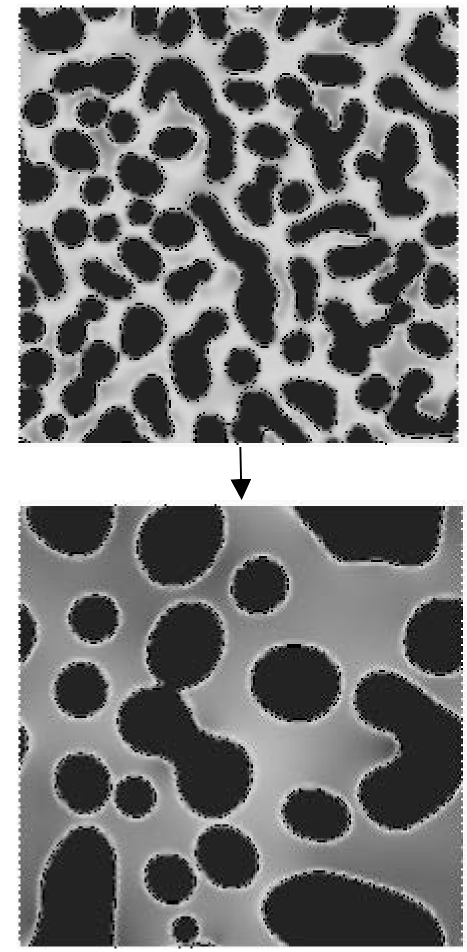
Polymer Blend Injection Molding



» Non-uniform properties due to skin-core structure

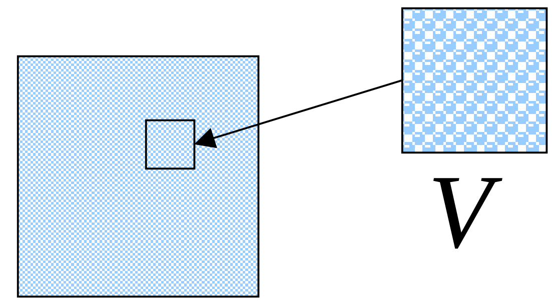
Multi-Component Flow Calculation

- **Direct Simulation**
  - » **e.g., Ginzburg-Landau, Lattice Boltzmann**
  - » **Difficulty: mismatched size scales**
    - ***Drops scale, microns***
    - ***Mold scale, cm to m***
  - » **Impractical for injection molding**
- **Volume Averaging**
  - » **Phase averaged properties for injection**
  - » **Predict microstructure from statistical averages or micro-model**
  - » **e.g. Doi-Ohta -- “Area Tensors”**
  - » **Tucker, Droplet Model**



Doi-Ohta Type Models

$$\underline{\underline{A}} = \frac{1}{V}\int_{\Gamma} \hat{n}\hat{n}\,dS$$

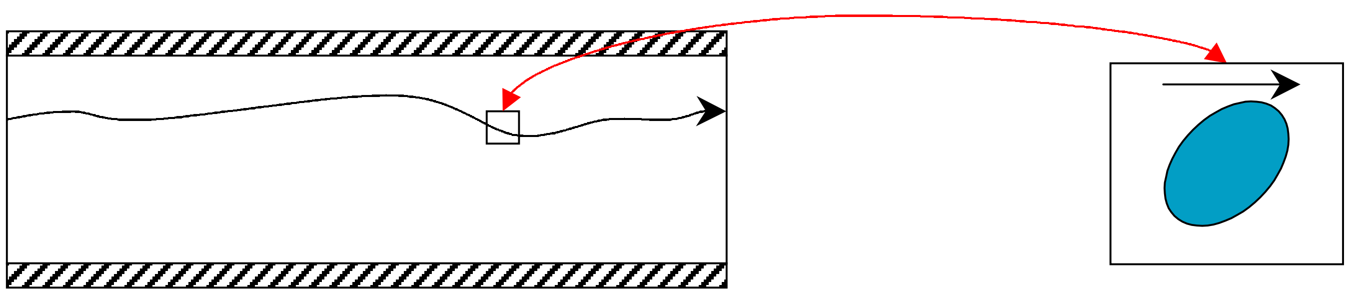


$$\dot{\underline{\underline{A}}} = \frac{1}{V}\int_{\Gamma} \dot{\hat{n}}\hat{n}\,dS + \frac{1}{V}\int_{\Gamma} \hat{n}\dot{\hat{n}}\,dS + \frac{1}{V}\int_{\Gamma} \hat{n}\hat{n}\,\dot{d}S$$

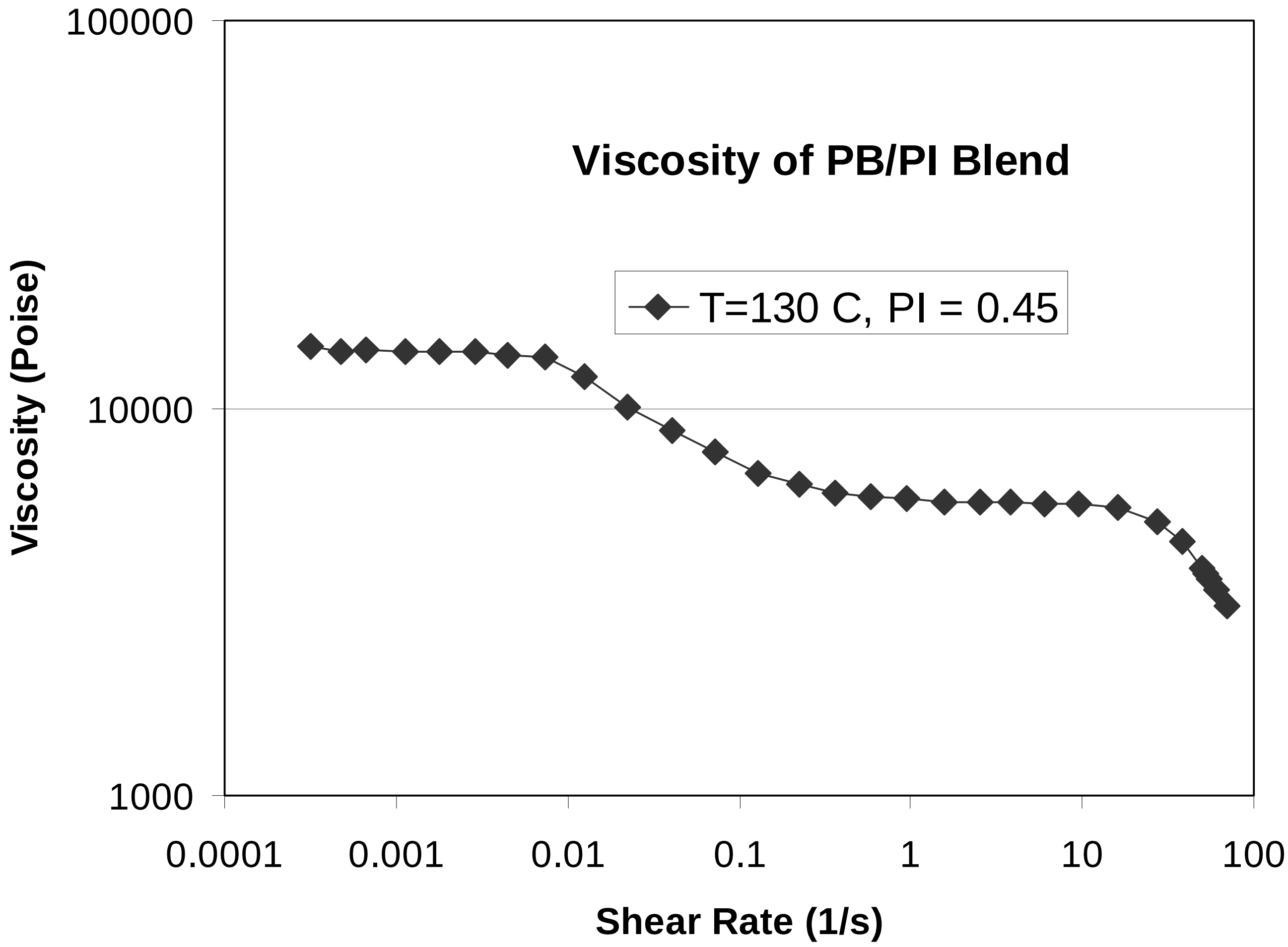
- **Computes microstructural averages**
- **Solve coupled evolution and flow equations**

Present Approach

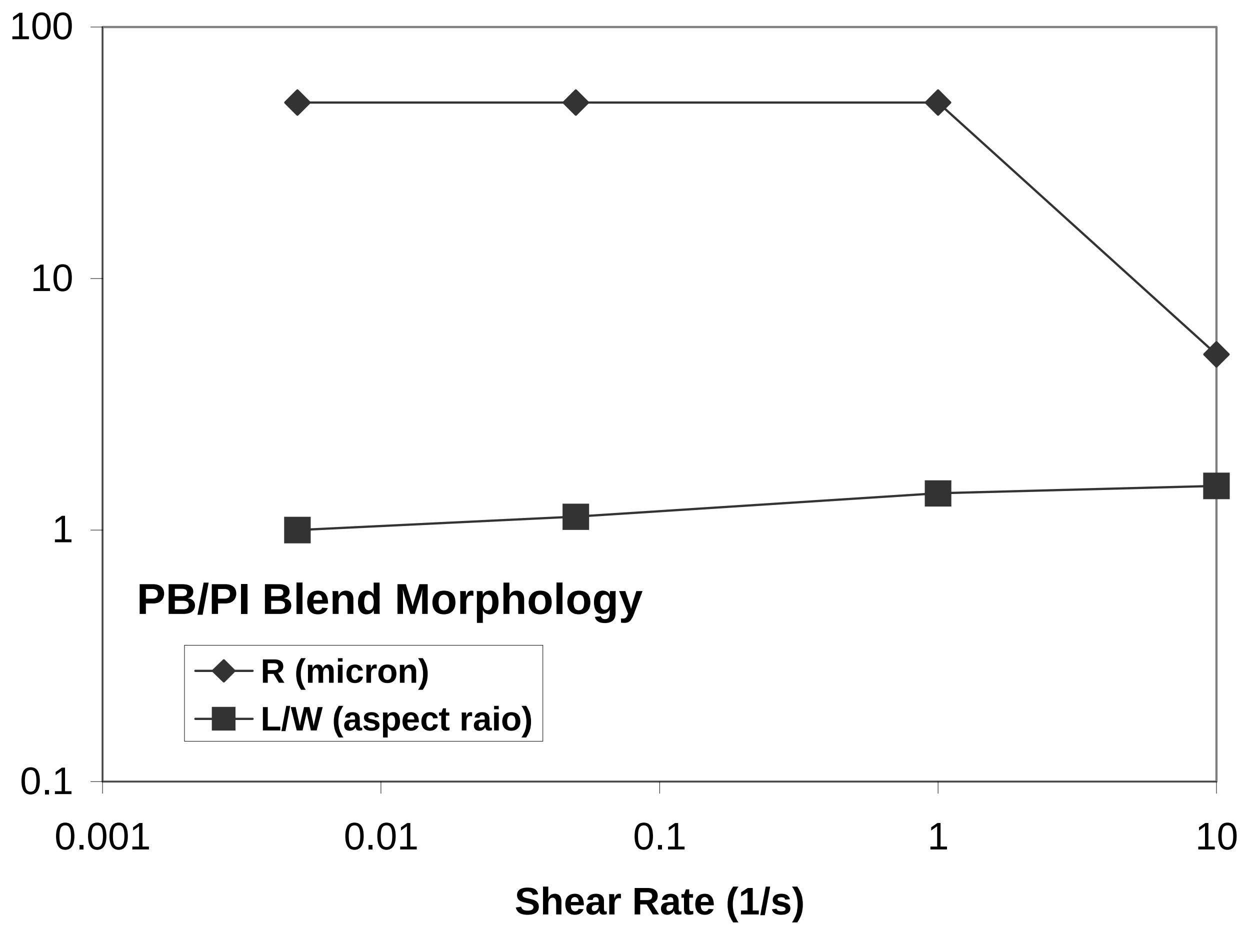
- "Customize" commercial code "FIDAP"
  - » Add user defined subroutines
    - *viscosity*
    - *microstructure evolution (average)*
  - » Compute flow field
  - » Determine drop size distribution in the injected part from shear distribution
- Direct two-phase calculations on "particle paths"
  - » Detailed microstructure prediction



PB/PI Blend Viscosity



PB/PI Flow Morphology



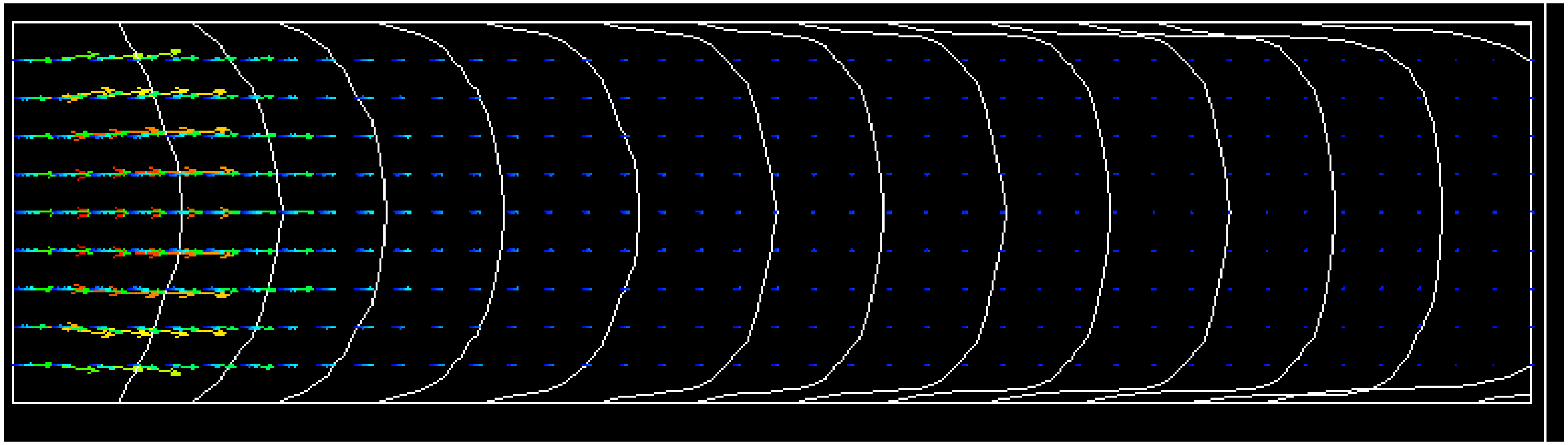
Drop Size Model

$$R_{drop} = \frac{50}{\sqrt{\frac{1}{2} tr\left(\underline{\underline{\dot{\gamma}}} \cdot \underline{\underline{\dot{\gamma}}}\right)}}, tr\left(\underline{\underline{\dot{\gamma}}} \cdot \underline{\underline{\dot{\gamma}}}\right) > 1$$

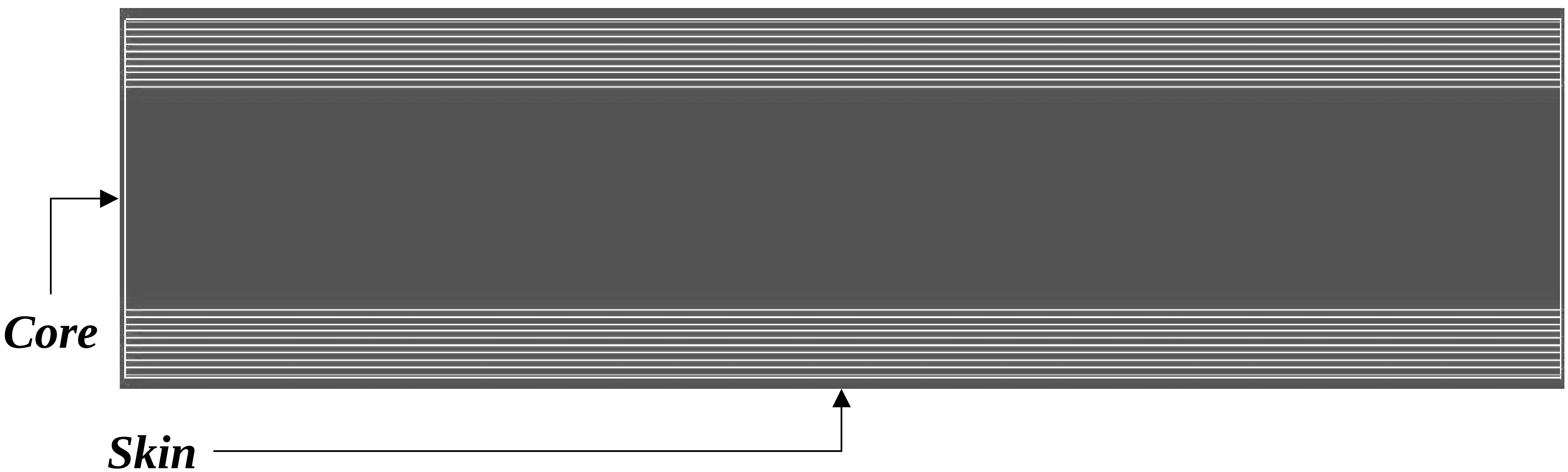
FIDAP Fill Simulation

Fill Pattern

PB/PI:55/45



Drop Size Distribution



Multi-Component Mesoscale Flow Model

- **Immediate Goals**
  - » **Modeling of phase separated polymer systems in flow**
  - » **Parameters easily attainable from experimental data**
  - » **Extensible to longer range goals**
- **Longer Range Goals**
  - » **Non-newtonian rheology**
    - ***e.g., "phase inversion" directly attributable to viscoelasticity***
  - » **Thermal Effects**
- **Approach**
  - » **Multi-component Navier-Stokes equation**
  - » **Ginzburg-Landau phase model**

Model Equations

Multi-component Momentum Balance

$$\mathrm{Re}\frac{D\vec{v}}{Dt} = -\nabla p + \nabla^2 \vec{v} + \frac{1}{Ca}\mu\nabla\phi$$

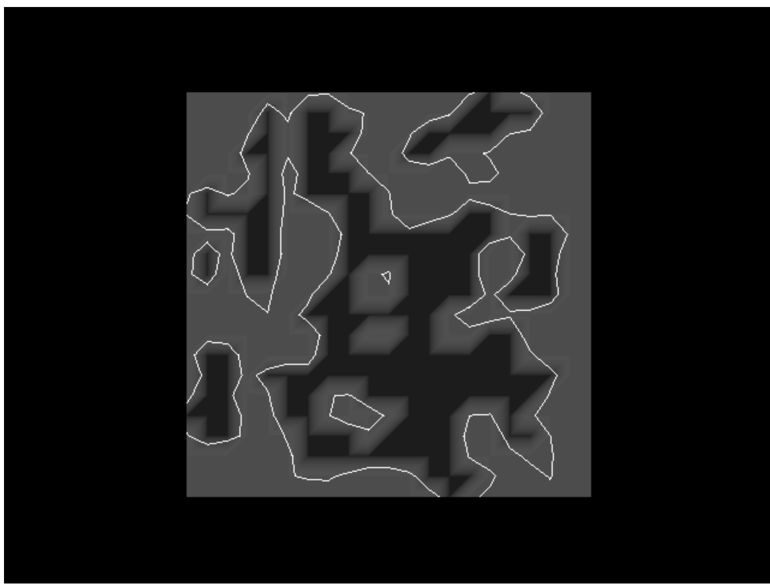
Order Parameter Transport Equation

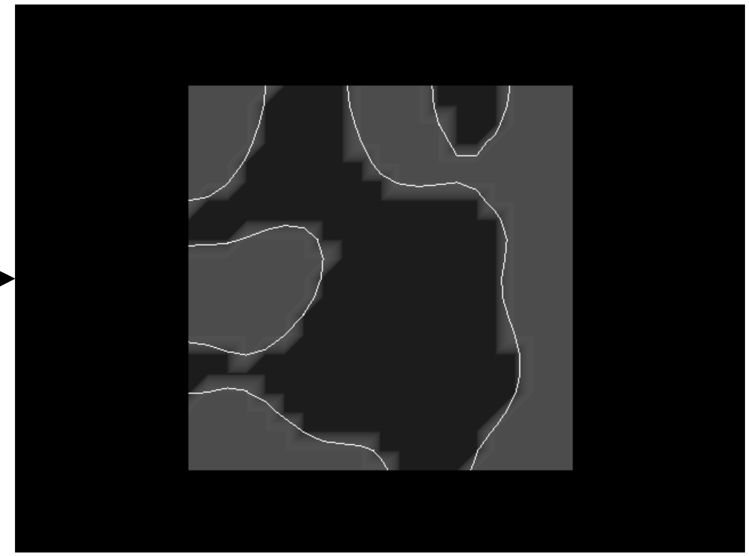
$$\frac{D\phi}{Dt} + \phi(\nabla\cdot\vec{v}) = \frac{1}{Pe}\nabla^2\mu$$

Chemical Potential

$$\mu = -Sr\nabla^2\phi - \phi + \phi^3$$

Examples





Coarsening

Flow: Coarsening and Orientation

Summary

- **Accomplishments**
  - » **FIDAP customized for polymer blends**
    - ***User defined routines for viscosity and drop size***
    - ***Predicts drop size distribution in the injected part from shear distribution***
  - » **Robust injection molding predictions, complex geometry, etc.**
  - » **Automatic calculation of particle paths**
- **In Progress**
  - » **Two-phase modeling**
    - ***FIDAP: Compute particle flow paths***
    - ***Ginzburg-Landau: Simulate drop evolution on flow path***

Future Work

- **FIDAP Level improvements**
  - » **Include effect of dynamics on drop size**
  - » **Thermal effects**
- **Doi-Ohta/Area tensor type models**
  - » **Need extensions**
    - ***drop breakup***
    - ***non-newtonian rheology***
- **Multiphase Modeling**
  - » **Non-Newtonian Rheology**