INTRODUCTION TO SOLIDIFICATION: PHYSICAL PHENOMENA AND MODELLING PRINCIPLES

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SCOPE

Introduction to Solid-Liquid Phase Change Phenomena

Introduction to Modeling of Solid-Liquid Systems

GOALS

Introduction & Overview

Enthusiasm, Further Study, Identification of Interest

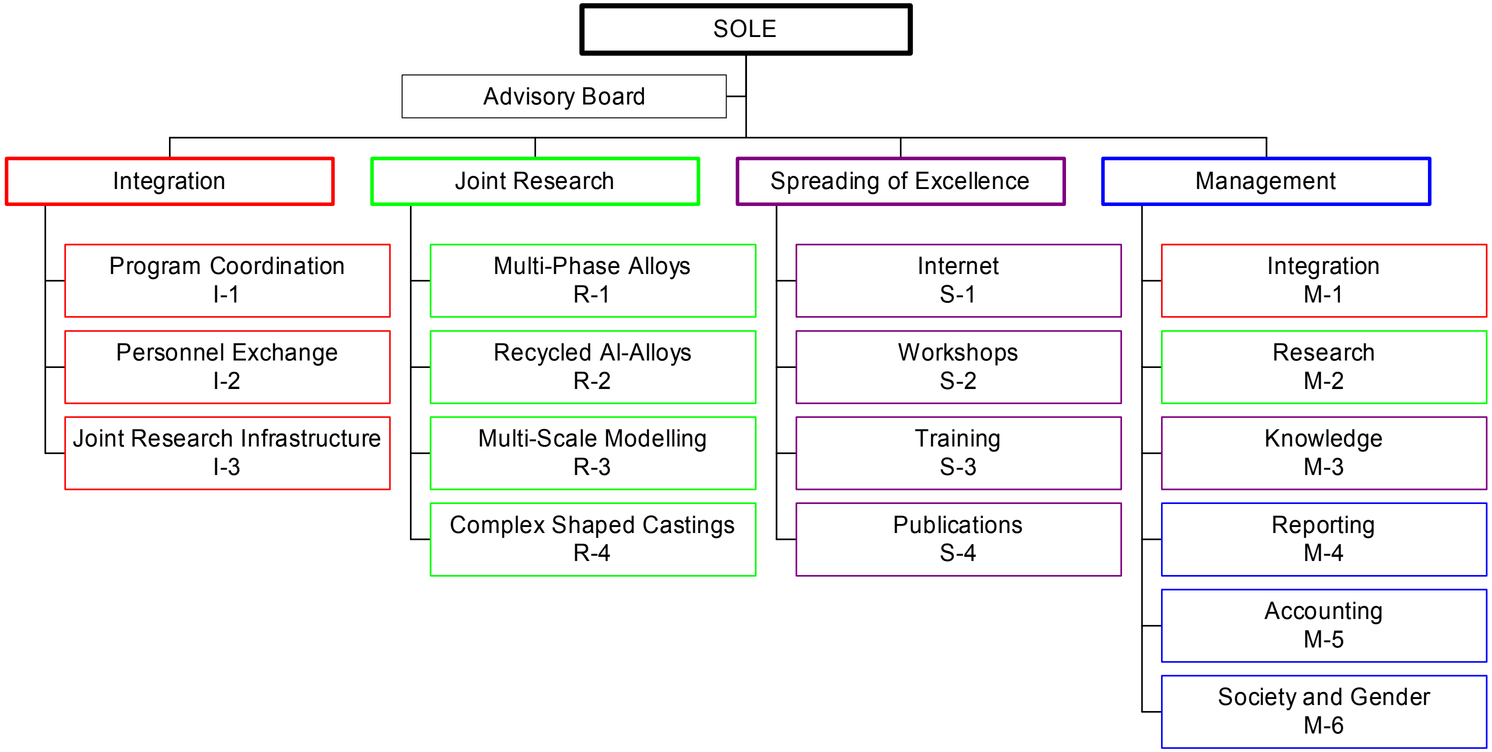
TECHNOLOGIES

Freezing of food
Freeze-drying
Purification of water
Criosurgery, preservation of transplants

Crystal growth
Casting (20% of mass, 40% of money)
Welding
Sintering

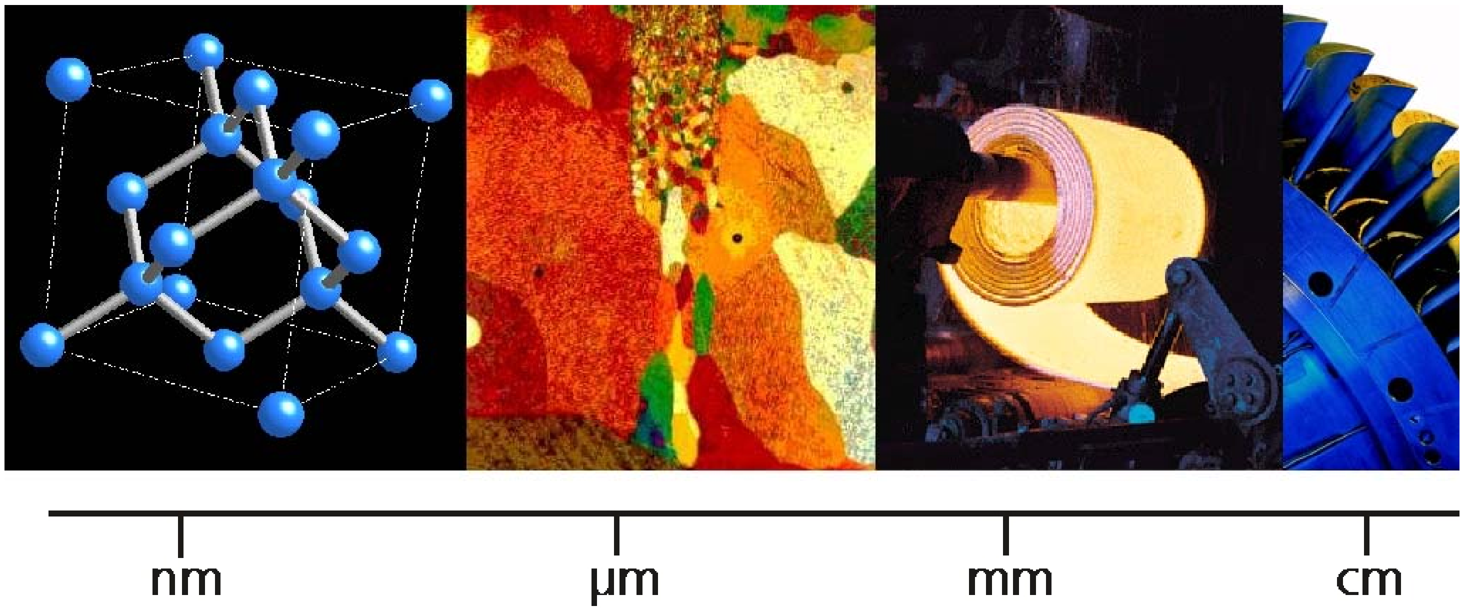
Vitrification of radioactive waste

6th Framework: solidification engineering network of excellence



ORGANISATION SCHEME OF THE SOLE NETWORK

COMPLEXITY OF THE SCALES

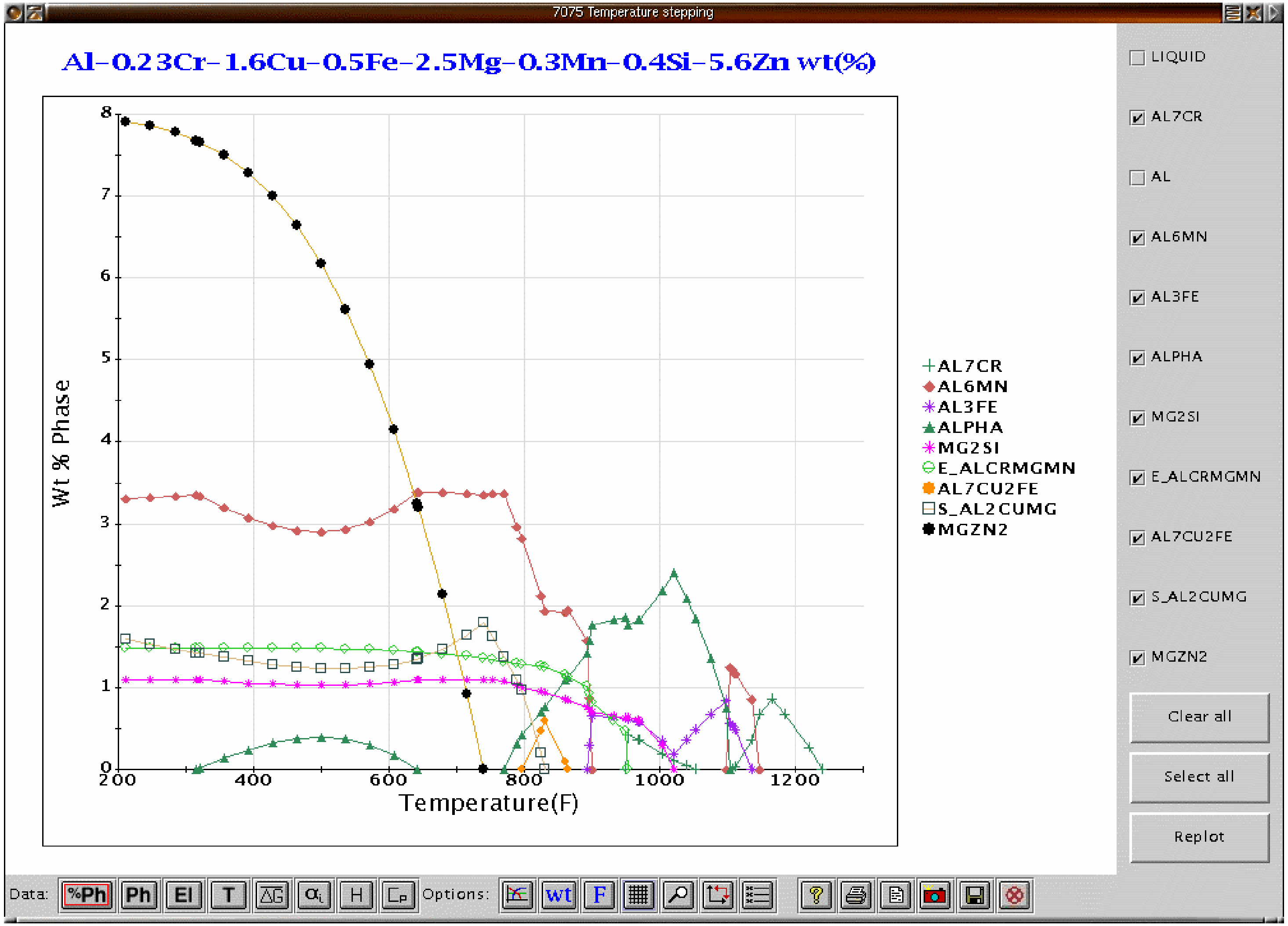


Nanometer scale: nucleation

Micron scale: microstructure, stresses, strains

Millimeter scale: shape, properties of semi-products and products

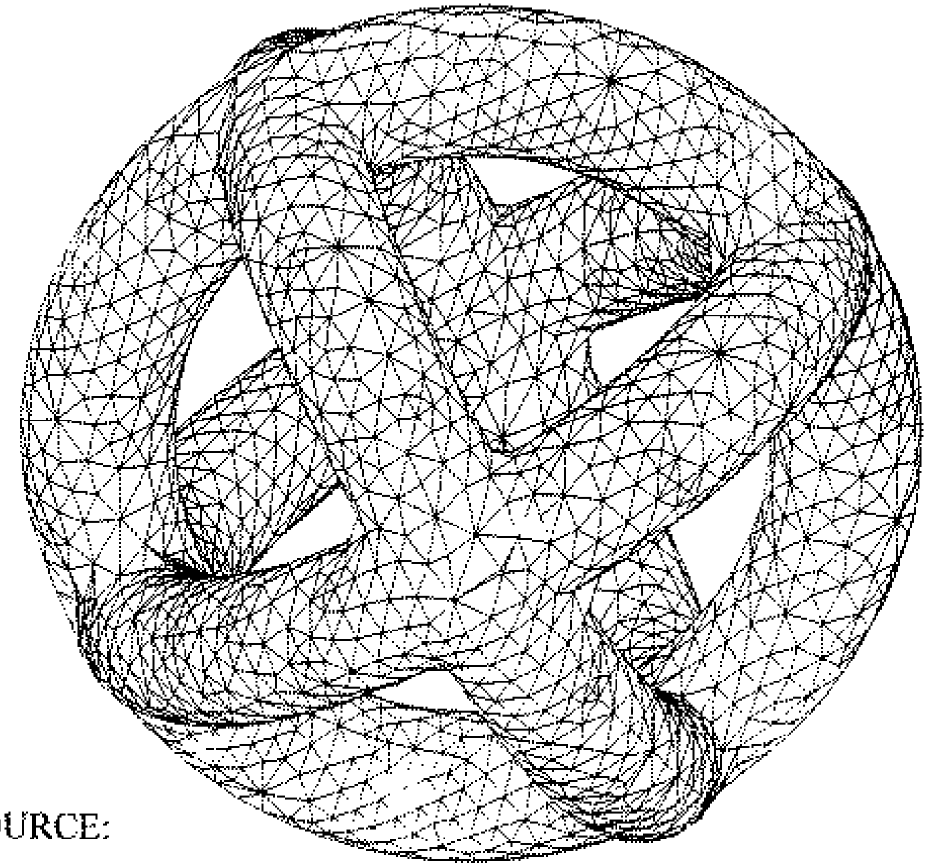
COMPLEXITY OF THE COMPOSITIONS



Jmatpro (2003), U.K.

COMPLEXITY OF THE SHAPES

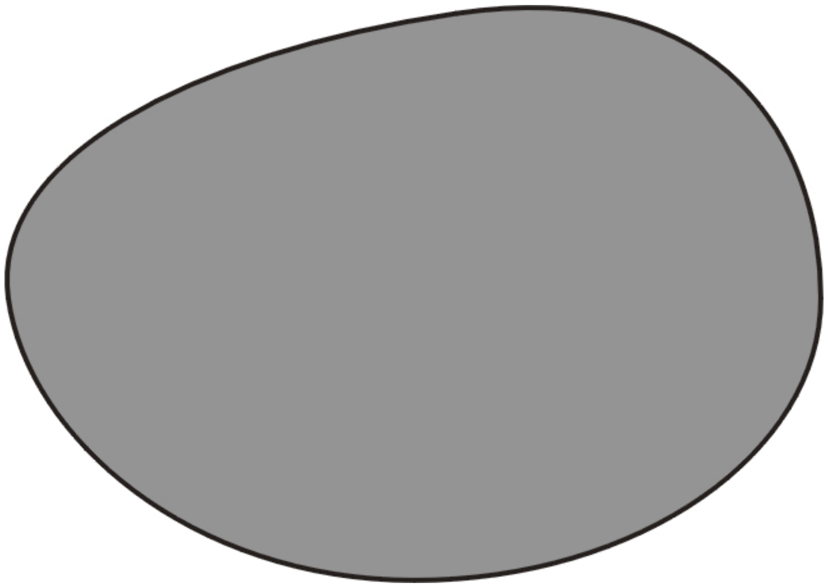
3 intersecting torii



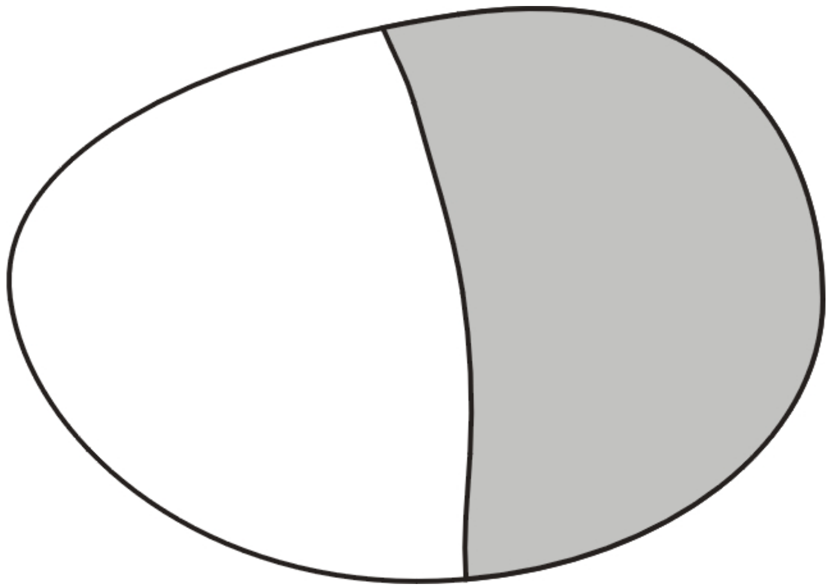
SOURCE:

R. Widman, **an efficient algorithm for the triangulation of surfaces in 3D.** Preprint-Math Dept. Colorado State University, 1991.

PHYSICAL PHENOMENA (1)



one-phase system

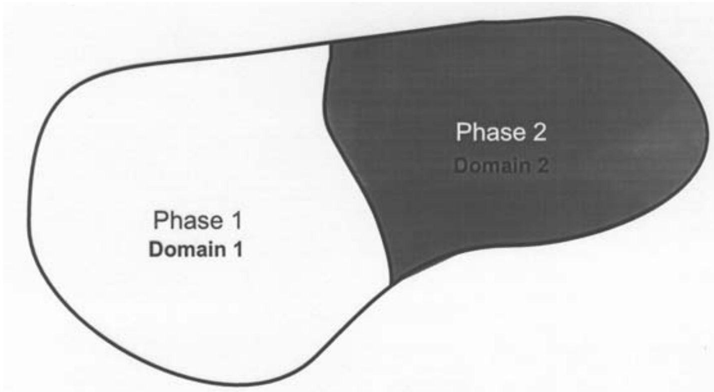


two-phase system

PHYSICAL PHENOMENA (2)

Free Boundary

Moving Boundary



solid phase 20 orders of magnitude higher viscosity as liquid phase

large jumps of other physical properties (thermal conductivity)

latent heat

PHYSICAL PHENOMENA (3)

Melting: solid - liquid (one-component)
Dissolving: solid - liquid (multi-component)

Freezing: liquid-solid (one-component)
Solidification: liquid-solid (multi-component)

PHYSICAL PHENOMENA (4)

NUCLEATION

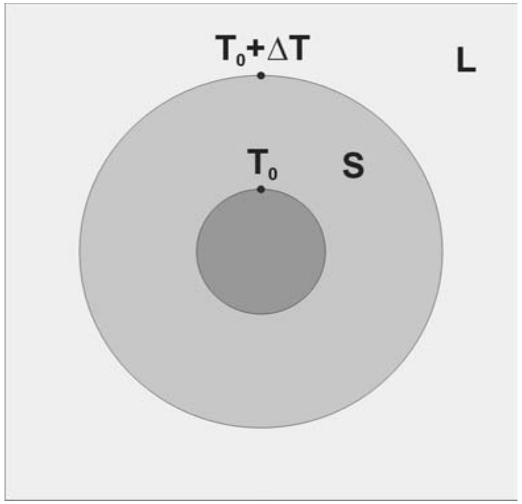
Homogenous Nucleation

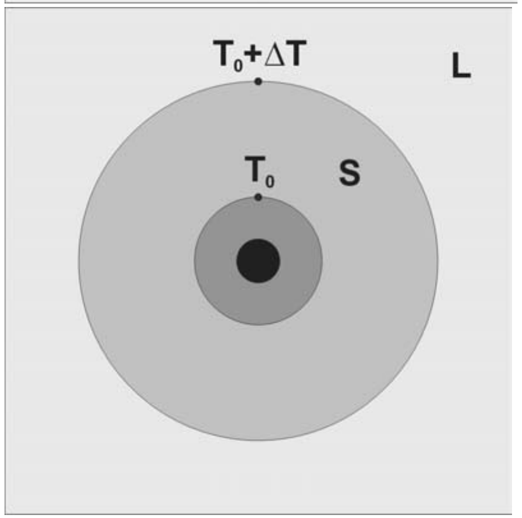
Heterogenous Nucleation

Nuclei 10e-8 m

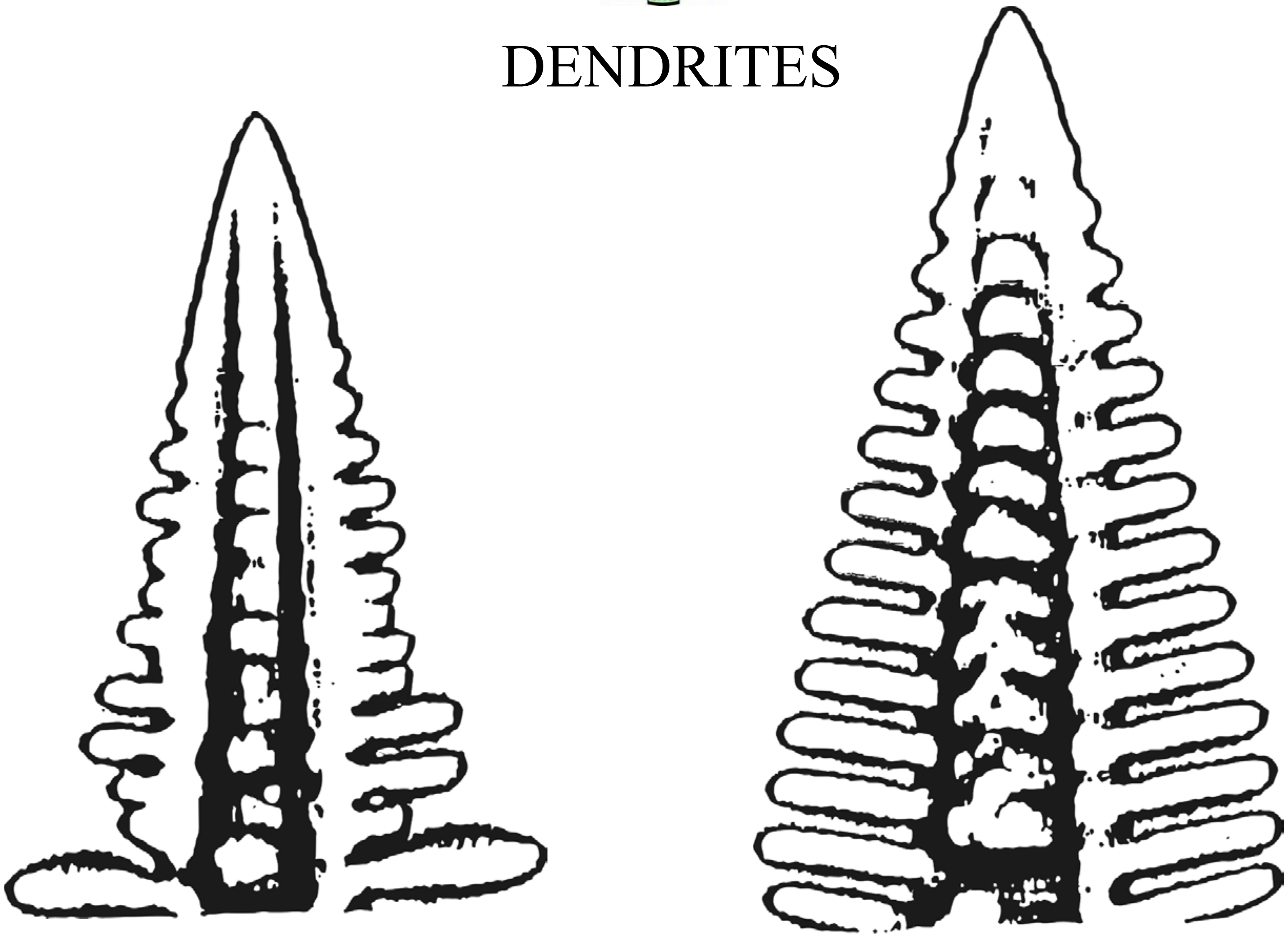
Fragments 10e-5 m

Orientation of cristallographic axes



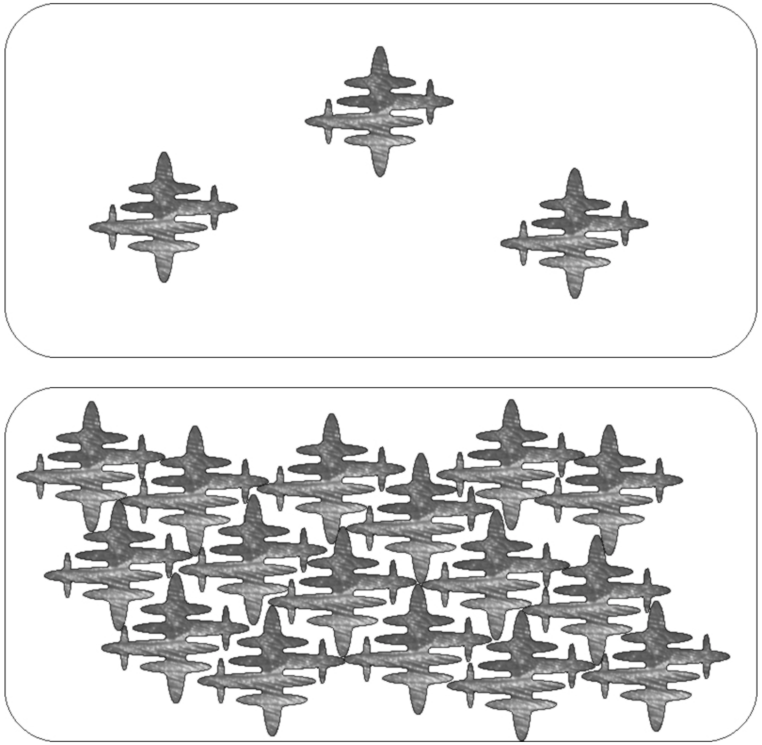


DENDRITES

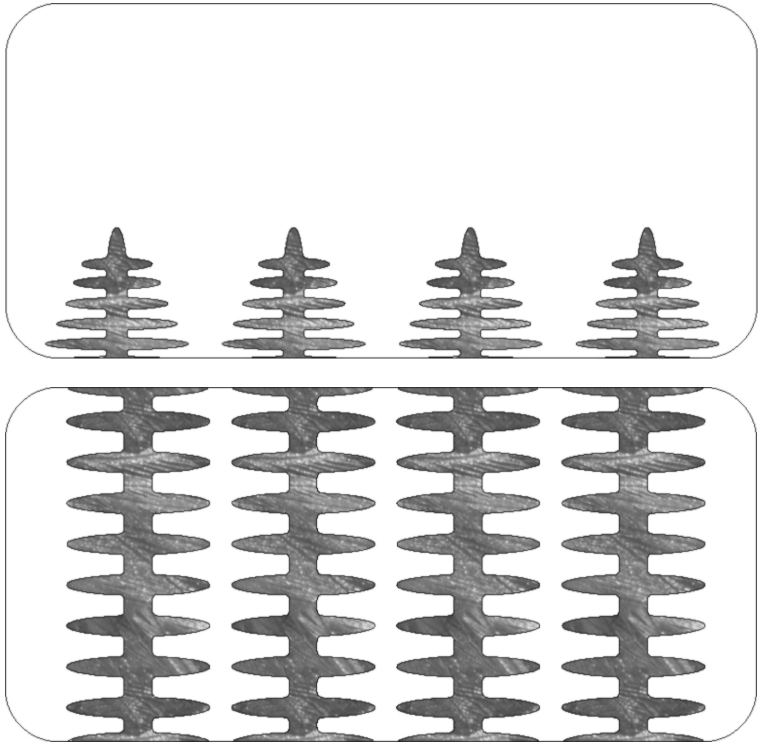


PHYSICAL PHENOMENA (5)

INTERPHASE BOUNDARY MORPHOLOGY



EQUIAXED



COLUMNAR

PHYSICAL PHENOMENA (6)

CONVECTION

Forced Internal, External

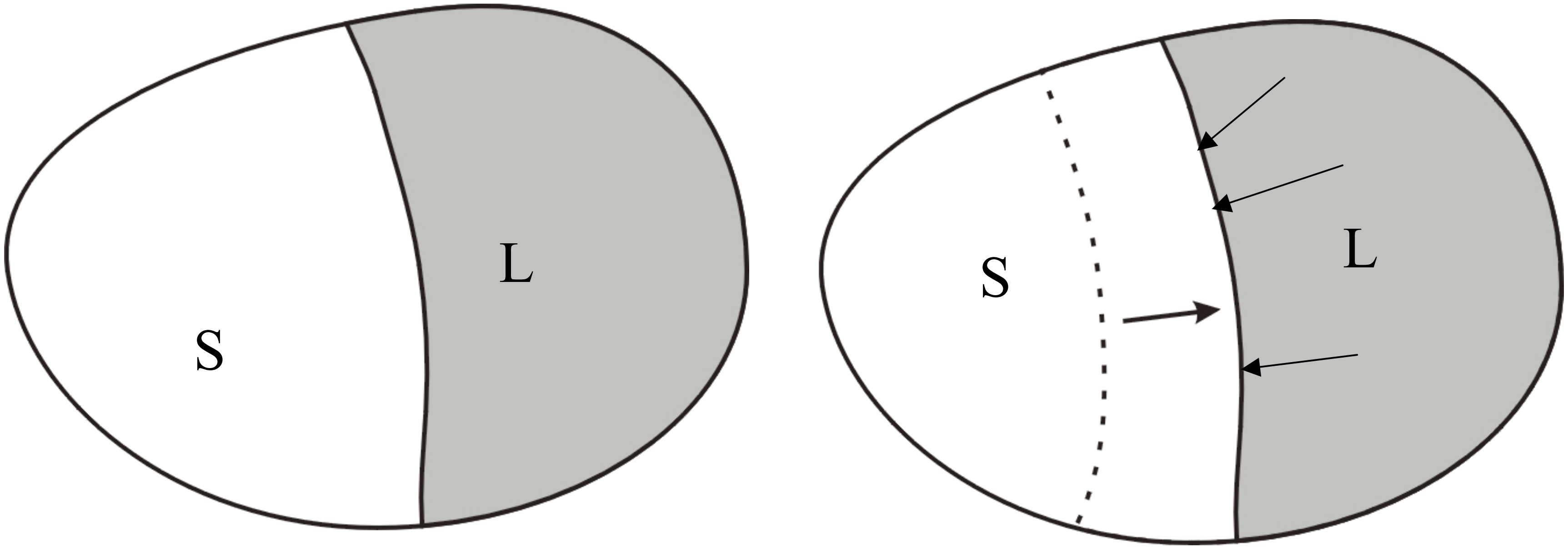
Interphase Movement Driven: Density Change

Bulk Driven: Thermal Gradients, Concentration Gradients

Interphase Properties Driven: Marangoni Convection

PHYSICAL PHENOMENA (7)

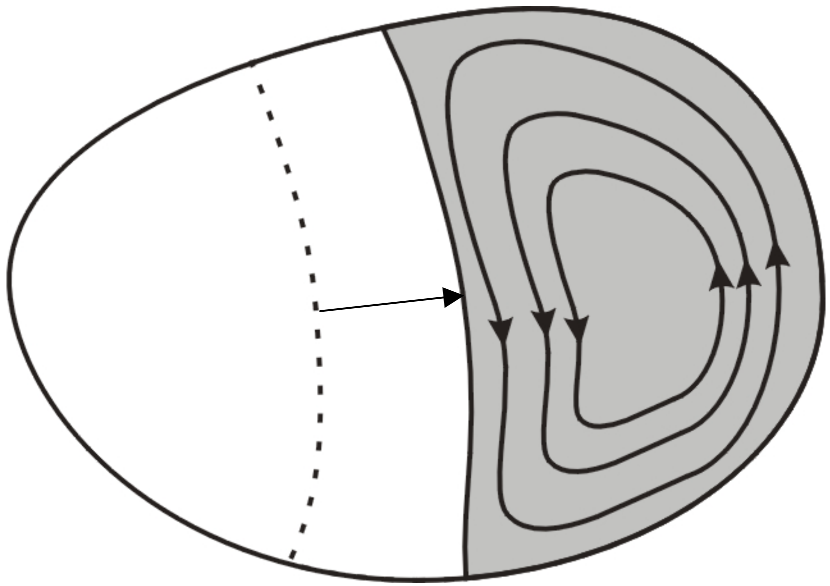
INTERPHASE MOVEMENT DRIVEN CONVECTION



pure iodine shrinks 21.6% during solidification !

PHYSICAL PHENOMENA (8)

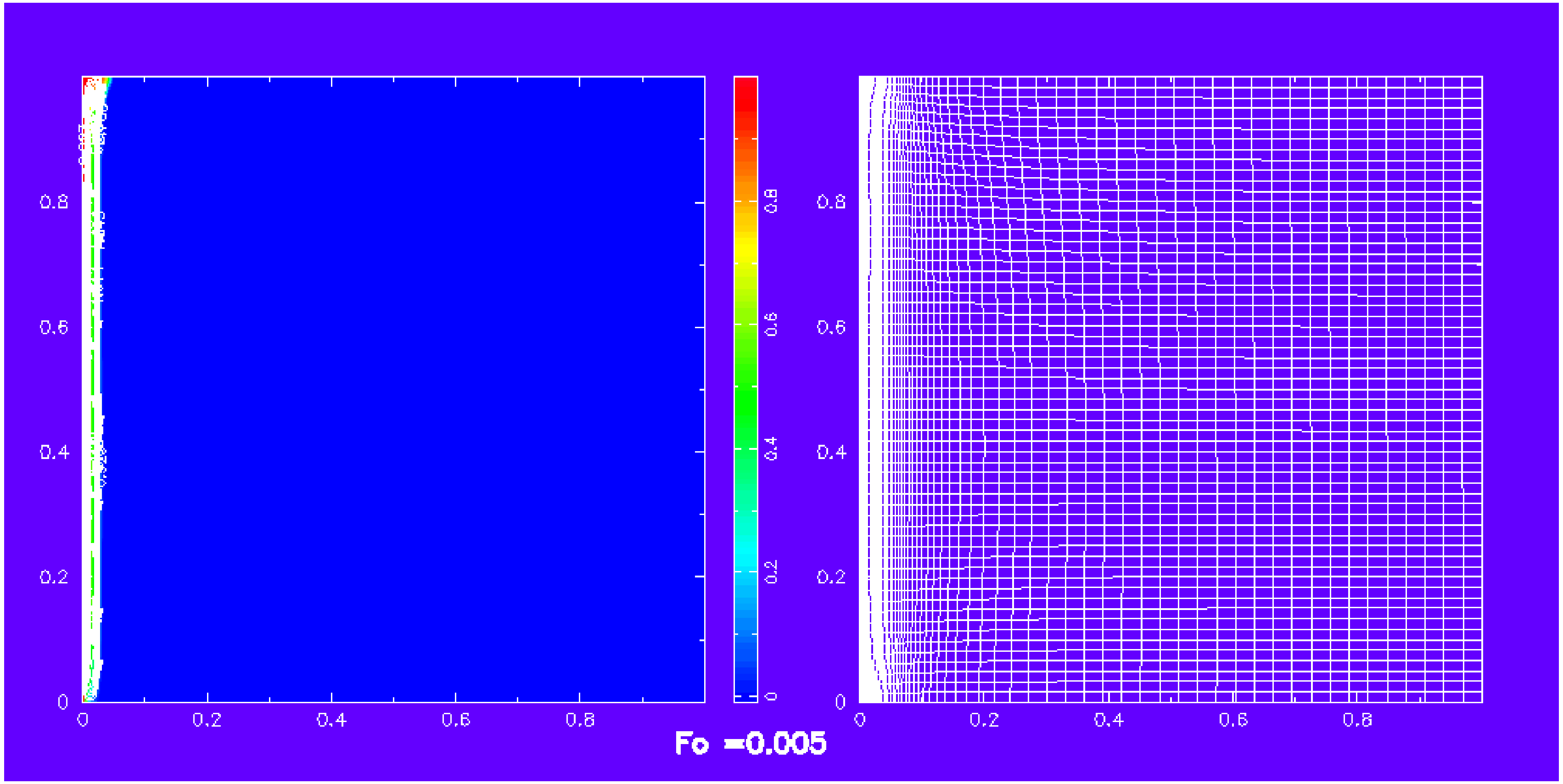
THERMAL CONVECTION



decrease the freezing rate
increase the melting rate

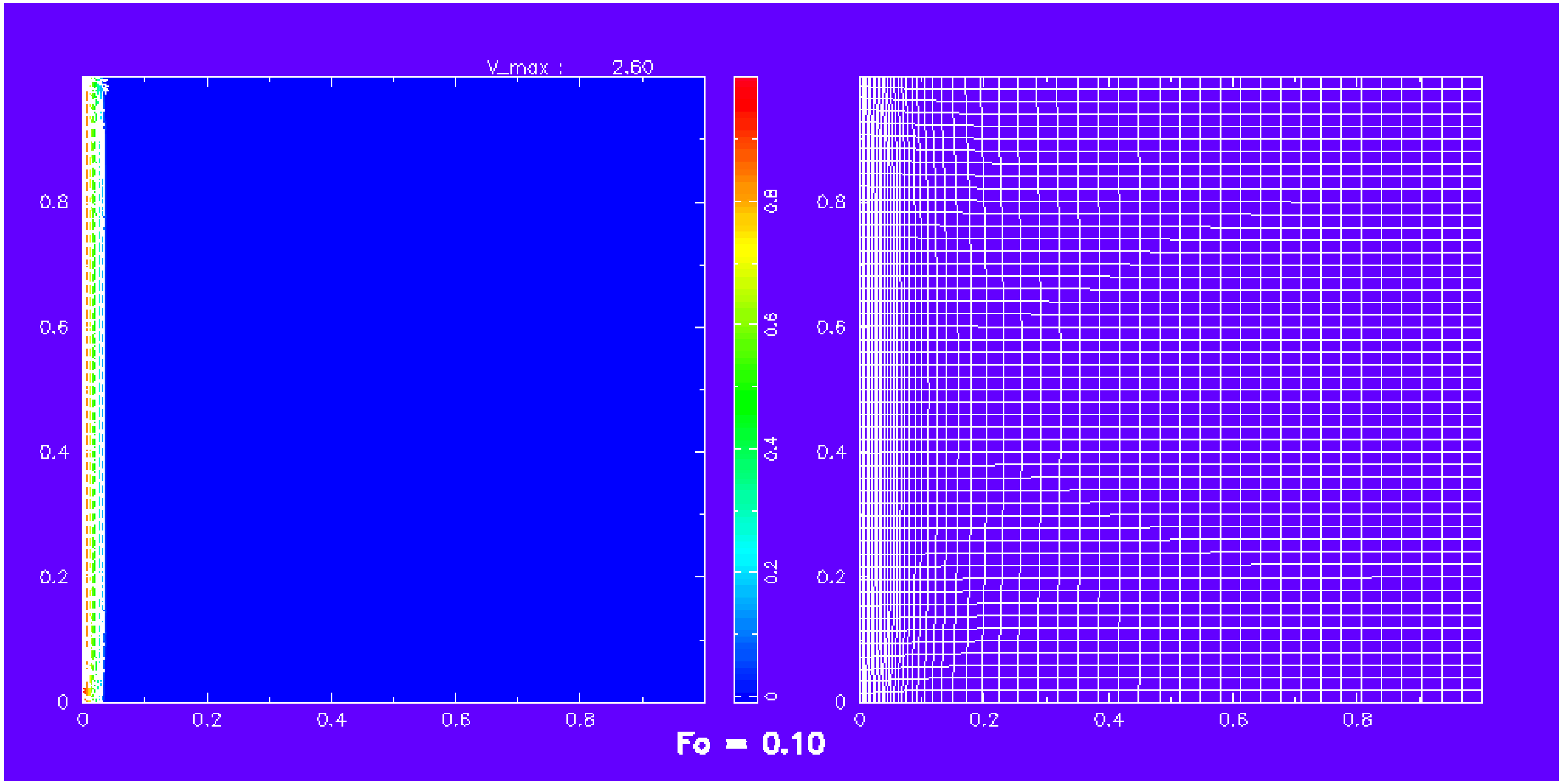
THERMAL CONVECTION PHENOMENA

Melting of system with high Prandtl number



J.Mencinger's contribution to Gobin-LeQuere benchmark test

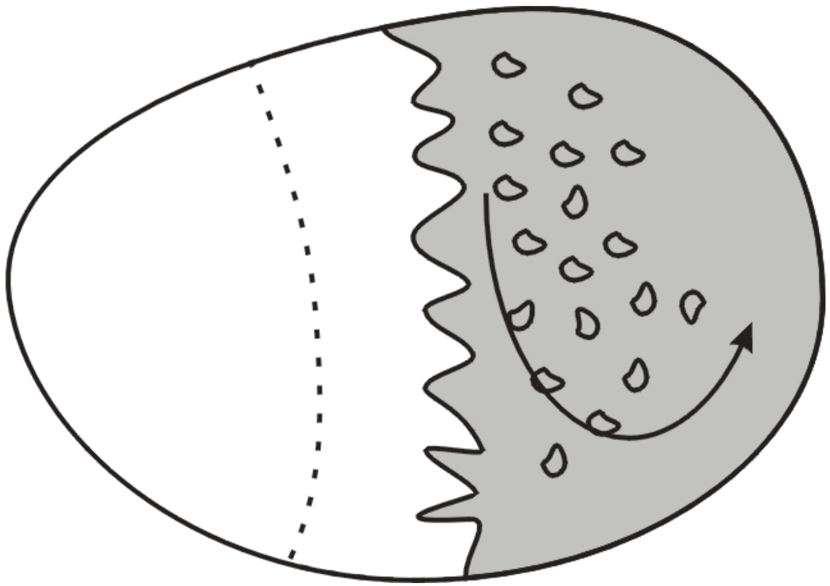
THERMAL CONVECTION PHENOMENA
Melting of system with low Prandtl number



J.Mencinger's contribution to Gobin-LeQuere benchmark test

PHYSICAL PHENOMENA (9)

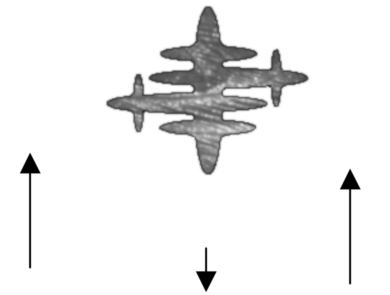
SOLID PHASE MOVEMENT



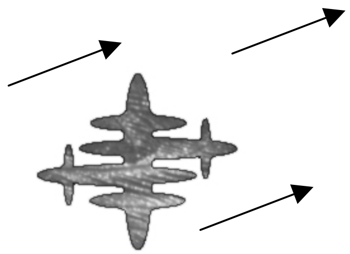
PHYSICAL PHENOMENA (10)

SOLID PHASE MOVEMENT

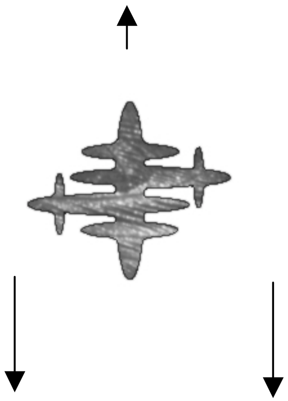
Settling
Floating
Movement with the melt



Settling when $\rho_S > \rho_1$ in a Gravitational Field



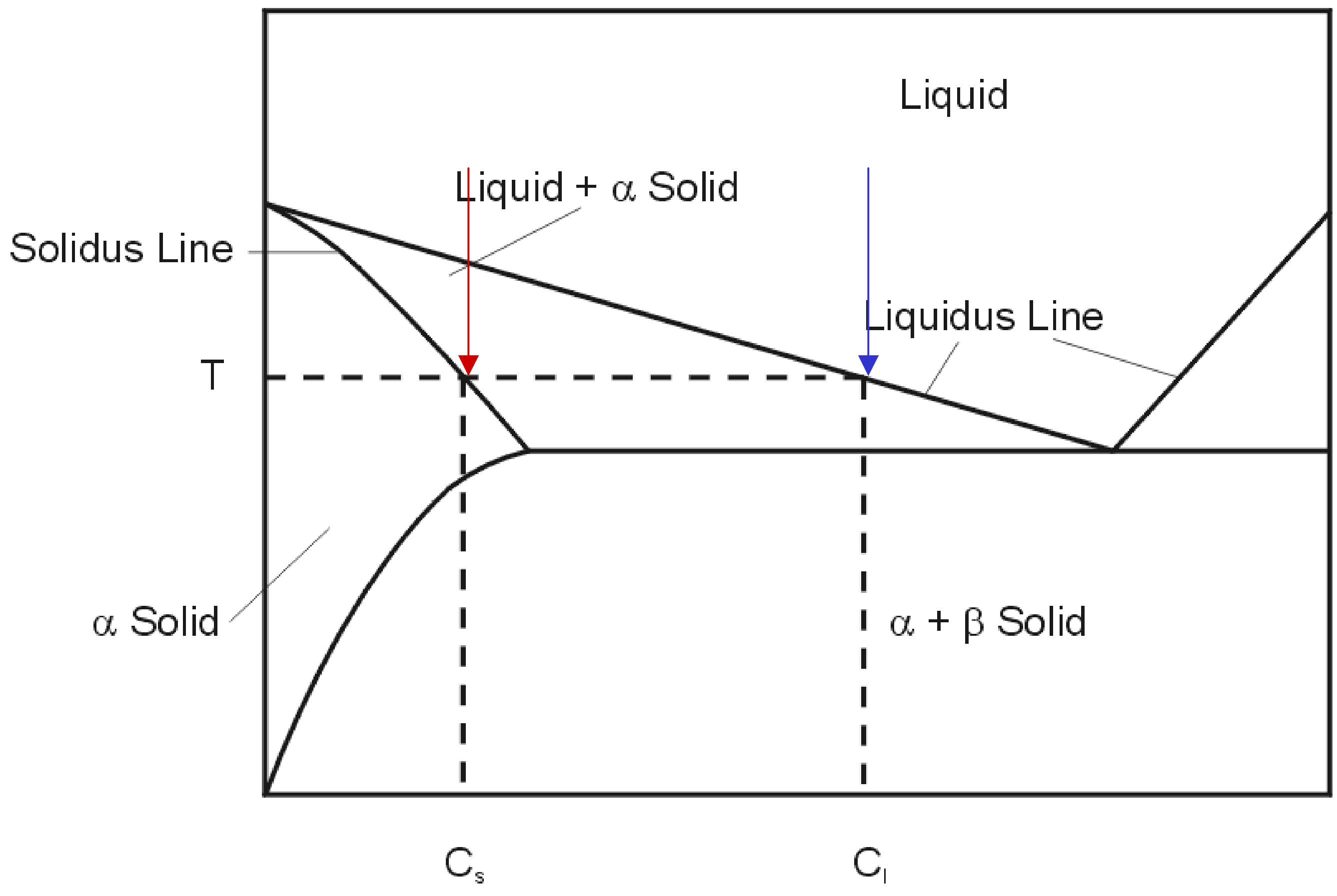
Movement within the Melt, when Viscous & Inertial Forces Dominate Buoyancy Forces



Floating when $\rho_S < \rho_1$ in a Gravitational Field

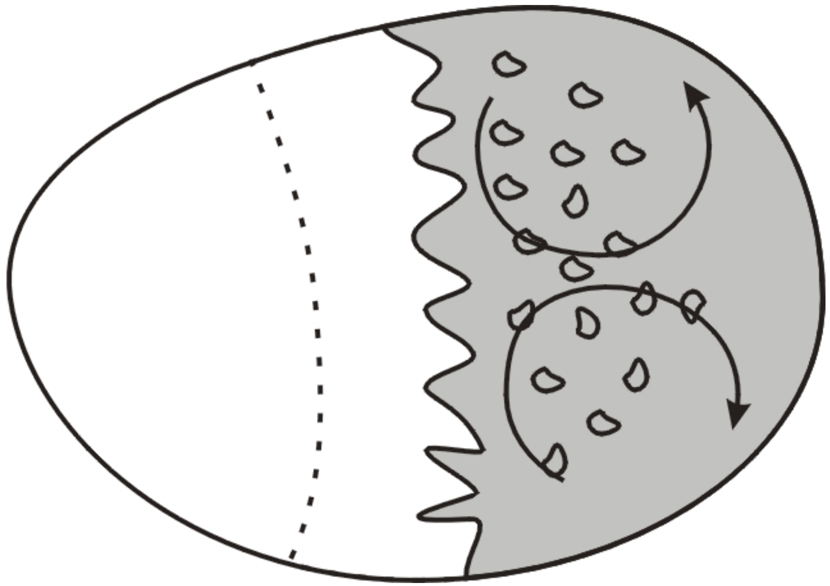
PHYSICAL PHENOMENA (11)

SEGREGATION



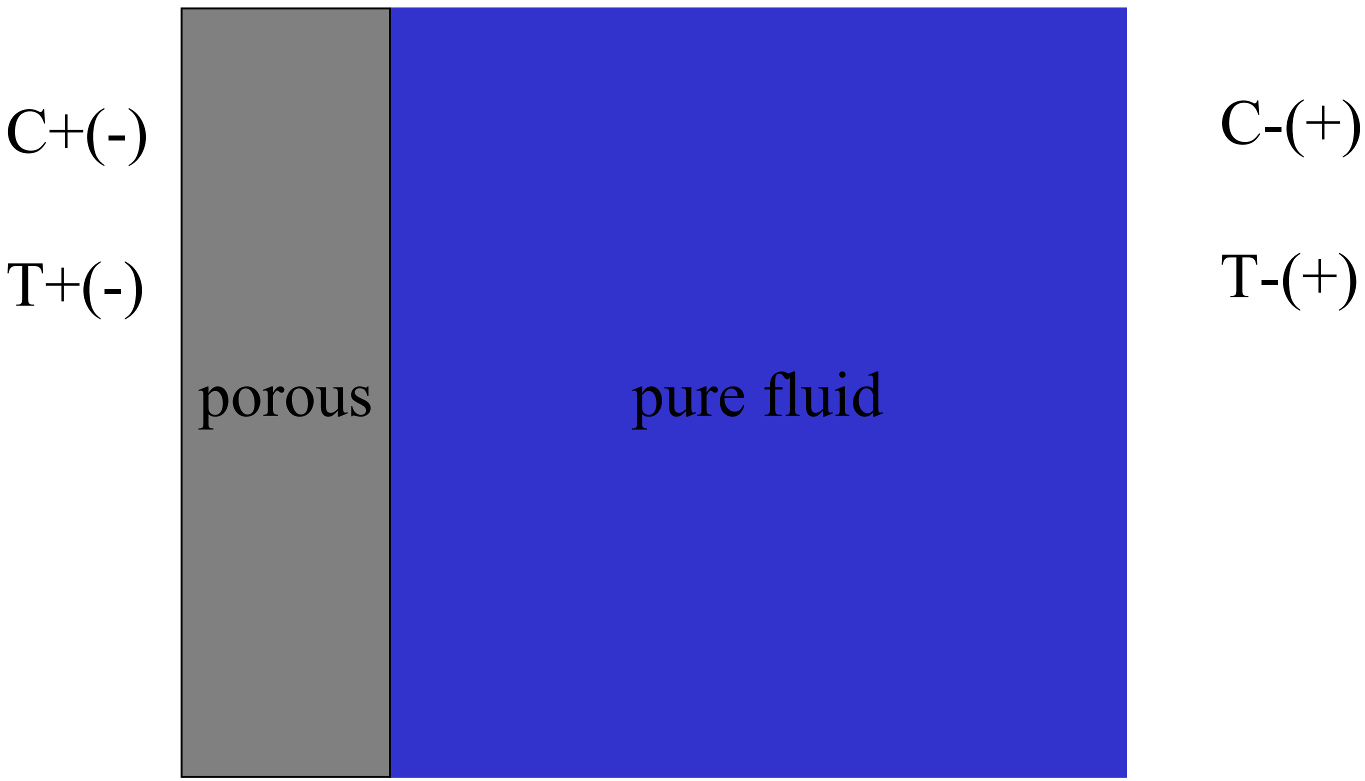
PHYSICAL PHENOMENA (12)

DOUBLE DIFFUSIVE CONVECTION



PHYSICAL PHENOMENA (12/b)

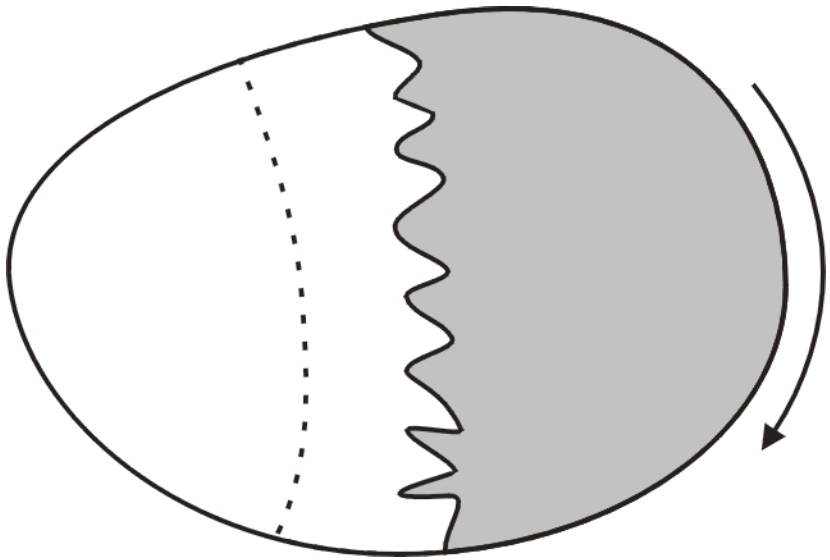
DOUBLE DIFFUSIVE CONVECTION



Gobin & Goyeau benchmark (2001)

PHYSICAL PHENOMENA (13)

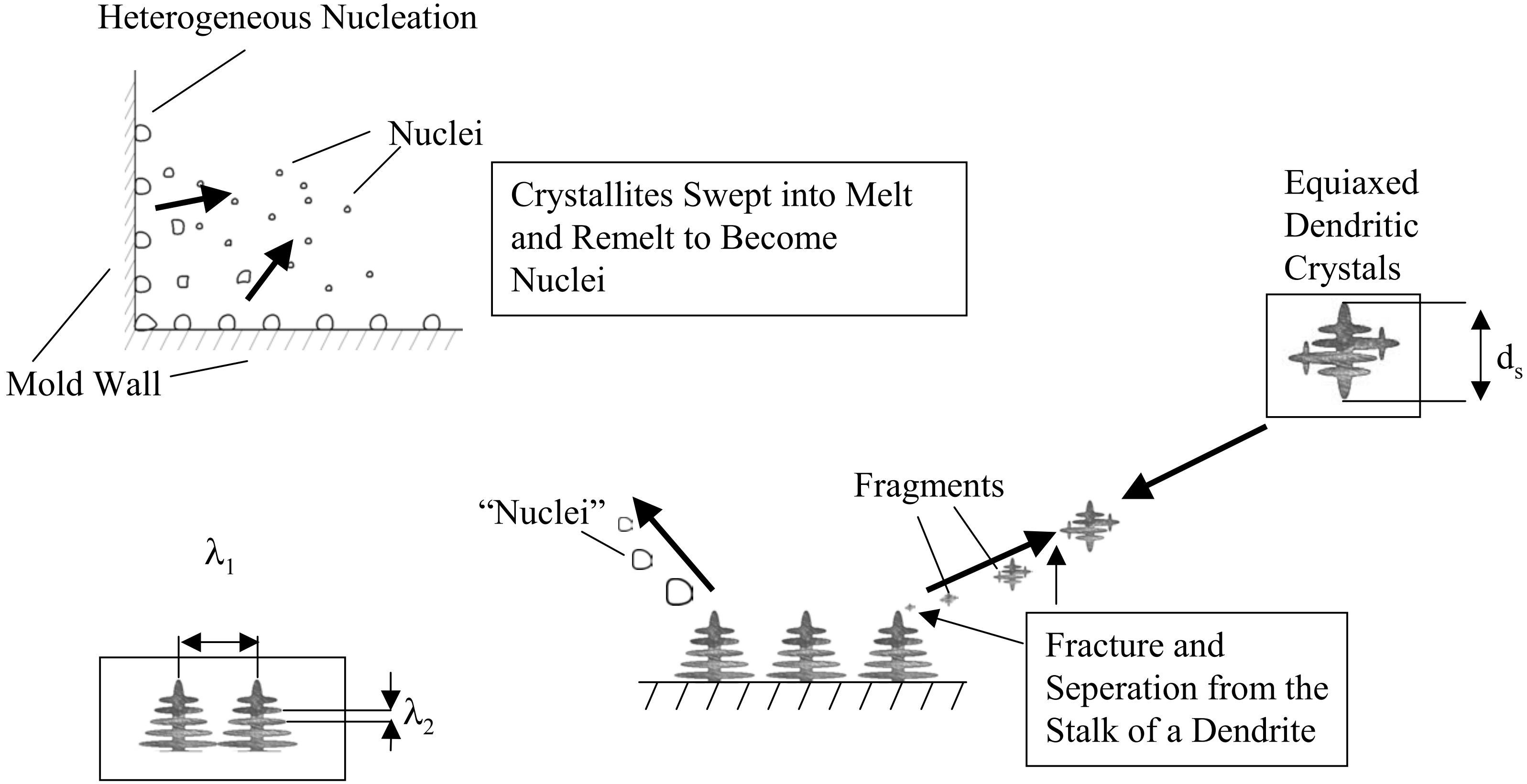
MARANGONI CONVECTION



welding
crystal growth
microgravity

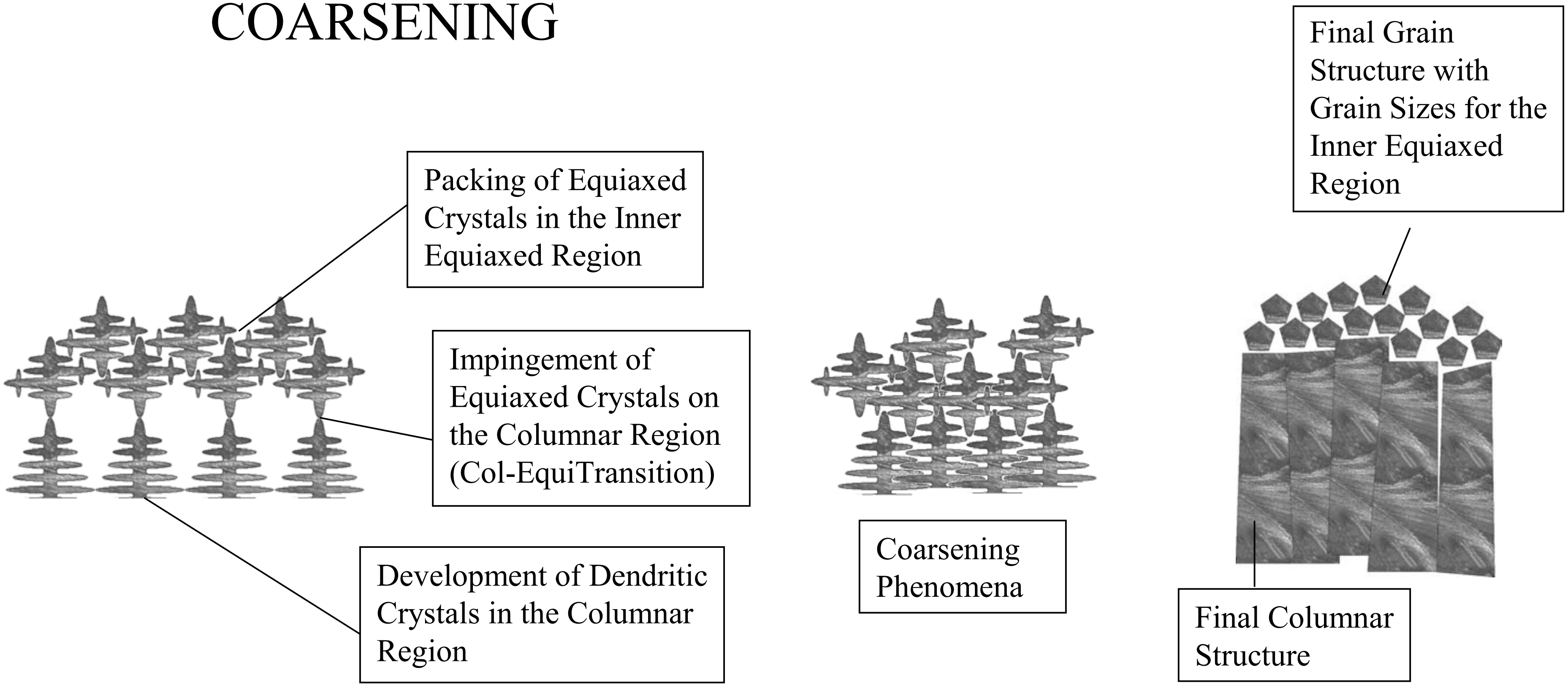
PHYSICAL PHENOMENA (14)

REMELTING, MECHANICAL INTERACTION

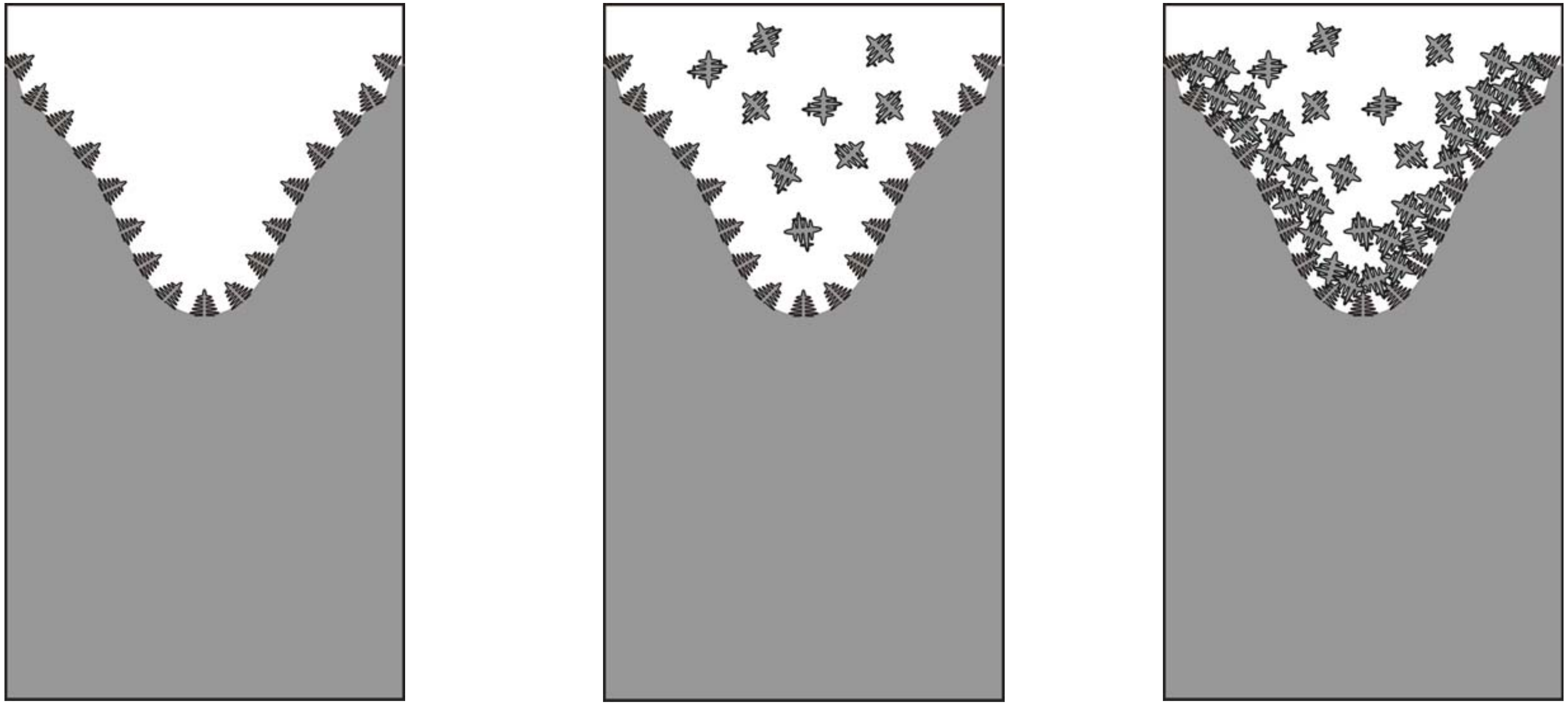


PHYSICAL PHENOMENA (15)

COARSENING



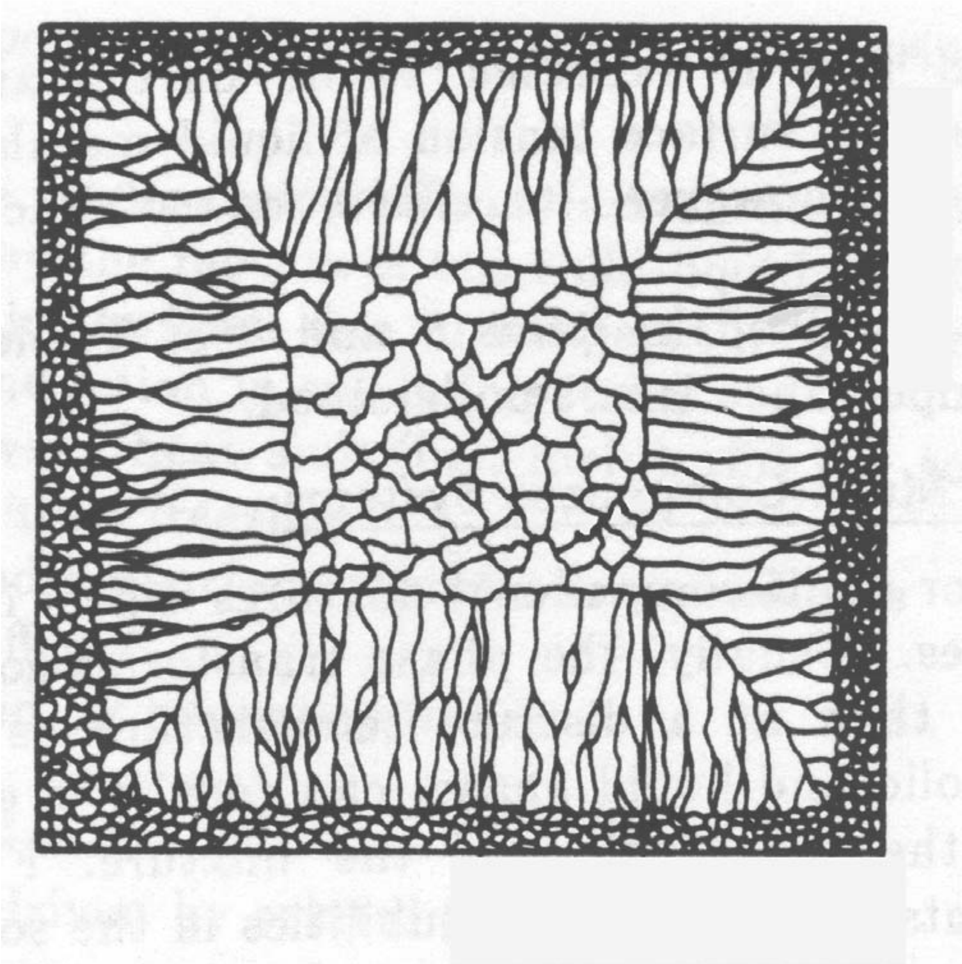
PHYSICAL PHENOMENA



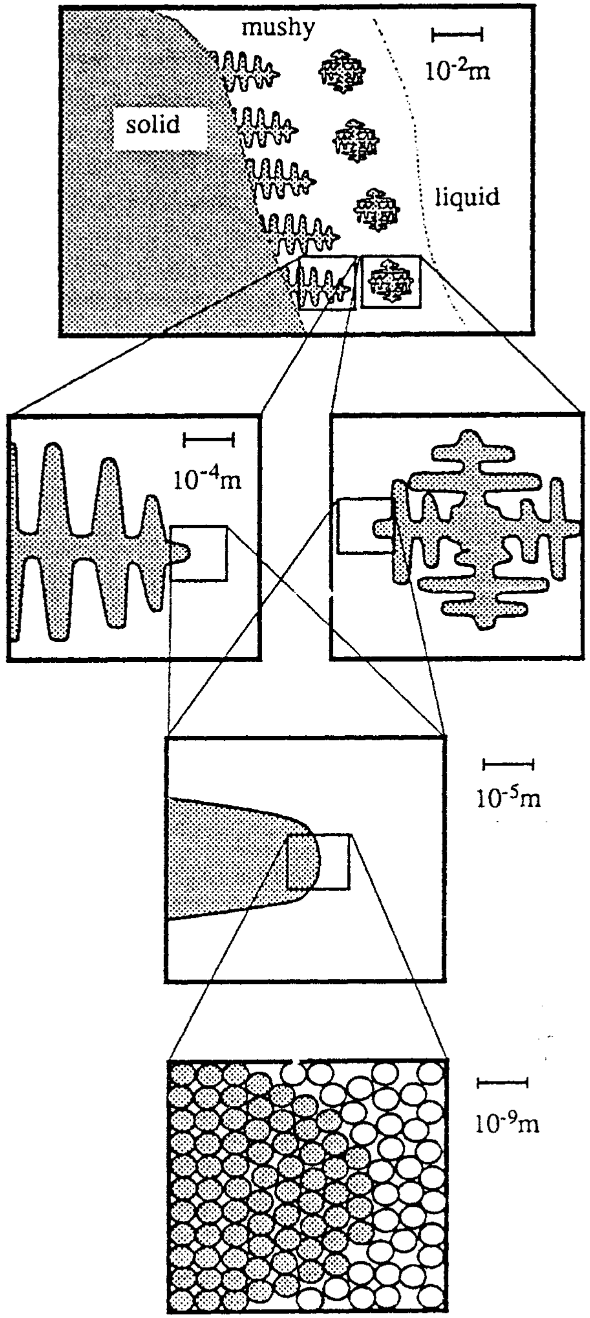
Interactions of solid and liquid phase

PHYSICAL PHENOMENA (16)

ANISOTROPY



PHYSICAL PHENOMENA (17)



MULTISCALES

1000000.000000000 m

10.000000000 m

0.000000001 m

MODELLING PROCESS

Physical Concept

Mathematical Concept

Modelling Assumptions/Simplifications

Solution

Verification, Validation

Feedback

Model Refinements

PHYSICAL SYSTEM

General Relativity

Quantum Mechanics

Statistical Mechanics

Continuum Mechanics (Classical Field Theory)

…

CONTINUUM MECHANICS

CONTINUUM HYPOTHESIS

Many constitutive parts, average properties, infinitely divisible

NEWTON'S LAWS

First Law - mass, straight line motion

Second Law - momentum, momentum of momentum

Third Law - action-reaction

THERMODYNAMIC LAWS

Zeroth Law - temperature

First Law - conservation of mass, energy

Second Law - entropy

Third Law - lower temperature margin

MATHEMATICAL CONCEPT

GENERAL AXIOMS
mathematical description of physical laws

CONSTITUTIVE AXIOMS
mathematical description of specific matter behavior

FORMULATION
design of equation systems

FORM
differential equations
integral equations
integro-differential equations

MODELLING ASSUMPTIONS

SIMPLIFICATIONS OF GEOMETRY

SIMPLIFICATIONS OF BOUNDARY CONDITIONS

SIMPLIFICATIONS OF GENERAL AND CONSTITUTIVE AXIOMS

EVALUATION

ANALYTICAL SOLUTIONS

CORRELATIONS

DISCRETE APPROXIMATE SOLUTIONS

VALIDATION

Are the equations we are solving correct ?

VALIDATION

BASIC LOGIC:

COMPARISON WITH OTHER METHODS

COMPARISON WITH EXPERIMENTS

SENSITIVITY STUDIES

VERIFICATION

Are we solving properly the equations ?

VERIFICATION

FINITE DIFFERENCE METHODS

FINITE VOLUME METHODS

FINITE ELEMENT METHODS

SPECTRAL METHODS

BOUNDARY ELEMENT METHODS

MESHLESS METHODS

VERIFICATION

CONSISTENCY
solving the proper equation
STABILITY
small changes in input - small changes in output
CONVERGENCE
mesh refinement - solution accuracy refinement
CONSERVATION
local, global - conservation of physical properties
BOUNDS
local, global - bounds of physical properties
REALIZATION
reasonable computer time, reasonable computer storage
ERROR
discretisation error, round-off error

CONTINUUM MODEL

TRANSPORT EQUATIONS

mass transport
energy transport
momentum transport
moment of momentum transport
entropy transport
species transport

GENERAL TRANSPORT EQUATION

$$\frac{\partial}{\partial t}\left(\rho\Upsilon(\Phi)\right)+\nabla\cdot\left(\rho\vec{v}\Upsilon(\Phi)\right)=\nabla\cdot\left(\underline{D}^{\Phi}\nabla\Phi\right)+S^{\Phi}$$

CONTINUUM MODEL

CONSTITUTIVE EQUATIONS

restrictions on the type of motion: irrotational, isochoric,...
specialisations of the transport equations: steady, creeping,...
constitutive relations: incompressible, newtonian,…
mechanical: stress tensor, body force
energetic: Fourier’s law, body heating
chemical: Fick’s law, body species generation
constitutive equations of state: entropy, internal energy, density

CONTINUUM MODEL

INITIAL + BOUNDARY CONDITIONS

SOLID PHASE
transport equations
constitutive equations

LIQUID PHASE
transport equations
constitutive equations

SOLID-LIQUID INTERFACE
jump conditions
interphase conditions

PROBLEM FORMULATIONS
MIXTURE THORY FORMULATION

A: solid phase

$$\frac{\partial}{\partial t}\left(\rho_S \Upsilon_S(\Phi_S)\right) + \nabla \cdot \left(\rho_S \vec{v}_S \Upsilon_S(\Phi_S)\right) = \nabla \cdot \left(\underline{D}_S^{\Phi} \nabla \Phi_S\right) + S_S^{\Phi}$$

B: liquid phase

$$\frac{\partial}{\partial t}\left(\rho_L \Upsilon_L(\Phi_L)\right) + \nabla \cdot \left(\rho_L \vec{v}_L \Upsilon_L(\Phi_L)\right) = \nabla \cdot \left(\underline{D}_L^{\Phi} \nabla \Phi_L\right) + S_L^{\Phi}$$

C: ideal mixture theory assumptions in mushy region

three regions, three equations

Flemings et.al., 1967

PROBLEM FORMULATIONS
MIXTURE CONTINUUM FORMULATION (1 REGION)

ideal mixture theory assumptions in whole domain

$$\frac{\partial}{\partial t}\Big(f_S \rho_S \Upsilon_S(\Phi_S) + f_L \rho_L \Upsilon_L(\Phi_L)\Big) +$$

$$+\nabla \cdot \Big(f_S \rho_S \vec{v}_S \Upsilon_S(\Phi_S) + f_L \rho_L \vec{v}_L \Upsilon_L(\Phi_L)\Big) =$$

$$= \nabla \cdot \Big(f_S \underline{D}_S^{\Phi} \nabla \Phi_S + f_L \underline{D}_L^{\Phi} \nabla \Phi_L \Big) + f_S S_S^{\Phi} + f_L S_L^{\Phi}$$

one region, one equation

Bennon & Incropera, 1987

PROBLEM FORMULATIONS
TWO-PHASE AVERAGED FORMULATION

solid phase

$$\frac{\partial}{\partial t}\left(f_S \rho_S \Upsilon_S(\Phi_S)\right) + \nabla \cdot \left(f_S \rho_S \vec{v}_S \Upsilon_S(\Phi_S)\right) =$$
$$= \nabla \cdot \left(f_S \underline{D}_S^{\Phi} \nabla \Phi_S\right) + f_S S_S^{\Phi} + Q_S$$

liquid phase

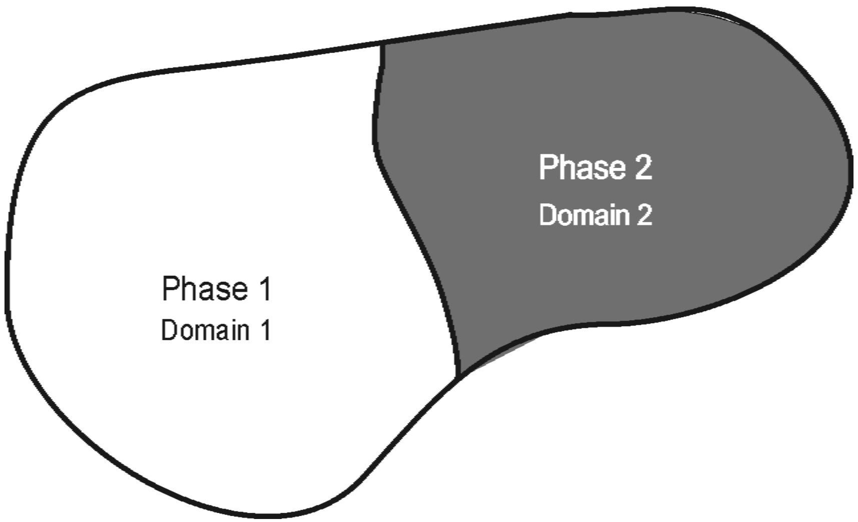
$$\frac{\partial}{\partial t}\left(f_L \rho_L \Upsilon_L(\Phi_L)\right) + \nabla \cdot \left(f_L \rho_L \vec{v}_L \Upsilon_L(\Phi_L)\right) =$$
$$= \nabla \cdot \left(f_L \underline{D}_L^{\Phi} \nabla \Phi_L\right) + f_L S_L^{\Phi} + Q_L$$

one region, two equations

Beckermann & Ni, 1990

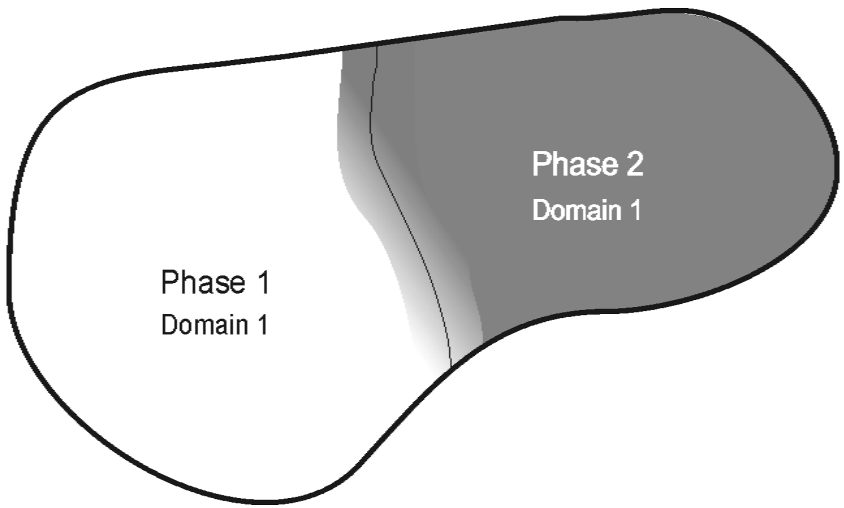
PROBLEM FORMULATIONS

two-domain



mixture theory

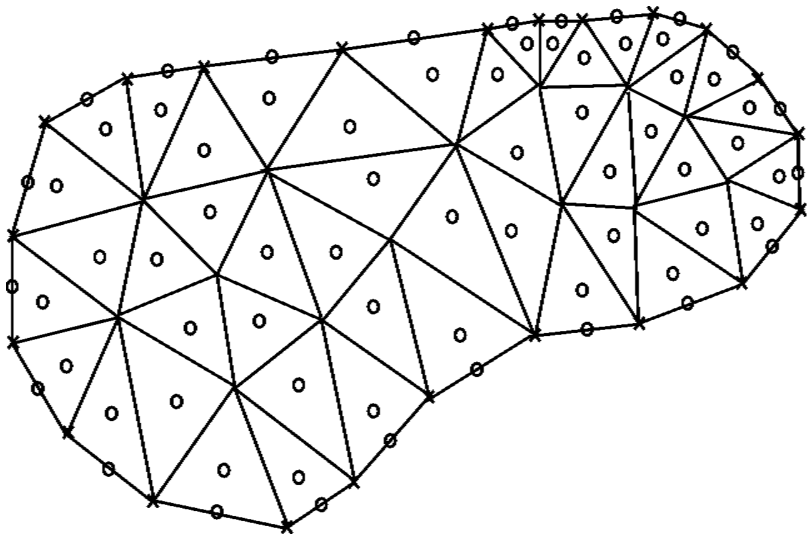
one-domain



mixture continuum
two-phase averaged

ONE-DOMAIN FORMULATION
POLYGON METHODS

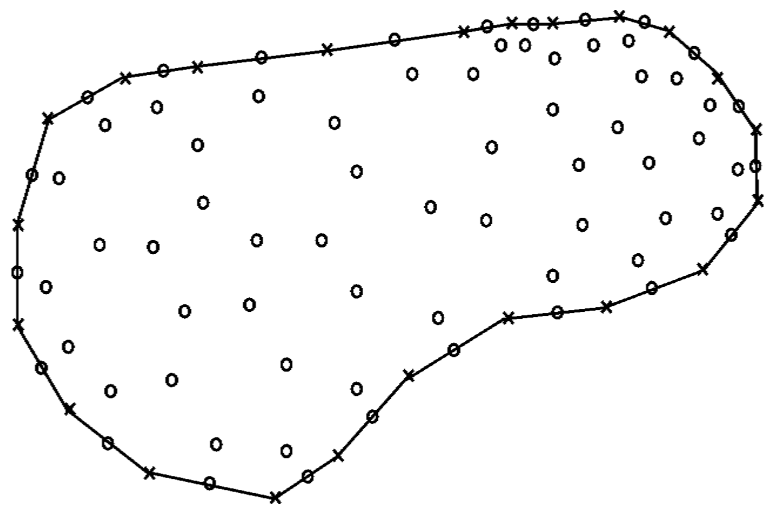
FEM, FVM, BDIM



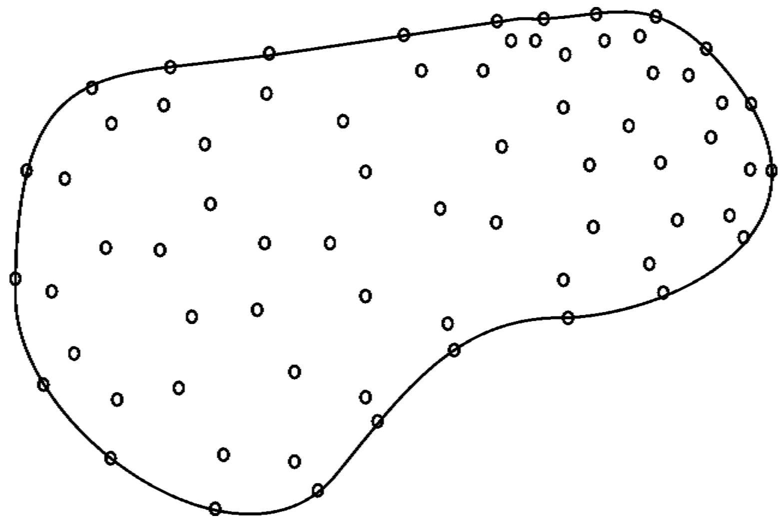
Refinement near the interphase !

ONE-DOMAIN FORMULATION
SEMI & COMPLETE MESH-FREE METHODS

DRBEM

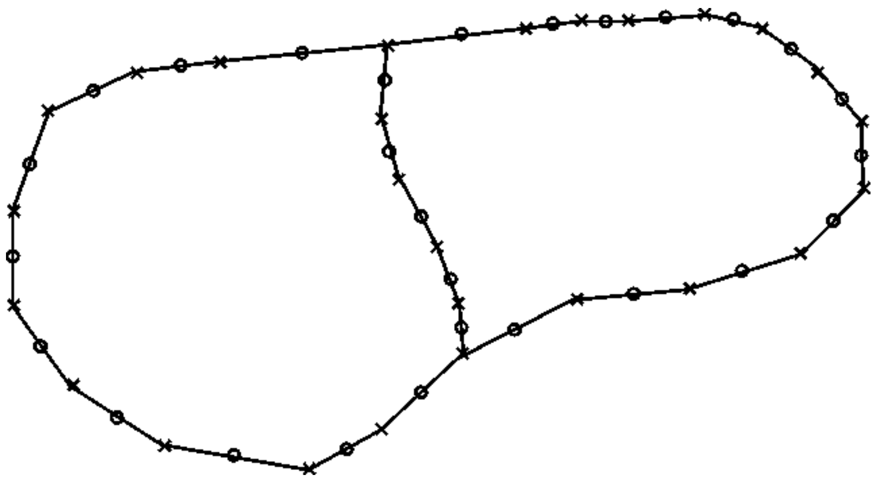


DRMFS, RBFCM

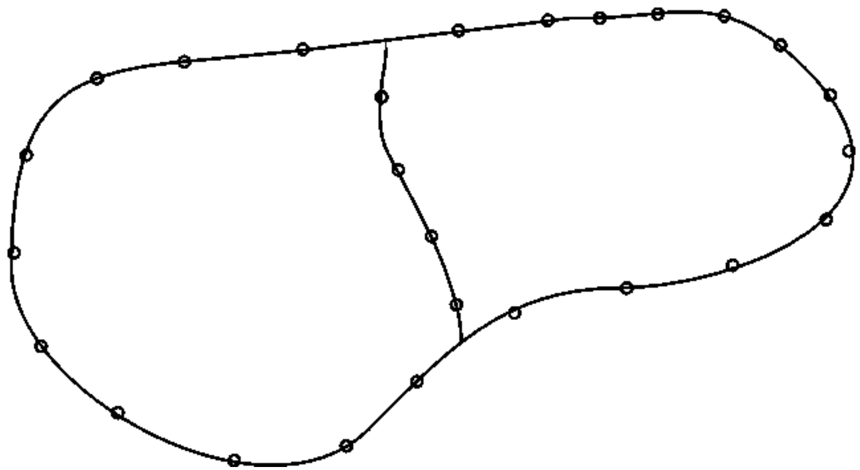


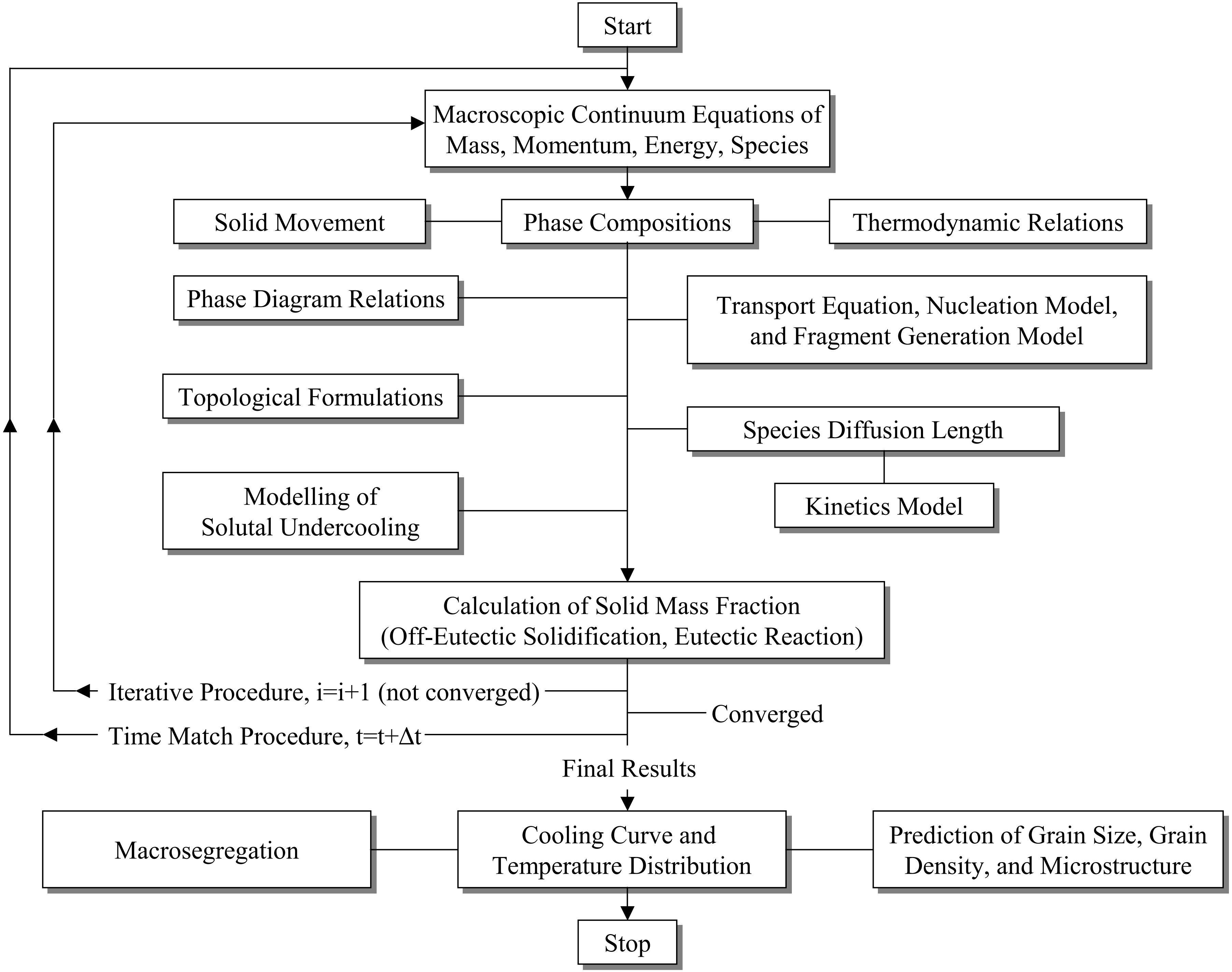
TWO-DOMAIN FORMULATION
SEMI & COMPLETE MESH-FREE METHODS

BEM



MFS




Start
Macroscopic Continuum Equations of Mass, Momentum, Energy, Species
Solid Movement
Phase Compositions
Thermodynamic Relations
Phase Diagram Relations
Transport Equation, Nucleation Model, and Fragment Generation Model
Topological Formulations
Species Diffusion Length
Kinetics Model
Modelling of Solutal Undercooling
Calculation of Solid Mass Fraction (Off-Eutectic Solidification, Eutectic Reaction)
Iterative Procedure, i=i+1 (not converged)
Converged
Time Match Procedure, t=t+Δt
Final Results
Macrosegregation
Cooling Curve and Temperature Distribution
Prediction of Grain Size, Grain Density, and Microstructure
Stop