COMSOL
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Combining Multiphysics Modeling and Solution Thermodynamics Using M4Dlib, an External Library

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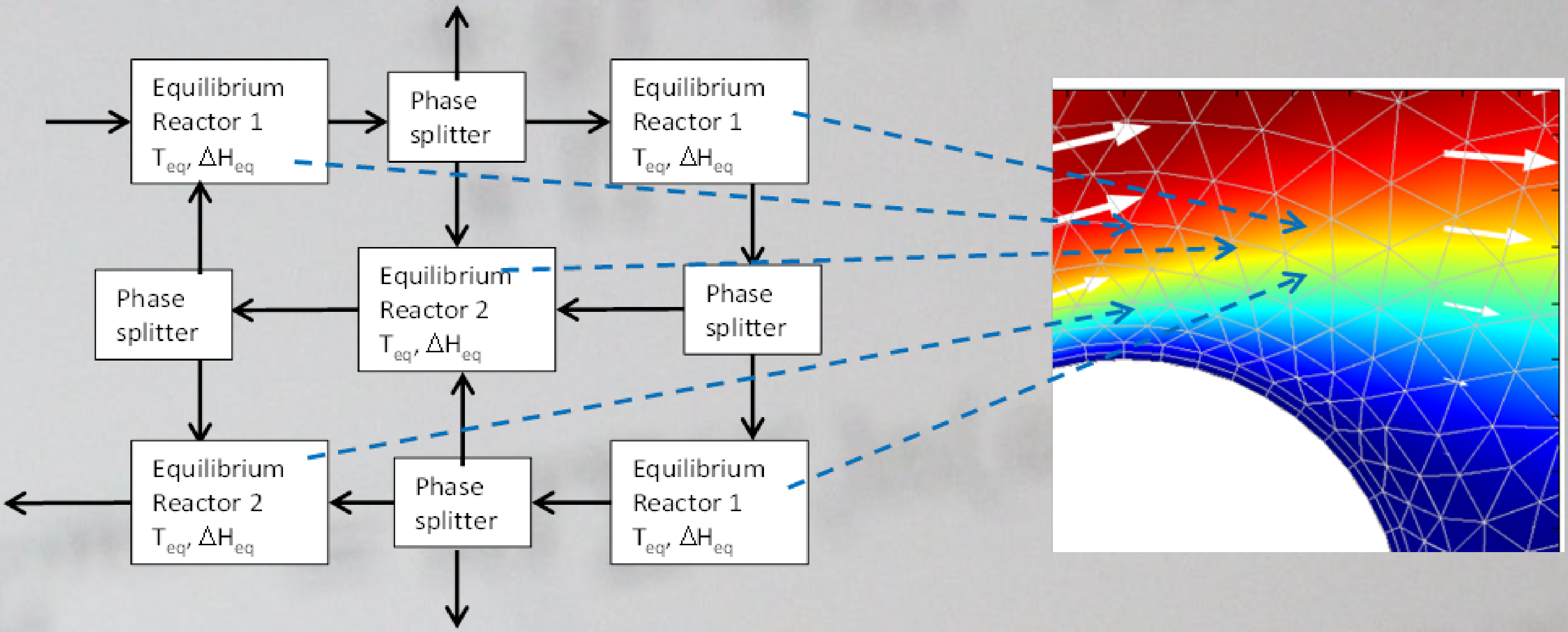
M4Dynamics

Introduction

- Why Multiphysics Simulation coupled to Solution Thermodynamics?
  - Modeling multicomponent chemical systems:
    - Alloys → Steelmaking, Light metals, Solar Energy, …
    - Matte / Metals → Smelting, Converting, Refining
    - Slags / Glass → Pyrometallurgy, glass industry, energy recovery
  - Phase change modeling of non-ideal system
  - Modeling reactive systems:
    - Corrosion
    - Combustion → energy generation, smelting, gas cleaning
    - High temperature vessel integrity

Approach

- Take the Local Equilibrium Concept (0D) from Thermodynamic Process Simulation experience and extend it to Multiphysics Modeling (0, 1, 2 and 3D)



Equilibrium Reactor 1 T_{eq}, ΔH_{eq}

Phase splitter

Equilibrium Reactor 1 T_{eq}, ΔH_{eq}

Phase splitter

Equilibrium Reactor 2 T_{eq}, ΔH_{eq}

Phase splitter

Equilibrium Reactor 2 T_{eq}, ΔH_{eq}

Phase splitter

Equilibrium Reactor 1 T_{eq}, ΔH_{eq}

The thermodynamic part – binary solution system

- Let's assume a binary system A-B
- Considering AB having solid and liquid solutions AB_S and AB_L
  - Integral Gibbs Free Energy of each solution is:

$$G^{int} = \sum G_i^o \cdot X_i + G^{mix}$$

$$G_i^o = a + bT + cTlnT + dT^2 + eT^3 + f/T + gT^i + hT^j + iT^k + jT^l + kT^m + lT^n \longleftarrow$$

For pure or stoichiometric compounds

$$G^{mix} = RT\sum(X_i \ln(a_i)) = G^{id} + G^{ex} \longleftarrow$$

Mixing contribution

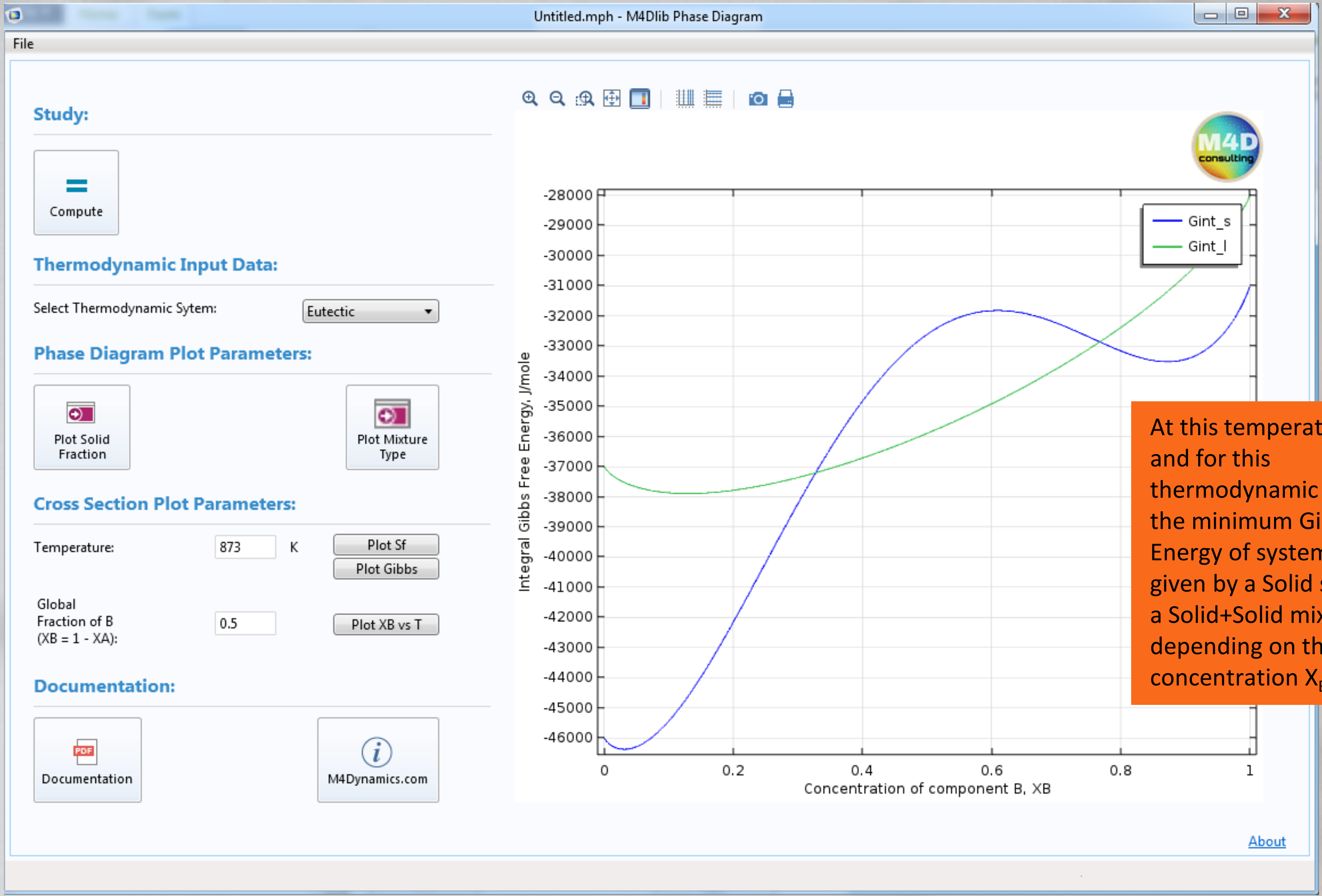
$$G^{id} = RT\sum(X_i \ln(X_i))$$

$$G^{ex} = RT\sum(X_i \ln(\gamma_i)) \longleftarrow$$

- Regular
- Wagner Interaction Parameters
- Darken Quadratic
- Redlich-Kistner (or polynomial)
- Associate Solution
- Modifier Quasi-Chemical
- Extended Modified Quasi-Chemical
- Compound Energy Formalism
- Sub-lattice
- Etc.

Non-ideal case: solid with strong positive deviation

- Depending on the parameters chosen for components A and B and their liquid and solid solutions models:



Untitled.mph - M4Dlib Phase Diagram

Study:

Thermodynamic Input Data:

Select Thermodynamic Sytem: Eutectic

Phase Diagram Plot Parameters:

Cross Section Plot Parameters:

Temperature: 873 K

Global Fraction of B (XB = 1 - XA): 0.5

Documentation:

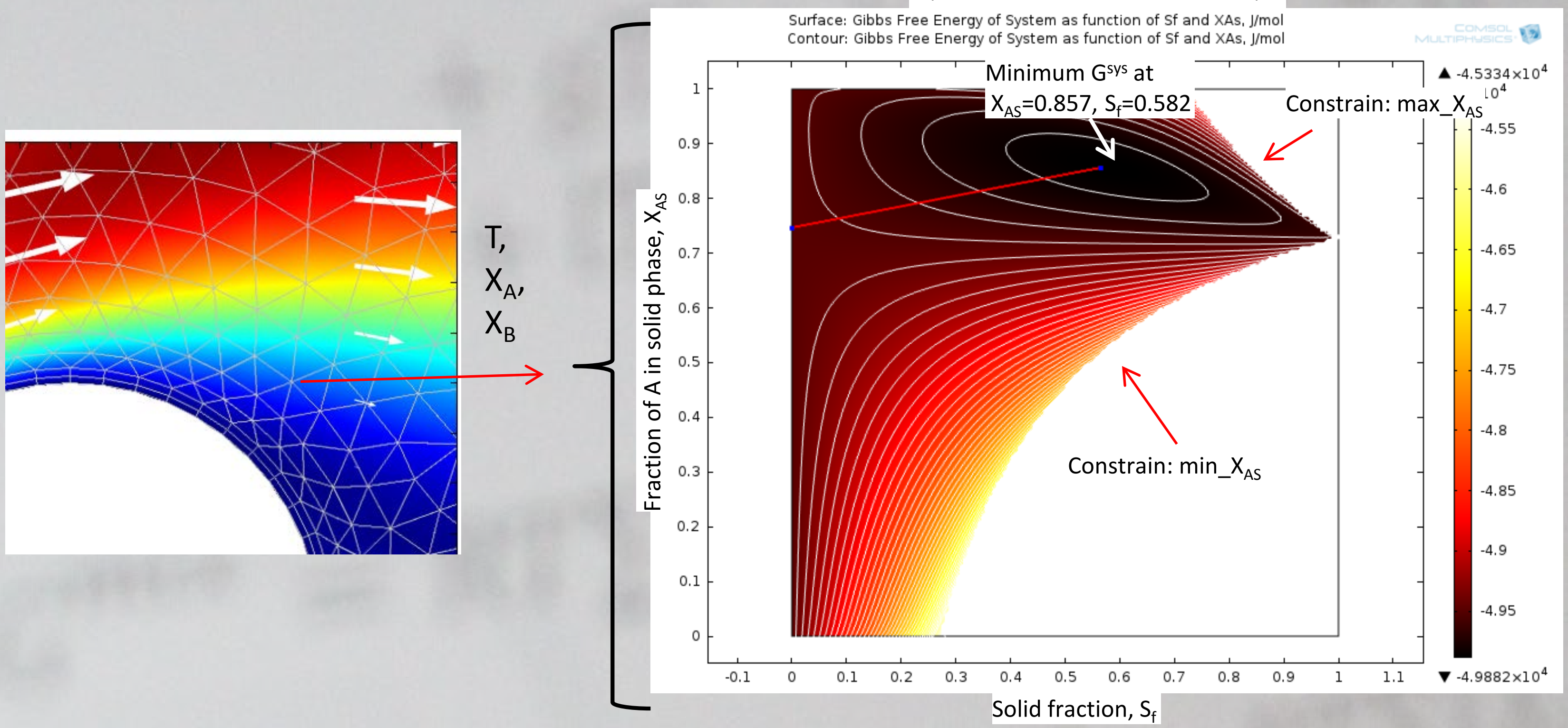
At this temperature (873 K) and for this thermodynamic system, the minimum Gibbs Free Energy of system will be given by a Solid solution or a Solid+Solid mixture, depending on the system's concentration X_B

Equilibrium calculation

- The problem require to minimize the System’s Gibbs Free Energy:

$$G^{sys} = \frac{G_L^{int} - G_S^{int}}{(X_{B,L} - X_{B,S})}(X_B - X_{B,S}) + G_S^{int}$$

(In this case: T=1143 K, XA=0.72)



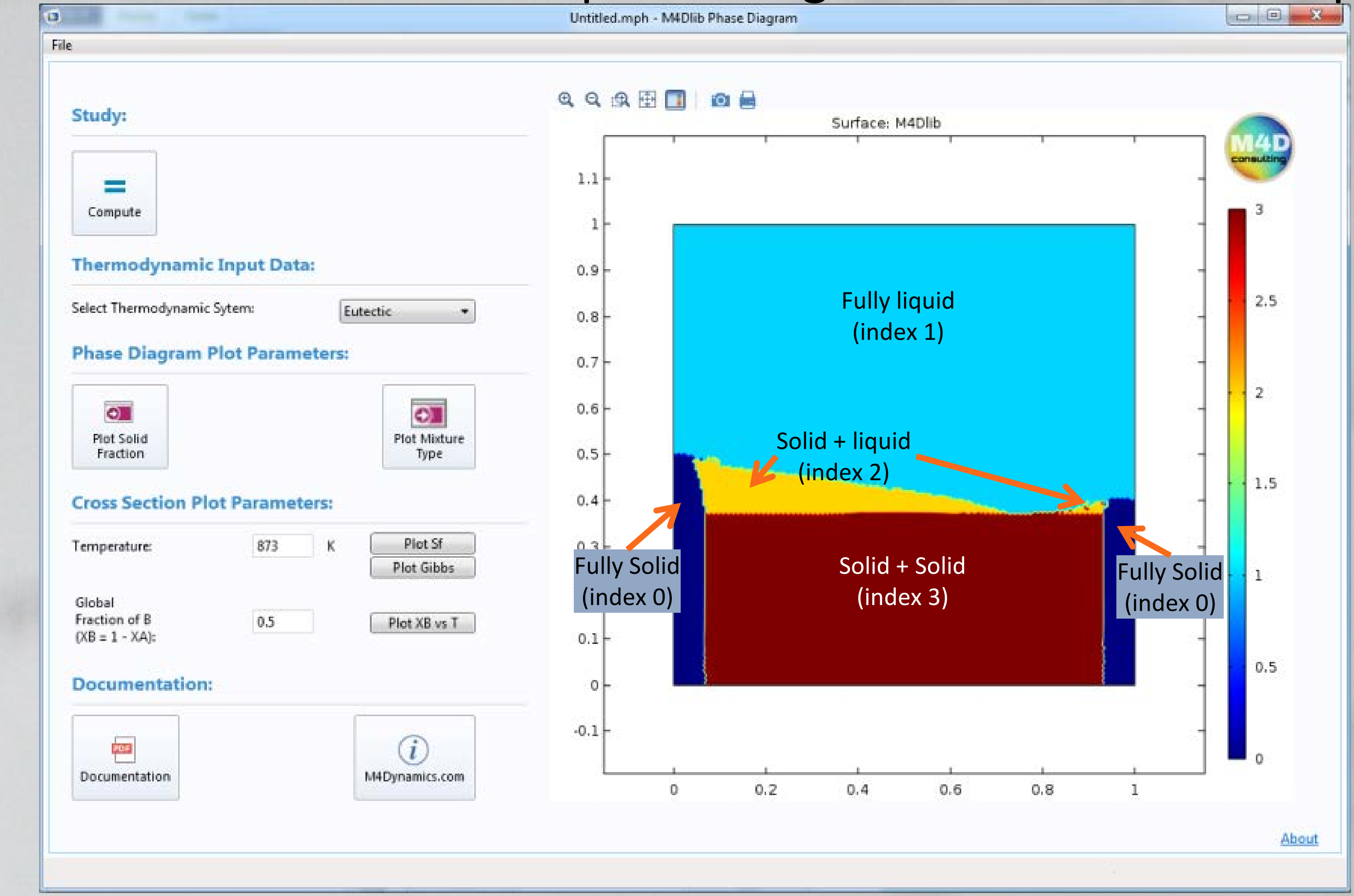
Minimum G^{sys} at X_{AS}=0.857, S_f=0.582

Constrain: max_X_{AS}

Constrain: min_X_{AS}

Thermodynamic part: Results

- By minimizing Gsys, the amount and composition of stable phases or mixtures are calculated. This is summarized in the calculation of Eutectic phase diagram in COMSOL Multiphysics



Untitled.mph - M4Dlib Phase Diagram

Select Thermodynamic Sytem: Eutectic

Temperature: 873 K

Global Fraction of B (XB = 1 - XA): 0.5

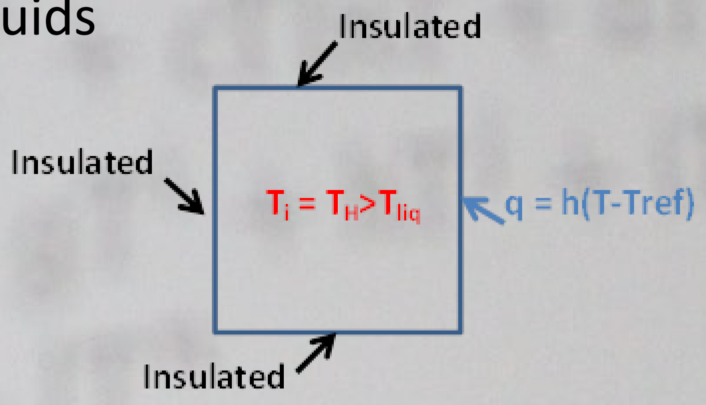
Application Example:

Multiphysics + Thermodynamics

- Let's consider the controlled solidification of a melt (system AB) inside a furnace or crucible
  - Vessel Integrity → for a protective layer on the surface of the hot phase of refractory or salamander → extend service life of furnace
  - Metal refining during controlled cooling → Solar Grade Silicon Refining (Cu-Si, Fe-Si)

Boundary and initial conditions

- Heat Transfer in fluids



Insulated

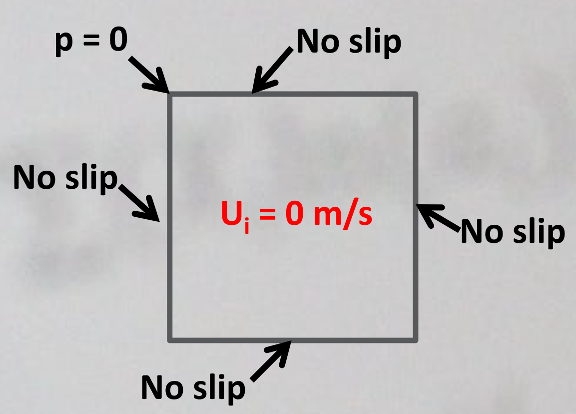
Insulated

$T_i = T_H > T_{liq}$

$q = h(T-T_{ref})$

Insulated

- Fluid Flow (laminar)



p = 0

No slip

No slip

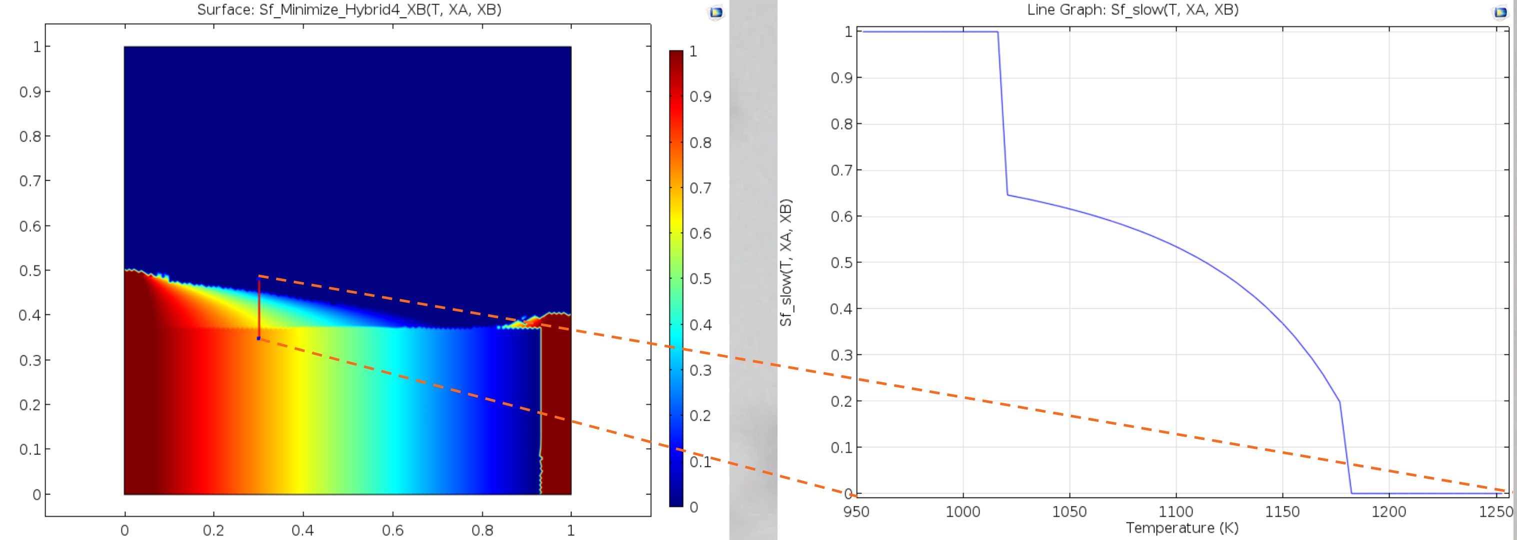
$U_i = 0$ m/s

No slip

No slip

Approach

- Based on the Solidification model by Voller and Prakash, Navier-Stokes Equations are coupled to Solidification process by Volume force terms depending on Solid Fraction

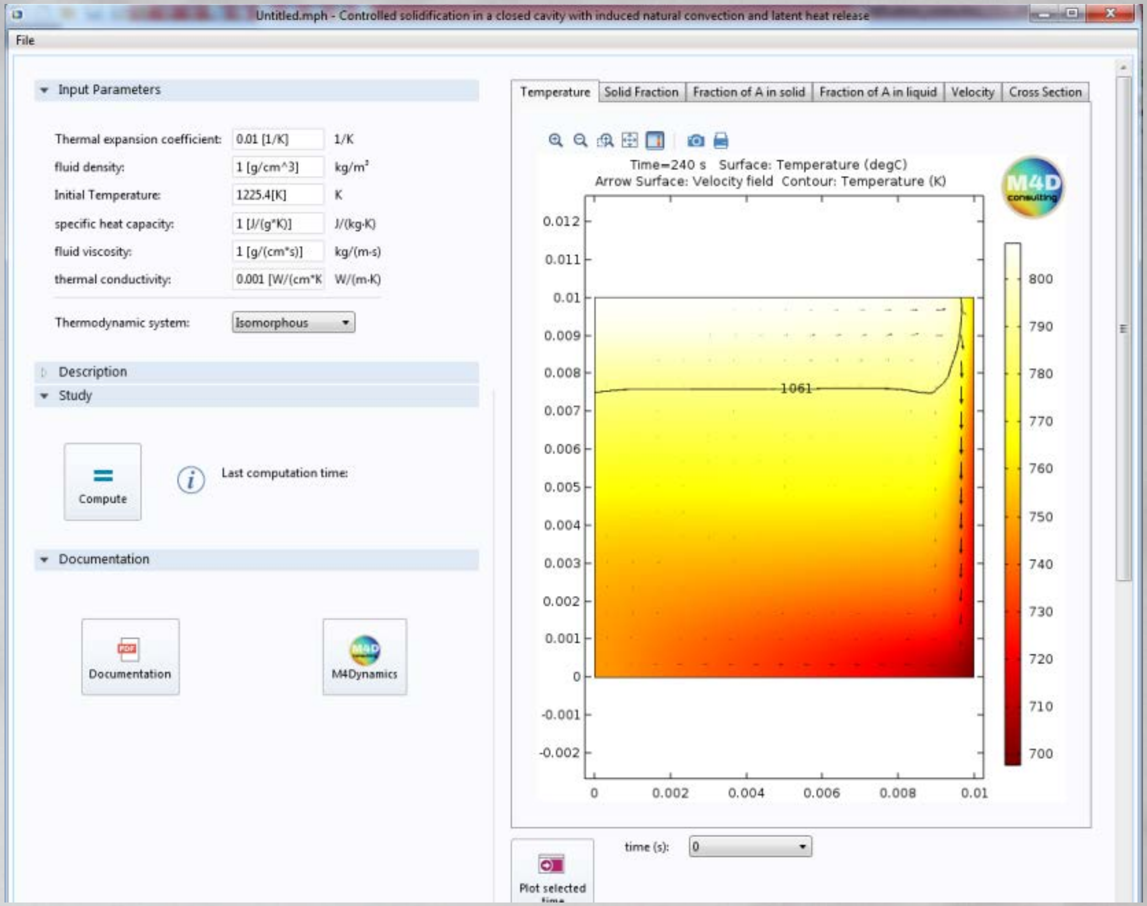


Solution model $\longrightarrow$ M4Dlib $\longrightarrow S_f \longrightarrow A = \dfrac{C(1-\lambda^2)}{\lambda^3 + q} \longrightarrow$

$$S_x = -A \cdot u$$
$$S_y = -A \cdot v$$
$$-\beta \cdot g \cdot \rho \cdot \left(T - T_{ref}\right)$$

Results

- Controlled Solidification of a binary melt in a closed cavity
- XA0 = 0.5; T liquidus = 1125 K, Tsolidus = 1060 K



Untitled.mph - Controlled solidification in a closed cavity with induced natural convection and latent heat release

Input Parameters

Thermal expansion coefficient: 0.01 [1/K] 1/K
fluid density: 1 [g/cm^3] kg/m³
Initial Temperature: 1225.4[K] K
specific heat capacity: 1 [J/(g*K)] J/(kg·K)
fluid viscosity: 1 [g/(cm*s)] kg/(m·s)
thermal conductivity: 0.001 [W/(cm*K W/(m·K)

Thermodynamic system: Isomorphous

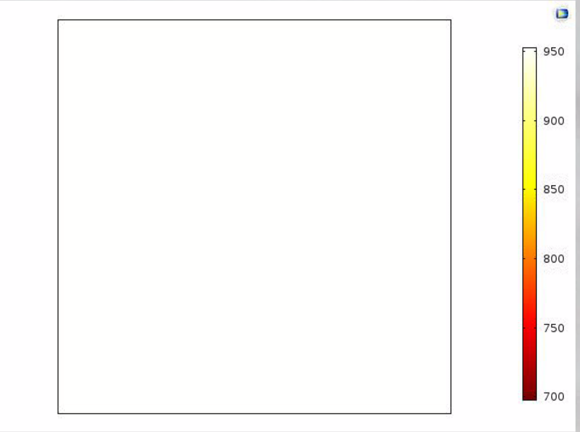
Last computation time:

time (s): 0

Time=240 s Surface: Temperature (degC)
Arrow Surface: Velocity field Contour: Temperature (K)

Results

Temperature



Solid Fraction

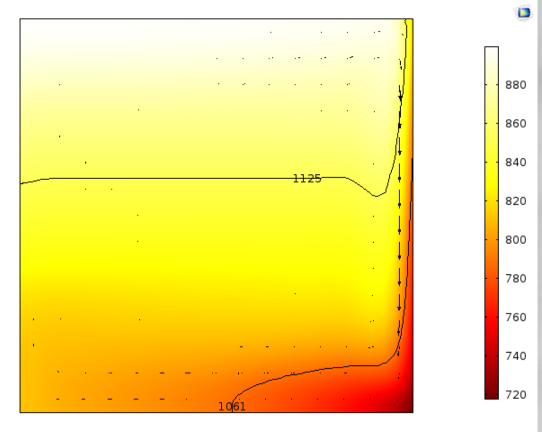
$X_{A,S}$ Composition of A in Solid

$X_{A,L}$ composition of A in Liquid

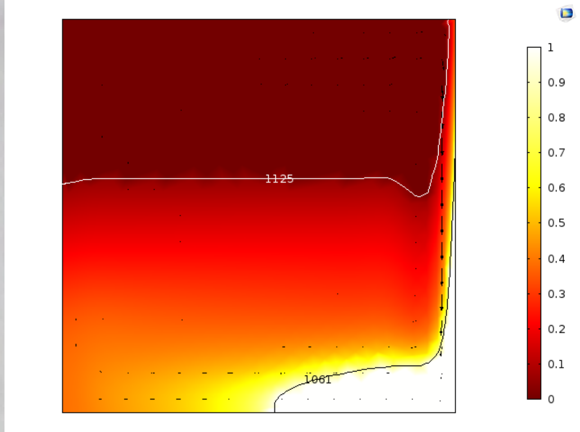
Results

t=100s

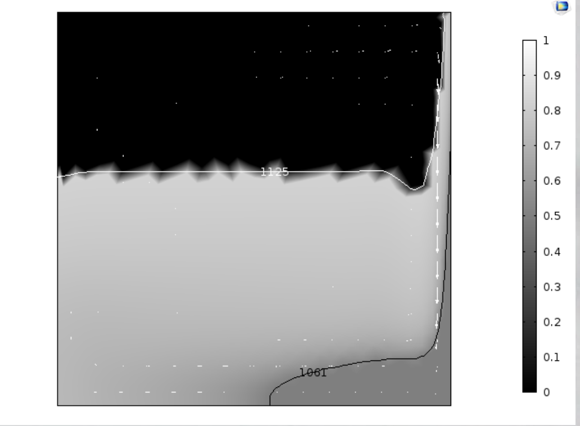
Temperature



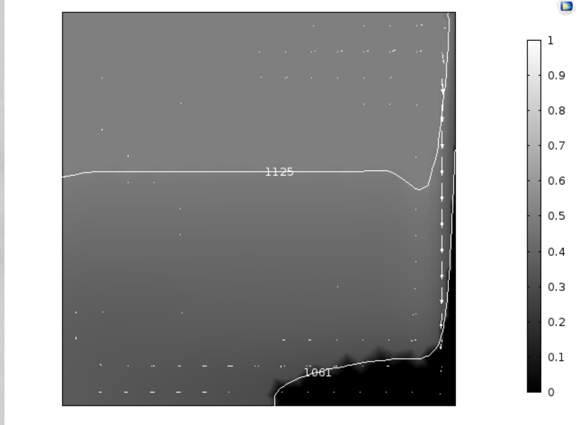
Solid Fraction



$X_{A,S}$ Composition of A in Solid



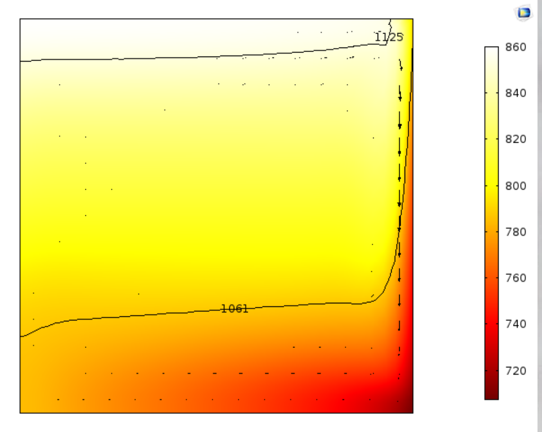
$X_{A,L}$ composition of A in Liquid



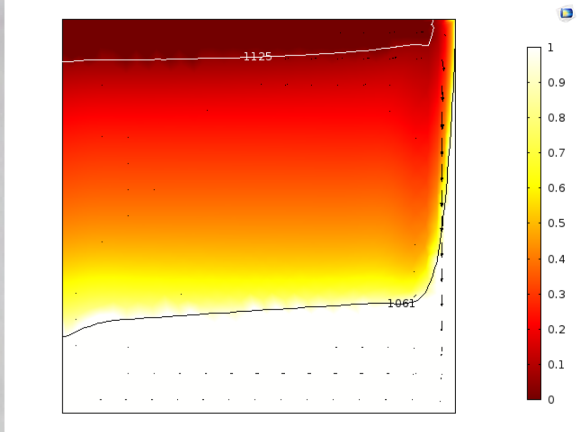
Results

t=150s

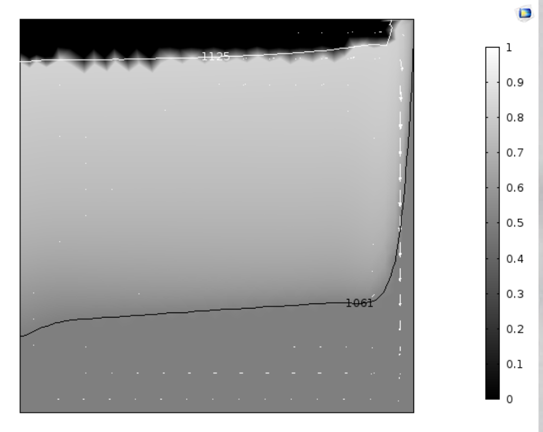
Temperature



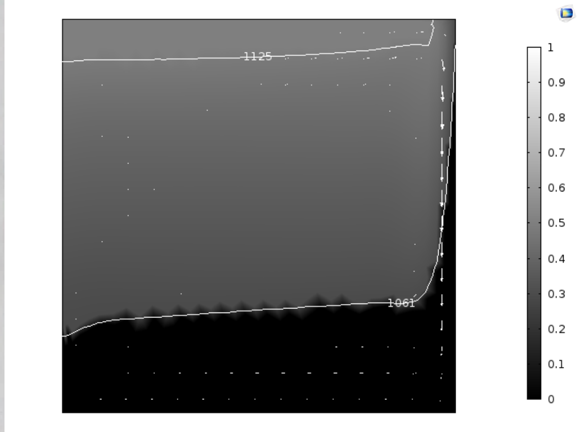
Solid Fraction



$X_{A,S}$ Composition of A in Solid



$X_{A,L}$ composition of A in Liquid



Summary

- Coupling Multiphysics and Solution Thermodynamics can be accomplish by the use of M4Dlib, an external function library
  - M4Dlib is available as a dynamic link library for Windows (*.dll), Mac OS X (*.dylib) and Linux (*.so)
  - An input thermodynamic system description is necessary:
    - A database needs to be created for each specific problem based on available data or experimental information
  - M4Dlib calculates composition and amounts of stable phases at given global conditions (T, composition) it also provides system information for:
    - Enthalpy, heat capacity, density, or other properties defined on the input thermodynamic file.

Thanks!

http://m4dynamics.com

contact@m4dynamics.com