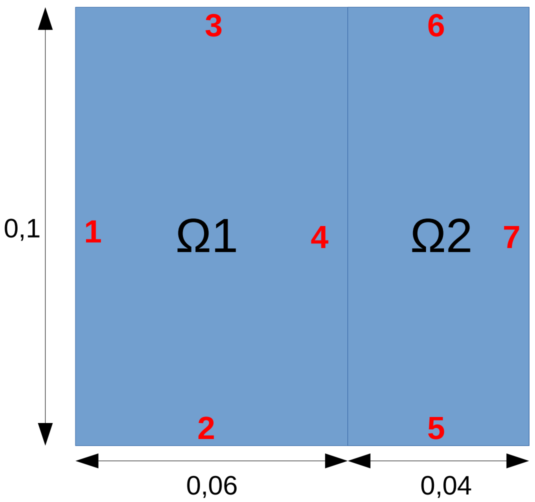
Elmer :Heat transfert with phase change solid-solid in transient problem
Application to silicon properties



1. Tb=1750 [K] → $T = T_b.$

2 & 5. q=-10000 [W/m²] → $-k\dfrac{\partial T}{\partial n} = q.$

3 & 6. α=15 [W/(m²K)] Text=300 [K] → $-k\dfrac{\partial T}{\partial n} = \alpha(T - T_{ext}).$

4. internal boundary (automatic) → $-\mathbf{n}_{\mathrm{dst}} \cdot (k\nabla T)_{\mathrm{dst}} = \mathbf{n}_{\mathrm{src}} \cdot (k\nabla T)_{\mathrm{src}}$

$T_{\mathrm{dst}} = T_{\mathrm{src}}$

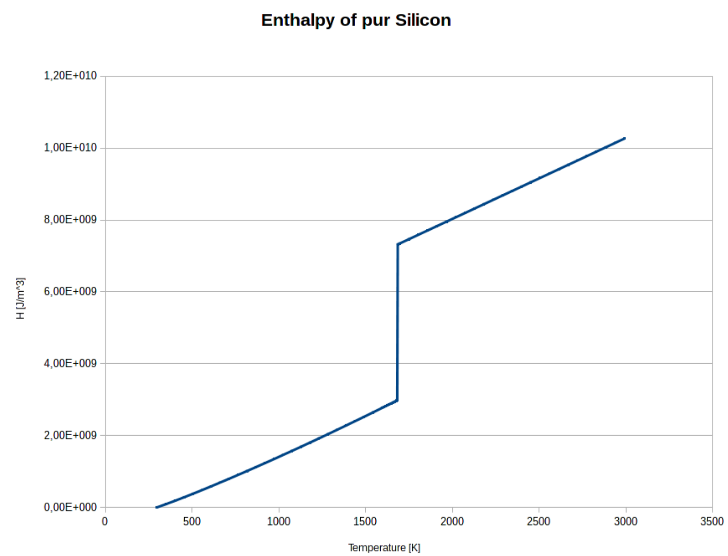
7. thermal insulation → $-k\dfrac{\partial T}{\partial n} = 0.$

<u>Heat transfert equation in solid (u=0)</u>

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \mathbf{u} \cdot \nabla T = \nabla \cdot (k \nabla T) + Q$$

Enthalpy [J/m³] used by Elmer to compute effective heat capacity
(-DeltaT width = 8 K)

$$c_{p,\mathrm{eff}} = \frac{\partial H / \partial t}{\partial T / \partial t}.$$



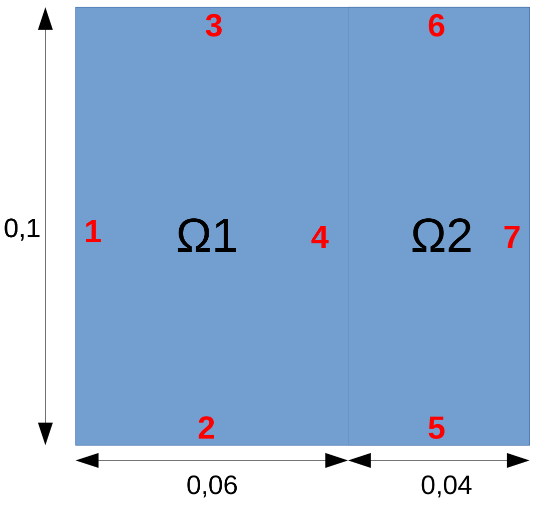
<u>Initial Condition :</u>
Ω1 → T0=300 [K]
Ω2 → T0=300 [K]

<u>Mesh :</u>
Mapped 40 x 40

SIF file : phasechange solid-solid

Julien Givernaud

Comsol :Heat transfert with phase change solid-solid in transient problem
Application to silicon properties



1. Tb=1750 [K] → $T = T_b.$

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7. thermal insulation → $-k\frac{\partial T}{\partial n} = 0.$

Heat transfert equation in solid (u=0)

Comsol used apparent heat capacity [J/(kg.K)]
(-DeltaT width = 20 K (if lower deltaT no convergence))

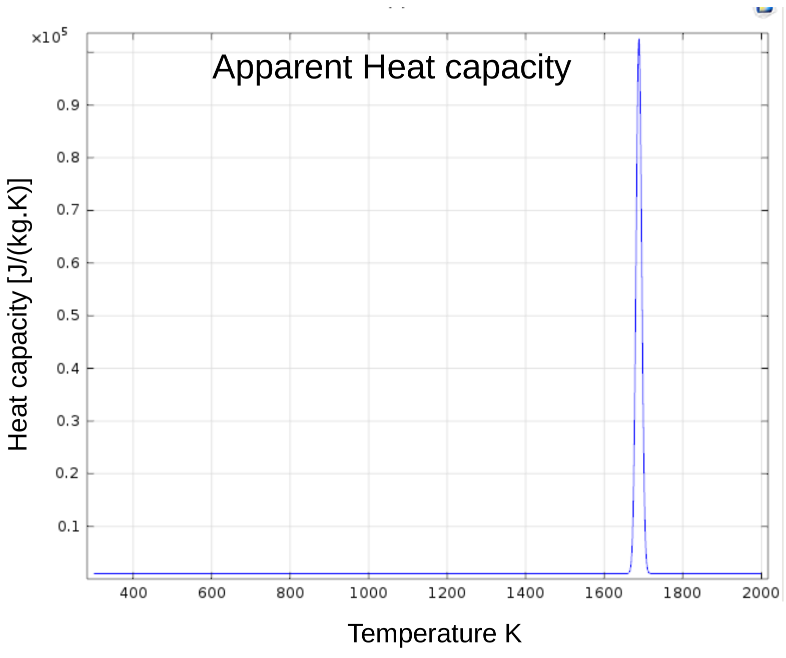
$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \mathbf{u} \cdot \nabla T = \nabla \cdot (k \nabla T) + Q + Q_{vd} + Q_p$$

$$\rho = \theta \rho_{\text{phase1}} + (1 - \theta) \rho_{\text{phase2}}$$

$$C_p = \frac{1}{\rho}\left(\theta \rho_{\text{phase1}} C_{p,\text{phase1}} + (1 - \theta) \rho_{\text{phase2}} C_{p,\text{phase2}}\right) + L \frac{\partial \alpha_m}{\partial T}$$

$$k = \theta k_{\text{phase1}} + (1 - \theta) k_{\text{phase2}}$$

$$\alpha_m = \frac{1}{2} \frac{(1 - \theta)\rho_{\text{phase2}} - \theta \rho_{\text{phase1}}}{\theta \rho_{\text{phase1}} + (1 - \theta)\rho_{\text{phase2}}}$$



Initial Condition :
Ω1 → T0=300 [K]
Ω2 → T0=300 [K]

Mesh :
Mapped 40 x 40

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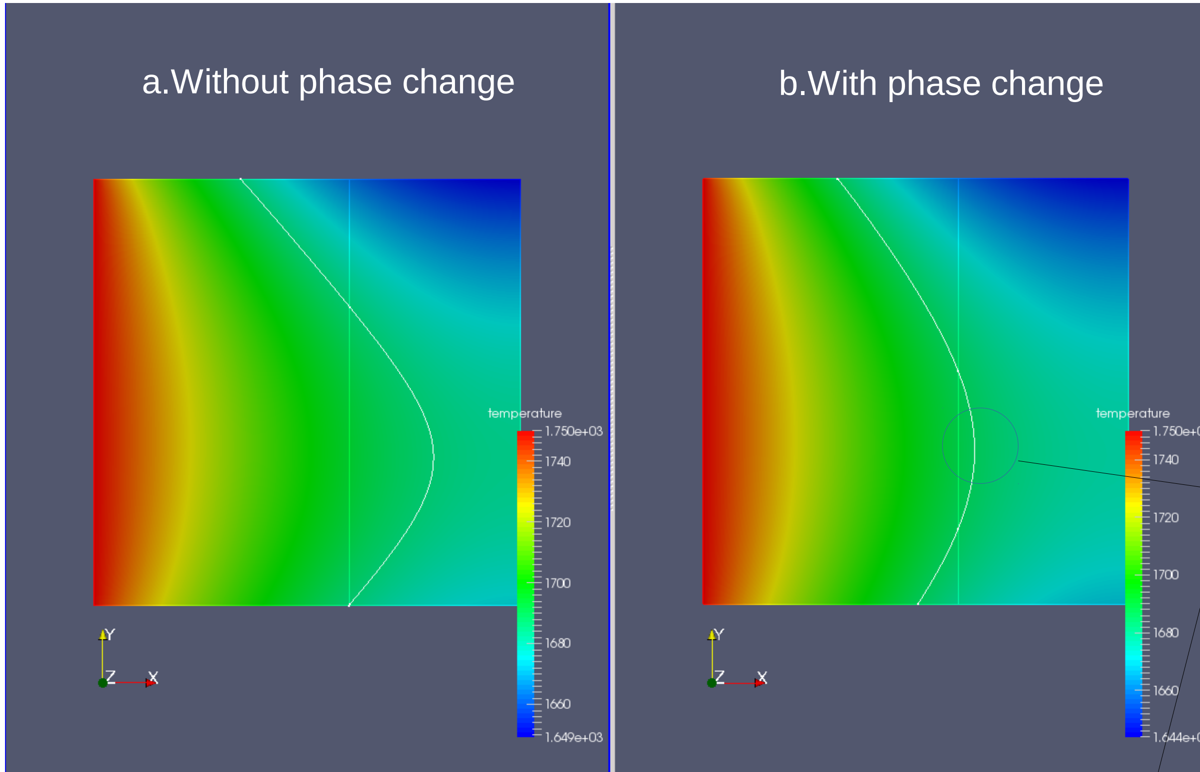
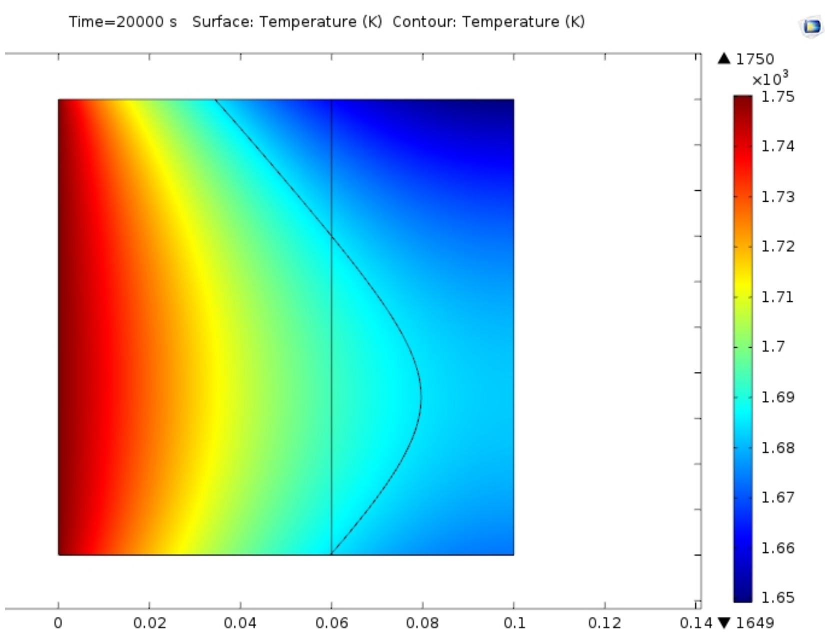
Heat transfert with phase change solid-solid in transient problem
Application to silicon properties - Results

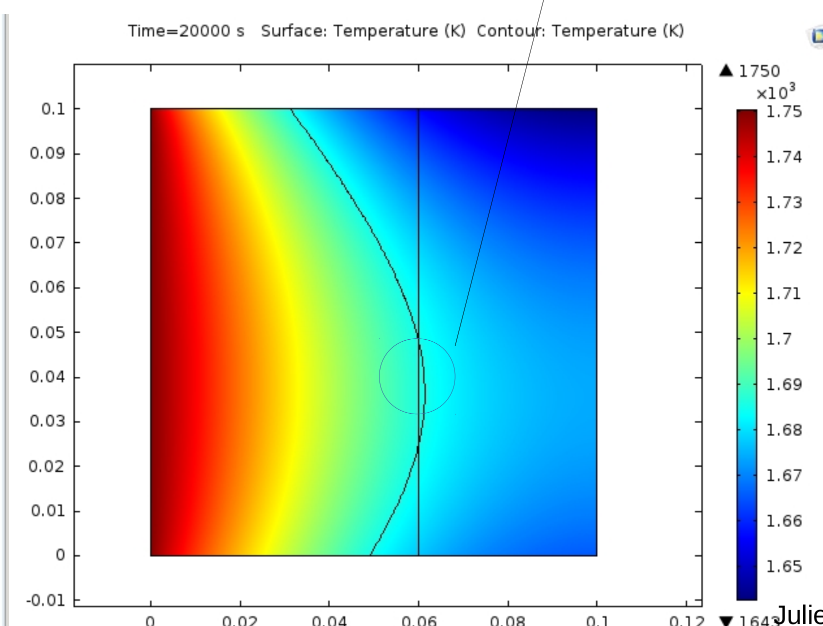
Elmer results at t=20000s



Little difference due to DeltaT Comsol larger than DeltaT Elmer

Comsol results at t=20000s





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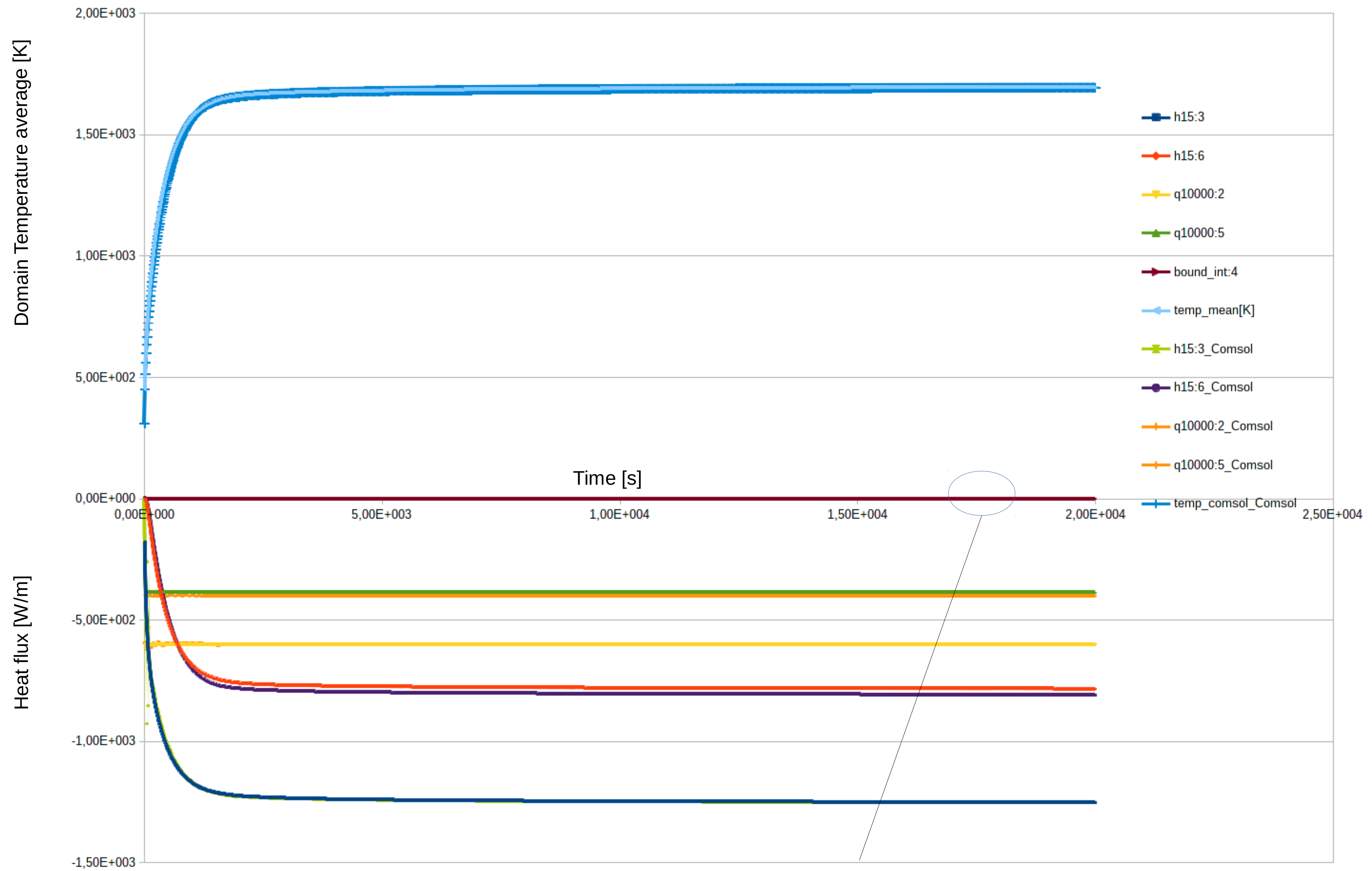
Heat transfert with phase change solid-solid in transient problem
Application to silicon properties - Results

Flux computation (savescalars) (flux comsol=x(-1))



No scalar computation on internal boundary with Elmer found

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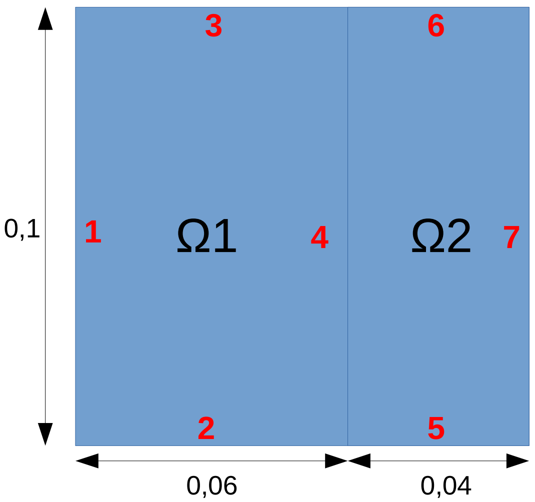
Elmer :Heat transfert with phase change solid-liquid in transient problem
Application to silicon properties



1. Tb=1715 [K]+ no slip → $T = T_b.\quad \mathbf{u} = 0$

2 & 5. q=-10000 [W/m²] + no slip → $-k\dfrac{\partial T}{\partial n} = q.\quad \mathbf{u} = 0$

3 & 6. α=15 [W/(m²K)] Text=300 [K] + no slip → $-k\dfrac{\partial T}{\partial n} = \alpha(T - T_{ext}).\quad \mathbf{u} = 0$

4. internal boundary (automatic) → $-\mathbf{n}_{dst} \cdot (k\nabla T)_{dst} = \mathbf{n}_{src} \cdot (k\nabla T)_{src}$

$T_{dst} = T_{src}$

7. Tb=1655 [K] + no slip → $T = T_b.\quad \mathbf{u} = 0$

Heat transfert equation in fluid + Imcompressible Navier-Stockes equation

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \mathbf{u} \cdot \nabla T = \nabla \cdot (k \nabla T) + Q$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} =$$

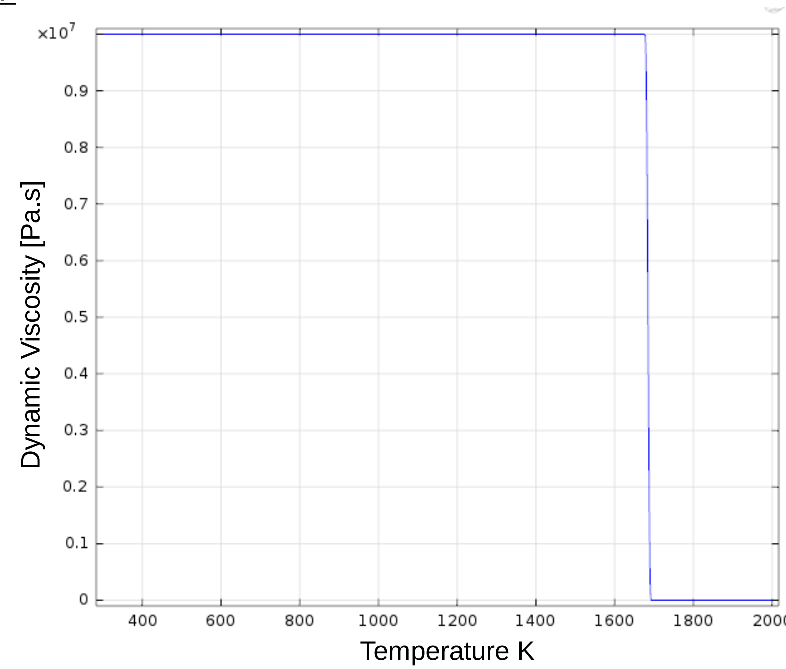
$$\nabla \cdot \left[-p\mathbf{I} + \mu\left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T\right)\right] + \mathbf{F}$$

$$\frac{\partial \rho}{\partial t} + \rho \nabla \cdot (\mathbf{u}) = 0$$

Enthalpy [J/m³] used by Elmer to compute effective heat capacity
(-DeltaT width = 8 K)

$$c_{p,\text{eff}} = \frac{\partial H/\partial t}{\partial T/\partial t}.$$

Change in viscosity to describe transition between solid and liquid
(-DeltaT width = 8 K)



Initial Condition :
Ω1 → T0=1715 [K] ; u=0 v=0 p=0
Ω2 → T0=1655 [K] ; u=0 v=0 p=0

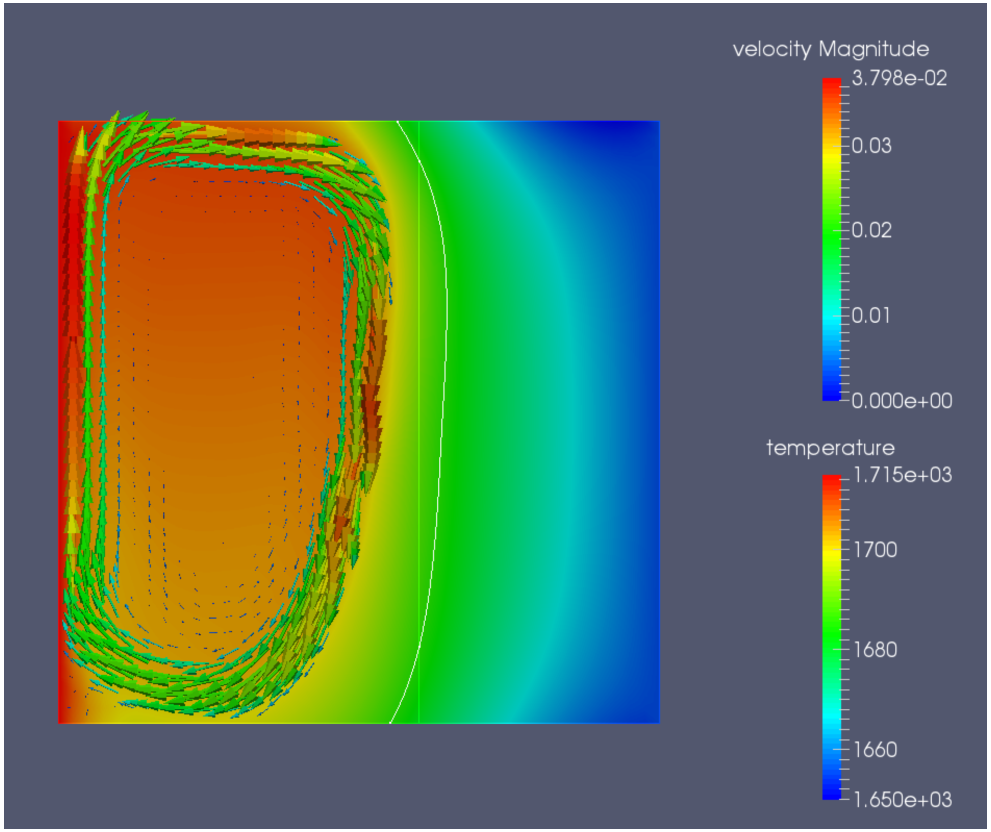
Body Force :
Boussinesq approximation
$F_y = -\rho_0(1 - \alpha(T - T_0)) \times g$

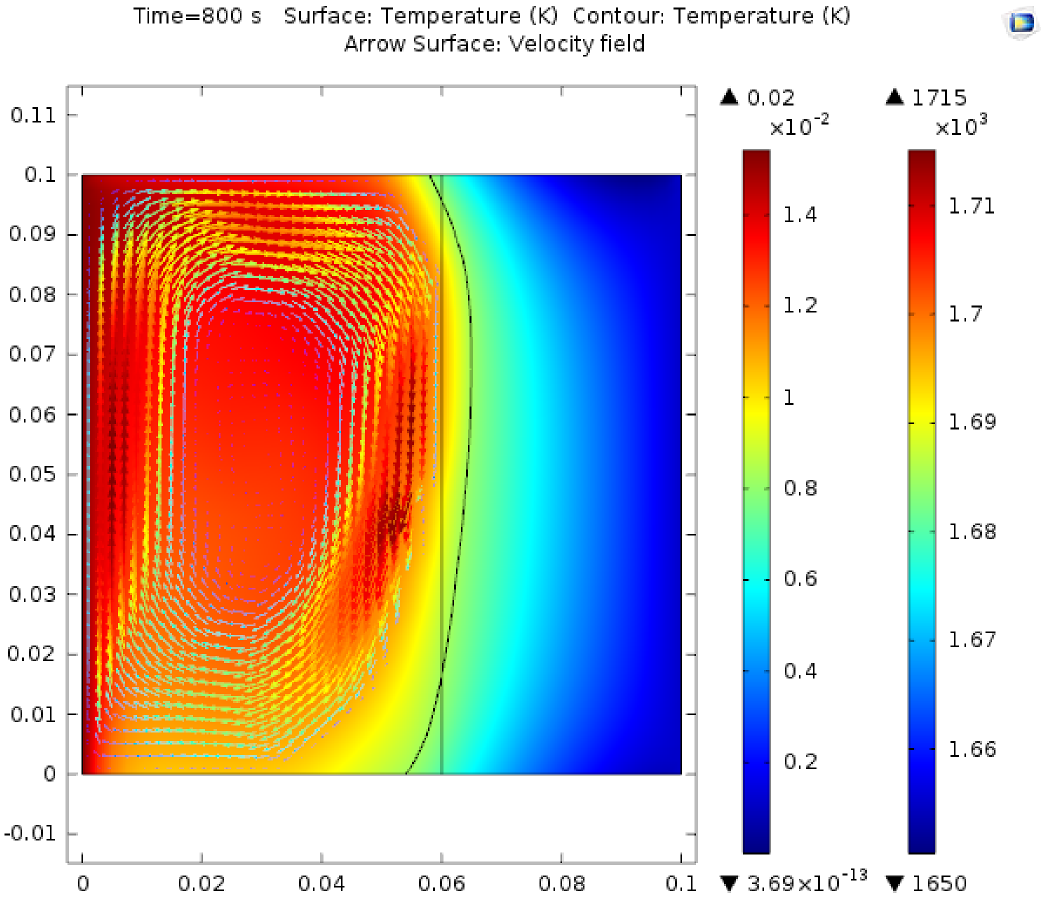
Mesh :
Mapped 40 x 40

SIF file : phasechange solid-liquid

Julien Givernaud

Elmer :Heat transfert with phase change solid-liquid in transient problem
Application to silicon properties : Results





Elmer results at t=800s

Comsol results at t=800s

- Interfaces position are quite similar (deltaT mushy zone different and stabilisation Comsol employed)

- Velocity is higher in Elmer because the use of inconsistent stabilisation term in Heat transfert and Navier Stockes equation in Comsol in increasing diffusion term in order to reduce locally Peclet number.

- Simulation time

Elmer simulation time 260 s

Comsol simulation time > 2000 s

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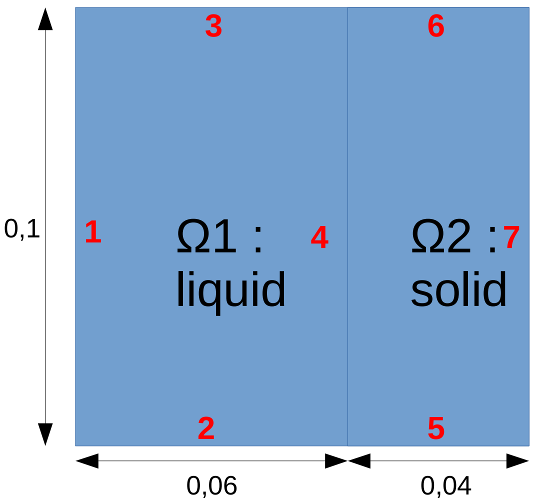
Elmer :Heat transfert with phase change solid-liquid in transient problem (ALE method) Application to silicon properties



1. Tb=1745 [K] ; d1=0 d2=0 ; → $T = T_b.$ $d_i = d_i^b$

2,3,5 & 6. thermal insulation ; d2=0 ; → $-k\dfrac{\partial T}{\partial n} = 0.$ $d_i = d_i^b$

4. Tb=1685 [K] ; d1=disp d2=0 → $T = T_b.$ $d_i = d_i^b$

7. Tb=1550 [K] ; d1=0 d2=0 → $T = T_b.$ $d_i = d_i^b$

1,2,3 & 4. no slip → u=0

<u>Heat transfert equation in fluids + NS</u>

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \mathbf{u} \cdot \nabla T = \nabla \cdot (k \nabla T) + Q$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} =$$

$$\nabla \cdot \left[-p\mathbf{I} + \mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right] + \mathbf{F} \longrightarrow F_y = -\rho_0 (1 - \alpha (T - T_0)) \times g$$

$$\frac{\partial \rho}{\partial t} + \rho \nabla \cdot (\mathbf{u}) = 0$$

<u>Elastic deformation of the mesh equation</u>

$$\tau = 2\mu\varepsilon + \lambda \nabla \cdot \vec{d} I$$

$$\varepsilon = \frac{1}{2}(\nabla \vec{d} + (\nabla \vec{d})^T). \quad \mu = \frac{Y\kappa}{(1-\kappa)(1-2\kappa)}, \quad \lambda = \frac{Y}{2(1+\kappa)}$$

τ : stress tensor
d : displacement
I : unit tensor
ε : linearized strain
μ & λ : first and second Lame parameters
Y & κ : Youngs Modulus & poisson ratio (conditionning the « rigidity » of the interface) → very low influence

<u>Phasechange solver compute the Stephan condition of the interface boundary</u>

$$L\rho \vec{v} \cdot \vec{n} = (\kappa_s \nabla T_s - \kappa_l \nabla T_l) \cdot \vec{n},$$

$$\vec{q} = \kappa_s \nabla T_s - \kappa_l \nabla T_l.$$

<u>If Phasechange occurs in x direction :</u>

$$\rho L n_x (v_x - D_v \nabla^2 v_x) = \vec{q} \vec{n} \qquad D_v << h^2$$

- Dv is an artificial diffusion term to avoid numerical oscillations
- h cell size

<u>Corresponding displacement calculed by phasechange solver</u>

$$disp_x = v_x \, dt$$

<u>Initial Conditions :</u>

Ω1 & 2 → Temperature = Variable Coordinate 1
Real
0.0 1745
0.1 1645
End ;

Ω1
d1 = 0 d2 = 0
u1 = 0 u2 = 0 p=0
disp = 0 (phasechange value)

Ω2
d1 = 0 d2 = 0

<u>Mesh :</u>
Mesh boundary layers

SIF file : phasechangesolver solid-liquid

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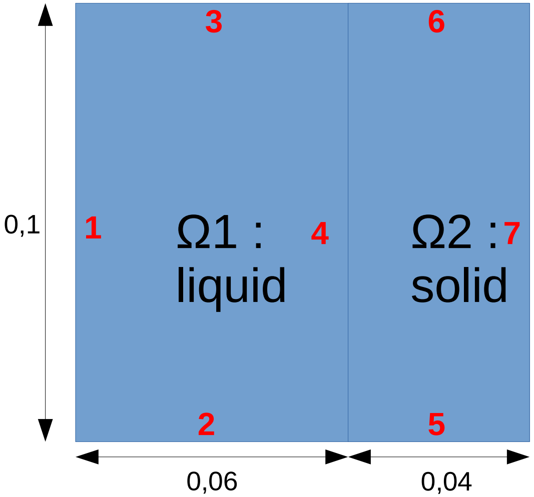
Comsol :Heat transfert with phase change solid-liquid in transient problem (ALE method)
Application to silicon properties



1. Tb=1745 [K] ; d1=0 d2=0 ; → $T = T_b.$ $d_i = d_i^b$

2,3,5 & 6. thermal insulation ; d2=0 ; → $-k\frac{\partial T}{\partial n} = 0.$ $d_i = d_i^b$

4. Tb=1685 [K] ; $v_n = \frac{T_{lm}}{\rho\, Lf}$ d2=0 → $T = T_b.$ $d_i = d_i^b$

7. Tb=1550 [K] ; d1=0 d2=0 → $T = T_b.$ $d_i = d_i^b$

1,2,3 & 4. no slip → u=0

<u>Heat transfert equation in fluids + NS</u>

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \mathbf{u} \cdot \nabla T = \nabla \cdot (k \nabla T) + Q$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} =$$

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$$\frac{\partial \rho}{\partial t} + \rho \nabla \cdot (\mathbf{u}) = 0$$

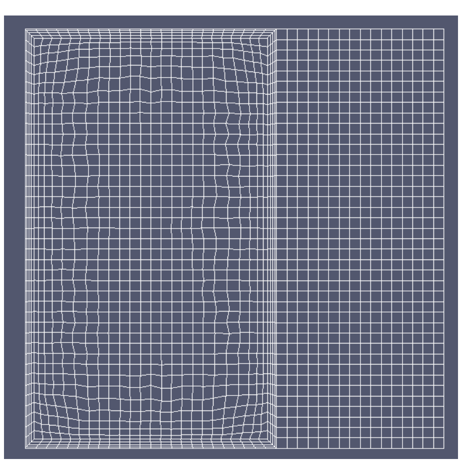
$$L\rho\vec{v} \cdot \vec{n} = (\kappa_s \nabla T_s - \kappa_l \nabla T_l) \cdot \vec{n},$$

$$\vec{q} = \kappa_s \nabla T_s - \kappa_l \nabla T_l.$$

<u>Heat flux difference across interface evaluated with Lagrange multiplier for temperature</u> : T_lm

$$v_n = \frac{T_{lm}}{\rho\, Lf}$$

<u>Deformed geometry used</u>



<u>Initial Conditions :</u>

Ω1 & 2 → Temperature = Variable Coordinate 1

Real
0.0 1745
0.1 1645
End ;

Ω1	Ω2
d1 = 0 d2 = 0	d1 = 0 d2 = 0
u1 = 0 u2 = 0 p=0	
disp = 0 (phasechange value)	

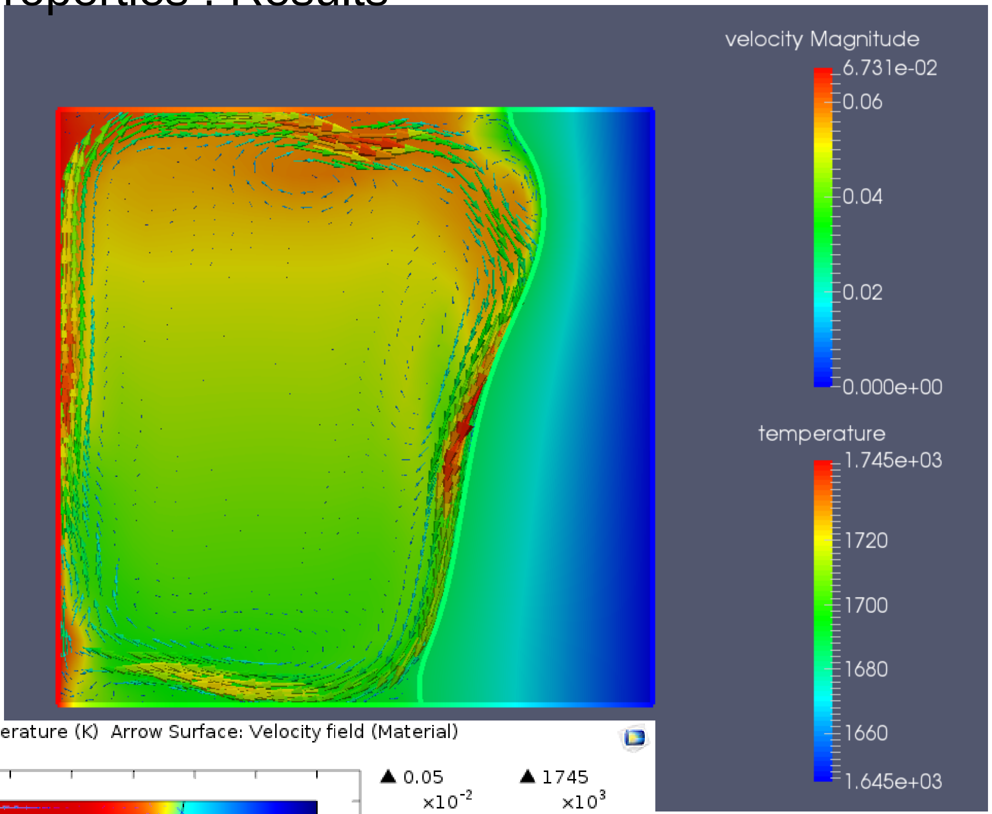
<u>Mesh :</u>
Mesh boundary layers

Julien Givernaud

Elmer :Heat transfert with phase change solid-liquid in transient problem (ALE method)
Application to silicon properties : Results

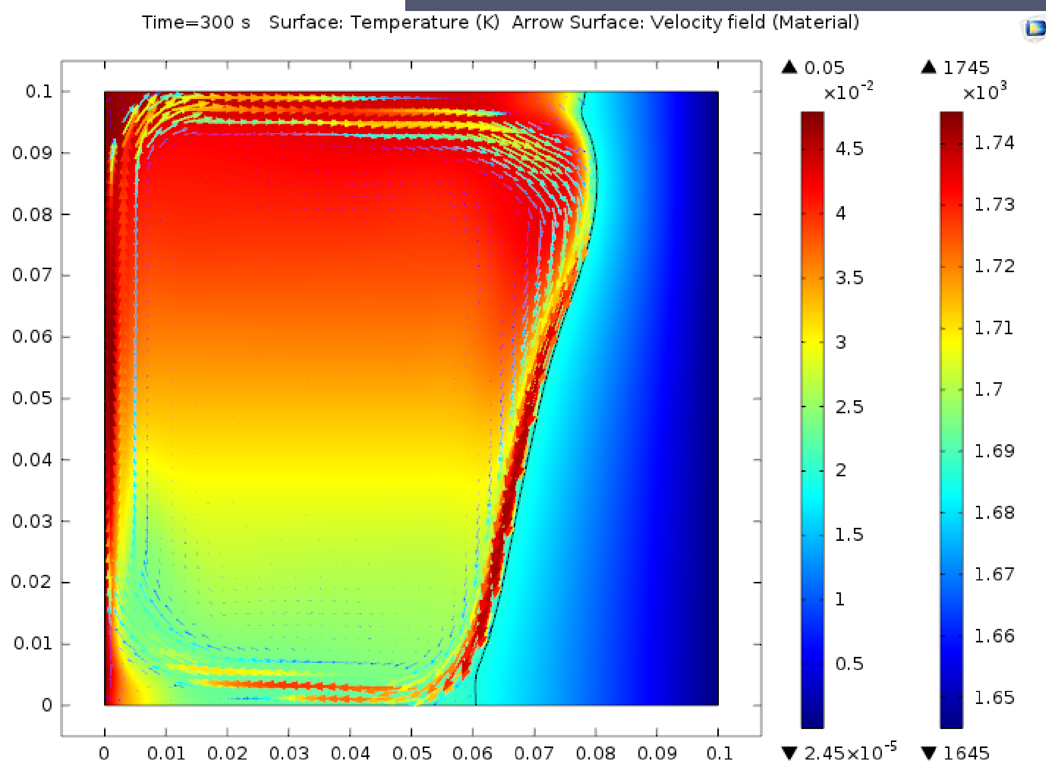
Elmer results at t=300s

Vortex visible
Interface position close to Comsol



Comsol results at t=300s

inconsistent stabilisation term used
Velocity lower than Elmer
Vortex not visible



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