An Enrichment Scheme for Solidification Problems

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Outline

- Mathematical setting of the problem

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- Numerical strategies to solve the problem

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- The proposed 1D solution

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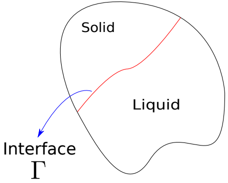
- Two dimensional extension
- Conclusions and observations

Mathematical setting

Equation

$$\rho\dot{\mathcal{H}} = Q + \nabla \cdot (k\nabla T) \qquad (1)$$



Initial Condition and boundary conditions

$$T = T_0$$
$$T = T_d$$
$$-(k\nabla T)\cdot \mathbf{n} = q_w$$
$$-(k\nabla T)\cdot \mathbf{n} = h_f(T - T_f)$$

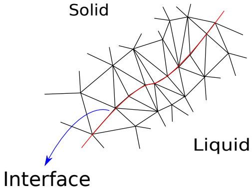
Constraints on the interface

$$T = T_m \qquad (2)$$
$$[-(k\nabla T)\cdot \mathbf{n}]_\Gamma = \rho\mathcal{L}\mathbf{u}_\Gamma \qquad (3)$$

$\mathcal{L}$: Latent Heat
$\mathbf{u}_\Gamma$: Velocity of Γ
f_l: Liquid fraction
(a Heaviside step)
c: Heat Capacity
$\mathcal{H}$: Specific Enthalpy
Q: Heat Source
ρ: density

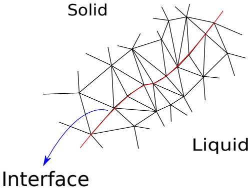
Numerical strategies to solve the problem

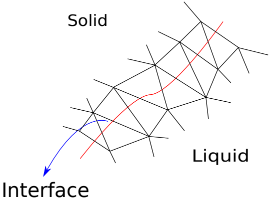
- Moving mesh or front tracking methods



Numerical strategies to solve the problem

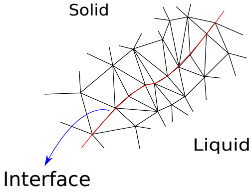
- Moving mesh or front tracking methods
- Fixed mesh methods
  - Enthalpy Methods
  - Capacitance Methods
  - Temperature Based Methods

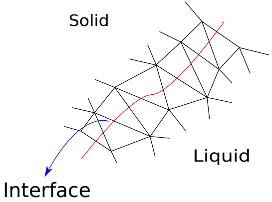




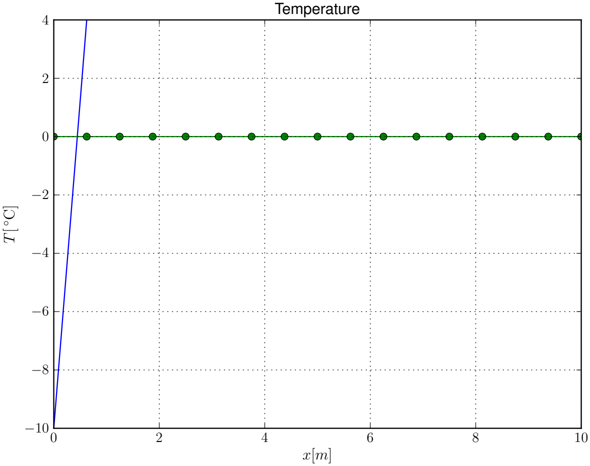
Numerical strategies to solve the problem

- Moving mesh or front tracking methods
- Fixed mesh methods
  - Enthalpy Methods
  - Capacitance Methods
  - Temperature Based Methods
- Our Objective: enrich the space.
  Literature: an auxiliary formulation to evolve the interface is used
  - Chessa, Smolinsky and Belytschko (2002)
  - Ji, Chopp and Dolbow (2002)
  - Merle and Dolbow (2002)
  - Bernauer and Herzog (2011)





Example: fixed mesh method without representing the gradient discontinuity

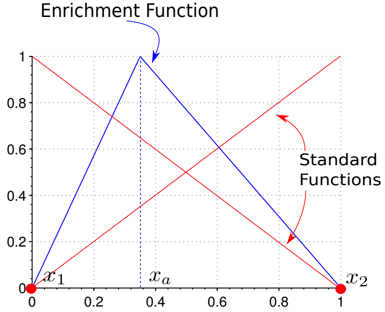


The proposed Enrichment Function

Enrichment DOF (internal)

$$T(x,t) = \sum_i N_i(x) T_i + E(x,t) a$$

Nodal amplitude DOFs



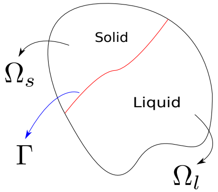
$$\phi = x - x_a$$

$$x_a = x_1 + s(x_2 - x_1) = x_1 + sh$$

$$E(x) = \begin{cases} \dfrac{x - x_1}{x_a - x_1} = \dfrac{\phi_1 - \phi}{\phi_1} & x \leq x_a \\ \dfrac{x_2 - x}{x_2 - x_a} = \dfrac{\phi_2 - \phi}{\phi_2} & x > x_a \end{cases}$$

Variational Formulation

$$\Omega = \Omega_s \cup \Omega_l$$



$$\boxed{\sum_{i\in[s,l]} \int_{\Omega_i} w \left[\rho\dot{\mathcal{H}} - \nabla\cdot(k\nabla T) - Q\right] \, d\Omega_i = 0}$$

$\mathcal{L}$: Latent Heat
f_l: Liquid fraction
(a Heaviside step)
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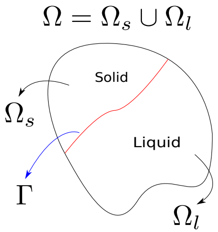
Variational Formulation



$$\sum_{i \in [s,l]} \int_{\Omega_i} w \left[\rho \dot{\mathcal{H}} - \nabla \cdot (k \nabla T) - Q \right] \, d\Omega_i = 0$$

Then, making use of

- $\mathcal{H} = \mathcal{H}^{\text{sen}} + \mathcal{H}^{\text{lat}} = \int_{T_{\text{ref}}}^{T} c(\tau) d\tau + \mathcal{L} f_l(T)$

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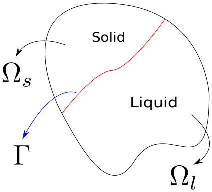

$$\boxed{\sum_{i\in[s,l]} \int_{\Omega_i} w \left[\rho\dot{\mathcal{H}} - \nabla\cdot(k\nabla T) - Q\right] \, d\Omega_i = 0}$$

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- $\mathcal{H} = \mathcal{H}^{\text{sen}} + \mathcal{H}^{\text{lat}} = \int_{T_{\text{ref}}}^{T} c(\tau)d\tau + \mathcal{L}f_l(T)$
- The Reynolds Theorem

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Variational Formulation

Find $T \in \mathcal{S}$ *such that* $\forall w \in \mathcal{V}$

Term coming from $\dot{\mathcal{H}}$

Standard stiffness term

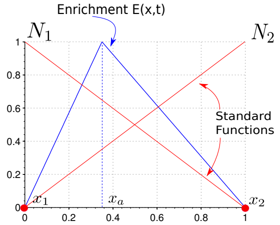
$$\int_\Omega w \left[\boxed{\rho c \frac{\partial T}{\partial t} + \rho \mathcal{L} \frac{\partial f_l}{\partial t}} - Q\right] \, d\Omega + \int_\Omega \nabla w \cdot (k \nabla T) \, d\Omega +$$

$$\int_{\Gamma_c} w h_f (T - T_f) \, d\Gamma_c + \int_{\Gamma_q} w q_w \, d\Gamma_q = 0$$

Robin BC

Neumman BC

Time and Spatial Discretisations: one dimensional case



Taking

$$T^h = \mathbf{N}^T \mathbf{T}$$

where

$$\mathbf{N} = \begin{bmatrix} N_1(x) \\ N_2(x) \\ E(x,t) \end{bmatrix} \quad \text{and} \quad \mathbf{T} = \begin{bmatrix} T_1 \\ T_2 \\ a \end{bmatrix}$$

Time and Spatial Discretisations

We have

$$\boxed{\boldsymbol{\Pi} = \frac{\mathbf{C}\mathbf{T}_{n+1}}{\Delta t} - \frac{\mathbf{C}^*\mathbf{T}_n}{\Delta t} + \frac{\mathbf{L}_{n+1} - \mathbf{L}_n}{\Delta t} + \mathbf{K}\mathbf{T}_{n+1} + \mathbf{F} - \mathbf{Q}}$$

where

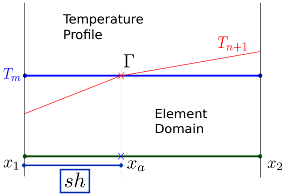
$$\mathbf{C}^* = \int_\Omega \rho c_{n+1} \mathbf{N}_{n+1} \mathbf{N}_n^T \, d\Omega$$

$$\mathbf{L}_{n+1} = \int_\Omega \rho \mathcal{L} \mathbf{N}_{n+1} f_{l(n+1)} \, d\Omega$$

$$\mathbf{L}_n = \int_\Omega \rho \mathcal{L} \mathbf{N}_{n+1} f_{l(n)} \, d\Omega$$

Interface Position Determination

Phase Change Element



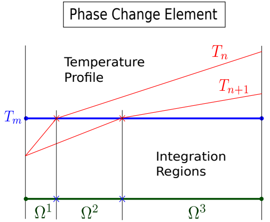
Basically we make use of the constraint

$$\boxed{T|_{\Gamma} = T_m}$$

and using the introduced enrichment function, we have

$$\boxed{s = \frac{T_m - T_1^{(i)} - a^{(i)}}{T_2^{(i)} - T_1^{(i)}}} \qquad (4)$$

Discontinuous Integration

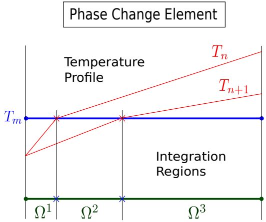


We take as an example the term $\mathbf{C}^*$

$$\mathbf{C}^* = \int_{\Omega} \rho c \mathbf{N}_{n+1} \mathbf{N}_n^T \, d\Omega =$$

$$\sum_{p=1}^{3} \sum_{g=1}^{n_g} \rho c \mathbf{N}_{n+1}(x_g^{(p)}) \mathbf{N}_n^T(x_g^{(p)}) w_g \Omega^{(p)}$$

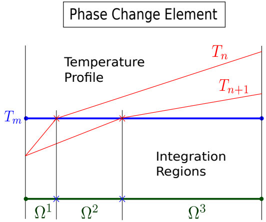
Tangent Matrix



From the previous slide we can detect three sources where $\mathbf{C}^*$ depends on $\mathbf{T}$:

- Evaluation dependency

Tangent Matrix



From the previous slide we can detect three sources where $\mathbf{C}^*$ depends on $\mathbf{T}$:

- Evaluation dependency
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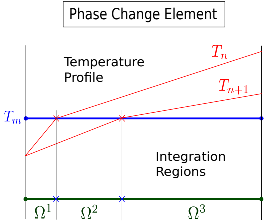
Tangent Matrix



From the previous slide we can detect three sources where $\mathbf{C}^*$ depends on $\mathbf{T}$:

- Evaluation dependency
- Enrichment definition dependency
- Integration region dependency

Tangent Matrix

In the following p represents the number of subdomains and n_g the number of Gaussian points. To take an idea of the needed derivatives, take a glance to $(\frac{\partial \mathbf{C}^*}{\partial \mathbf{T}})$:

$$
\begin{aligned}
\frac{\partial C^*_{rk}}{\partial T_j} = \sum_{p=1}^{3}\sum_{g=1}^{n_g} \rho c \Bigg[& \frac{\partial N_{n+1(r)}}{\partial x_g^{(p)}} \frac{\partial x_g^{(p)}}{\partial s} \frac{\partial s}{\partial T_j} N_{n(k)} w_g \Omega^{(p)} + \\
& N_{n+1(r)} \frac{\partial N_{n(k)}}{\partial x_g^{(p)}} \frac{\partial x_g^{(p)}}{\partial s} \frac{\partial s}{\partial T_j} w_g \Omega^{(p)} + \\
& \frac{\partial N_{n+1(r)}}{\partial x_a} \frac{\partial x_a}{\partial s} \frac{\partial s}{\partial T_j} N_{n(k)} w_g \Omega^{(p)} + \\
& N_{n+1(r)} N_{n(k)} w_g \frac{\partial \Omega^{(p)}}{\partial s} \frac{\partial s}{\partial T_j} \Bigg]
\end{aligned}
$$

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$$\frac{\partial C^*_{rk}}{\partial T_j} = \sum_{p=1}^{3}\sum_{g=1}^{n_g} \rho c \left[\frac{\partial N_{n+1(r)}}{\partial x_g^{(p)}} \frac{\partial x_g^{(p)}}{\partial s} \frac{\partial s}{\partial T_j} N_{n(k)} w_g \Omega^{(p)} + N_{n+1(r)} \frac{\partial N_{n(k)}}{\partial x_g^{(p)}} \frac{\partial x_g^{(p)}}{\partial s} \frac{\partial s}{\partial T_j} w_g \Omega^{(p)} + \frac{\partial N_{n+1(r)}}{\partial x_a} \frac{\partial x_a}{\partial s} \frac{\partial s}{\partial T_j} N_{n(k)} w_g \Omega^{(p)} + N_{n+1(r)} N_{n(k)} w_g \frac{\partial \Omega^{(p)}}{\partial s} \frac{\partial s}{\partial T_j} \right]$$

Tangent Matrix

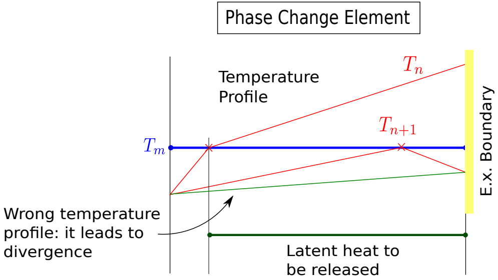
The **core of the idea**: the derivative $\frac{\partial s}{\partial T_j}$

After some computations, we have

$$\boxed{\frac{\partial s}{\partial \mathbf{T}} = -\left(\sum_{i=1}^{2} h \frac{\partial N_i}{\partial x}(x_a)\ T_i \right)^{-1} \begin{bmatrix} N_1(x_a) \\ N_2(x_a) \\ 1 \end{bmatrix}} \tag{5}$$

Algorithmic Implementation

Some special treatment must be considered when one of following situations is detected:



- Once an element is enriched and as the simulation evolves, careful attention must be paid to the elemental latent heat contribution in order to accurately determine the element state.

Algorithmic Implementation

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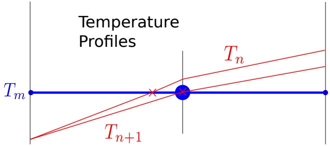

- If the parameter s and the parameter associated to the enrichement a are below or above certain thresholds, the element is not enriched.

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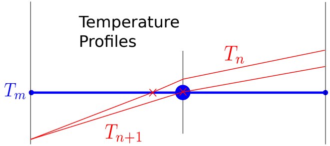


- If the parameter s and the parameter associated to the enrichement a are below or above certain thresholds, the element is not enriched.
- When the parameter s is outside the range $(0, 1)$, the element is considered liquid or solid depending on which state is most likely.

Application: Example I

Example I: we study the frezzing of a long slab of length L with two Dirichlet boundary conditions at its ends. Parameters of the problem:

$$T_m = 0\,^\circ\mathrm{C}$$

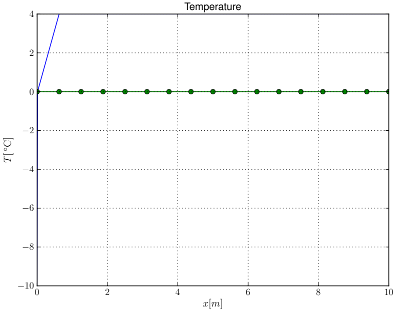
$$\mathcal{L} = 190.26\,\frac{\mathrm{J}}{\mathrm{kg}}$$

$-10\,^\circ\mathrm{C}$ $4\,^\circ\mathrm{C}$

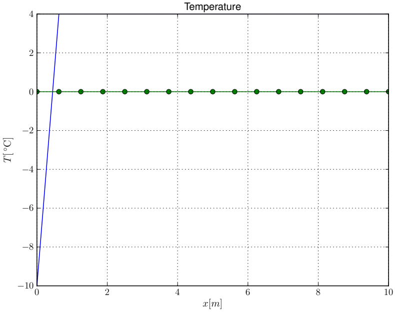
$$T_0 = 4\,^\circ\mathrm{C}$$

Application: Example I

With Enrichment



Without Enrichment



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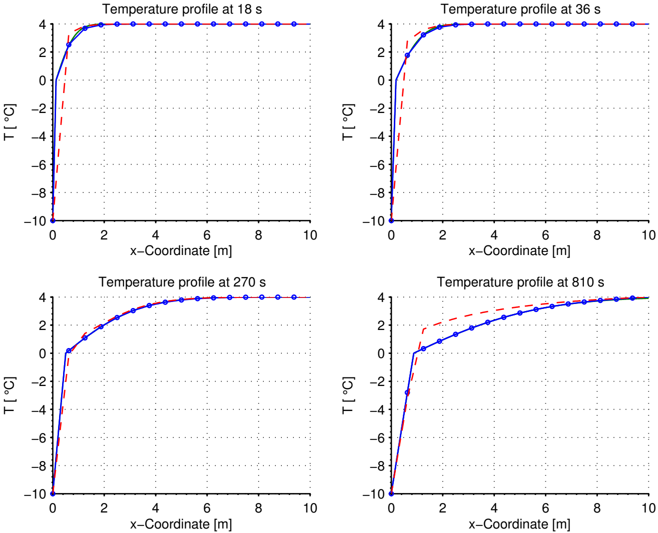

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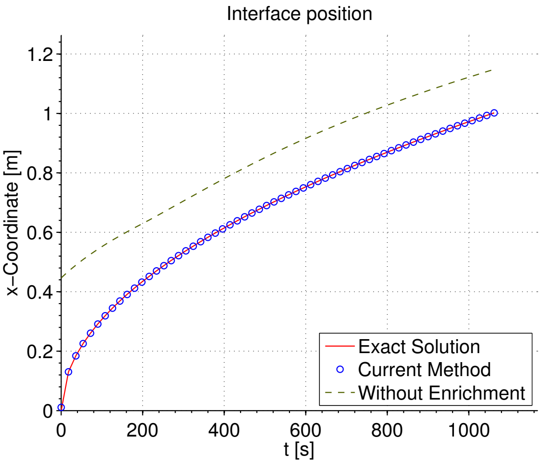

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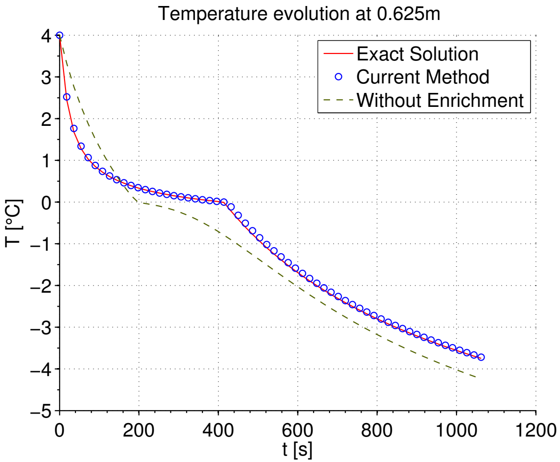

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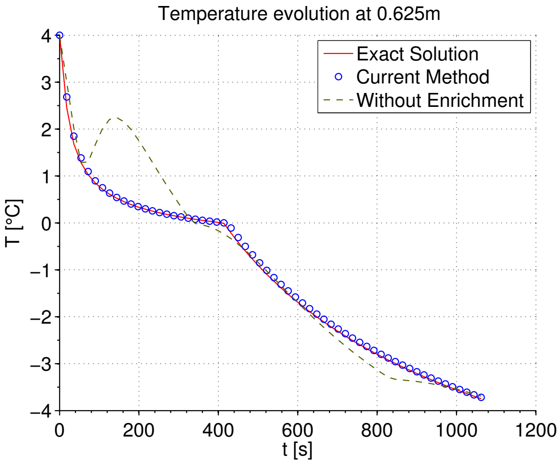


Application: Example II

Example II: we study the melting of a long slab of length L with one Dirichlet condition and one Neumann boundary condition.
Parameters of the problem:

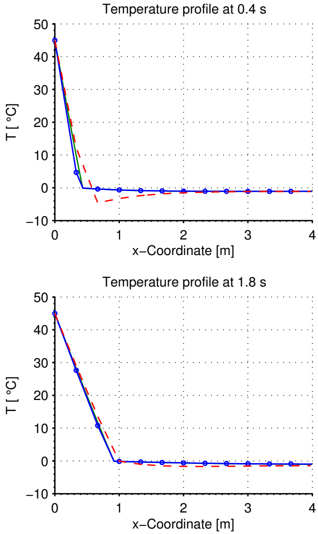
$$T_m = -0.1\,^\circ\mathrm{C}$$

$$\mathcal{L} = 190.26\,\frac{\mathrm{J}}{\mathrm{kg}}$$

$45\,^\circ\mathrm{C}$ $\qquad$ $0\,\frac{W\,K}{^\circ\mathrm{C}\mathrm{m}^2}$

$$T_0 = -1.1\,^\circ\mathrm{C}$$

Application: Example II



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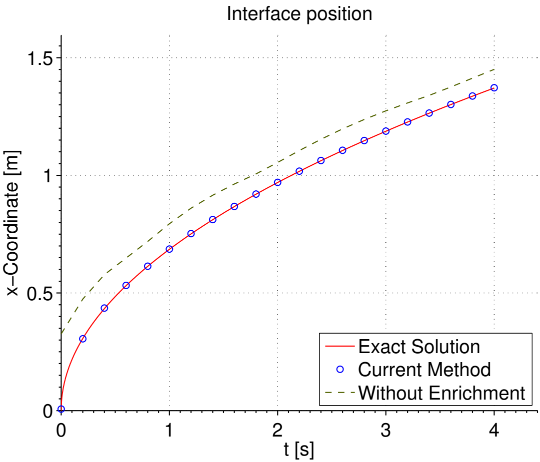
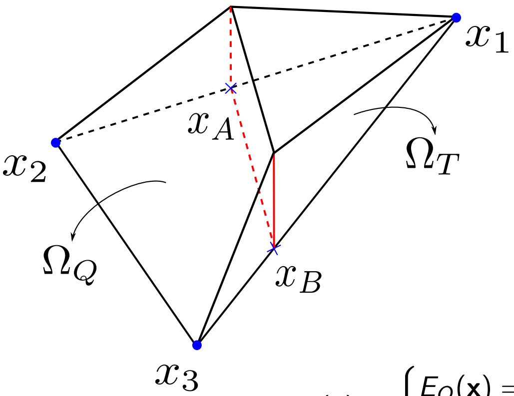
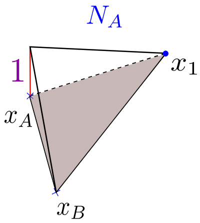
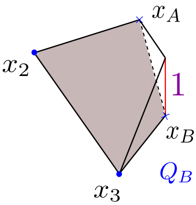


Two Dimensional Extension







$$E(\mathbf{x}) = \begin{cases} E_Q(\mathbf{x}) = Q_A(\mathbf{x}) + Q_B(\mathbf{x}) & \mathbf{x} \in \Omega_Q \\ E_T(\mathbf{x}) = N_A(\mathbf{x}) + N_B(\mathbf{x}) & \mathbf{x} \in \Omega_T \end{cases}$$

Conclusions and observations

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  - Besides, when the temperature profile is close to the melting temperature, we approach to the one phase problem.

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- Accurate solutions were obtained.
- The nonlinearity of the problem increases.
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- Work in progress: two dimensional extension.

Thanks for your attention

Questions?