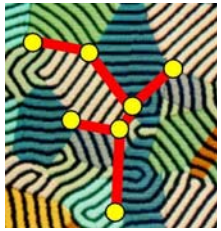


METRO
MEtallurgical TRaining On-line

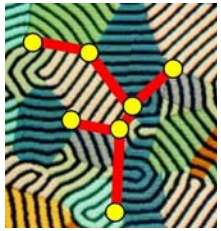
IPPT PAN

Numerical modelling of macroscopic transport phenomena

Control Volume and FE models for solidification controlled by diffusion

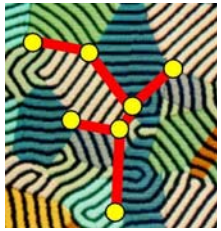
Jerzy Banaszek
WUT

Education and Culture



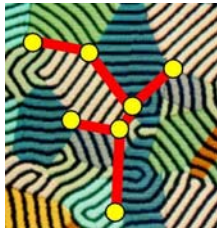
Computer simulation – what is this all about?

- Need for efficient calculation tool to reduce laboratory testing and prototyping in foundry engineering
- Challenge: complex, multi-scale, multi-phase and mutually coupled phenomena
- Fully microscopic calculation impossible due to formidable computer facilities needed
- **Remedy**: macroscopic computer simulation models with included detailed information on developing micro-structures



What is macroscopic computer simulation ?

- Volume- or ensemble-averaging techniques to replace a real medium by the one of smoothly varying effective properties
- Two approaches:
  - **Two-domain** – moving grid, front tracking, suitable for discrete interface
  - **Single-domain** – fixed grid, suitable for multi-component system without sharp interface

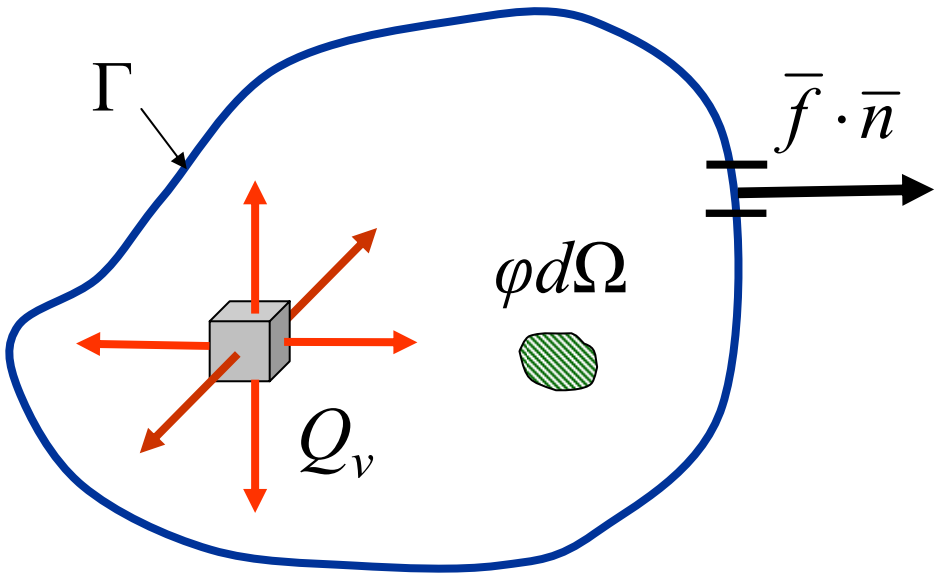


Single-domain approach – reasonable choice

- Single set of mass, momentum, energy and species conservation equations valid in the whole domain
- Fixed grid, no need for front tracking
- Computationally effective – moderate requirements for computer facilities
- Satisfactory representation of columnar and equiaxed solidification when correctly coupled with information of microscopic phenomena

Conservation of scalar quantity

Integral form – basis for CV methods

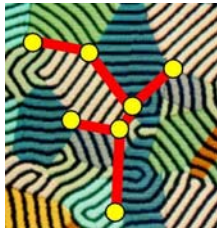


Ω - volume

Γ - boundary surface

$\varphi = \frac{\Phi}{\Omega}$ - density of scalar quantity

$$\frac{\partial}{\partial t}\int_{\Omega} \varphi d\Omega + \oint_{\Gamma} \bar{f}\,\bar{n} d\Gamma = \int_{\Omega} Q_v d\Omega$$



Conservation of scalar quantity

$$\overline{f} = \overline{f}_{conv.} + \overline{f}_{dyf.}$$

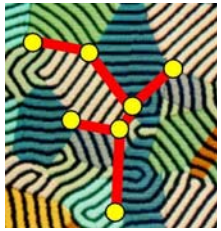
Convective flux

$$\overline{f}_{conv.} = \overline{v}\varphi; \qquad \overline{v} = \left(v_1, v_2, v_3\right)$$ - velocity vector

Diffusive flux – general Fick's law

$$\overline{f}_{dyf.} = -\chi \nabla \varphi; \qquad \chi$$ - diffusivity

$$\frac{\partial}{\partial t}\int_{\Omega} \varphi d\Omega + \oint_{\Gamma} \left(\overline{v}\varphi - \chi \nabla \varphi\right)\overline{n} d\Gamma = \int_{\Omega} Q_v d\Omega$$



Conservation of scalar quantity

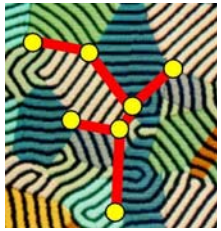
Einstein summation rule

$$\sum_{j=1}^{n} A_j \varphi_j = A_j \varphi_j \qquad \text{for } j = 1, 2, \ldots n$$

$$\sum_{j=1}^{n} A_{ij} \varphi_j = A_{ij} \varphi_j \qquad \text{for } i = \text{const}$$

$$\sum_{j=1}^{3} \frac{\partial v_j}{\partial x_j} = \frac{\partial v_j}{\partial x_j}$$

$$\frac{\partial}{\partial t} \int_{\Omega} \varphi d\Omega + \oint_{\Gamma} \left(v_j \varphi - \chi \frac{\partial \varphi}{\partial x_j} \right) n_j d\Gamma = \int_{\Omega} Q_v d\Omega$$

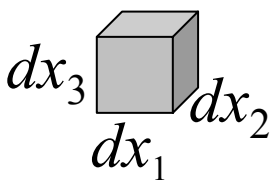


Conservation of scalar quantity

Differential form – basis for FE Method

$$\frac{\partial}{\partial t}\int_{\Omega}\varphi d\Omega+\oint_{\Gamma}\left(v_j\varphi-\chi\frac{\partial\varphi}{\partial x_j}\right)n_j d\Gamma=\int_{\Omega}Q_v d\Omega$$

Infinitesimal control volume

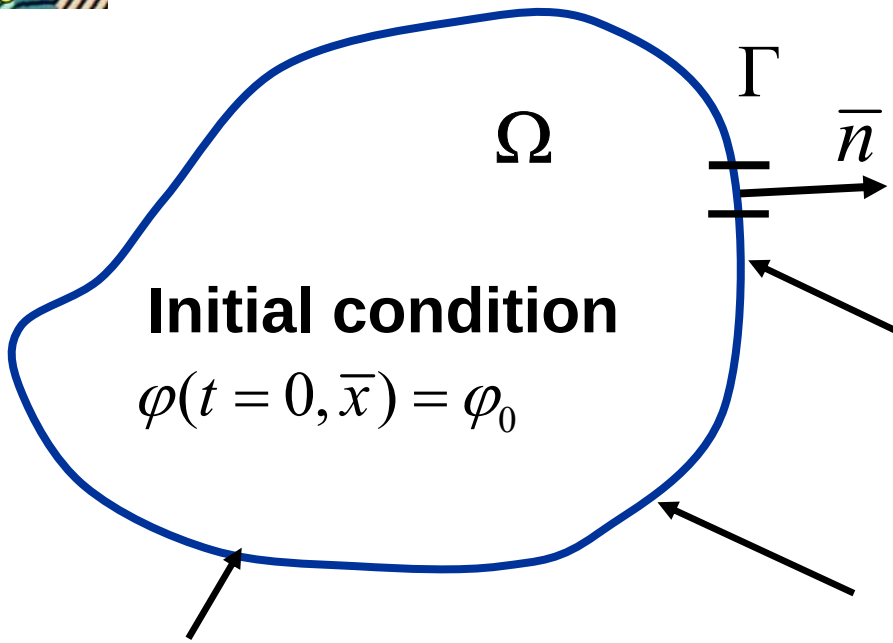


Gauss Divergence Theorem

$$\oint_{\Gamma}\overline{f}\,\overline{n}d\Gamma=\int_{\Omega}\frac{\partial f_j}{\partial x_j}d\Omega$$

$$\frac{\partial\varphi}{\partial t}+\frac{\partial}{\partial x_j}\left(v_j\varphi-\chi\frac{\partial\varphi}{\partial x_j}\right)=Q_v$$

Initial & boundary conditions



Initial condition

$$\varphi(t=0,\bar{x})=\varphi_0$$

Dirichlet condition

$$\varphi=\varphi_b \quad \text{(known)}$$

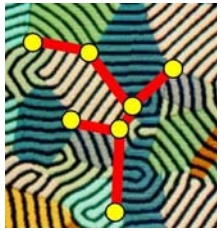
Neumann condition

$$\chi\frac{\partial\varphi}{\partial n}=q_b \quad \text{(flux known)}$$

Mixed (Cauchy) condition

$$\chi\frac{\partial\varphi}{\partial n}=k\left(\varphi_a-\varphi\right)$$

k and φ_a known



Diffusive – type problem

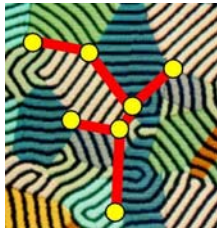
$$v_j = 0$$

Integral form – basis for CV Method

$$\frac{\partial}{\partial t}\int_{\Omega}\varphi d\Omega - \oint_{\Gamma}\chi\frac{\partial\varphi}{\partial x_j}n_j d\Gamma = \int_{\Omega}Q_v d\Omega$$

Differential form – basis for FE Method

$$\frac{\partial\varphi}{\partial t} - \frac{\partial}{\partial x_j}\left(\chi\frac{\partial\varphi}{\partial x_j}\right) = Q_v$$



Commonly used spatial discretization methods

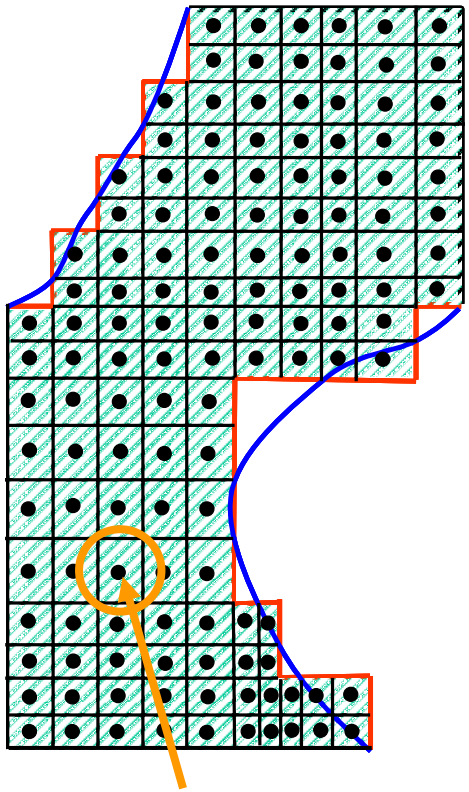
- Control Volume Finite Difference Method (CVFDM) based on the integral conservation equation

$$\frac{\partial}{\partial t}\int_{\Omega}\varphi d\Omega - \oint_{\Gamma}\chi\frac{\partial\varphi}{\partial x_j}n_j d\Gamma = \int_{\Omega}Q_v d\Omega$$

- Finite Element Method (FEM) based on the differential conservation equation

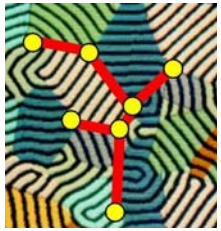
$$\frac{\partial\varphi}{\partial t} - \frac{\partial}{\partial x_j}\left(\chi\frac{\partial\varphi}{\partial x_j}\right) = Q_v$$

Idea of Control Volume discretization procedure



control volume and its node

- Divison of the domain of interest into non-overlapping sub-domains – control volumes
- Node located in the centre of a control-volume to represent averaged properties associated with these balance sub-domain
- Integral balance of a scalar quantity within a control volume

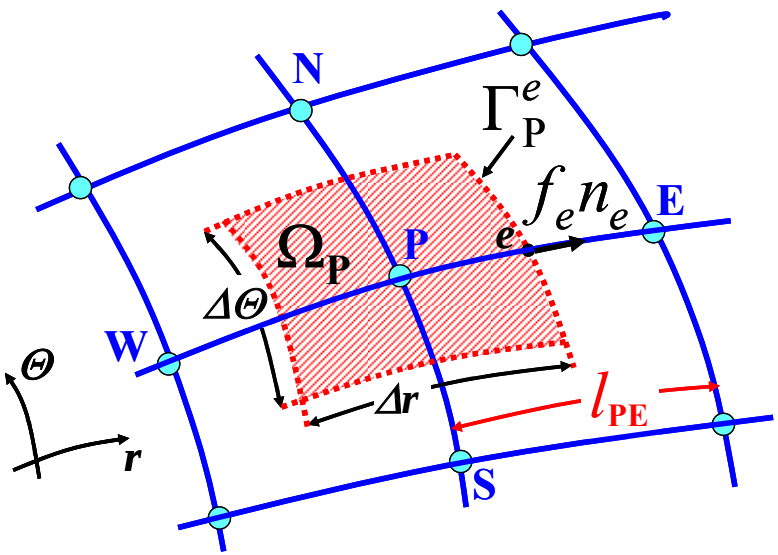


Appealing features of Control Volume approach

- Assures the interpretation of the final model equations fulfillment of conservation law for the scalar quantity within each control volume and in the whole analysed domain - **local and global conservation property** of a discretization model;
- Simple, clear and convincing for those not deeply involved in mathematics;
- Permits direct physical interpretation of final model equations

Control Volume method – basic assumptions

1. Spatial derivatives replaced by respective difference quotients



Example:

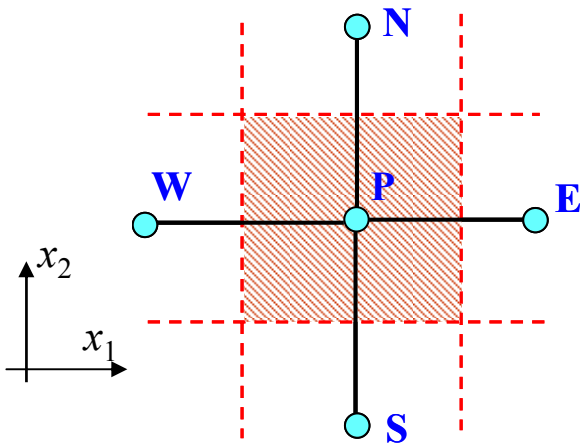
diffusive flux on eastern, ‘e’ , boundary of CV

$$f_e n_e = -\chi_e \frac{\partial \varphi}{\partial x_j} n_j \cong -\chi_e \frac{\varphi_E - \varphi_P}{l_{PE}} n_e$$

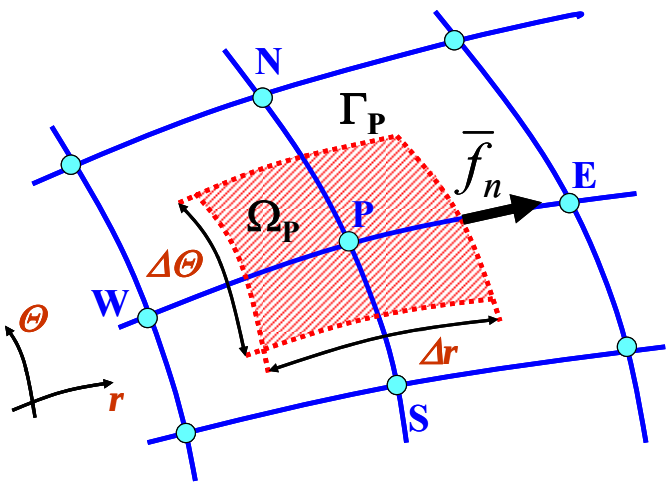
with $n_e = 1$

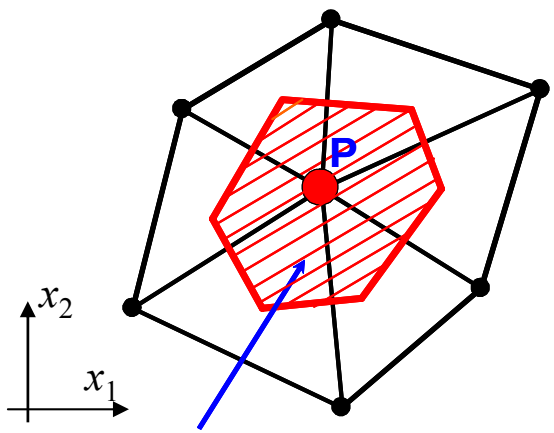
CVFDM – Control Volume Finite Difference Method

Control Volume method – basic assumptions



2. Control-Volume (CV) boundary segments orthogonal to grid lines

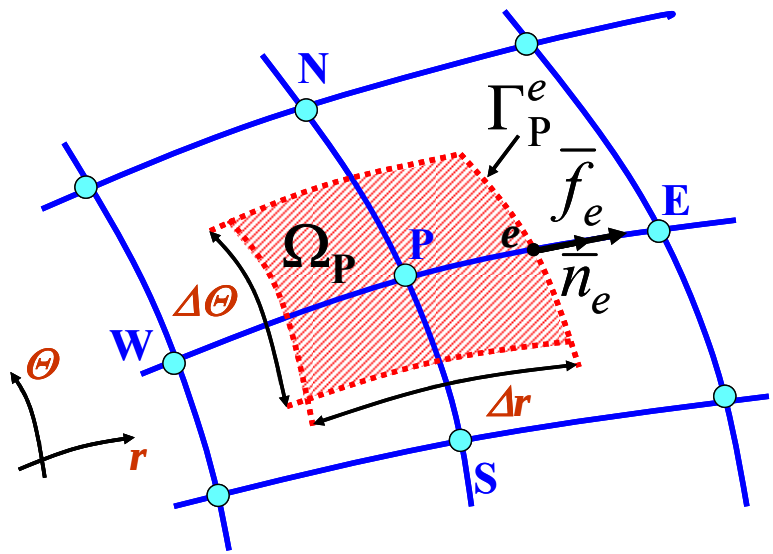




Control volume of node P

Control Volume method – basic assumptions

3. Averaged properties within a CV volume and on its boundary segment



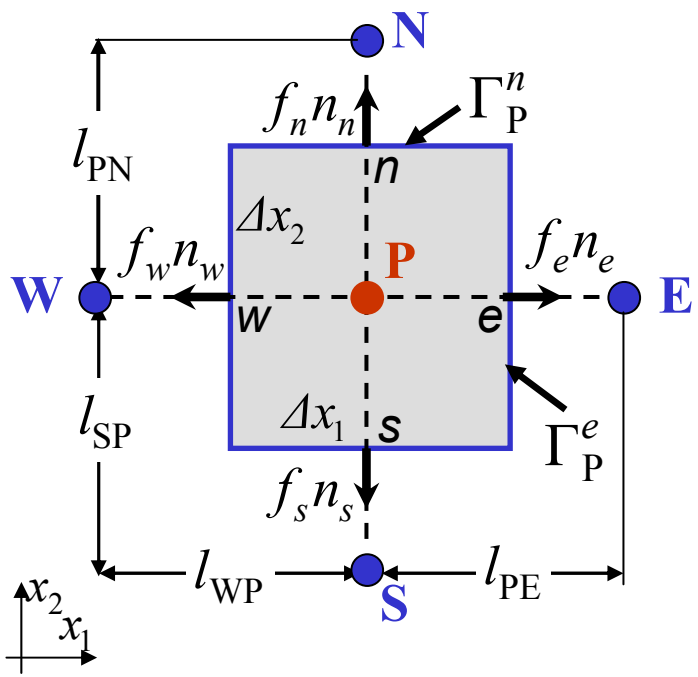
$$\frac{\partial}{\partial t}\int_{\Omega_P}\varphi d\Omega \cong \Omega_P \frac{d\varphi_P}{dt}$$

$$\int_{\Omega_P} Q_v d\Omega \cong \left(Q_v\right)_P \Omega_P$$

$$\int_{\Gamma_P^e} f_j n_j d\Gamma \cong f_e n_e \Gamma_P^e$$

CVFDM – balance in an internal control volume

Balance of scalar φ in 2D Control Volume



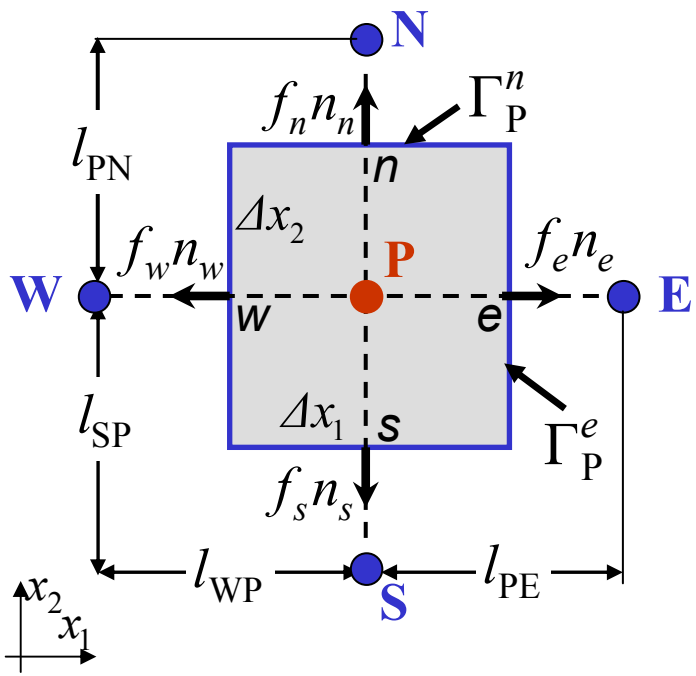
$$\Omega_P \frac{d\varphi_P}{dt} + \sum_{i=e,n,w,s} f_i n_i \Gamma_P^i = (Q_v)_P \Omega_P$$

where

$$\begin{cases} \Omega_P = \Delta x_1 \Delta x_2 \cdot (1) \\ \Gamma_P^i = \Delta x_i \cdot (1) \\ n_i = \pm 1 \end{cases}$$

CVFDM – balance in an internal control volume

Balance of scalar φ in 2D Control Volume



$$\Delta x_1 \Delta x_2 \frac{d\varphi_P}{dt} - \chi_e \frac{\varphi_E - \varphi_P}{l_{PE}} \Delta x_2 (1) +$$

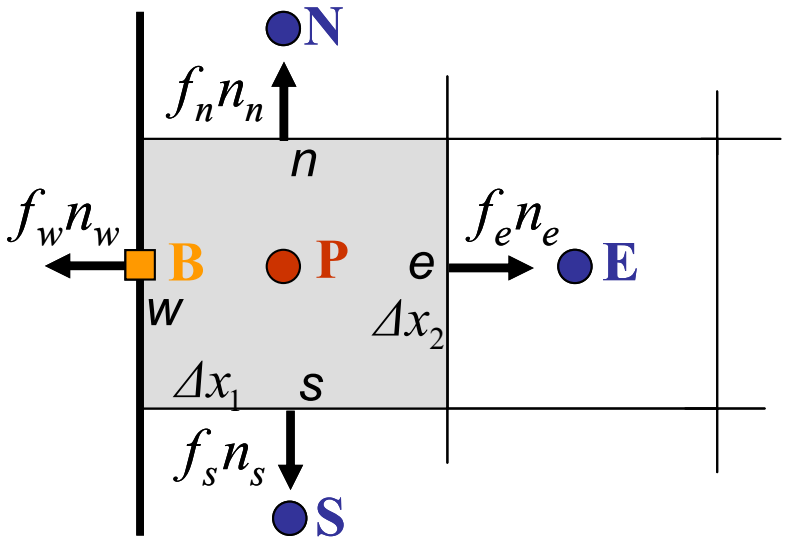
$$\chi_w \frac{\varphi_P - \varphi_W}{l_{WP}} \Delta x_2 (-1) + \chi_n \frac{\varphi_N - \varphi_P}{l_{PN}} \Delta x_1 (1)$$

$$+ \chi_n \frac{\varphi_P - \varphi_S}{l_{SP}} \Delta x_1 (-1) = \Delta x_1 \Delta x_2 \left(Q_v\right)_P$$

CVFDM – balance in a boundary control volume

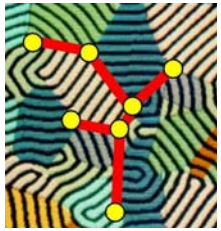
Example: Control volume adjacent to west boundary surface

$$\Delta x_1 \Delta x_2 \frac{d\varphi_{\mathrm{P}}}{dt} + \sum_{i=e,n,s} f_i n_i \Delta x_i + f_w n_w \Delta x_2 = \Delta x_1 \Delta x_2 \left(Q_v\right)_{\mathrm{P}}$$



where

$$f_w n_w = \chi_w \frac{\varphi_{\mathrm{P}} - \varphi_{\mathrm{B}}}{\Delta x_1 / 2}(-1) = k\left(\varphi_a - \varphi_{\mathrm{B}}\right) + q_b$$



CVFDM – boundary conditions

All boundary conditions modelled as general mixed ones:

$$f_w n_w = \chi_w \frac{\varphi_\mathrm{P} - \varphi_\mathrm{B}}{\Delta x_1 / 2}(-1) = k\left(\varphi_a - \varphi_\mathrm{B}\right) + q_b$$

1. Dirichlet boundary condition

   $k =$ huge value; $q_b = 0 \quad \Rightarrow \quad \varphi_\mathrm{B} = \varphi_a$

2. Neumann boundary condition

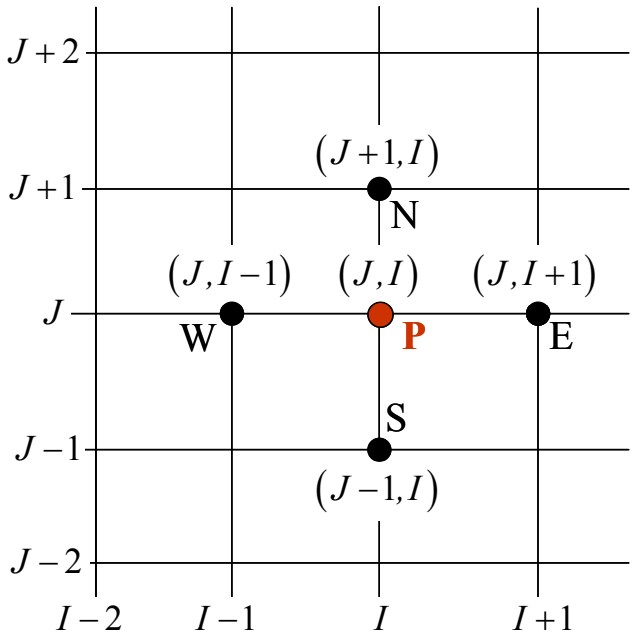
   $k = 0;\ q_b = 0$ (adiabatic) or $q_b \neq 0$

3. Cauchy boundary condition

   $k > 0;\ q_v = 0;\ \varphi_b$ - given

CVFDM – double index notation

Index notation of grid nodes



Balance of scalar φ

$$\Delta x_1 \Delta x_2 \frac{d\varphi_{J,I}}{dt} - \chi_e \frac{\varphi_{J,I+1} - \varphi_{J,I}}{l_{\mathrm{PE}}} \Delta x_2 (1) +$$

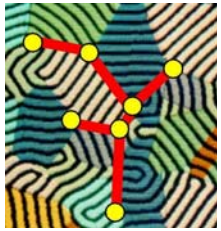
$$\chi_w \frac{\varphi_{J,I} - \varphi_{J,I-1}}{l_{\mathrm{WP}}} \Delta x_2 (-1) + \chi_n \frac{\varphi_{J+1,I} - \varphi_{J,I}}{l_{\mathrm{PN}}} \Delta x_1 (1)$$

$$+ \chi_n \frac{\varphi_{J,I} - \varphi_{J-1,I}}{l_{\mathrm{SP}}} \Delta x_1 (-1) = \Delta x_1 \Delta x_2 \left(Q_v \right)_{\mathrm{P}}$$

OR after simple rearrangements

$$C_{J,I} \frac{d\varphi_{J,I}}{dt} + K_{J-1,I}\varphi_{J-1,I} + K_{J,I-1}\varphi_{J,I-1} +$$

$$K_{J,I}\varphi_{J,I} + K_{J,I+1}\varphi_{J,I+1} + K_{J+1,I}\varphi_{J+1,I} = R_{J,I}$$



CVFDM – matrix notation

$$[\mathbf{C}]\left\{\frac{d\varphi(t)}{dt}\right\}+[\mathbf{K}]\{\varphi(t)\}=\{\mathbf{R}\}$$

where: $C_{J,I}=\Delta x_1\Delta x_2$ terms of the **Capacity Matrix**

$$K_{J-1,I}=-\chi_s\frac{\Delta x_1}{l_{\mathrm{SP}}};\ K_{J,I-1}=-\chi_w\frac{\Delta x_2}{l_{\mathrm{WP}}}$$

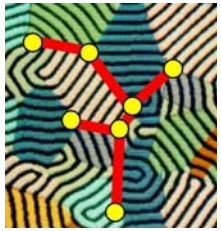
$$K_{J,I+1}=-\chi_e\frac{\Delta x_2}{l_{\mathrm{PE}}};\ K_{J+1,I}=-\chi_n\frac{\Delta x_1}{l_{\mathrm{PN}}}$$

$$K_{J,I}=-\left(K_{J-1,I}+K_{J,I-1}+K_{J,I+1}+K_{J+1,I}\right)$$

} terms of the **Diffusive Matrix**

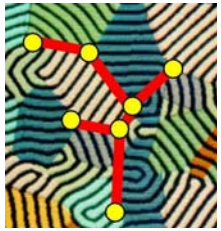
$R_{J,I}=\Delta x_1\Delta x_2\left(Q_v\right)_{\mathrm{P}}$ **RHS** vector component

and $\{...\}$ - vector of nodal values



Finite Element Method (FEM) – a powerful engineering tool

- Basic idea - a solution region modelled by replacing it with an assemblage of discrete elements
- These elements can be put together in a variety of ways - exceedingly complex shapes of a domain can be quite precisely represented
- Within each element its geometry and a field quantity sought interpolated using simple functions (polynomials)
- Ability to formulate solutions for each individual elements before putting them together to represent the entire problem



Weighted Residual Method (WRM) – a basis for FEM

Starting point:

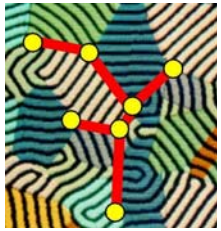
- Differential operator of diffusive transport

$$\mathbf{A}\left(\varphi_{ex.}\right)=\frac{\partial\varphi_{ex.}}{\partial t}-\frac{\partial}{\partial x_j}\left(\chi\frac{\partial\varphi_{ex.}}{\partial x_j}\right)-Q_v=0$$

- Operator of boundary conditions

$$\mathbf{B}\left(\varphi_{ex.}\right)=\chi\frac{\partial\varphi_{ex.}}{\partial n}-k\left(\varphi_a-\varphi_{ex.}\right)-q_b=0$$

where $\varphi_{ex.}$ - exact solution for scalar field quantity



Weighted Residual Method (WRM) – a basis for FEM

Residuals:

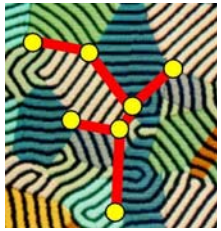
- Assumed spatial approximation of $\varphi_{ex.}$

$$\varphi_{ex.}\left(x_1, x_2, x_3, t\right) \approx \varphi\left(x_1, x_2, x_3, t\right)$$

- Residuals of **A** and **B** operators

$$\mathbf{REZ_A} = \mathbf{A}\left(\varphi\right) = \frac{\partial \varphi}{\partial t} - \frac{\partial}{\partial x_j}\left(\chi \frac{\partial \varphi}{\partial x_j}\right) - Q_v \neq 0$$

$$\mathbf{REZ_B} = \mathbf{B}\left(\varphi\right) = \chi \frac{\partial \varphi}{\partial n} - k\left(\varphi_a - \varphi\right) - q_b \neq 0$$



Weighted Residual Method – integral formulation

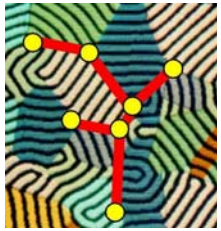
Weighting of residuals through spatial distribution

$$\int_{\Omega} W_k \mathbf{REZ_A}\, d\Omega + \int_{\Gamma} W_k \mathbf{REZ_B}\, d\Gamma = 0$$

where $W_k(x_1,x_2,x_3)$ - assumed weighting function, $k = 1,2,\ldots N$

$$\int_{\Omega} W_k \left(\frac{\partial \varphi}{\partial t} - \frac{\partial}{\partial x_j}\left(\chi \frac{\partial \varphi}{\partial x_j} \right) - Q_v \right) d\Omega +$$

$$\int_{\Gamma} W_k \left(\chi \frac{\partial \varphi}{\partial n} - k\left(\varphi_a - \varphi\right) - q_b \right) d\Gamma = 0$$



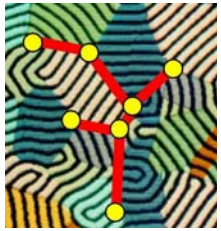
Weighted Residual Method – weak formulation

- Green's Identity

$$\int_{\Omega} W_k \frac{\partial}{\partial x_j}\left(\chi \frac{\partial \varphi}{\partial x_j}\right) d\Omega = \int_{\Omega} \frac{\partial}{\partial x_j}\left(W_k \chi \frac{\partial \varphi}{\partial x_j}\right) d\Omega - \int_{\Omega} \frac{\partial W_k}{\partial x_j} \chi \frac{\partial \varphi}{\partial x_j} d\Omega$$

- Gauss Divergence Theorem

$$\int_{\Omega} \frac{\partial}{\partial x_j}\left(W_k \chi \frac{\partial \varphi}{\partial x_j}\right) d\Omega = \oint_{\Gamma} W_k \chi \frac{\partial \varphi}{\partial x_j} n_j \, d\Gamma$$



Weighted Residual Method – weak formulation

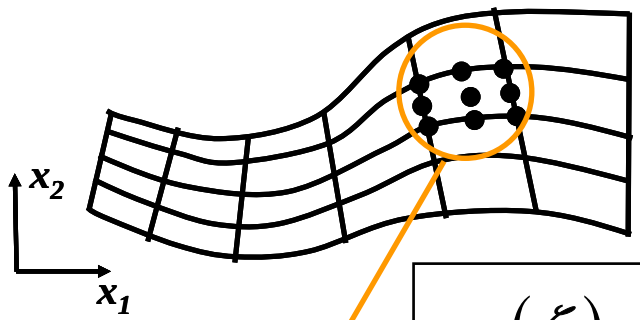
‘Weak’ form of WRM formulation

$$\int_{\Omega} W_k \frac{\partial \varphi}{\partial t} d\Omega + \int_{\Omega} \frac{\partial W_k}{\partial x_j} \chi \frac{\partial \varphi}{\partial x_j} d\Omega = \int_{\Gamma} W_k \left(k\left(\varphi_a - \varphi\right) + q_b \right) d\Gamma + \int_{\Omega} W_k Q_v \, d\Omega$$

$$\text{for } \; k = 1, 2, \ldots, N$$

Finite Element Method – piece-wise spatial interpolation

Finite element approximation of domain geometry

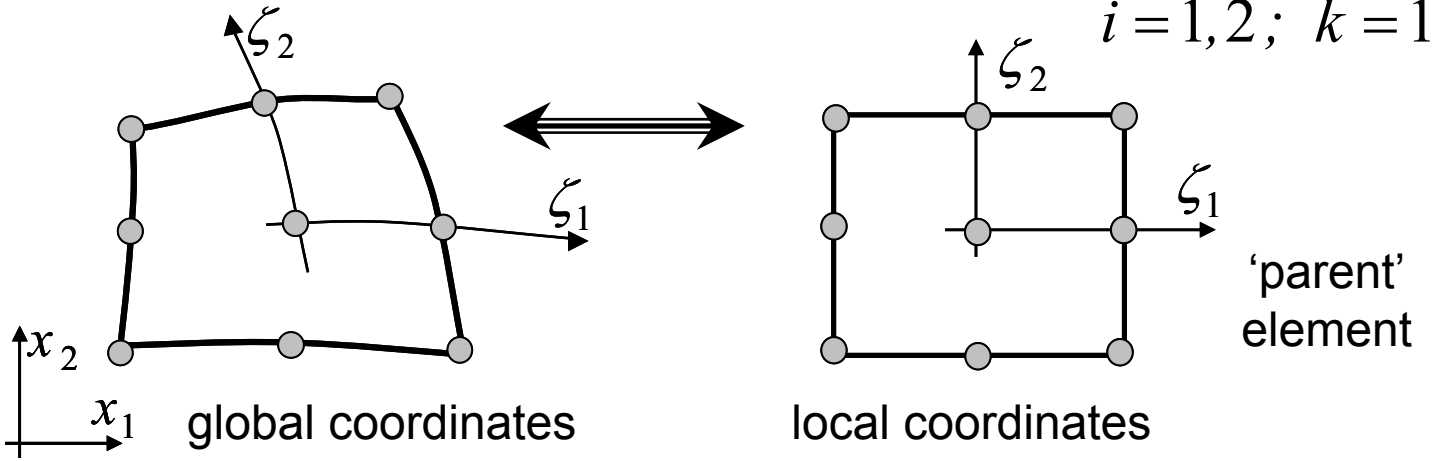


$$\Omega = \sum_{e=1}^{NE} \Omega_e$$

$$x_i(\zeta) = N_k(\zeta)(x_i)_k$$

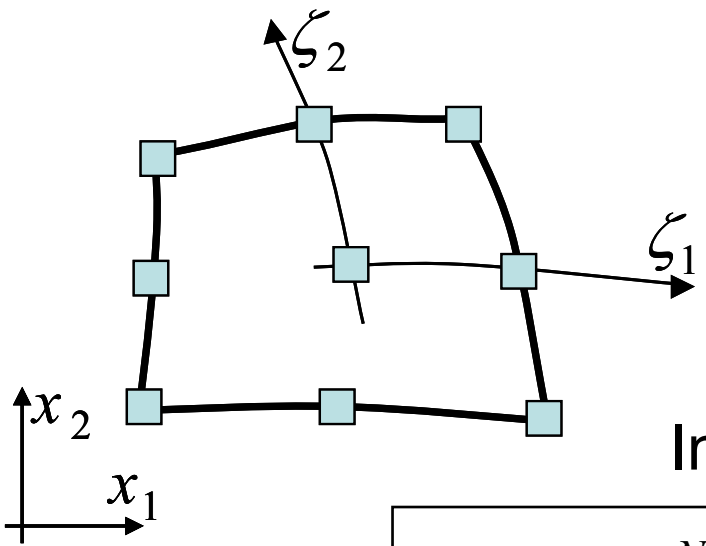
where: $\zeta = (\zeta_1, \zeta_2)$

$i = 1,2;\ k = 1,2,\ldots N_g$



Finite Element Method – piece-wise spatial interpolation

Finite element interpolation of scalar quantity



Interpolation within *e* element

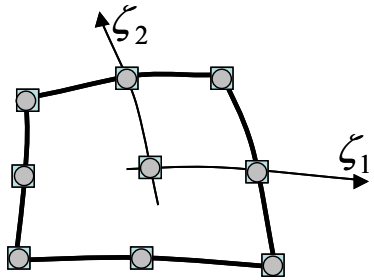
$$\varphi^{(e)}(\mathbf{x},t) = M_k^{(e)}\left(\zeta\left(\mathbf{x}\right)\right)\varphi_k(t)$$

Interpolation over a whole domain

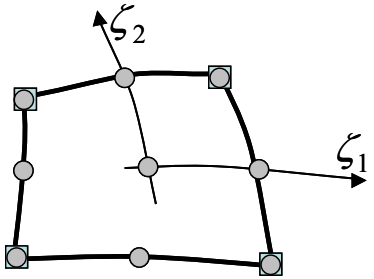
$$\varphi(\mathbf{x},t) = \sum_{e=1}^{NE}\varphi^{(e)}(\mathbf{x},t) = \sum_{e=1}^{NE} M_k^{(e)}\left(\zeta\left(\mathbf{x}\right)\right)\varphi_k(t)$$

$$\text{for } k = 1,2,...,N_\varphi$$

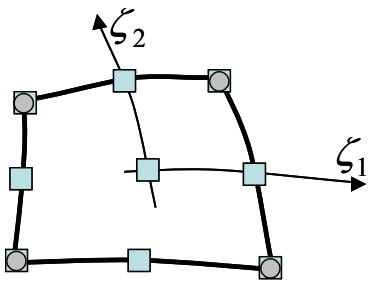
Finite Element Method – concept of parametric elements



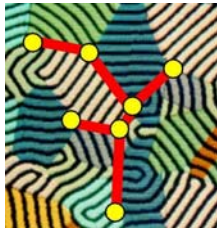
Iso-parametric element – the same nodes used for both interpolations with identical M_k and N_k functions, and $N_g=N_\varphi$



Super-parametric element – order of polynomial N_k higher than order of M_k, and $N_g>N_\varphi$



Sub-parametric element – order of polynomial N_k lower than order of M_k, and $N_g<N_\varphi$



Finite Element Method – nodal equations

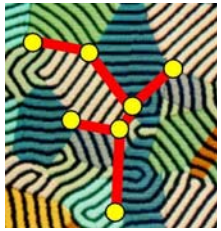
$$\left.\begin{aligned} x_i(\zeta) &= N_m(\zeta)(x_i)_m \\ \varphi(\mathbf{x},t) &= \sum_{e=1}^{NE} M_k^{(e)}\left(\zeta(\mathbf{x})\right)\varphi_k(t) \end{aligned}\right\} \quad \text{for} \quad \begin{cases} m = 1,2,\ldots,N_g \\ k = 1,2,\ldots,N_\varphi \end{cases}$$

$$\int_\Omega W_k \frac{\partial \varphi}{\partial t} d\Omega + \int_\Omega \frac{\partial W_k}{\partial x_j} \chi \frac{\partial \varphi}{\partial x_j} d\Omega = \int_\Gamma W_k \left(k(\varphi_a - \varphi) + q_b\right) d\Gamma + \int_\Omega W_k Q_v \, d\Omega$$

$$\text{for} \quad k = 1,2,\ldots,N$$

Bubnov-Galerkin WRM – the best approximation

$$W_k \equiv M_k; \quad N = N_\varphi$$



Finite Element Method – nodal equations

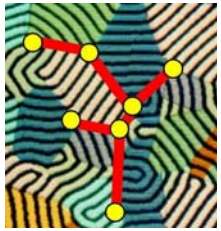
Galerkin FEM (GFEM) equations

$$\sum_{e=1}^{NE} \int_{\Omega_e} M_k^{(e)} M_m^{(e)} \frac{d\varphi_m}{dt} d\Omega + \sum_{e=1}^{NE} \int_{\Omega_e} \frac{\partial M_k^{(e)}}{\partial x_i} \chi^{(e)} \frac{\partial M_m^{(e)}}{\partial x_i} \varphi_m d\Omega +$$

$$\sum_{eb=1}^{NE_b} \int_{\Gamma_e} k^{(eb)} M_k^{(eb)} \varphi_k d\Gamma = \sum_{e=1}^{NE} \int_{\Omega_e} M_k^{(e)} Q_v^{(e)} d\Omega +$$

$$\sum_{eb=1}^{NE_b} \int_{\Gamma_e} M_k^{(eb)} \left(k^{(eb)} \varphi_a^{(eb)} + q_b \right) d\Gamma$$

$$\text{for} \begin{cases} i = 1,2,3 \\ k,m = 1,2,\ldots,N_\varphi \end{cases}$$



Matrix GFEM equations

$$[\mathbf{C}]\left\{\frac{d\varphi(t)}{dt}\right\}+[\mathbf{K}]\varphi(t)=\{\mathbf{R}\}$$

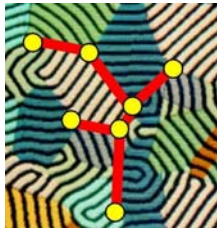
Capacity ('mass') matrix

$$C_{km}=\sum_{e=1}^{NE}C_{km}^{(e)}=\sum_{e=1}^{NE}\int_{\Omega_e}M_k^{(e)}M_m^{(e)}d\Omega$$

CMM – Consistent 'Mass' Matrix Model

$$C_{kk}=\sum_{e=1}^{NE}\int_{\Omega_e}M_k^{(e)}d\Omega;\ C_{km}=0 \quad \text{for } m\neq k$$

LMM – Lumped 'Mass' Matrix Model



Matrix GFEM equations

$$[\mathbf{C}]\left\{\frac{d\varphi(t)}{dt}\right\}+[\mathbf{K}]\varphi(t)=\{\mathbf{R}\}$$

Diffusion Matrix (symmetrical)

$$K_{km}=\sum_{e=1}^{NE}\int_{\Omega_e}\frac{\partial M_k^{(e)}}{\partial x_i}\chi^{(e)}\frac{\partial M_m^{(e)}}{\partial x_i}d\Omega+\sum_{eb=1}^{NE_b}\int_{\Gamma_e}k^{(eb)}M_k^{(eb)}d\Gamma$$

Right Hand Side (RHS) Vector

$$R_k=\sum_{e=1}^{NE}\int_{\Omega_e}M_k^{(e)}Q_v^{(e)}d\Omega+\sum_{eb=1}^{NE_b}\int_{\Gamma_e}M_k^{(eb)}\left(k^{(eb)}\varphi_a^{(eb)}+q_b\right)d\Gamma$$

Time integration procedure

Semi-discrete CVFDM and GFEM equations

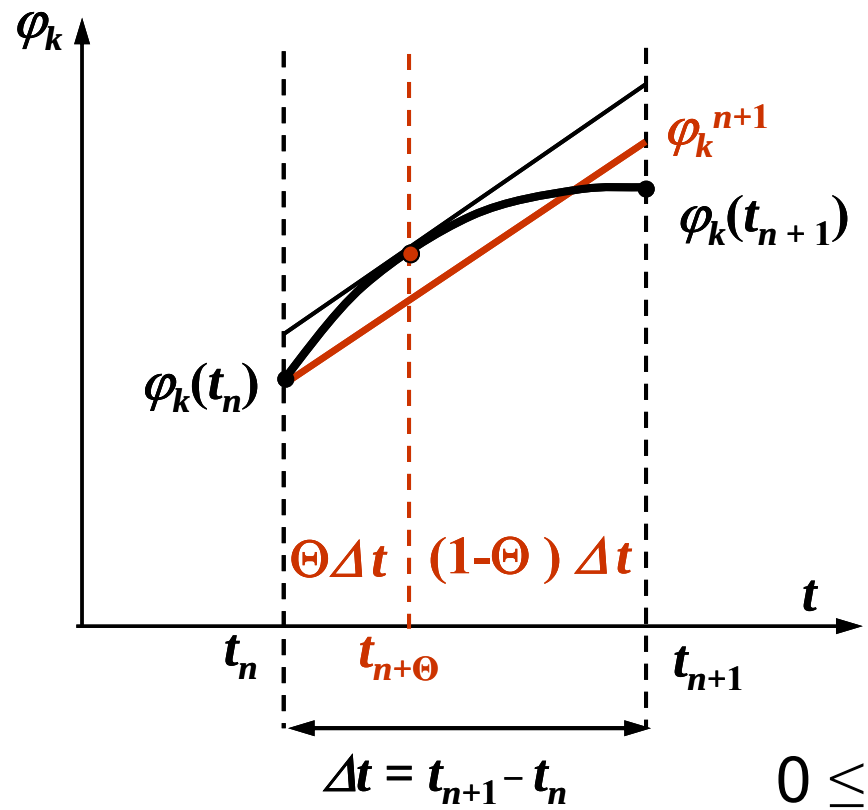
$$[\mathbf{C}]\left\{\frac{d\varphi(t)}{dt}\right\}+[\mathbf{K}]\varphi(t)=\{\mathbf{R}\}$$

Need for time integration

Characteristic feature:

One-way coordinate – marching in time

One-step explicit / implicit time marching scheme



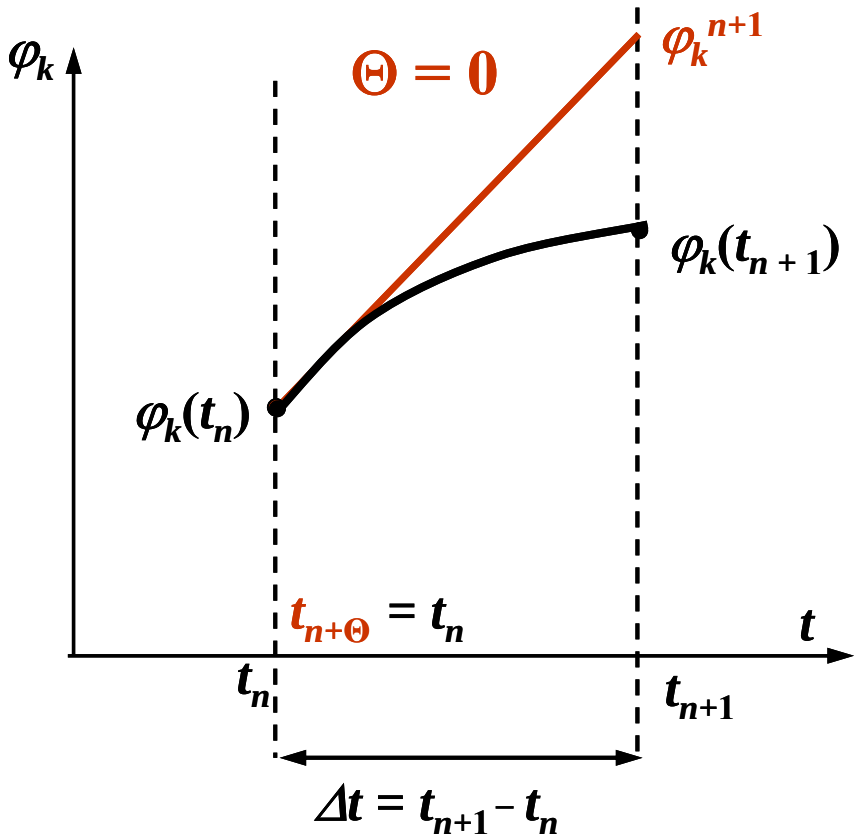
Taylor series expansion – time derivative replaced by difference quotient:

$$\left(\frac{d\varphi_k}{dt}\right)^{n+\Theta} = \frac{\varphi_k^{n+1} - \varphi_k^{n}}{\Delta t} + \frac{1}{2}(2\Theta - 1)\Delta t\left(\frac{d^2\varphi_k}{dt^2}\right)^{n+\Theta} + 0\left(\Delta t^2\right)$$

$0 \le \Theta \le 1$ - parameter of the scheme

One-step explicit / implicit time marching scheme

Explicit Euler Scheme



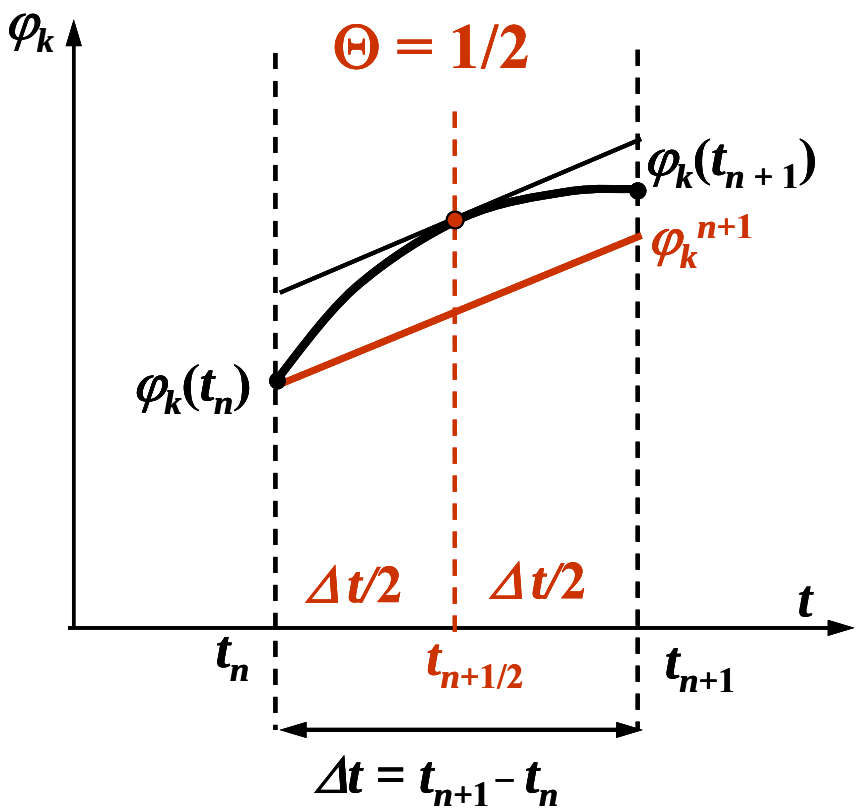
$$\left(\frac{d\varphi_k}{dt}\right)^{n+\Theta} = \left(\frac{d\varphi_k}{dt}\right)^{n} = \frac{\varphi_k^{n+1} - \varphi_k^{n}}{\Delta t} + 0(\Delta t)$$

First order accuracy

Conditionally stable

One-step explicit / implicit time marching scheme

Crank-Nicolson Scheme



$$\left(\frac{d\varphi_k}{dt}\right)^{n+\Theta} = \left(\frac{d\varphi_k}{dt}\right)^{n+1/2} =$$

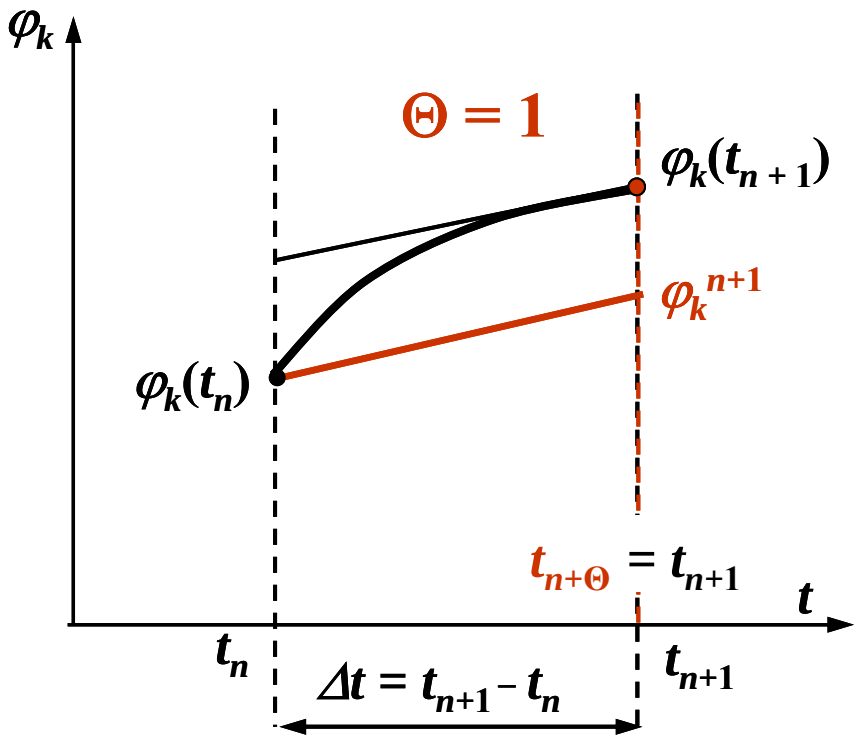
$$\frac{\varphi_k^{n+1} - \varphi_k^n}{\Delta t} + 0\left(\Delta t^2\right)$$

Second order accuracy

Unconditionally stable

One-step explicit / implicit time marching schemes

Implicit Backward Euler Scheme



$$\left(\frac{d\varphi_k}{dt}\right)^{n+\Theta} = \left(\frac{d\varphi_k}{dt}\right)^{n+1} =$$

$$\frac{\varphi_k^{n+1} - \varphi_k^n}{\Delta t} + 0(\Delta t)$$

First order accuracy

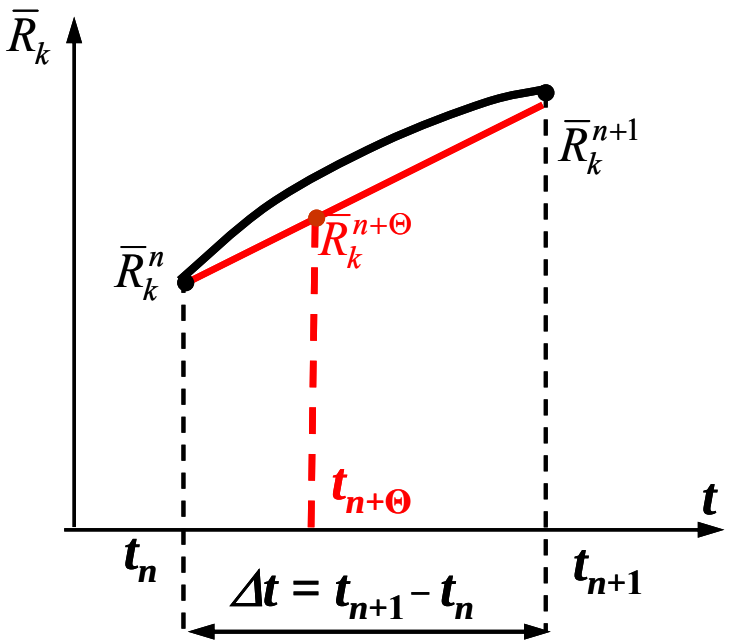
Unconditionally stable

Fully discrete GFEM and CVFDM models of diffusion

Balance equation for node k at time $t_{n+\Theta}$

$$C_{kk}\frac{d\varphi_k^{n+\Theta}}{dt} = \bar{R}_k^{n+\Theta}$$

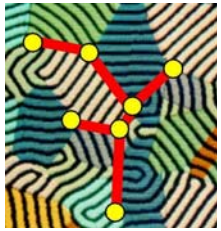
where: $\bar{R}_k^{n+\Theta} = R_k - K_{kj}\varphi_j^{n+\Theta}$



Assumptions:

$$\bar{R}_k^{n+\Theta} = (1-\Theta)\bar{R}_k^{n} + \Theta\bar{R}_k^{n+1}$$

$$\left(\frac{d\varphi_k}{dt}\right)^{n+\Theta} = \frac{\varphi_k^{n+1} - \varphi_k^{n}}{\Delta t}$$



Fully discrete GFEM and CVFDM models

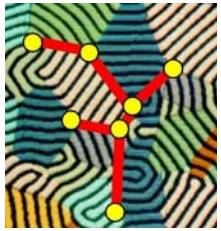
$$C_{kk}\frac{\varphi_k^{n+1}-\varphi_k^n}{\Delta t}=\left(1-\Theta\right)\bar{R}_k^n+\Theta\bar{R}_k^{n+1}$$

OR

$$\left(C_{kk}+\Theta\Delta tK_{kj}\right)\varphi_j^{n+1}=\left(C_{kk}+\left(1-\Theta\right)\Delta tK_{kj}\right)\varphi_j^n+\left(1-\Theta\right)R_k^n+\Theta R_k^{n+1}$$

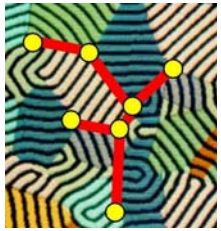
Matrix equation of fully-discrete CVFDM or GFEM

$$\left(\left[\mathbf{C}\right]+\Theta\Delta t\left[\mathbf{K}\right]\right)\left\{\varphi^{n+1}\right\}=\left(\left[\mathbf{C}\right]-\left(1-\Theta\right)\Delta t\left[\mathbf{K}\right]\right)\left\{\varphi^n\right\}+\Delta t\left(\left(1-\Theta\right)\left\{\mathbf{R}\right\}^n+\Theta\left\{\mathbf{R}\right\}^{n+1}\right)$$



Solution of CVFDM or GFEM algebraic equation system

- DIRECT METHODS:
  - Gauss and Gauss-Jordan elimination
  - LU decomposition
  - Special techniques for banded matrices (eg. Thomas algorithm)
- ITERATIVE METHODS:
  - Jacobi and Gauss-Seidel methods
  - Successive Over-Relaxation (SOR)
  - Conjugate Gradient Method



Fixed grid models of diffusion-controlled alloy solidification

Assumption:

with no convection at the macroscopic scale solidification of alloys is controlled only by heat diffusion (conduction)

Crucial issue:

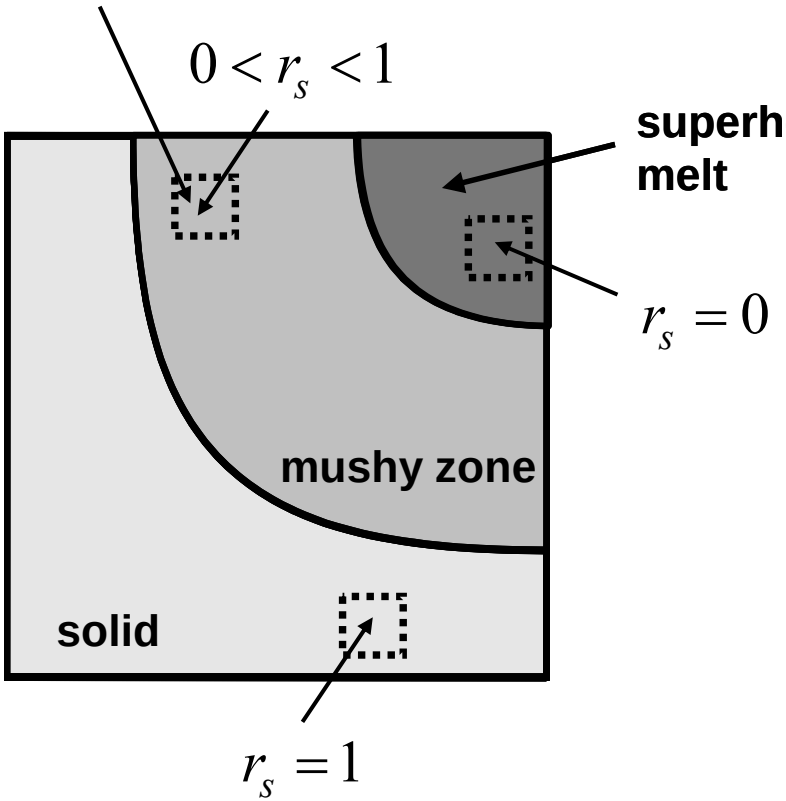
modelling of latent heat effect on a fixed grid

Methods:

- General Enthalpy method
- Apparent Heat Capacity method
- Latent Heat Source based formulation

Fixed grid models of diffusion-controlled alloy solidification

Representative **E**lementary **V**olume [Beckermann, 1987]



Volumetric and mass fractions of solid (s) and liquid (l)

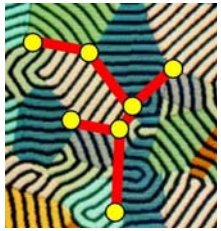
$$r_i = V_i / \left(V_s + V_l \right)$$

$$f_i = m_i / \left(m_s + m_l \right)$$

with $i=s$ or $i=l$

and, saturation condition:

$$\left. \begin{aligned} r_s + r_l &= 1 \\ f_s + f_l &= 1 \end{aligned} \right\}$$



Single-domain enthalpy formulation

$$\frac{\partial\left(r_s H_s\right)}{\partial t}-\frac{\partial}{\partial x_j}\left(r_s \lambda_s \frac{\partial T}{\partial x_j}\right)+\left(\textit{interface term}\right)=0$$

Conduction in the solid phase

$$\frac{\partial\left(r_l H_l\right)}{\partial t}-\frac{\partial}{\partial x_j}\left(r_l \lambda_l \frac{\partial T}{\partial x_j}\right)-\left(\textit{interface term}\right)=0$$

Conduction in the liquid phase

where:

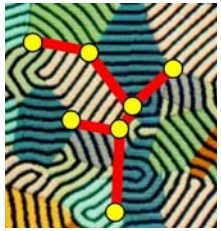
H_s and H_l - volumetric enthalpy of solid and liquid

λ_s and λ_l - thermal conductivity of solid and liquid

$$\boxed{\frac{\partial\left(H\right)}{\partial t}-\frac{\partial}{\partial x_j}\left(\lambda \frac{\partial T}{\partial x_j}\right)=0}$$

General Enthalpy Method

[Swaminathan & Voller, 1992]



Averaged parameters of solid-liquid mixture

Mixture volumetric enthalpy

$$H = r_s H_s + r_l H_l$$

Mixture thermal conductivity

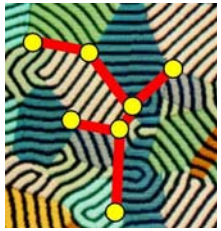
$$\lambda = r_s \lambda_s + r_l \lambda_l$$

Mixture density

$$\rho = r_s \rho_s + r_l \rho_l \qquad \text{and} \qquad \left.\begin{aligned} \rho f_s &= \rho_s r_s \\ \rho f_l &= \rho_l r_l \end{aligned}\right\}$$

Mixture heat capacitance

$$\rho c = r_s \rho_s c_s + r_l \rho_l c_l = \rho\left(f_s c_s + f_l c_l\right)$$



Phase enthalpies and enthalpy of solid/liquid mixture

Assumptions: constant phase densities and latent heat, L, specific heats are functions of temperature only

$$H = \rho h = r_s \rho_s h_s + r_l \rho_l h_l = \rho \left(f_s h_s + f_l h_l \right)$$

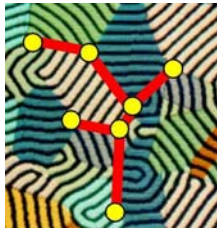
with

$$h_s = h_{s,ref.} + \int_{T_{ref.}}^{T} c_s \left(T \right) dT$$

$$h_l = h_{l,ref.} + \int_{T_{ref.}}^{T} c_l \left(T \right) dT + L$$

For: $c_s = \text{const.}$; $c_l = \text{const.}$; $h_{s,ref} = c_s T_{ref.}$; $h_{l,ref} = c_l T_{ref.}$

$$H = r_s \rho_s c_s T + r_l \rho_l \left(c_l T + L \right) = \rho \left(f_s c_s + f_l c_l \right) T + \rho f_l L$$



Apparent Heat Capacity formulation

$$c_{app.}(T) = \frac{dH}{dT} = \rho\left(f_s c_s + f_l c_l\right) + \rho\left(\left(c_l - c_s\right)T + L\right)\frac{df_l}{dT}$$

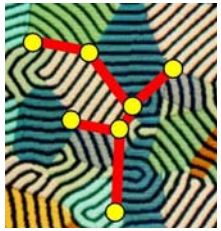
or

$$c_{app.}(T) = \frac{dH}{dT} = \left(\rho_s r_s c_s + \rho_l r_l c_l\right) + \left(\left(\rho_l c_l - \rho_s c_s\right)T + \rho_l L\right)\frac{dr_l}{dT}$$

$$\frac{\partial H}{\partial t} = \frac{dH}{dT}\frac{\partial T}{\partial t} = c_{app.}(T)\frac{\partial T}{\partial t}$$

$$\frac{\partial H}{\partial t} - \frac{\partial}{\partial x_j}\left(\lambda \frac{\partial T}{\partial x_j}\right) = 0 \longrightarrow c_{app.}\frac{\partial T}{\partial t} - \frac{\partial}{\partial x_j}\left(\lambda \frac{\partial T}{\partial x_j}\right) = 0$$

(e.g. Voller et al., 1990)



Latent Heat Source method

$$c_{app.}(T) = \rho c + \Delta h_{sl} \frac{dr_l}{dT}$$

where

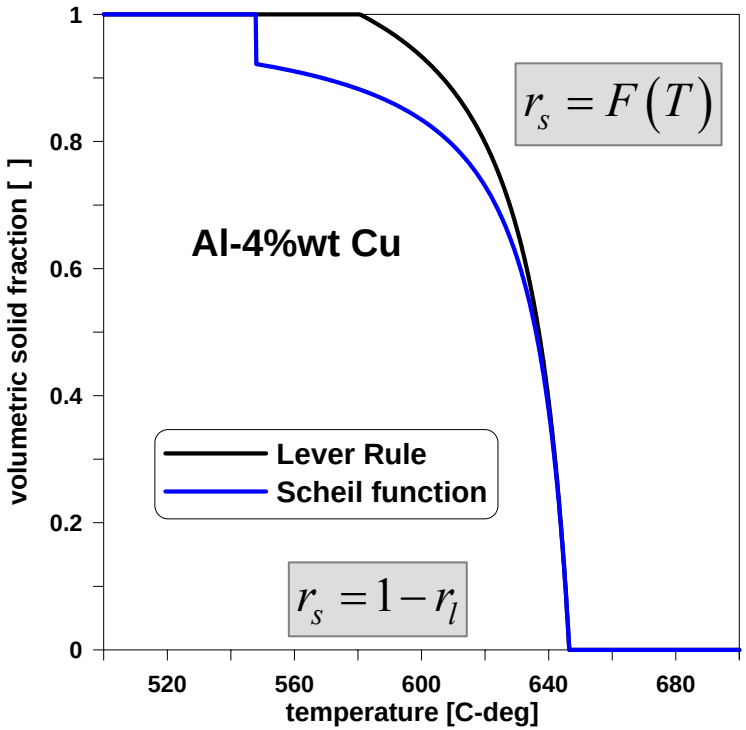
$$\rho c = \rho_s r_s c_s + \rho_l r_l c_l$$

$$\Delta h_{sl} = (\rho_l c_l - \rho_s c_s) T + \rho_l L$$

$$\left(\rho c + \Delta h_{sl} \frac{dr_l}{dT} \right) \frac{\partial T}{\partial t} - \frac{\partial}{\partial x_j} \left(\lambda \frac{\partial T}{\partial x_j} \right) = 0$$

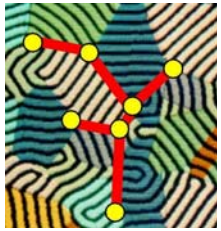
$$\boxed{\rho c \frac{\partial T}{\partial t} - \frac{\partial}{\partial x_j} \left(\lambda \frac{\partial T}{\partial x_j} \right) = -\Delta h_{sl} \frac{\partial r_l}{\partial t}}$$

Fraction solid – temperature relationship



Example of fraction solid – temperature relationship

- Two uknown fields: T and r_s:
  - function $r_s = F(T)$ – a key issue
- Common assumption in macroscopic calculations of diffusion-controlled solidification: r_s a function of T only
- Commonly used relations based on microscopic solutal diffusion models of complete solute mixing in the liquid



CVFDM and GFEM for conduction-driven solidification

All equations of single-domain models of solidification controlled by conduction coincide with the generic form of diffusion transport equation of scalar quantity φ:

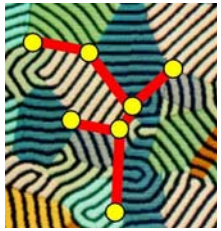
$$\frac{\partial \varphi}{\partial t} - \frac{\partial}{\partial x_j}\left(\chi \frac{\partial \varphi}{\partial x_j} \right) = Q_v$$

where

$\varphi \equiv h_{sens.} = \rho c T$ volumetric sensible enthalpy

$\chi \equiv \lambda / (\rho c)$ thermal diffusivity

$Q_v \equiv S_h$ latent heat source term



CVFDM and GFEM for conduction-driven solidification

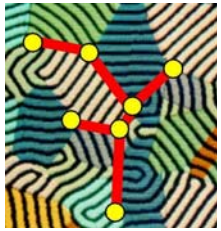
latent heat source term:

$$S_h = 0$$ for apparent heat capacity method

$$S_h = -\Delta h_{sl} \frac{\partial r_l}{\partial t} = \Delta h_{sl} \frac{\partial r_s}{\partial t}$$ for latent heat source method

CONCLUSION:

Follow all consecutive steps of CVFDM or GFEM spatial and temporal discretization (discussed in this lecture) to get a final set of algebraic equations for fully discrete models of alloy solidification



CVFDM and GFEM for conduction-driven solidification

IPPT PAN

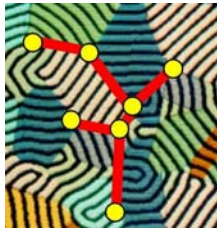
Matrix equation

$$\left(\left[\mathbf{C}(T)\right]+\Theta\Delta t\left[\mathbf{K}(T)\right]\right)\left\{T^{n+1}\right\}=\left(\left[\mathbf{C}(T)\right]-(1-\Theta)\Delta t\left[\mathbf{K}(T)\right]\right)\left\{T^{n}\right\}+$$
$$\Delta t\left((1-\Theta)\left\{\mathbf{R}(T)\right\}^{n}+\Theta\left\{\mathbf{R}(T)\right\}^{n+1}\right)$$

Nodal equation

$$\left(C_{kj}(T)+\Theta\Delta tK_{kj}(T)\right)T_j^{n+1}=\left(C_{kj}(T)+(1-\Theta)\Delta tK_{kj}(T)\right)T_j^{n}+$$
$$(1-\Theta)R_k^{n}(T)+\Theta R_k^{n+1}(T)$$

Nonlinearity due to the fraction solid/enthalpy – temperature coupling – need for iterative solution strategy



Fully implicit CVFDM and GFEM model equations

Backward Euler scheme, and LMM

$$\theta = 1,\ C_{kj} = 0 \quad \text{for} \quad j \neq k$$

- Source Based Method - nodal energy equation

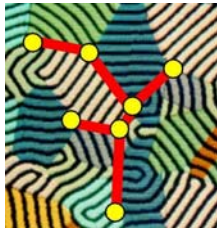
with $T_j \equiv T_j^{n+1}$, $\left(r_l\right)_k \equiv \left(r_l\right)_k^{n+1}$ and known $r_l = F\left(T\right)$

$$C_{kk}\left(T\right)\left(T_k - T_k^n\right) + \Delta t K_{kj}\left(T\right)T_j = S_k \Delta h_{sl}\left(T\right)\left(\left(r_l\right)_k^n - \left(r_l\right)_k\right)$$

where

$$S_k = \Omega_k \qquad \text{for CVFDM}$$

$$S_k = \sum_{e=1}^{NE} \int_{\Omega_e} M_k^{(e)} d\Omega \qquad \text{for GFEM}$$



Fully implicit CVFDM and GFEM equations

- General Enthalpy Method - nodal energy equation

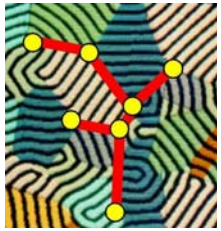
with $T_j \equiv T_j^{n+1}$, $H_k \equiv H_k^{n+1}$, and known $H = G(T)$

$$\boxed{\Delta t K_{kj}(T) T_j = S_k \left(H_k^n - H_k \right)}$$

where

$$S_k = \Omega_k \qquad \text{for CVFDM}$$

$$S_k = \sum_{e=1}^{NE} \int_{\Omega_e} M_k^{(e)} d\Omega \qquad \text{for GFEM}$$



Iterative adjustment of solid fraction / enthalpy and temperature

Source Based Method (SBM)

Taylor series expansion of r_l [Voller & Swaminathan, 1991]:

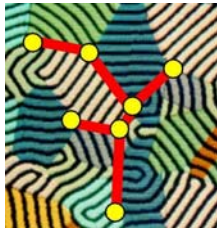
$$\left(r_l\right)_k^{(m+1)} = \left(r_l\right)_k^{(m)} + \frac{dF}{dT}\left(T_k^{(m+1)} - T_k^{(m)}\right) =$$

$$\left(r_l\right)_k^{(m)} + \frac{dF}{dT}\left(T_k^{(m+1)} - F^{-1}\left(\left(r_l\right)_k^{(m)}\right)\right)$$

where:

$r_l = F\left(T\right)$ - known function

$T = F^{-1}\left(r_l\right)$ - its inverse



Iterative adjustment of solid fraction / enthalpy and temperature

General Enthalpy Method (GEM)

Taylor series expansion of H [Swaminathan & Voller, 1992]:

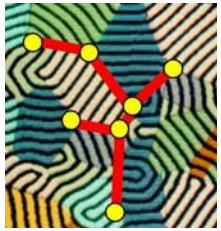
$$H_k^{(m+1)} = H_k^{(m)} + \frac{dG}{dT}\left(T_k^{(m+1)} - T_k^{(m)}\right) =$$

$$H_k^{(m)} + \frac{dG}{dT}\left(T_k^{(m+1)} - G^{-1}\left(H_k^{(m)}\right)\right)$$

where:

$H = G(T)$ - a known function

$T = G^{-1}(H)$ - its inverse



Iterative adjustment of solid fraction / enthalpy and temperature

Iterative solution algorithm [Voller & Swaminathan,1991,1992]:

1. At the start of each consecutive, (n+1), time step Δt:

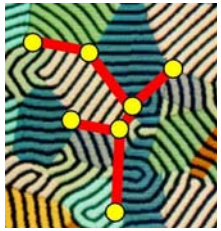
   for $m = 0$: $T_k^{(m)} = T_k^n$ and $\left(r_l\right)_k^{(m)} = \left(r_l\right)_k^n$ in SBM

   or $H_k^{(m)} = H_k^n$ in GEM

2. For known m – iteration of all $T_k, \left(r_l\right)_k$ or H_k calculate

   $K_{ij}\left(T^{(m)}\right); C_{kk}\left(T^{(m)}\right); \dfrac{dF}{dT}\left(T^{(m)}\right)$ and $F^{-1}\left(\left(r_l\right)^{(m)}\right)$ in SBM

   or $K_{ij}\left(T^{(m)}\right); \dfrac{dG}{dT}\left(T^{(m)}\right)$ and $G^{-1}\left(H^{(m)}\right)$ in GEM



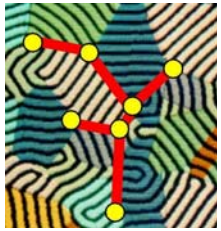
Iterative adjustment of solid fraction / enthalpy and temperature

3. Solve linearized energy conservation equation to get a new approximation of nodal values of temperature $T_k^{(m+1)}$
4. Update nodal values of r_l or H according to their Taylor series expansions to get a new iteration

$$\left(r_l\right)_k^{(m+1)} = \left(r_l\right)_k^{(m)} + \frac{dF}{dT}\left(T_k^{(m+1)} - F^{-1}\left(\left(r_l\right)_k^{(m)}\right)\right) \quad \text{in SBM}$$

or

$$H_k^{(m+1)} = H_k^{(m)} + \frac{dG}{dT}\left(T_k^{(m+1)} - G^{-1}\left(H_k^{(m)}\right)\right) \quad \text{in GEM}$$



Iterative adjustment of solid fraction / enthalpy and temperature

5. Check convergence – compare two consecutive iterations of H and:

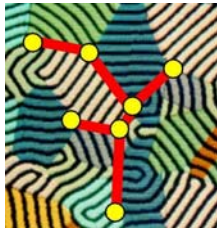
IF: $$\max_k \left| \frac{H_k^{(m+1)} - H_k^{(m)}}{H_k^{(m)}} \right| < \text{tolerance}$$

go to the next time step

OTHERWISE:

$$T_k^{(m)} = T_k^{(m+1)};\ \left(r_l\right)_k^{(m)} = \left(r_l\right)_k^{(m+1)} \quad \text{or} \quad H_k^{(m)} = H_k^{(m+1)}$$

And continue procedure outlined in steps from 2 to 5 till convergence



Examples of GFEM and CVFDM calculations

- EXAMPLE 1:

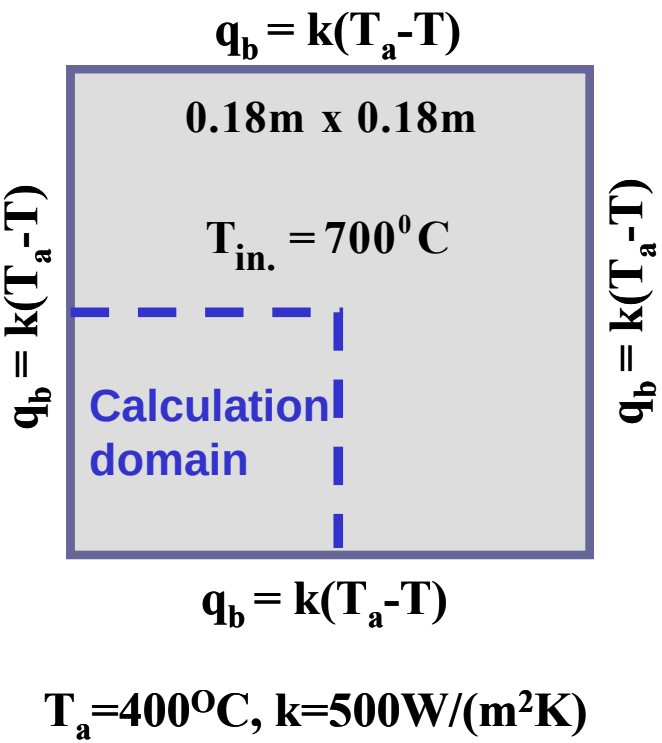
  Galerkin FEM simulation of Al-2%wt.Cu solidification in a square mould

- EXAMPLE 2:

  CVFDM calculations of directional solidification in a longitudinal sample of Al-7%wt.Si

EXAMPLE 1: problem specification

Geometry and boundary conditions



T_a=400^{O}C, k=500W/(m^{2}K)

Physical properties

Al–2%wt.Cu

T_S= 610^{O}C, T_L=655^{O}C

λ_s=150W/(mK), λ_l=75W/(mK)

c_s=c_l=1360J/(kg K), L=408kJ/kg

Scheil's solute diffusion model

Numerical model

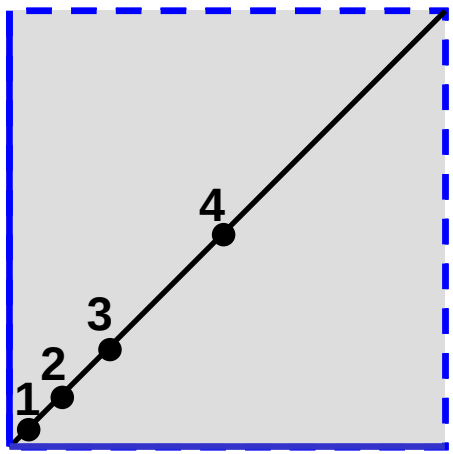
GFEM with General Enthalpy Method

50*50 bilinear elements

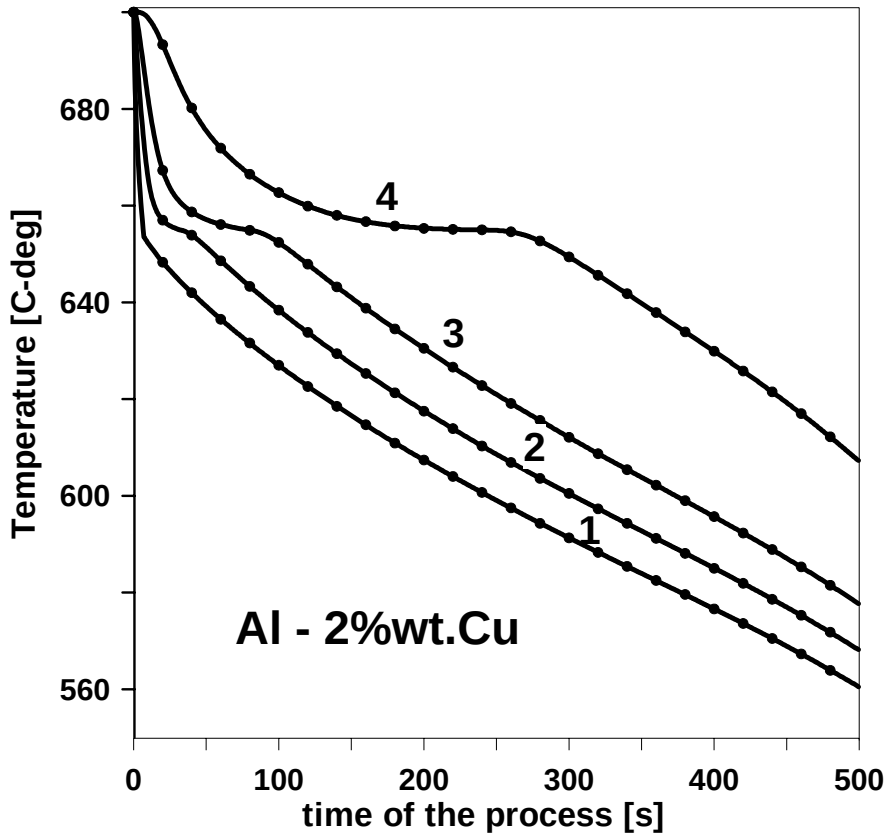
Implicit scheme, Δt=0.5s

EXAMPLE 1: Results

Cooling curves at selected locations along the mould diagonal

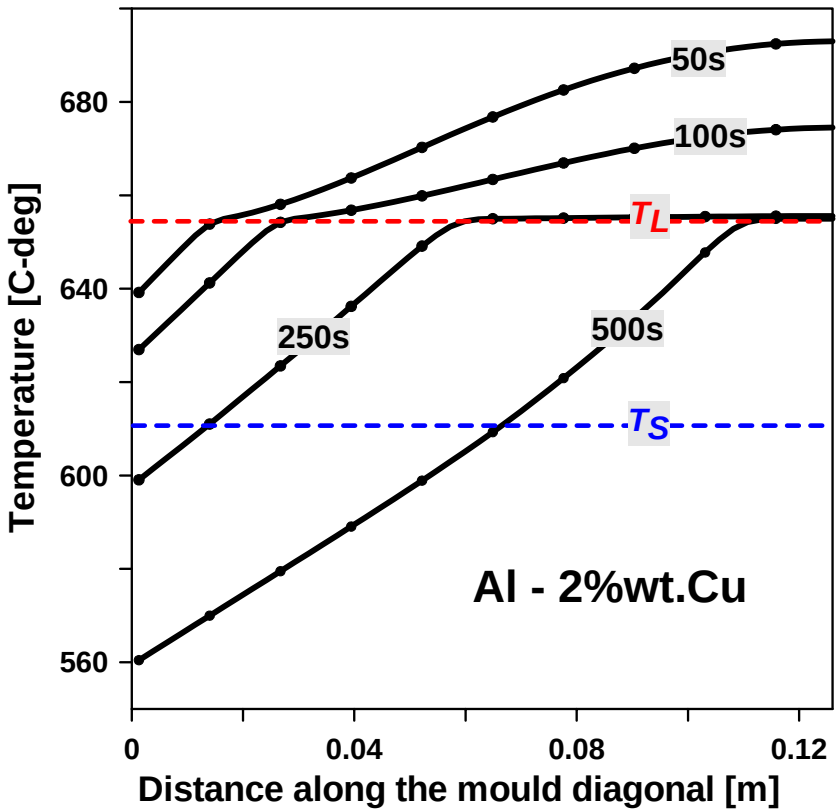


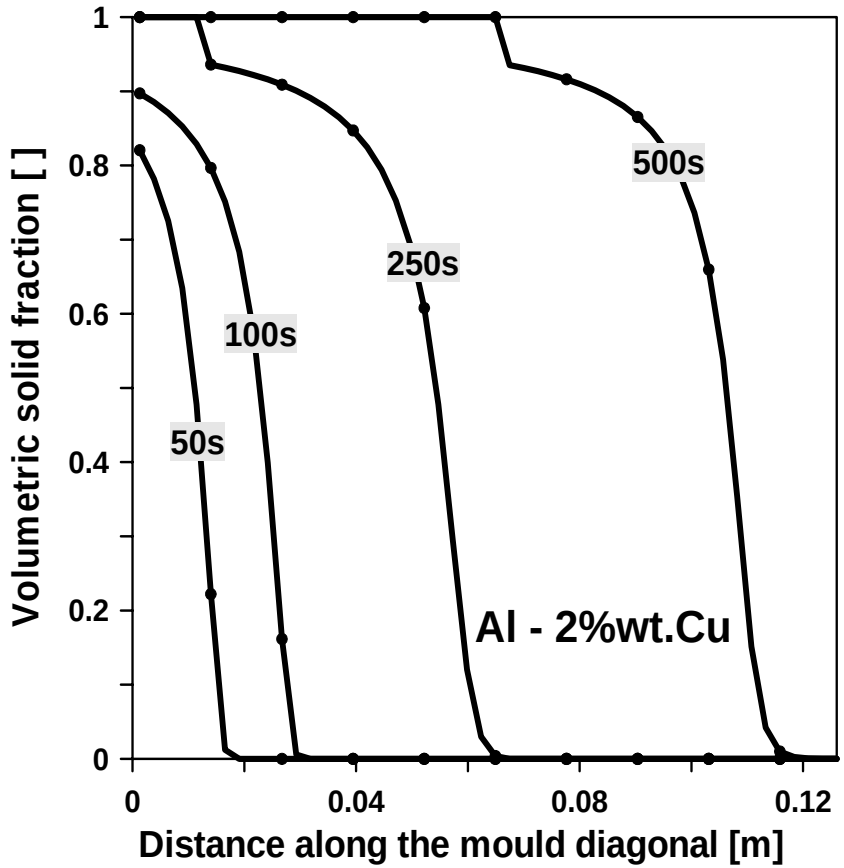
Calculation domain and selected nodes positions



EXAMPLE 1: Results

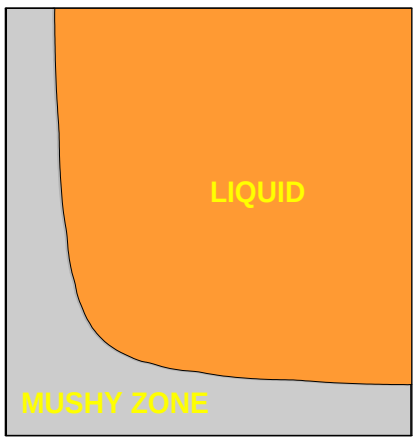
Temperature and fraction solid along the mould diagonal at different times



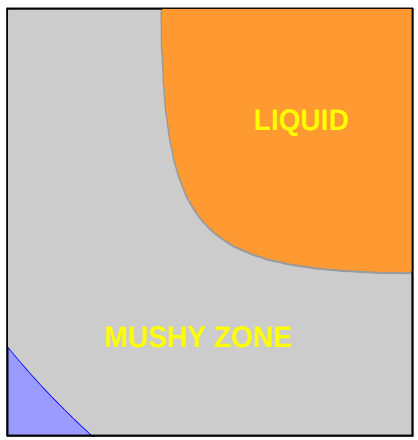


EXAMPLE 1: Results

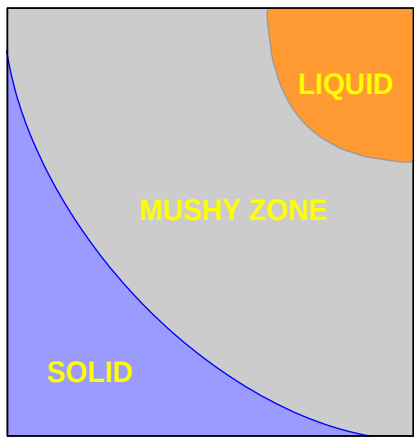
Evolution of solid, mushy zone and superheated liquid



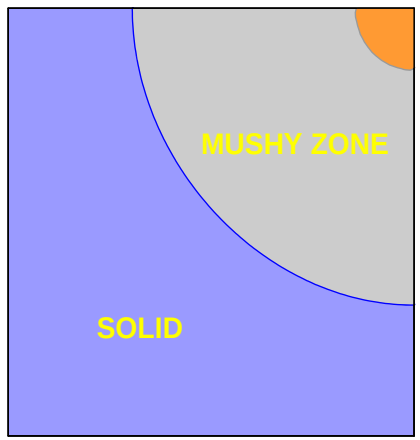
time = 100s



time = 250s

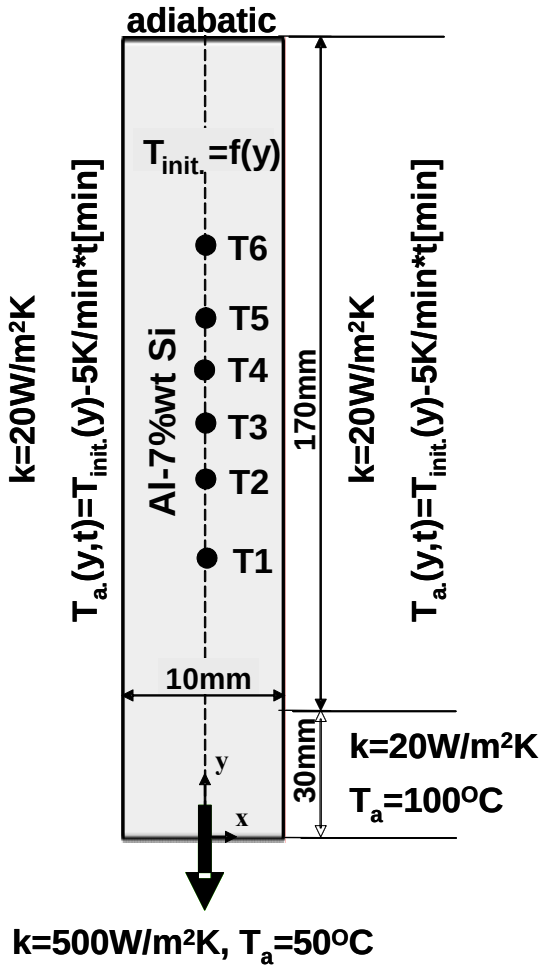


time = 400s



time = 500s

EXAMPLE 2: problem specification



Physical properties

Al–7%wt.Si

T_E= 577°C, T_L=614°C

λ_s=170W/(mK), λ_l=70W/(mK)

c_s=920 J/(kg K), c_l=1140 J/(kg K),

ρ=2530kg/m^3, L=397kJ/kg

Scheil's solute diffusion model

Numerical model

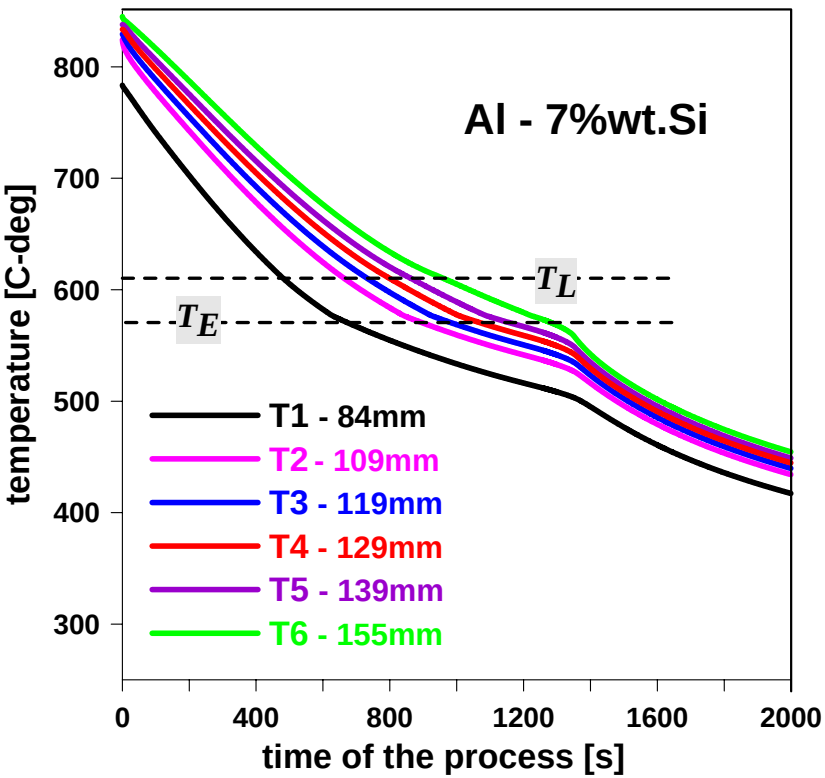
CVFDM with Source Based Method

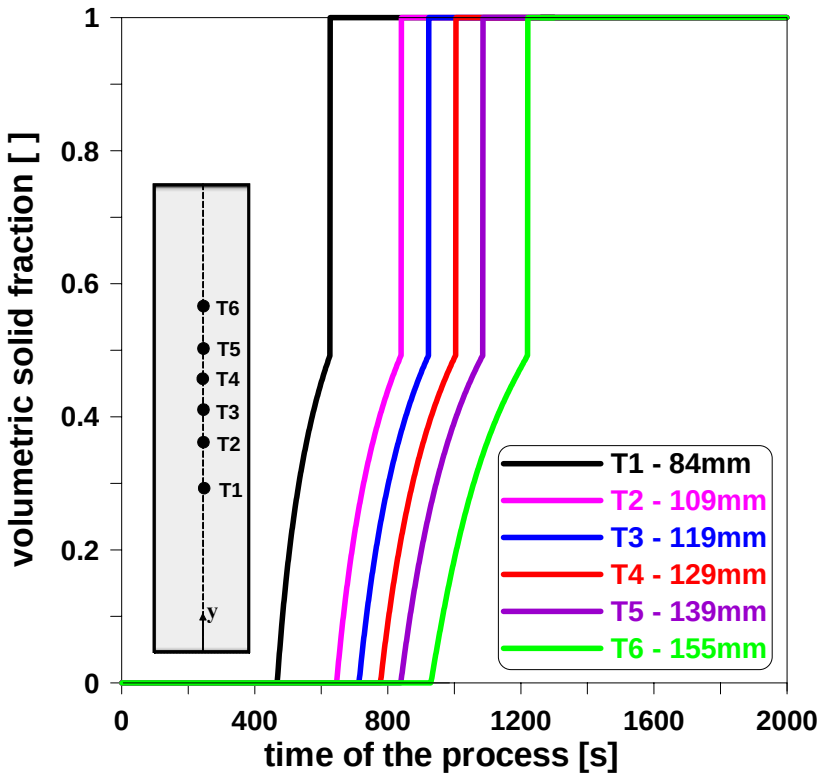
11*220 regular CVs

Implicit scheme, Δt=1s

EXAMPLE 2: Results

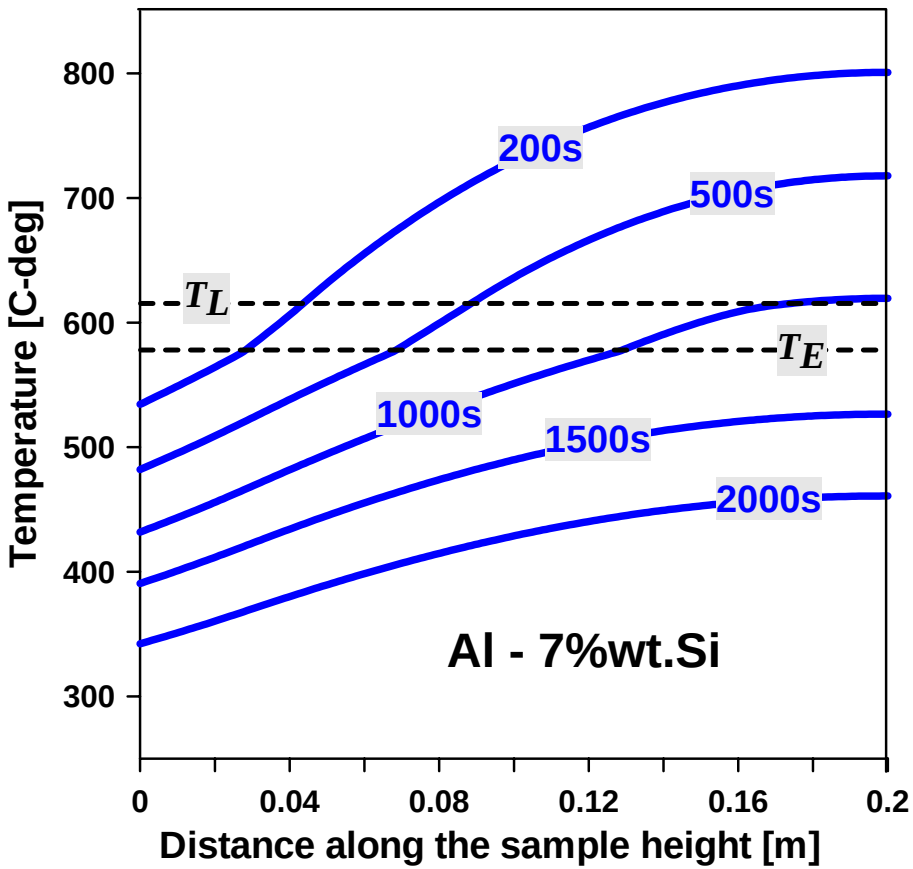
Cooling curves and time changes of fraction solid at selected locations

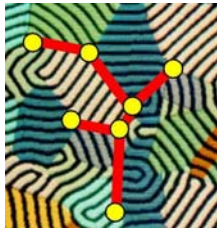




EXAMPLE 2: Results

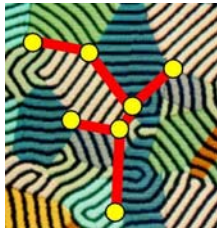
Temperature along the sample height





CLOSURE – some comments on more enhanced problems

- Effective macroscopic properties are dependent on microscopic transport phenomena and developing microstructure
- Coupling between micro- and macro-scales phenomena possible through the latent heat evolution – through careful definition of the solid fraction
- Complete solute mixing models (*lever rule, Scheil's model*) are commonly used in macroscopic calculations



CLOSURE – some comments on more enhanced problems

Macroscopic calculations that include solute diffusion and solutal undercooling possible by:

- improved models of solid fraction
  (for review see: M.Rappaz, *Int. Mat. Rev.,*vol.34,1989)
- simultaneous solution of macroscopic heat conduction and microscopic solute diffusion equations
  (C.Y. Wang & C.Beckermann, *Metall. Mater.Trans*. **25A**,1994)
- fixed grid front tracking technique based on assumed dendrite tip kinetics
  (D.J.Browne & J.D.Hunt, *Num.Heat Transfer*, Part B, **45,** 2004)