University of Ljubljana
Faculty of Mechanical Engineering

Univerza v Ljubljani
Fakulteta za strojništvo

Laboratory for Fluid Dynamics and Thermodynamics

Laboratorij za dinamiko fluidov in termodinamiko

A meshless approch for solving solidification with moving grains for two-dimensional binary alloy

Katarina Mramor[1], Vanja Hatić[2], and Božidar Šarler[1,2]

[1]*University of Ljubljana, Faculty for Mechanical Engineering, Laboratory for Fluid Dynamics and Thermodynamics, Aškerčeva cesta 6, 1000 Ljubljana, Slovenia*

[2]*Institute of Metals and Technology, Laboratory for Simulation of Materials and Processes, Lepi pot 11, 1000 Ljubljana, Slovenia*

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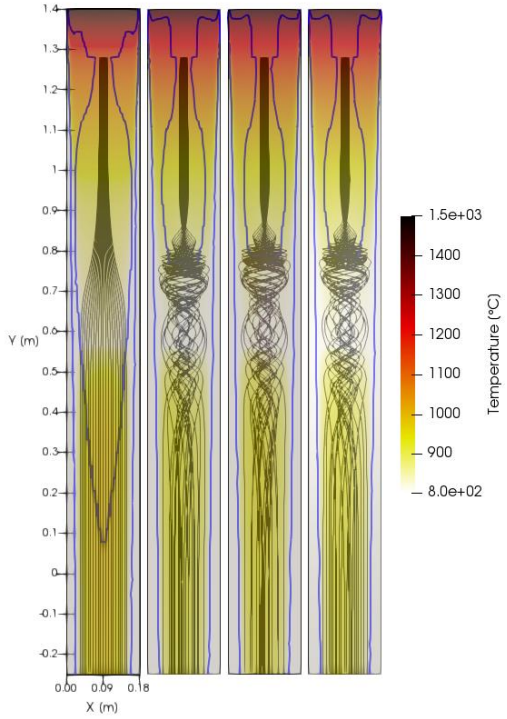
Introduction
General

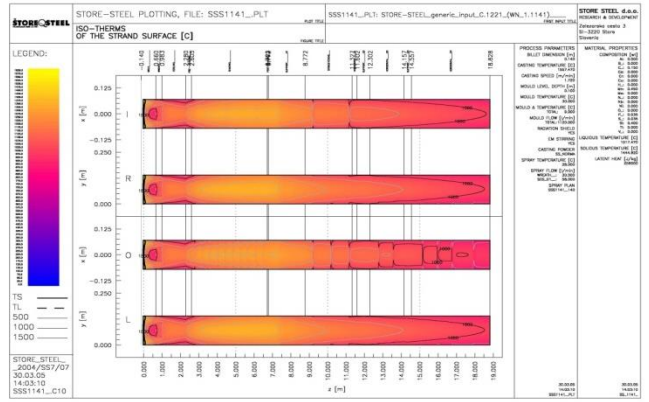
INDUSTRY (casting, remelting, ...) demends materials with BETTER STRUCTUAL QUALITY and ADVANCED PHYSICAL PROPERTIES.

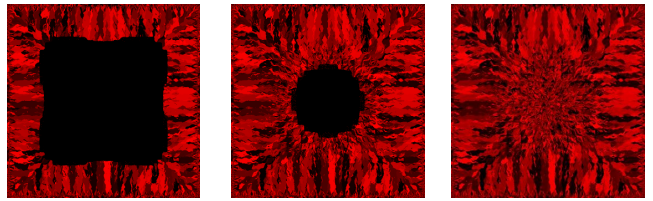
SOLIDIFICATION is a phase change transformation process that is accompanied by undesired side effects such as:

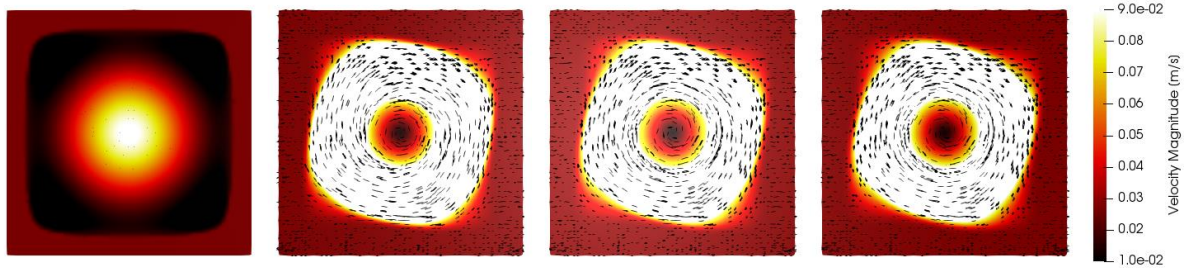
- MACROSEGREGATION
- inclusions
- porosity
- shrinkage
- …

Such effects can greatly affect the quality of manufactured material.







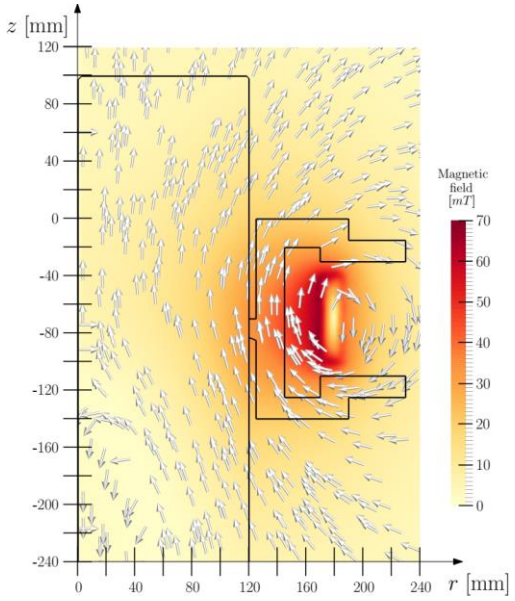


Vertnik, Mramor, Guštin, Maček

Introduction
Numerical modelling

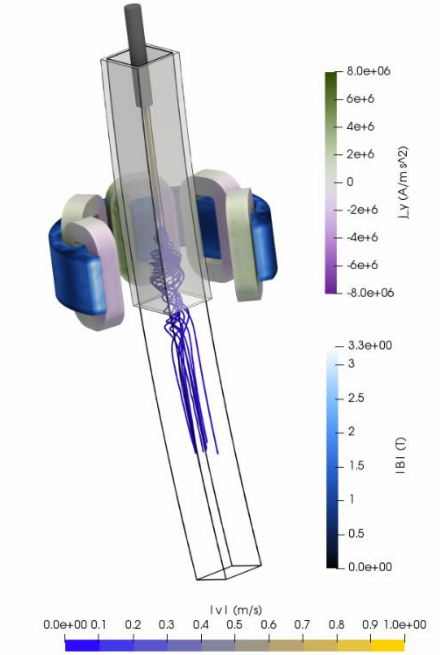
The experimental work in complex industrial examples (Continuous casting, Direct chill casting) can be very **expensive** and **time consuming**. Some of the key mechanism of fluid transport and solidification are difficult to measure and observe.

These processes can be predicted by NUMERICAL MODELLING.



Direct chill casting of aluminium

Hatić et al. *App. math. model. (2018)*

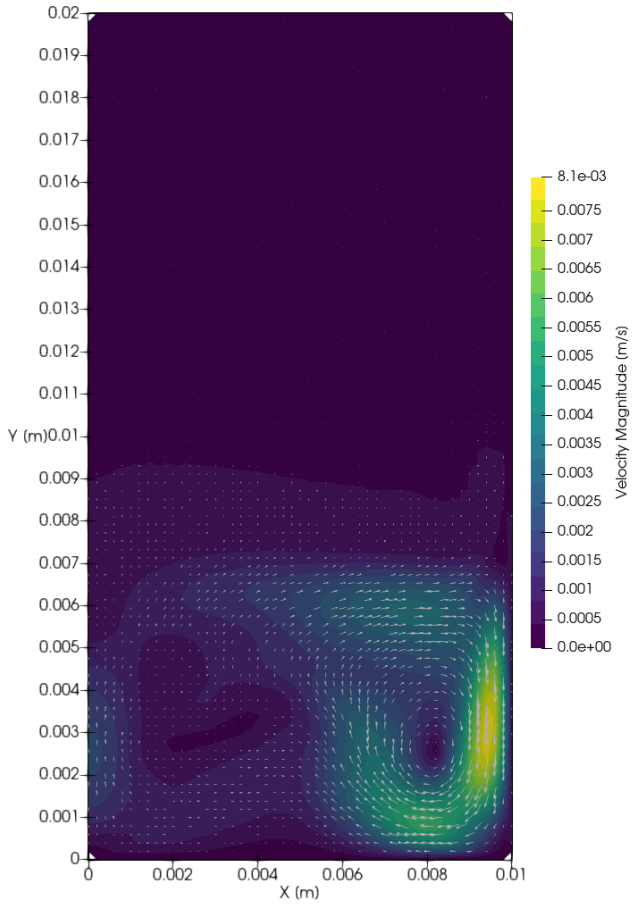


Continuous casting of steel

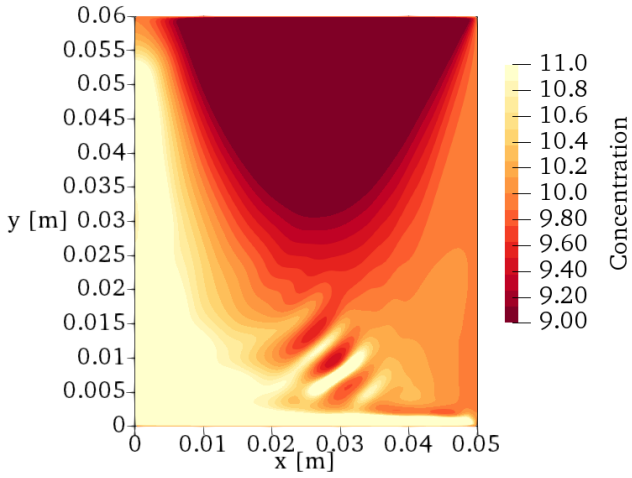
Vertnik et al. *EABE* (2019)

Introduction Diffuse Approximate Method

DIFFUSE APPROXIMATE METHOD is a meshless technique based on WEIGHTED LEAST SQUARES FUNCTIONS and locally SMOOTH and DIFFERENTIABLE APPROXIMATION in the computational nodes.



TEST CASE – solidification of binary alloy (Al 4.5 wt % Cu) with moving grains



TEST CASE – solidification of binary alloy (Sn 10% Pb)

Problem description

- Solidification of binary alloy with moving grains
- Al 4.5 wt% Cu
- Domain size: 0.02 m x 0.02 m
- Computational domain size: 0.01 m x 0.02 m
- Solidification of binary alloy without the motion of grains [Kosec et al. CMC, 2011, Hatič et al. J. *Num. Meth. Heat & Fluid Flow* (2018)]

Property	Symbol	Value	Unit
Specific heat capacity	c_p	$1 \cdot 10^3$	J/kg/K
Thermal conductivity	λ	$1.92 \cdot 10^2$	W/m/K
Density	ρ	$2.45 \cdot 10^3$	kg/m^3
Dynamic viscosity	μ	$1.2 \cdot 10^{-3}$	kg/m/s
Gravity acceleration	g	9.80	m/s^2
Darcy constant	K_0	$5.56 \cdot 10^{-11}$	m^2
Latent heat	L_f	$4.00 \cdot 10^{-5}$	J/kg
Fusion temperature	T_f	933.15	K
Eutectic temperature	T_e	821.15	K
Reference temperature	T_{ref}	738.15	K
Eutectic concentration	C_{eut}	32.60	wt%
Reference concentration	C_{ref}	4.50	wt%
Liquidus slope	m_L	3.43	K/wt%
Partition coefficient	k_p	0.173	/
Thermal expansion coefficient	β_T	$1.3 \cdot 10^{-4}$	1/K
Solutal expansion coefficient	β_C	$-7.3 \cdot 10^{-3}$	1/wt%
Initial grain radius	r_g	$1 \cdot 10^{-6}$	m
Dendrite arm spacing	λ_{DAS}	$100.035 \cdot 10^{-6}$	m

Model formulation
Volume averaged model

Porous region: grains form porous matrix

$$g_S > g_S^C \qquad \mathbf{v}_S = 0$$

Mass

$$\frac{\partial(g_L\rho_L + g_S\rho_S)}{\partial t} + \nabla\cdot\left(\rho_L g_L \mathbf{v}_L\right) = 0$$

Energy

$$\frac{\partial(\rho_L g_L h_L + \rho_S g_S h_S)}{\partial t} + \nabla\cdot(g_L\mathbf{v}_L h_L) = \lambda_T\nabla^2 T$$

Species

$$\frac{\partial(\rho_L g_L C_L + \rho_S g_S C_S)}{\partial t} + \nabla\cdot(\rho_L g_L \mathbf{v}_L C_L) = 0$$

Slurry region: grains move freely in the fluid

$$g_S \leq g_S^C \qquad \mathbf{v}_S \neq 0$$

Mass

$$\frac{\partial(g_L\rho_L + g_S\rho_S)}{\partial t} + \nabla\cdot\left(\rho_L g_L \mathbf{v}_L + \rho_S g_S \mathbf{v}_S\right) = 0$$

Energy

$$\frac{\partial(\rho_L g_L h_L + \rho_S g_S h_S)}{\partial t} + \nabla\cdot(\rho_L g_L \mathbf{v}_L h_L + \rho_S g_S \mathbf{v}_S h_S) = \lambda_T\nabla^2 T$$

Species

$$\frac{\partial(\rho_L g_L C_L + \rho_S g_S C_S)}{\partial t} + \nabla\cdot(\rho_L g_L \mathbf{v}_L C_L + \rho_S g_S \mathbf{v}_S C_S) = 0$$

Model formulation
Volume averaged model

Porous region: grains form porous matrix

$$g_S > g_S^C \qquad \mathbf{v}_S = 0$$

Momentum

$$\begin{aligned}\frac{\partial(\rho_L g_L \mathbf{v}_L)}{\partial t} &+ \nabla\cdot(\rho_L g_L \mathbf{v}_L \mathbf{v}_L) = -g_L\nabla p + \nabla\cdot(\mu g_L \nabla(\mathbf{v}_L)) \\ &+ g_L \mathbf{g}\rho_{ref}(1-\beta_T(T-T_{ref})-\beta_C(C-C_{ref})) \\ &+ g_L\frac{g_L\mu(\mathbf{v}_L)}{K}\end{aligned}$$

Slurry region: grains move freely in the fluid

$$g_S \leq g_S^C \qquad \mathbf{v}_S \neq 0$$

Momentum

$$\begin{aligned}\frac{\partial}{\partial t}\left(\rho_L g_L \mathbf{v}_L\right) &+ \nabla\cdot\left(\rho_L g_L \mathbf{v}_L \mathbf{v}_L\right) = -\nabla p \\ &+ \nabla\cdot\left[(\mu_L) g_L\left(\nabla \mathbf{v}_L\right)\right] \\ &+ g_L \mathbf{g}\rho_{ref}(1+\beta_T(T-T_{ref})+\beta_C(C-C_{ref})) \\ &+ g_S\mathbf{g}\frac{\rho_{ref}}{1-\beta_{SL}}\end{aligned}$$

$$\mathbf{v}_S = \mathbf{v}_L + \frac{4d_g^2 g_L}{3C_d\mu_L Re}\left(-\nabla p + \frac{\rho_S}{1-\beta_{SL}}\mathbf{g}\right)$$

Model formulation
Volume averaged model

Slurry region: grains move freely in the fluid

$$g_S \leq g_S^C \qquad \mathbf{v}_S \neq 0$$

$$\mathbf{v}_S = \mathbf{v}_L + \frac{4 d_g^2 g_L}{3 C_d \mu_L Re}\left(-\nabla p + \frac{\rho_S}{1-\beta_{SL}}\mathbf{g}\right)$$

$$C_d = \frac{48 C_{ke}(1-g_L)}{Re} + C_{ie}$$
$$Re = \frac{\rho_L g_L d_g}{\mu_L}|\mathbf{v}_L - \mathbf{v}_S|$$
$$E = 0.261 Re^{0.369} - 0.105 Re^{0.431} - \frac{0.124}{1+(log_{10} Re)^2}$$

$$C_{ke} = \begin{cases} \frac{25}{6}, & g_L \leq 0.5; \\ \frac{1}{2}\left(\frac{g_L^3}{1-g_L}\right)\frac{1+4.7(1-g_L)}{1-1.83(1-g_L)}, & g_L > 0.5; \end{cases}$$

$$C_{ie} = \begin{cases} \frac{7}{3}, & g_L \leq 0.5; \\ \frac{24(10^E-1)}{Re(1-0.9(g_L-0.25)^{1/3}(1-g_L)^{2/3})^3}, & g_L > 0.5; \end{cases}$$

$$d_g = min\left(2r_g, 2\left(\frac{3}{4}\frac{g_S}{\pi N}\right)^{1/3}\right)$$

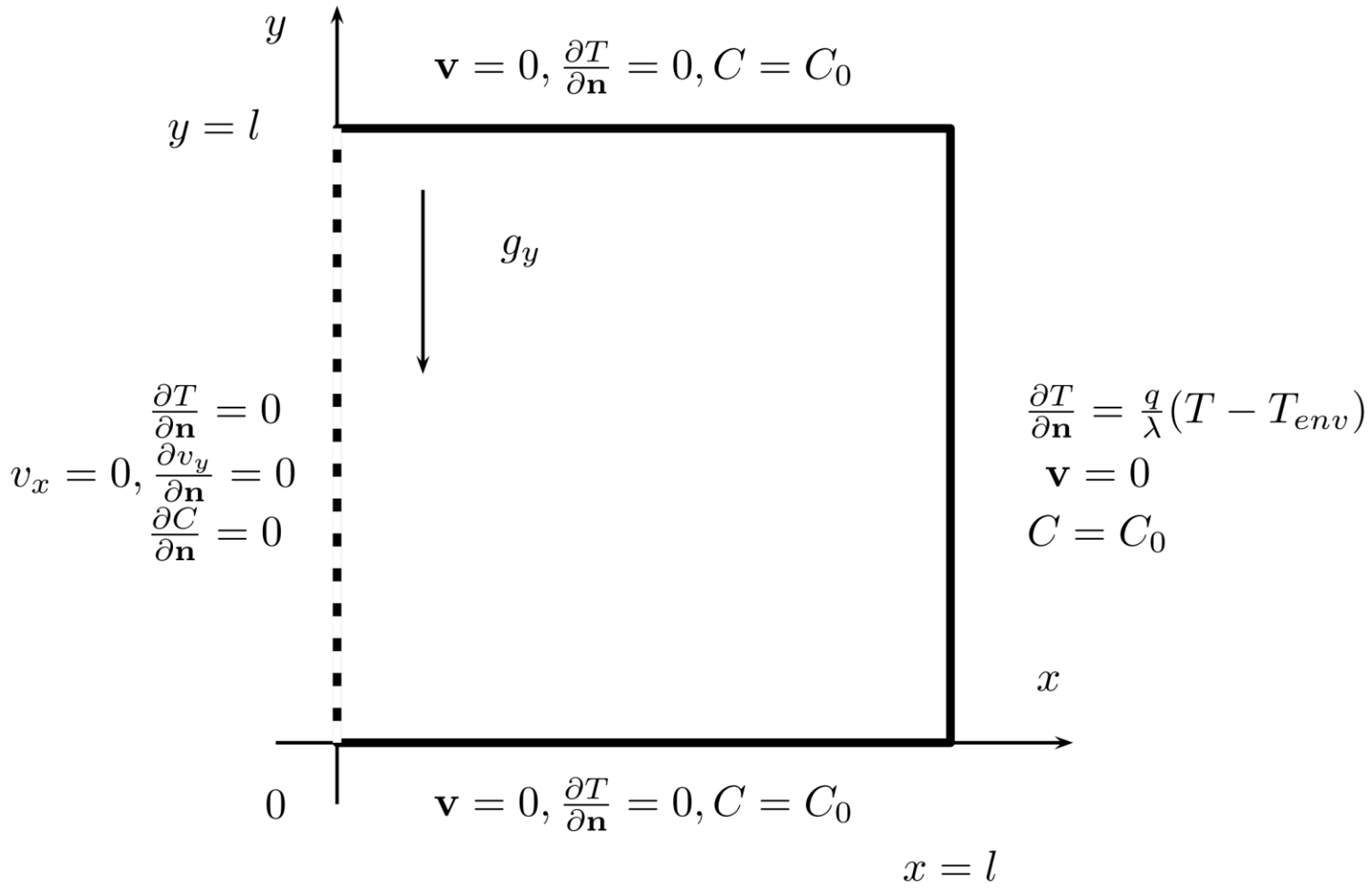
$$\frac{\partial N}{\partial t} + \nabla \cdot (\mathbf{v}_S N) = 0$$

Coupling between macroscopic model and grain growth
Založnik PhD thesis (2006), Založnik et al. Comput Mater Sci (2010)

Model formulation

Boundary and initial conditions

Schematic representation of boundary conditions



Model formulation
Microscopic model

Microsegregation model

Lever rule

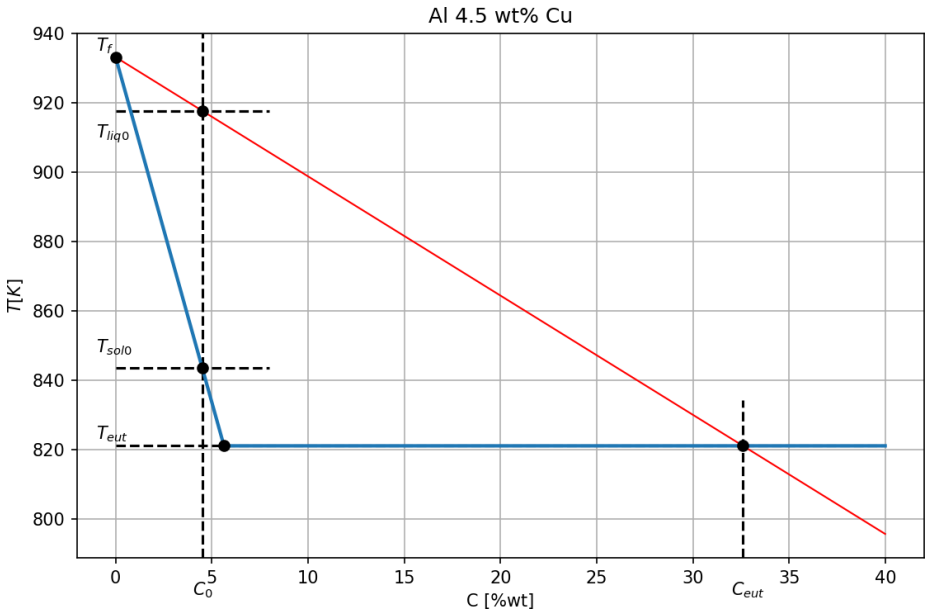
$$T_S = max(T_f - m_S C_0, T_{eut})$$

$$T_L = max(T_f - m_L C_0, T_{eut})$$

$$C_S = k_p C_L$$

$$k_p = \frac{m_L}{m_S}$$

Linearized phase diagram for Al 4.5 wt% Cu



Numerical model
Discretization

Time disretization

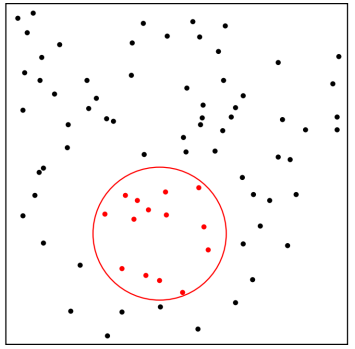
Euler explicit method

$$\frac{\partial(\rho\phi)}{\partial t} \approx \frac{\rho\phi - \rho_0\phi_0}{\Delta t}$$

Space disretization

Diffuse approximate method

$$\hat{f}_l(\mathbf{r}) = \mathbf{p}(\mathbf{r}, \mathbf{r}_l) \cdot \boldsymbol{\alpha}_l = \sum_{j=1}^{J} p_j(\mathbf{r}, \mathbf{r}_l)\alpha_{l,j}$$



Numerical model DAM

GLOBAL DOMAIN is devided into k LOCAL SUBDOMAINS.

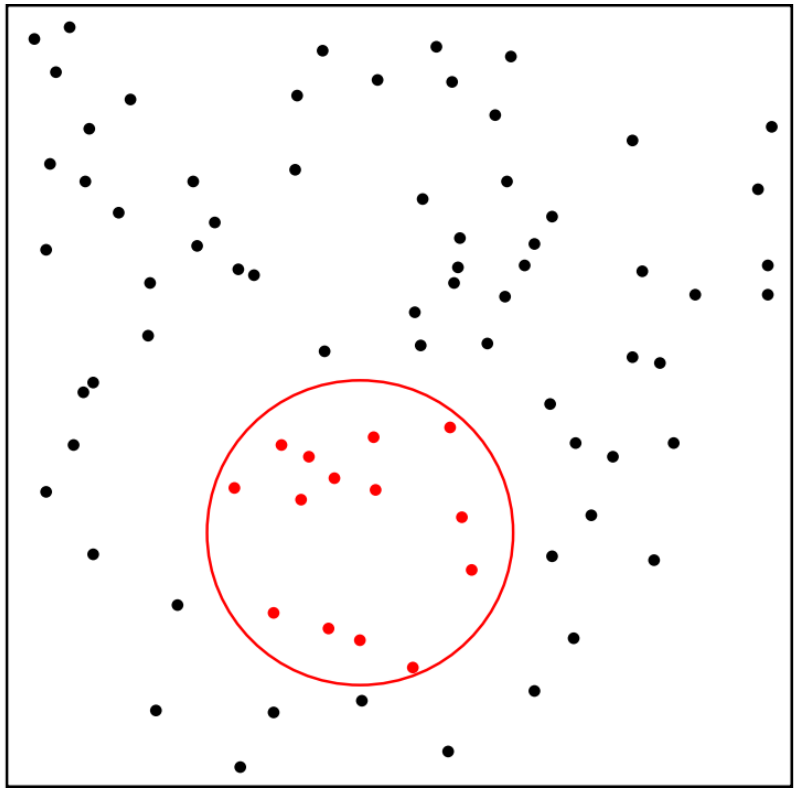
Local subdomain has N computational nodes and J basis functions (N ≥ J); N = 14, J = 6

$$\mathbf{p}(\mathbf{r},\mathbf{r}_l) = [1,(x_1-\tilde{x}_{1_l}),(x_2-\tilde{x}_{2_l}),$$
$$(x_1-\tilde{x}_{1_l})(x_2-\tilde{x}_{2_l}),(x_1-\tilde{x}_{1_l})^2,(x_2-\tilde{x}_{2_l})^2]$$

Approximation function

$$\hat{f}_l(\mathbf{r}) = \mathbf{p}(\mathbf{r},\mathbf{r}_l)\cdot\boldsymbol{\alpha}_l = \sum_{j=1}^{J} p_j(\mathbf{r},\mathbf{r}_l)\alpha_{l,j}$$

Gaussian weight function $\theta(\mathbf{r}_i,\mathbf{r}_l) = \exp\left(-c_0\frac{\|\mathbf{r}_i-\mathbf{r}_l\|^2}{{c_\sigma}^2}\right)$

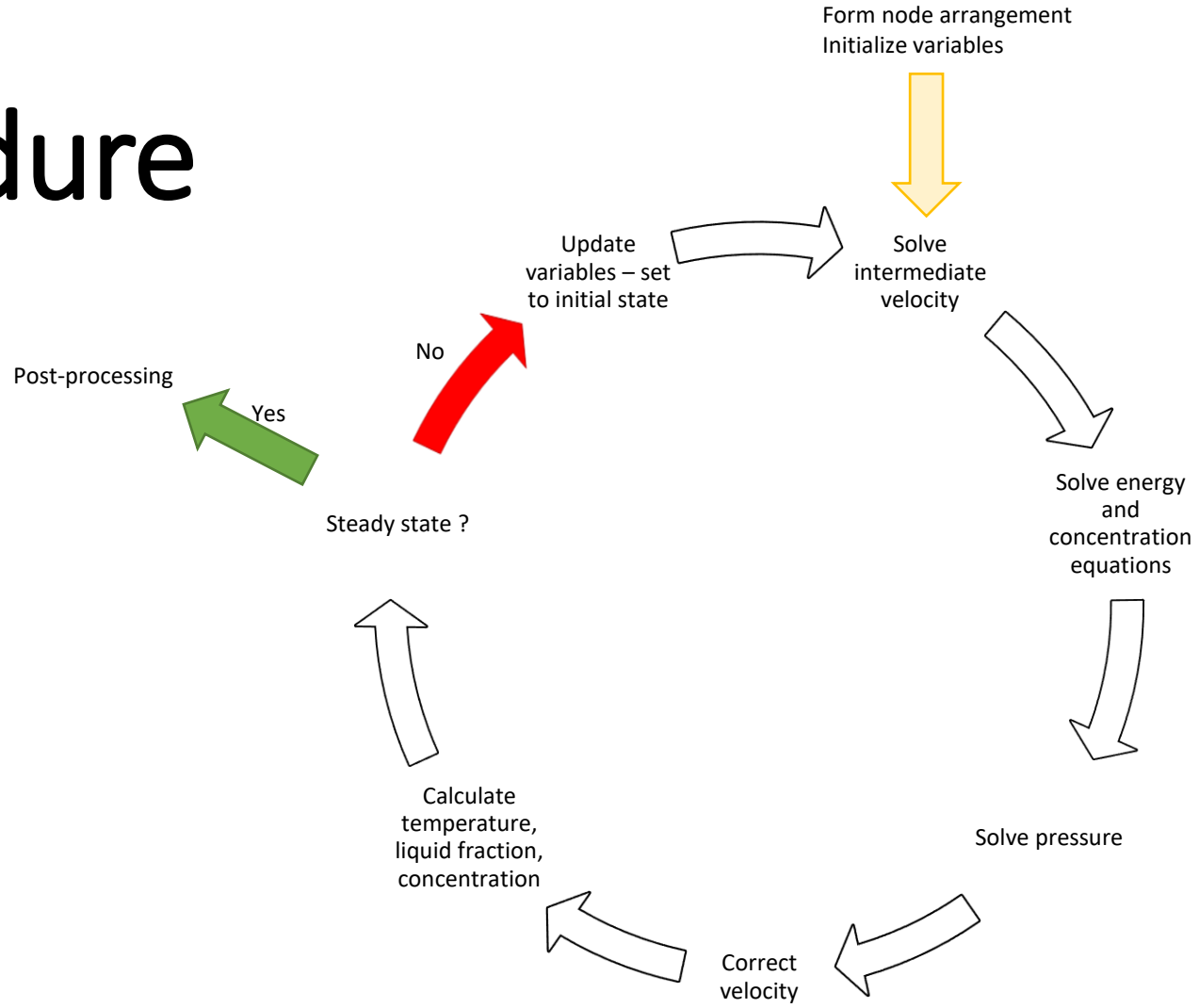


Solution procedure

Pressure-velocity coupling

Fractional step method

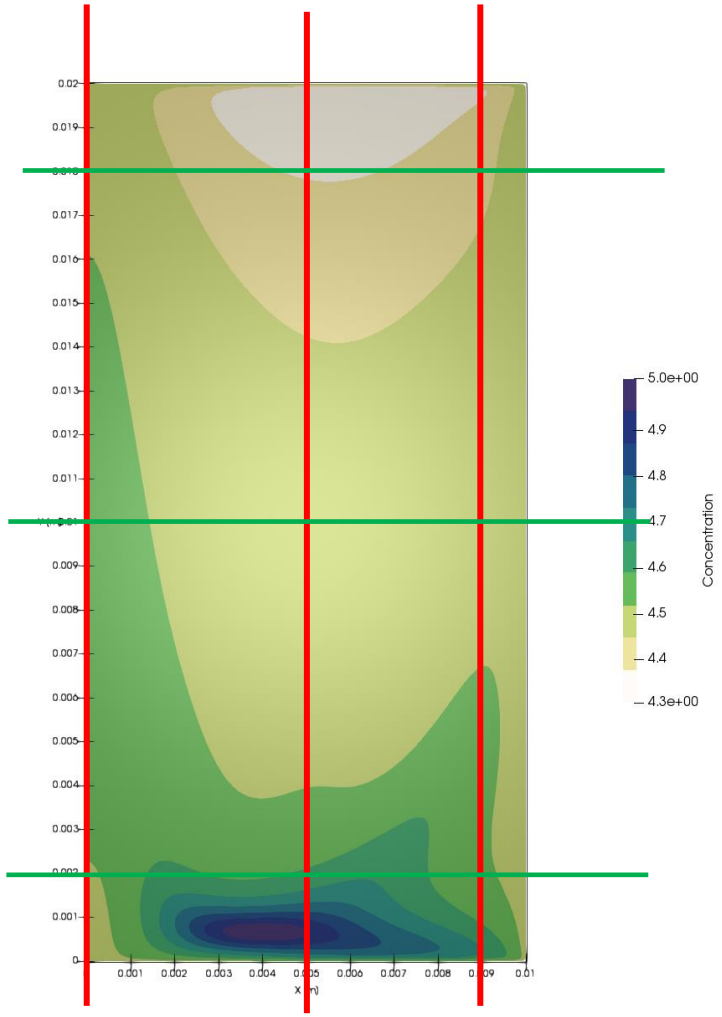
- Calculate velocity without pressure
- Solve Poisson equation for pressure
- Update velocity with pressure

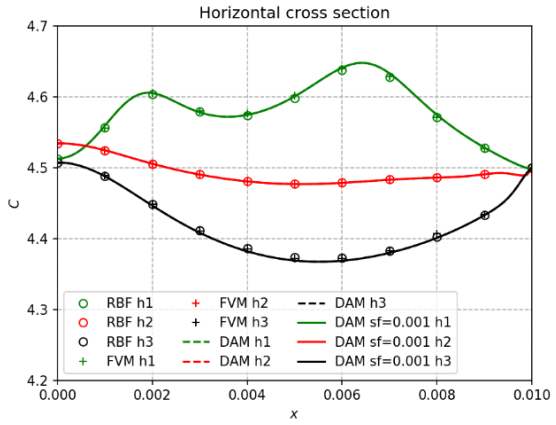


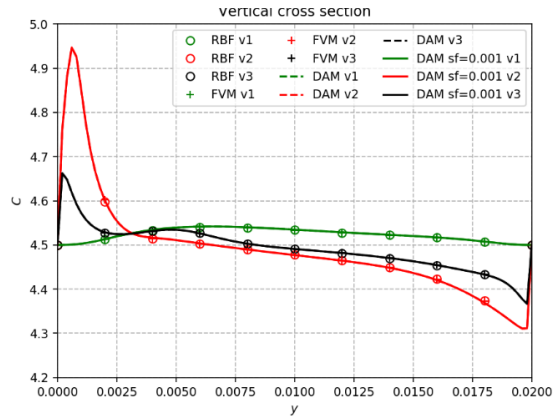
Results

The test case solidification of binary alloy with moving grains has previously been compared to the solidification of binary alloy test case.

In this presentation we focus on node arrangement density.







Solidification of binary alloy without the motion of grains
COMPARISON with
RBF, FVM: [Kosec et al. CMC, 2011]
DAM: [Hatič et al. J. *Num. Meth. Heat & Fluid Flow* (2018)]

Results

Node arrangements construction

The points in the calculational domain are constructed in such a way that we have

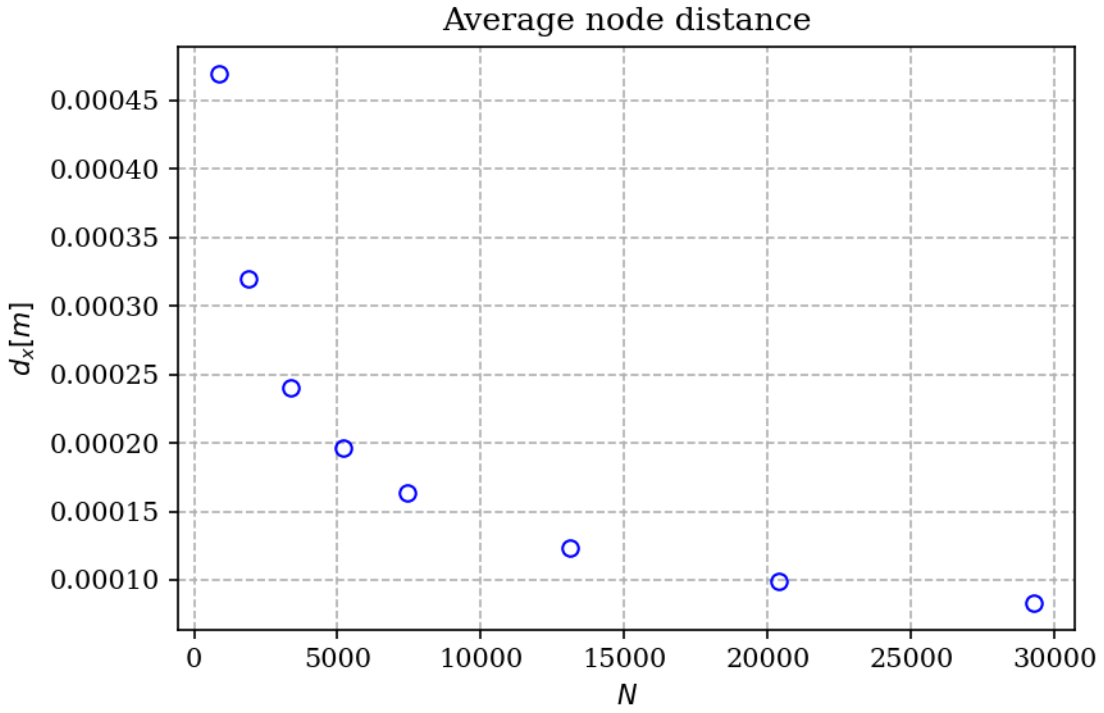
Nx points in **x direction** and

2Nx points in **y direction**.

The 4 corner points are **not included** due to the specifics of the numerical procedure.

Node arrangements

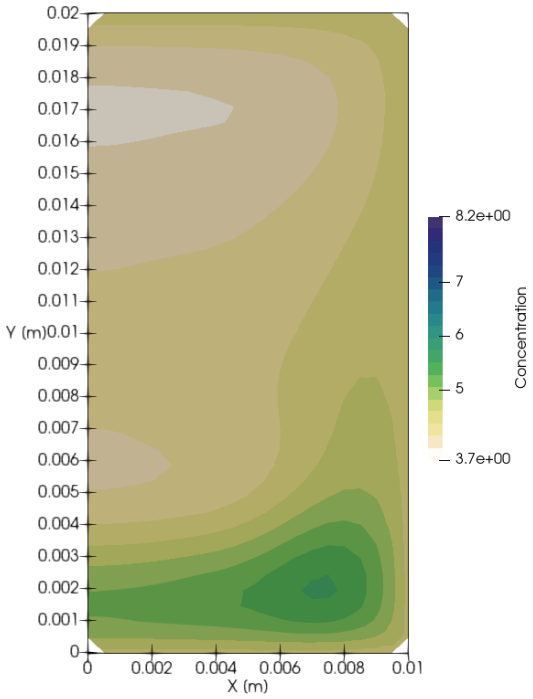
- 878
- 1918
- 3358
- 5198
- 7438
- 13118
- 20398
- 29278



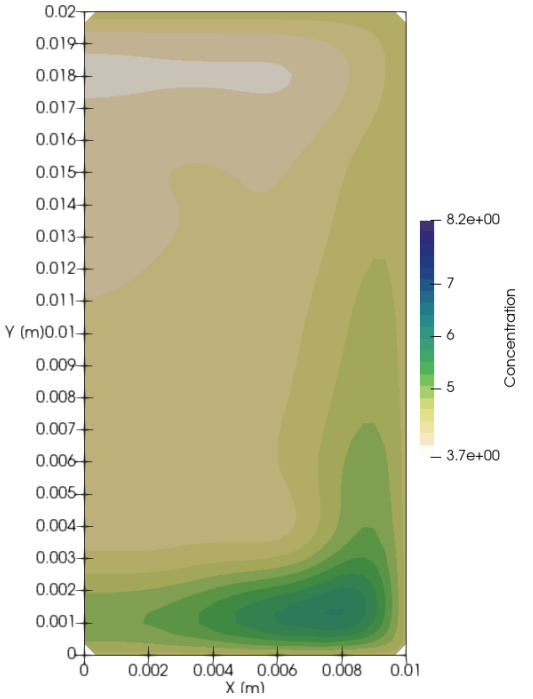
Results

Parametric study for node arrangements

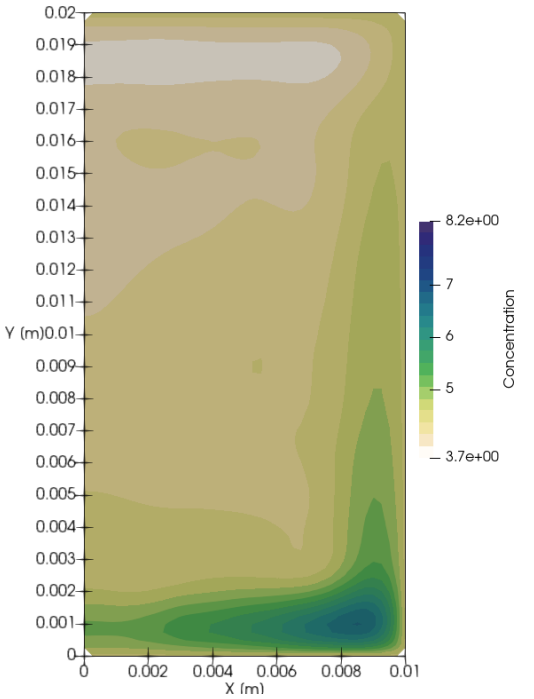
878



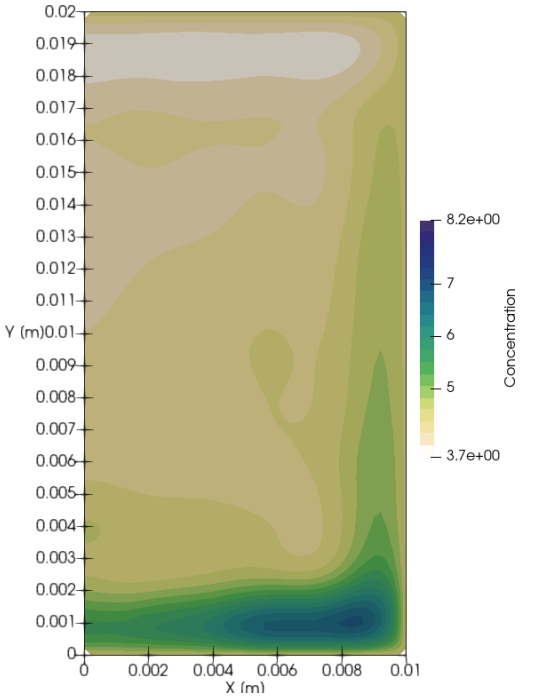
1918



3358



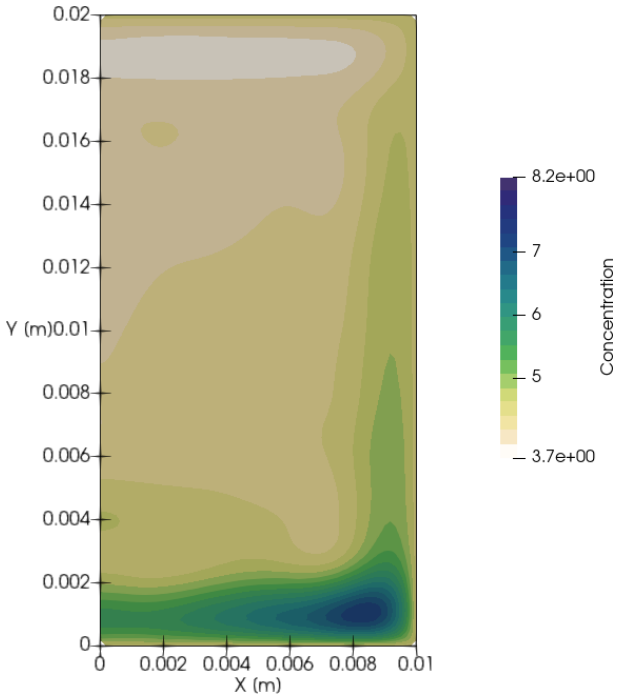
5198



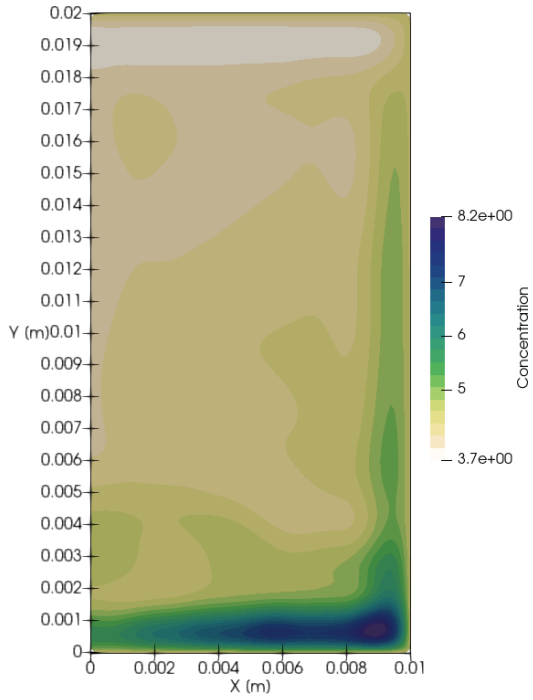
Results

Parametric study for node arrangements

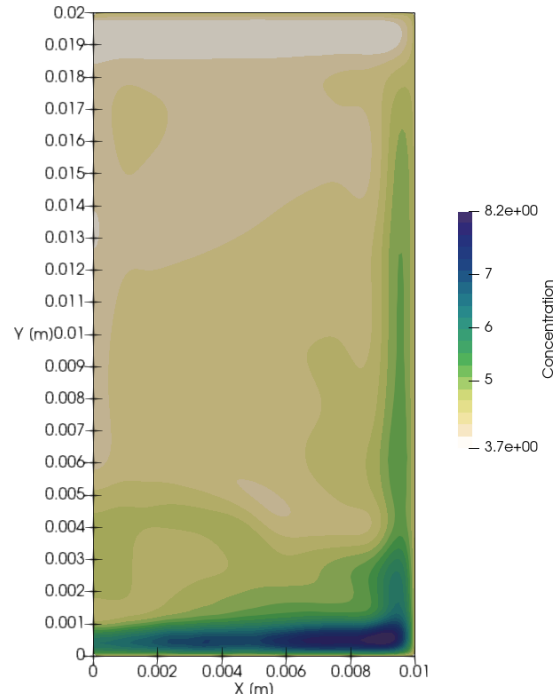
7438



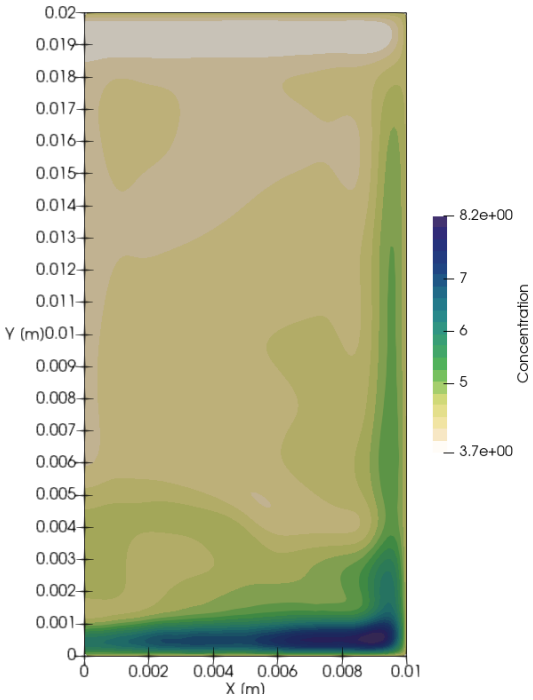
13118



20398



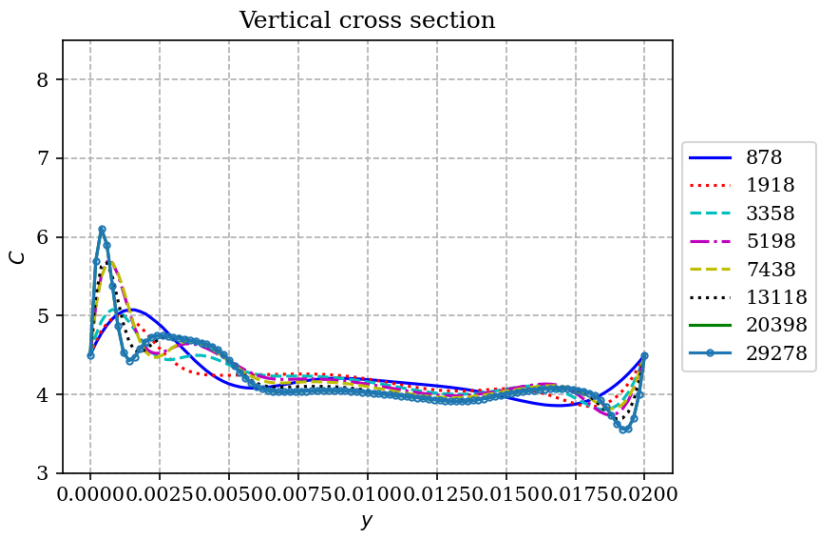
29278



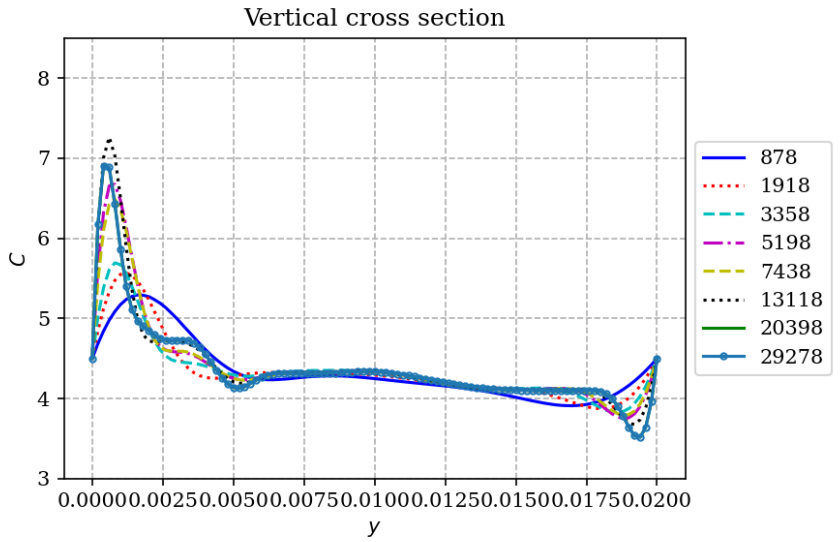
Results

Vertical cross - sections

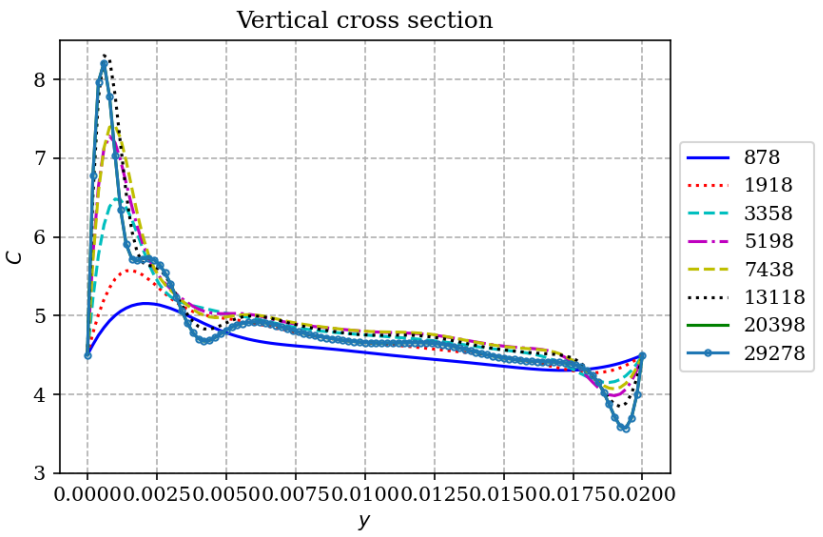
v1



v2



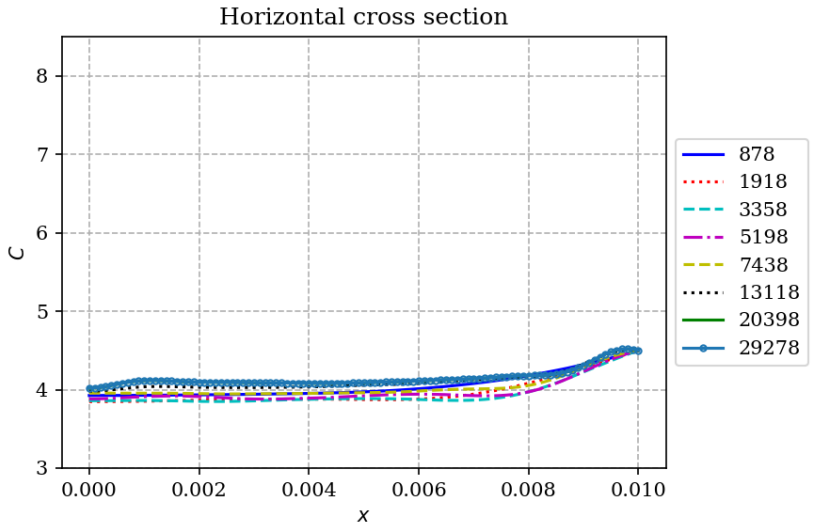
v3



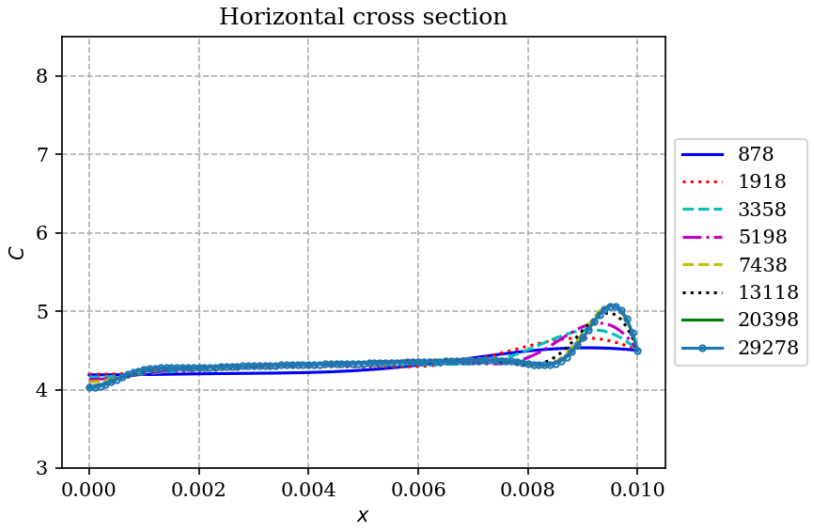
Results

Horizontal cross - sections

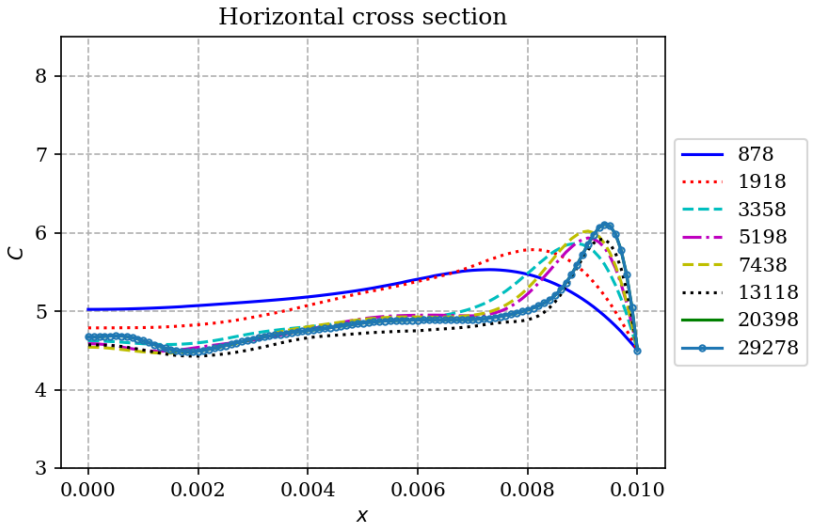
h1



h2



h3



Conclusions

Conclusions

- A meshless method has been applied to the solidification of binary alloy with moving grains
- A parametric study has been performed for various node arrangements
- In comparison to the binary alloy solidification without the moving grains, a finer node arrangement is needed to achieve node convergence
- Smaller node arrangements give a general idea of the final macrosegregation
- A finer node arrangement needs to be applied for more accurate results

Future work

Test the method on industrial cases:

- Apply the method to the DCC of aluminum and CC of steel

Acknowledegement

This research has been supported by Slovenian Grant Agency (ARRS) through program P2-0162 and project L2-9246.

Thank you for your attention!

Submitted ABSTRACT

This work describes the application of the discrete approximate meshless method with an explicit Euler time scheme for simulating grain motion during solidification of binary alloy in a square cavity. The performance of the method has previously been verified by comparing the results with reference results from literature. The volume averaged scheme based physical model couples mass, momentum, species, and energy transport equations by dividing the flow into porous region with stationary solid phase and into slurry region with free motion of solid grains. On the microscopic scale the assumption of infinitely slow diffusion is made by using the lever rule model. The coupling between pressure and velocity is solved by using the fractional step method. The effect of node arrangement density on macrosegregation pattern is analysed and discussed for the presented case.