Phase change heat and mass transfer simulation with MFEM

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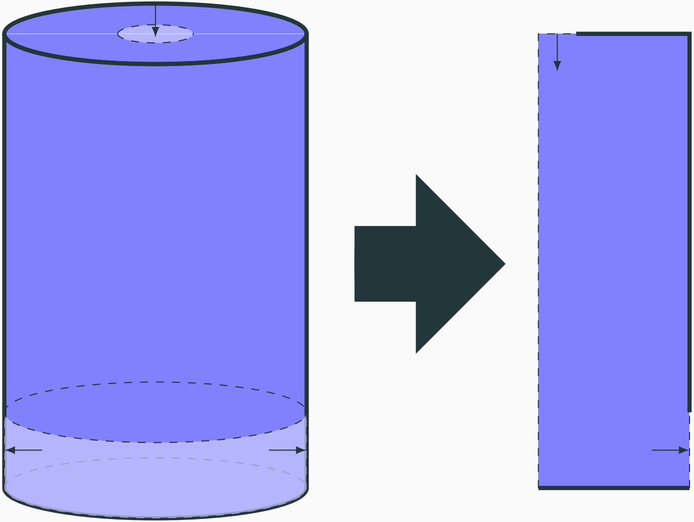
Index

1. What is a brinicle?
2. What is our mathematical model?
3. What is the structure of our implementation?
4. Which results did we obtain?

Physical phenomenon[1]

[1] BBC. Finger of death. BBC One. 2011. URL: *https://www.bbc.co.uk/programmes/p00l817b*.

Physical domain



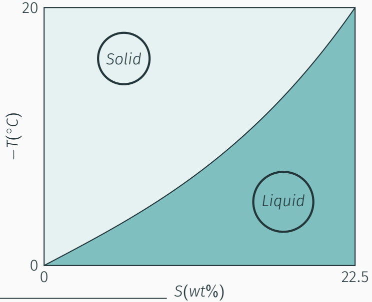
Transport equations

Heat convection-diffusion equation[2]

$$\left(\rho c + \rho L \delta(T - T_f)\right) \left(\frac{\partial T}{\partial t} + \vec{V} \cdot \vec{\nabla} T\right) - \vec{\nabla} \cdot \left(k \vec{\nabla} T\right) = 0$$

Salinity convection-diffusion equation

$$\left(\frac{\partial S}{\partial t} + \vec{V} \cdot \vec{\nabla} S\right) - \vec{\nabla} \cdot \left(d \vec{\nabla} S\right) = 0$$



[2] G. Comini, S. Del Guidice, R. W. Lewis, and O. C. Zienkiewicz. Finite element solution of non-linear heat conduction problems with special reference to phase change. International Journal for Numerical Methods in Engineering, 8(3):613–624, 1974

Flow equations

Stokes' equations [3]

$$\vec{\boldsymbol{\nabla}} \cdot \vec{V} = 0$$

$$\frac{\nu}{\eta}\vec{V} - \nu\nabla^2\vec{V} + \vec{\boldsymbol{\nabla}} p = -g\rho'\,\hat{\boldsymbol{e}}_{\boldsymbol{z}}$$

Using vorticity formulation

$$\vec{V} = -\vec{\boldsymbol{\nabla}} \times \left(\frac{\psi}{r}\hat{\boldsymbol{e}}_{\boldsymbol{\theta}}\right) \qquad \frac{\omega}{r}\hat{\boldsymbol{e}}_{\boldsymbol{\theta}} = \vec{\boldsymbol{\nabla}} \times \vec{V}$$

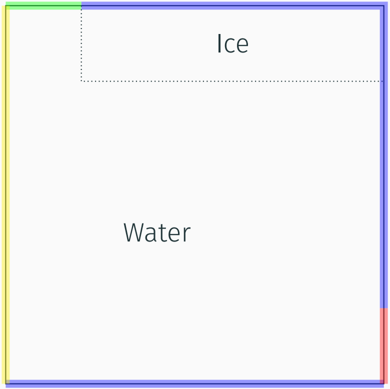
$$\omega - r^2\vec{\boldsymbol{\nabla}} \cdot \left(\frac{1}{r^2}\vec{\boldsymbol{\nabla}}\psi\right) = 0$$

$$-r^2\vec{\boldsymbol{\nabla}} \cdot \left(\frac{1}{r^2}\vec{\boldsymbol{\nabla}}\omega\right) + r^2\vec{\boldsymbol{\nabla}} \cdot \left(\frac{1}{\eta r^2}\vec{\boldsymbol{\nabla}}\psi\right) = r\frac{g}{\nu}\frac{\partial\rho'}{\partial r}$$

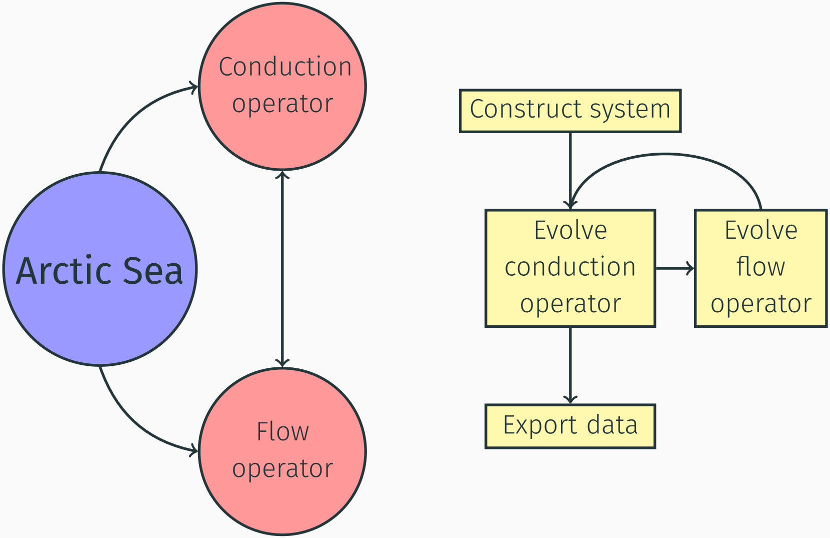
[3] H. Brinkman. A calculation of the viscous force exerted by a flowing fluid on a dense swarm of particles. Applied Scientific Research, A1:27–34, 1947.

Boundary conditions

- Closed boundary
  - $T, S \rightarrow$ Zero Neumann
  - $\psi \rightarrow$ Constant Dirichlet
  - $\omega \rightarrow$ Zero Neumann
- Symmetry boundary
  - $T, S \rightarrow$ Zero Neumann
  - $\psi, \omega \rightarrow$ Zero Dirichlet
- Inflow boundary
  - $T, S \rightarrow$ Non-zero Dirichlet
  - $\psi \rightarrow$ Non-constant Dirichlet
  - $\omega \rightarrow$ Zero Neumann
- Outflow boundary
  - $T, S \rightarrow$ Zero Neumann
  - $\psi \rightarrow$ Non-constant Dirichlet
  - $\omega \rightarrow$ Zero Neumann



Implementation diagram



Conduction operator construction

$$T = \sum_{i}^{N} \alpha_i \cdot u_i^{(T)} \qquad S = \sum_{i}^{N} \alpha_i \cdot u_i^{(S)}$$

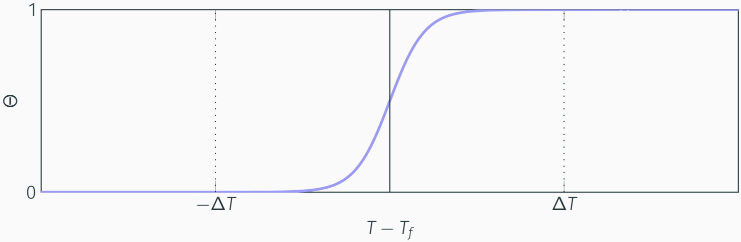
$$\overline{\overline{M}}^{(T)} \dot{\overline{u}}^{(T)} + \overline{\overline{K}}^{(T)} \overline{u} = \overline{0}$$
$$\overline{\overline{M}}^{(S)} \dot{\overline{u}}^{(S)} + \overline{\overline{K}}^{(S)} \overline{u} = \overline{0}$$

- M $\rightarrow$ Mass integrator (Latent heat)
- K $\rightarrow$ Convection and diffusion integrators

Latent heat term

Phase indicator

$$\Theta\left(T-T_f\right)=\frac{1}{2}\left(1+\tanh\left(\frac{5}{\Delta T}\left(T-T_f\right)\right)\right)$$



Dirac approximation

$$\rho L\delta\left(T-T_f\right)=\rho L\frac{\vec{\nabla}\left(T-T_f\right)\cdot\vec{\nabla}\Theta\left(T-T_f\right)}{\|\vec{\nabla}\left(T-T_f\right)\|^2+\epsilon_T}$$

Flow operator construction

$$\omega = \sum_{i}^{N} \alpha_i \cdot u_i^{(\omega)} \qquad \psi = \sum_{i}^{N} \alpha_i \cdot u_i^{(\psi)}$$

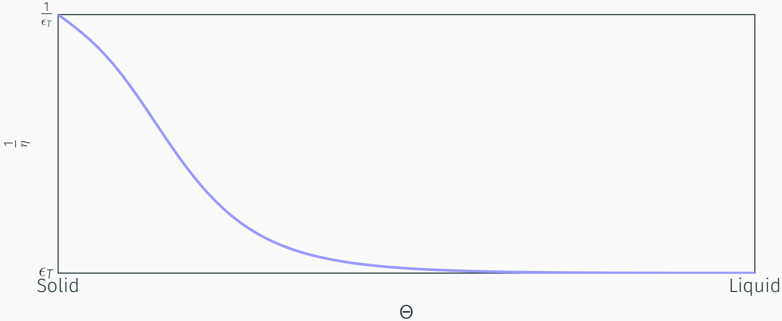
$$\begin{bmatrix} \overline{\overline{M}} & \overline{\overline{C}} \\ \overline{\overline{C}}^t & \overline{\overline{D}} \end{bmatrix} \begin{bmatrix} \overline{u}^{(\omega)} \\ \overline{u}^{(\psi)} \end{bmatrix} = \begin{bmatrix} \overline{0} \\ \overline{F} \end{bmatrix}$$

- M $\rightarrow$ Mass integrator
- C $\rightarrow$ Convection and diffusion integrators
- D $\rightarrow$ Convection and diffusion integrators from Brinkman term
- F $\rightarrow$ RHS integrator from buoyant force

Brinkman term

Carman-Kozeny equation[4]

$$\frac{1}{\eta} = \epsilon_V + \frac{\left(1 - \Theta\left(T - T_f\right)\right)^2}{\Theta\left(T - T_f\right)^3 + \epsilon_V}$$



[4] P. Carman. Fluid flow through granular beds. Transactions of the Institution of Chemical Engineers, 15:S32–S48, 1937.

Operators solvers

Conduction operator

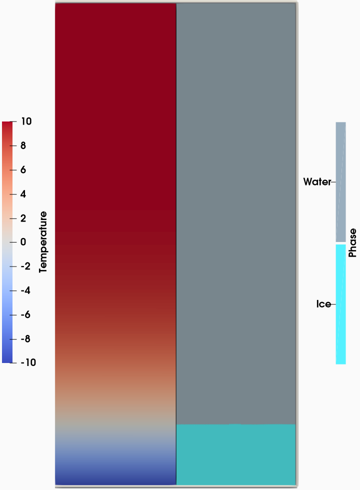
- SUNDIALS
  - ARKODE (Runge-Kutta method)
  - Variable time step
- HYPRE
  - PCG solver
  - BoomerAMG preconditioner

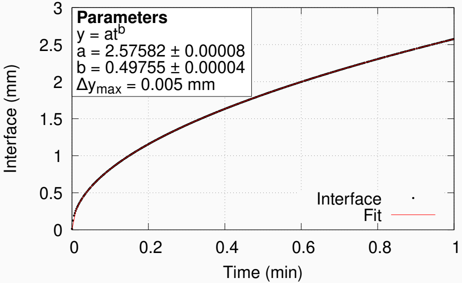
Flow operator

- SuperLU-dist
  - HypreParMatrixFromBlocks
  - Memory leak[5]
- Gradient interpolator
  - $H^1 \to ND$
  - $r\vec{V} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \vec{\boldsymbol{\nabla}}\psi$

[5] https://github.com/mfem/mfem/pull/2420.

Stefan problem[6]



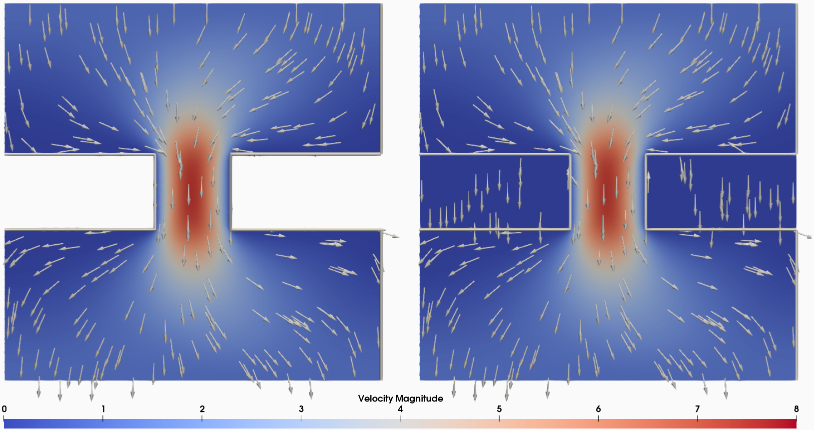


Percentage error of $a \to 0.8\%$

Percentage error of $b \to 0.5\%$

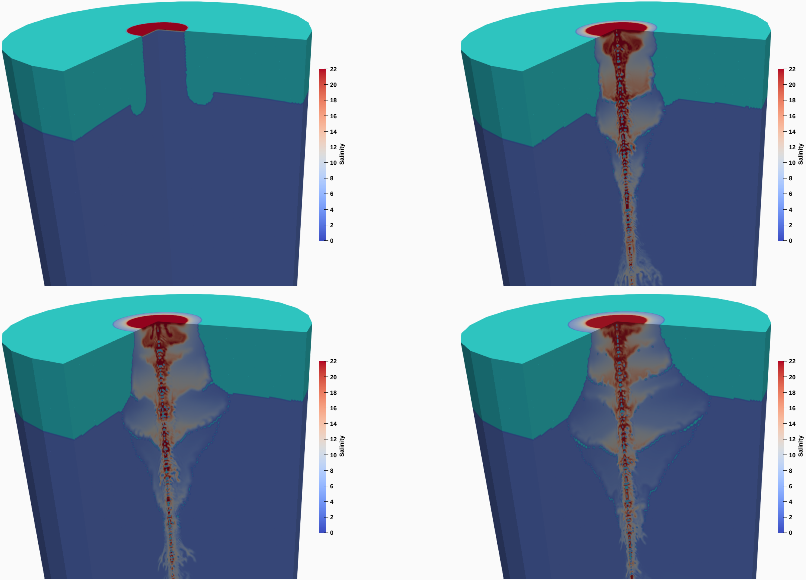
6 S. Kakaç, Y. Yener, and C. Naveira-Cotta. Heat Conduction. Fifth Edition. CRC Press. 2018. p. 393,394.

Flow with obstacles



Percentage difference $\rightarrow$ 0.0001%

Brinicle



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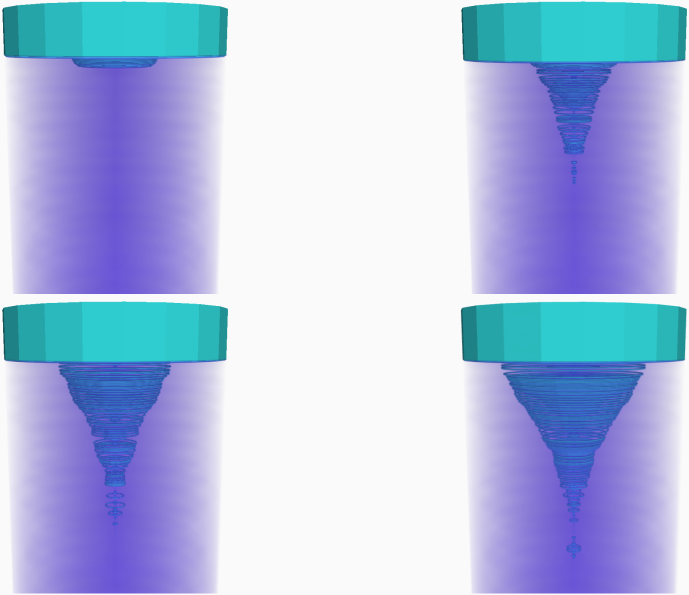
Salinity

Brinicle



Thank you for your attention!

Questions?

Operators

$$\vec{\nabla}' f(r,z) = \frac{\partial f}{\partial r}\hat{e}_r + \frac{\partial f}{\partial z}\hat{e}_z$$

$$\vec{\nabla}' \cdot \vec{f}(r,z) = \frac{\partial f_r}{\partial r} + \frac{\partial f_z}{\partial z}$$

$$\mathcal{C}(\vec{f}(r,z)) = \frac{\partial f_r}{\partial z} - \frac{\partial f_z}{\partial r}$$

$$\vec{\nabla} f(r,z) = \vec{\nabla}' f$$

$$\vec{\nabla} \cdot \vec{f}(r,z) = \frac{1}{r}\vec{\nabla}' \cdot \left(r\vec{f}\right)$$

$$\vec{\nabla} \times \vec{f}(r,z) = \frac{1}{r}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\vec{\nabla}'\left(rf_\theta\right) + \mathcal{C}(\vec{f})\hat{e}_\theta$$

Transformed equations

$$r\left(\rho c + \rho L \delta(T - T_f)\right)\left(\frac{\partial T}{\partial t} + \vec{V} \cdot \vec{\nabla}' T\right) - \vec{\nabla}' \cdot \left(r k \vec{\nabla}' T\right) = 0$$

$$r\left(\frac{\partial S}{\partial t} + \vec{V} \cdot \vec{\nabla}' S\right) - \vec{\nabla}' \cdot \left(r d \vec{\nabla}' S\right) = 0$$

$$\omega - r\vec{\nabla}' \cdot \left(\frac{1}{r}\vec{\nabla}' \psi\right) = 0$$

$$-r\vec{\nabla}' \cdot \left(\frac{1}{r}\vec{\nabla}' \omega\right) + r\vec{\nabla}' \cdot \left(\frac{1}{\eta r}\vec{\nabla}' \psi\right) = r\frac{g}{\nu}\frac{\partial \rho'}{\partial r}$$

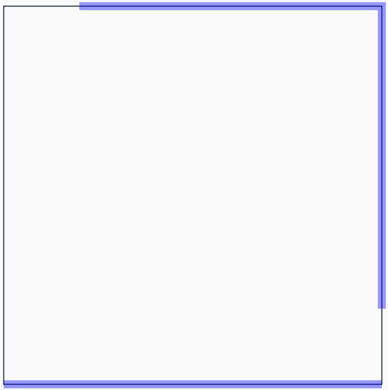
Closed boundary

$$\vec{\boldsymbol{\nabla}}' T \cdot \hat{\boldsymbol{n}} = 0$$

$$\vec{\boldsymbol{\nabla}}' S \cdot \hat{\boldsymbol{n}} = 0$$

$$\psi = 0$$

$$\vec{\boldsymbol{\nabla}}' \omega \cdot \hat{\boldsymbol{n}} = 0$$



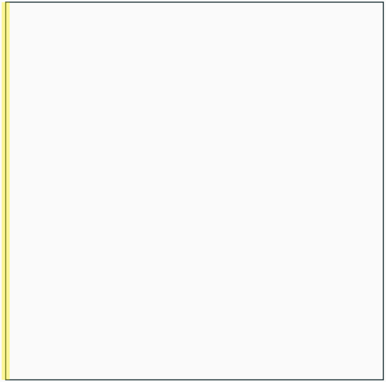
Symmetry boundary

$$\vec{\boldsymbol{\nabla}}' T \cdot \hat{\boldsymbol{n}} = 0$$

$$\vec{\boldsymbol{\nabla}}' S \cdot \hat{\boldsymbol{n}} = 0$$

$$\psi = 0$$

$$\omega = 0$$



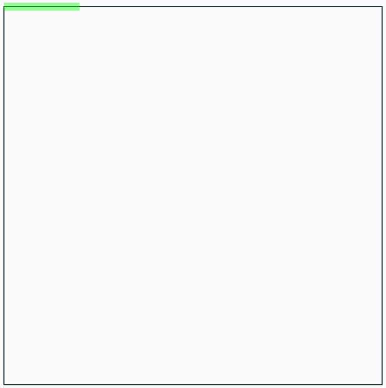
Inflow boundary

$$T = T_{brine}$$

$$S = S_{brine}$$

$$\psi = Q \left(\frac{r}{l_{in}} \right)^2 \left(2 - \left(\frac{r}{l_{in}} \right)^2 \right)$$

$$\vec{\nabla}' \omega \cdot \hat{n} = 0$$



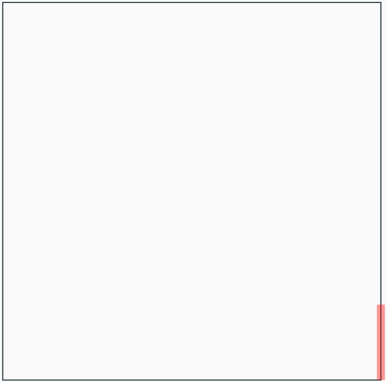
Outflow boundary

$$\vec{\nabla}' T \cdot \hat{n} = 0$$

$$\vec{\nabla}' S \cdot \hat{n} = 0$$

$$\psi = Q \left(\frac{z}{l_{out}} \right)^2 \left(3 - 2 \frac{z}{l_{out}} \right)$$

$$\vec{\nabla}' \omega \cdot \hat{n} = 0$$



Conduction operator integrators

$$\overline{\overline{M}}^{(T)}\dot{\overline{u}}^{(T)} + \overline{\overline{K}}^{(T)}\overline{u} = \overline{0}$$

$$\overline{\overline{M}}^{(S)}\dot{\overline{u}}^{(S)} + \overline{\overline{K}}^{(S)}\overline{u} = \overline{0}$$

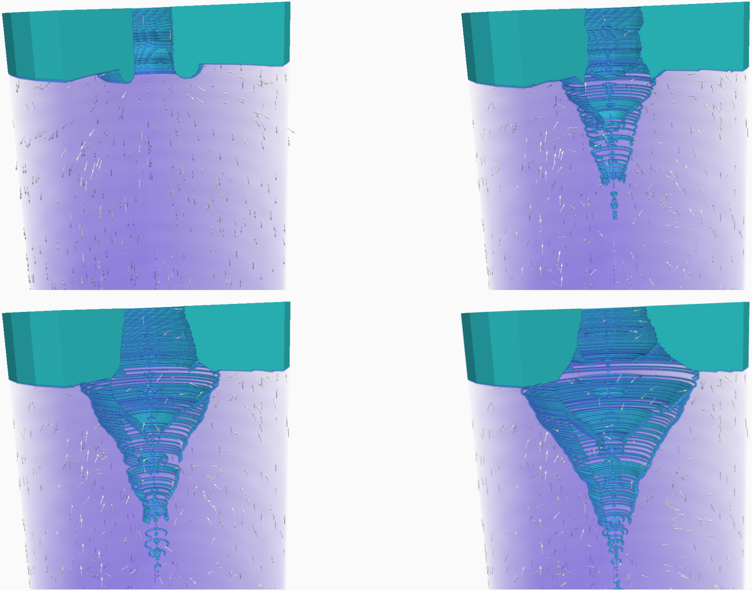
$$\begin{aligned}
M_{i,j}^{(T)} &= \left\langle r\left(\rho c + \rho L \delta\left(T - T_f\right)\right)\alpha_j,\, \alpha_i\right\rangle_{\Omega'} \\
M_{i,j}^{(S)} &= \left\langle r\alpha_j,\, \alpha_i\right\rangle_{\Omega'} \\
K_{i,j}^{(T)} &= \left\langle r\left(\rho c + \rho L \delta\left(T - T_f\right)\right)\vec{V}\cdot\vec{\boldsymbol{\nabla}}'\alpha_j,\, \alpha_i\right\rangle_{\Omega'} + \left\langle rk\vec{\boldsymbol{\nabla}}'\alpha_j,\, \vec{\boldsymbol{\nabla}}'\alpha_i\right\rangle_{\Omega'} \\
K_{i,j}^{(S)} &= \left\langle r\vec{V}\cdot\vec{\boldsymbol{\nabla}}'\alpha_j,\, \alpha_i\right\rangle_{\Omega'} + \left\langle rd\vec{\boldsymbol{\nabla}}'\alpha_j,\, \vec{\boldsymbol{\nabla}}'\alpha_i\right\rangle_{\Omega'}
\end{aligned}$$

Flow operator integrators

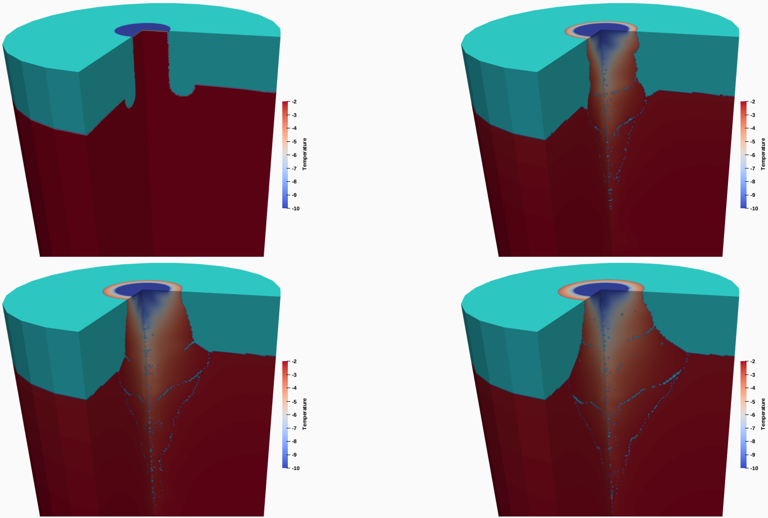
$$\begin{bmatrix} \overline{\overline{M}} & \overline{\overline{C}} \\ \overline{\overline{C}}^t & \overline{\overline{D}} \end{bmatrix} \begin{bmatrix} \overline{u}^{(\omega)} \\ \overline{u}^{(\psi)} \end{bmatrix} = \begin{bmatrix} \overline{0} \\ \overline{F} \end{bmatrix}$$

$$\begin{aligned}
M_{i,j} &= \left\langle \alpha_j,\, \alpha_i \right\rangle_{\Omega'} \\
C_{i,j} &= \left\langle \vec{\nabla}' \alpha_j,\, \vec{\nabla}' \alpha_i \right\rangle_{\Omega'} + \left\langle \frac{\hat{r}}{r} \cdot \vec{\nabla}' \alpha_j,\, \alpha_i \right\rangle_{\Omega'} \\
D_{i,j} &= \left\langle -\frac{1}{\eta} \vec{\nabla}' \alpha_j,\, \vec{\nabla}' \alpha_i \right\rangle_{\Omega'} + \left\langle -\frac{\hat{r}}{\eta r} \cdot \vec{\nabla}' \alpha_j,\, \alpha_i \right\rangle_{\Omega'} \\
F_i &= \left\langle r \frac{g}{\nu} \frac{\partial \rho'}{\partial r},\, \alpha_i \right\rangle_{\Omega'}
\end{aligned}$$

Brinicle



Brinicle



Equipment

- System $\rightarrow$ Debian 9
- Compiler $\rightarrow$ GCC 11.1.0
- Proccesors $\rightarrow$ Intel(R) Xeon(R) Gold 6130 CPU @ 2.10GHz
- RAM $\rightarrow$ 256 Gb