HPC @LMRS: on superfluids and phase change materials.

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Outline

Quantum turbulence exploration

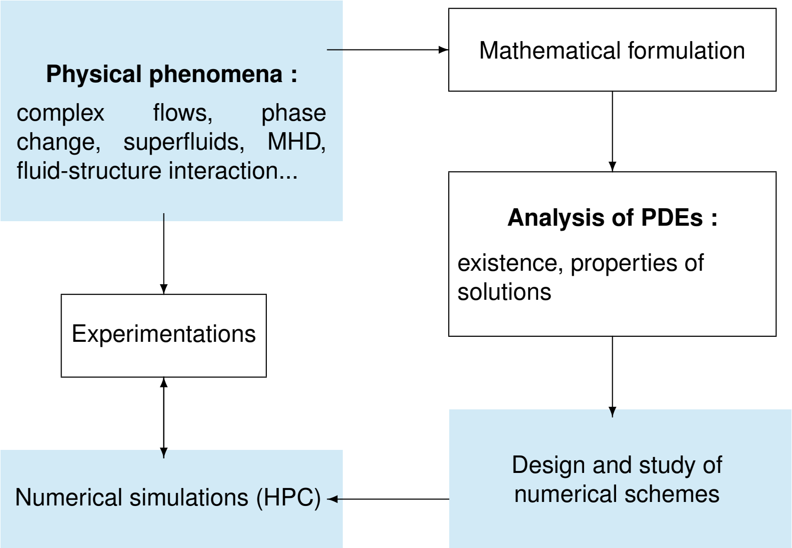
- Our project
- Gross-Pitaevskii equation
- Real time problem
- Imaginary time problem

Phase change materials

- Our project
- Model and equations
- Solution method
- Validations and simulations

Conclusion

Numerical simulation of complex physical phenomena



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Quantum turbulence exploration
- Our project
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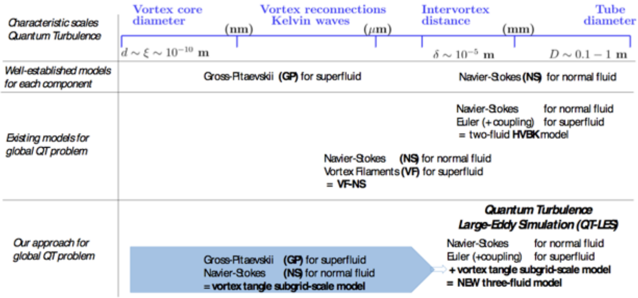
Conclusion

Quantum turbulence exploration

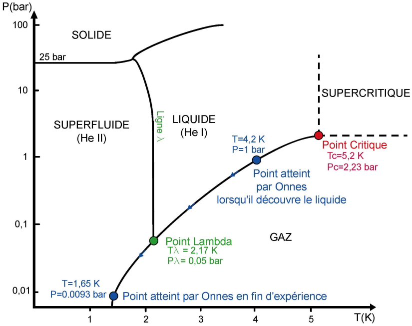
- Different successive projects/collaborations...
  - ANR project BECASIM (2013-2017), more focused on Bose-Einstein condensate)
  - ANR project QUTE-HPC (2019-2022)
- ... involving many people from different communities
  - I. Danaila, I. Ciotir, C. Lothodé, F. L. ,
  - M. Brachet, L. Danaila, E. Lévêque, Ph.-E. Roche.



ANR Project QUTE-HPC : QUantum Turbulence Exploration by High-Performance Computing

Quantum Turbulence (QT) :

- multi-scale, multi-physics phenomenon,
- in (super) cold systems (Bose-Einstein condensate, superfluid Helium),
- coexistence of a "normal" fluid (viscous) and a superfluid (no viscosity).



Framework

Superfluid (very small scales) :

- Gross-Pitaevskii equation (non linear Schrödinger)

$$i\partial_t \psi = -\frac{1}{2}\Delta\psi + V(\mathbf{x})\psi + \beta|\psi|^2\psi - i\Omega L_z\psi$$

- GPS code (for Gross-Pitaevskii Simulator) : spectral or high-order compact FD scheme.

"Normal" fluid :

- Navier-Stokes equations

$$\nabla \cdot u = 0$$
$$\partial_t u + u\nabla u - \nu\Delta u = -\nabla p$$

Is it possible to design models and numerical methods to couple all possible scales ?

Superfluid = fluid without viscosity ?

Gross-Pitaevskii equation (for QT) :

$$i\partial_t\psi = -\frac{1}{2}\Delta\psi + \beta|\psi|^2\psi$$

Where are the hydrodynamic quantities ?

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$$i\partial_t\psi = -\frac{1}{2}\Delta\psi + \beta|\psi|^2\psi$$

Where are the hydrodynamic quantities ?

Madelung transformation

$$\psi = \sqrt{\rho}e^{i\theta}$$

- ρ is the density of the fluid,
- $\mathbf{u} := \nabla\theta$ is the velocity,
- creation of vortices in the superfluid (topological defects),
- circulation is quantized,
- recover Euler-like equations

$$\partial_t\rho + \nabla\cdot(\rho\mathbf{u}) = 0,$$
$$\partial_t(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\mathbf{u}) = \mathbf{g},$$

g more complicated than in Euler equations.

First step : GP only

GPS code :

- spatial : spectral method with periodic BC, or 6th order compact FD scheme (periodic or Dirichlet BC),
- real-time simulations : second order ADI time-splitting,
- imaginary-time simulations : full Newton method or semi-implicit backwards Euler,
- two levels of parallelization : MPI and OpenMP,
- pencil distribution of the grid.

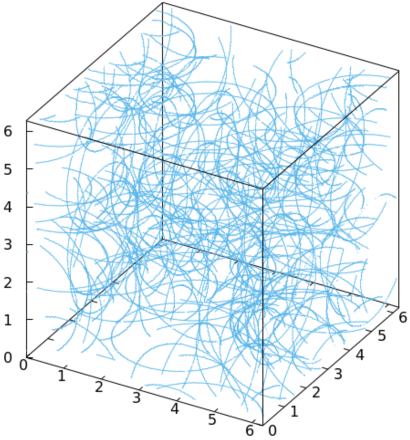
Generation of QT

Are there connections, similarities between QT and classical turbulence ?

- Test different initial conditions (with or without vortices),
- Run GPS code,
- Get accurate and relevant diagnostics : energy spectra, structure functions, helicity,...
- Comparison between physical settings ?
- Need for benchmarks !

Random vortex rings

At $t = 0$, ψ is made of 50 pairs of vortex rings (randomly set in the domain)



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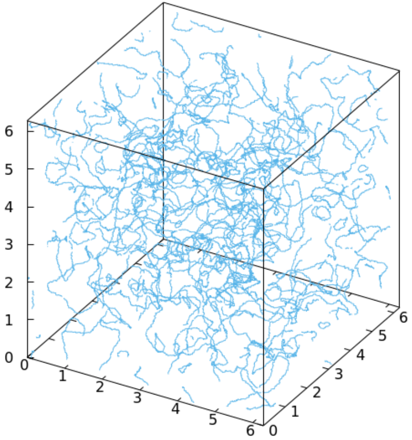

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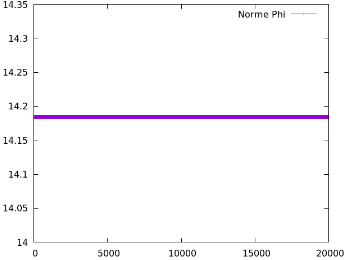

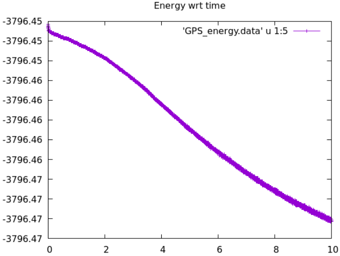

Good conservation of norm and energy !

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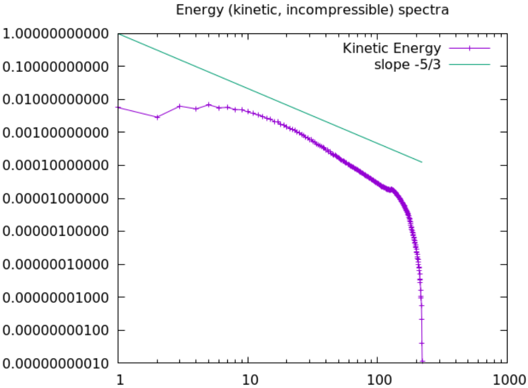
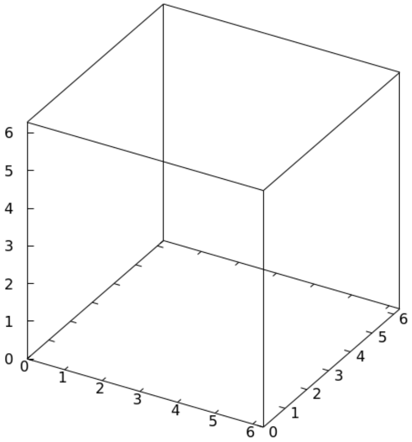


Comparisons in progress with M. Kobayashi (Kyoto).

Smooth random phase

At $t = 0$, $\psi = e^{i\theta}$ with θ cubic splines from 64 random values. **No vortex at $t = 0$!**



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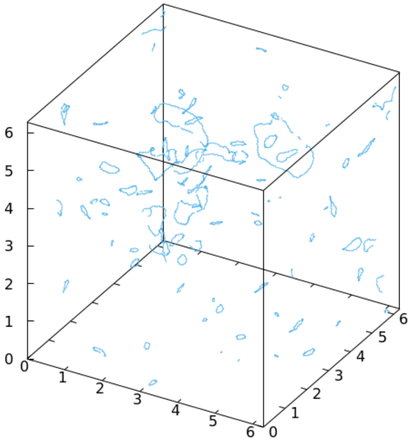

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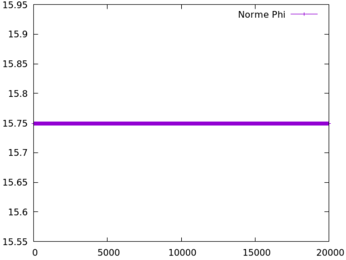

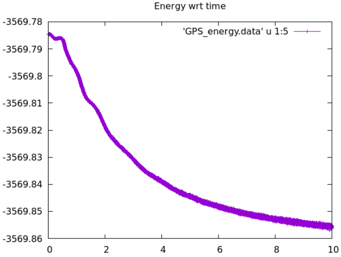

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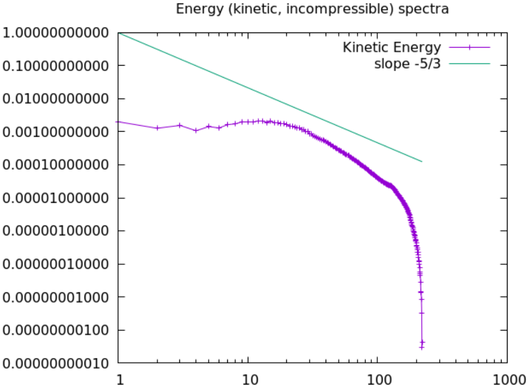

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Mimicking classical flows

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Set $\mathbf{u}^{adv}$ a "target velocity" and minimize the energy

$$\mathcal{J}(\psi) := \int_\Omega \frac{1}{2}|\nabla\psi - i\, u^{adv}\psi|^2 + \frac{\beta}{2}\left(|\psi|^2 - 1\right)^2.$$

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Gradient flow method : introduce imaginary-time (pseudo time) and solve the problem until steady state is achieved :

$$\partial_t\phi - \frac{1}{2}\Delta\phi + \beta|\phi|^2\phi - \beta\phi + \frac{\|\mathbf{u}^{adv}\|^2}{2}\phi - i\mathbf{u}^{adv}\cdot\nabla\phi = 0.$$

Then use ϕ as initial state for real-time GP.

Imaginary time scheme

Originally in GPS :

- Semi-implicit backwards Euler (Bao et al.)

$$\frac{\phi_{n+1}-\phi_n}{\delta t}-\frac{1}{2}\Delta\phi_{n+1}+\beta|\phi_n|^2\phi_{n+1}-\beta\phi_{n+1}+\frac{\|\mathbf{u}^{adv}\|^2}{2}\phi_{n+1}-i\mathbf{u}^{adv}\cdot\nabla\phi_{n+1}=0.$$

- Full Newton method

$$\frac{\phi_{n+1}-\phi_n}{\delta t}-\frac{1}{2}\Delta\phi_{n+1}+\beta|\phi_{n+1}|^2\phi_{n+1}-\beta\phi_{n+1}+\frac{\|\mathbf{u}^{adv}\|^2}{2}\phi_{n+1}-i\mathbf{u}^{adv}\cdot\nabla\phi_{n+1}=0.$$

- Systems preconditionned by diagonal terms in physical space (Antoine & Dubosq),
- + renormalization (for BEC).

For our cases, sufficient to use simpler semi-implicit scheme, and no renormalization :

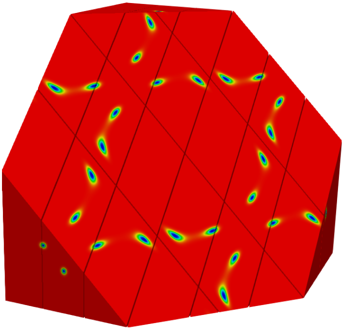
$$\frac{\phi_{n+1}-\phi_n}{\delta t}-\frac{1}{2}\Delta\phi_{n+1}+\beta|\phi_n|^2\phi_n-\beta\phi_n+\frac{\|\mathbf{u}^{adv}\|^2}{2}\phi_n-i\mathbf{u}^{adv}\cdot\nabla\phi_n=0.$$

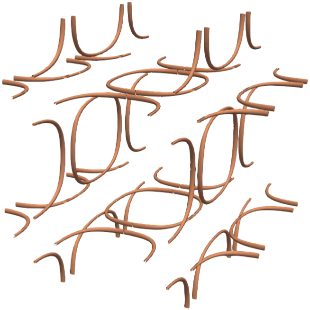
Taylor-Green flow

$\mathbf{u}^{adv}$ defined by :

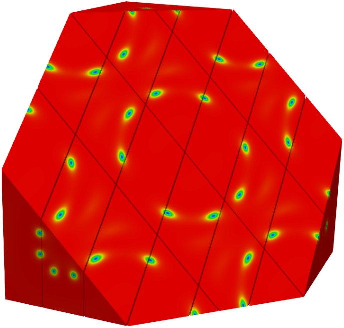
$$\mathbf{u}^{adv} = \begin{pmatrix} \sin(x)\cos(y)\cos(z) \\ \cos(x)\sin(y)\cos(z) \\ 0 \end{pmatrix}$$

$\psi_{|t=0}$ contains vortices with winding number 3.





Taylor-Green flow (cont'd)



	E_k^i	E_k^c	E_q	E_i
GPS	0.129 567	0.000 272	0.007 804 1	0.013 0279
MB	0.129 570	0.000 272	0.007 804	0.013 028

Energies computed at the end of imaginary time run : GPS computation (top) vs. data from M. Brachet (bottom).

Perspectives

This work was performed using computing resources of CRIANN (Normandie)

- GPS will be able to run interesting cases of QT,
- resolution up to 4096^3,
- good agreement with other codes (MK, MB).

A lot of ongoing work :

- check energy spectra, structure function, ...
- link between QT and CT ?
- how to integrate GP+NS ? (at different scales)

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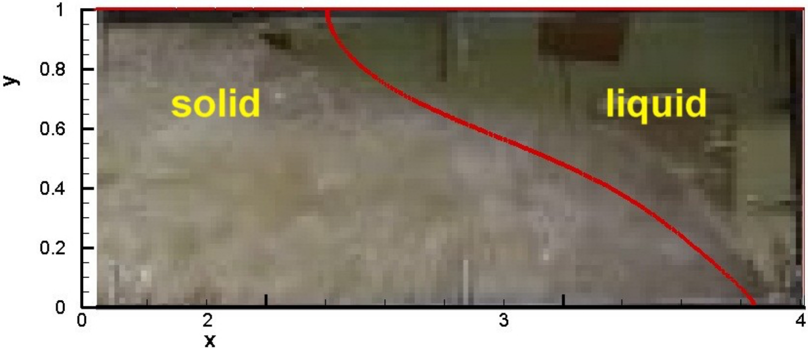
Phase change materials

- Different successive projects/collaborations...
  - (Regional) project M2NUM (2015-2019)
  - RIN M2SiNUM (2018-2021)
  - Collaborations with Orange Labs
- ... involving many people from different communities
  - I. Danaila, P. Jolivet, C. Lothodé, F. L., A. Rakotondrandisa, G. Sadaka, P-H. Tournier,
  - L. Danaila, E. Varea,
  - S. Le Masson.

Phase changing materials (PCM) : what for ?



Orange labs, Lannion, France.

- passive thermal regulation (buildings, tablets e.g.),
- energy storage ?
- need a better understanding of the mechanisms.

Navier-Stokes-Boussinesq approximation + Enthalpy model

Single domain approach (dimensionless equations)

$$
\begin{aligned}
\nabla \cdot \mathbf{u} &= 0, \\
\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p - \frac{1}{\mathrm{Re}} \nabla^2 \mathbf{u} - f_B(\theta)\, \mathbf{e}_y &= A(\theta)\mathbf{u}, \\
\frac{\partial (C\theta)}{\partial t} + \nabla \cdot (C\theta \mathbf{u}) - \frac{K}{\mathrm{Pr}\ \mathrm{Re}} \nabla^2 \theta + \frac{\partial (CS(\theta))}{\partial t} &= 0.
\end{aligned}
$$

Navier-Stokes-Boussinesq approximation + Enthalpy model

Single domain approach (dimensionless equations)

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- *liquid-solid interface at* $\theta = 0$*,*
- $f_B(\theta)$ *: linearized Boussinesq force*
- $A(\theta)$ *: penalty term*
- C, K *possibly depend on* θ
- *S, A discontinuous functions* $\rightsquigarrow$ *regularization for the simulations (*tanh*)*
- *huge variations in the coefficients* $\rightsquigarrow$ *stiff problems*
- $A = -C_{CK}\dfrac{(1-\lambda(\theta))^2}{\lambda(\theta)^3 + b}$

Numerical methods

Space and time discretization

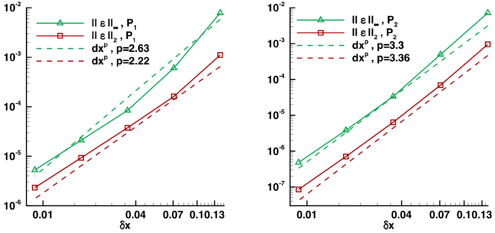
- Taylor-Hood triangular finite elements, i.e. $\mathbb{P}_2$ for the velocity, $\mathbb{P}_1$ for the pressure and $\mathbb{P}_1/\mathbb{P}_2$ for the temperature,
- Second-order in time : Gear implicit scheme :

$$\frac{\partial \phi}{\partial t} \simeq \frac{3\phi^{n+1} - 4\phi^{n} + \phi^{n-1}}{2\delta t},$$

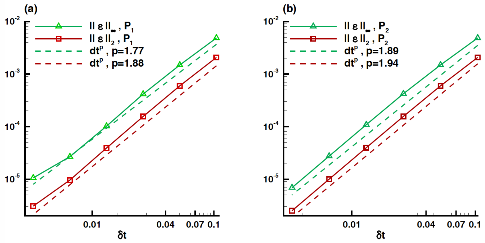
- Newton method for the nonlinear terms,
- Mesh adaptation at each step,
- Implementation with FreeFem++.

Academic test cases (natural convection solver)

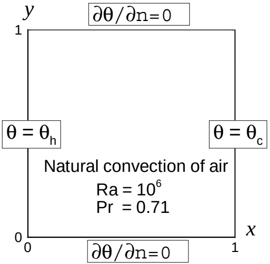
Space accuracy (Burggraf manufactured solution)

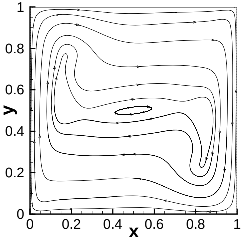


Time accuracy (Nourgaliev time-dependent solution)

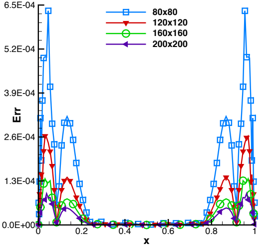


Natural convection only

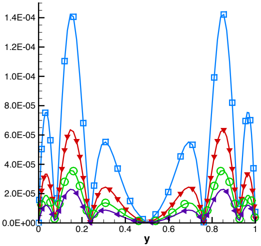




(a)

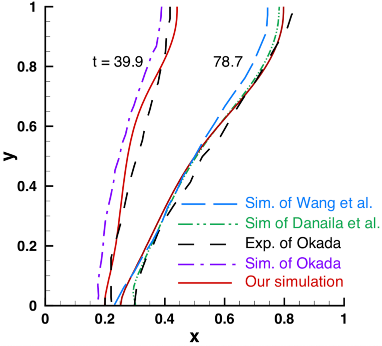


(b)



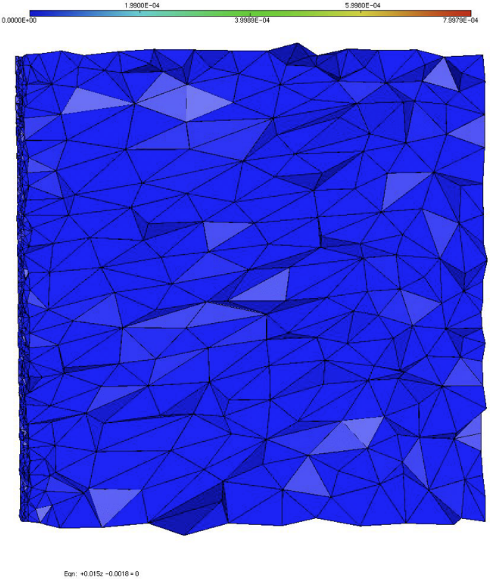
2D melting of PCM

Same setting, but adding phase change

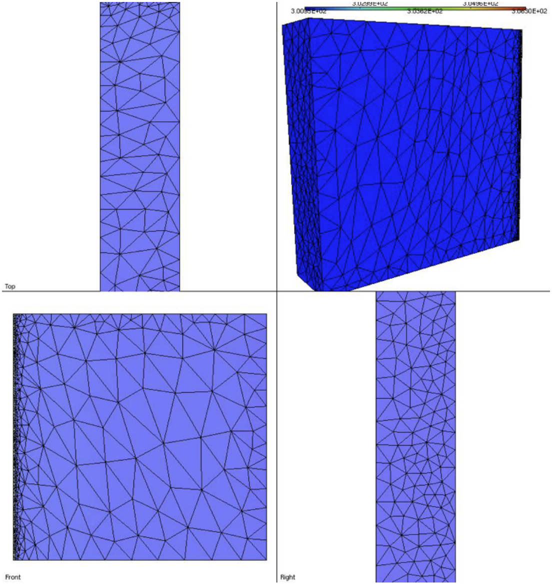


⇒ Good quantification of the position of the interface, the liquid fraction, transferred heat...

3D melting


1.9900E-04
5.9980E-04
0.0000E+00
3.9989E-04
7.9979E-04
Eqn: +0.015z -0.0018 = 0

3D melting



Perspectives

This work was performed using computing resources of CRIANN (Normandie) and MATRICS (Picardie).

- Phase change is well-treated, interface is correctly captured,
- Possibility to treat more complex density variations (e.g. water freezing),
- Parallelization done using FFDDM,

To do list :

- More 3D validation needed (complex geometries),
- Homogenization problems ?
- Influence on PCM on a convection cell,
- More physics in the solidification process (dendrites),
- Limitations of the FE approach ?

Thank you !