

# Kick off meeting of INTERFROST, 18/10/14 Paris

## INTERFROST : First test cases treated with OpenFOAM®

**Laurent Orgogozo<sup>1</sup>, Christophe Grenier<sup>2</sup>, Nicolas Roux<sup>2</sup>, Quentin Chanzy<sup>2</sup>.**

<sup>1</sup>Geosciences Environment Toulouse, Toulouse, France

<sup>2</sup>Laboratory of the Sciences of Climate and Environment, Paris, France



# INTERFROST: A benchmark of Thermo-Hydraulic codes for cold regions hydrology



LSCE

Christophe Grenier<sup>1</sup>, Nicolas Roux<sup>1,2</sup>, François Costard<sup>2</sup>, Marc Pessel<sup>2</sup>

Contact : [christophe.grenier@lsce.ipsl.fr](mailto:christophe.grenier@lsce.ipsl.fr) and site at <https://wiki.lsce.ipsl.fr/interfrost/>

LSCE - UMR 8212 CEA-CNRS-UVSQ, Orme des Merisiers, 91191 Gif sur Yvette Cedex 16GEOPS, UMR 8148 CNRS - Université Paris Sud, 91405 Orsay Cedex, France



## Context and objectives

Large focus was put recently on the impact of climate changes in boreal regions due to the large amplitudes expected. Large portions of these regions, corresponding to permafrost areas, are covered by water bodies (lakes, rivers) with very specific evolution and water budget. These water bodies generate taliks (unfrozen zones below) that may play a key role in the context of climate change. Recent studies and modeling exercises showed that a fully coupled 2D or 3D Thermo-Hydraulic (TH) approach is required to understand and model the evolution of river and lake systems in a changing climate.

However, 3D studies are still scarce while all numerical approaches can only be validated against analytical solutions for a purely thermic equation with phase change (e.g. Neumann/Stefan, Lunardini). When it comes to the coupled TH system (coupling two highly non-linear equations), the only possible approach is to compare different codes on provided test cases and/or to have controlled experiments for validation and/or model discussions to try and improve the code performances.

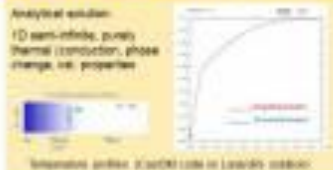
We propose here a benchmark exercise, detail some of its planned test cases and invite other research groups to join. The benchmark will consist of some test cases inspired by existing literature (e.g. Mc Kerrel et al., 2007) as well as new ones. Some experimental cases in cold room will complement the validation approach. The benchmark is open as well to new or alternative cases reflecting a numerical or a process oriented interest or answering a more general concern among the cold region community.

A further purpose of the benchmark exercise is to propel discussions for the optimization of codes and numerical approaches in order to develop validated and optimized simulation tools allowing in the end for 3D realistic applications.

## Strategy, work plan

- For the test cases we will proceed from simple to complex, progressively including:
  - The various terms of the system of equations (pure thermal transfers to full coupling)
  - 1D to 2D and finally 3D problems
  - Simple geometries with homogeneous properties to more realistic systems
- Simple performance measurements will be chosen to inter-compare the simulation results among participants
- Validation is expected from analytical solutions (1D purely thermal cases) or from experiments in cold room. Evaluation of codes will come from an inter-comparison of simulation results
- The inter-comparison exercise is open to anybody willing to join. The present first phase of the benchmark considers simple cases. The extension to more complex and realistic cases is considered and will be discussed in the course of the first phase. A first set of test cases will be provided by Spring 2014. A kick off meeting is planned October 2014

### T1: Lunardini/Osterkamp



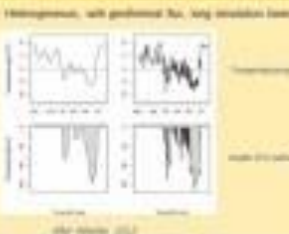
### T→P: 1D P↑



### T2: Heterogeneous



### T3: geological times



### Experiments in cold room



Facility at GEOPS with controlled room temperature



### Coupled system of TH equations

Darcy water flow equation

$$\left( \frac{\partial \rho_w}{\partial t} \right) \frac{\partial p}{\partial t} = \nabla \cdot [ \rho_w K_v \nabla p ] + \nabla \cdot [ \rho_w K_h \nabla z ] - \left( \rho_w - \rho_i \right) \frac{\partial S}{\partial t} + Q$$

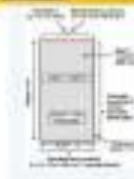
Heat transfer equation

$$(\rho_s c_s + \rho_i c_i + \rho_w c_w) \frac{\partial T}{\partial t} =$$

$$\nabla \cdot ( \lambda \nabla T ) + \nabla \cdot ( \rho_w K_v \nabla p + \rho_w K_h \nabla z ) - \frac{\partial S}{\partial t} ( \rho_w L ) - \left( \rho_s \frac{\partial m_s}{\partial t} \right) \frac{\partial p}{\partial t} + Q$$

The system is similar to the one of Mc Kerrel et al., 2007

### TH1: Kurylyk & Lunardini

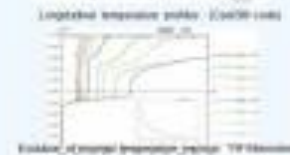


Analytical solutions including constant advection

### TH2: Frozen inclusion

An initially 2D cold ( $T < 0^\circ\text{C}$ ) permafrost inclusion is present within a uniform water flow ( $T = 0^\circ\text{C}$ )

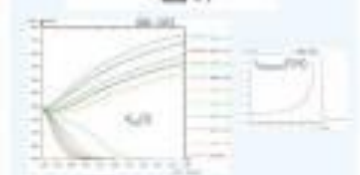
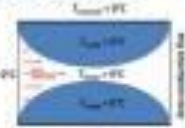
Performance measurements are: 1°) time for the maximum system temperature to reach  $0^\circ\text{C}$ , 2°) temperature profiles along main axis for a set of control times



### TH3: Talik evolution

An initially 2D cold ( $T < 0^\circ\text{C}$ ) permafrost zone is present within a uniform water flow ( $T = 0^\circ\text{C}$ ). Imposed  $T < 0^\circ\text{C}$  for upper and lower boundaries

Performance measurements are: 1°) equivalent permeability evolution, 2°) time for the talik to close (talik advection levels)



Please join! ... and come to discuss the cases!



Contact [christophe.grenier@lsce.ipsl.fr](mailto:christophe.grenier@lsce.ipsl.fr) Site at <https://wiki.lsce.ipsl.fr/interfrost/> Financial support from INSU/EC2CO and CIC ([www.climate-cryosphere.org](http://www.climate-cryosphere.org))



# INTERFROST: A benchmark of Thermo-Hydraulic codes for cold regions hydrology



LSCE

Christophe Grenier<sup>1</sup>, Nicolas Roux<sup>1,2</sup>, François Costard<sup>2</sup>, Marc Pessel<sup>2</sup>

Contact : [christophe.grenier@lcea.ipsl.fr](mailto:christophe.grenier@lcea.ipsl.fr) and site at <https://wiki.lcea.ipsl.fr/interfrost/>

<sup>1</sup>LSCE - UMR 8212 CEA-CNRS-UVSQ, Orme des Merisiers, 91191 Gif sur Yvette Cedex <sup>2</sup>GEOPS, UMR 8148 CNRS - Université Paris Sud, 91405 Orsay Cedex, France



## Context and objectives

Large focus was put recently on the impact of climate changes in boreal regions due to the large amplitudes expected. Large portions of these regions, corresponding to permafrost areas, are covered by water bodies (lakes, rivers) with very specific evolution and water budget. These water bodies generate taliks (unfrozen zones below) that may play a key role in the context of climate change. Recent studies and modeling exercises showed that a fully coupled 2D or 3D Thermo-Hydraulic (TH) approach is required to understand and model the evolution of river and lake systems in a changing climate.

However, 3D studies are still scarce while all numerical approaches can only be validated against analytical solutions for a purely thermic equation with phase change (e.g. Neumann/Stefan, Lunardini). When it comes to the coupled TH system (coupling two highly non-linear equations), the only possible approach is to compare different codes on provided test cases and/or to have controlled experiments for validation and/or to improve the code performances.

We propose here a benchmark exercise, detail some of its planned test cases and invite other research groups to join. The benchmark will consist of some test cases inspired by existing literature (e.g. Mc Kerrel et al., 2007) as well as new ones. Some experimental cases in cold room will complement the validation approach. The benchmark is open as well to new or alternative cases reflecting a numerical or a process oriented interest or answering a more general concern among the cold region community.

A further purpose of the benchmark exercise is to propel discussions for the optimization of codes and numerical approaches in order to develop validated and optimized simulation tools allowing in the end for 3D realistic applications.

## Strategy, work plan

- For the test cases we will proceed from simple to complex, progressively including:
  - The various terms of the system of equations (pure thermal transfers to full coupling)
  - 1D to 2D and finally 3D problems
  - Simple geometries with homogeneous properties to more realistic systems
- Simple performance measurements will be chosen to inter-compare the simulation results among participants
- Validation is expected from analytical solutions (1D purely thermal cases) or from experiments in cold room. Evaluation of codes will come from an inter-comparison of simulation results
- The inter-comparison exercise is open to anybody willing to join. The present first phase of the benchmark considers simple cases. The extension to more complex and realistic cases is considered and will be discussed in the course of the first phase. A first set of test cases will be provided by Spring 2014. A kick off meeting is planned October 2014

### T1: Lunardini/Osterkamp

Analytical solution:  
1D semi-infinite, pure thermal (conduction, phase change, ice properties)

Experimental setup: 1D semi-infinite, pure thermal (conduction, phase change, ice properties)

### T2: Heterogeneous

Multi-layered, bounded, with geothermal flux, include field monitoring data.

### T3: geological times

Heterogeneous, with geothermal flux, long simulation times

### Experiments in cold room

Facility at GEOPS with controlled room temperature

Lunardini et al., 2011

### T → P: 1D P ↑



### TH1: Kurylyk & Lunardini

Analytical solutions including constant advection

### Coupled system of TH equations

Darcy water flow equation

$$\left( \frac{\partial \rho_w}{\partial t} \right) \frac{\partial p}{\partial t} = \nabla \cdot \left[ \rho_w K_r \nabla p \right] + \nabla \cdot \left[ \rho_w K_r \nabla z \right] - \left( \rho_w - \rho_i \right) \frac{\partial S}{\partial t} - Q$$

Heat transfer equation

$$\left( \rho_s C_s + \rho_i C_i + \rho_w C_w \right) \frac{\partial T}{\partial t} = \nabla \cdot \left[ \lambda \nabla T \right] + \nabla \cdot \left[ \rho_w K_r \nabla p + \rho_w K_r \nabla z \right] - \frac{\partial S}{\partial t} \left( \rho_w L \right) - \left( \rho_s \frac{\partial H_s}{\partial t} \right) \frac{\partial T}{\partial t} - Q$$

The system is similar to the one of Mc Kerrel et al., 2007.

### TH2: Frozen inclusion

An initially 2D cold ( $T < 0^\circ\text{C}$ ) permafrost inclusion is present within a uniform water flow ( $T = 0^\circ\text{C}$ )

Performance measurements are: 1°) time for the maximum system temperature to reach  $0^\circ\text{C}$ , 2°) temperature profiles along main axis for a set of control times

Logarithmic temperature profiles (20000 cont)

Evolution of maximum temperature (permafrost) (10000 cont)

### TH3: Talik evolution

An initially 2D cold ( $T < 0^\circ\text{C}$ ) permafrost zone is present within a uniform water flow ( $T > 0^\circ\text{C}$ ). Imposed  $T < 0^\circ\text{C}$  for upper and lower boundaries

Performance measurements are: 1°) equivalent permeability evolution, 2°) time for the talik to close (talik advection levels)

Please join! ... and come to discuss the cases!

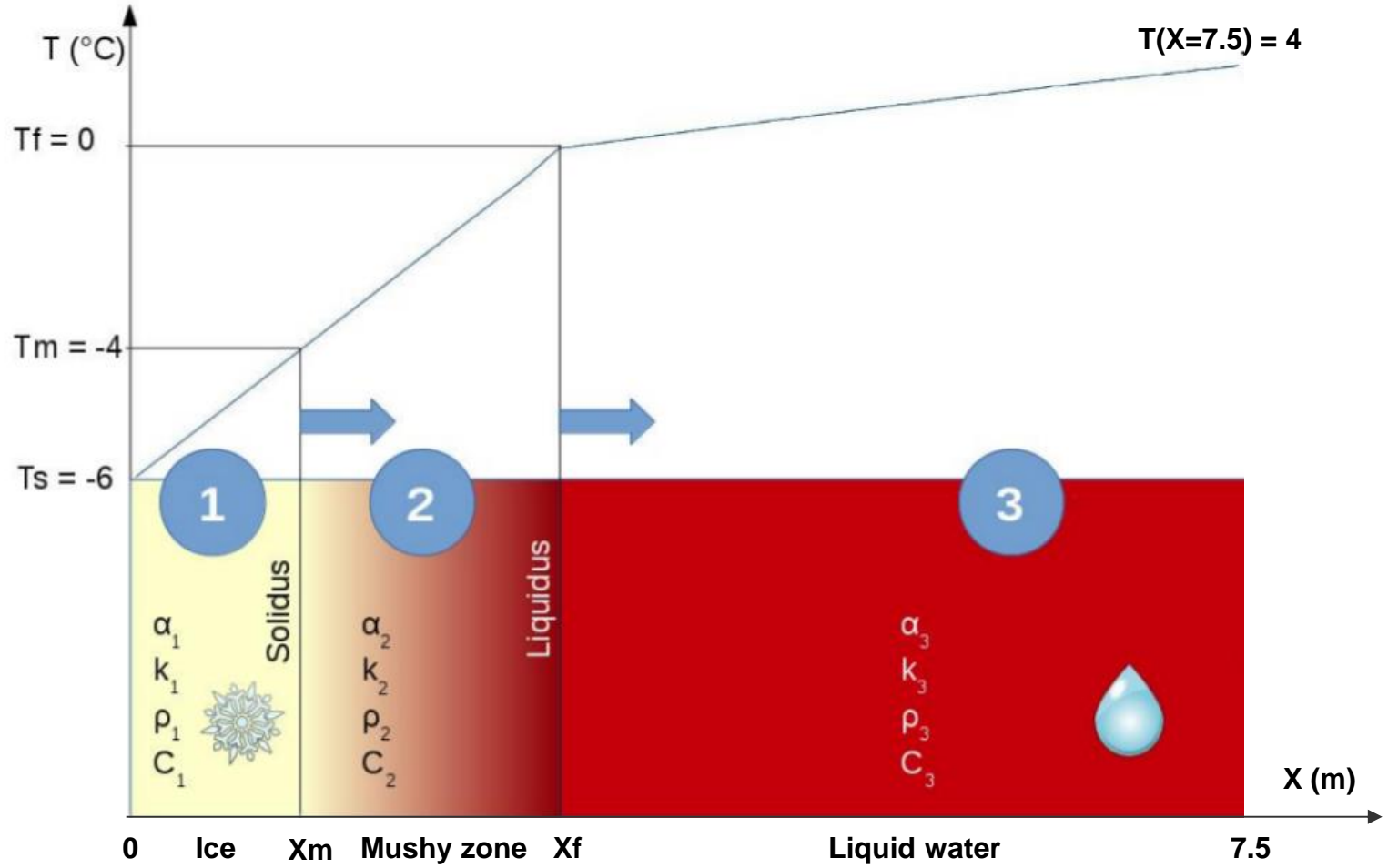
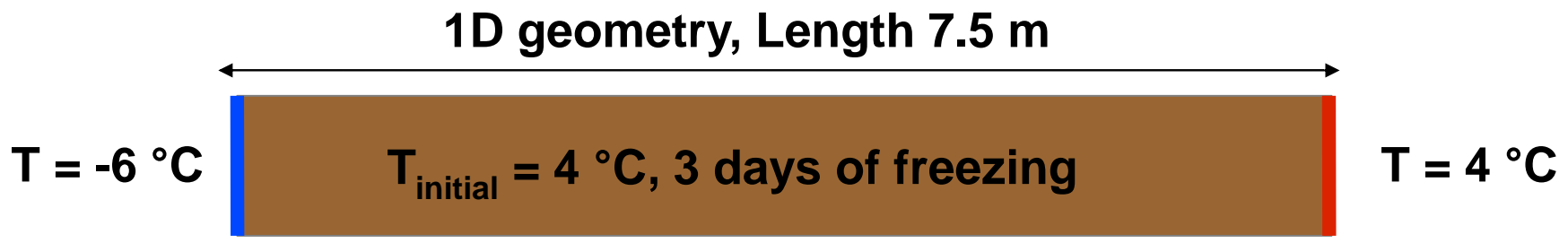


Contact [christophe.grenier@lcea.ipsl.fr](mailto:christophe.grenier@lcea.ipsl.fr) Site at <https://wiki.lcea.ipsl.fr/interfrost/> Financial support from INSU/EC2CO and CIC ([www.climate-cryosphere.org](http://www.climate-cryosphere.org))



# The purely conductive Lunardini case, McKenzie et al. 2007

## 1D transient analytical solution for thermal transfer / phase changes



(Interfrost website, <https://wiki.lscce.ipsl.fr/interfrost/doku.php?id=home>)

# The purely conductive Lunardini case, McKenzie 2007

## 1D transient analytical solution for thermal transfer / phase changes

Conservation equation:

$$C_n \frac{\partial T}{\partial t} = K_n \Delta T + L \frac{\partial \theta_{ice}}{\partial t}, \quad n = \text{liquid zone} / \text{mushy zone} / \text{icy zone}$$

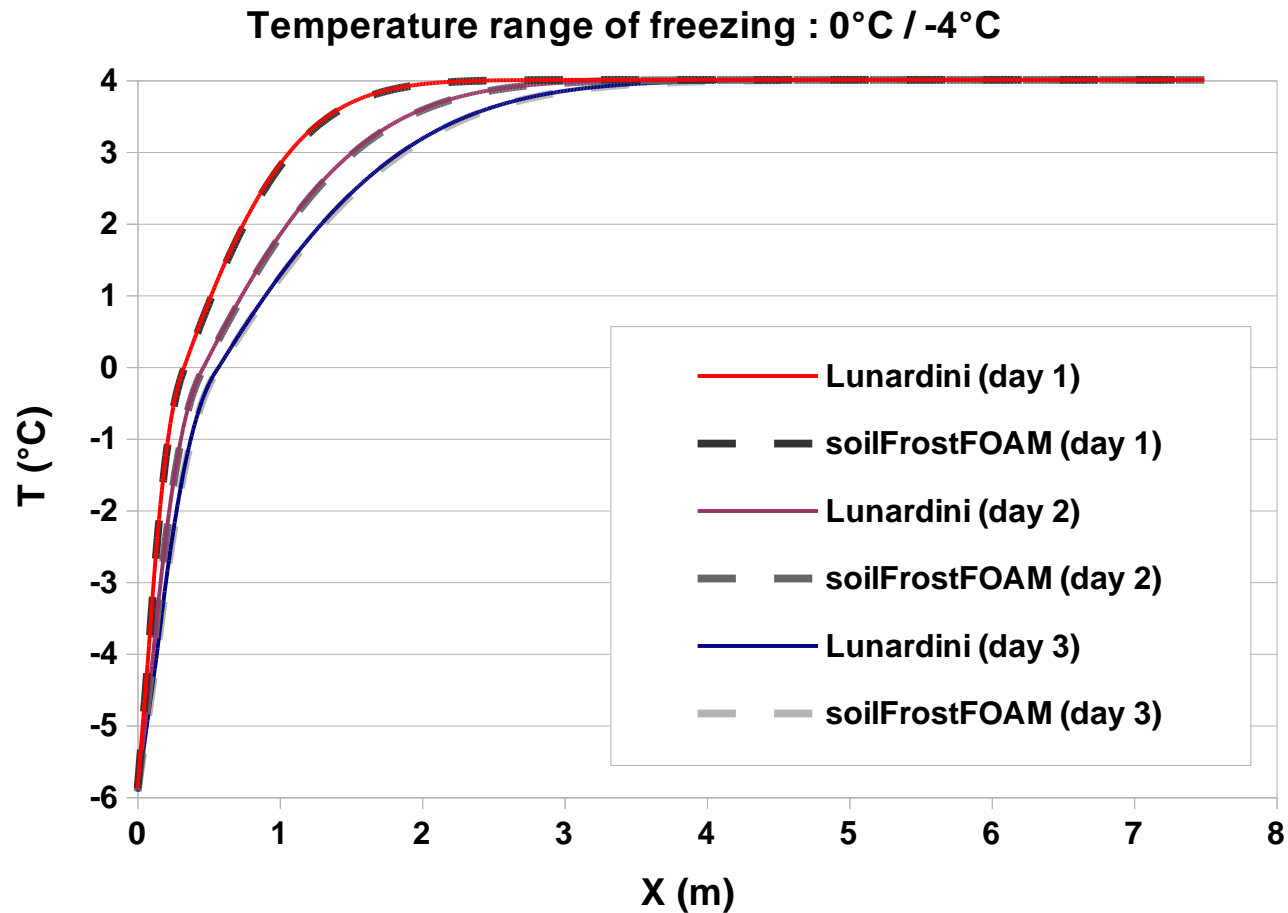
Phase changes:

$$\theta_{liquid} + \theta_{ice} = \theta_s$$

$$\theta_{ice} = \begin{cases} 0 & \text{if } T > T_f \\ (\theta_s - \theta_r) \left( \frac{T - T_f}{T_f - T_m} \right) & \\ \theta_s & \text{if } T < T_m \end{cases}$$

$T$  temperature [K],  $T_f$  starting temperature of water freezing [K],  $T_m$  starting temperature of ice melting [K],  $t$  time [s],  $C_n$  volumetric heat capacity [ $\text{kg.m.s}^{-3}.\text{K}^{-1}$ ] of zone  $n$ ,  $K_n$  thermal conductivity [ $\text{kg.m.s}^{-3}.\text{K}^{-1}$ ],  $L$  latent heat of fusion of ice [ $\text{kg.m}^{-1}.\text{s}^{-2}$ ],  $\theta_{liquid}$  volumetric fraction of liquid water [-],  $\theta_{ice}$  volumetric fraction of ice [-],  $\theta_s$  saturated volumetric fraction of liquid water [-],  $\theta_r$  residual volumetric fraction of liquid water [-].

# The purely conductive Lunardini case: 1D transient analytical solution for thermal transfer / phase changes



Error max (T, °C) : <0.04

Dt0 = 1e-2 s Dtmax = 1 h

Mesh cell size : 1e-2 m (750 cells)

Tfact = 1.3

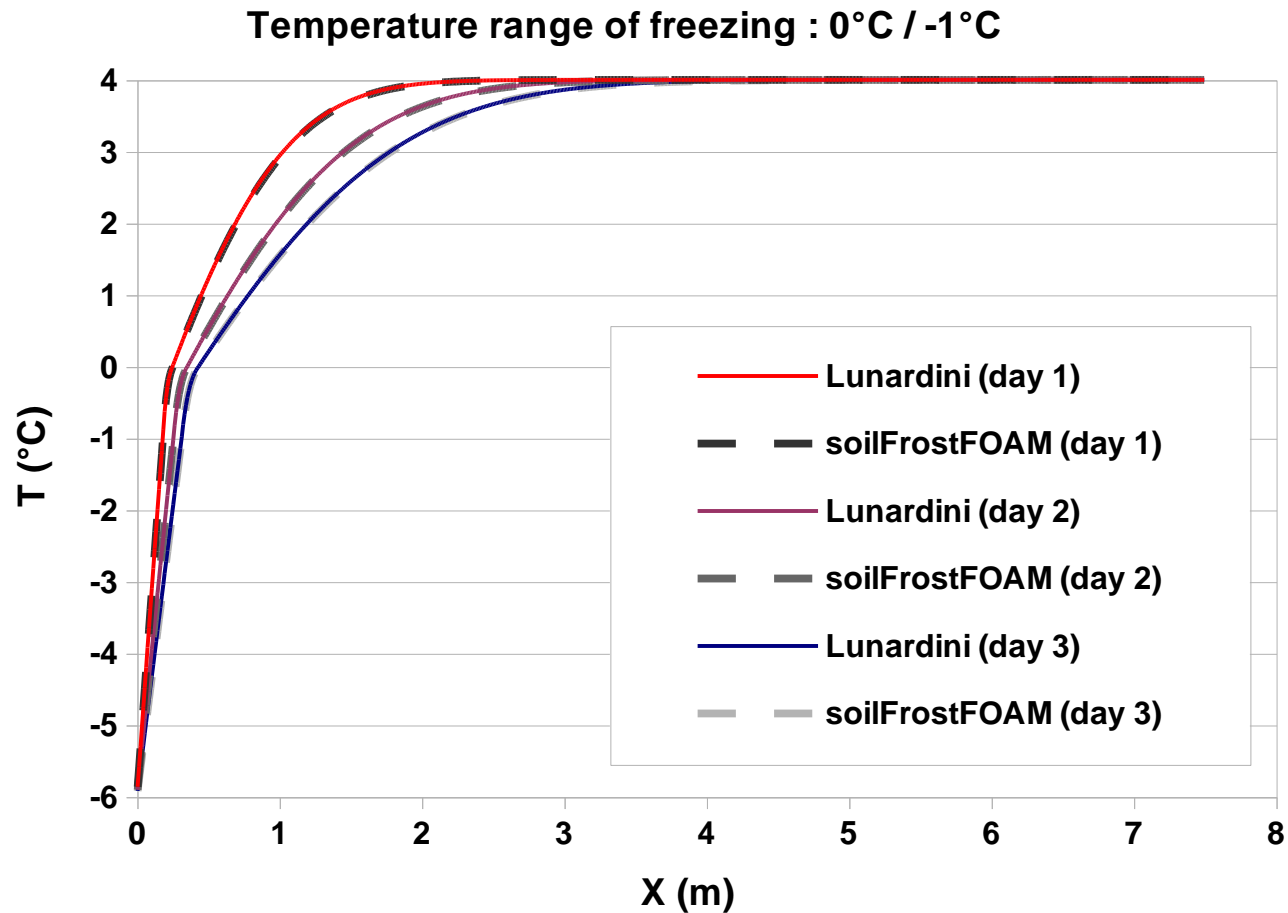
Execution time : ~ 1 s

DIC-PCG precision : 1e-6 m

(Intel® Core™ i7-2760QM CPU @ 2.40GHz × 8 )

Picard precision : 1e-4 m

# The purely conductive Lunardini case: 1D transient analytical solution for thermal transfer / phase changes



Error max (T, °C) : <0.05

$Dt_0 = 0.5$  s  $Dt_{max} = 15$  mn

Mesh cell size :  $1e-2$  m (750 cells)

$T_{fact} = 1.3$

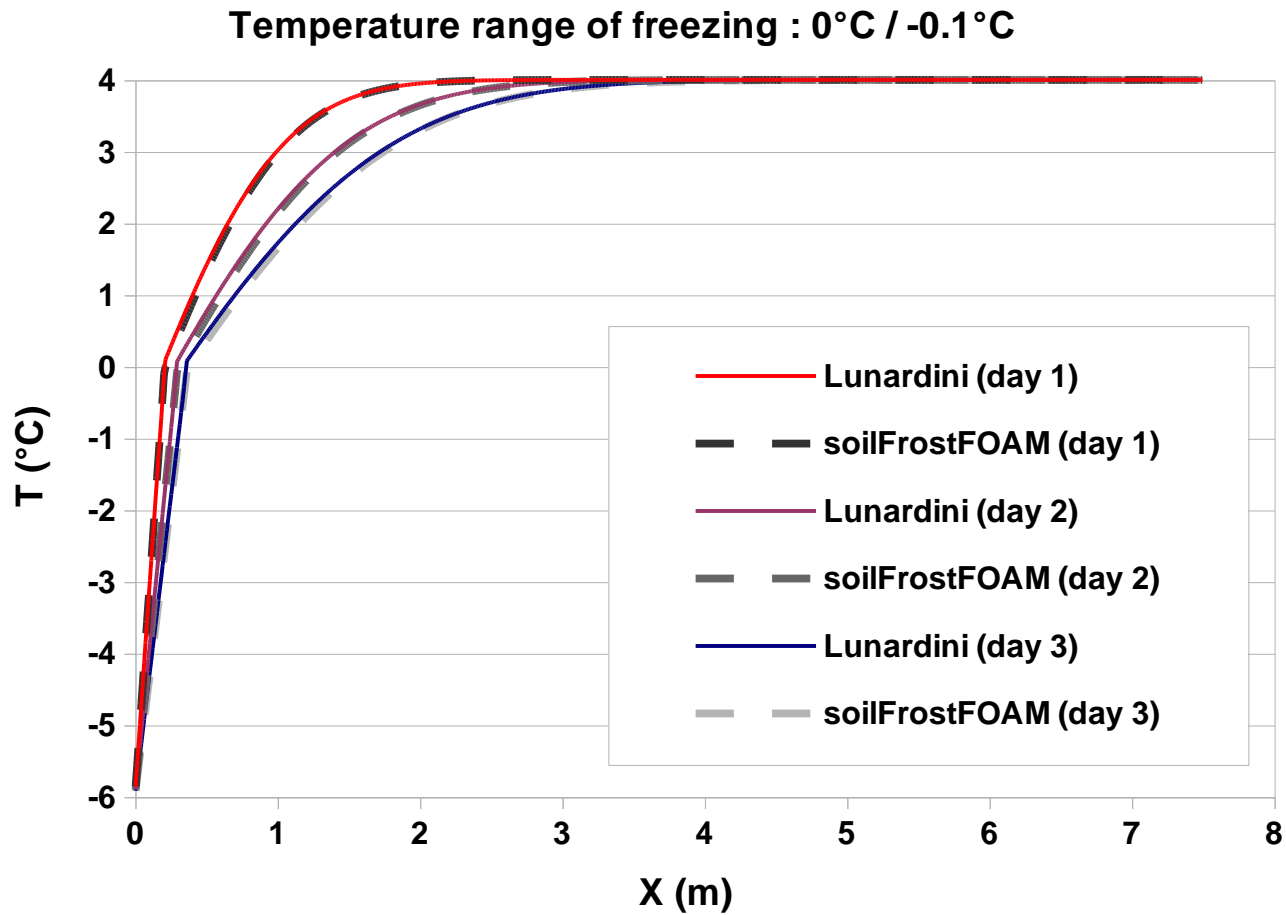
Execution time : ~ 2 s

DIC-PCG precision :  $1e-6$  m

(Intel® Core™ i7-2760QM CPU @ 2.40GHz × 8 )

Picard precision :  $1e-3$  m

# The purely conductive Lunardini case: 1D transient analytical solution for thermal transfer / phase changes



Error max (T, °C) : <0.15

Dt0 =1e-7 s Dtmax = 10 s

Mesh cell size : 1e-2 m (750 cells)

Tfact = 1.5

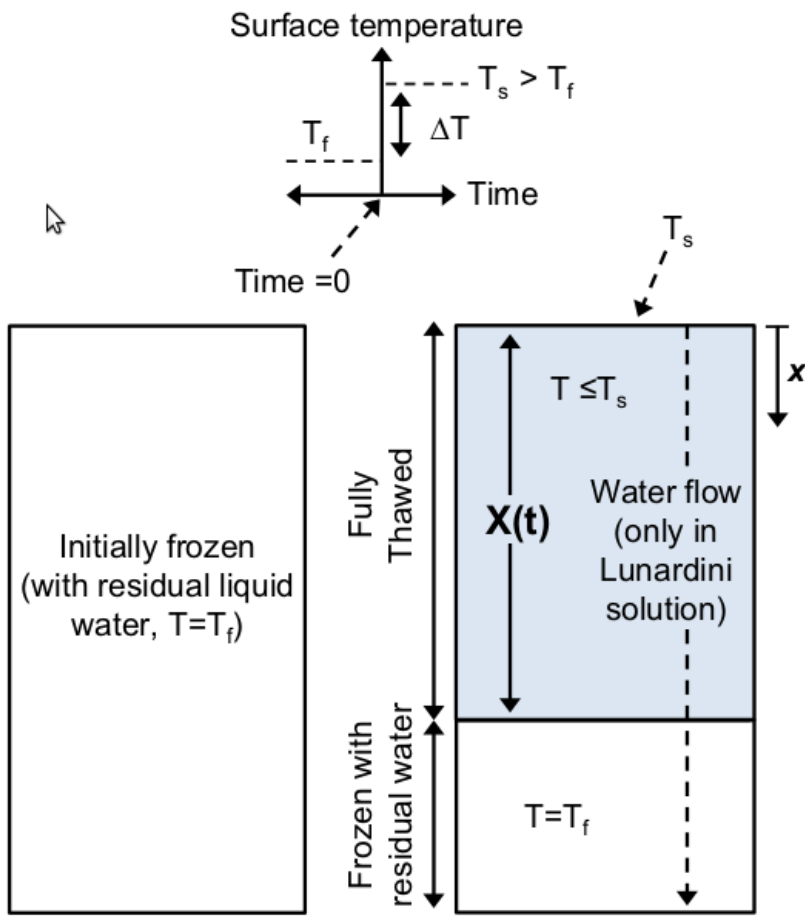
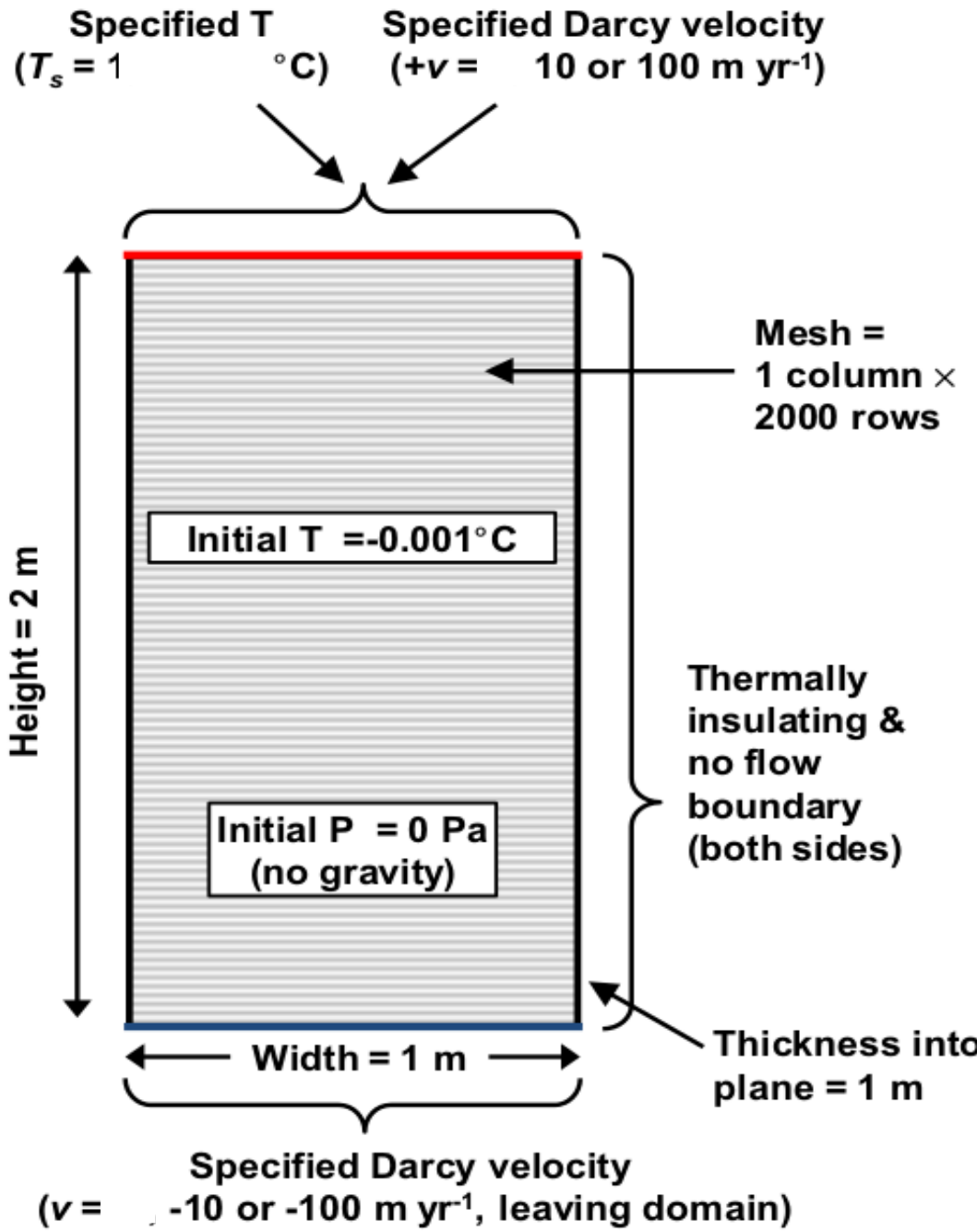
Execution time : ~ 28 mn  
(Intel® Core™ i7-2760QM CPU @ 2.40GHz × 8 )

DIC-PCG precision : 1e-8 m  
Picard precision : 1e-6 m



# The advective-conductive Lunardini case, Kurylyk et al. 2014

## 1D transient analytical solution for thermal transfer / phase changes



(a) Initial conditions      (b) After thawing period

(Figures extracted from Kurylyk et al. 2014)

# The advective-conductive Lunardini case, Kurylyk et al. 2014

## 1D transient analytical solution for thermal transfer / phase changes

Conservation equation :

$$C_n \frac{\partial T}{\partial t} + C_w v \nabla T = K_n \Delta T + L \frac{\partial \theta_{ice}}{\partial t}, \quad n = \text{thawed zone ( / mushy zone / icy zone)}$$

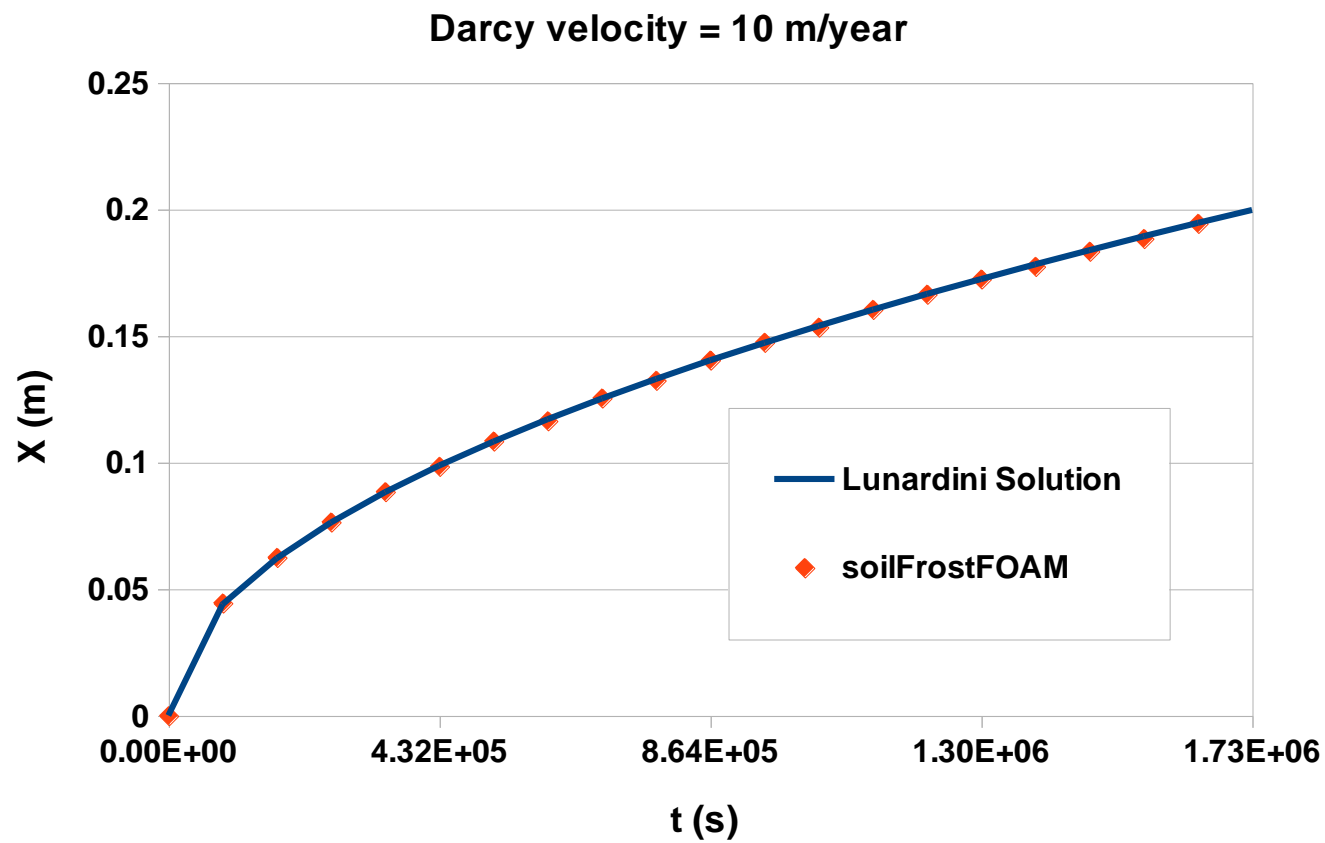
Phase changes:

$$\theta_{liquid} + \theta_{ice} = \theta_s$$

$$\theta_{ice} = \begin{cases} 0 & \text{if } T > T_f \\ (\theta_s - \theta_r) \left( \frac{T - T_f}{T_f - T_m} \right) & \\ \theta_s & \text{if } T < T_m \end{cases}$$

$T$  temperature [K],  $T_f$  starting temperature of water freezing [K],  $T_m$  starting temperature of ice melting [K], with  $T_f$  and  $T_m$  very close from each other ( $T_f - T_m = 0.0005$ ),  $t$  time [s],  $C_n$  volumetric heat capacity [ $\text{kg.m.s}^{-3}.\text{K}^{-1}$ ] of zone  $n$ ,  $C_w$  volumetric heat capacity [ $\text{kg.m.s}^{-3}.\text{K}^{-1}$ ] of water,  $v$  Darcy velocity of water flow [ $\text{m.s}^{-1}$ ],  $K_n$  thermal conductivity [ $\text{kg.m.s}^{-3}.\text{K}^{-1}$ ] of zone  $n$ ,  $L$  latent heat of fusion of ice [ $\text{kg.m}^{-1}.\text{s}^{-2}$ ],  $\theta_{liquid}$  volumetric fraction of liquid water [-],  $\theta_{ice}$  volumetric fraction of ice [-],  $\theta_s$  saturated volumetric fraction of liquid water [-],  $\theta_r$  residual volumetric fraction of liquid water [-].

# The advective-conductive Lunardini case: 1D transient analytical solution for thermal transfer / phase changes



Max rel. error (%) : < 1.4

Dt0 = 1e-5 s Dtmax = 100 s

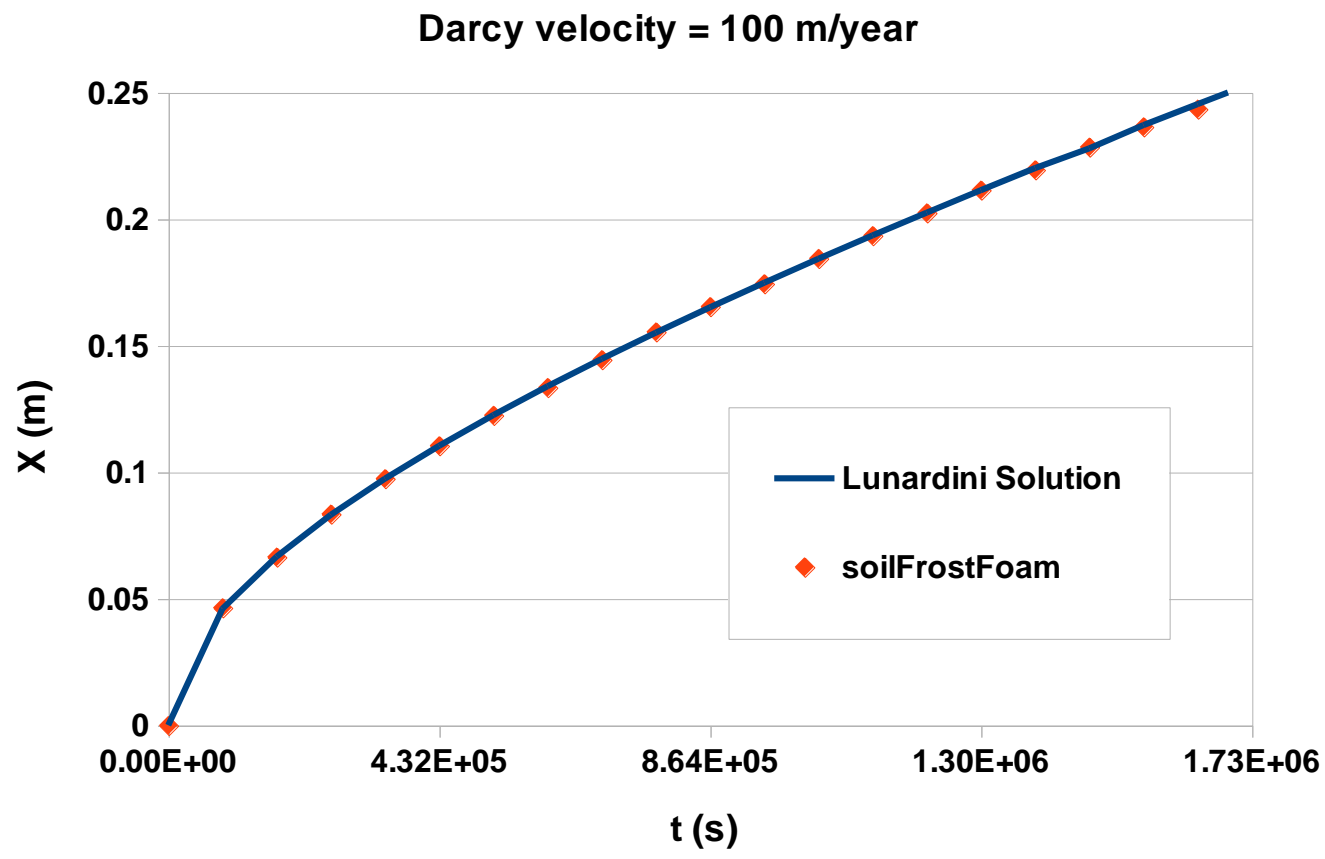
Mesh cell size : 1e-3 m (2000 cells)

Tfact = 1.1

Execution time : ~ 63 s  
(Intel® Core™ i7-2760QM CPU @ 2.40GHz x 8 )

DILU-PBiCG precision : 1e-8 m  
Picard precision : 1e-6 m

# The advective-conductive Lunardini case: 1D transient analytical solution for thermal transfer / phase changes



Max rel. error (%) : < 1.1

Dt0 = 1e-5 s Dtmax = 100 s

Mesh cell size : 1e-3 m (2000 cells)

Tfact = 1.1

Execution time : ~ 63 s  
(Intel® Core™ i7-2760QM CPU @ 2.40GHz x 8 )

DILU-PBiCG precision : 1e-8 m  
Picard precision : 1e-6 m

# Conclusions

**A validated implementation for advective-conductive thermal transport with phase change in porous medium has been set up in the framework of OpenFOAM®.**

**OpenFOAM solver: directly 3D, parallel**

**Perspectives :**

**coupling with RichardsFOAM (Orgogozo et al., CPC 2014)**

**Next steps of INTERFROST benchmark**

**Application to field data sets**

**Study of the parallel performances**

# Kick off meeting of INTERFROST, 18/10/14 Paris

**Thank you for your attention.**

**Contact : [laurent.orgogozo@get.obs-mip.fr](mailto:laurent.orgogozo@get.obs-mip.fr)**

