Contribution to certain physical and Numerical Aspects of the study of the heat transfer in a granular medium

Salwa Mansour
SAGE- INRIA- RENNES

Advisor: Édouard Canot

Co-Advisors: N. Nassif and M. Muhieddine

December 8, 2015 – PhD Thesis Defense.

Evolution of Human Behavior and Fire

Archaeologists try to answer these questions:

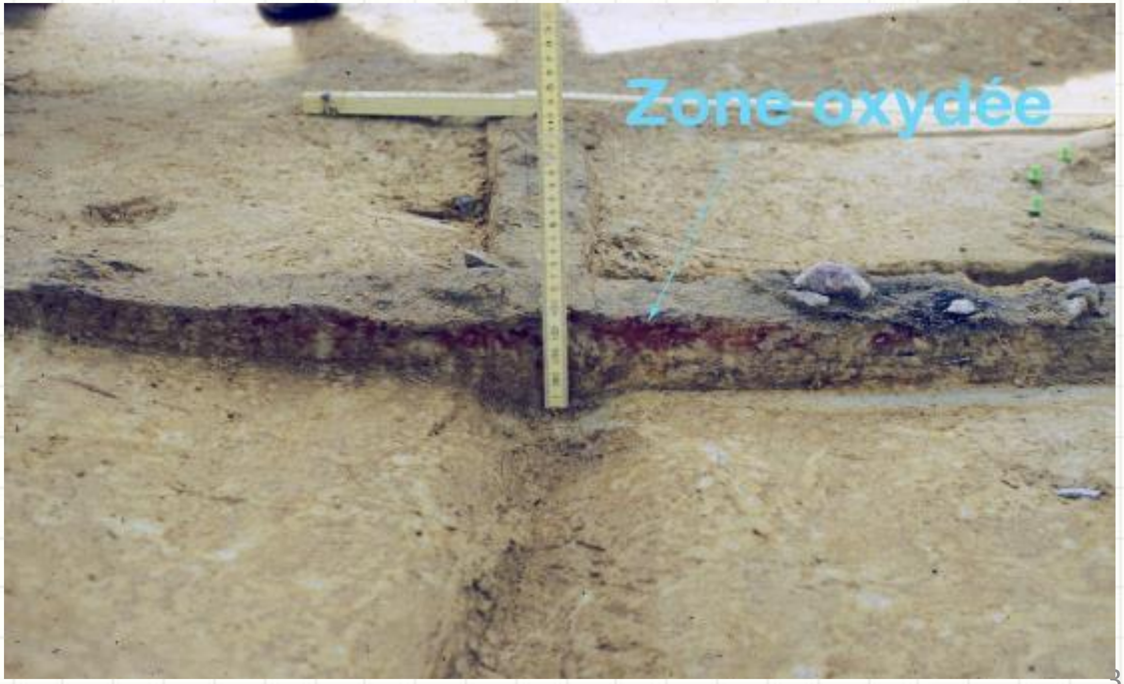
- What was the form of the fire?
- What was their mode of functioning?
- What was their utility?
- What was the minimal duration of fire?

Clay-silt soil (Pincevent): change in soil color due to temperature.

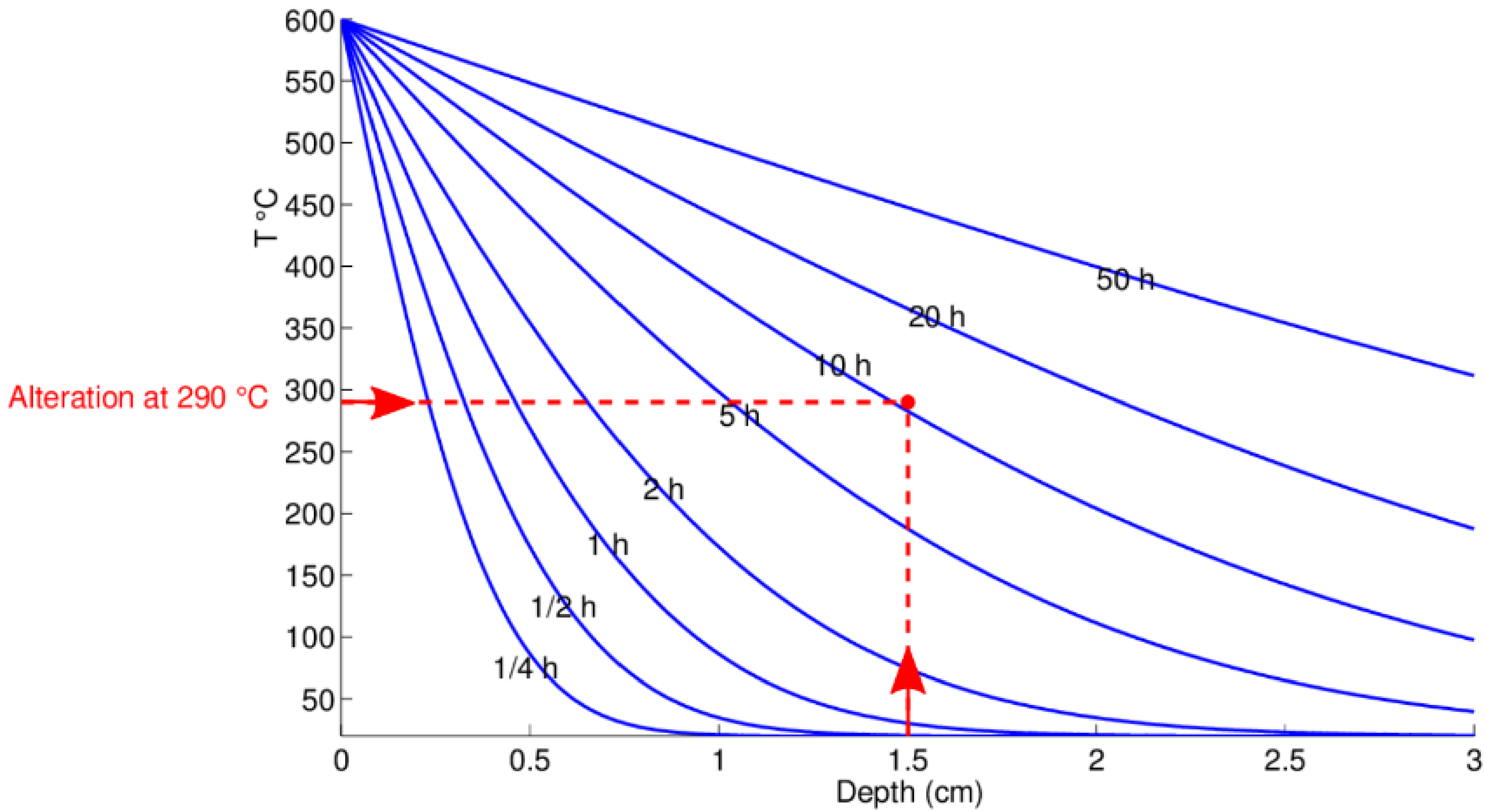
Yellow ------→ Red (oxides at 290°C)

Paleothermometer

Courtesy: Ramiro March (CREAAH, Rennes)



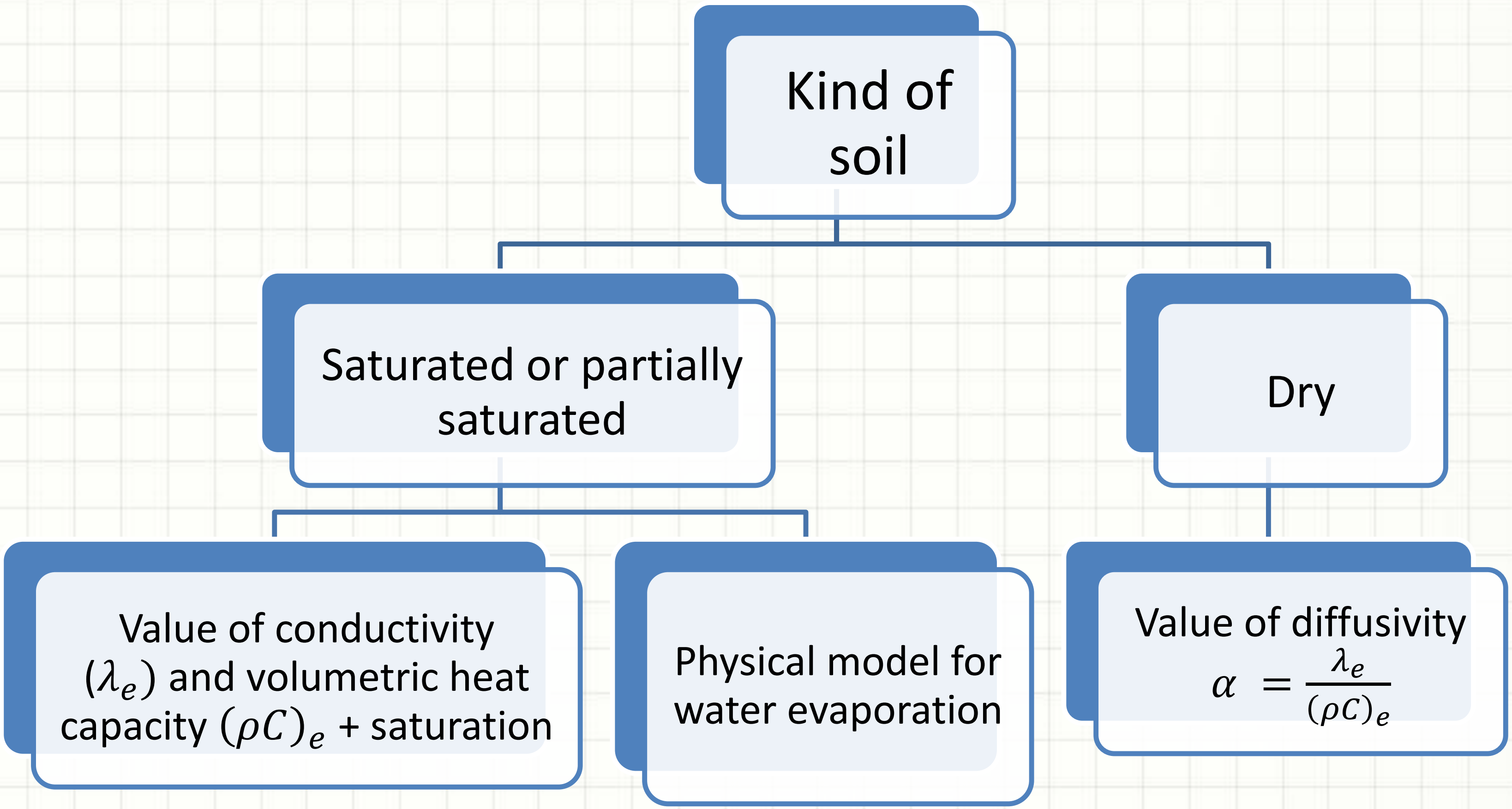
Minimal duration of fire (Dry soil)

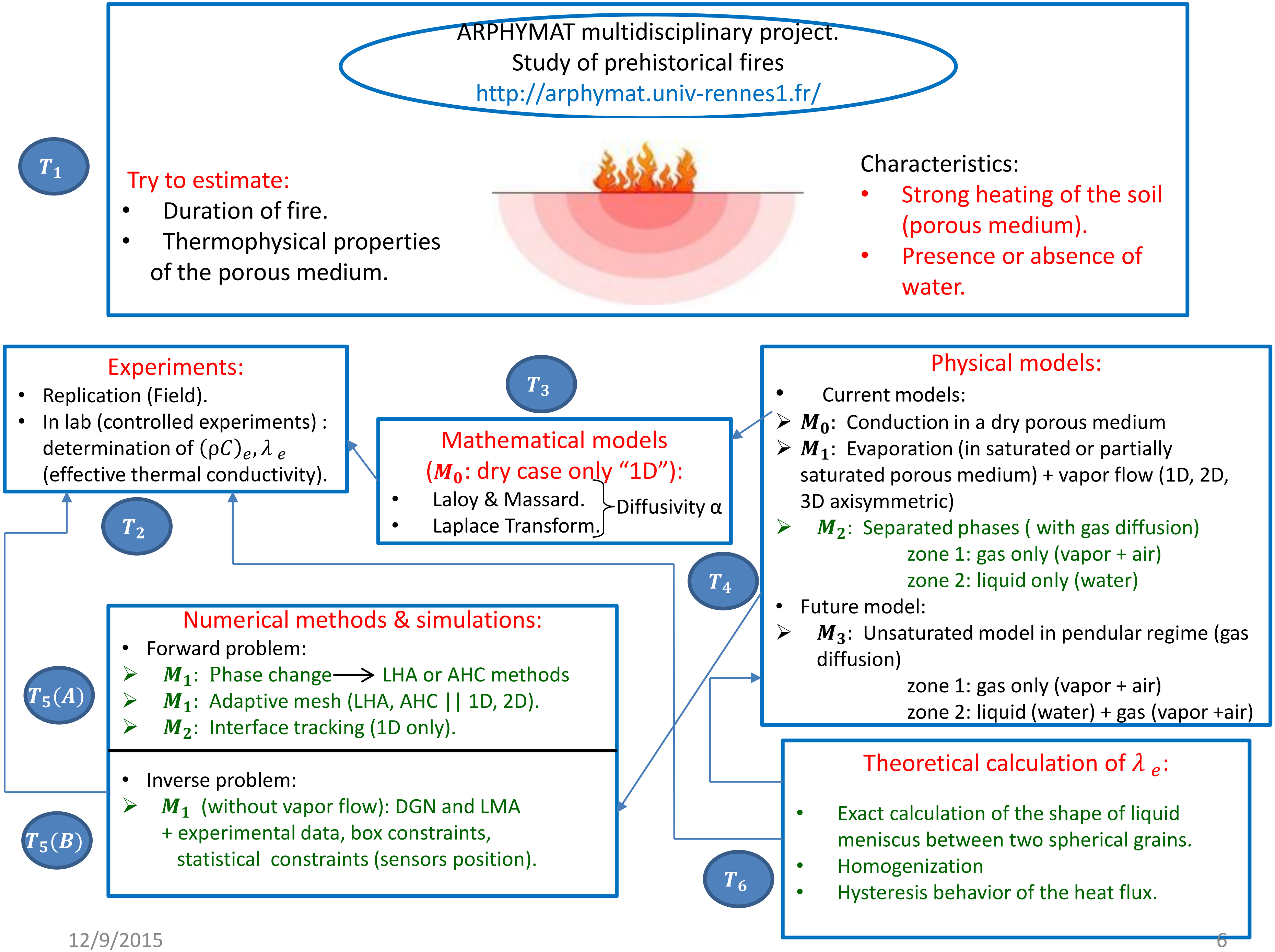


Assumptions:
- Homogeneous and isotropic medium
- Thermal diffusivity is known

What happens in case of wet soil?

To help Archaeologists :





An overview diagram representing the framework of my thesis with my main contributions in green.

Outline:

1. Solving the Heat equation with phase change in 1D and 2D coordinate systems.
2. Identification of the thermophysical properties of the soil by inverse problem.
3. A simplified physical model for phase change in presence of air.
4. Conclusions and Perspectives.

Outline:

1. **Solving the Heat equation with phase change in 1D and 2D coordinate systems.**
2. Identification of the thermophysical properties of the soil by inverse problem.
3. A simplified physical model for phase change in presence of air.
4. Conclusions and Perspectives.

Resolution of the heat diffusion equation with phase change

$$(\rho C)_e(T)\frac{\partial T(x,t)}{\partial t} = \mathrm{div}\big(\lambda_e(T)\nabla T(x,t)\big) \text{ in } \Omega \times (0, t_{end}]$$

Stefan Problem (Melting of a semi-infinite slab of ice "1D"):

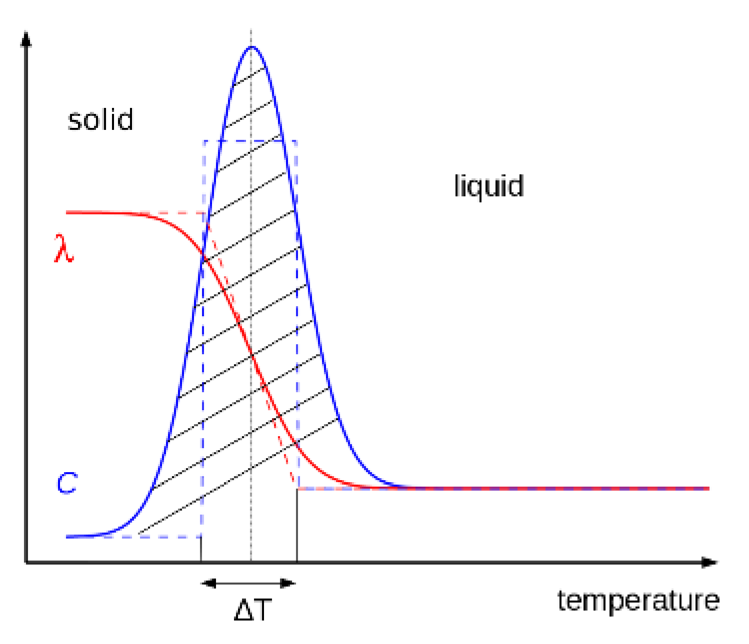
- Simplest Mathematical model of phenomenon of phase change
- An Analytical solution exists assuming that ice and water have same density ($\rho_s = \rho_l$).

Method of Resolution:

- Apparent Heat capacity (AHC).
  * Enthalpy method where no front tracking.
  * Can be easily applied to 2D or 3D coordinate systems.

Apparent Heat Capacity Method (AHC)

- The heat capacity is calculated knowing that its integration over the temperature is equal to the Latent heat.
- Computational domain is considered as one region,
- Suffers from singularity in the physical properties.

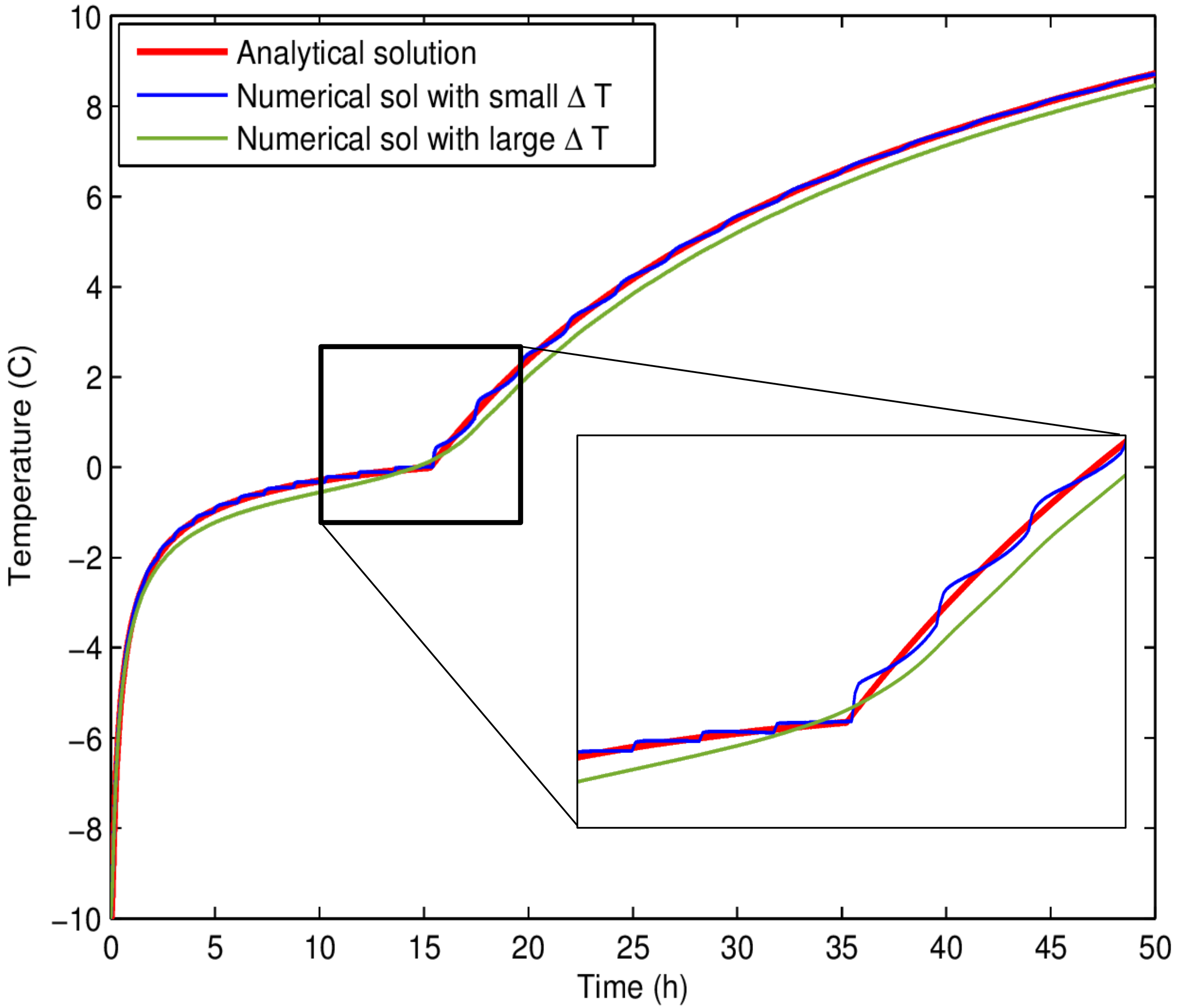


❖ **The phase transition takes place at a fixed temperature so:**

- $\int C\, dT = U(T - T_f)$ ⟶ **step function**
- $\boldsymbol{C = \delta(T - T_f)}$ ⟶ **Dirac delta function**

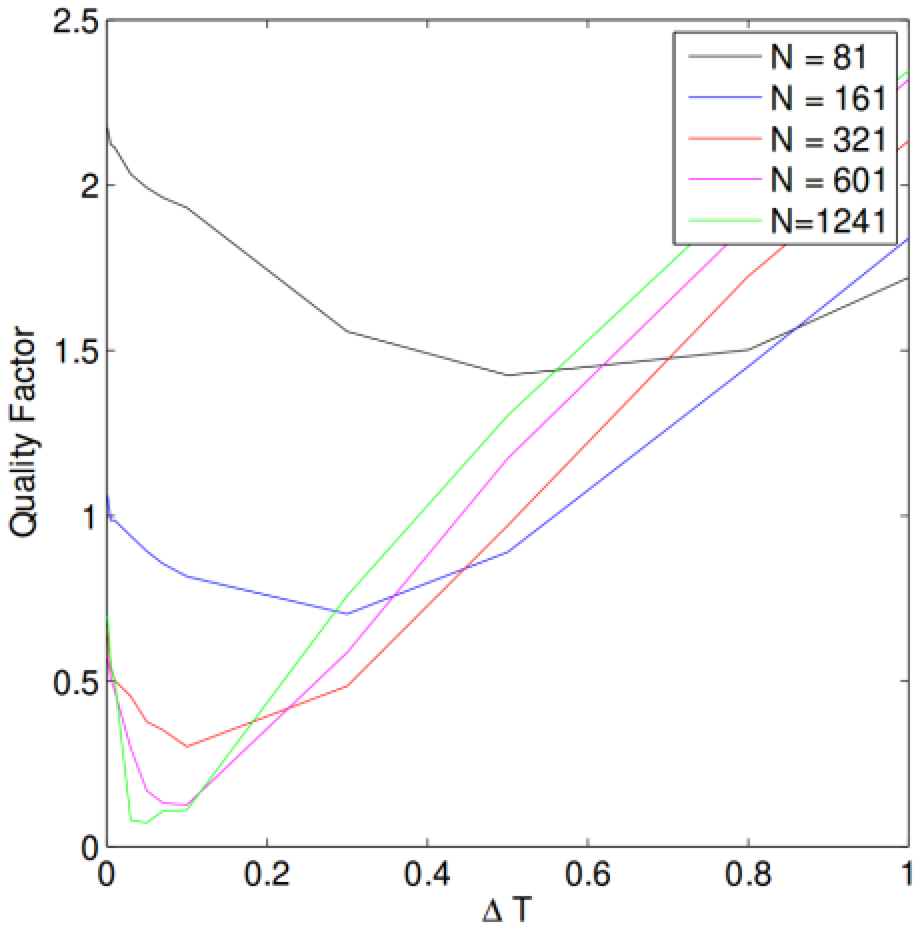
Apparent Heat Capacity method (Bonacina et al., 1973):
No front tracking
ΔT : Temperature phase change interval

Effect of value of ΔT in AHC method



Choice of ΔT in AHC:

$\Delta T_{optimum}$ → insures accuracy of solution with few fluctuations



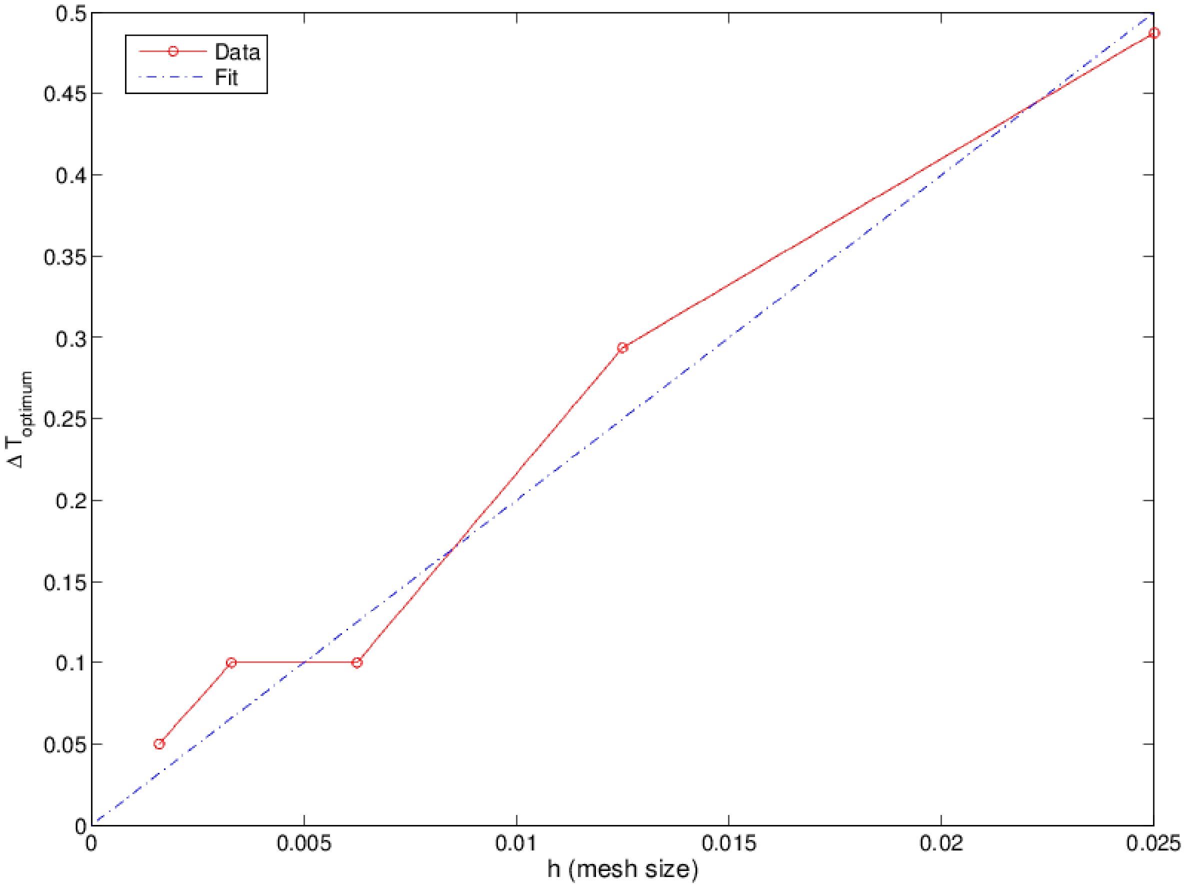
Accuracy

Smooth

Quality factor = Error(T) + 0.025 Error(T')

ΔT corresponding to minimum quality factor → $\Delta T_{optimum}$

Choice of ΔT in AHC:



$$\Delta T_{optimum} \approx K\ h$$

$$Constant \times (T_{max} - T_{min})$$

Numerical Strategy (AHC using $\Delta T_{optimum}$)

- Discretization using the **method of lines.**
- Spatial discretization **(Finite Volume Method).**
- After discretization, we get a system of first order implicit ODEs:

$$\begin{cases} F(t, T, T') = 0 \\ T(t_0) = T_0 \end{cases}$$

- Use an automatic ODE **solver "Backward Differentiation Formula"**

- **Two kinds of errors (between numerical and analytical solutions):**

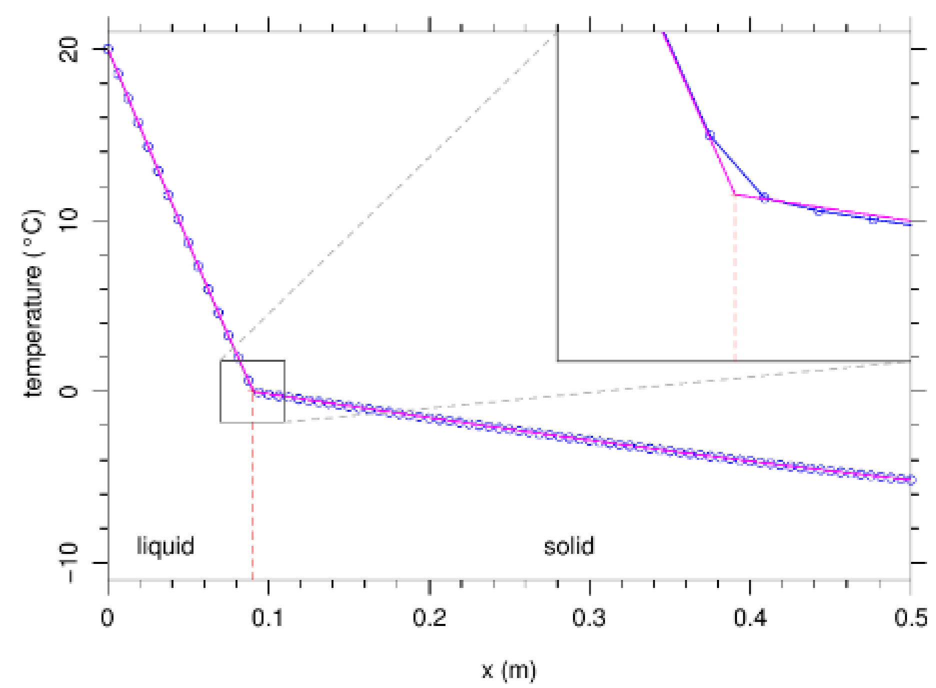
L^2 average norm error in temperature profile at final time**:**

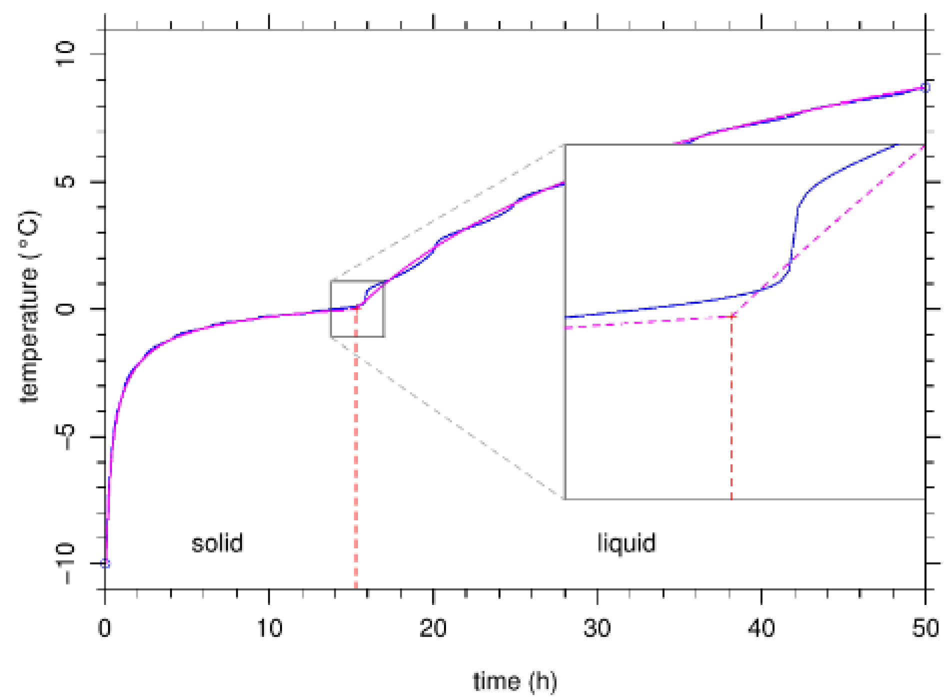
$$\boldsymbol{e_x = \frac{\left(\sum_i [T_i - T_{exact}(x_i)]^2 \Delta x_i\right)^{\frac{1}{2}}}{l}}$$

L^2 average norm error in temperature history at precise position:

$$\boldsymbol{e_t = \frac{\left(\sum_k \left[T^k - T_{exact}\left(t^k\right)\right]^2 \Delta t^k\right)^{\frac{1}{2}}}{t_{max}}}$$

Results AHC with uniform mesh





$At\ t_{final}\ \ with\ \ h = 6.25 \times 10^{-3}$
$e_x = 1.63 \times 10^{-2}\%$

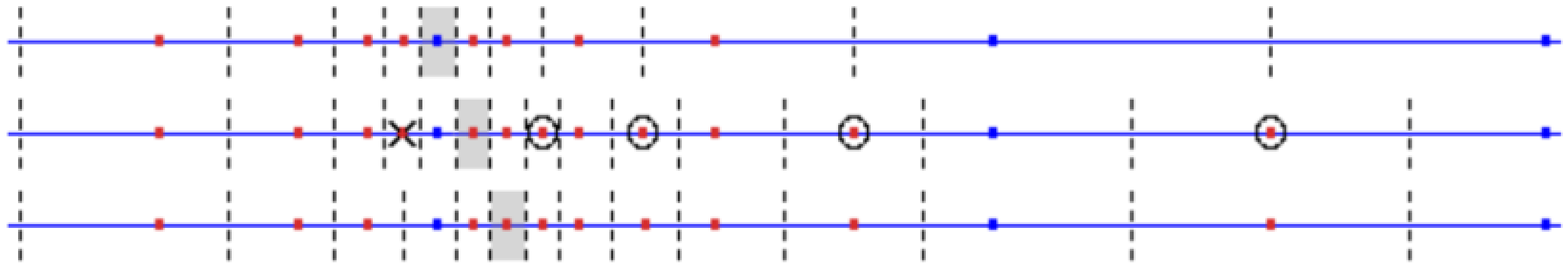
$At\ \ x = 5\ cm\ \left(\frac{1}{80}\ l_{max}\right) with$
$h = 6.25 \times 10^{-3}: \ \ e_t = 3.04 \times 10^{-1}\%$

Fluctuations are more visible near phase change zone ⟶ A more refined mesh near the interface ⟶ An adaptive mesh refinement technique

Adaptive Mesh

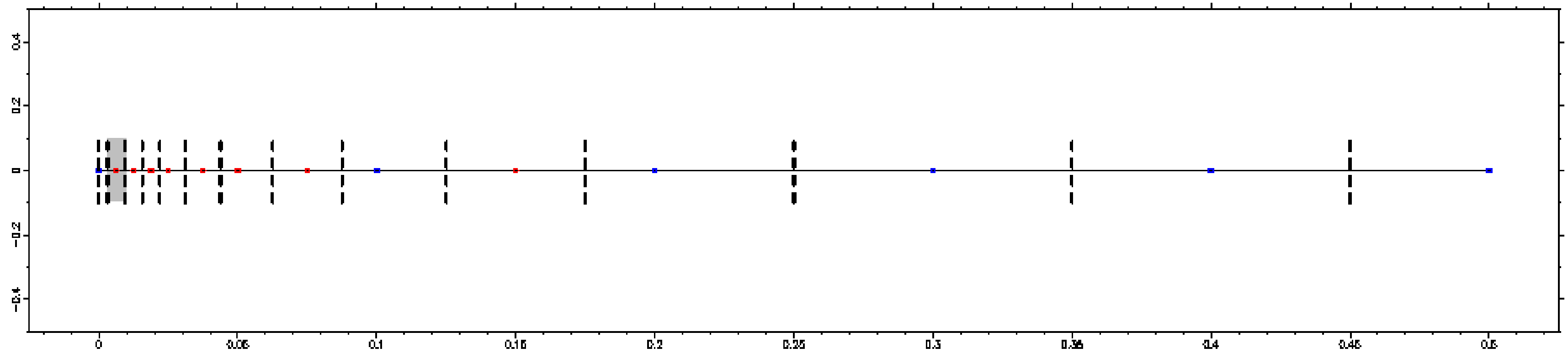
- Reducing the spatial step size uniformly over the whole domain → Method will be computationally expensive.

- Refinement is needed around the position of interface.
- Our refinement technique is based on adding and removing nodes recursively for the basic initial mesh.



Blue dots represents the nodes of the basic mesh. Circles are the new nodes (between step 1 and 2).

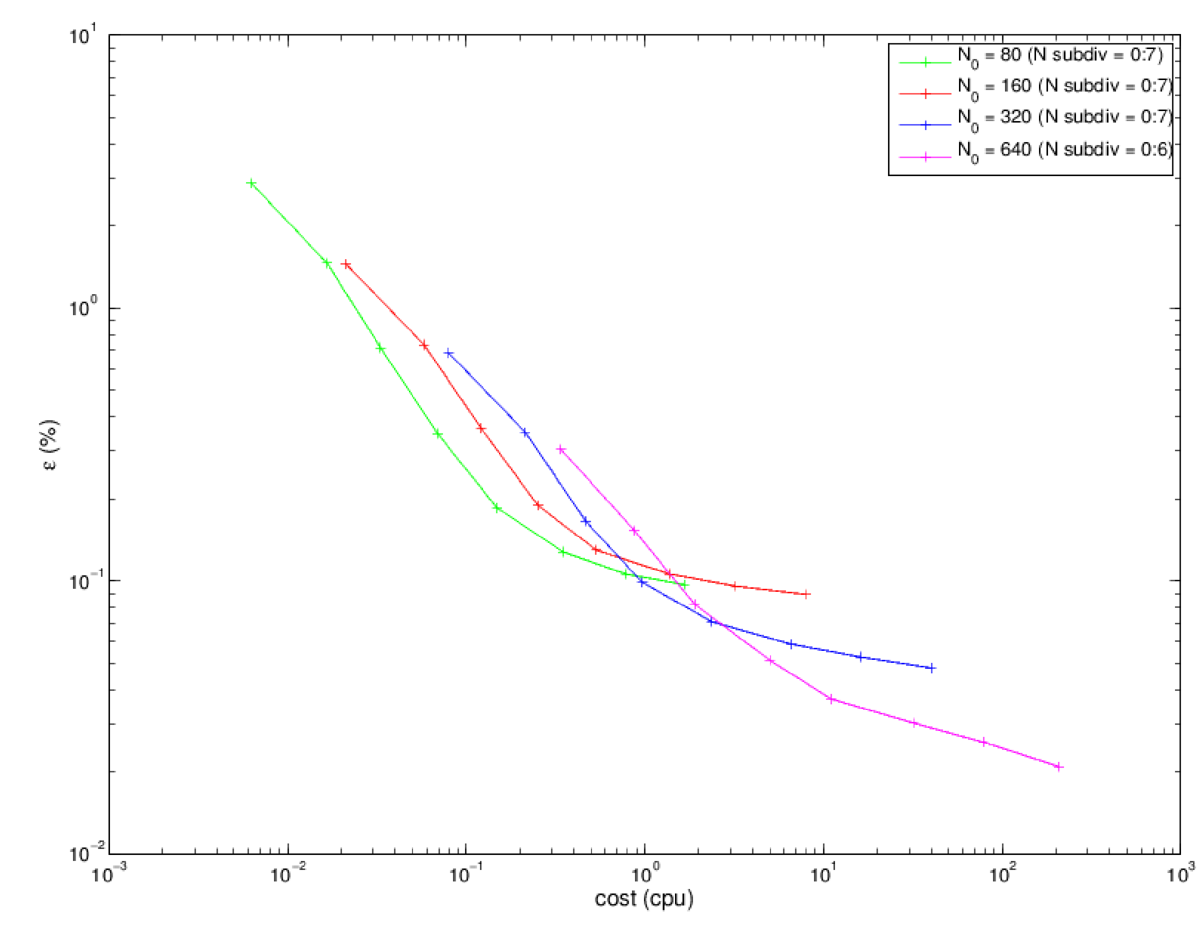
Adaptive Mesh



Kind of mesh	e_x	e_t	CPU
Uniform ($h = 6.25 \times 10^{-3}$ m)	$1.63 \times 10^{-2}\%$	$3.04 \times 10^{-1}\%$	3.39×10^{-1}
Adaptive ($h_{basic} = 5 \times 10^{-2}$ m) $N_{subdivisions}$= 3	$2.06 \times 10^{-2}\%$	$3.47 \times 10^{-1}\%$	6.90×10^{-2}

CPU gain
80%

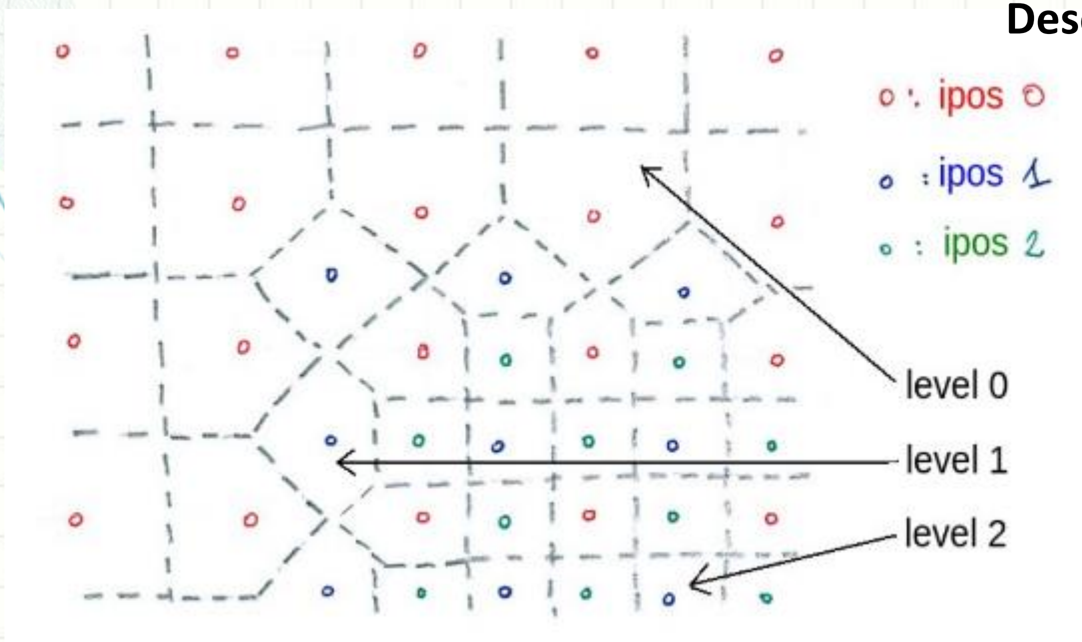
Error/CPU diagram



Seeking efficiency with accuracy → Small number of basic mesh cells with few subdivisions.

The ideal number of subdivisions is 3 or 4

Zohour: A node-based adaptive 2D mesh algorithm



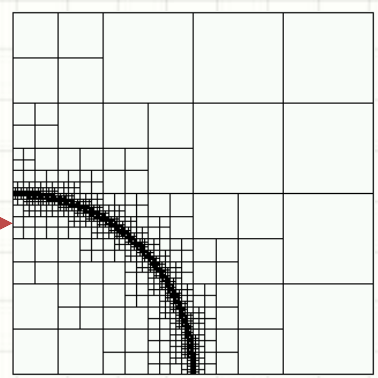
Description:

- Node based conformal mesh.
- Initial mesh : Regular squared set.
- At each level of subdivision: new nodes are added or removed according to some criteria → few interpolations

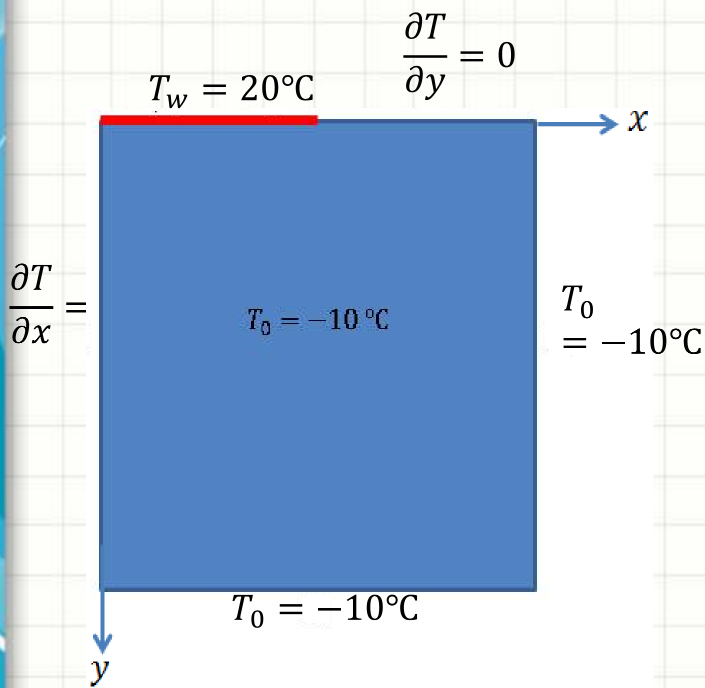
Advantages of Zohour:

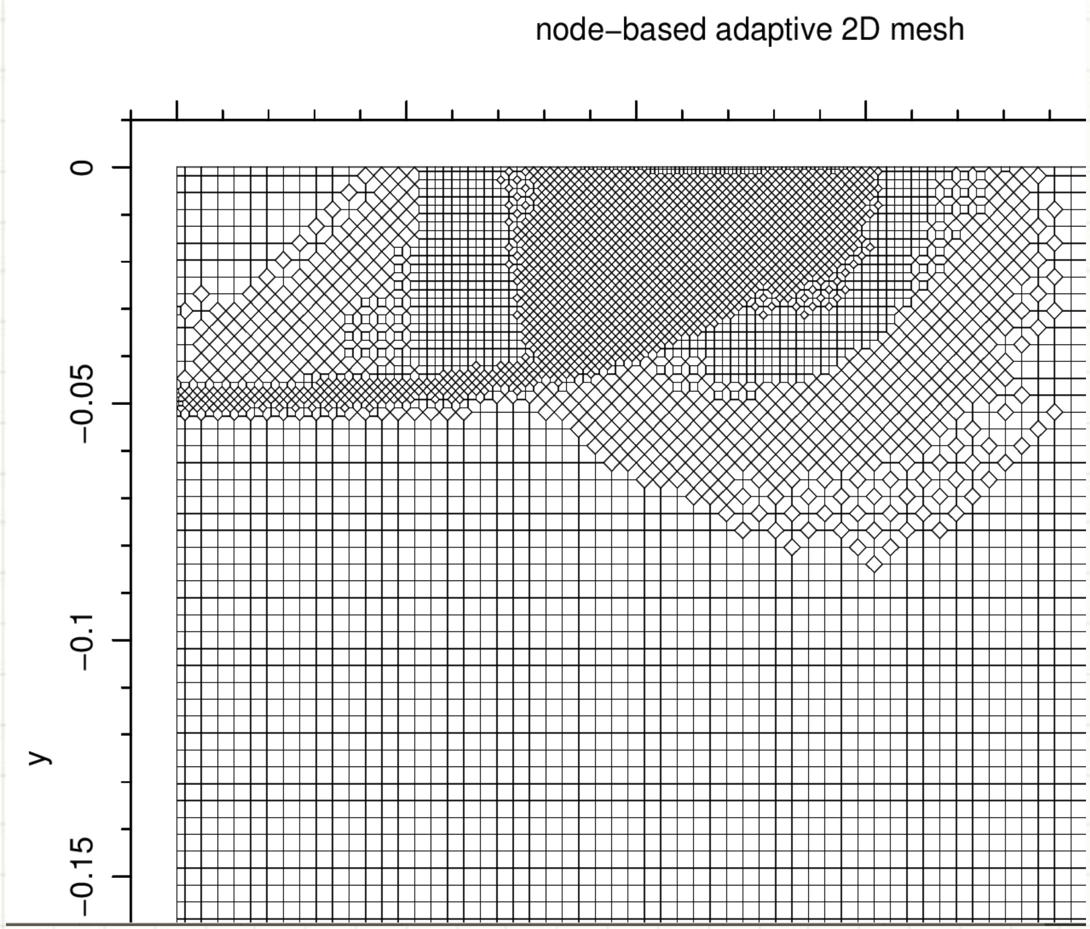
- Being a Voronoi mesh: ∇T can be easily approximated and is more precise.
- Efficiency of Hessian estimation.
- Refinement factor $\sqrt{2}$ more progressive than classical divided squares

Non-conformal mesh



Phase change problem in 2D coordinate system





$N_{basic} = 70 \times 70$ *with* 3 *levels of subdivision*

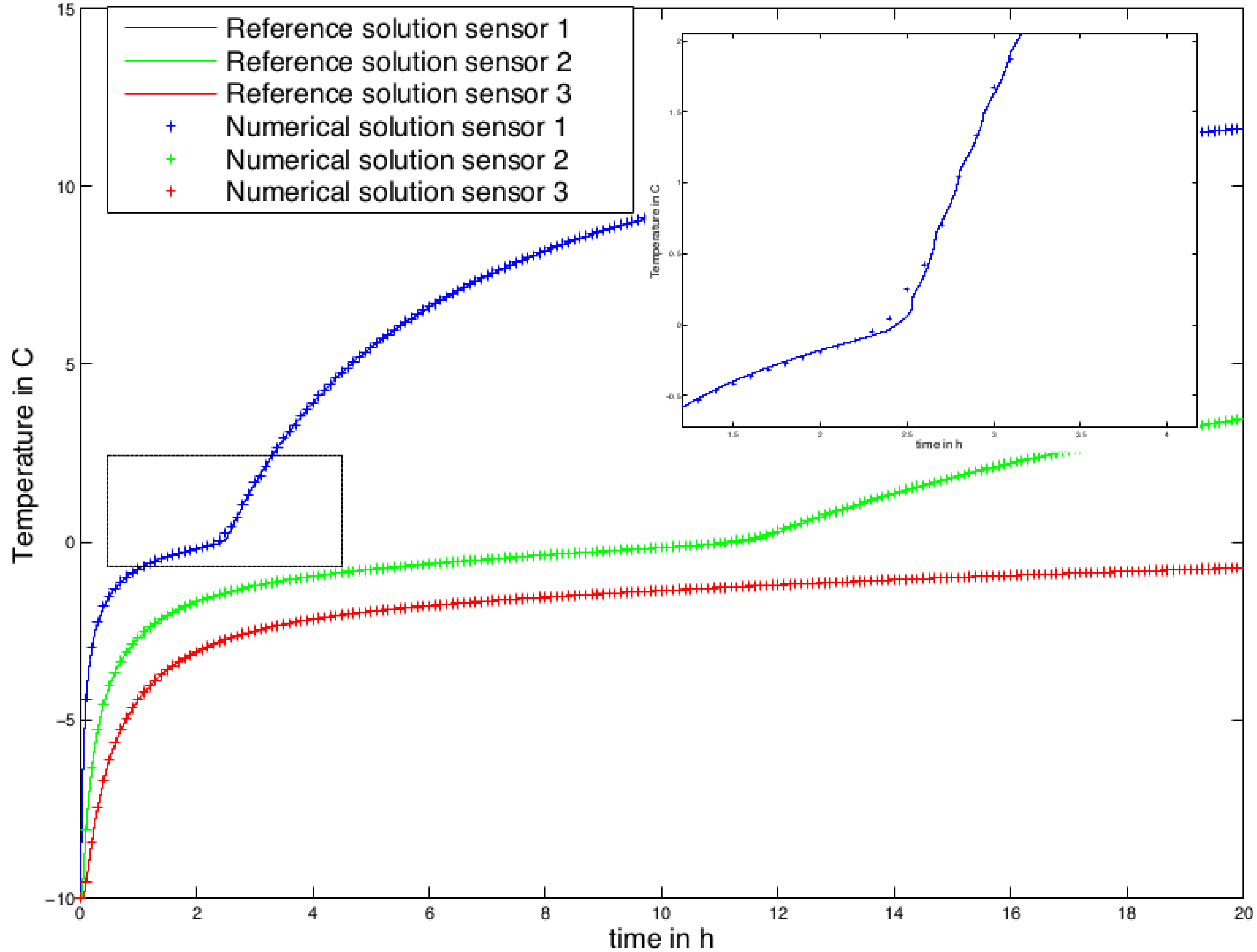
Refinement Criteria:

- Phase change region:

$$h = k_1 \left| T(x, y) - T_{fusion} \right|$$

- Local Hessian matrix "H"

$$h = \frac{k_2}{|H|}$$

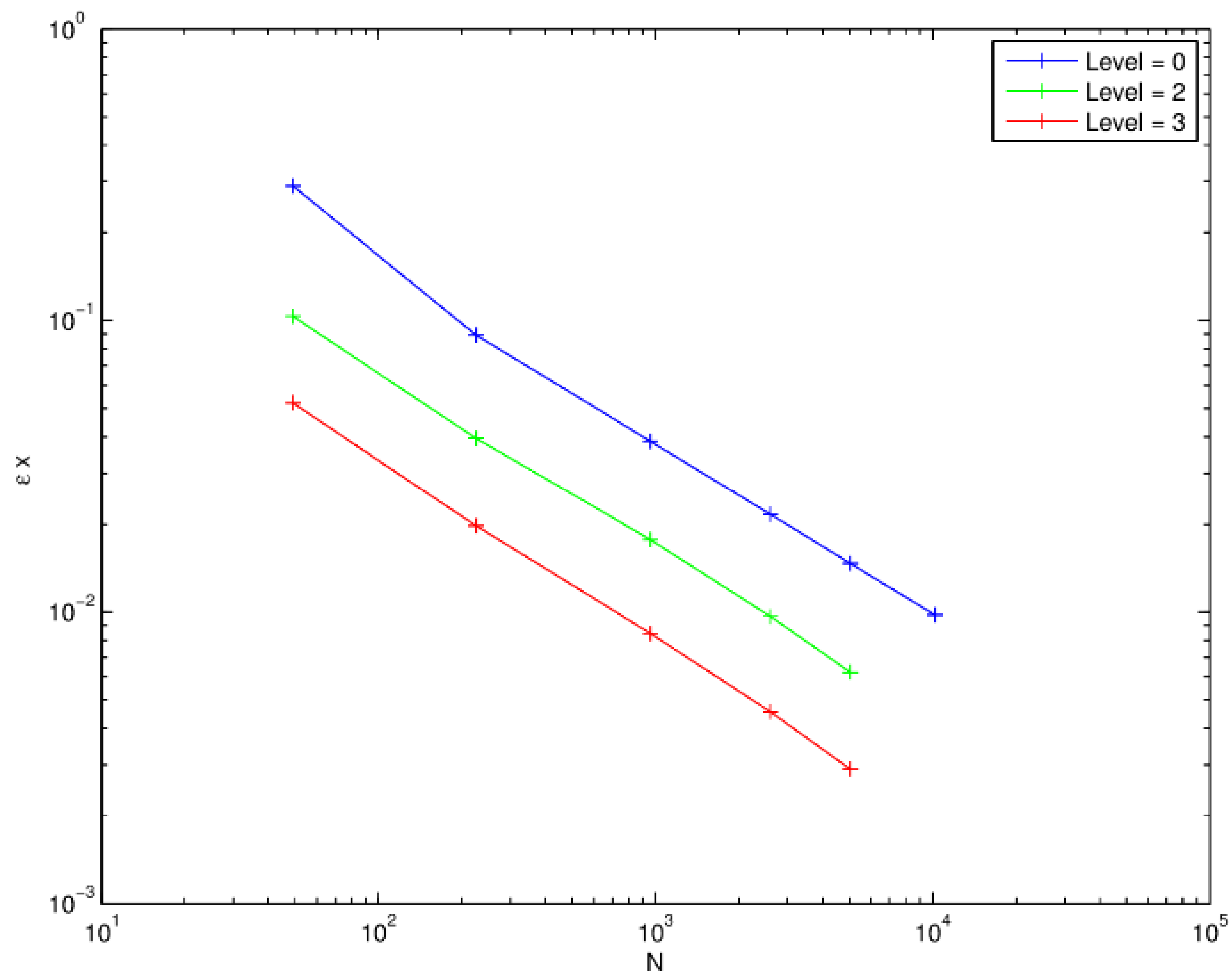


Reference Solution:

- 500×500 mesh cells

Numerical solution with Zohour:

- 70×70 mesh cells with $N_{subdivisions} = 3$



For same number of basic mesh cells → The error decreases as number of subdivisions increase.

Outline:

1. Solving the Heat equation with phase change in 1D and 2D coordinate systems.
2. **Identification of the thermophysical properties of the soil by inverse problem.**
3. A simplified physical model for phase change in presence of air.
4. Conclusions and Perspectives.

Identification of the thermophysical properties of the soil (dry case)

Objective: : Estimation of the thermal diffusivity α of the soil by inverse problem knowing the history of heat curves at selected points (few sensors) of the domain.

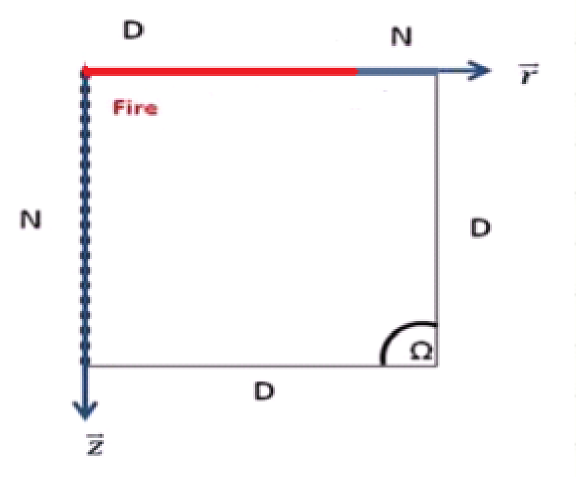
Dry Soil

Forward Problem:

Modeling: Replacing the soil by a perfect porous medium heated from above by a strong temperature.

$$\frac{\partial T(x,t)}{\partial t} = \alpha \, \mathrm{div}\big(\nabla T(x,t)\big) \text{ where } \alpha \text{ is the diffusivity}$$

Resolution of the heat diffusion equation in 3D axi-symmetric coordinate system.



Inverse Problem:

Use the **least square criterion** where we try to minimize the error function S (difference between experimental and numerical temperature):

$$S(\alpha) = \frac{1}{2}\sum_{i=1}^{M}\sum_{f=1}^{F}\left(T_{i,num}^{f} - T_{i,exp}^{f}\right)^2$$

- **Differentiate the main heat equation w.r.t to the parameter :**

$$\frac{\partial}{\partial \alpha}\left(\frac{\partial T(x,t)}{\partial t}\right) = \frac{\partial}{\partial \alpha}\left(\alpha \ \operatorname{div}\left(\nabla T(x,t)\right)\right)$$

- **Obtaining a PDE having a sensitivity coefficient as unknown:**

$$\frac{\partial U_\alpha(x,t)}{\partial t} = \alpha \ \operatorname{div}\left(\nabla U_\alpha(x,t)\right) + \operatorname{div}\left(\nabla T(x,t)\right)$$

Where $U_\alpha = \frac{\partial T}{\partial \alpha}$ is the sensitivity coefficient.

- **The problem is composed of solving 2 partial differential equations (Heat Equation + a sensitivity equation).**

Numerical Strategy

- Discretization using the **method of lines.**
- Spatial discretization **(Finite Volume Method).**
- After discretization, the system of coupled equations can be written in the form of a system of first order implicit ODEs:

$$\begin{cases} F(t, Y, Y') = 0 \\ Y(t_0) = Y_0 \end{cases} \qquad Y = [T, U_\alpha]^T$$

- Use an **automatic ODE solver.**
- Obtain the values of **T** and the sensitivity coefficient $\boldsymbol{U}_\alpha$.
- Solve the nonlinear least square problem by the Levenberg-Marquardt Algorithm (LMA)

Inverse Problem (Estimation of diffusivity)

Using experimental data (A. Cordero), the values of obtained using different mesh sizes are as follows:

Mesh	Diffusivity α (m^2/s)	Residue
30x50	3.909×10^{-5}	6.581×10^3
120x200	3.203×10^{-5}	6.584×10^3
300x500	3.060×10^{-5}	6.582×10^3

Same sand with different method in 1D: $10^{-7} \leq \alpha \leq 4 \times 10^{-7}$

List of difficulties:

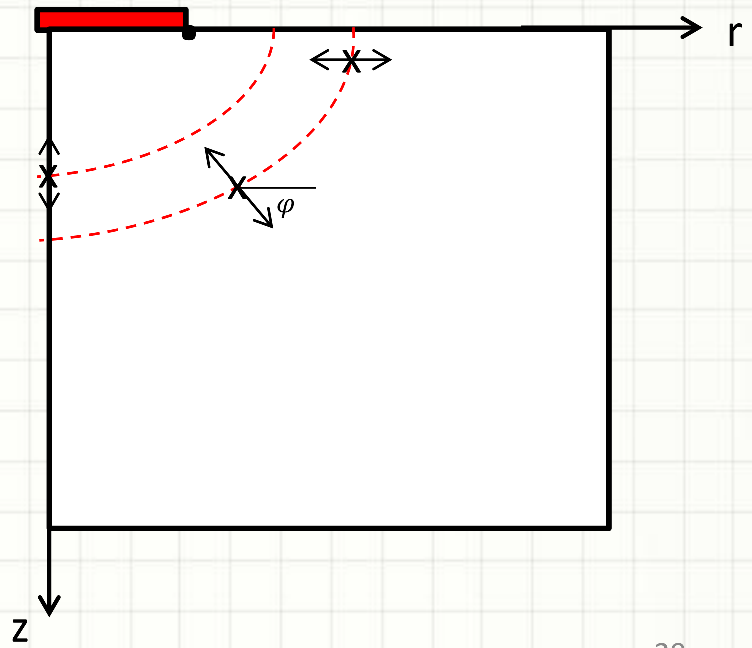
- Suspections on the measurement of sensors' positions ⟶ to be treated as unknowns
- Non-uniform initial temperature across sensors ⟶ Use a fit
- Non-uniform heating plate temperature ⟶ Preliminary tests show an important role... to be taken into account in future.
- The value of α is very sensitive w.r.t sensors' positions: a change of 1 mm of a sensor "close to the fire" will cause a change of approximately 100 in the value of α.

Inverse Problem (Estimation of α and sensors' positions)

1. This inverse problem (without any constraint) has infinitely many solutions:
   - The analytical solution in 1D $\approx \operatorname{erf}\left(\frac{z}{\sqrt{\alpha t}}\right)$

2. To obtain a unique solution: a constraint is needed
   - Experiments with large number of sensors.
   - Statistically: we can assume that the sum of the measurement error in sensors' positions (δ_{r_i} and δ_{z_i}) is zero. (i.e. $\sum_{i=1}^{n} \delta_{r_i}=0$ and $\sum_{i=1}^{n} \delta_{z_i}=0$).

3. In 3D-axisymmetric coordinate system:
   - The isotherms has a shape close to an ellipse.
   - Each sensor is constrained to move only in the direction normal to the isotherm.



- Constraints:
  1. $\sin\varphi_i \delta_{r_i} = \cos\varphi_i\, \delta_{z_i}$
  2. $\sum_{i=1}^{n} \delta_{r_i} = 0$
  3. $\sum_{i=1}^{n} \delta_{z_i} = 0$

4. An error in measurement method

A bias represented by a shift in both directions should be added as unknowns

Inverse Problem: Reformulation

A sensor new position can be defined as follows:

$$\tilde{r}_i = r_i + \delta_{r_i} + \beta_r$$
$$\tilde{z}_i = z_i + \delta_{z_i} + \beta_z$$
$$i = 1, 2, \dots, n$$

The unknowns in our inverse problem are:

- Diffusivity α
- Change in r-position and z-position of each sensor (δ_{r_i} *and* δ_{z_i})
- The bias in both r and z directions (β_r *and* β_z)

The constraints are:

- $\sum_{i=1}^{n} \delta_{r_i} = 0$ and $\sum_{i=1}^{n} \delta_{z_i} = 0.$
- For each sensor, $\sin\varphi_i \delta_{r_i} = \cos\varphi_i \delta_{z_i}$
- Box constraints to insure: $\begin{cases} New\ sensor's\ position\ belongs\ to\ physical\ domain \\ \alpha\ attains\ a\ positive\ value \end{cases}$

How to Solve the Constrained Inverse Problem?

Constrained non-linear least square problem with linear constraints (Equality constraints)

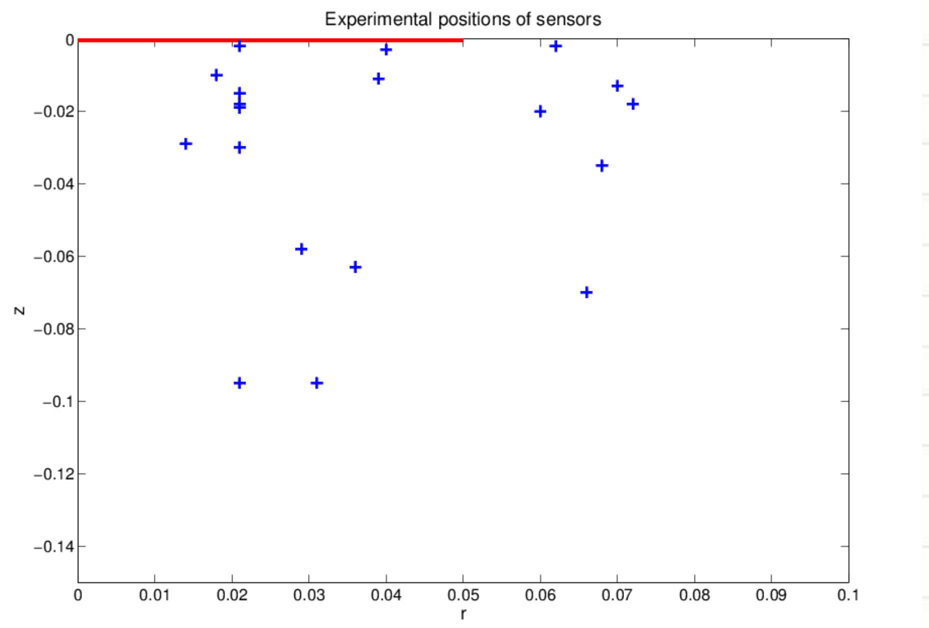
↓ Using variable substitution

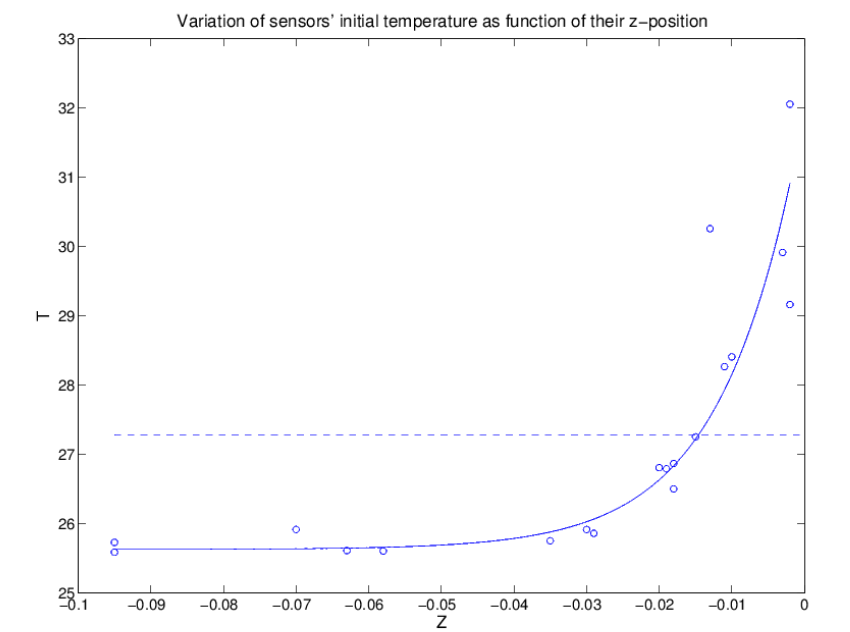
Unconstrained non-linear least square problem with less number of unknowns

↓

Use Levenberg Marquardt algorithm with parameters' scaling

Experiment





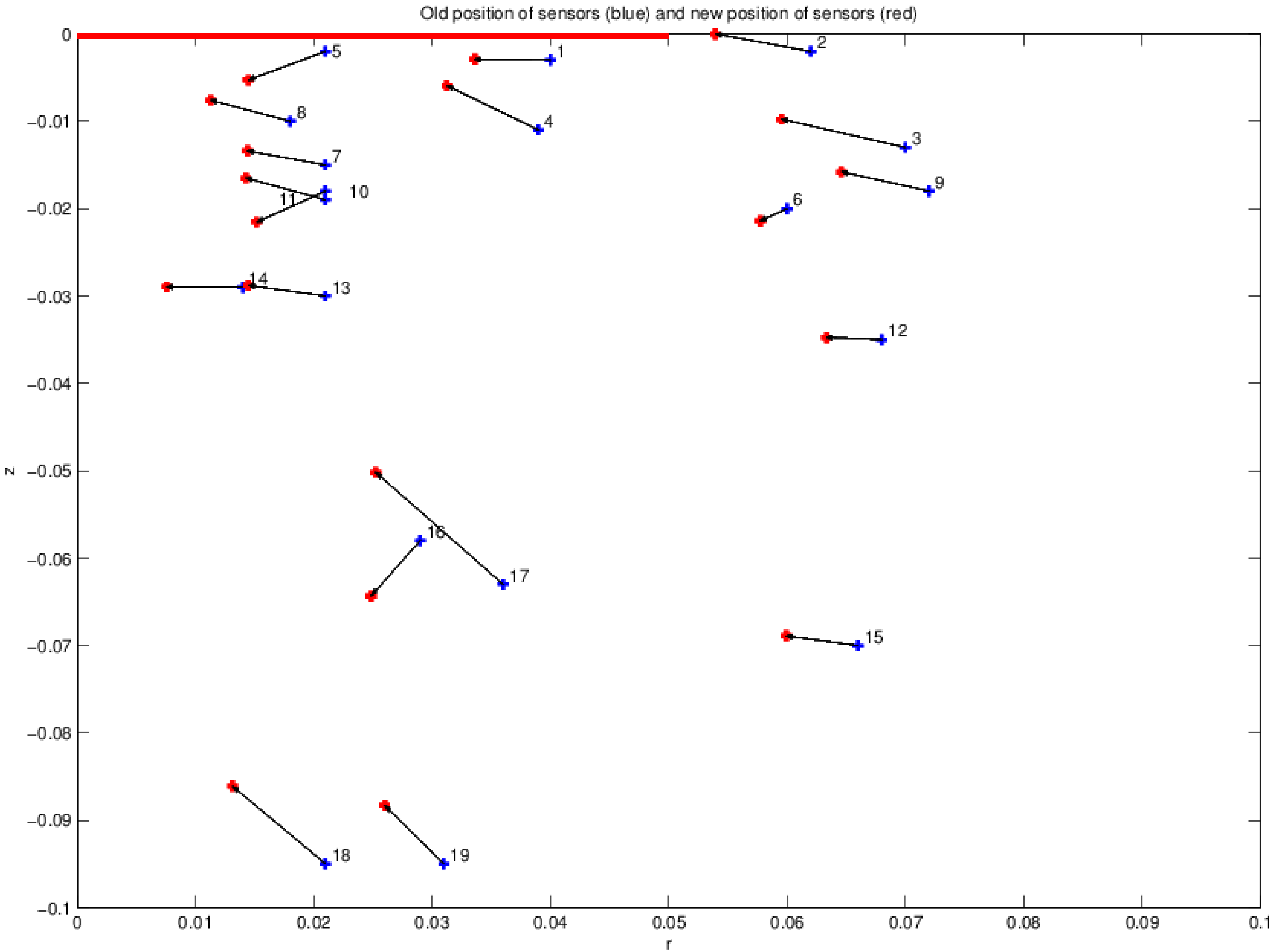
- Sensors on the top-right are more sensitive in r-direction
- Sensors close to the axis of symmetry are more sensitive in the z-direction.

- Initial temperature ≠ homogenous
- Exponential fit

Comparison between uniform & non-uniform initial temperature (Mesh: 300x500)

	Uniform	Non-Uniform
α (m^2/s)	2.1×10^{-7}	2.42×10^{-7}
β_r (cm)	-0.014	-0.664
β_z (cm)	0.473	0.187
Standard deviation of δ_r (cm)	0.658	0.197
Standard deviation of δ_z (cm)	0.544	0.440
Residual	816.5	787.6

Displacement of sensors

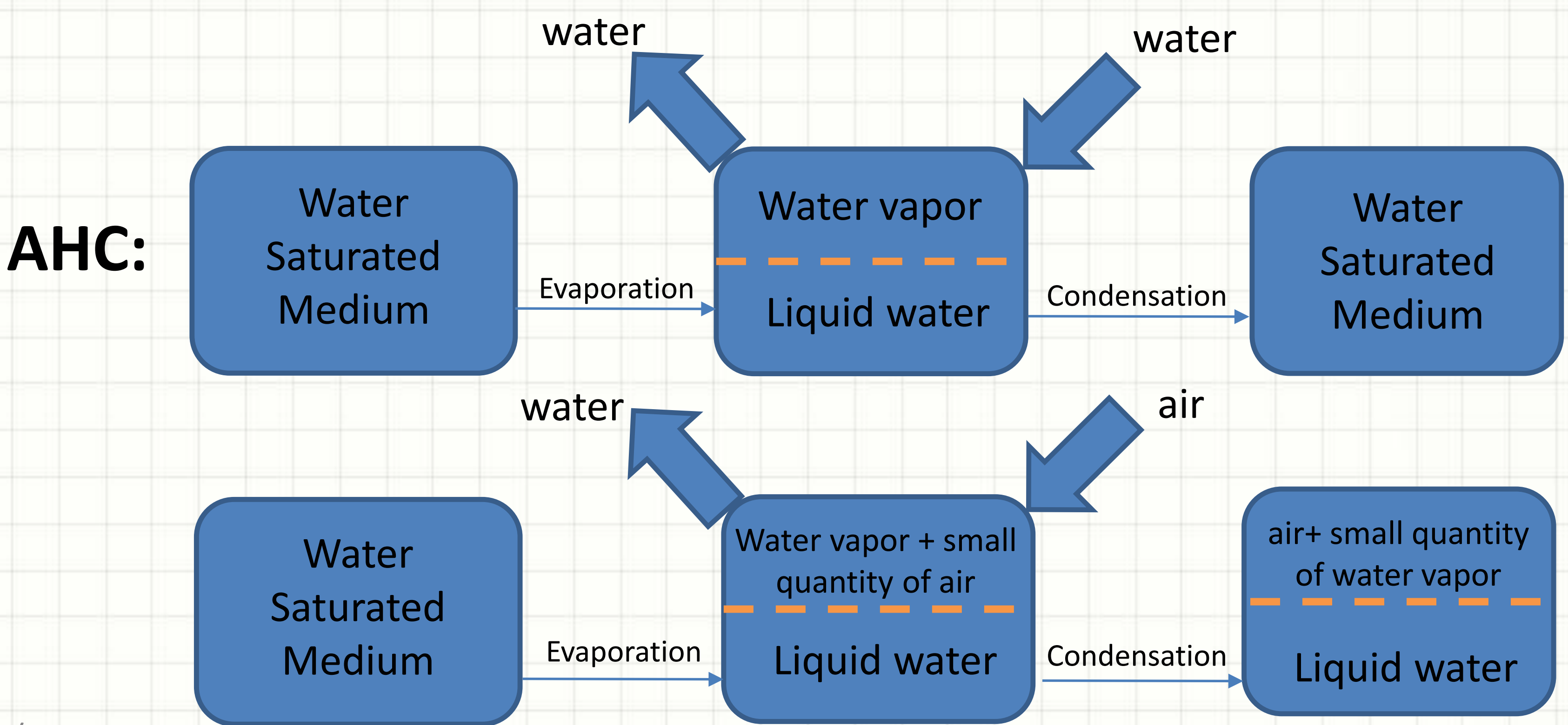


Outline:

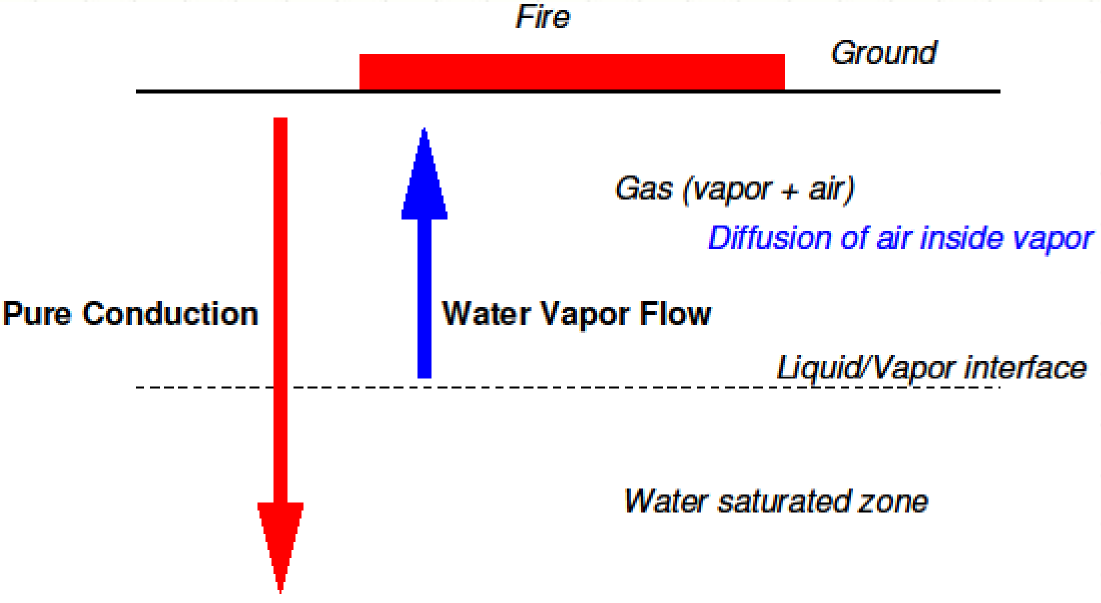
1. Solving the Heat equation with phase change in 1D and 2D coordinate systems.
2. Identification of the thermophysical properties of the soil by inverse problem.
3. **A simplified physical model for phase change in presence of air.**
4. Conclusions and Perspectives.

Phase change in a porous medium in presence of dry air

- Archaeologists are interested in studying the heating and cooling stages of prehistoric hearths.
- The old model based on the AHC method can’t be used to describe the cooling stage.



Physical Model



A separated phase model.

→ Liquid zone

→ Gaseous zone

The interface position is calculated explicitly

Governing Equations:

The main Variables are :

Temperature (T), Pressure (P) and the molar density of water vapor (n_w)

1. The energy conservation in the two zones:

$$(\rho C)_e \frac{\partial T}{\partial t} - \frac{K(\rho C)_f}{\mu_f} \nabla P \nabla T = \mathrm{div}(\lambda_e \nabla T) + \text{energy source term}$$

2. The mass conservation of the gaseous mixture in the gaseous zone:

$$\emptyset \left[\frac{1}{\beta T}\frac{\partial P}{\partial t} - \frac{P}{\beta T^2}\frac{\partial T}{\partial t}\right] + \mathrm{div}\left(- \frac{\rho_f K}{\mu_f} \nabla P \right) = 0 + \text{mass flux at interface}$$

3. The mass conservation of the water vapor in the gaseous zone:

$$\frac{\partial(\emptyset n_w)}{\partial t} + \mathrm{div}\left(n_w v_g - D_{w,a} \nabla n_w \right) = 0$$

4. Explicit interface tracking:

$$\rho_l \frac{\partial \xi}{\partial t} = n_w M_w \frac{K}{\mu_g} \nabla P + M_w D_{w,a} \nabla n_w$$

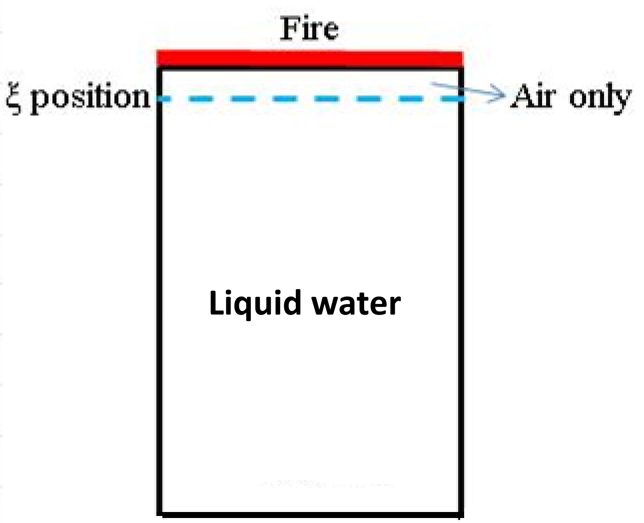
3 PDEs and 1 ODE

$$
\begin{cases}
\dfrac{\partial T}{\partial t} = f(t,x,T,P) + energy\ source\ term \\
\begin{cases}
A\dfrac{\partial T}{\partial t} + B\dfrac{\partial P}{\partial t} = g(t,x,T,P) + mass\ flux\ at\ interface\ (gaseous\ zone) \\
\dfrac{\partial P}{\partial x} = 0\ (liquid\ zone)
\end{cases} \\
\dfrac{\partial n_w}{\partial t} = h(t,x,T,P,n_w)\ \ only\ for\ \ 0 < x < \xi \\
\dfrac{d\xi}{dt} = q(t,P,n_w)
\end{cases}
$$

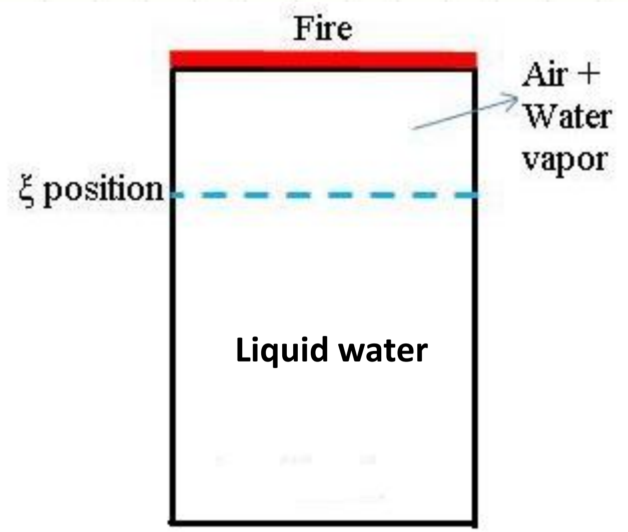
Method of lines: spatial discretization “Finite volume method“

→ ODE system → ODE solver “BDF scheme”

Numerical Example



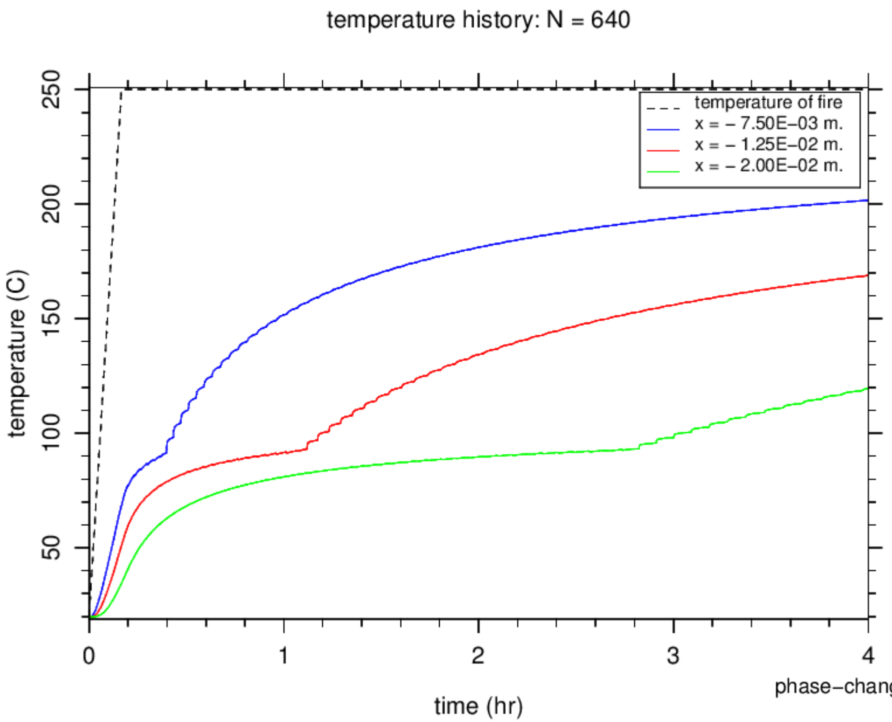
At $t_0 = 0$

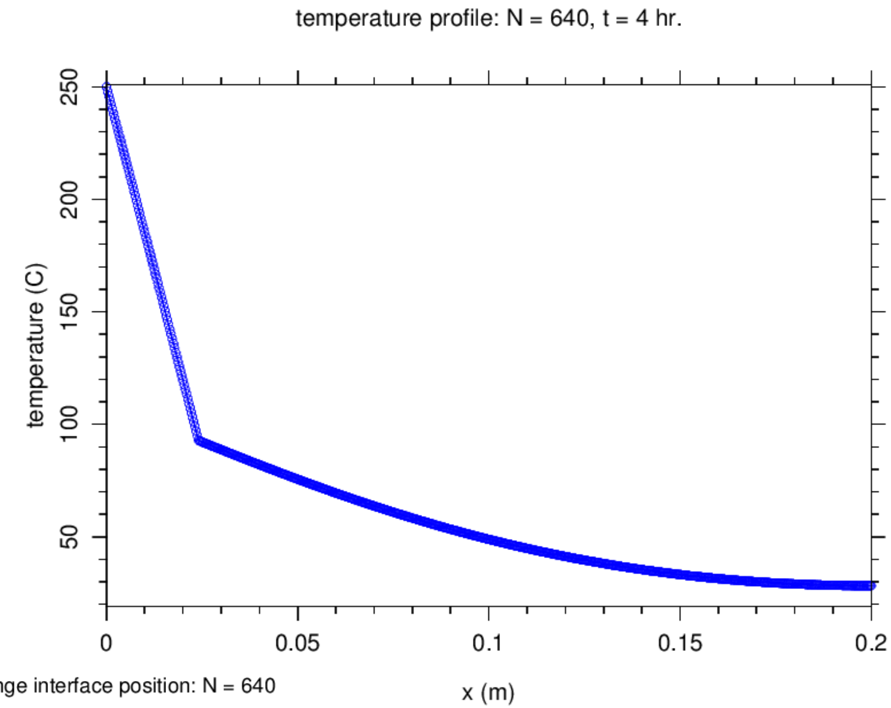


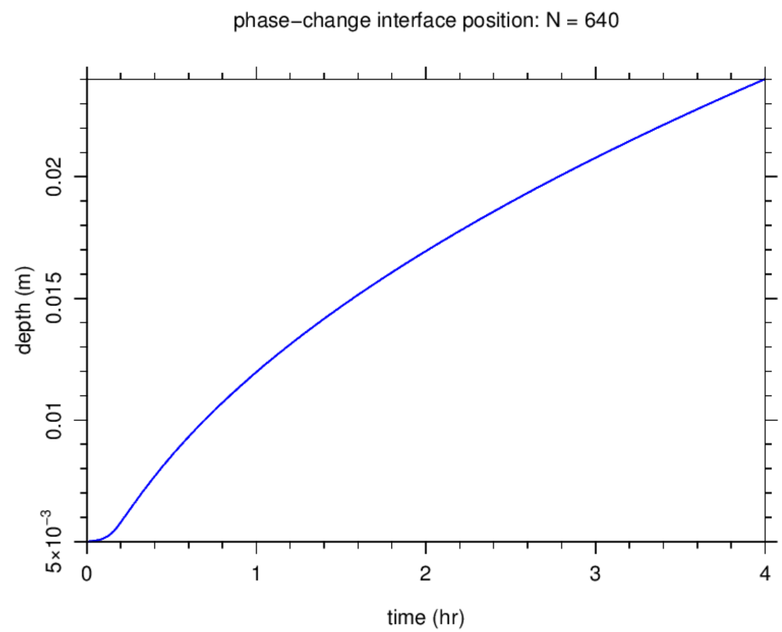
At $t_{final} = 4\ h$

- 20 cm 1D Domain
- Initially interface at 5 mm
- $T_{fire} = 250^0\ C$
- Final position of interface ($\xi = 23.3\ mm$)

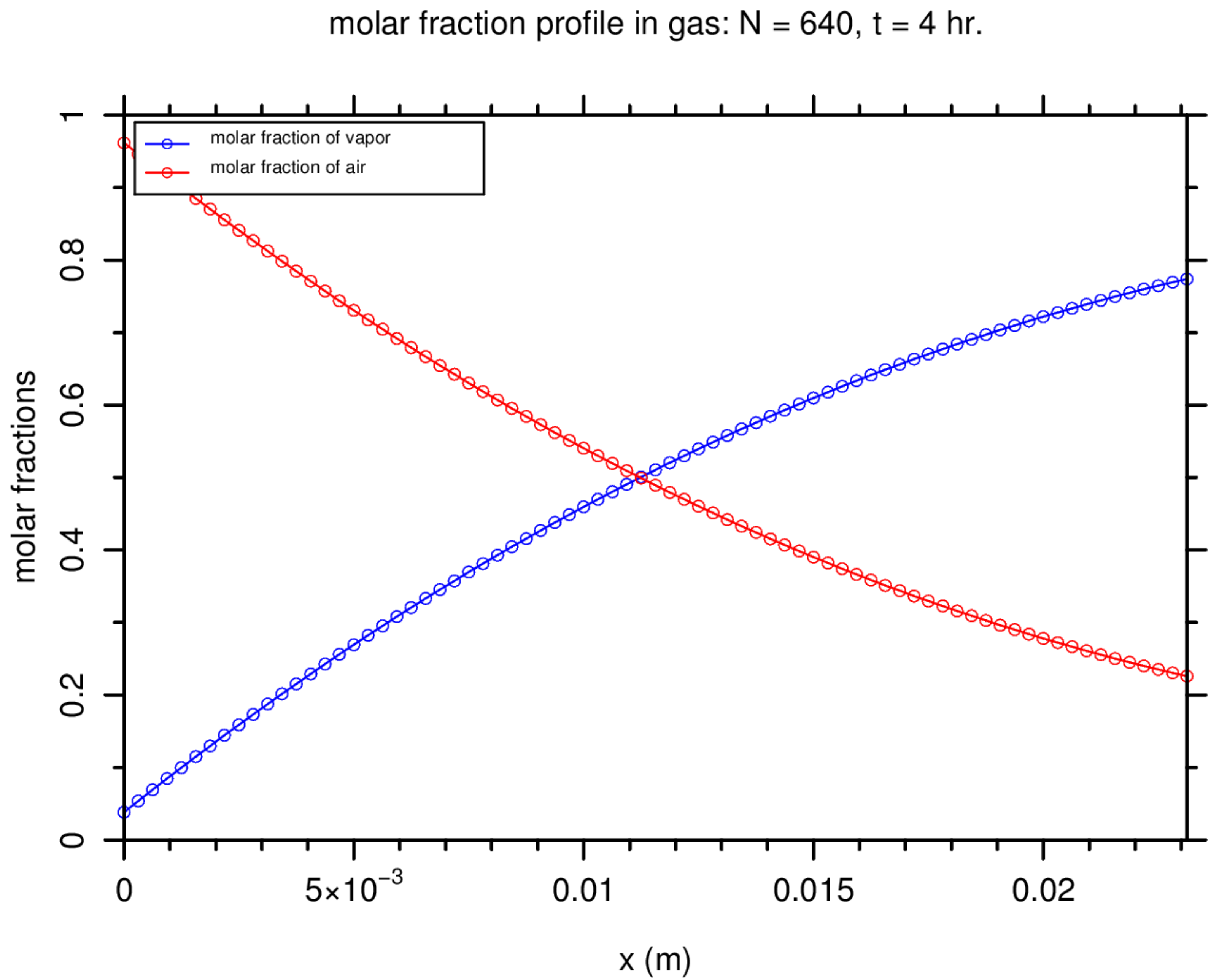
Results


temperature history: N = 640
temperature of fire
x = – 7.50E–03 m.
x = – 1.25E–02 m.
x = – 2.00E–02 m.
temperature (C)
250
200
150
100
50
0
1
2
3
4
time (hr)

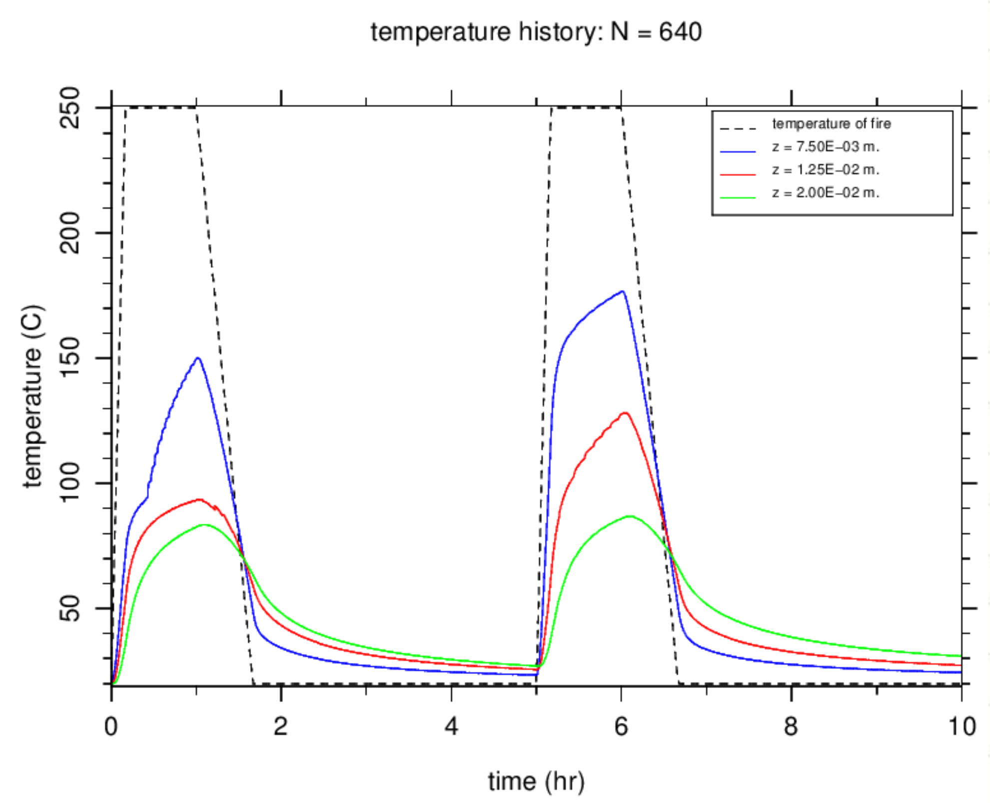

temperature profile: N = 640, t = 4 hr.
temperature (C)
250
200
150
100
50
0
0.05
0.1
0.15
0.2
x (m)


phase–change interface position: N = 640
depth (m)
0.02
0.015
0.01
5×10⁻³
0
1
2
3
4
time (hr)

Components' distribution in the gaseous zone

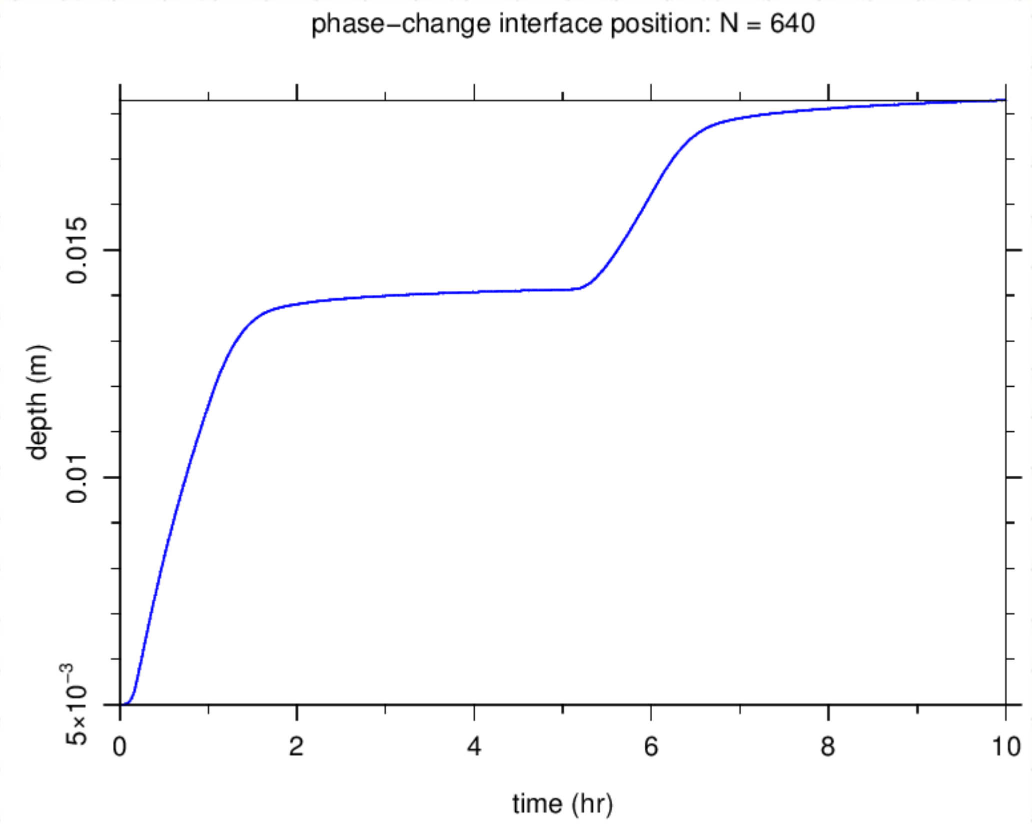


A sequence of heating and cooling stages



Stages	The temperature of the closest sensor to heating source
1st heating stage Maximum Temperature	150 °C
2nd heating stage Maximum Temperature	178 °C
1st cooling stage Minimum Temperature	23 °C
2nd cooling stage Minimum Temperature	24.5 °C

A sequence of heating and cooling stages



Sequence	Change in interface position
1st sequence	9.15 mm
2nd sequence	4.15 mm

Outline:

1. Solving the Heat equation with phase change in 1D and 2D coordinate systems.
2. Identification of the thermophysical properties of the soil by inverse problem.
3. A simplified physical model for phase change in presence of air.
4. **Conclusions and Perspectives.**

Conclusion

- Importance of the choice of ΔT in the AHC method (Direct and Inverse Problems)
- A phase change problem using 2D home-made adaptive mesh.
- Inverse problem in 3D axisymmetric coordinate system (synthetic and experimental data)
- A new separated phase model was presented. (interface tracking):
  - Presence of air
  - Alternating heating/cooling stages can be simulated.

Perspectives

- The application of a new model which deals with phase change in a wet unsaturated porous medium.
  - Calculate the value of λ_e for a realistic grains' distribution in a wet porous medium using statistical information.
  - Use this value of λ_e as an input parameter in the new physical model.

- Taking radiation, gravity and capillary forces into account in the future models.

- Studying the effect of the variation of the parameters related to the use of Zohour (phase change and Hessian coefficients).