STEFAN PROBLEM EVALUATED UNDER DIFFERENT BOUNDARY CONDITIONS USING A FINITE DIFFERENCE SCHEME AND A CRANK-NICOLSON SCHEME

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Stefan's problem corresponds to a range of problems of differential equations with the particularity of having a mobile border condition. In the following work, Stefan's condition is raised after obtaining it considering the diffusion in a specific region. Together with Stefan's condition, a heat equation is proposed in the region that progressively expands in the problem, so that these two equations are the starting point for a dimensionless problem that will facilitate the elimination of one of the most important characteristics of the problem in a Cartesian coordinate system: there is a singularity at the beginning of the time coordinate for the problem. This singularity is resolved by making a change of coordinates, which makes it clear that the singularity corresponds to the coordinates used to model the problem but not to the physical problem. Once this change of coordinates is made, the problem is solved numerically by proposing three types of boundary conditions: a constant, a time-dependent and a periodic condition. Finally, the results are presented in heat maps and graphs of the interface advance profile.

PDE's Model [1]

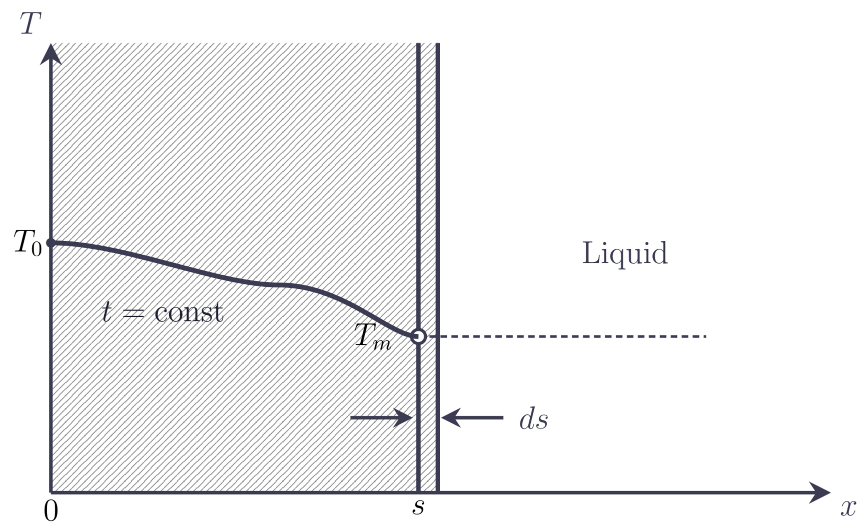
The Stefan condition is obtained considering an initial material going through a phase change, in this region a differential equation of heat can be used:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad \begin{cases} T(x=0) = T_0(t) \\ T(x=s) = T_m \end{cases}$$

$$-h_E \rho \frac{ds}{dt} = \lambda_L \frac{\partial T}{\partial x} \quad \{ s = 0, t = 0 \ .$$

$$\frac{\partial^2 \theta}{\partial q^2} = \frac{\partial \theta}{\partial \tau} \quad \begin{cases} \theta(0,\tau) = \theta_0(\tau) \\ \theta(\xi, \tau) = 0 \end{cases}$$

$$\frac{d\xi(\tau)}{d\tau} = \pm Ste \frac{\partial \theta}{\partial q}\bigg|_{s=\xi(\tau)} .$$



Temperature profile (for t = constant) for the solidifying of a plane solid. s is the distance between the phase boundary and the cooled surface $x = 0$.

Numerical Schemes:

The numerical schemes implemented are a semi-implicit scheme and the Crank-Nicholson Scheme. Where we discretize implicit in time and explicit in terms of χ

Analysis for times near zero [2]

Considering that in the numerical solution of problems that involve a phase change, a crucial problem is in how to start the computational work for a region with thickness 0. A solution to this coordinate problem is sought by establishing a change of variables where the variable χ will represent the spatial coordinate of the problem, and two functions $h(\tau)$ and $F(\chi,\tau)$ such that the function $h(\tau)$ is an auxiliary function to get rid of the singularities of the beginning of the problem

$$\chi = \frac{q}{\xi(\tau)} \ , \quad \theta = h(\tau) F(\chi, \tau) \ .$$

Furthermore, as the change of coordinates is assessed, a new set of equations is set, a partial differential equation involving F, h and the interface term ξ. Along with a Stefan condition which is consistent with the new coordinates

$$h \frac{\partial F}{\partial \chi} = \xi \left[\xi \frac{dh}{dt} F + \xi h \frac{\partial F}{\partial \tau} - \chi \frac{d\xi}{d\tau} h \frac{\partial F}{\partial \chi} \right] \begin{cases} F = \frac{\theta(0,\tau)}{h(\tau)} \text{ at } \chi = 0 \\ F = 0 \text{ at } \chi = 1 \end{cases} ,$$

$$\beta \chi \frac{d\xi}{d\tau} = -h \frac{\partial F}{\partial \chi} \text{ at } \chi = 1.$$

Constant boundary condition

The first boundary condition established for the general Stefan Problem is the constante condition $\theta(\chi = 0, \tau) = 0$. Near zero the equation

$$\frac{\partial^2 F}{\partial \chi^2} = -2\gamma^2 \chi \frac{\partial F}{\partial \chi} \ , \longrightarrow \frac{\partial^2 F}{\partial \chi^2} = z \frac{\partial F}{\partial \tau} - \chi \frac{1}{2} \frac{dz}{d\tau} \frac{\partial F}{\partial \chi} \begin{cases} F(\chi=0) = 1 \\ F(\chi=1) = 0 \\ F(\chi, \tau=0) = 1 - \frac{\text{erf}(\gamma\chi)}{\text{erf}(\gamma)} \end{cases} ,$$

$$\frac{\beta}{2} \frac{dz}{d\tau} = -\frac{\partial F}{\partial \chi}$$

Semi-Implicit Scheme's Equations

$$\left[r + \frac{\nu}{4} \chi_i \left(\frac{dz}{d\tau} \right)^n \right] F_{i+1}^{n+1} - (2r + z^n) F_i^{n+1} + \left[r - \frac{\nu}{4} \chi_i \left(\frac{dz}{d\tau} \right)^n \right] F_{i-1}^{n+1} = -z^n F^n \ ,$$

$$\left(\frac{dz}{d\tau} \right)^n = -\frac{3F_I^n - 4F_{I-1}^n + F_{I-2}^n}{\beta \Delta \chi} \ ,$$

Crank-Nicholson Scheme's Equations

$$\frac{\beta \chi_I}{2\Delta t} (z^{n+1})^2 + \left[-\frac{\beta \chi_I}{\Delta \tau} z^n + \frac{2\beta}{\nu} r F_I^{n+1} - F_I^n \right] z^{n+1} + \frac{\beta \chi_I}{2\Delta \tau} (z^n)^2 - 2\frac{2\beta r}{\nu} z^n$$
$$+ (2r + z^n) F_I^{n+1} + (2r - z^n) F_I^n - 2r \left(F_{I-1}^{n+1} + F_{I-1}^n \right) = 0 \ .$$

$$(A + I' + z'B) F^{n+1} = \left(-\frac{z^{n+\frac{1}{2}}}{k} I - z'B - A \right) ,$$

Exponential boundary condition

We now introduce a time dependent boundary condition, such that our approach for times near zero can be applied. This boundary is expressed as $\theta(\chi, \tau = 0) = e^\tau - 1$.

$$\frac{\partial^2 F}{\partial \chi^2} = 0 \begin{cases} F(\chi=0) = 1 \\ F(\chi=1) = 0 \end{cases} \longrightarrow \tau \frac{\partial^2 F}{\partial \chi^2} = \xi \left[\xi F + \xi \tau \frac{\partial F}{\partial \tau} - \chi \tau \frac{d\xi}{d\tau} \frac{\partial F}{\partial \chi} \right] \begin{cases} F(\chi=0) = 1 \\ F(\chi=1) = 0 \\ F(\chi,0) = 1 - \chi \end{cases}$$

$$\gamma^2 \beta = -\frac{\partial F}{\partial \xi} \text{ at } \chi = 1. \qquad \beta \chi \frac{d\xi}{d\tau} = -\tau \frac{\partial F}{\partial \chi}$$

Semi-Implicit Scheme's Equations

$$\left[r + \frac{\nu}{2} \chi_i \xi^n \left(\frac{d\xi}{d\tau} \right)^n \right] F_{i+1}^{n+1} - \left[2r + (\xi^n)^2 + \Delta\tau \right] F_i^{n+1} +$$
$$\left[r - \frac{\nu}{2} \chi_i \xi^n \left(\frac{d\xi}{d\tau} \right)^n \right] F_{i-1}^{n+1} = -(s^n) F_i^n \ ,$$

$$\left(\frac{ds}{d\tau} \right)^n = -\frac{t^n}{s^n} \cdot \frac{(3F^n I - 4F^n I - 1 + F_{I-2}^n)}{2\beta s^n \Delta \chi} \ .$$

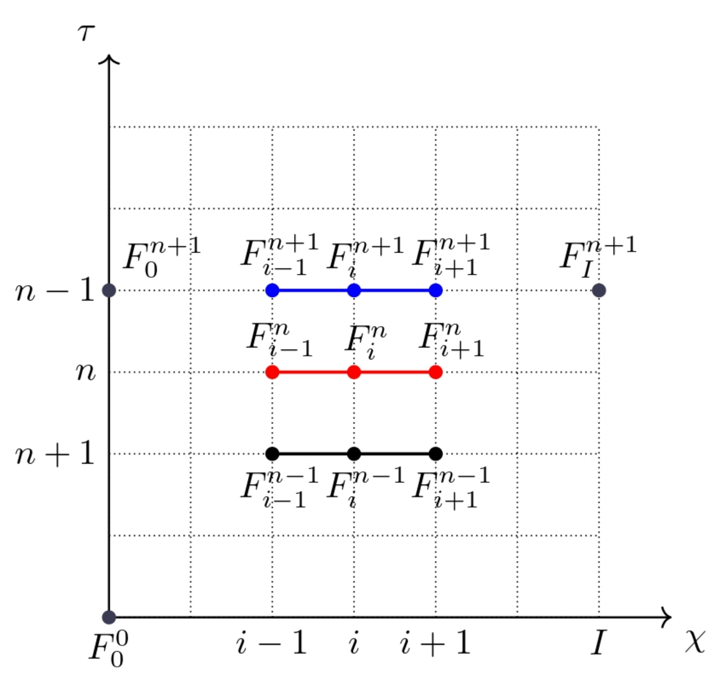
Crank-Nicholson Scheme's Equations

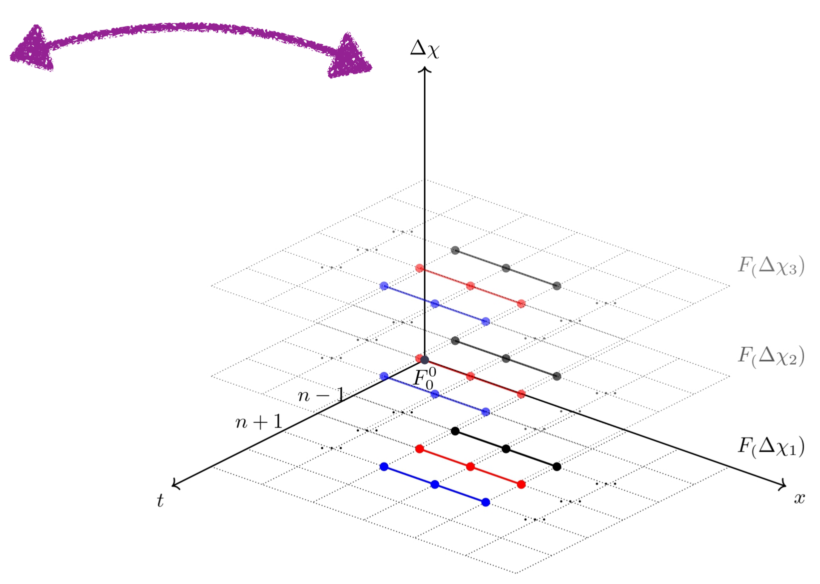
$$2r(\tau^{n+1} + \tau^n) \left(F_{I-1}^{n+1} + F_{I+1}^{n+1} \right) -$$
$$\frac{4\beta}{\nu} \left[r + \frac{\xi_I}{4\Delta\xi} \left((\xi^{n+1})^2 - (\xi^n)^2 \right) \right] \left((\xi^{n+1})^2 - (\xi^n)^2 \right) = 0$$

$$\left[\tau^{n+1/2} A - (\xi^{n+1/2})^2 \left(\frac{1}{2} + \frac{\tau^{n+1/2}}{k} I + \tau^{n+1/2} \xi^{n+1/2} \xi' B \right) \right] F^{n+1} =$$
$$\left[\tau^{n+1/2} A - (\xi^{n+1/2})^2 \left(\frac{1}{2} - \frac{\tau^{n+1/2}}{k} I - \tau^{n+1/2} \xi^{n+1/2} \xi' B \right) \right] F^n + D(\tau) \ ,$$

Error measurement

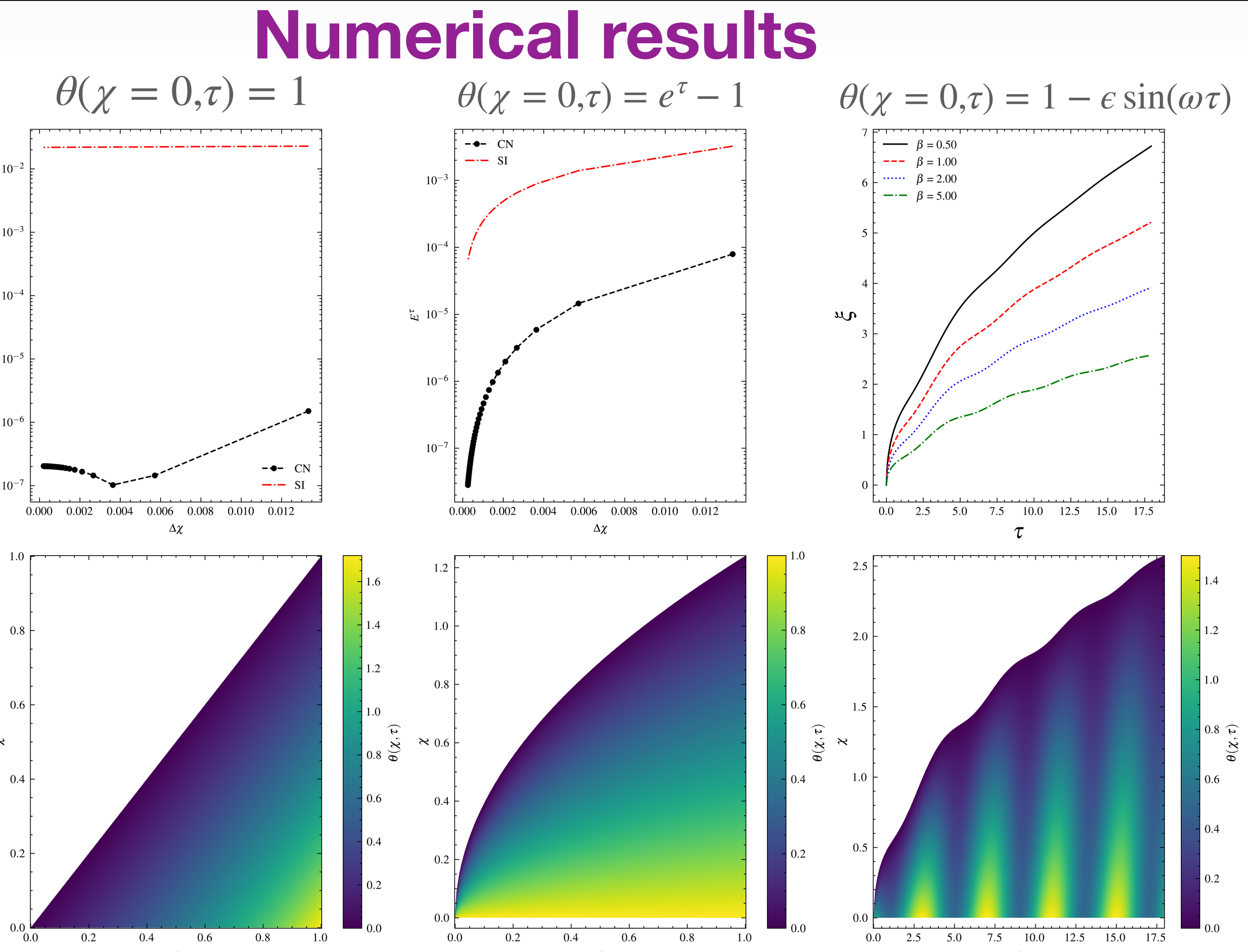
$$E_k^n = \left(\Delta_k \sum_{i=1}^{I-1} \left(F(\chi_i, \tau^n) - F_i^n \right)^2 \right)$$





The error measurement is done with k runs of the numerical scheme. Then, to quantize this error, a curve fit algorithm is implemented. This, to obtain a relation between the error E_k^n and the space separation or number of nodes.

Numerical results



Outlook & Conclusions

- The method proposed shows to be successful at addressing the singularity at $\tau \to 0$
- The approximation error with the Crank-Nicholson is lower than the error with the Semi-Implicit Scheme.
- Each temperatura distribution is strongly changed by the boundary conditions.
- The approach for the periodic boundary condition can be extender to more functions.

References

[1]Dieter Hans, Stephan Karl. Heat and mass transfers. Springer, Berling, third edition, 2014

[2] S.L. Mitchell and M. Vynnycky. Finite-difference methods with increased accuracy and correct initialization for one-dimensional Stefan problems.

[3] Svetislav Savović, James Caldwell, Finite difference solution of one-dimensional Stefan problem with periodic boundary conditions.

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