ASSESSMENT OF TWO DISCRETIZATION SCHEMES FOR HEAT CONDUCTION AND PHASE CHANGE MODELING

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Abstract. *Heat conduction and phase change problems are discretized in space by means of finite elements based on Ritz and collocation methods, while the time discretization stems*

from a fully implicit scheme. These formulations have their performances assessed by comparing the numerical results with the exact solutions of problems in semi-infinite media, either in pure diffusion without phase change - one-phase Stefan problem - or in conduction with phase change - two-phase Stefan problem. Convergence analyses reveal that the Ritz method is better suited to one-phase Stefan problem, while the two-phase Stefan problem is better treated by the collocation method.

Keywords: *Convergence, Eigenvalue bound, Finite element, Heat conduction*

1 INTRODUCTION

In recent years, PCM (Phase Change Materials) have become important in several aplications involving thermal insulation. Nowadays, modern construcions often use building envelopes with PCM in order to provide thermal comfort to occupants, together with energy efficiency (Kośny, 2015). As phase change is a nonlinear phenomenon, energy savings obtained by using these materials will change in dfferent situations, depending on climate, material properties, thermal loads, among other issues. Hence, building project with PCM should involve careful modeling of phase change and heat transfer between internal and external environments.

Several studies have been performed in order to assess the importance of material selection for thermal performance of building envelopes. Halford & Boehm (2007) modeled via finite differences peak load shift of air conditioning caused by the use of various PCM solutions as insulation for walls and ceilings. Those authors observed reductions on HVAC (heating, ventilating and air conditioning) peak load that vary from 11 to 57%, in relation to usual materials. On the other side, several recent implementations of PCM modeling showed numerical errors which varied from 5 to 20% in thermal loads (Barbour & Hittle, 2006; Al-Saadi & Zhai, 2013; Tabares-Velasco et al., 2012). This overlap between error margins and supposed energy savings justify the research on efficiency and accuracy of numerical methods for PCM modeling (Al-Saadi & Zhai, 2013; Dutil et al., 2014).

This work presents a convergence analysis of the method proposed by Rolph III & Bathe (1982) to model heat conduction and phase change. This method is implemented together with collocation method (which was the original implementation) and with linear interpolation of temperatures. Numerical results are compared to exact solutions for both one-phase and two-phase Stefan problems.

2 THE STEFAN PROBLEM

The one-dimensional Stefan problem consists of a semi-infinite solid medium at an initial constant temperature ($T = T_l$ for $x > 0$). The boundary at $x = 0$ is suddenly heated and the temperature at this surface raises to a constant value $T_h > T_l$.

In the one-phase Stefan problem, T_h is lower than the melting point T_m of the medium, which preserves their thermal properties, like its density ρ, specific heat c_s and thermal conductivity k_s. This problem is ruled by the heat conduction equation,

$$\frac{\partial T}{\partial t} = \alpha_s \frac{\partial^2 T}{\partial x^2}, \tag{1}$$

where $\alpha_s = k_s/\rho\, c_s$ is the thermal diffusivity. This equation is equal to the mass diffusion equation and may be solved by Laplace Transform (Crank, 1975):

$$T(x,t) = T_h + (T_l - T_h)\,\mathrm{erf}\left[\frac{x}{\sqrt{\alpha_s\, t}}\right], \tag{2}$$

where erf is the error function.

In the two-phase Stefan problem, $T_h > T_m > T_l$ and the heating of the boundary surface will melt the material. In this case, after melting the material is supposed to have the same

density ρ, but different specific heat c_l and thermal conductivity k_l; the material have a latent heat c_{sl}, which is absorved during the melting and is released during solitification. The melting front is considered planar and has position given by a function $s(t)$. The heat conduction in the melted zone ($0 < x < s(t)$) is ruled by diffusion equation

$$\frac{\partial T}{\partial t} = \alpha_l \frac{\partial^2 T}{\partial x^2}, \tag{3}$$

where $\alpha_l = k_l/\rho\, c_l$ is the thermal diffusivity. At $s(t)$, energy conservation is warranted by Stefan condition (Alexiades & Solomon, 1993)

$$\rho\, c_{sl} \frac{\mathrm{d}s}{\mathrm{d}t} = -k_l \left.\frac{\partial T}{\partial x}\right|_{x=s(t)^-} + k_s \left.\frac{\partial T}{\partial x}\right|_{x=s(t)^+}. \tag{4}$$

The exact solution of this problem is obtained by similarity, and involves the liquid-solid interface location

$$s(t) = 2\lambda\sqrt{\alpha_l\, t}, \tag{5}$$

where λ is the solution of the transcendental equation

$$\frac{St_l}{\exp(\lambda^2)\,\mathrm{erf}(\lambda)} - \frac{St_s}{\nu\exp(\nu^2\lambda^2)\,\mathrm{erfc}(\nu\lambda)} = \lambda\sqrt{\pi}, \tag{6}$$

with erfc being the complementary error function and

$$St_l = \frac{c_l(T_h - T_m)}{c_{sl}} \qquad St_s = \frac{c_s(T_m - T_l)}{c_{sl}} \qquad \nu = \sqrt{\frac{\alpha_l}{\alpha_s}}. \tag{7}$$

At any time, the material will be liquid for $x < s(t)$ and the temperature will be given by

$$T(x,t) = T_h - (T_h - T_m)\frac{\mathrm{erf}\left(\dfrac{x}{2\sqrt{\alpha_l\, t}}\right)}{\mathrm{erf}(\lambda)}. \tag{8}$$

The material will be solid for $x > s(t)$ and the temperature will be given by

$$T(x,t) = T_l + (T_m - T_l)\frac{\mathrm{erfc}\left(\dfrac{x}{2\sqrt{\alpha_s\, t}}\right)}{\mathrm{erfc}(\nu\lambda)}. \tag{9}$$

3 ALGORITHM FOR MODELING PHASE CHANGE

Rolph III & Bathe (1982) proposed an iterative algorithm for modeling phase change as a modified Newton-Raphson iteration, which is described in the following, with minor modifications. The calculation is performed as an incremental and iterative process. At initial instant of a time step Δt, nodal temperatures are given by the vector ${}^t\mathbf{T}$. For each iteration (i), nodal temperatures are incremented by the vector $\mathbf{\Delta T}^{(i)}$

$${}^{t+\Delta t}\mathbf{T}^{(i)} = {}^{t+\Delta t}\mathbf{T}^{(i-1)} + \mathbf{\Delta T}^{(i)} = {}^{t}\mathbf{T} + \mathbf{T}^{(i)}, \tag{10}$$

that is, $\mathbf{T}^{(i)}$ is the sum of all previous temperature increments along the time step Δt:

$$\mathbf{T}^{(i)} = \sum_{j=1} \boldsymbol{\Delta}\mathbf{T}^{(j)}. \tag{11}$$

Each iterative temperature increment is calculated by

$$\left({}^{t}\mathbf{K}^{k} + {}^{t}\mathbf{K}^{c} + {}^{t}\mathbf{K}^{r}\right)\boldsymbol{\Delta}\mathbf{T}^{(i)} = {}^{t+\Delta t}\mathbf{Q}^{(i)} + {}^{t+\Delta t}\mathbf{Q}^{c(i-1)} + {}^{t+\Delta t}\mathbf{Q}^{r(i-1)} - {}^{t+\Delta t}\mathbf{Q}^{k(i-1)}, \tag{12}$$

where ${}^{t}\mathbf{K}^{k}$, ${}^{t}\mathbf{K}^{c}$ and ${}^{t}\mathbf{K}^{r}$ are the conductivity, convection and radiation matrices, respectively. The vectors ${}^{t+\Delta t}\mathbf{Q}^{(i)}$, ${}^{t+\Delta t}\mathbf{Q}^{c(i-1)}$, ${}^{t+\Delta t}\mathbf{Q}^{r(i-1)}$ and ${}^{t+\Delta t}\mathbf{Q}^{k(i-1)}$ are the nodal point heat flows, corresponding to heat loads, convection, radiation and conduction effects, respectively.

It is worth noting that the RHS (right-hand side) should be zero and the components of the matrices ${}^{t}\mathbf{K}^{k}$, ${}^{t}\mathbf{K}^{c}$ and ${}^{t}\mathbf{K}^{r}$ may be viewed as derivatives of heat flows, as functions of nodal temperatures:

$${}^{t}K^{k}_{ij} = -\frac{\partial\, {}^{t+\Delta t}Q^{k(i-1)}_{i}}{\partial T^{(i)}_{j}} \quad {}^{t}K^{c}_{ij} = \frac{\partial\, {}^{t+\Delta t}Q^{c(i-1)}_{i}}{\partial T^{(i)}_{j}} \quad {}^{t}K^{r}_{ij} = \frac{\partial\, {}^{t+\Delta t}Q^{r(i-1)}_{i}}{\partial T^{(i)}_{j}}. \tag{13}$$

Hence, (12) might be taken as a Newton-Raphson procedure, except to the fact that ${}^{t+\Delta t}\mathbf{Q}^{(i)}$ contains heat loads due to phase change, which is a discondinuous function of $T^{(i)}_{j}$; this forbirds the existence of a matrix ${}^{t}\mathbf{K}$ for thermal loads.

The nodal point heat load vector is given by

$$\begin{aligned} {}^{t+\Delta t}\mathbf{Q}^{(i)} \;=\; & \int_{V} \mathbf{H}^{T}\; {}^{t+\Delta t}\mathbf{q}^{B}\mathrm{d}V + \int_{S_q} \left(\mathbf{H}^{\mathbf{S}}\right)^{T}\; {}^{t+\Delta t}\mathbf{q}^{S}\mathrm{d}S \\ & - \left(\int_{V} \boldsymbol{\rho}\; {}^{t+\Delta t}\mathbf{c}^{(i-1)}\mathbf{H}^{T}\mathbf{H}\mathrm{d}V\right)\dot{\mathbf{T}}^{(i)} + {}^{t+\Delta t}\,\mathbf{Q}^{(i-1)}_{l}, \end{aligned} \tag{14}$$

where $\mathbf{H}$ and $\mathbf{H}^{\mathbf{S}}$ are matrices of interpolation funcions in the volume and at the boundary surface, respectively, ${}^{t+\Delta t}\mathbf{q}^{B}$ is the vector of bulk heat generation, ${}^{t+\Delta t}\mathbf{q}^{S}$ is the vector of surface heat load, $\boldsymbol{\rho}$ is the material density ${}^{t+\Delta t}\mathbf{c}^{(i-1)}$ is the specific heat, which is calculated for ${}^{t+\Delta t}\mathbf{T}^{(i)}$, $\dot{\mathbf{T}}^{(i)}$ is the sum of all iterative temperature increments $\mathbf{T}^{(i)}$ divided by time step Δt and ${}^{t+\Delta t}\mathbf{Q}^{(i-1)}_{l}$ is the latent heat contribution.

In the case of phase change of a pure substance, for each node k with melting point $T_{m,k}$, latent heat contribution is calculated following one of these two cases:

1. Temperature is outside phase change:

   if

   $${}^{t}T_{k} < T_{m,k} \quad \text{and} \quad {}^{t+\Delta t}T^{(i)}_{k} < T_{m,k} \tag{15}$$

   or

   $${}^{t}T_{k} > T_{m,k} \quad \text{and} \quad {}^{t+\Delta t}T^{(i)}_{k} > T_{m,k}, \tag{16}$$

   then[1]

   $$\begin{aligned} \overline{T}^{(i)}_{k} &= T^{(i)}_{k} \\ Q^{(i)}_{l,k} &= 0. \end{aligned} \tag{17}$$

[1] According to Rolph III & Bathe (1982), the second equation reads $\Delta Q^{(i)}_{l,k} = 0$

2. Temperature passes through phase change temperature:

   if

$$ {}^{t}T_k < T_{m,k} \quad \text{and} \quad {}^{t+\Delta t}T_k^{(i)} \geq T_{m,k} \tag{18} $$

   or

$$ {}^{t}T_k > T_{m,k} \quad \text{and} \quad {}^{t+\Delta t}T_k^{(i)} \leq T_{m,k}, \tag{19} $$

   then

$$ \begin{aligned} \overline{T}_k^{(i)} &= T_m - {}^{t}T_k \\ \Delta Q_{l,k}^{(i)} &= -\int_{V_k} \frac{1}{\Delta t}\rho_k \ {}^{t+\Delta t}c_k^{(i-1)}(T_k^{(i)} - \overline{T}_k^{(i)})\mathrm{d}V. \end{aligned} \tag{20} $$

The volume integration is performed over the volume V_k associated (in a finite element sense) with node k, until

$$ {}^{t+\Delta t}Q_{l,k}^{(i)} = \sum \Delta Q_{l,k}^{(i)} = \pm Q_{l,total,k} \tag{21} $$

where we sum over all iterations ("+" refers to solidification; "−" refers to melting). For both cases, one has

$$ {}^{t+\Delta t}T_k^{(i)} = {}^{t}T_k + \overline{T}_k^{(i)} \tag{22} $$

while only for the second case,[2]

$$ {}^{t+\Delta t}Q_{l,k}^{(i)} = {}^{t+\Delta t}Q_{l,k}^{(i-1)} + \Delta Q_{l,k}^{(i)}. \tag{23} $$

4 HEAT CONDUCTION FORMULATION

Two formulations are used in this work for modeling heat conduction in space: the Ritz method and the collocation method. For the Ritz method, a linear interpolation of temperatures was chosen. In order to avoid eventual numerical instabilities caused by phase change, a fully implicit scheme was employed in time integration for both methods.

The development of the Ritz method with linear interpolation is detailed by Ramis et al. (2016) and it is beyond the scope of this work. Essentially, for a simple general purpose, heat conduction equation may be written in the form

$$ \rho c \frac{\partial T}{\partial t} - \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) - q^B = 0, \tag{24} $$

where q^B is an volumetric internal source of heat. The finite element equation for a fully implicit formulation is

$$ \frac{\rho c L_e}{6}\mathbf{A}\left\{\begin{array}{c} {}^{n+1}\dot{T}_1 \\ {}^{n+1}\dot{T}_2 \end{array}\right\} + \frac{k}{L_e}\mathbf{B}\left\{\begin{array}{c} {}^{n+1}T_1 \\ {}^{n+1}T_2 \end{array}\right\} = \frac{L_e}{2}q^B\left\{\begin{array}{c} 1 \\ 1 \end{array}\right\} + \left\{\begin{array}{c} q_1^S \\ q_2^S \end{array}\right\} \tag{25} $$

[2]Rolph III & Bathe (1982) state that this is valid for both cases.

where L_e is the element length, q^B is supposed to be uniformly distributed over L_e, q_i^S is the heat flow into the element at the nodes, $\dot{(\ )} = \mathrm{d}(\ )/\mathrm{d}t$ and

$$\mathbf{A} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}. \tag{26}$$

It is easy to identify that the first term of (25) is the third term on the RHS of (14) (sensible heat), the second term of (25) is ${}^{t+\Delta t}\mathbf{Q}^{k(i-1)}$ (i.e., conduction term of equation (12)), the third term of (25) is the first term on the RHS of (14) (bulk heat generation) and the fourth term of (25) is the second term on the RHS of equation (14) (surface heat load).

The collocation method uses the same formulation, except to the fact that sensible heat is calculated by a scheme of "lumped mass", which causes matrix $\mathbf{A}$ to be redefined as

$$\mathbf{A} = \begin{bmatrix} 3 & 0 \\ 0 & 3 \end{bmatrix}. \tag{27}$$

5 CONVERGENCE ANALYSIS

5.1 Statement of the Reference Problem

The problem chosen for convergence analysis was considered earlier by Comini et al. (1974, apud Rolph III & Bathe, 1982); this work preserves the original figures of numerical values, written in SI consistent units, without conversion. A uniform infinite slab of liquid is considered initially at $T = 0°$C. At time $t = 0^+$, the temperature of the surface of the liquid is reduced to $-45°$C and maintained constant. The conductivity, specific heat and density of the liquid and solid phases are assumed equal and constant:

- $k_s = k_l = 1.08$ J/m s K
- $\rho = 1$ kg/m^3
- $c_s = c_l = 1$ J/kg K
- $c_{sl} = 70.26$ J/kg

In the two-phase Stefan problem, $T_m = -0.1°$C, while freezing/melting point is higher than $0°$C for the one-phase Stefan problem.

The domain modeled by finite elements is $0 < x < 4$ m, and temperatures are imposed at both boundaries (Dirichlet condition), so that they coincide with the exact solutions of the Stefan problem (Section 2). The domain was subdivided in 8, 16, 32, 64 and 128 elements of same length.

Total time interval for analysis is taken to be $0 < t < 1$ s. Time domain as subdivided in 1, 4, 16, 64 and 256 time increments.

This problem is "inverted" in relation to Stefan original problem, as the medium is not melting, but it is freezing. This solution is almost the same solution presented in Section 2, except for the fact that St_s and St_l should be taken in modulus (positive sign), T_l is the medium initial temperature and T_h is the boundary temperature.

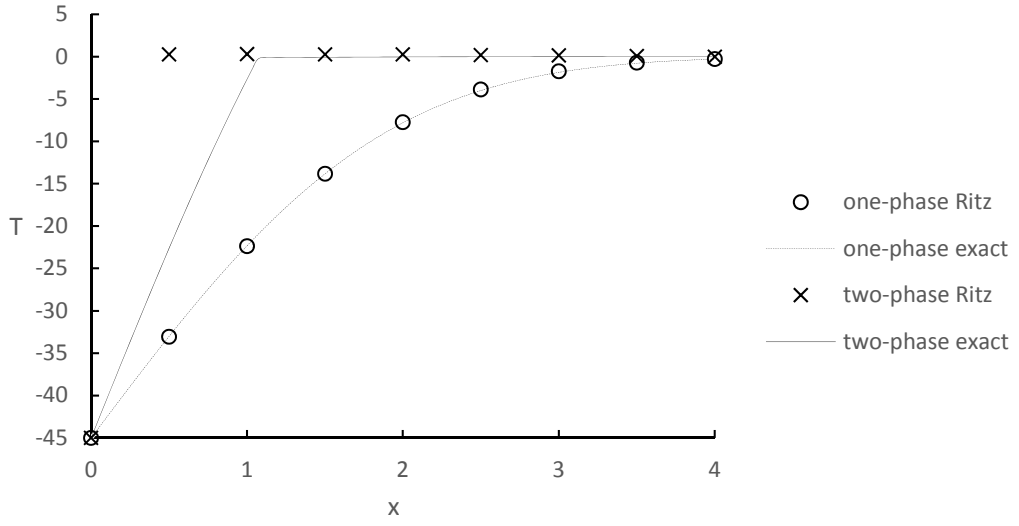

Figure 1: Results obtained with Ritz method for $t = 1$ s using 8 elements and 256 time increments.

5.2 Some Numerical Results

Figure 1 presents the results for $t = 1$ s obtained with Ritz method using 8 elements and 256 time increments. While the one-phase analysis shows very good agreement with the exact solution, the two-phase analysis did not converge after 55 iterations of Rolph III & Bathe's method.

Figure 2 presents the same analysis, but now using the collocation method with 128 elements and 256 time increments. In this case, both one-phase and two-phase analyses converged to the exact solutions.

5.3 Error Analysis

Table 1 presents the relative quadratic error

$$\varepsilon = \sqrt{\frac{\sum_{i=1}^{n} \left({}^{t+\Delta t}\tilde{T}_i - {}^{t+\Delta t} T_i \right)^2}{\sum_{i=1}^{n} {}^{t+\Delta t}T_i^2}} \tag{28}$$

for all analyses performed in this work, where ${}^{t+\Delta t}\tilde{T}_i$ is the temperature calculated at each node (contributions of the nodes constrained by Dirichlet boundary condition are not considered in (28)) and ${}^{t+\Delta t}T_i$ is the exact solution for the Stefan problem. As expected, most results show lower errors for higher discretization in space and time. Moreover, most results of collocation and Ritz method are similar. A very clear exception for these rules is the two-phase Stefan problem calculated with the Ritz method, which has three points at the up right corner (coarse space mesh with small time increments), that have the highest errors of the whole table, as

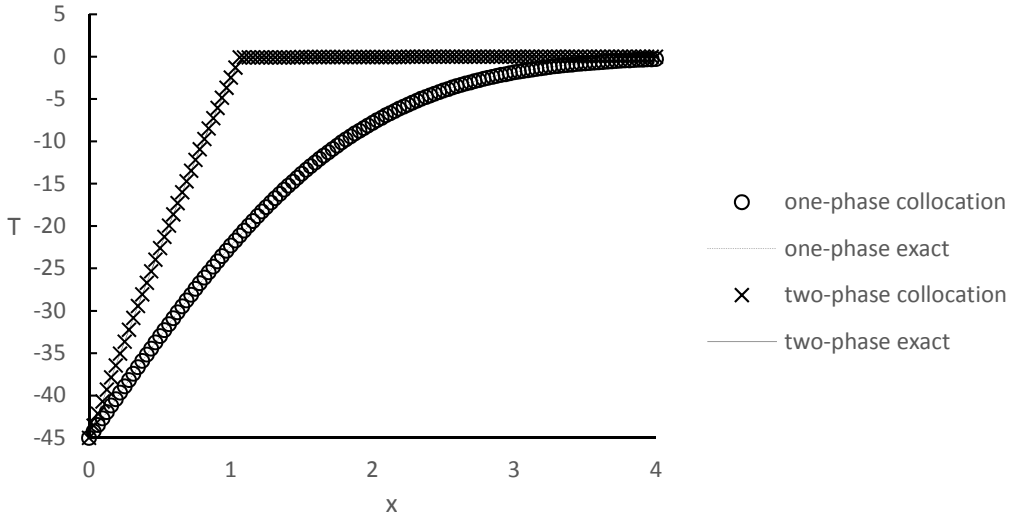

Figure 2: Results obtained with collocation method for $t = 1$ s using 128 elements and 256 time increments.

shown in Figure 1. This result suggests that application of Rolph III & Bathe (1982)'s algorithm to Ritz method may have convergence limitations, probably related to the melting front advance; this limitation can be estimated by some limit value of $\frac{\lambda^2 \alpha_l \Delta t}{\Delta x^2}$.

Figure 3 shows errors in numerical analyses with 128 elements (fifth line of each portion of Table 1). Almost all results suggest a first-order convergence, with similar accuracy. The only exception are the results for two-phase with 256 time steps, which suggest a limit for accuracy on phase change caused by the number of elements.

Figure 4 shows errors in numerical analyses with 256 time steps (fifth column of Table 1). It is worth noting that, for the one-phase Stefan problem, analyses with 32, 64 and 128 elements seem to have its accuracy controled by time discretization; analyses with 8 and 16 elements slightly suggest a second order convergence. For the two-phase problem with 128 elements, accuracy seems to be controlled by time discretization; analyses with 32 and 64 elements suggest second order convergence. At last, for analyses of two-phase Stefan problem with 8 or 16 elements, Ritz method leads to much worse results than those obtained with collocation method, as discussed in the beginning of this section.

6 CONCLUDING REMARKS

This paper presented a comparison between Ritz and collocation methods for heat conduction and phase change modeling. For problem involving only linear heat conduction (one-phase Stefan problem), both methods presented very similar performances and convergence, with very slightly better results for Ritz method in finer meshes. On the other side, Ritz method with coarser meshes in space showed very poor results for phase change problem (two-phase Stefan problem). Aparently, there is an implicit degree of regularity in Ritz formulation, which is based

Table 1: Relative quadratic error ε of Ritz and collocation methods for Stefan problems at $t = 1$ s.

number of	number of time increments				
elements	1	4	16	64	256
one-phase					
8	0.19539 †	0.05429	0.01393	0.00550	0.00479
	0.18357 ‡	0.05393	0.01544	0.00668	0.00534
16	0.17262	0.04869	0.01238	0.00313	0.00125
	0.16996	0.04862	0.01274	0.00355	0.00151
32	0.16348	0.04634	0.01188	0.00296	0.00074
	0.16285	0.04632	0.01196	0.00306	0.00085
64	0.15945	0.04525	0.01163	0.00292	0.00072
	0.15929	0.04525	0.01165	0.00294	0.00075
128	0.15756	0.04473	0.01150	0.00289	0.00072
	0.15752	0.04473	0.01151	0.00290	0.00073
two-phase					
8	0.45511	0.12008	0.11288	1.03516	1.01409
	0.44046	0.13003	0.11373	0.11303	0.11294
16	0.35218	0.09264	0.06756	0.06550	1.02605
	0.34819	0.09569	0.06847	0.06604	0.06560
32	0.30378	0.06530	0.02089	0.01385	0.01590
	0.30179	0.06554	0.01960	0.01251	0.01497
64	0.29223	0.06160	0.01319	0.00451	0.00398
	0.29206	0.06135	0.01470	0.00456	0.00398
128	0.28404	0.06338	0.01432	0.00508	0.00359
	0.28434	0.06361	0.01582	0.00521	0.00359

† - Ritz method ‡ - collocation method

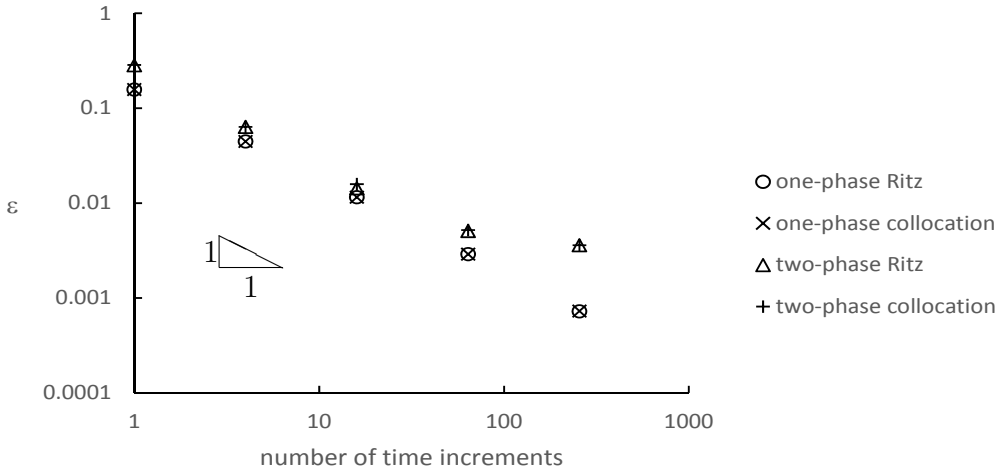

Figure 3: Quadratic error of Stefan problem numerical solutions with 128 elements

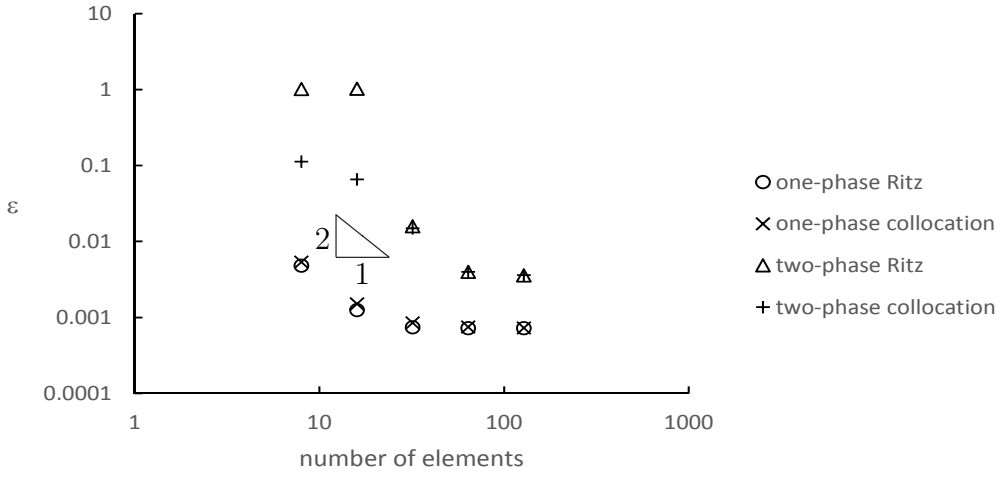

Figure 4: Quadratic error of Stefan problem numerical solutions with 256 time increments

on the derivative of temperature; this regularity does not take place in phase change problems. This might explain why collocation method shows better performance in phase change analyses involving short time steps. This trial explanation might be investigated in future researches, as, for example, with hybrid formulations, that require a lower degree of regularity in temperature.

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