ADAPTIVE SOLUTION OF PARABOLIC FREE BOUNDARY PROBLEMS WITH ERROR CONTROL

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Abstract

We derive *a posteriori* error estimates in natural energy norms with weights. They are useful in localizing the error extraction in regions of interest, and form the basis of an adaptive procedure. We use them to study the evolution of a persistent corner singularity and elucidate the issue of critical angle for instantaneous smoothing.

1 Introduction

The presence of interfaces, and associated lack of regularity, is responsible for global numerical pollution effects for parabolic free boundary problems. A cure consists of equidistributing discretization errors in adequate norms by means of highly graded meshes and varying time steps. Their construction relies on *a posteriori* error estimates, which are a fundamental component for the design of reliable and efficient adaptive algorithms for PDEs. These issues have been recently tackled in [6], [7], [8], [9], and are briefly discussed here.

We consider for simplicity the classical two-phase Stefan problem for an ideal material with constant thermal properties and unit latent heat

$$\partial_t u - \Delta\beta(u) = f \quad \text{in } Q = \Omega \times (0,T), \quad u(\cdot,0) = u_0(\cdot) \quad \text{in } \Omega, \tag{1}$$

where $\beta(s) = \min(s,0) + \max(s-1,0)$. A discrete solution U of (1) satisfies

$$\partial_t U - \Delta\beta(U) = f - \mathcal{R} \quad \text{in } Q, \quad U(\cdot,0) = U_0(\cdot) \quad \text{in } \Omega, \tag{2}$$

where $\mathcal{R}$, a distribution with singular components and oscillatory behavior, is the so-called *parabolic residual*. Its size is to be determined in negative norms which entail averaging and thus quantify oscillations better.

In §2 we show how to represent the errors $e_u = u - U$ and $e_{\beta(u)} = \beta(u) - \beta(U)$ in terms of $\mathcal{R}$, and in §§3 and 4 we derive error estimates in *weighted norms*

$$\|e_u(\cdot,T)\|_{H^{-1}_{-\omega}(\Omega)} + \|e_{\beta(u)}\|_{L^2_{-\omega}(Q)} \le \mathcal{E}(u_0, f, T, \Omega, \omega; U, h, \tau), \tag{3}$$

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with computable right hand side; hereafter h stands for the meshsize and τ for the time step. The weight ω is space dependent and serves to localize the errors in regions of interest. These formulas are the basis of the adaptive algorithm of [6], [7], [8], [9]. We present in §5 an application to a persistent corner singularity, and elucidate the question of critical angle for instantaneous smoothing. We conclude in §6 with some remarks on the hyperbolic structure of (1) along with the essential role of adaptivity in this study.

2 Error Representation Formulas

Upon subtracting (2) from (1), the error e_u satisfies the equation

$$\partial_t e_u - \Delta(b e_u) = \mathcal{R} \tag{4}$$

in the sense of distributions, where

$$0 \le b(x,t) = \int_0^1 \beta'(su(x,t) + (1-s)U(x,t))\, ds \le 1$$

is discontinuous. To express e_u in suitable norms we resort to *parabolic duality*. We multiply (4) by a smooth test function ϕ and integrate by parts

$$\langle e_u(\cdot,T), \phi(\cdot,T)\rangle - \int_0^T \langle e_u, \partial_t\phi + b\Delta\phi\rangle = \langle u_0 - U^0, \phi(\cdot,0)\rangle + \mathcal{R}(\phi), \tag{5}$$

where $\langle\cdot,\cdot\rangle$ stands for the usual $L^2(\Omega)$ inner product. We are thus led to study the backward parabolic problem in *nondivergence* form [3], with vanishing diffusion coefficient b and regularization parameter $\delta \downarrow 0$,

$$\partial_t\phi + (b+\delta)\Delta\phi = -b^{1/2}\chi \quad \text{in } Q, \quad \phi(\cdot,T) = \rho \quad \text{in } \Omega. \tag{6}$$

Let $\omega \in C^{0,1}(\bar\Omega)$ be a weight satisfying $\omega(x) \ge \omega_0 > 0$ and

$$\frac{|\nabla\omega(x)|}{\omega(x)} \le W \quad \forall\, x \in \Omega. \tag{7}$$

We introduce the following weighted norms over a generic domain Ξ

$$\|v\|_{L^2_{\pm\omega}(\Xi)} = \Big(\int_\Xi v^2\omega^{\pm 2}\Big)^{1/2}, \quad \|v\|_{H^{-1}_{-\omega}(\Xi)} = \sup_{\eta\in H^1_0(\Xi)} \|\nabla\eta\|^{-1}_{L^2_\omega(\Xi)} \int_\Xi v\eta.$$

These norms will serve to localize the error estimates, and thereby force extra refinement, in regions of interest. The theory of nonlinear strictly parabolic problems [2] yields existence of a unique solution ϕ, which satisfies

$$\max_{0\le t\le T} \|\nabla\phi(\cdot,t)\|_{L^2_\omega(\Omega)} + \|\partial_t\phi\|_{L^2_\omega(Q)} \le \mathrm{e}^{WT}\big(\|\nabla\rho\|_{L^2_\omega(\Omega)} + \|\chi\|_{L^2_\omega(Q)}\big) = D. \tag{8}$$

These bounds are proved in [3], [6] for $\omega = 1$. Their weighted counterpart result from multiplying (6) by $\omega^2\Delta\phi$, integrating by parts, and making proper use of

(7) to absorb an additional term via Gronwall. We thus realize that (6) does not exhibit a regularizing effect such as the heat equation since $\phi(\cdot,t)=\rho$ for all $0\leq t\leq T$ if $b=\delta=0$; hence $\|\Delta\phi\|_{L^2(Q)}$ is never bounded uniformly in δ. Duality combined with (5) as $\delta\downarrow 0$ thus yields

$$\chi=0: \quad \|e_u(\cdot,T)\|_{H^{-1}_{-\omega}(\Omega)} \leq \|u_0-U^0\|_{H^{-1}_{-\omega}(\Omega)} + \sup_{\rho\in H^1_0(\Omega)} \frac{|\mathcal{R}(\phi)|}{\|\nabla\rho\|_{L^2_\omega(\Omega)}}, \tag{9}$$

$$\rho=0: \quad \|e_{\beta(u)}\|_{L^2_{-\omega}(Q)} \leq \|u_0-U^0\|_{H^{-1}_{-\omega}(\Omega)} + \sup_{\chi\in L^2_\omega(Q)} \frac{|\mathcal{R}(\phi)|}{\|\chi\|_{L^2_\omega(Q)}}. \tag{10}$$

We stress that U need not be a finite element approximation of u. We use (9) and (10) below to study the time and full discretizations of (1).

3 Error Estimation for Time Discretization

We first illustrate the main ideas for an implicit time discretization of (1). Let $\tau_n=t^n-t^{n-1}$ be a variable time step and let U^n satisfy

$$\partial U^n-\Delta\beta(U^n)=f^n,$$

where $\partial U^n=(U^n-U^{n-1})/\tau_n$ and $f^n(\cdot)$ is an approximation of $f(\cdot,t)$ in $[t^{n-1},t^n]$ (e.g. $f^n(\cdot)=f(\cdot,t^n)$ or $f^n(\cdot)=\tau_n^{-1}\int_{t^{n-1}}^{t^n} f(\cdot,s)\,ds=\bar f^n(\cdot)$). If $U(\cdot,t)=U^n$ for $t^{n-1}<t\leq t^n$, then the residual $\mathcal{R}$ in (2) is given by

$$\mathcal{R}=\sum_{n=1}^N(\partial U^n+f-f^n)\,\chi_{[t^{n-1},t^n]}-(U^n-U^{n-1})\,\delta_{t^{n-1}},$$

where χ_I is the characteristic function of I and δ_s is a Dirac mass at $t=s$. Equivalently, we can split $\mathcal{R}$ into $\mathcal{R}_1$ and $\mathcal{R}_2$ as follows

$$\mathcal{R}_1(\phi)=\sum_{n=1}^N\int_{t^{n-1}}^{t^n}\langle\partial U^n,\phi-\phi(\cdot,t^{n-1})\rangle,\quad \mathcal{R}_2(\phi)=\sum_{n=1}^N\int_{t^{n-1}}^{t^n}\langle f-f^n,\phi\rangle. \tag{11}$$

If $f^n=\bar f^n$, we can exploit L^2 time orthogonality in conjunction with $\phi(\cdot,t)-\phi(\cdot,t^{n-1})=\int_{t^{n-1}}^t\partial_s\phi(\cdot,s)\,ds$ and (8), to deduce

$$|\mathcal{R}_1(\phi)|\leq\sum_{n=1}^N\int_{t^{n-1}}^{t^n}\|U^n-U^{n-1}\|_{L^2_{-\omega}(\Omega)}\|\partial_t\phi\|_{L^2_\omega(\Omega)}\leq D\mathcal{E}_1,$$
$$|\mathcal{R}_2(\phi)|=\Big|\sum_{n=1}^N\int_{t^{n-1}}^{t^n}\langle f-\bar f^n,\phi-\phi(\cdot,t^{n-1})\rangle\Big|\leq D\mathcal{E}_2,$$

where

$$\mathcal{E}_1=\Big(\sum_{n=1}^N\tau_n\|U^n-U^{n-1}\|^2_{L^2_{-\omega}(\Omega)}\Big)^{1/2} \qquad \textit{time residual,}$$
$$\mathcal{E}_2=\Big(\sum_{n=1}^N\tau_n^2\int_{t^{n-1}}^{t^n}\|f-\bar f^n\|^2_{L^2_{-\omega}(\Omega)}\Big)^{1/2} \qquad \textit{interpolation.}$$

If $\mathcal{E}_0 = \|u_0 - U^0\|_{H^{-1}_{-\omega}(\Omega)}$ denotes the *initial error*, on using (9) and (10), we immediately obtain

$$\|e_u(\cdot,T)\|_{H^{-1}_{-\omega}(\Omega)} + \|e_{\beta(u)}\|_{L^2_{-\omega}(Q)} \le \mathrm{e}^{WT}\big(\mathcal{E}_0 + \mathcal{E}_1 + \mathcal{E}_2\big);$$

the discretization error thus accumulates in time in the L^2 norm. To make it computable, we can replace $\mathcal{E}_1$ by the upper bound

$$\mathcal{E}_1 \le T^{1/2} \max_{1\le n\le N} \|U^n - U^{n-1}\|_{L^2_{-\omega}(\Omega)}.$$

Invoking H^1 space regularity of ϕ yields a weaker expression for $\mathcal{E}_2$ regardless of the choice of f^n [6]: $\mathcal{E}_2 = \sum_{n=1}^N \int_{t^{n-1}}^{t^n} \|f - f^n\|_{H^{-1}_{-\omega}(\Omega)}$.

4 Error Estimation for Full Discretization

Let $\mathcal{M}^n$ be a uniformly regular partition of Ω into simplices S with diameter h_S. Let $\mathbf{V}^n \subset H^1_0(\Omega)$ be the piecewise linear finite element space over $\mathcal{M}^n$ and I^n be the Lagrange interpolation operator.

The discrete problem can be written as follows. Let $U^0 \in \mathbf{V}^0$ be an approximation of u_0. Given $U^{n-1}, \Theta^{n-1} \in \mathbf{V}^{n-1}$, and having modified $\mathcal{M}^{n-1}$ and τ_{n-1} to get $\mathcal{M}^n$ and τ_n, we compute $U^n, \Theta^n \in \mathbf{V}^n$ according to $\Theta^n = I^n\beta(U^n)$ and

$$\langle \partial U^n, \varphi\rangle^n + \langle \nabla\Theta^n, \nabla\varphi\rangle = \langle f^n, \varphi\rangle^n \quad \forall\, \varphi \in \mathbf{V}^n. \tag{12}$$

Hereafter $\langle\cdot,\cdot\rangle^n$ is the vertex rule and $\partial U^n = (U^n - I^n U^{n-1})/\tau_n$ is the discrete time derivative. Mass lumping diagonalizes the mass matrix and, together with the constitutive relation $\Theta^n = I^n\beta(U^n)$ being only enforced at the nodes, leads to a monotone problem easy to implement and solved via nonlinear SOR [5].

On combining (12) with (11), we easily arrive at

$$\begin{aligned}
\mathcal{R}(\phi) = {} & \sum_{n=1}^N \int_{t^{n-1}}^{t^n} \langle R^n, \phi - \varphi\rangle - \sum_{n=1}^N \int_{t^{n-1}}^{t^n} \langle \nabla\Theta^n, \nabla(\phi - \varphi)\rangle \\
& + \sum_{n=1}^N \langle U^{n-1} - I^n U^{n-1}, \phi(\cdot, t^{n-1})\rangle + \sum_{n=1}^N \int_{t^{n-1}}^{t^n} \langle \partial U^n, \phi - \phi(\cdot, t^{n-1})\rangle \\
& + \sum_{n=1}^N \int_{t^{n-1}}^{t^n} \langle \nabla I^n\beta(U^n) - \nabla\beta(U^n), \nabla\phi\rangle \\
& + \sum_{n=1}^N \int_{t^{n-1}}^{t^n} \Big(\langle R^n, \varphi\rangle - \langle R^n, \varphi\rangle^n\Big) + \sum_{n=1}^N \int_{t^{n-1}}^{t^n} \langle f - I^n f^n, \phi\rangle
\end{aligned}$$

for all $\varphi(\cdot,t) \in \mathbf{V}^n$, $t^{n-1} < t < t^n$; hereafter R^n stands for the interior residual $R^n = I^n f^n - \partial U^n$. The last three terms account for consistency in the constitutive relation, quadrature, and interpolation of the source term; we will refer to them collectively as *consistency terms*. The forth term is similar to the time residual derived in §3, whereas the important new terms are the first three. They will be the focus of our next discussion.

In light of (8), we readily get

$$\sum_{n=1}^{N} \langle U^{n-1} - I^n U^{n-1}, \phi(\cdot, t^{n-1})\rangle \leq D \sum_{n=1}^{N} \|U^{n-1} - I^n U^{n-1}\|_{H^{-1}_{-\omega}(\Omega)}.$$

If we integrate by parts at the element level, and rearrange the contributions over each element edge, we obtain

$$-\langle \nabla\Theta^n, \nabla(\phi - \varphi)\rangle = \tfrac{1}{2} \sum_{S\in\mathcal{M}^n} \langle\!\langle J_S^n, \phi - \varphi\rangle\!\rangle_S,$$

where $\langle\!\langle\cdot,\cdot\rangle\!\rangle_S$ stands for the inner product in $L^2(\partial S)$ and $J_S^n = [\![\nabla\Theta^n \cdot \nu]\!]_S$ is the jump of temperature flux across ∂S. With the convention that the unit normal ν points outwards and $\nabla\Theta^n$ inside S is subtracted from $\nabla\Theta^n$ outside S, J_S^n is well defined. We next resort to approximation theory, and a nonoscillation property of ω at the element level, to select a piecewise linear φ satisfying

$$\|\phi - \varphi\|_{L^2_\omega(S)} + h_S\|\nabla(\phi - \varphi)\|_{L^2_\omega(S)} \leq C h_S \|\nabla\phi\|_{L^2_\omega(\hat{S})},$$

where $\hat{S}$ is the collection of all elements surrounding S; φ could be the Clément interpolant of ϕ. According to the regularity (8) of ϕ, we therefore deduce

$$\sum_{n=1}^{N}\int_{t^{n-1}}^{t^n} \langle R^n, \phi - \varphi\rangle \leq C_1 D \sum_{n=1}^{N} \tau_n \Big(\sum_{S\in\mathcal{M}^n} h_S^2 \|R^n\|^2_{L^2_{-\omega}(S)}\Big)^{1/2},$$

$$-\sum_{n=1}^{N}\int_{t^{n-1}}^{t^n} \langle \nabla\Theta^n, \nabla(\phi - \varphi)\rangle \leq C_2 D \sum_{n=1}^{N} \tau_n \Big(\sum_{S\in\mathcal{M}^n} h_S \|J_S^n\|^2_{L^2_{-\omega}(\partial S)}\Big)^{1/2}.$$

Collecting all previous estimates and using (9) and (10), we deduce the *a posteriori* error estimates of (3), namely

$$\|e_u(\cdot, T)\|_{H^{-1}_{-\omega}(\Omega)} + \|e_{\beta(u)}\|_{L^2_{-\omega}(Q)} \leq \mathrm{e}^{WT} \sum_{i=0}^{4} \mathcal{E}_i + \text{consistency terms}, \tag{13}$$

where

$$\mathcal{E}_1 = C_1 \sum_{n=1}^{N} \tau_n \Big(\sum_{S\in\mathcal{M}^n} h_S^2 \|R^n\|^2_{L^2_{-\omega}(S)}\Big)^{1/2} \qquad \textit{interior residual,}$$

$$\mathcal{E}_2 = C_2 \sum_{n=1}^{N} \tau_n \Big(\sum_{S\in\mathcal{M}^n} h_S \|J_S^n\|^2_{L^2_{-\omega}(\partial S)}\Big)^{1/2} \qquad \textit{jump residual,}$$

$$\mathcal{E}_3 = \sum_{n=1}^{N} \|U^{n-1} - I^n U^{n-1}\|_{H^{-1}_{-\omega}(\Omega)} \qquad \textit{coarsening,}$$

$$\mathcal{E}_4 = \Big(\sum_{n=1}^{N} \tau_n \|U^n - I^n U^{n-1}\|^2_{L^2_{-\omega}(\Omega)}\Big)^{1/2} \qquad \textit{time residual.}$$

5 Application

We study the evolution of a persistent corner singularity for a one-phase Stefan problem in two space dimensions. The example, still unpublished, is due to Athanasopoulos, Caffarelli, and Salsa. The key question is whether or not $\pi/2$ is the critical angle beyond which the interface immediately regularizes. To address this issue, the use of adaptive local refinements has been essential. Our simulations seem to indicate that the critical angle is actually larger than $\pi/2$.

Let $\Omega = (-0.1, 0.1)^2$, $T = 0.1$, and $g(t) = 2.1 - 10\,t$. If (ρ, ξ) denote polar coordinates, then the function

$$u^+(\rho, \xi, t) = 1 + \rho^{g(t)} \cos\big(\xi g(t)\big) \quad \text{if } 2g(t)|\xi| < \pi, \quad u^+ = 0 \quad \text{otherwise}, \tag{14}$$

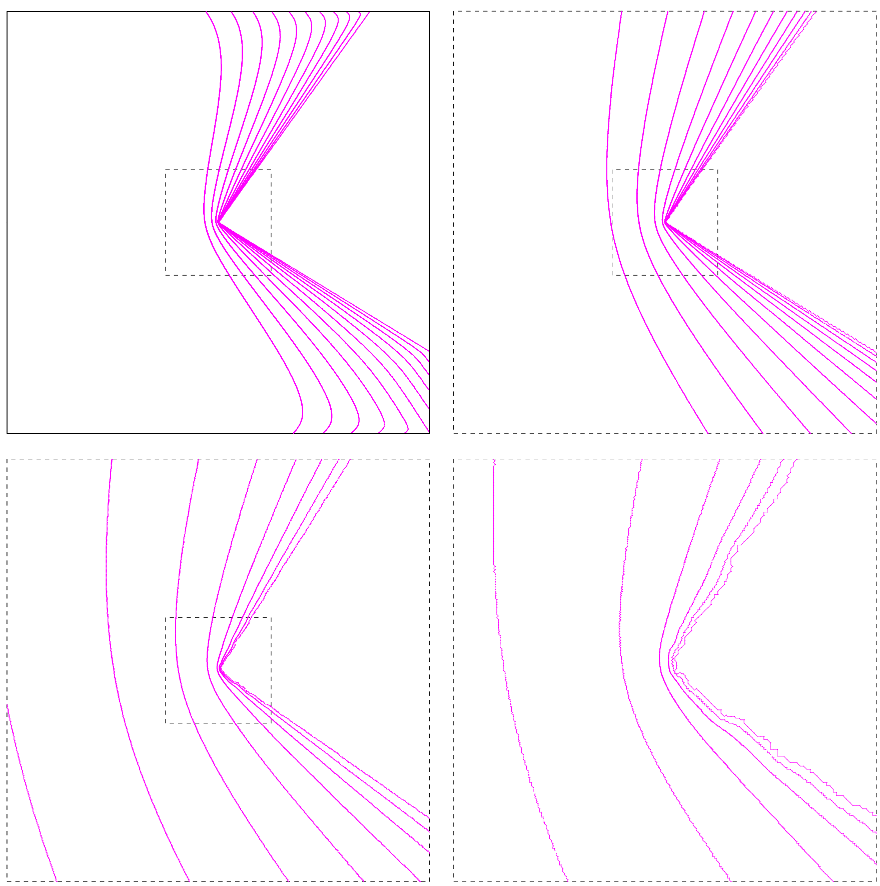

Figure 1: Zoom of interfaces with scaling factors 1, 4, 16, 64 for smallest tolerance $\varepsilon = 1$, at times $t = 0.01\,k$, $0 \le k \le 10$ (top) resp. $3 \le k \le 10$ (bottom).

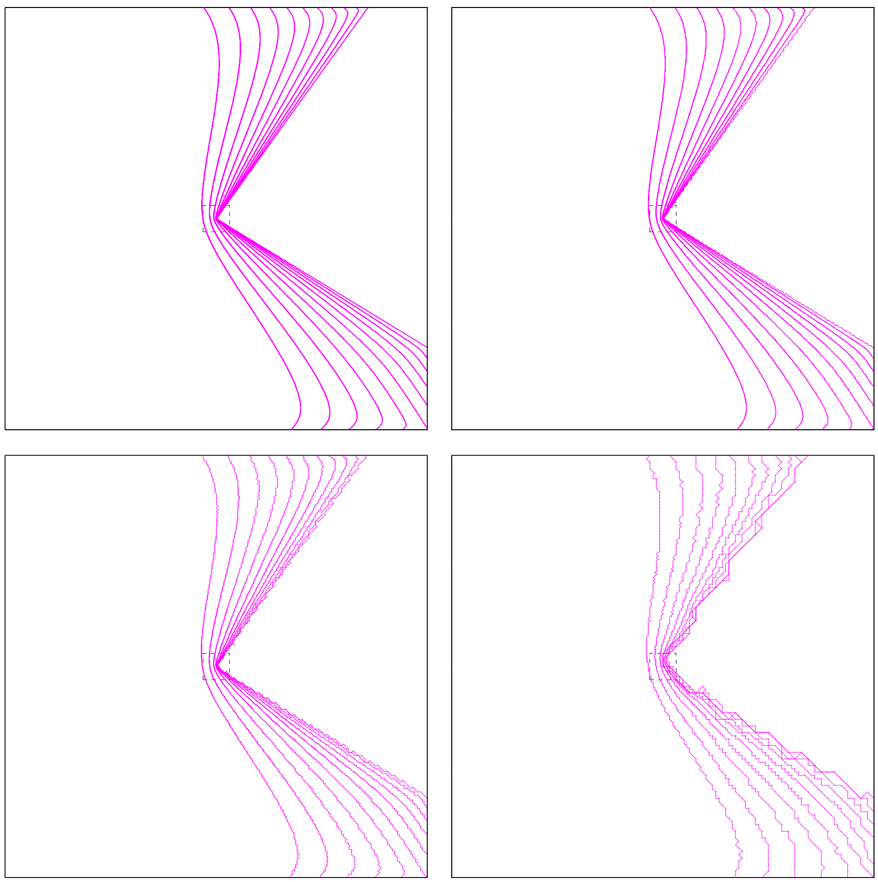

Figure 2: Interfaces for tolerances $\varepsilon = 1,\ 2,\ 4,\ 8$, at times $t = 0.01\,k$, $0 \le k \le 10$.

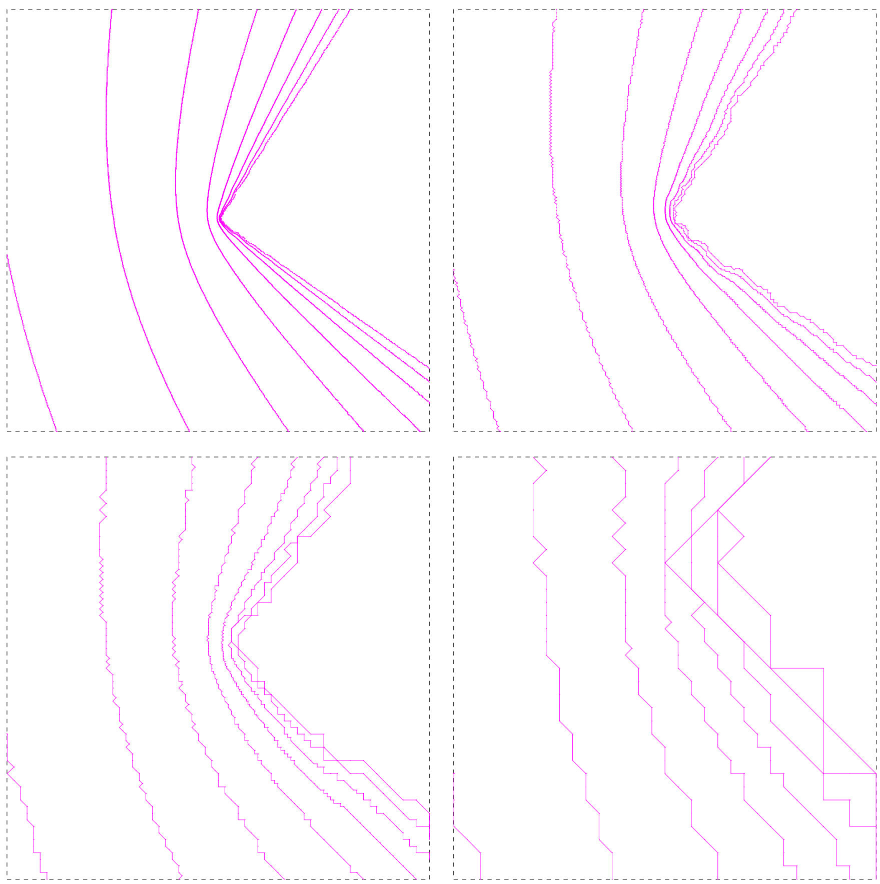

Figure 3: Zoom of interfaces with scaling factor 16 for tolerances $\varepsilon = 1,\ 2,\ 4,\ 8$, at times $t = 0.01\,k$, $3 \le k \le 10$.

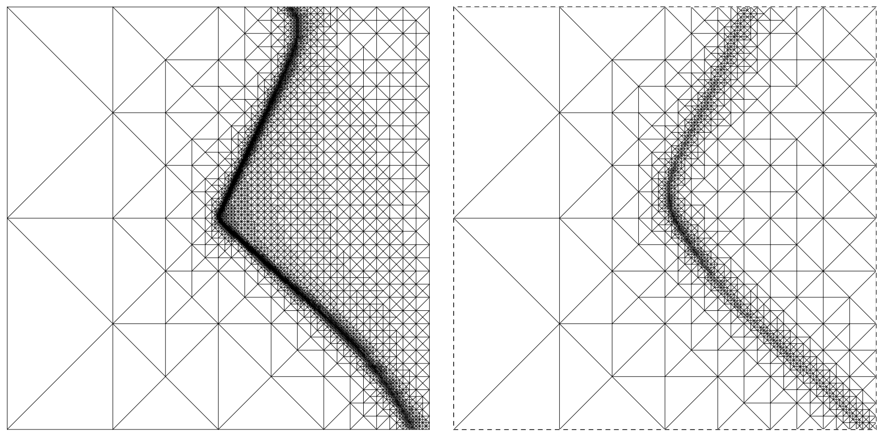

Figure 4: Mesh and Zoom with scaling factor 16 for tolerance $\varepsilon = 4$, at time $t = 0.06$ (number of triangles $M = 15,273$).

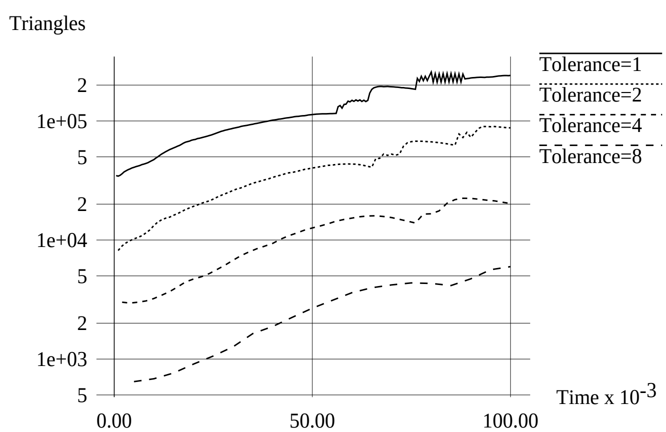

Figure 5: Number of triangles M vs. time for various tolerances; at $t = 0.05$, $M = 113,136$ for $\varepsilon = 1$, $M = 40,306$ for $\varepsilon = 2$, $M = 12,618$ for $\varepsilon = 4$, $M = 2,677$ for $\varepsilon = 8$.

is a supersolution provided $2\, g^3(t)\rho^{g(t)-2} + \pi\, g'(t) \le 0$. Such a condition is not satisfied for all $t \le T$ and can only be enforced for $g(t) > 2$ in a shrinking domain Ω as $g(t) \downarrow 2$. It also provides some support to the above conjecture that $\xi_0 = \pi/4$, and thus the opening $\pi/2 = 2\xi_0$, could be critical. We only use u^+ to set up the Dirichlet condition on the parabolic boundary of Q in our simulations. We also use an angle shift of 0.2, and thus consider $\xi - 0.2$ in (14), to avoid grid orientation effects.

Given an error tolerance ε, a local equidistribution strategy is used to enforce the bound

$$\mathcal{E}(u_0, f, T, \Omega, \omega; h, U, \tau) \le \varepsilon.$$

In view of (3), this guarantees error control; we refer to [6], [7], [8], [9] for details. We run simulations for various tolerances $\varepsilon = 1$, 2, 4, 8 and fixed time-steps $\tau = 0.5, 1, 2, 5 \times 10^{-3}$.

Figure 1 displays the interfaces and zooms with scaling factors 1, 4, 16, 64 for the most accurate run with $\varepsilon = 1$. The angle seems to regularize for $0.04 \le t \le 0.05$, when it is already larger than $\pi/2$. Figures 2 and 3 depict a mesh study for zoom scaling factors 1 and 16, respectively. The relative location of interfaces, as well as time of regularization, are consistent with mesh refinement. Finally, Figure 4 contains a representative locally refined mesh, along with its zoom with scaling factor 16. It is clear that the interface is correctly captured by the algorithm even though the solution is very degenerate near the origin. This is due to the additional weighting factor

$$\omega(\rho) = \sqrt{\max(\rho^2, h_{\min}, \beta(U))},$$

with $h_{\min}$ given, which is essentially proportional to ρ. Hence the weight ω^{-2} in (13) compensates for the behavior $\beta(u) \approx \rho^2$ of the solution near the origin.

The number of triangles M vs. time for various tolerances is plotted in Figure 5: reducing the tolerance ε by a factor 2 entails an increase of M by a factor 4. The oscillations of M for $\varepsilon = 1$ are due to the upper limit $M_{\max}$ of triangles that the Fortran code is allowed to generate; when $M_{\max}$ is exceeded, the code automatically increases the tolerance ε. For $\varepsilon = 1$, we set $M_{\max} = 160,000$ and observe that oscillations likely occur after the corner smooths out, thereby not affecting our conclusions.

6 Conclusions

It may seem surprising at first glance that a problem governed by a parabolic partial differential equation can exhibit a stationary corner singularity. This is a hyperbolic effect consistent with the scaling at the interface. We could infer that the Stefan problem possesses a hyperbolic behavior near the interface. This is a structural property already used in [4], [5] for *a priori* design of refined meshes and a consequence of the *a posteriori* mesh design of [6], [7], [8].

The example of §5 corroborates the theory of [1], namely that the following two factors may prevent smoothing: (a) the angle is not sufficiently large; (b) the heat fluxes of both phases vanish simultaneously. The theory predicts that failure of either (a) or (b) yields immediate smoothing, but it does not address the behavior for intermediate angles. This delicate question can only be explored numerically with a flexible and reliable adaptive technique: the critical angle appears to be larger than $\pi/2$.

The minimum value of meshsize is 1.2×10^{-5} for $\varepsilon = 1$ in §5. A comparable accuracy for a quasi-uniform mesh would require 10^8 elements to capture the singularity: adaptivity and local mesh refinement are thus essential in our study.

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