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Nyström method for BEM of the heat equation with moving boundaries

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Abstract

A direct boundary integral equation method for the heat equation based on Nyström discretization is proposed and analyzed. For problems with moving geometries, a weakly and strongly singular Green's integral equation is formulated. Here the hypersingular integral operator, i.e., the normal trace of the double-layer potential, must be understood as a Hadamard finite part integral. The thermal layer potentials are regarded as generalized Abel integral operators in time and discretized with a singularity-corrected trapezoidal rule. The spatial discretization is a standard quadrature rule for smooth surface integrals. The discretized systems lead to an explicit time stepping scheme and is effective for solving the Dirichlet and Neumann boundary value problems based on both the weakly and/or strongly singular integral equations.

Keywords Moving boundary problem · Boundary integral equation · Heat equation · Nyström method · Finite part integral

Mathematics Subject Classification (2010) 58J35 · 35K05 · 65N38 65R20

1 Introduction

Solving time-dependent partial differential equations with boundary integral equation methods has been a topic of several recent investigations; they are surveyed in [5]. Integral operators for time-dependent problems involve integrals over the space-time boundary which demands the development of suitable discretization and fast evaluation methods.

For the heat equation, several options for the fast evaluation of layer potentials are available, which are either based on spectral expansions of the heat kernel [7, 8, 14],

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a space-time version of the fast multipole method [17], sparse grids [9], or on parallel implementations [6].

In addition, one can choose between several discretization methods, such as convolution quadrature, Galerkin, collocation, and Nyström methods [11, 13, 15]. Variational methods are better understood from a theoretical viewpoint and are applicable to a wider range of operator equations [1, 4]. However, they require the calculation of complicated surface integrals and lead to implicit time stepping methods [12].

The Nyström method on the other hand is explicit and involves much simpler quadrature rules. It is well known that the numerical analysis is limited to the classical case of second-kind integral equations on smooth surfaces (see, e.g., [2, 5, 10]). Even though much less is known about the stability of Nyström methods in more general cases, we will also present numerical results below for first-kind and hypersingular equations.

The approach taken in the present paper is based on the earlier work in [18]. There the thermal layer potentials are treated as generalized Abel integral operators in time where the space dependence is expressed in terms of smooth surface potentials. The time discretization is a singularity-corrected trapezoidal rule, and the spatial discretization is a standard quadrature rule for smooth surface integrals. The goal of the present article is to extend this work to handle moving geometries and hypersingular integral operators.

We are primarily interested in the direct integral formulation based on weakly and strongly singular Green's formula. The two integral formulations present options to solve both the Dirichlet and Neumann problems as an integral equation of either the first or the second kind. More on this and the connection with indirect integral formulations can be found in [5].

A moving surface implies that an additional term appears in Green's representation formula that involves the normal velocity. In addition, a moving surface changes the nature of the singularity of the double-layer operator. We will show that by introducing a space-time version of the normal trace, this complication can be avoided.

In the context of Galerkin methods, the hypersingular operator can be expressed as a weakly singular potential of the surface curl of the ansatz and test function [4]. Since this trick is not available for the Nyström method, we will show that the normal trace of the double-layer potential can be interpreted in the sense of a Hadamard finite part integral in time. We then derive a singularity-corrected quadrature rule to evaluate the finite part integral with a high order of convergence.

We conclude with numerical results solving the Dirichlet and Neumann problems with the weakly and strongly singular integral formulation. The results obtained are consistent with the convergence rate of the quadrature rules used.

2 Integral formulation for moving domain problems

We consider the heat equation in a domain $\Omega(t)$ of $\mathbb{R}^3$ with boundary $\Gamma(t) = \partial\Omega(t)$ that may change in the time interval $0 \leq t \leq T$. Here

$$\begin{aligned} Q &= \{(\Omega(t), t),\ 0 \leq t \leq T\}, \\ \partial Q &= \Sigma \cup \big(\bar{\Omega}(0) \times \{0\}\big) \cup \big(\bar{\Omega}(T) \times \{T\}\big), \end{aligned}$$

denotes the space-time domain and the space-time boundary, and Σ is the lateral boundary

$$\Sigma = \{(\Gamma(t), t),\ 0 < t < T\}.$$

The goal is to solve the heat equation

$$\partial_t u(\mathbf{x}, t) - \Delta u(\mathbf{x}, t) = 0, \quad (\mathbf{x}, t) \in Q, \tag{1}$$

with suitable boundary conditions on Σ and initial conditions on $\Omega(0)$. To motivate the following discussion, we briefly review the derivation of the representation formula with particular attention to a moving geometry.

We will use the arrow notation to denote a vector in space-time and a boldface character to denote a vector in space. Thus, $\vec{\nabla} = [\nabla, \partial_t]$ is the space-time gradient and $\vec{\nabla} \cdot \vec{\mathbf{F}} = \nabla \cdot \mathbf{F}_s + \partial_t F_t$ is the space-time divergence of a space-time vector field $\vec{\mathbf{F}} = [\mathbf{F}_s, F_t]$. In these notations, the divergence theorem is

$$\int_Q \vec{\nabla}\cdot\vec{\mathbf{F}}\, dQ = \int_\Sigma \vec{\mathbf{F}}\cdot\vec{\mathbf{n}}\, d\Sigma + \int_{\Omega(T)} F_t\, d\mathbf{x} - \int_{\Omega(0)} F_t\, d\mathbf{x},$$

where $\vec{\mathbf{n}} = [\mathbf{n}_s, n_t] \in \mathbb{R}^4$ is the space-time normal of Σ. Suppose now that u and v are scalar functions in Q that vanish in $\Omega(0) \times \{0\}$ and $\Omega(T) \times \{T\}$, respectively; then the choice of $\vec{\mathbf{F}} = [u\nabla v - v\nabla u, uv]$ gives the second Green's identity

$$\int_Q (\Delta v + \partial_t v)\, u - (\Delta u - \partial_t u)\, v\, dQ = \int_\Sigma \frac{\partial v}{\partial \mathbf{n}_s} u - \frac{\partial u}{\partial \mathbf{n}_s} v + uvn_t\, d\Sigma.$$

Specializing the above result to a solution u of (1) with homogeneous initial conditions and v, Green's function of the heat equation

$$G(\mathbf{x}, \mathbf{y}, t, \tau) = \begin{cases} \frac{1}{(4\pi(t-\tau))^{\frac{3}{2}}} \exp\left(-\frac{|\mathbf{x}-\mathbf{y}|^2}{4(t-\tau)}\right), & \text{if } \tau < t, \\ 0, & \text{if } \tau \geq t, \end{cases}$$

results in the representation formula

$$\begin{aligned} u(\widetilde{\mathbf{x}}, t) = & \int_\Sigma G(\widetilde{\mathbf{x}}, \mathbf{y}, t, \tau) \frac{\partial u}{\partial \mathbf{n}_s}(\mathbf{y}, \tau)\, d\Sigma_{y,\tau} \\ & - \int_\Sigma \frac{\partial G}{\partial \mathbf{n}_{sy}}(\widetilde{\mathbf{x}}, \mathbf{y}, t, \tau) u(\mathbf{y}, \tau)\, d\Sigma_{y,\tau} \\ & - \int_\Sigma G(\widetilde{\mathbf{x}}, \mathbf{y}, t, \tau) n_\tau(\mathbf{y}, \tau) u(\mathbf{y}, \tau)\, d\Sigma_{y,\tau}, \end{aligned} \tag{2}$$

where $(\widetilde{\mathbf{x}}, t) \in Q$. The third term is specific for a moving surface. We will see in Eq. 13 that the n_t-component of the space-time normal corresponds to the normal velocity of $\Gamma(t)$. This form of the representation formula has appeared without derivation earlier [3].

We define the normal traces of a function φ in Q as

$$\gamma_1^{\pm}\varphi := \frac{\partial \varphi}{\partial \mathbf{n}_s} \pm \frac{1}{2} n_t \varphi. \tag{3}$$

To motivate the additional $n_t\varphi$ term, let $\vec{\mathbf{x}} = [\mathbf{x}, t] \in \Sigma$ and $\vec{\mathbf{y}} = [\mathbf{y}, \tau] \in \Sigma$, then

$$\gamma_{1,(y,\tau)}^{+} G(\mathbf{x}, \mathbf{y}, t, \tau) = G(\mathbf{x}, \mathbf{y}, t, \tau) \frac{(\vec{\mathbf{x}} - \vec{\mathbf{y}}) \cdot \vec{\mathbf{n}}}{2(t - \tau)}.$$

If Σ is smooth, it follows from the orthogonality of the space-time normal to Σ that

$$(\vec{\mathbf{x}} - \vec{\mathbf{y}}) \cdot \vec{\mathbf{n}} = O\left(|\mathbf{x} - \mathbf{y}|^2 + (t - \tau)^2\right). \tag{4}$$

Note that in the case of a moving surface, the usual $(\mathbf{x} - \mathbf{y}) \cdot \mathbf{n}_s = O(|\mathbf{x} - \mathbf{y}|^2)$ holds only if $\mathbf{x}$ and $\mathbf{y}$ have the same time coordinates. In general, we get

$$(\mathbf{x} - \mathbf{y}) \cdot \mathbf{n}_s = O\left(|\mathbf{x} - \mathbf{y}|^2 + (t - \tau)\right). \tag{5}$$

For a function φ on Σ, we define the single- and double-layer potentials as

$$\widetilde{\mathcal{V}}\varphi(\widetilde{\mathbf{x}}, t) = \int_\Sigma G(\widetilde{\mathbf{x}}, \mathbf{y}, t, \tau)\varphi(\mathbf{y}, \tau)\, d\Sigma_{y,\tau} ,$$

$$\widetilde{\mathcal{K}}\varphi(\widetilde{\mathbf{x}}, t) = \int_\Sigma \gamma_{1,(y,\tau)}^{+} G(\widetilde{\mathbf{x}}, \mathbf{y}, t, \tau)\varphi(\mathbf{y}, \tau)\, d\Sigma_{y,\tau} .$$

Then the representation formula (2) appears in the familiar form with a single- and double-layer potential

$$u(\widetilde{\mathbf{x}}, t) = \widetilde{\mathcal{V}}\gamma_1^{-} u(\widetilde{\mathbf{x}}, t) - \widetilde{\mathcal{K}} u(\widetilde{\mathbf{x}}, t), \quad (\widetilde{\mathbf{x}}, t) \in Q. \tag{6}$$

Note that the third term of (2) is incorporated in equal parts in the single- and double-layer terms.

The four boundary integral operators for moving surfaces are obtained by taking the interior trace γ_0 and the normal trace as defined above.

$$\mathcal{V}\varphi(\mathbf{x}, t) = \gamma_0\widetilde{\mathcal{V}}\varphi(\mathbf{x}, t) = \int_\Sigma G(\mathbf{x}, \mathbf{y}, t, \tau)\varphi(\mathbf{y}, \tau)\, d\Sigma_{y,\tau}, \tag{7}$$

$$\mathcal{K}\varphi(\mathbf{x}, t) = \gamma_0\widetilde{\mathcal{K}}\varphi(\mathbf{x}, t) = -\frac{1}{2}\varphi(\mathbf{x}, t) + \int_\Sigma \gamma_{1,(y,\tau)}^{+} G(\mathbf{x}, \mathbf{y}, t, \tau)\varphi(\mathbf{y}, \tau)\, d\Sigma_{y,\tau}, \tag{8}$$

$$\mathcal{K}'\varphi(\mathbf{x}, t) = \gamma_1^{-}\widetilde{\mathcal{V}}\varphi(\mathbf{x}, t) = \frac{1}{2}\varphi(\mathbf{x}, t) + \int_\Sigma \gamma_{1,(x,t)}^{-} G(\mathbf{x}, \mathbf{y}, t, \tau)\varphi(\mathbf{y}, \tau)\, d\Sigma_{y,\tau}, \tag{9}$$

$$\mathcal{D}\varphi(\mathbf{x}, t) = \gamma_1^{-}\widetilde{\mathcal{K}}\varphi(\mathbf{x}, t) = \int_\Sigma \gamma_{1,(x,t)}^{-}\gamma_{1,(y,\tau)}^{+} G(\mathbf{x}, \mathbf{y}, t, \tau)\varphi(\mathbf{y}, \tau)\, d\Sigma_{y,\tau}, \tag{10}$$

where $(\mathbf{x}, t) \in \Sigma$. It is not difficult to verify that the jump relations of the thermal double-layer potentials hold for both fixed as well as moving geometries. The hypersingular integral operator $\mathcal{D}$ requires more care because it has a strong singularity. We will see below that the Hadamard finite part of this integral is the normal trace of the double-layer potential.

Taking traces in (6) results in the weakly and strongly singular Green's integral formulations

$$\frac{1}{2}u(\mathbf{x},t) = \mathcal{V}\gamma_1^- u(\mathbf{x},t) - \mathcal{K}u(\mathbf{x},t), \tag{11}$$

$$\frac{1}{2}\gamma_1^- u(\mathbf{x},t) = \mathcal{K}'\gamma_1^- u(\mathbf{x},t) - \mathcal{D}u(\mathbf{x},t), \tag{12}$$

where $(\mathbf{x},t) \in \Sigma$. Thanks to the extra term in the space-time normal trace, these integrals have the same form as in the well-known case of a fixed geometry.

3 Thermal layer potentials in Abel integral form

We now consider surfaces that are the image of a time-dependent parameterization $\mathbf{x}(\cdot,t) : X \subset \mathbb{R}^2 \to \Gamma(t)$ where the Jacobian $|\partial_1 \mathbf{x}(\boldsymbol{\xi},t) \times \partial_2 \mathbf{x}(\boldsymbol{\xi},t)|$ is a smooth function and bounded away from zero. Note that this assumption is somewhat restrictive as it excludes topology changes of $\Gamma(t)$. The parameterization of Σ is

$$\Sigma = \left\{ \vec{\mathbf{x}}(\boldsymbol{\xi},t) := \begin{bmatrix} \mathbf{x}(\boldsymbol{\xi},t) \\ t \end{bmatrix} \; : \; (\boldsymbol{\xi},t) \in X \times [0,T] \right\}.$$

The normal and normal velocity of $\Gamma(t)$ are given by

$$\mathbf{n} = \frac{\partial_1 \mathbf{x} \times \partial_2 \mathbf{x}}{|\partial_1 \mathbf{x} \times \partial_2 \mathbf{x}|} \quad \text{and} \quad v_n = \partial_t \mathbf{x} \cdot \mathbf{n}, \tag{13}$$

where ∂_1 and ∂_2 denote differentiation with respect to the variables ξ_1 and ξ_2. In a slight change from terminology introduced in the previous section, we call the vector

$$\vec{\mathbf{n}} = \begin{bmatrix} \mathbf{n} \\ -v_n \end{bmatrix}$$

the space-time normal. This vector is, up to the normalization factor $\sqrt{1+v_n^2}$, the normal of Σ, because it is $\mathbb{R}^4$-orthogonal to all partial derivatives of $\vec{\mathbf{x}}(\boldsymbol{\xi},t)$. The surface measure on Σ is

$$d\Sigma = \sqrt{1+v_n^2}\,|\partial_1 \mathbf{x} \times \partial_2 \mathbf{x}|\, d\boldsymbol{\xi} dt = \sqrt{1+v_n^2}\, d\Gamma dt,$$

where $d\Gamma$ is the surface measure on $\Gamma(t)$. We will write

$$\gamma_1^{\pm}\varphi := \frac{\partial \varphi}{\partial \mathbf{n}} \mp \frac{1}{2} v_n \varphi$$

for the normal trace. This is, up to the factor $\sqrt{1+v_n^2}$, the normal trace of Section 2.

The integral operators (7)–(10) can be written in the form

$$\mathcal{V}\varphi(\mathbf{x},t) = \frac{1}{\sqrt{4\pi}}\int_0^t \frac{1}{\sqrt{t-\tau}} V\varphi(\mathbf{x},t,\tau)\,d\tau, \tag{14}$$

$$\mathcal{K}\varphi(\mathbf{x},t) = \frac{1}{\sqrt{4\pi}}\int_0^t \frac{1}{\sqrt{t-\tau}} K\varphi(\mathbf{x},t,\tau)\,d\tau, \tag{15}$$

$$\mathcal{K}'\varphi(\mathbf{x},t) = \frac{1}{\sqrt{4\pi}}\int_0^t \frac{1}{\sqrt{t-\tau}} K'\varphi(\mathbf{x},t,\tau)\,d\tau, \tag{16}$$

$$\mathcal{D}\varphi(\mathbf{x},t) = \frac{1}{\sqrt{4\pi}}\mathrm{pf}\int_0^t \frac{1}{(t-\tau)^{\frac{3}{2}}} D\varphi(\mathbf{x},t,\tau)\,d\tau, \tag{17}$$

where

$$V\varphi(\mathbf{x},t,\tau) = \int_{\Gamma(\tau)} \frac{1}{4\pi(t-\tau)} \exp\left(-\frac{|\mathbf{x}-\mathbf{y}|^2}{4(t-\tau)}\right) \varphi(\mathbf{y},\tau)\,d\Gamma_y\,, \tag{18}$$

$$K\varphi(\mathbf{x},t,\tau) = \int_{\Gamma(\tau)} \frac{1}{4\pi(t-\tau)} \exp\left(-\frac{|\mathbf{x}-\mathbf{y}|^2}{4(t-\tau)}\right) \frac{(\vec{\mathbf{x}}-\vec{\mathbf{y}})\cdot\vec{\mathbf{n}}_y}{2(t-\tau)} \varphi(\mathbf{y},\tau)\,d\Gamma_y\,, \tag{19}$$

$$K'\varphi(\mathbf{x},t,\tau) = \int_{\Gamma(\tau)} \frac{1}{4\pi(t-\tau)} \exp\left(-\frac{|\mathbf{x}-\mathbf{y}|^2}{4(t-\tau)}\right) \frac{(\vec{\mathbf{x}}-\vec{\mathbf{y}})\cdot\vec{\mathbf{n}}_x}{2(t-\tau)} \varphi(\mathbf{y},\tau)\,d\Gamma_y\,, \tag{20}$$

$$D\varphi(\mathbf{x},t,\tau) = \int_{\Gamma(\tau)} \frac{1}{4\pi(t-\tau)} \exp\left(-\frac{|\mathbf{x}-\mathbf{y}|^2}{4(t-\tau)}\right) \cdot \left[\frac{\mathbf{n}_x\cdot\mathbf{n}_y}{2} - \frac{(\vec{\mathbf{x}}-\vec{\mathbf{y}})\cdot\vec{\mathbf{n}}_x}{2(t-\tau)}\frac{(\vec{\mathbf{x}}-\vec{\mathbf{y}})\cdot\vec{\mathbf{n}}_y}{2(t-\tau)}\right]\varphi(\mathbf{y},\tau)\,d\Gamma_y\,. \tag{21}$$

The kernel in the above time-dependent surface potentials is Green's function of the two-dimensional heat equation. Thus, they may be regarded as Poisson-Weierstrass integrals defined on a surface instead of the usual plane. As in the planar case, these integrals are smooth functions in all variables. The limiting behavior of these functions as $\tau \to t$ is

$$\begin{aligned}
V\varphi(\mathbf{x},t,\tau) &= \varphi(\mathbf{x},t) + O(t-\tau),\\
K\varphi(\mathbf{x},t,\tau) &= H(\mathbf{x},t)\varphi(\mathbf{x},t) + O(t-\tau),\\
K'\varphi(\mathbf{x},t,\tau) &= H(\mathbf{x},t)\varphi(\mathbf{x},t) + O(t-\tau),\\
D\varphi(\mathbf{x},t,\tau) &= \frac{1}{2}\varphi(\mathbf{x},t) + O(t-\tau),
\end{aligned}$$

where $H(\mathbf{x}, t)$ is the mean curvature of the surface $\Gamma(t)$. The derivation of this expansion for the single- and double-layer potentials with a fixed surface can be found in [18]. The modifications for the other layer potentials and for a time-dependent surface are not significant, and hence, we only state the final result here. For boundary curves, expansions of a similar nature can also be found in [20].

4 Hypersingular Operator

In this section, we show that the hypersingular operator can be understood as a strongly singular integral in the Hadamard finite part sense. We briefly recall the definition. A smooth function f can be decomposed as

$$f(t,\tau) = f(t,t) + (t-\tau) f_1(t,\tau),$$

where f_1 is another smooth function. Thus, for $\epsilon > 0$, we can calculate

$$\begin{aligned}\int_0^{t-\epsilon} \frac{1}{(t-\tau)^{\frac{3}{2}}} f(t,\tau)\,d\tau &= f(t,t)\int_0^{t-\epsilon} \frac{1}{(t-\tau)^{\frac{3}{2}}}\,d\tau + \int_0^{t-\epsilon} \frac{1}{(t-\tau)^{\frac{1}{2}}} f_1(t,\tau)\,d\tau \\ &= \frac{2}{\sqrt{\epsilon}} f(t,t) - \frac{2}{\sqrt{t}} f(t,t) + \int_0^{t-\epsilon} \frac{1}{(t-\tau)^{\frac{1}{2}}} f_1(t,\tau)\,d\tau\end{aligned}$$

The finite part integral is the convergent part of this expression. Since the integral on the right hand side is weakly singular, we get

$$\mathrm{pf}\int_0^{t} \frac{1}{(t-\tau)^{\frac{3}{2}}} f(t,\tau)\,d\tau = -\frac{2}{\sqrt{t}} f(t,t) + \int_0^{t} \frac{1}{(t-\tau)^{\frac{3}{2}}} \big(f(t,\tau) - f(t,t)\big) d\tau. \quad (22)$$

Since $D\varphi(\cdot)$ is a smooth function in t and τ, the integral (17) can be understood as a Hadamard finite part integral in time. What remains to verify is that the normal trace of the double-layer potential is indeed given by (17). This is the statement of the following:

Theorem 4.1 *For a smooth function φ on Σ*

$$\gamma_1^- \mathcal{K}\varphi(\mathbf{x}, t) = \mathcal{D}\varphi(\mathbf{x}, t)$$

holds.

Before we give the proof of this result, we note that a point $\widetilde{\mathbf{x}}$ in a sufficiently small neighborhood of $\Gamma(t)$ has a unique nearest point $\mathbf{x} \in \Gamma(t)$ such that $\widetilde{\mathbf{x}} = \mathbf{x} + \lambda \mathbf{n}_x$. Here $\mathbf{n}_x$ is the normal at $\mathbf{x}$ and λ is the Euclidean distance of $\widetilde{\mathbf{x}}$ to the surface.

For some $\lambda > 0$, let

$$w(\mathbf{x}, t, \lambda) := \gamma_{1,x}^- \mathcal{K}(\widetilde{\mathbf{x}}, t) = \mathbf{n}_x \cdot \nabla_x \mathcal{K}(\widetilde{\mathbf{x}}, t) + \frac{v_{nx}}{2} \mathcal{K}(\widetilde{\mathbf{x}}, t).$$

If the limit $\lambda \to 0$ exists, then $w(\mathbf{x}, t, 0)$ is the normal trace of the double-layer potential, that is, the left-hand side in Theorem 4.1. For the right-hand side, simple differentiation shows the explicit form of this function is

$$w(\mathbf{x}, t, \lambda) = \int_0^t \int_{\Gamma(\tau)} \frac{1}{(4\pi\delta)^{\frac{3}{2}}} \exp\left(-\frac{|\widetilde{\mathbf{x}} - \mathbf{y}|^2}{4\delta}\right) \left[\frac{\mathbf{n}_x \cdot \mathbf{n}_y}{2\delta^2} - \frac{(\vec{\widetilde{\mathbf{x}}} - \vec{\mathbf{y}}) \cdot \vec{\mathbf{n}}_y}{2\delta} \frac{(\vec{\widetilde{\mathbf{x}}} - \vec{\mathbf{y}}) \cdot \vec{\mathbf{n}}_x}{2\delta}\right] \times \varphi(\mathbf{y}, \tau)\, d\Gamma_y d\tau \tag{23}$$

where $\delta := t - \tau$ and $\vec{\widetilde{\mathbf{x}}} = [\widetilde{\mathbf{x}}, t]$. Mind that the first term in the angle bracket is an $\mathbb{R}^3$-inner product, while the second term consists of $\mathbb{R}^4$-inner products. Expanding $\widetilde{\mathbf{x}} = \mathbf{x} + \lambda \mathbf{n}_x$ gives

$$\exp\left(-\frac{|\widetilde{\mathbf{x}} - \mathbf{y}|^2}{4\delta}\right) = \exp\left(-\frac{\lambda^2}{4\delta}\right) \exp\left(-\lambda \frac{(\mathbf{x} - \mathbf{y}) \cdot \mathbf{n}_x}{2\delta}\right) \exp\left(-\frac{|\mathbf{x} - \mathbf{y}|^2}{4\delta}\right) \tag{24}$$

and analogous expressions can be found for the inner products with the space-time normals. Thus, the function w can be expanded into three parts $w = w_1 + \lambda w_2 + w_3$, where

$$w_1(\mathbf{x}, t, \lambda) = \frac{1}{\sqrt{4\pi}} \int_0^t \frac{1}{\delta^{\frac{3}{2}}} \exp\left(-\frac{\lambda^2}{4\delta}\right) \left(\frac{1}{2} - \frac{\lambda^2}{4\delta}\right) \Phi_1(\mathbf{x}, t, \tau, \lambda)\, d\tau,$$

and

$$\Phi_1(\mathbf{x}, t, \tau, \lambda) = \int_{\Gamma(\tau)} \frac{1}{4\pi\delta} \exp\left(-\frac{|\mathbf{x} - \mathbf{y}|^2}{4\delta}\right) \exp\left(-\lambda \frac{(\mathbf{x} - \mathbf{y}) \cdot \mathbf{n}_x}{2\delta}\right) \mathbf{n}_x \cdot \mathbf{n}_y\, \varphi(\mathbf{y}, \tau)\, d\Gamma_y.$$

That is, w_1 contains the first and the λ^2-term in the angle bracket of (23). Moreover,

$$w_2(\mathbf{x}, t, \lambda) = \int_0^t \int_{\Gamma(\tau)} \frac{1}{(4\pi\delta)^{\frac{3}{2}}} \exp\left(-\frac{|\widetilde{\mathbf{x}} - \mathbf{y}|^2}{4\delta}\right) \frac{(\vec{\mathbf{x}} - \vec{\mathbf{y}}) \cdot \vec{\mathbf{n}}_y - (\vec{\mathbf{x}} - \vec{\mathbf{y}}) \cdot \vec{\mathbf{n}}_y\, \vec{\mathbf{n}}_x \cdot \vec{\mathbf{n}}_y}{4\delta^2} \times \varphi(\mathbf{y}, \tau)\, d\Gamma_y d\tau$$

contains the linear terms in λ and

$$w_3(\mathbf{x}, t, \lambda) = \int_0^t \int_{\Gamma(\tau)} \frac{1}{(4\pi\delta)^{\frac{3}{2}}} \exp\left(-\frac{|\widetilde{\mathbf{x}} - \mathbf{y}|^2}{4\delta}\right) \frac{(\vec{\mathbf{x}} - \vec{\mathbf{y}}) \cdot \vec{\mathbf{n}}_y\, (\vec{\mathbf{x}} - \vec{\mathbf{y}}) \cdot \vec{\mathbf{n}}_x}{4\delta^2} \varphi(\mathbf{y}, \tau)\, d\Gamma_y d\tau$$

contains the remainder. The following lemmas examine the properties of these three functions.

Lemma 4.2 *There is a constant* $C > 0$ *such that*

$$|w_2(\mathbf{x}, t, \lambda)| \le C \|\varphi\|_{C^\infty(\Sigma)}.$$

Proof If λ is small enough, then the middle term in (24) can be estimated by

$$\exp\left(-\lambda\frac{(\mathbf{x}-\mathbf{y})\cdot\mathbf{n}_x}{2\delta}\right) \le c_1 \exp\left(c_2\lambda\frac{|\mathbf{x}-\mathbf{y}|^2}{2\delta}\right) \le c_1 \exp\left(\frac{|\mathbf{x}-\mathbf{y}|^2}{8\delta}\right),$$

where the first step follows from (5). Moreover, it follows from (4) that

$$\frac{(\vec{\mathbf{x}}-\vec{\mathbf{y}})\cdot\vec{\mathbf{n}}_y - (\vec{\mathbf{x}}-\vec{\mathbf{y}})\cdot\vec{\mathbf{n}}_y\,\vec{\mathbf{n}}_x\cdot\vec{\mathbf{n}}_y}{\delta^2} \le C\left(\frac{|\mathbf{x}-\mathbf{y}|^2}{\delta^2}+1\right).$$

The rest of the argument relies on the estimate

$$e^{-z} \le c_\mu z^{-\mu}, \qquad z>0,\ \mu>0 \tag{25}$$

(see [10, Eq. 9.15]). Thus,

$$\begin{aligned}
&|w_2(\mathbf{x},t,\lambda)| \\
&\le c\int_0^t \frac{1}{\delta^{\frac{3}{2}}}\exp\left(-\frac{\lambda^2}{4\delta}\right)\int_{\Gamma(\tau)}\exp\left(-\frac{|\mathbf{x}-\mathbf{y}|^2}{8\delta}\right)\left(\frac{|\mathbf{x}-\mathbf{y}|^2}{\delta^2}+1\right)d\Gamma_y d\tau\,\|\varphi\|_{C^\infty(\Sigma)} \\
&\le c\int_0^t \frac{1}{\delta^{\frac{3}{2}}}\exp\left(-\frac{\lambda^2}{4\delta}\right)\int_{\Gamma(\tau)}\frac{\delta^{\mu-2}}{|\mathbf{x}-\mathbf{y}|^{2\mu-2}}+\frac{\delta^\mu}{|\mathbf{x}-\mathbf{y}|^{2\mu}}\,d\Gamma_y d\tau\,\|\varphi\|_{C^\infty(\Sigma)}.
\end{aligned}$$

For $\lambda \neq 0$, this integral is weakly singular if the exponent of $|\mathbf{x}-\mathbf{y}|$ is less than two or $\mu < 2$. In addition, the τ integral should be bounded independently of μ which is the case when the combined exponent of δ is less than unity. This can be accomplished by setting $\mu = 7/4$ for the first term and by setting $\mu = 3/4$ for the second term. Then

$$|w_2(\mathbf{x},t,\lambda)| \le c\int_{\Gamma(\tau)}\left(\frac{1}{\delta^{\frac{7}{4}}}+\frac{1}{\delta^{\frac{3}{4}}}\right)\exp\left(-\frac{\lambda^2}{4\delta}\right)d\tau\,\|\varphi\|_{C^\infty(\Sigma)} \le c\|\varphi\|_{C^\infty(\Sigma)}.$$

□

Lemma 4.3 *The function w_3 is a continuous function of λ. In particular,*

$$\begin{aligned}
\lim_{\lambda\to 0} w_3(\mathbf{x},t,\lambda) = &\int_0^t\int_{\Gamma(\tau)}\frac{1}{(4\pi\delta)^{\frac{3}{2}}}\exp\left(-\frac{|\mathbf{x}-\mathbf{y}|^2}{4\delta}\right)\frac{(\vec{\mathbf{x}}-\vec{\mathbf{y}})\cdot\vec{\mathbf{n}}_y\,(\vec{\mathbf{x}}-\vec{\mathbf{y}})\cdot\vec{\mathbf{n}}_x}{4\delta^2} \\
&\times\varphi(\mathbf{y},\tau)\,d\Gamma_y d\tau.
\end{aligned}$$

Proof We first show that the integral $w_3(\mathbf{x},t,0)$ is weakly singular. From (4) and (25), it follows that

$$w_3(\mathbf{x},t,0) \le c\int_0^t\int_{\Gamma(\tau)}\frac{1}{(4\pi\delta)^{\frac{3}{2}}}\frac{\delta^\mu}{|\mathbf{x}-\mathbf{y}|^{2\mu}}\left(\frac{|\mathbf{x}-\mathbf{y}|^4}{\delta^2}+|\mathbf{x}-\mathbf{y}|^2+\delta^2\right)d\Gamma_y d\tau.$$

Similar to the proof in the previous lemma, the choices $\mu = 11/4$, $7/4$, and $3/4$ show that both the space and time integrals are weakly singular. The rest is a standard argument: If w_{3a} is defined as w_3 but with time integration from $\tau = 0$ to $t - a$, then the reminder is $O(\sqrt{a})$ because the integrand is $O(1/\sqrt{\delta})$ in time. Then

$$\lim_{\lambda\to 0}[w_3(\mathbf{x}, t, \lambda) - w_3(\mathbf{x}, t, 0)] = \lim_{\lambda\to 0}[w_{3a}(\mathbf{x}, t, \lambda) - w_{3a}(\mathbf{x}, t, 0)] + O(\sqrt{a}).$$

The first limit vanishes because the integrand is a smooth function. This implies that the limit on the left-hand side also vanishes because a can be arbitrarily small. □

Lemma 4.4

$$\lim_{\lambda\to 0} w_1(\mathbf{x}, t, \lambda) = \frac{1}{2} pf\int_0^t \frac{1}{\sqrt{4\pi}} \frac{1}{\delta^{\frac{3}{2}}} \Phi_1(\mathbf{x}, t, \tau, 0)\, d\tau.$$

Proof We first note that the function Φ_1 is a smooth function in all variables. This follows in a similar manner as the smoothness of the surface potentials in (18)–(21). To get some insight into the properties of w_1, consider first the case $\Phi_1 = 1$ where a closed-form analytic expression can be found

$$\frac{1}{\sqrt{4\pi}} \int_0^t \frac{1}{\delta^{\frac{3}{2}}} \exp\left(-\frac{\lambda^2}{4\delta}\right)\left(\frac{1}{2} - \frac{\lambda^2}{4\delta}\right) d\tau = \frac{-1}{\sqrt{4\pi t}} \exp\left(-\frac{\lambda^2}{4t}\right). \tag{26}$$

Thus, the integral is not defined for $\lambda = 0$ but has an analytic extension. Since Φ_1 is smooth, we have $\Phi_1(\mathbf{x}, t, \tau, \lambda) = \Phi_1(\mathbf{x}, t, \tau, 0) + O(\lambda)$, and hence, it follows that for fixed $t > 0$,

$$w_1(\mathbf{x}, t.\lambda) = \frac{1}{\sqrt{4\pi}} \int_0^t \frac{1}{\delta^{\frac{3}{2}}} \exp\left(-\frac{\lambda^2}{4\delta}\right)\left(\frac{1}{2} - \frac{\lambda^2}{4\delta}\right) \Phi_1(\mathbf{x}, t, \tau, 0)\, d\tau + O(\lambda). \tag{27}$$

Since Φ_1 is a smooth function in the τ-variable,

$$\Phi_1(\mathbf{x}, t, \tau, 0) = \Phi_1(\mathbf{x}, t, t, 0) + \delta\Psi(\mathbf{x}, t, \tau), \tag{28}$$

where $\Psi(\mathbf{x}, t, \tau)$ is another smooth function. From (26), the contribution of the first term to (27) is

$$\frac{1}{\sqrt{4\pi}} \int_0^t \frac{1}{\delta^{\frac{3}{2}}} \exp\left(-\frac{\lambda^2}{4\delta}\right)\left(\frac{1}{2} - \frac{\lambda^2}{4\delta}\right) d\tau\, \Phi_1(\mathbf{x}, t, t, 0) = \frac{-1}{\sqrt{4\pi t}} \Phi_1(\mathbf{x}, t, t, 0) + O(\lambda) \tag{29}$$

The Ψ-term in (28) cancels one power of δ, and thus, its contribution to (27) is

$$\begin{aligned} &\int_0^t \frac{1}{\sqrt{4\pi\delta}} \exp\left(-\frac{\lambda^2}{4\delta}\right)\left(\frac{1}{2} - \frac{\lambda^2}{4\delta}\right) \Psi(\mathbf{x}, t, \tau)\, d\tau \\ &= \frac{1}{2}\int_0^t \frac{1}{\sqrt{4\pi\delta}} \exp\left(-\frac{\lambda^2}{4\delta}\right) \Psi(\mathbf{x}, t, \tau)\, d\tau + O\left(\lambda^2 \int_0^t \frac{1}{\delta^{\frac{3}{2}}} \exp\left(-\frac{\lambda^2}{4\delta}\right) d\tau\right). \end{aligned}$$

Analytic integration shows that the last integral is $O\left(\lambda^{-1}\right)$; hence, the last term simplifies to $O(\lambda)$. Moreover, since the first integral is weakly singular when $\lambda = 0$, we see that its limiting value can be simply obtained by substituting $\lambda = 0$. Combining this result with (27), (28), and (29) shows that

$$\lim_{\lambda\to 0} w_1(\mathbf{x}, t, \lambda) = \frac{-1}{\sqrt{4\pi t}}\Phi_1(\mathbf{x}, t, \tau, 0) + \frac{1}{2}\int_0^t \frac{1}{\sqrt{4\pi}}\frac{1}{\delta^{\frac{3}{2}}} \times \big(\Phi_1(\mathbf{x}, t, \tau, 0) - \Phi_1(\mathbf{x}, t, t, 0)\big)d\tau.$$

The assertion follows from (22). □

Proof of Theorem 4.1 Since the w_2-term is multiplied by λ, it does not contribute to the limit; thus, it follows from the previous lemmas and the definitions of Φ_1 and w_3 that

$$\begin{aligned}\lim_{\lambda\to 0} w(\mathbf{x}, t, \lambda) &= \frac{1}{2}\mathrm{pf}\int_0^t \frac{1}{\sqrt{4\pi}}\frac{1}{\delta^{\frac{3}{2}}}\Phi_1(\mathbf{x}, t, \tau, 0)\, d\tau + w_3(\mathbf{x}, t, 0)\\ &= \mathrm{pf}\int_0^t \int_{\Gamma(\tau)} \frac{1}{(4\pi\delta)^{\frac{3}{2}}}\exp\left(-\frac{|\mathbf{x}-\mathbf{y}|^2}{4\delta}\right)\\ &\quad\times\left[\frac{\mathbf{n}_x\cdot\mathbf{n}_y}{2\delta^2} - \frac{(\vec{\mathbf{x}}-\vec{\mathbf{y}})\cdot\vec{\mathbf{n}}_y}{2\delta}\frac{(\vec{\mathbf{x}}-\vec{\mathbf{y}})\cdot\vec{\mathbf{n}}_x}{2\delta}\right]d\Gamma_y d\tau,\end{aligned}$$

which is the assertion of Theorem 4.1. □

5 Discretization

In [18], a quadrature rule is obtained for weakly singular integrals by singularity subtraction as follows:

$$\begin{aligned}&\int_0^{t_n} \frac{1}{\sqrt{t_n-\tau}} f(t,\tau)\, d\tau\\ &= 2\sqrt{t_n} f(t_n, t_n) + \int_0^{t_n}\frac{1}{\sqrt{t_n-\tau}}\big(f(t_n,\tau) - f(t_n,t_n)\big)\, d\tau\\ &= 2\sqrt{t_n} f(t_n, t_n) + \sum_{j=0}^{n-1}\frac{h_t}{\sqrt{t_n-t_j}}\big(f(t_n,t_j) - f(t_n,t_n)\big) + O\left(h_t^{\frac{3}{2}}\right)\\ &= \mu_n f(t_n, t_n) + \sum_{j=0}^{n-1}\frac{h_t}{\sqrt{t-\tau}} f(t_n,t_j) + O\left(h_t^{\frac{3}{2}}\right),\end{aligned} \tag{30}$$

where h_t is the time step size, $t_n = nh_t$, and $\sum'$ indicates that the first term in the sum is multiplied by the factor $\frac{1}{2}$. Further,

$$\mu_n = 2\sqrt{t_n} - h_t \sum_{j=0}^{n-1}{}' \frac{1}{\sqrt{t_n - t_j}}.$$

The second integral in the above calculation is order $\sqrt{t-\tau}$ which implies that the quadrature error of the trapezoidal rule is order $h_t^{\frac{3}{2}}$. Higher order versions of this rule can be obtained by subtracting more terms. Moreover, a stability analysis for the case that the quadrature rule is applied to solve Abel integral equations of the first and second kind can be found in [19] and in [16].

This rule can be modified to approximate the weakly singular integral in the finite part integral. Using the notations of Section 4

$$\begin{aligned}\text{pf}\int_0^{t_n} \frac{1}{(t_n-\tau)^{\frac{3}{2}}} f(t_n,\tau)\,d\tau &= -\frac{2}{\sqrt{t_n}} f(t_n,t_n) + \int_0^{t_n} \frac{1}{(t_n-\tau)^{\frac{1}{2}}} f_1(t,\tau)\,d\tau \\ = -\frac{2}{\sqrt{t_n}} f(t_n,t_n) + \mu_n f_1(t_n,t_n) &+ \sum_{j=0}^{n-1}{}' \frac{h_t}{\sqrt{t-\tau}} f_1(t_n,t_j) + O\left(h_t^{\frac{3}{2}}\right).\end{aligned}$$

Replacing $f_1(t_n,t_n) = \partial_\tau f(t_n,t_n)$ by a forward difference adds another $O(h_t^{\frac{3}{2}})$ to the error because of the first-order approximation multiplied by $\mu_n = O(h_t^{\frac{1}{2}})$. Thus,

$$\begin{aligned}\text{pf}\int_0^{t_n} \frac{1}{(t_n-\tau)^{\frac{3}{2}}} f(t_n,\tau)\,d\tau \;&=\; \mu_n^{(0)} f(t_n,t_n) + \mu_n^{(1)} f(t_n,t_{n-1}) \\ &+ \sum_{j=0}^{n-2}{}' \frac{h_t}{(t_n-t_j)^{\frac{3}{2}}} f(t_n,t_j) + O\left(h_t^{\frac{3}{2}}\right),\end{aligned} \tag{31}$$

where

$$\begin{aligned}\mu_n^{(0)} &= \frac{\mu_n}{h_t} - \frac{2}{\sqrt{t_n}} - \sum_{j=0}^{n-2}{}' \frac{h_t}{(t_n-t_j)^{\frac{3}{2}}} \\ \mu_n^{(1)} &= -\frac{\mu_n}{h_t} + \frac{1}{\sqrt{h_t}}.\end{aligned}$$

When the quadrature rules (30) and (31) are applied to the integrals in (14)–(17), then the function values $f(t_n,t_n)$ are replaced by the asymptotic values $\tau \to t$ of the Poisson-type integrals (18)–(21). On the other hand, the evaluation of $f(t_n,t_j)$, $j < n$ in the temporal quadrature involves surface integrals. Since the surface integral operators in (18)–(21) have smooth kernels, standard surface quadrature rules can be applied, which have the form

$$\int_{\Gamma(t_j)} \varphi(\mathbf{y})\, d\Gamma_y \approx \sum_{k\in N_j} \varphi(\mathbf{x}_k) w_k^j \,,$$

where $\mathbf{x}_k^j$, $k \in N_j$ are nodes on $\Gamma(t_j)$ and w_k^j are the weights. Here we use rules based on a triangulation of $\Gamma(t_j)$ that integrates piecewise polynomials of a given degree exactly. The construction of such rules is described, for instance, in Atkinson [2, Sec 5.3].

Since the heat kernel becomes increasingly peaked when t_j approaches t_n, the mesh width of the surface triangulation must be decreased as the mesh is refined. In [18], it is shown that if the relation of the spatial mesh width h_s to the time step size is

$$\frac{h_s}{\sqrt{h_t}} \to 0 \quad \text{as } h_t \to 0, \tag{32}$$

then the convergence rate of the fully discrete formula is still $O(h_t^{\frac{3}{2}})$. Thus, the fully discrete approximation for the single-layer potential is

$$\mathcal{V}\varphi(\mathbf{x}_m^n, t_n) = \mu_n \varphi(\mathbf{x}, t_n) + h_t \sum_{j=0}^{n-1} \sum_{k\in N_j} G\Big(\mathbf{x}_m^n, \mathbf{x}_k^j, t_n, t_j\Big)\varphi\Big(\mathbf{x}_k^j, t_j\Big) w_k^j + O\Big(h_t^{\frac{3}{2}}\Big),$$

where $m \in N_n$. The other operators are similar.

6 Numerical Example

Both the weakly and strongly singular integral formulas can be used to solve the Dirichlet or Neumann problem of the heat equation. This gives a total of four different integral formulations:

P1. The Dirichlet problem using the weakly singular equation. Solving (11) for $\gamma_1^- u$ results in an integral equation of the first kind.

P2. The Neumann problem using the weakly singular equation. Solving (11) for u results in an integral equation of the second kind.

P3. The Neumann problem using the strongly singular equation. Solving (12) for u results in a hypersingular integral equation of the first kind.

Table 1 Mesh parameters

Mesh number	h_t	Points
M1	0.02	288
M2	0.01	1152
M3	0.005	4608
M4	0.0025	18432

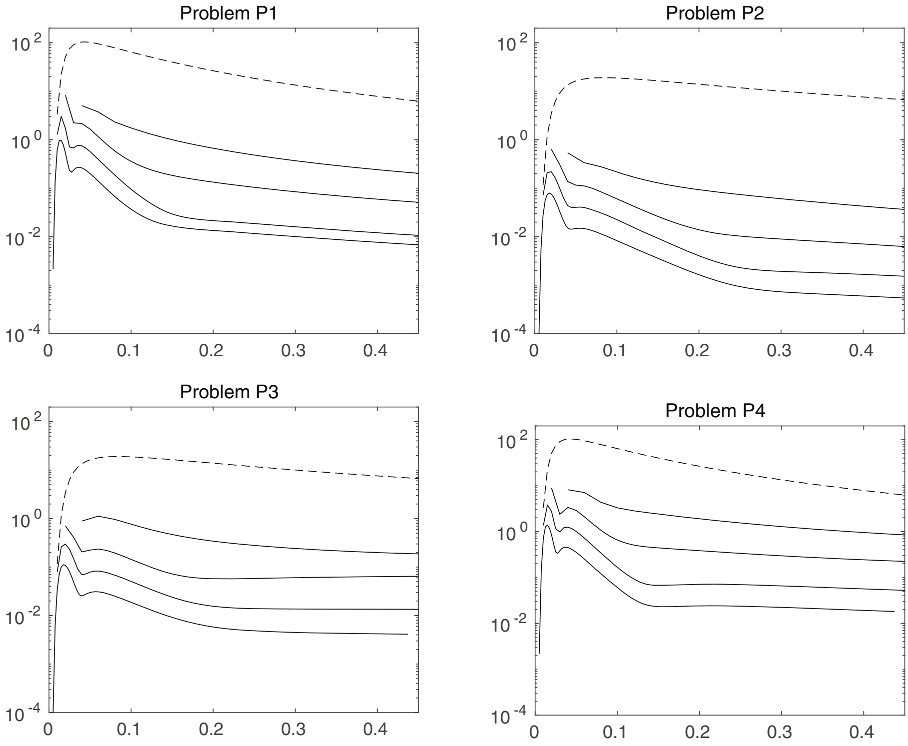

Fig. 1 $L_2(\Gamma)$-norms of the solution (dashed line) and the errors (solid lines) for the four meshes versus time

P4. The Dirichlet problem using the strongly singular equation. Solving (12) for $\gamma_1^- u$ results in an integral equation of the second kind.

In the Nyström method, the integral operators are replaced by their fully discrete counter part. This leads to a time stepping method where in the nth step the approximate solution is computed at the quadrature nodes. Because of the special form of the fully discrete operators, this is an explicit scheme.

For second-kind formulations, the classical convergence theory of Nyström methods applies as was performed in the context of fixed geometries in [18]. The

Table 2 Convergence rates for the four problems at two selected times

Time	Mesh	P1	P2	P3	P4
	M1-2	2.2885	1.8368	2.4148	2.3285
0.1	M2-3	1.9037	1.4419	1.5111	1.9629
	M3-4	1.3740	1.4261	1.4301	1.4740
	M1-2	2.0230	2.5955	1.6498	1.9753
0.4	M2-3	2.3005	2.0781	2.2324	2.1053
	M3-4	0.6523	1.4829	1.6880	1.5545

modifications for moving geometries are not presented here as they do not require essential modifications of the argument. We are not aware of a stability analysis for the first-kind formulations, but our experimentations suggest that the discretization methods described are at least conditionally stable.

To illustrate the behavior of the discretization scheme for the four different formulations, we solve a problem in the outside of the ellipse

$$\left(\frac{x}{1.2}\right)^2 + \left(\frac{y}{0.8}\right)^2 + \left(\frac{z}{0.7}\right)^2 = 1$$

that rotates about the z-axis. The rate of rotation is such that one revolution is completed in the time interval $t \in [0, 2]$.

The boundary condition is such that the solution is given by $u(x, t) = G(x - x_0, t)$, where $x_0 = [0.1, 0.2, -0.05]$ is slightly off centered to avoid symmetries in the solution. The spatial quadrature rule in this experiment is chosen to have degree of precision $p = 2$. In order to satisfy (32), we keep the ratio of the spatial and temporal mesh constant. We have computed four refinements; their parameters are listed in Table 1.

Figure 1 displays the $L_2(\Gamma)$-norm of the solution together with the errors for the different meshes as functions of time. Table 2 displays the convergence rate of two consecutive meshes $\log_2(\|e_m\|/\|e_{m+1}\|)$ at times $t = 0.1$ and $t = 0.4$ (m is the mesh number). With the exception of P1, the convergence rates of the finer meshes are in good agreement with the theoretical rate of 1.5. For P1, the initial convergence is rapid but deteriorates for the finest mesh.

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