A numerical method for solving heat equations involving interfaces *

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Abstract

In 1993, Li and Mayo [3] gave a finite-difference method with second
order accuracy for solving the heat equations involving interfaces with
constant coefficients and discontinuous sources. In this paper, we expand
their result by presenting a finite-difference method which allows each
coefficient to take different values in different sub-regions of the interface.
Our method is useful in physical applications, and has also second order
accuracy.

1 Introduction

Consider the heat equation

$$u_t = (\beta u_x)_x + (\beta u_y)_y + f(x, y, t), \tag{1}$$

where t is in $[a, \infty)$ and (x, y) in an open region $\Omega \subset R^2$ which is divided into
two sub-regions Ω^+, Ω^- by an irregular interface Γ.

Let $\Omega = \Omega^+ \cup \Gamma \cup \Omega^-$ be an open rectangular region in R^2, and let

$$\beta(x, y) = \begin{cases} \beta^+, & \text{if } (x, y) \in \Omega^+, \\ \beta^-, & \text{if } (x, y) \in \Omega^-, \end{cases}$$

where β^+ and β^- are positive constants. Assume that f is continuous in each
sub-region, and may have jumps of discontinuty across Γ. The solution $u(x, y, t)$
and its normal derivative $u_n(x, y, t)$ crossing the curve Γ have prescribed jumps

$$[u] \equiv u^+(x(s), y(s), t) - u^-(x(s), y(s), t) = \omega(s, t), \tag{2}$$

$$[u_n] \equiv u_n^+(x(s), y(s), t) - u_n^-(x(s), y(s), t) = g(s, t), \tag{3}$$

where s is a parameter of Γ, the superscripts $+$ and $-$ denote the limiting
values of a function from one side in Ω^+ and another side in Ω^- respectively.
Throughout this paper, we use $[G] = G^+ - G^-$ to denote the difference of the

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limiting values of a function G from different sides of the interface as in (2), (3). We also assume that the initial condition at $t = a$ and the boundary condition on ∂B are known. In 1993, Li and Mayo [3] gave a finite-difference method with second accuracy for solving (1), assuming that f is discontinuous but β is constant. In this paper, we present a finite-difference method for solving (1), which allows β to be taken different values in different sub-regions of the interface. This feature is useful in physical applications.

We organize this paper as follows: In Section 2, we establish local coordinate systems around the interface. In Section 3, we give the correction terms for the finite-difference method. In Section 4, we show that our method is second order accurate. Finally, in Section 5, we give some numerical examples, in which the actual solutions are known, to confirm the theoretical result.

2   Local Coordinate Systems

We first give local coordinate systems along the interface Γ, as in [2, 3]. When a point (x_0, y_0) on the interface is fixed for the origin, we use the normal direction as the ξ-direction, which has an angle θ with the x-axis. Rotating the ξ-direction by ninety degrees counter-clockwise, we obtain the η-direction. Now we express the curve Γ as a function of the independent variable η locally.

$$\xi = \chi(\eta). \tag{4}$$

We express (2),(3) locally by using the η coordinate.

$$[u] \equiv u^+ - u^- = \omega(\eta, t), \tag{5}$$

$$[u_n] \equiv u_n^+ - u_n^- = g(\eta, t), \tag{6}$$

where ω and g are known in advance. From (4) and (6), we have

$$g = [u_n] = \frac{-[u_\eta]\chi_\eta + [u_\xi]}{\sqrt{1 + \chi_\eta^2}}.$$

Using differentiation with respect to η, noting $\chi_\eta(0) = 0$, we have

$$[u_\eta] = \omega_\eta, \tag{7}$$

$$[u_\xi] = g, \tag{8}$$

$$[u_{\eta\eta}] = -g\chi_{\eta\eta} + \omega_{\eta\eta}, \tag{9}$$

$$[u_{\xi\eta}] = \omega_\eta\chi_{\eta\eta} + g_\eta. \tag{10}$$

Changing (1) locally, using

$$\xi = (x - x_0)cos\theta + (y - y_0)sin\theta, \tag{11}$$

$$\eta = -(x - x_0)sin\theta + (y - y_0)cos\theta, \tag{12}$$

we have

$$u_{xx} + u_{yy} = u_{\xi\xi} + u_{\eta\eta},$$

therefore,

$$u_t = \beta u_{\xi\xi} + \beta u_{\eta\eta} + \widetilde{f}(\xi, \eta, t), \tag{13}$$

where $\widetilde{f}(\xi, \eta, t) = f(x(\xi, \eta), y(\xi, \eta), t)$. (13) implies

$$[u_{\xi\xi}] = [u_{\xi\xi}]_1 + \left[\frac{u_t}{\beta} \right], \tag{14}$$

where

$$[u_{\xi\xi}]_1 = g\chi_{\eta\eta} - \omega_{\eta\eta} - \left[\frac{\widetilde{f}}{\beta} \right]. \tag{15}$$

In (7)-(10)and (14)-(15), all functions in the right-hand sides are known except for $[u_t/\beta]$ in (14) which will be explored in the next section.

3   Correction Terms

We first discretize in both of the x-direction and the y-direction with a mesh of size h.

$$u_{xx} \quad \approx \quad \delta_x u_{i,j} \equiv \frac{1}{h^2}(u_{i-1,j} - 2u_{i,j} + u_{i+1,j}), \tag{16}$$

$$u_{yy} \quad \approx \quad \delta_y u_{i,j} \equiv \frac{1}{h^2}(u_{i,j-1} - 2u_{i,j} + u_{i,j+1}). \tag{17}$$

We group all the grid points in Ω into two sets. The set S_{reg} consists the regular points, each point in one sub-region has no neighbor point in the another sub-region. The set S_{irr} consists the irregular points, each point in one sub-region has at least one neighbor point in the other sub-region. For a regular grid point, the local truncation error of (16),(17) from $\beta u_{xx} + \beta_{yy} + f$ is $O(h^2)$.

For an irregular grid point, we need add some correction terms in (16),(17) such that the local truncation error is $O(h)$, therefore the global error of the solution for solving the heat equation is $O(h^2)$ after the discretization of time t in certain way. At first, we relate the jumps with respect to x and y to the jumps with respect to ξ and η by (11) and (12).

$$
\begin{aligned}
{}[u_x] &= [u_\xi]\cos\theta - [u_\eta]\sin\theta, \\
[u_y] &= [u_\xi]\sin\theta + [u_\eta]\cos\theta, \\
[u_{xx}] &= [u_{xx}]_1 + \left[\frac{u_t}{\beta} \right]\cos^2\theta,
\end{aligned}
\tag{18}
$$

where

$$
\begin{aligned}
{}[u_{xx}]_1 &= [u_{\xi\xi}]_1\cos^2\theta - 2[u_{\xi\eta}]\cos\theta\sin\theta + [u_{\eta\eta}]\sin^2\theta, \\
[u_{yy}] &= [u_{yy}]_1 + \left[\frac{u_t}{\beta} \right]\sin^2\theta,
\end{aligned}
\tag{19}
$$

where
$$[u_{yy}]_1 = [u_{\xi\xi}]_1 \sin^2 \theta + 2[u_{\xi\eta}] \cos \theta \sin \theta + [u_{\eta\eta}] \cos^2 \theta.$$
By (7)-(10) and (14)-(15), all the terms in the right-hand sides of (18)-(19) are known except for $[u_t/\beta]$.

Now we consider an irregular grid point in the x-direction, there are four cases:

(a) $(x_i, y_j) \in \Omega^-, (x_{i+1}, y_j) \in \Omega^+$

(b) $(x_i, y_j) \in \Omega^+, (x_{i-1}, y_j) \in \Omega^-$

(c) $(x_i, y_j) \in \Omega^+, (x_{i+1}, y_j) \in \Omega^-$

(d) $(x_i, y_j) \in \Omega^-, (x_{i-1}, y_j) \in \Omega^+$

For case (a), let the intersection of the line segment connecting (x_i, y_j), (x_{i+1}, y_j) and Γ be (x^*, y_j). Using Taylor's series around x^*, we have

$$\frac{1}{h^2}(u(x_{i-1}, y_j) - 2u(x_i, y_j) + u(x_{i+1}, y_j))$$
$$= \frac{1}{h^2}\left\{ [u] + [u_x](x_{i+1} - x^*) + \frac{[u_{xx}]}{2!}(x_{i+1} - x^*)^2 \right\} + u_{xx}^- + O(h),$$

which implies

$$u_{xx} = \delta_x u_{i,j} + C_x u_{i,j} - \frac{[\frac{u_t}{\beta}](x_{i+1} - x^*)^2}{2h^2} + O(h), \tag{20}$$

where

$$C_x u_{i,j} = -\frac{1}{h^2}\left\{ [u] + [u_x](x_{i+1} - x^*) + \frac{[u_{xx}]_1}{2!}(x_{i+1} - x^*)^2 \right\}.$$

Similarly, for case (b), we have

$$u_{xx} = \delta_x u_{i,j} + C_x u_{i,j} + \frac{[\frac{u_t}{\beta}](x_{i-1} - x^*)^2}{2h^2} + O(h), \tag{21}$$

where

$$C_x u_{i,j} = \frac{1}{h^2}\left\{ [u] + [u_x](x_{i-1} - x^*) + \frac{[u_{xx}]_1}{2!}(x_{i-1} - x^*)^2 \right\}.$$

For case (c), we have

$$u_{xx} = \delta_x u_{i,j} + C_x u_{i,j} + \frac{[\frac{u_t}{\beta}](x_{i+1} - x^*)^2}{2h^2} + O(h), \tag{22}$$

where

$$C_x u_{i,j} = \frac{1}{h^2}\left\{ [u] + [u_x](x_{i+1} - x^*) + \frac{[u_{xx}]_1}{2!}(x_{i+1} - x^*)^2 \right\}.$$

For case (d), we have

$$u_{xx} = \delta_x u_{i,j} + C_x u_{i,j} - \frac{[\frac{u_t}{\beta}](x_{i-1} - x^*)^2}{2h^2} + O(h), \tag{23}$$

where

$$C_x u_{i,j} = -\frac{1}{h^2}\left\{[u] + [u_x](x_{i-1} - x^*) + \frac{[u_{xx}]_1}{2!}(x_{i-1} - x^*)^2\right\}.$$

Analogously, in the y-direction, we also have four cases. We add correction terms such that the local truncation is $O(h)$.

Now using these correction terms in both x-and y-directions, we obtain a system of ordinary differential equations

$$\begin{aligned}
(u_{i,j})_t &= \beta(\delta_x u_{i,j} + \delta_y u_{i,j}) + f_{i,j} \\
&+\beta \sum_{(x_{i_0},y^*)\in S_{\text{irr}}} \left\{C_x u_{i,j} + \left[\frac{u_t}{\beta}\right]\frac{\tau_{x_0}(x_{i_0} - x^*)^2 \cos^2\theta}{2h^2}\right\} \\
&+\beta \sum_{(x^*,y_{j_0})\in S_{\text{irr}}} \left\{C_y u_{i,j} + \left[\frac{u_t}{\beta}\right]\frac{\tau_{y_0}(y_{j_0} - y^*)^2 \sin^2\theta}{2h^2}\right\} + O(h),
\end{aligned} \tag{24}$$

where $i_0 = i - 1$ or $i + 1$, $j_0 = j - 1$ or $j + 1$. τ_{x_0}, $\tau_{y_0} = 1$ or -1 according to (20)-(23). We have

$$\left[\frac{u_t}{\beta}\right] = u_t^- \left[\frac{1}{\beta}\right] + \frac{[u_t]}{\beta^+} = u_t^+ \left[\frac{1}{\beta}\right] + \frac{[u_t]}{\beta^-},$$

which imply

$$\left[\frac{u_t}{\beta}\right] = (u_{i,j})_t \left[\frac{1}{\beta}\right] + \frac{\omega_t}{\widetilde{\beta}} + O(h), \tag{25}$$

where $\widetilde{\beta} = \beta^-$ if $\beta = \beta^+$, $\widetilde{\beta} = \beta^+$ if $\beta = \beta^-$, and ω is defined in (5). Using (25), we have the following system of ordinary differential equations

$$(u_{i,j})_t = F(u_{i,j-1}, u_{i-1,j}, u_{i,j}, u_{i+1,j}, u_{i,j+1})$$

with the right-hand side F is equal to

$$\frac{\beta(\delta_x u_{i,j} + \delta_y u_{i,j} + \sum_{(x_{i_0},y^*)\in S_{\text{irr}}} \widetilde{C}_x u_{i,j} + \sum_{(x^*,y_{j_0})\in S_{\text{irr}}} \widetilde{C}_y u_{i,j}) + f_{i,j}}{1 - \sum_{(x_{i_0},y^*)\in S_{\text{irr}}} \beta[\frac{1}{\beta}]\frac{\tau_{x_{i_0}}(x_{i_0}-x^*)^2\cos^2\theta}{2h^2} - \sum_{(x^*,y_{j_0})\in S_{\text{irr}}} \beta[\frac{1}{\beta}]\frac{\tau_{y_{j_0}}(y_{j_0}-y^*)^2\sin^2\theta}{2h^2}}, \tag{26}$$

where

$$\widetilde{C}_x u_{ij} = C_x u_{ij} + \frac{\omega_t}{\widetilde{\beta}}\frac{\tau_{x_{i_0}}(x_{i_0} - x^*)^2 \cos^2\theta}{2h^2}$$

and

$$\widetilde{C}_y u_{ij} = C_y u_{ij} + \frac{\omega_t}{\widetilde{\beta}}\frac{\tau_{y_{j_0}}(y_{j_0} - y^*)^2 \sin^2\theta}{2h^2}.$$

At a regular grid point, the local truncation error of the right-hand side of (26) from $\beta u_{xx} + \beta_{yy} + f$ is $O(h^2)$. In the next section, we will show that at an irregular grid point, the local truncation error is $O(h)$.

Finally, we discretize time t by choosing $\Delta t = h$. We use Crank-Nicholson method.

$$
\begin{aligned}
u_{i,j,k+1} &= u_{i,j,k} + \Delta t (0.5 F(u_{i,j-1,k}, u_{i-1,j,k}, u_{i,j,k}, u_{i+1,j,k}, u_{i,j+1,k}) \quad (27) \\
&\quad + 0.5 F(u_{i,j-1,k+1}, u_{i-1,j,k+1}, u_{i,j,k+1}, u_{i+1,j,k+1}, u_{i,j+1,k+1})),
\end{aligned}
$$

which implies the local truncation error for discretizing on t is $O((\Delta t)^2)$, [1, 4]. To solve for $u_{i,j,k+1}$, from (27), we use S.O.R. iteration with a certain parameter λ. Set

$$
u_{i,j,k+1}^{(0)} = u_{i,j,k},
$$

and for $n = 1, 2, \ldots$, set

$$
\begin{aligned}
u_{i,j,k+1}^{(n+1)} &= (1 - \lambda) u_{i,j,k+1}^{(n)} + \lambda (u_{i,j,k} \\
&\quad + 0.5 F(u_{i,j-1,k}, u_{i-1,j,k}, u_{i,j,k}, u_{i+1,j,k}, u_{i,j+1,k}) \quad (28) \\
&\quad + 0.5 F(u_{i,j-1,k+1}^{(n+1)}, u_{i-1,j,k+1}^{(n+1)}, u_{i,j,k+1}^{(n)}, u_{i+1,j,k+1}^{(n)}, u_{i,j+1,k+1}^{(n)})).
\end{aligned}
$$

4 Accuracy Analysis

We first show that the denominator of the right-hand side of (26) is bounded below and above by positive constants. Let

$$
\begin{aligned}
D_{i,j} &\equiv 1 - \sum_{(x_{i_0}, y^*) \in S_{\text{irr}}} \beta \left[\frac{1}{\beta} \right] \frac{\tau_{x_{i_0}} (x_{i_0} - x^*)^2 \cos^2 \theta}{2h^2} \quad (29) \\
&\quad - \sum_{(x^*, y_{j_0}) \in S_{\text{irr}}} \beta \left[\frac{1}{\beta} \right] \frac{\tau_{y_{j_0}} (y_{j_0} - y^*)^2 \sin^2 \theta}{2h^2}.
\end{aligned}
$$

and

$$
\begin{aligned}
E_{i,j} &\equiv 1 + \sum_{(x_{i_0}, y^*) \in S_{\text{irr}}} \left| \beta \left[\frac{1}{\beta} \right] \frac{\tau_{x_{i_0}} (x_{i_0} - x^*)^2 \cos^2 \theta}{2h^2} \right| \quad (30) \\
&\quad + \sum_{(x^*, y_{j_0}) \in S_{\text{irr}}} \left| \beta \left[\frac{1}{\beta} \right] \frac{\tau_{y_{j_0}} (y_{j_0} - y^*)^2 \sin^2 \theta}{2h^2} \right|.
\end{aligned}
$$

Lemma 4.1 *Let $D_{i,j}$ and $E_{i,j}$ be as defined above. Then*

$$
D_{i,j} \geq \frac{\min(\beta^+, \beta^-)}{\max(\beta^+, \beta^-)} \quad \text{and} \quad E_{i,j} \leq 1 + \max(\beta^+, \beta^-) \left| \left[\frac{1}{\beta} \right] \right|, \quad (31)
$$

where $i_0 = i - 1$ or $i + 1$, $j_0 = j - 1$ or $j + 1$. $\tau_{x_{i_0}}$, $\tau_{y_{j_0}} = 1$ or -1 according to (20)-(23).

Proof: At first we prove the lower bound. Look at the first summation. In x-direction, we have four cases.

(a) $(x_i, y_j) \in \Omega^-$, $(x_{i+1}, y_j) \in \Omega^+$. Then $x_{i_0} = x_{i+1}$, $\tau_{x_{i_0}} = -1$, $\beta = \beta^-$, and $\beta \left[\frac{1}{\beta}\right] \tau_{x_{i_0}} = 1 - \frac{\beta^-}{\beta^+}$ which is positive iff $\beta^- < \beta^+$.

(b) $(x_i, y_j) \in \Omega^+$, $(x_{i-1}, y_j) \in \Omega^-$. Then $x_{i_0} = x_{i-1}$, $\tau_{x_{i_0}} = 1$, $\beta = \beta^+$, and $\beta \left[\frac{1}{\beta}\right] \tau_{x_{i_0}} = 1 - \frac{\beta^+}{\beta^-}$ which is positive iff $\beta^+ < \beta^-$.

(c) $(x_i, y_j) \in \Omega^+$, $(x_{i+1}, y_j) \in \Omega^-$. Then $x_{i_0} = x_{i+1}$, $\tau_{x_{i_0}} = 1$, $\beta = \beta^+$, and $\beta \left[\frac{1}{\beta}\right] \tau_{x_{i_0}} = 1 - \frac{\beta^+}{\beta^-}$ which is positive iff $\beta^+ < \beta^-$.

(d) $(x_i, y_j) \in \Omega^-$, $(x_{i+1}, y_j) \in \Omega^+$. Then $x_{i_0} = x_{i-1}$, $\tau_{x_{i_0}} = -1$, $\beta = \beta^-$, and $\beta \left[\frac{1}{\beta}\right] \tau_{x_{i_0}} = 1 - \frac{\beta^-}{\beta^+}$ which is positive iff $\beta^- < \beta^+$.

For all cases, a term in the first summation is positive iff $\beta = \min\{\beta^+, \beta^-\}$. Similarly we can show that a term in the second summation is positive iff $\beta = \min\{\beta^+, \beta^-\}$ too. Only the positive terms will reduce the lower bound of the left-hand side of (29). So the left-hand side is bounded below by

$$D_{i,j} \geq 1 - 0.5\left(1 - \frac{\min(\beta^+, \beta^-)}{\max(\beta^+, \beta^-)}\right) - 0.5\left(1 - \frac{\min(\beta^+, \beta^-)}{\max(\beta^+, \beta^-)}\right) = \frac{\min(\beta^+, \beta^-)}{\max(\beta^+, \beta^-)}.$$

Now we turn to the upper bound which can be proved directly from (30).

$$E_{i,j} \leq 1 + 0.5\beta \left|\left[\frac{1}{\beta}\right]\right| + 0.5\beta \left|\left[\frac{1}{\beta}\right]\right| \leq 1 + \max(\beta^+, \beta^-) \left|\left[\frac{1}{\beta}\right]\right|.$$

The lower bound (31) is useful for the stability of the numerical scheme and the upper bound (31) will be used in the proof of the following theorem.

Theorem 4.2 *At irregular grid points (x_i, y_j) in Ω,*

$$F(u_{i,j-1}, u_{i-1,j}, u_{i,j}, u_{i+1,j}, u_{i,j+1}) - (\beta u_{xx} + \beta u_{yy} + f)(x_i, y_j) = O(h). \quad (32)$$

Proof: From (24), (25), (26), and (31), we have

$$F(u_{i,j-1}, u_{i-1,j}, u_{i,j}, u_{i+1,j}, u_{i,j+1}) = (u_{i,j})_t$$
$$= \beta\left(\delta_x u_{i,j} + \delta_y u_{i,j} + \sum_{(x_{i_0},y^*)\in S_{\text{irr}}} \widetilde{C}_x u_{i,j} + \sum_{(x^*,y_{j_0})\in S_{\text{irr}}} \widetilde{C}_y u_{i,j}\right)$$
$$+ f_{i,j} + (u_{i,j})_t\left\{\sum_{(x_{i_0},y^*)\in S_{\text{irr}}} \beta\left[\frac{1}{\beta}\right]\frac{\tau_{x_{i_0}}(x_{i_0} - x^*)^2 \cos^2\theta}{2h^2}\right.$$
$$\left.+ \sum_{(x^*,y_{j_0})\in S_{\text{irr}}} \beta\left[\frac{1}{\beta}\right]\frac{\tau_{y_{j_0}}(y_{j_0} - y^*)^2 \sin^2\theta}{2h^2}\right\}$$

$$
\begin{aligned}
= \quad & \beta(\delta_x u_{i,j} + \delta_y u_{i,j}) + f_{i,j} \\
& +\beta \sum_{(x_{i_0},y^*)\in S_{\mathrm{irr}}} \left\{ C_x u_{i,j} + \left[\frac{u_t}{\beta}\right] \frac{\tau_{x_{i_0}} (x_{i_0} - x^*)^2 \cos^2\theta}{2h^2} \right\} \\
& +\beta \sum_{(x^*,y_{j_0})\in S_{\mathrm{irr}}} \left\{ C_y u_{i,j} + \left[\frac{u_t}{\beta}\right] \frac{\tau_{y_{j_0}} (y_{j_0} - y^*)^2 \sin^2\theta}{2h^2} \right\} + O(h) \\
= \quad & (\beta u_{xx} + \beta u_{yy} + f)(x_i, y_j) + O(h),
\end{aligned}
$$

which proves (32).

At a regular grid point, the local truncation error is $O(h^2)$. At an irregular grid point, the local truncation error is $O(h)$ by Theorem 4.2. The local truncation error from the discretization of time is $O((\Delta t)^2) = O(h^2)$. All these imply that the numerical solution has global error $O(h^2)$.

5   Numerical Examples

We choose some examples in which the actual solutions are known; therefore, numerical error computations can be obtained to confirm the theoretical result of our method. We choose

$$
\begin{aligned}
\Omega &= (-1,1) \times (-1,1), \quad t \in [1,\infty), \\
\Omega^+ &= \{(x,y) \in \Omega \quad |x^2 + y^2 > 1/4\}, \\
\Omega^- &= \{(x,y) \in \Omega \quad |x^2 + y^2 < 1/4\}, \\
\Gamma &= \{(x,y) \in \Omega \quad |x^2 + y^2 = 1/4\}.
\end{aligned}
$$

The exact solution for $f = 0$ is

$$
u(x,y,t) = \frac{1}{t} e^{-(x^2+y^2)/(4\beta t)}. \tag{33}
$$

We give the initial condition when $t = 1$, and the Dirichlet boundary condition when x and y are equal to 1 or -1. We choose $\lambda=1.75$ in (28). For different pairs β^+ and β^-, in t from 1.0 to 1.5, we obtain the data shown in Table 1.

The error is computed using the infinity norm. It shows that when h is divided by 2, the error becomes approximately a quarter of its previous value, which confirms that the numerical solution has second order accuracy.

h	β^+	β^-	error	ratio
0.100	1000	1	2.227782D-04	–
0.050	1000	1	5.391984D-05	4.13
0.025	1000	1	1.307318D-05	4.12
0.100	1	1000	2.392997D-05	–
0.050	1	1000	6.703319D-06	3.57
0.025	1	1000	1.766744D-06	3.79
0.100	5	1	2.629529D-04	–
0.050	5	1	6.351060D-05	4.14
0.025	5	1	1.550294D-05	4.10
0.100	1	5	5.461059D-05	–
0.050	1	5	1.309861D-05	4.17
0.025	1	5	3.263757D-06	4.01

Table 1: Accuracy of computations

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