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On a highly accurate approximation of the first and pure second derivatives of the Laplace equation in a rectangular parallelpiped

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Abstract

We propose and justify difference schemes for the approximation of the first and pure second derivatives of a solution of the Dirichlet problem in a rectangular parallelepiped. The boundary values on the faces of the parallelepiped are supposed to have six derivatives satisfying the Hölder condition, to be continuous on the edges, and to have second- and fourth-order derivatives satisfying the compatibility conditions resulting from the Laplace equation. We prove that the solutions of the proposed difference schemes converge uniformly on the cubic grid of order $O(h^4)$, where h is a grid step. Numerical experiments are presented to illustrate and support the analysis made.

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Keywords: finite difference method; approximation of derivatives; uniform error; Laplace equation

1 Introduction

A highly accurate method is one of the powerful tools reducing the number of unknowns, which is the main problem in the numerical solution of differential equations, to get reasonable results. This becomes more valuable in 3D problems when we are looking for the derivatives of the unknown solution by the finite difference or finite element methods for a small discretization parameter h.

The derivative problem was investigated in [1], in which it was proved that the high-order difference derivatives uniformly converge to the corresponding derivatives of the solution for the 2D Laplace equation in any strictly interior subdomain with the same order h as in the given domain. The uniform convergence of the difference derivatives over the whole grid domain to the corresponding derivatives of the solution for the 2D Laplace equation with order $O(h^2)$ was proved in [2]. In [3], for the first and pure second derivatives of the solution for the 2D Laplace equation, special finite difference problems were investigated. It is proved that the solution of these problems converge to the exact derivatives with order $O(h^4)$.

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In [4], for the 3D Laplace equation, the convergence of order $O(h^2)$ of the difference derivatives to the corresponding first-order derivatives of the exact solution is proved. It was assumed that the boundary values have the third derivatives on the faces and satisfy the Hölder condition. Furthermore, they are continuous on the edges, and their second derivatives satisfy the compatibility condition that is implied by the Laplace equation. Whereas in [5], when the boundary values on the faces of a parallelepiped are supposed to have the fourth derivatives satisfying the Hölder condition, the constructed difference schemes converge with order $O(h^2)$ to the first and pure second derivatives of the exact solution.

In this paper, we consider the Dirichlet problem for the Laplace equation on a rectangular parallelepiped. We assume that the boundary values on the faces have the sixth-order derivatives satisfying the Hölder condition, and the second- and fourth-order derivatives satisfy some compatibility conditions on the edges. We construct three different schemes on a cubic grid with mesh size h, whose solutions separately approximate the solution of the Dirichlet problem with order $O(h^6|\ln h|)$ and its first and pure second derivatives with order $O(h^4)$. We show that, for the same boundary functions, if we use fifth-order numerical differentiation formulae to construct the finite-difference problem for the first derivatives, then the accuracy can be increased up to $O(h^5|\ln h|)$. Finally, numerical experiments are given to support the theoretical results.

2 The Dirichlet problem on a rectangular parallelepiped

Let $R = \{(x_1, x_2, x_3) : 0 < x_i < a_i, i = 1,2,3\}$ be an open rectangular parallelepiped, Γ_j ($j = 1,2,\ldots,6$) be its faces including the edges such that Γ_j for $j = 1,2,3$ (for $j = 4,5,6$) belong to the plane $x_j = 0$ (to the plane $x_{j-3} = a_{j-3}$), let $\Gamma = \bigcup_{j=1}^{6} \Gamma_j$ be the boundary of R, and let $\gamma_{\mu\nu} = \Gamma_\mu \cap \Gamma_\nu$ be the edges of the parallelepiped R. We say that $f \in C^{k,\lambda}(D)$ if f has kth derivatives on D satisfying the Hölder condition with exponent $\lambda \in (0,1)$.

We consider the boundary value problem

$$\Delta u = 0 \quad \text{on } R, \qquad u = \varphi_j \quad \text{on } \Gamma_j, j = 1,2,\ldots,6, \tag{2.1}$$

where $\Delta \equiv \partial^2/\partial x_1^2 + \partial^2/\partial x_2^2 + \partial^2/\partial x_3^2$, and φ_j are given functions. Assume that

$$\varphi_j \in C^{6,\lambda}(\Gamma_j), \quad 0 < \lambda < 1, j = 1,2,\ldots,6, \tag{2.2}$$

$$\varphi_\mu = \varphi_\nu \quad \text{on } \gamma_{\mu\nu}, \tag{2.3}$$

$$\frac{\partial^2 \varphi_\mu}{\partial t_\mu^2} + \frac{\partial^2 \varphi_\nu}{\partial t_\nu^2} + \frac{\partial^2 \varphi_\mu}{\partial t_{\mu\nu}^2} = 0 \quad \text{on } \gamma_{\mu\nu}, \tag{2.4}$$

$$\frac{\partial^4 \varphi_\mu}{\partial t_\mu^4} + \frac{\partial^4 \varphi_\mu}{\partial t_\mu^2 \, \partial t_{\mu\nu}^2} = \frac{\partial^4 \varphi_\nu}{\partial t_\nu^4} + \frac{\partial^4 \varphi_\nu}{\partial t_\nu^2 \, \partial t_{\nu\mu}^2} \quad \text{on } \gamma_{\mu\nu}, \tag{2.5}$$

where $1 \le \mu < \nu \le 6$, $\nu - \mu \neq 3$, $t_{\mu\nu}$ is an element in $\gamma_{\mu\nu}$, and t_μ and t_ν are elements of the normal to $\gamma_{\mu\nu}$ on the face Γ_μ and Γ_ν, respectively.

Lemma 2.1 *The solution u of problem* (2.1) *is from* $C^{5,\lambda}(\overline{R})$.

The proof of Lemma 2.1 follows from Theorem 2.1 in [6].

Lemma 2.2 *We have the inequality*

$$\max_{0\le p\le 3}\max_{0\le q\le 3-p}\sup_{(x_1,x_2,x_3)\in R}\left|\frac{\partial^6 u}{\partial x_1^{2p}\,\partial x_2^{2q}\,\partial x_3^{6-2p-2q}}\right|\le c<\infty, \tag{2.6}$$

where u is the solution of problem (2.1).

Proof From Lemma 2.1 it follows that the functions $\frac{\partial^4 u}{\partial x_1^4}$, $\frac{\partial^4 u}{\partial x_2^4}$, and $\frac{\partial^4 u}{\partial x_3^4}$ are continuous on $\overline{R}$. We put $w=\frac{\partial^4 u}{\partial x_1^4}$. The function w is harmonic in R and is the solution of the problem

$$\Delta w=0 \quad \text{on } R, \qquad w=\Psi_j \quad \text{on } \Gamma_j, j=1,2,\ldots,6,$$

where

$$\Psi_\tau=\frac{\partial^4\varphi_\tau}{\partial x_2^4}+\frac{\partial^4\varphi_\tau}{\partial x_3^4}+2\frac{\partial^4\varphi_\tau}{\partial x_2^2\,\partial x_3^2}, \quad \tau=1,4,$$
$$\Psi_\nu=\frac{\partial^4\varphi_\nu}{\partial x_1^4}, \quad \nu=2,3,5,6.$$

From conditions (2.2)-(2.5) it follows that

$$\Psi_j\in C^{2,\lambda}(\Gamma_j), \quad 0<\lambda<1, j=1,2,\ldots,6,$$
$$\Psi_\mu=\Psi_\nu \quad \text{on } \gamma_{\mu\nu}, 1\le\mu<\nu\le 6, \nu-\mu\ne 3.$$

Hence, by Theorem 4.1 in [6] we have

$$\sup_{(x_1,x_2,x_3)\in R}\left|\frac{\partial^6 u}{\partial x_1^6}\right|=\sup_{(x_1,x_2,x_3)\in R}\left|\frac{\partial^2 w}{\partial x_1^2}\right|<\infty, \tag{2.7}$$

$$\sup_{(x_1,x_2,x_3)\in R}\left|\frac{\partial^6 u}{\partial x_1^4\,\partial x_2^2}\right|=\sup_{(x_1,x_2,x_3)\in R}\left|\frac{\partial^2 w}{\partial x_2^2}\right|<\infty, \tag{2.8}$$

$$\sup_{(x_1,x_2,x_3)\in R}\left|\frac{\partial^6 u}{\partial x_1^4\,\partial x_3^2}\right|=\sup_{(x_1,x_2,x_3)\in R}\left|\frac{\partial^2 w}{\partial x_3^2}\right|<\infty. \tag{2.9}$$

Similarly, it is proved that

$$\sup_{(x_1,x_2,x_3)\in R}\left\{\left|\frac{\partial^6 u}{\partial x_2^6}\right|,\left|\frac{\partial^6 u}{\partial x_3^6}\right|,\left|\frac{\partial^6 u}{\partial x_1^2\,\partial x_2^4}\right|,\left|\frac{\partial^6 u}{\partial x_1^2\,\partial x_3^4}\right|,\left|\frac{\partial^6 u}{\partial x_2^2\,\partial x_3^4}\right|,\left|\frac{\partial^6 u}{\partial x_2^4\,\partial x_3^2}\right|\right\}<\infty. \tag{2.10}$$

From (2.7)-(2.10) estimate (2.6) follows. □

Lemma 2.3 *Let* $\rho(x_1,x_2,x_3)$ *be the distance from the current point of the open parallelepiped R to its boundary, and let* $\partial/\partial l\equiv\alpha_1\partial/\partial x_1+\alpha_2\partial/\partial x_2+\alpha_3\partial/\partial x_3$, $\alpha_1^2+\alpha_2^2+\alpha_3^2=1$. *Then we have the inequality*

$$\left|\frac{\partial^8 u(x_1,x_2,x_3)}{\partial l^8}\right|\le c\rho^{-2}(x_1,x_2,x_3), \quad (x_1,x_2,x_3)\in R, \tag{2.11}$$

where c is a constant independent of the direction of differentiation $\partial/\partial l$, *and u is a solution of problem* (2.1).

Proof Since the sixth-order derivatives of the solution u of the form $\partial^6/\partial x_1^{2p}\,\partial x_2^{2q}\,\partial x_3^{6-2p-2q}$, $p+q+s=3$, are harmonic and by Lemma 2.2 are bounded in R, any eighth-order derivative can be obtained by twice differentiating some of these derivatives, on the basis of Lemma 3 from [7] (see Chapter 4, Section 3), we have

$$\max_{0\le\mu\le 8}\max_{0\le\upsilon\le 8-\mu}\left|\frac{\partial^8 u(x_1,x_2,x_3)}{\partial x_1^{\mu}\,\partial x_2^{\upsilon}\,\partial x_3^{8-\mu-\upsilon}}\right|\le c_1\rho^{-2}(x_1,x_2,x_3),\quad (x_1,x_2,x_3)\in R. \tag{2.12}$$

Inequality (2.11) follows from inequality (2.12). □

Let $h>0$ and $a_i/h\ge 6$, $i=1,2,3$. We assign R^h, a cubic grid on R, with step h, obtained by the planes $x_i=0,h,2h,\ldots$, $i=1,2,3$. Let D_h be the set of nodes of this grid, $R_h=R\cap D_h$, $\Gamma_{jh}=\Gamma_j\cap D_h$, and $\Gamma_h=\Gamma_{1h}\cup\Gamma_{2h}\cup\cdots\cup\Gamma_{6h}$.

Let the operator $\Re$ be defined as follows (see [8]):

$$\Re u(x_1,x_2,x_3)=\frac{1}{128}\left(14\sum_{p=1}^{6}{}_{(1)}u_p+3\sum_{q=7}^{18}{}_{(2)}u_p+\sum_{r=19}^{26}{}_{(3)}u_r\right),\quad (x_1,x_2,x_3)\in R, \tag{2.13}$$

where the sum $\sum_{(k)}$ is taken over the grid nodes that are at a distance of $\sqrt{k}h$ from the point (x_1,x_2,x_3), and u_p, u_q, and u_r are the values of u at the corresponding grid points.

We consider the following finite difference approximations of problem (2.1):

$$u_h=\Re u_h\quad\text{on } R^h,\qquad u_h=\varphi_j\quad\text{on } \Gamma_{jh}, j=1,2,\ldots,6. \tag{2.14}$$

By the maximum principle (see [9], Chapter 4), problem (2.14) has a unique solution.

In what follows and for simplicity, we denote by $c,c_1,c_2,\ldots$ constants that are independent of h and the nearest factor, and the identical notation will be used for various constants.

Let R^{kh} be the set of nodes of the grid R^h whose distance from Γ is kh. It is obvious that $1\le k\le N(h)$, where

$$N(h)=\left[\min\{a_1,a_2,a_3\}/(2h)\right]. \tag{2.15}$$

We define, for $1\le k\le N(h)$,

$$f_h^k=\begin{cases}1, & (x_1,x_2,x_3)\in R^{kh},\\ 0, & (x_1,x_2,x_3)\in R^h\backslash R^{kh}.\end{cases}$$

Lemma 2.4 *The solution of the system*

$$v_h^k=\Re v_h^k+f_h^k\quad\textit{on } R^h,\qquad v_h^k=0\quad\textit{on } \Gamma_h,$$

satisfies the inequality

$$\max_{(x_1,x_2,x_3)\in R^h} v_h^k\le 6k,\quad 1\le k\le N(h).$$

Proof For the proof, see Lemma 2 in [10]. □

Lemma 2.5 *Let u be a solution of problem* (2.1). *Then*

$$\max_{(x_1,x_2,x_3)\in R^{kh}} |\Re u - u| \le c\frac{h^6}{k^2}, \quad k = 1,2,\ldots,N(h). \tag{2.16}$$

Proof Let (x_{10}, x_{20}, x_{30}) be a point of R^{1h}, and let

$$R_0 = \{(x_1,x_2,x_3) : |x_i - x_{i0}| < h, i = 1,2,3\} \tag{2.17}$$

be an elementary cube, some faces of which lie on the boundary of the rectangular parallelepiped R. On the vertices of R_0 and on the center of its faces and edges. there lie the nodes of which the function values are used to evaluate $\Re u(x_{10}, x_{20}, x_{30})$. We represent a solution of problem (2.1) in some neighborhood of $x_0 = (x_{10}, x_{20}, x_{30}) \in R^{1h}$ by Taylor's formula

$$u(x_1,x_2,x_3) = p_7(x_1,x_2,x_3;x_0) + r_8(x_1,x_2,x_3;x_0), \tag{2.18}$$

where $p_7(x_1,x_2,x_3)$ is the seventh-order Taylor polynomial, and $r_8(x_1,x_2,x_3)$ is the remainder term. Taking into account that the function u is harmonic, we have

$$\Re p_7(x_{10},x_{20},x_{30};x_0) = u(x_{10},x_{20},x_{30}). \tag{2.19}$$

Now, we estimate r_8 at the nodes of the operator $\Re$. We take a node $(x_{10} + h, x_{20}, x_{30} + h)$, which is one of the twenty six nodes of $\Re$, and consider the function

$$\tilde{u}(s) = u\left(x_{10} + \frac{s}{\sqrt{2}}, x_{20}, x_{30} + \frac{s}{\sqrt{2}}\right), \quad -\sqrt{2}h \le s \le \sqrt{2}h, \tag{2.20}$$

of single variable s, which is the arc length along the straight line through the points $(x_{10} - h, x_{20}, x_{30} - h)$ and $(x_{10} + h, x_{20}, x_{30} + h)$. By Lemma 2.3 we have

$$\left|\frac{d^8\tilde{u}(s)}{ds^8}\right| \le c(\sqrt{2}h - s)^{-2}, \quad 0 \le s < \sqrt{2}h. \tag{2.21}$$

We represent the function (2.20) around the point $s = 0$ by Taylor's formula

$$\tilde{u}(s) = \tilde{p}_7(s) + \tilde{r}_8(s),$$

where $\tilde{p}_7(s) \equiv p_7(x_{10} + \frac{s}{\sqrt{2}}, x_{20}, x_{30} + \frac{s}{\sqrt{2}})$ is the seventh-order Taylor polynomial of the variable s, and

$$\tilde{r}_8(s) \equiv r_8\left(x_{10} + \frac{s}{\sqrt{2}}, x_{20}, x_{30} + \frac{s}{\sqrt{2}}; x_0\right), \quad |s| < \sqrt{2}h, \tag{2.22}$$

is the remainder term. By the continuity of $\tilde{r}_8(s)$ on the interval $[-\sqrt{2}h, \sqrt{2}h]$ and estimate (2.21) we obtain

$$\begin{aligned} &r_8(x_{10} + h, x_{20}, x_{30}h; x_0) \\ &\quad = \lim_{\varepsilon\to+0} \tilde{r}_8(\sqrt{2}h - \varepsilon) \end{aligned}$$

$$\leq \lim_{\varepsilon\to+0}\left[c\frac{1}{7!}\int_0^{\sqrt{2}h-\varepsilon}(\sqrt{2}h-\varepsilon-t)^7(\sqrt{3}h-t)^{-2}\,dt\right]$$
$$\leq c_1h^6, \quad 0<\varepsilon\leq\frac{\sqrt{2}h}{2}, \tag{2.23}$$

where c_1 is a constant independent of the choice of $(x_{10},x_{20},x_{30})\in R^{kh}$.

Estimate (2.23) is obtained analogously for the remaining twenty five nodes on the closed cube (2.17). Since the norm of the operator $\Re$ in the uniform metric is equal to one, by (2.23) we have

$$\left|\Re r_8(x_{10},x_{20},x_{30})\right|\leq c_2h^6. \tag{2.24}$$

From (2.18), (2.19), and (2.24) we obtain

$$\left|\Re u(x_{10},x_{20},x_{30})-u(x_{10},x_{20},x_{30})\right|\leq ch^6$$

for any $(x_{10},x_{20},x_{30})\in R^{1h}$.

Now, let (x_{10},x_{20},x_{30}) be a point of R^{kh} for $2\leq k\leq N(h)$. By Lemma 2.3 for any k, $2\leq k\leq N(h)$, we obtain

$$\left|\Re r_8(x_{10},x_{20},x_{30})\right|\leq c_3\frac{h^6}{k^2}, \tag{2.25}$$

where c_3 is a constant independent of k, $2\leq k\leq N(h)$, and the choice of $(x_{10},x_{20},x_{30})\in R^{kh}$. From (2.18), (2.19), and (2.25) estimate (2.16) follows. □

Lemma 2.6 *Assume that the boundary functions φ_j, $j=1,2,\ldots,6$, satisfy conditions* (2.2)-(2.5). *Then*

$$\max_{\overline{R}^h}|u_h-u|\leq ch^6\bigl(1+|\ln h|\bigr), \tag{2.26}$$

where u_h is the solution of the finite difference problem (2.14), *and u is the exact solution of problem* (2.1).

Proof Let

$$\varepsilon_h=u_h-u \quad \text{on } \overline{R}^h. \tag{2.27}$$

By (2.14) and (2.27) the error function satisfies the system of equations

$$\varepsilon_h=\Re\varepsilon_h+(\Re u-u) \quad \text{on } R^h, \qquad \varepsilon_h=0 \quad \text{on } \Gamma^h. \tag{2.28}$$

We represent a solution of system (2.28) as follows:

$$\varepsilon_h=\sum_{k=1}^{N(h)}\varepsilon_h^k, \tag{2.29}$$

where ε_h^k, $1 \le k \le N(h)$, with $N(h)$ defined by (2.15), is a solution of the system

$$\varepsilon_h^k = \Re\varepsilon_h^k + \nu^k \quad \text{on } R^h, \qquad \varepsilon_h^k = 0 \quad \text{on } \Gamma^h, \tag{2.30}$$

where

$$\nu^k = \begin{cases} \Re u - u & \text{on } R^{kh}, \\ 0 & \text{on } R^h \backslash R^{kh}. \end{cases}$$

Then for the solution of (2.30) by applying Lemmas 2.4 and 2.5 we have

$$\max_{(x_1,x_2,x_3)\in R^h} \left|\varepsilon_h^k\right| \le c\frac{h^6}{k}, \quad 1 \le k \le N(h). \tag{2.31}$$

By (2.27), (2.29), and (2.31) we obtain

$$\max_{(x_1,x_2,x_3)\in R^h} |u_h - u| \le ch^6\bigl(1 + |\ln h|\bigr). \qquad \square$$

Let ω be a solution of the problem

$$\Delta\omega = 0 \quad \text{on } R, \qquad \omega = \psi_j \quad \text{on } \Gamma_j, j = 1,2,\ldots,6, \tag{2.32}$$

where ψ_j, $j = 1,2,\ldots,6$, are given functions, and

$$\psi_j \in C^{4,\lambda}(\Gamma_j), \quad 0 < \lambda < 1, j = 1,2,\ldots,6, \tag{2.33}$$

$$\psi_\mu = \psi_\nu \quad \text{on } \gamma_{\mu\nu}, \tag{2.34}$$

$$\frac{\partial^2\psi_\mu}{\partial t_\mu^2} + \frac{\partial^2\psi_\nu}{\partial t_\nu^2} + \frac{\partial^2\psi_\mu}{\partial t_{\mu\nu}^2} = 0 \quad \text{on } \gamma_{\mu\nu}. \tag{2.35}$$

Lemma 2.7 *We have the estimate*

$$\max_{\overline{R}^h} |\omega_h - \omega| \le ch^4, \tag{2.36}$$

where ω is the exact solution of problem (2.32), *and ω_h is the exact solution of the finite difference problem*

$$\omega_h = \Re\omega_h \quad \text{on } R^h, \qquad \omega_h = \psi_j \quad \text{on } \Gamma_{jh}, j = 1,2,\ldots,6. \tag{2.37}$$

Proof It follows from Lemma 1.2 in [5] that

$$\max_{0\le p\le q}\max_{0\le q\le 2-p}\sup_{(x_1,x_2,x_3)\in R}\left|\frac{\partial^4\omega(x_1,x_2,x_3)}{\partial x_1^{2p}\,\partial x_2^{2q}\,\partial x_3^{4-2p-2q}}\right| < \infty,$$

where u is the solution of problem (2.32). Then, instead of inequality (2.12), we have

$$\max_{0\le\mu\le 8}\max_{0\le\nu\le 8-\mu}\left|\frac{\partial^8\omega(x_1,x_2,x_3)}{\partial x_1^{\mu}\,\partial x_2^{\nu}\,\partial x_3^{8-\mu-\nu}}\right| \le c\rho^{-4}(x_1,x_2,x_3), \quad (x_1,x_2,x_3) \in R, \tag{2.38}$$

where $\rho(x_1,x_2,x_3)$ is the distance from $(x_1,x_2,x_3) \in R$ to the boundary Γ.

By estimate (2.38) and Taylor's formula, by analogy with the proof of Lemma 2.5 we have

$$\max_{(x_1,x_2,x_3)\in R^{kh}} |\Re\omega - \omega| \le c\frac{h^4}{k^4}, \quad k = 1,2,\ldots,N(h).$$

We put

$$\epsilon_h = \omega_h - \omega \quad \text{on } R^h \cup \Gamma_h.$$

Then, as in the proof of Lemma 2.6, we obtain

$$\max_{\overline{R}^h} |\omega_h - \omega| \le c_4 h^4 \sum_{k=1}^{N(h)} \frac{1}{k^3} \le ch^4. \qquad \square$$

3 Approximation of the first derivative

Let $\nu = \frac{\partial u}{\partial x_1}$, and let $\Phi_j = \frac{\partial u}{\partial x_1}$ on Γ_j, $j = 1,2,\ldots,6$, and consider the boundary value problem

$$\Delta\nu = 0 \quad \text{on } R, \qquad \nu = \Phi_j \quad \text{on } \Gamma_j, j = 1,2,\ldots,6, \tag{3.1}$$

where u is a solution of the boundary value problem (2.1).

We define the following operators $\Phi_{\nu h}$, $\nu = 1,2,\ldots,6$:

$$\begin{aligned}\Phi_{1h}(u_h) = {}& \frac{1}{12h}\bigl(-25\varphi_1(x_2,x_3) + 48u_h(h,x_2,x_3) - 36u_h(2h,x_2,x_3) \\ & + 16u_h(3h,x_2,x_3) - 3u_h(4h,x_2,x_3)\bigr) \quad \text{on } \Gamma_1^h,\end{aligned} \tag{3.2}$$

$$\begin{aligned}\Phi_{4h}(u_h) = {}& \frac{1}{12h}\bigl(25\varphi_4(x_2,x_3) - 48u_h(a_1-h,x_2,x_3) + 36u_h(a_1-2h,x_2,x_3) \\ & - 16u_h(a_1-3h,x_2,x_3) + 3u_h(a_1-4h,x_2,x_3)\bigr) \quad \text{on } \Gamma_4^h,\end{aligned} \tag{3.3}$$

$$\Phi_{ph}(u_h) = \frac{\partial\varphi_p}{\partial x_1} \quad \text{on } \Gamma_p^h, p = 2,3,5,6, \tag{3.4}$$

where u_h is the solution of finite difference problem (2.14).

Lemma 3.1 *We have the inequality*

$$\bigl|\Phi_{kh}(u_h) - \Phi_{kh}(u)\bigr| \le c_3 h^5\bigl(1 + |\ln h|\bigr), \quad k = 1,4, \tag{3.5}$$

where u_h is the solution of problem (2.14), *and u is the solution of problem* (2.1).

Proof It is obvious that $\Phi_{ph}(u_h) - \Phi_{ph}(u) = 0$ for $p = 2,3,5,6$. For $k = 1$, by (3.2) and Lemma 2.6 we have

$$\begin{aligned}\bigl|\Phi_{1h}(u_h) - \Phi_{1h}(u)\bigr| \le {}& \frac{1}{12h}\bigl(48\bigl|u_h(h,x_2,x_3) - u(h,x_2,x_3)\bigr| \\ & + 36\bigl|u_h(2h,x_2,x_3) - u(2h,x_2,x_3)\bigr| \\ & + 16\bigl|u_h(3h,x_2,x_3) - u(3h,x_2,x_3)\bigr|\end{aligned}$$

$$\begin{aligned} &+ 3\left|u_h(4h,x_2,x_3) - u(4h,x_2,x_3)\right|\bigr) \\ &\le c_5 h^5\bigl(1 + |\ln h|\bigr). \end{aligned}$$

The same inequality is also true when $k = 4$. □

Lemma 3.2 *We have the inequality*

$$\max_{(x_1,x_2,x_3)\in\Gamma_k^h} \left|\Phi_{kh}(u_h) - \Phi_k\right| \le c_4 h^4, \quad k = 1,4, \tag{3.6}$$

where Φ_{kh}, $k = 1,4$, *are defined by* (3.2), (3.3), *and* $\Phi_k = \frac{\partial u}{\partial x_1}$ *on* Γ_k, $k = 1,4$.

Proof From Lemma 2.1 it follows that $u \in C^{5,0}(\overline{R})$. Then, at the end points $(0,\nu h,\omega h) \in \Gamma_1^h$ and $(a_1,\nu h,\omega h) \in \Gamma_4^h$ of each line segment

$$\bigl\{(x_1,x_2,x_3) : 0 \le x_1 \le a_1, 0 < x_2 = \nu h < a_2, 0 < x_3 = \omega h < a_3\bigr\},$$

expressions (3.2) and (3.3) give the fourth-order approximation of $\frac{\partial u}{\partial x_1}$, respectively. From the truncation error formulas (see [11]) it follows that

$$\max_{(x_1,x_2,x_3)\in\Gamma_k^h} \left|\Phi(u) - \Phi_k\right| \le c_5 h^4, \quad k = 1,4. \tag{3.7}$$

By Lemma 3.1 and estimate (3.7), (3.6) follows. □

We consider the finite difference boundary value problem

$$\nu_h = \Re\nu_h \quad \text{on } R^h, \qquad \nu_h = \Phi_{jh} \quad \text{on } \Gamma_j^h, j = 1,2,\ldots,6, \tag{3.8}$$

where Ψ_{jh}, $j = 1,2,\ldots,6$, are defined by (3.2)-(3.4).

Theorem 3.3 *We have the estimate*

$$\max_{(x_1,x_2,x_3)\in\overline{R}^h} \left|\nu_h - \frac{\partial u}{\partial x_1}\right| \le ch^4, \tag{3.9}$$

where u is the solution of problem (2.1), *and ν_h is the solution of the finite difference problem* (3.8).

Proof Let

$$\varepsilon_h = \nu_h - \nu \quad \text{on } \overline{R}^h, \tag{3.10}$$

where $\nu = \frac{\partial u}{\partial x_1}$. From (3.8) and (3.10) we have

$$\begin{aligned} &\varepsilon_h = \Re\varepsilon_h + (\Re\nu - \nu) \quad \text{on } R^h, \\ &\varepsilon_h = \Phi_{kh}(u_h) - \nu \quad \text{on } \Gamma_k^h, k = 1,4, \qquad \varepsilon_h = 0 \quad \text{on } \Gamma_p^h, p = 2,3,5,6. \end{aligned}$$

We represent

$$\varepsilon_h = \varepsilon_h^1 + \varepsilon_h^2, \tag{3.11}$$

where

$$\varepsilon_h^1 = \Re\varepsilon_h^1 \quad \text{on } R^h, \tag{3.12}$$

$$\varepsilon_h^1 = \Phi_{kh}(u_h) - \nu \quad \text{on } \Gamma_k^h, k = 1,4, \qquad \varepsilon_h^1 = 0 \quad \text{on } \Gamma_p^h, p = 2,3,5,6; \tag{3.13}$$

$$\varepsilon_h^2 = \Re\varepsilon_h^2 + (\Re\nu - \nu) \quad \text{on } R^h, \qquad \varepsilon_h^2 = 0 \quad \text{on } \Gamma_j^h, j = 1,2,\ldots,6. \tag{3.14}$$

By Lemma 3.2 and by the maximum principle, for the solution of system (3.12)-(3.13), we have

$$\max_{(x_1,x_2,x_3)\in \overline{R}^h} \left|\varepsilon_h^1\right| \leq \max_{q=1,4} \max_{(x_1,x_2,x_3)\in \Gamma_q^h} \left|\Phi_{qh}(u_h) - \nu\right| \leq c_4 h^4. \tag{3.15}$$

The solution ε_h^2 of system (3.14) is the error of the approximate solution obtained by the finite difference method for problem (3.1) when on the boundary nodes Γ_{jh}, the approximate values are defined as the exact values of the functions Φ_j in (3.1). It is obvious that Φ_j, $j = 1,2,\ldots,6$, satisfy the conditions

$$\Phi_j \in C^{5,\lambda}(\Gamma_j), \quad 0 < \lambda < 1, j = 1,2,\ldots,6, \tag{3.16}$$

$$\Phi_\mu = \Phi_\nu \quad \text{on } \gamma_{\mu\nu}, \tag{3.17}$$

$$\frac{\partial_\mu^2 \Phi}{\partial t_\mu^2} + \frac{\partial_\nu^2 \Phi}{\partial t_\nu^2} + \frac{\partial_\mu^2 \Phi}{\partial t_{\mu\nu}^2} = 0 \quad \text{on } \gamma_{\mu\nu}. \tag{3.18}$$

Since the function $\nu = \frac{\partial u}{\partial x_1}$ is harmonic on R with the boundary functions Ψ_j, $j = 1,2,\ldots,6$, by (3.16)- (3.18) and Lemma 2.7 we obtain

$$\max_{(x_1,x_2,x_3)\in \overline{R}^h} \left|\epsilon_h^2\right| \leq c_6 h^4. \tag{3.19}$$

By (3.11), (3.15), and (3.19), inequality (3.9) follows. □

Remark 1 By Lemma 2.2 the sixth-order pure derivatives are bounded in R. Therefore, if we replace formulae (3.2) and (3.3) by the fifth-order forward and backward numerical differentiation formulae (see Chapter 2 in [12]), then by analogy with the proof of estimate (3.9) we obtain

$$\max_{(x_1,x_2,x_3)\in \overline{R}^h} \left|\nu_h - \frac{\partial u}{\partial x_1}\right| \leq ch^5\bigl(1 + |\ln h|\bigr).$$

4 Approximation of the pure second derivatives

We denote by $\omega = \frac{\partial^2 u}{\partial x_1^2}$. The function ω is harmonic on R, by Lemma 2.1 is continuous on $\overline{R}$, and is a solution of the following Dirichlet problem:

$$\Delta\omega = 0 \quad \text{on } R, \qquad \omega = \chi_j \quad \text{on } \Gamma_j, j = 1,2,\ldots,6, \tag{4.1}$$

where

$$\chi_\tau = \frac{\partial^2 \varphi_\tau}{\partial x_1^2}, \quad \tau = 2,3,5,6, \tag{4.2}$$

$$\chi_\nu = -\left(\frac{\partial^2 \varphi_\nu}{\partial x_2^2} + \frac{\partial^2 \varphi_\nu}{\partial x_3^2}\right), \quad \nu = 1,4. \tag{4.3}$$

Let ω_h be the solution of the finite difference problem

$$\omega_h = \Re\omega_h \quad \text{on } R^h, \qquad \omega_h = \chi_j \quad \text{on } \Gamma_j^h, j = 1,2,\ldots,6, \tag{4.4}$$

where χ_j, $j = 1,2,\ldots,6$, are the functions determined by (4.2) and (4.3).

Theorem 4.1 *We have the estimate*

$$\max_{\overline{R}^h} |\omega_h - \omega| \le ch^4, \tag{4.5}$$

where $\omega = \frac{\partial^2 u}{\partial x_1^2}$, *u is the solution of problem* (2.1), *and* ω_h *is the solution of the finite difference problem* (4.4).

Proof By the continuity of the function ω on $\overline{R}$, from (2.2)-(2.5) and (4.2), (4.3) it follows that

$$\chi_j \in C^{4,\lambda}(\Gamma_j), \quad 0 < \lambda < 1, j = 1,2,\ldots,6, \tag{4.6}$$

$$\chi_\mu = \chi_\nu \quad \text{on } \gamma_{\mu\nu}, \tag{4.7}$$

$$\frac{\partial^2 \chi_\mu}{\partial t_\mu^2} + \frac{\partial^2 \chi_\nu}{\partial t_\nu^2} + \frac{\partial^2 \chi_\mu}{\partial t_{\mu\nu}^2} = 0 \quad \text{on } \gamma_{\mu\nu}. \tag{4.8}$$

The boundary functions χ_j, $j = 1,2,\ldots,6$, in (4.1) by (4.6)-(4.8) satisfy all conditions of Lemma 2.7, from which the proof of the error estimate (4.5) follows. □

5 Numerical results

Let $R = \{(x_1,x_2,x_3) : 0 < x_i < 1, i = 1,2,3\}$, and let Γ be the boundary of R. We consider the following problem:

$$\Delta u = 0 \quad \text{on } R, \qquad u = \varphi(x_1,x_2,x_3) \quad \text{on } \Gamma_j, j = 1,2,\ldots,6, \tag{5.1}$$

where

$$\theta = \arctan\left(\frac{x_2}{x_1}\right),$$

$$\varphi(x_1,x_2,x_3) = \left(x_3 - \frac{1}{2}\right)^2 - \left(\frac{x_1^2 + x_2^2}{2}\right) + \left(x_1^2 + x_2^2\right)^{\frac{(6+\frac{1}{30})}{2}} \cdot \cos\left(6 + \frac{1}{30}\right)\theta$$

is the exact solution of this problem.

Table 1 Results for the solution

$\frac{1}{h}$	$\Vert u - u_h \Vert_{\overline{R}^h}$	E_u^m
$\frac{1}{8}$	1.3642E–9	54.95
$\frac{1}{16}$	2.4828E–11	62.64
$\frac{1}{32}$	3.9637E–13	63.14
$\frac{1}{64}$	6.2773E–15	63.77
$\frac{1}{128}$	9.8437E–17	

Table 2 First derivative approximation results with the fourth-order accurate formulae

$\frac{1}{h}$	$\Vert v - v_h \Vert_{\overline{R}^h}$	E_v^m
$\frac{1}{8}$	1.4993E–2	9.78
$\frac{1}{16}$	1.5327E–3	12.93
$\frac{1}{32}$	1.1854E–4	14.50
$\frac{1}{64}$	8.1771E–6	15.25
$\frac{1}{128}$	5.3605E–7	

Table 3 Second pure derivative approximation results

$\frac{1}{h}$	$\Vert w - w_h \Vert_{\overline{R}^h}$	E_w^m
$\frac{1}{8}$	9.8243E–7	15.21
$\frac{1}{16}$	6.4587E–8	16.21
$\frac{1}{32}$	3.9850E–9	16.36
$\frac{1}{64}$	2.4361E–10	16.37
$\frac{1}{128}$	1.4879E–11	

Table 4 First derivative approximation results with the fifth-order accurate formulae

$\frac{1}{h}$	$\Vert v - v_h \Vert_{\overline{R}^h}$	E_v^m
$\frac{1}{8}$	2.0469E–3	22.08
$\frac{1}{16}$	9.2725E–5	27.35
$\frac{1}{32}$	3.3903E–6	29.78
$\frac{1}{64}$	1.1382E–7	30.91
$\frac{1}{128}$	3.6823E–9	

Let U be the exact solution of the continuous problem, and U_h be its approximate values on $\overline{R}^h$. We denote $\Vert U - U_h \Vert_{\overline{R}^h} = \max_{\overline{R}^h} |U - U_h|$ and $E_U^m = \frac{\Vert U - U_{2^{-m}} \Vert_{\overline{R}^h}}{\Vert U - U_{2^{-(m+1)}} \Vert_{\overline{R}^h}}$.

In Tables 1 and 2, the maximum errors and the order of convergence of the approximate solution for different step sizes h are given, which corresponds to order of accuracy $O(h^6|\ln h|)$. In Tables 2 and 3, the results for the first and pure second derivatives of problem (5.1) are presented, which correspond to $O(h^4)$. The results presented in Table 4 show that the accuracy is improved by using the fifth-order accurate formulae for the same conditions imposed on the given boundary functions.

6 Conclusion

A highly accurate difference schemes are proposed and investigated under the conditions imposed on the given boundary values to approximate the solution of the 3D Laplace equation and its first and pure second derivatives on a cubic grid. The uniform convergence for the approximate solution at the rate of $O(h^6|\ln h|)$ and for the first and pure second derivatives at the rate of $O(h^4)$ is proved. It is shown that the accuracy for the approximate value of the first derivatives can be improved up to $O(h^5|\ln h|)$ for the same boundary functions by using the fifth-order formulae on some faces of the parallelepiped.

The obtained results can be used to justify finding the above-mentioned derivatives of the solution of 3D Laplace boundary value problems on domains described as unions or as intersections of a finite number of rectangular parallelepipeds by the difference method, using the Schwarz or Schwarz-Neumann iterations (see [13–19]).

Competing interests
The authors declare that they have no competing interests.

Authors' contributions
All authors contributed equally to the writing of this paper. All authors read and approved the final manuscript.

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