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Parallel algorithms for three-dimensional parabolic and pseudoparabolic problems with different boundary conditions*

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Abstract. In this paper, three-dimensional parabolic and pseudo-parabolic equations with classical, periodic and nonlocal boundary conditions are approximated by the full approximation backward Euler method, locally one dimensional and Douglas ADI splitting schemes. The stability with respect to initial conditions is investigated. We note that the stability of the proposed numerical algorithms can be proved only if the matrix of discrete operator can be diagonalized and eigenvectors make a complete basis system.

Parallel versions of all algorithms are constructed and scalability analysis is done. It is shown that discrete one-dimensional problems with periodic and nonlocal boundary conditions can be efficiently solved with similar modifications of the parallel Wang algorithm.

Keywords: parallel algorithms, three-dimensional paraboloic and pseudoparabolic equations, finite-difference method.

1 Introduction

Let us consider domain $D = (0,1)^3$. We formulate an initial boundary value parabolic problem with different local, periodic and nonlocal boundary conditions on different parts of the boundary:

$$\frac{\partial u}{\partial t} + \sum_{\alpha=1}^{3} A_\alpha u = 0, \quad X = (x_1, x_2, x_3) \in D,\ t > 0, \tag{1}$$

$$A_\alpha u := \frac{\partial}{\partial x_\alpha}\left(k_\alpha(x_\alpha)\frac{\partial u}{\partial x_\alpha}\right) - q_\alpha(x_\alpha)u, \quad \alpha = 1,2,3,$$

$$u(X,0) = \varphi(X), \quad X \in \bar{D} := [0,1]^3, \tag{2}$$

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$$
\begin{aligned}
&u(0,x_2,x_3,t)=0, \quad u(1,x_2,x_3,t)=0, \quad 0<x_2,x_3<1,\ t>0,\\
&u(x_1,x_2,x_3,t)=u(x_1,x_2+1,x_3,t), \quad X\in D,\ t>0;\\
&u(x_1,x_2,0,t)=\gamma_1 u(x_1,x_2,a,t), \quad u(x_1,x_2,1,t)=\gamma_2 u(x_1,x_2,b,t),\\
&\quad 0<x_1,x_2<1,\ t>0.
\end{aligned}
\tag{3}
$$

Here k_α, q_α and φ are given functions, which satisfy estimates

$$
k_\alpha \geqslant c_0>0, \quad q_\alpha \geqslant 0, \quad \alpha=1,2,3. \tag{4}
$$

We also consider a pseudoparabolic equation with the same initial and boundary conditions

$$
\left(I+\eta\sum_{\alpha=1}^{3}A_\alpha\right)\frac{\partial u}{\partial t}+\sum_{\alpha=1}^{3}A_\alpha u=0, \quad X=(x_1,x_2,x_3)\in D,\ t>0. \tag{5}
$$

The main aim of this paper is to construct efficient parallel algorithms to solve the given multidimensional problems. Two classes of integration methods are investigated. First, we use stability results obtained in [1], where unconditionally stable approximations of the pseudoparabolic problem were constructed only using the full approximation backward Euler method. Therefore this method is also used to construct parallel algorithms. The backward Euler method is combined with the Fast Fourier Transform (FFT). A set of one-dimensional systems with tridiagonal matrices are solved in the x_3 direction, where nonlocal boundary conditions are formulated. For pseudoparabolic problems an alternative to the backward or symmetrical Euler method can be three-level explicit schemes. Examples of such methods and spectral stability analysis results are presented in [1, 2]. The parallelization properties of such schemes are very favorable, but for all known explicit schemes the convergence of a discrete solution to the exact solution of pseudoparabolic problems is proved under severely limiting constraints on discretization parameters.

Second, splitting type schemes are constructed for the three-dimensional parabolic problem with different boundary conditions. We apply the LOD and Douglas ADI methods to develop parallel algorithms. Unconditional stability with respect to initial condition of both schemes is proved. The blocks of systems with tridiagonal matrices are solved by using modifications of Wang algorithm tailored to different types of boundary conditions. Scalability analysis of all parallel algorithms shows the efficiency of three-dimensional block distribution of the grid among processors. We note, that a new class of additive schemes is proposed in [3], the parallelization of these schemes can be done in a similar way.

The rest of this paper is organized as follows. In Section 2, the implicit backward Euler finite difference scheme is constructed for approximation of the parabolic (1) and pseudoparabolic (5) equations. The stability regions of the finite difference schemes are derived and investigated. A parallel version of this scheme is constructed by using the domain decomposition method. The parallel algorithm combines FFT and the Wang method for solving systems with tridiagonal matrices. Some results of the scalability analysis are presented. In Section 3, the three-dimensional parabolic problem with local, periodic

and nonlocal boundary conditions is solved by using LOD method. Stability of the finite difference scheme is investigated. A parallel version of the algorithm is constructed and the scalability analysis is done. In Section 4, the three-dimensional parabolic problem is solved by using the Douglas ADI method. Some final conclusions are done in Section 5.

2 Full approximation finite difference schemes

The domain $\bar{D}$ is covered by the discrete uniform grid

$$\bar{D}_h = \big\{X_{j_1,j_2,j_3} = (x_{\alpha,j_\alpha},\ \alpha = 1,\dots,3),\ x_{\alpha,j} = jh,\ j = 0,\dots,J\big\}, \quad Jh = 1,$$

$\bar{D}_h = D_h \cup \partial D_h$. Let ω_τ be a uniform time grid

$$\omega_\tau = \big\{t^n\colon\ t^n = n\tau,\ n = 0,\dots,N,\ N\tau = T\big\},$$

where τ is the time step. Although the constant time step is taken here, the following studies can be easily extended to the case when τ varies.

Let us introduce notations $j = (j_1, j_2, j_p)$, $\ell_\alpha = (\delta_{k,\alpha},\ k = 1,2,3)$. We consider numerical approximations U_j^n to the exact solution values $u_j^n = u(x_{j_1}, x_{j_2}, x_{j_3}, t^n)$ at the grid points $(X_j, t^n) \in \bar{D}_h \times \omega_\tau$. For functions defined on the grid, we introduce the forward and backward difference quotients with respect to x_α

$$\partial_{x_\alpha} U_j^n = \frac{U_{j+\ell_\alpha}^n - U_j^n}{h}, \qquad \partial_{\bar{x}_\alpha} U_j^n = \frac{U_j^n - U_{j-\ell_\alpha}^n}{h}$$

and the backward difference quotient with respect to t

$$\partial_{\bar{t}} U_j^n = \frac{U_j^n - U_j^{n-1}}{\tau}.$$

Let us define discrete approximations of differential operators $A_\alpha u$:

$$A_{h\alpha} U_j := -\partial_{x_\alpha}\big(k_\alpha(x_{\alpha,j_\alpha - 1/2})\partial_{\bar{x}_\alpha} U_j\big) + q_\alpha(x_{\alpha,j_\alpha}) U_j, \quad \alpha = 1,2,3.$$

Periodic boundary conditions (3) are approximated as follows:

$$U_{j_1,j_2,j_3} = U_{j_1,j_2+J,j_3}, \quad j_2 = -1, 0, \tag{6}$$

and nonlocal boundary conditions are approximated as

$$U_{j_1,j_2,0} = \gamma_1 U(x_{1,j_1}, x_{2,j_2}, a), \qquad U_{j_1,j_2,J} = \gamma_2 U(x_{1,j_1}, x_{2,j_2}, b), \tag{7}$$

where $U(x_{1,j_1}, x_{2,j_2}, a)$, $U(x_{1,j_1}, x_{2,j_2}, b)$ are linear interpolants of U_j at appropriate points. Finally, we introduce notation of discrete operators

$$\mathcal{A}_{h\alpha} U := \begin{cases} A_{h\alpha} U, & X_j \in D_h, \\ \text{b.c.}, & X_j \in \partial D_{h\alpha}, \end{cases}$$

where the domains D_h, $\partial D_{h\alpha}$, $\alpha = 1, 2, 3$, are defined as

$$\begin{aligned} D_h &= \{X_j\colon\ 0 < j_1, j_3 < J,\ 0 \leqslant j_2 < J\},\\ \partial D_{h1} &= \{X_j\colon\ j_1 = 0, J,\ 0 \leqslant j_2 < J,\ 0 < j_3 < J\},\\ \partial D_{h2} &= \{X_j\colon\ j_2 = -1, J,\ 0 < j_1, j_3 < J\},\\ \partial D_{h3} &= \{X_j\colon\ j_3 = 0, J,\ 0 < j_1 < J,\ 0 \leqslant j_2 < J\}. \end{aligned}$$

By using the backward Euler method the parabolic problem (1)–(3) is approximated by the following full approximation finite difference scheme (FAFDS):

$$\begin{aligned} &\partial_{\bar{t}} U^n + \sum_{\alpha=1}^{3} \mathcal{A}_{h\alpha} U^n = 0, \quad n > 0,\ X_j \in D_h,\\ &U^0(X_j) = \varphi(X_j), \quad X_j \in \bar{D}_h. \end{aligned} \tag{8}$$

Similarly the pseudoparabolic problem (5) is approximated by FAFDS

$$\begin{aligned} &\left(I + \eta \sum_{\alpha=1}^{3} \mathcal{A}_{h\alpha}\right) \partial_{\bar{t}} U^n + \sum_{\alpha=1}^{3} \mathcal{A}_{h\alpha} U^n = 0, \quad n > 0,\\ &U^0(X_j) = \varphi(X_j), \quad X_j \in \bar{D}_h. \end{aligned} \tag{9}$$

2.1 Stability analysis

We restrict to the analysis of the stability of discrete solutions with respect to the initial condition. The spectral method is used as the main technique. Here we apply the same stability analysis template as in [1]. It consists of two steps. First, the stability of a numerical time integration method is investigated. This analysis should be done only once and the result is defined in a form of simple stability conditions, which should be checked for given discrete operators. An example of such conditions can be the stability region in complex space. Second, eigenvalues of discrete operators of interest (including specific boundary conditions) should be determined and then the stability conditions of the given integration method can be applied.

It is well known that the stability region of the backward Euler integration method is defined by [4]

$$|1 + \tau\lambda| \geqslant 1, \tag{10}$$

where λ are eigenvalues of discrete operator $\mathcal{A}_h$. The stability region of the integration method (9) for a pseudoparabolic problem is defined in [1]

$$\big((2\eta + \tau)\lambda_R + 1\big)^2 + (2\eta + \tau)^2 \lambda_I^2 \geqslant 1, \tag{11}$$

where $\lambda = \lambda_R + \mathrm{i}\lambda_I$. Thus the stability region of the backward Euler method for the pseudoparabolic problem is larger than the stability region of the parabolic problem. We note that the first stability results on finite difference schemes applied to solve pseudoparabolic problems were obtained in [5, 6].

Now, according to the proposed template of the stability analysis, we should estimate the eigenvalues of the discrete operator $\mathcal{A}_h := \sum_{\alpha=0}^{3} \mathcal{A}_{h\alpha}$. Due to properties of coefficients in (1), boundary conditions and geometry D_h the eigenvectors of $\mathcal{A}_h$ can be written as $\Psi_k^1(x_1)\Psi_\ell^2(x_2)\Psi_m^3(x_3)$, where $\Psi_\ell^\alpha(x_\alpha)$ are eigenvectors of 1D restrictions of operators $\mathcal{A}_{h\alpha}$ (we are using the same notation for these operators). The properties of eigenvalue problems of $\mathcal{A}_{h1}$, $\mathcal{A}_{h2}$ are well-known. Both problems are symmetric, thus there exist complete orthonormal systems of eigenvectors

$$\mathcal{A}_{h\alpha}\Psi_\ell^\alpha = \lambda_\ell^\alpha \Psi_\ell^\alpha, \quad \ell \in S_\alpha,\ \alpha = 1, 2.$$

Let us assume that coefficients of the differential operators A_α are bounded functions and satisfy the ellipticity conditions (4). Then for the Dirichlet boundary conditions (i.e. $\alpha = 1$), the eigenvalues are real-valued, positive and bounded from above

$$0 < m_0 \leqslant \lambda_\ell^1 \leqslant \frac{m_1}{h^2}, \quad \ell \in S_1 := \{1, \dots, J-1\}.$$

For the periodic boundary conditions (i.e. $\alpha = 2$), the eigenvalues are real-valued, non-negative and bounded from above

$$0 \leqslant \lambda_\ell^2 \leqslant \frac{m_2}{h^2}, \quad \ell \in S_2 := \{0, \dots, J-1\}.$$

If the coefficient $q_2 > 0$, then all eigenvalues λ_ℓ^2 are also positive.

In the case of nonlocal boundary conditions, the matrix of discrete operator $\mathcal{A}_{h3}$ is non-normal. The spectral stability analysis is still can be used for such operators if these matrices can be diagonalized

$$\mathcal{A}_{h3} = \Psi^3 \Lambda (\Psi^3)^{-1}, \quad \Lambda = \operatorname{diag}\bigl(\lambda_\ell^3\bigr),\ \ell \in S_3,$$

and eigenvectors Ψ^3 make a complete basis system. In our paper, we always assume that this property is valid for the considered problems (see [7,8] for a spectral analysis of some discrete operators with various nonlocal boundary conditions).

Since the discrete operators $\mathcal{A}_{h\alpha}$ commute

$$\mathcal{A}_{h\alpha}\mathcal{A}_{h\beta} = \mathcal{A}_{h\beta}\mathcal{A}_{h\alpha}, \quad 1 \leqslant \alpha, \beta \leqslant 3,$$

the eigenvalue problem for the operator $\mathcal{A}_h$ is solved trivially:

$$\mathcal{A}_h \Psi_k^1 \Psi_\ell^2 \Psi_m^3 = \bigl(\lambda_k^1 + \lambda_\ell^2 + \lambda_m^3\bigr)\Psi_k^1 \Psi_\ell^2 \Psi_m^3, \quad (k, \ell, m) \in S_1 \times S_2 \times S_3.$$

Now we can use the derived general stability conditions (10) and (11). As an interesting conclusion, it follows from the given stability estimates that the backward Euler FAFDS is still may be stable even if the discrete operator $\mathcal{A}_{h3}$ (corresponding to nonlocal boundary conditions) has some negative eigenvalues. In this case, it is sufficient to guarantee that eigenvalues of operator $\mathcal{A}_{h1} + \mathcal{A}_{h2}$ compensate these negative eigenvalues of $\mathcal{A}_{h3}$.

2.2 Parallel FAFDS

In this section, we construct parallel versions of FAFDS (8) and (9). Let us assume that coefficients k_α, q_α, $\alpha = 1, 2$, are constant. Then the solution U^n can be written as the Fourier sum

$$U_j^n = \sum_{k\in S_1} \sum_{\ell\in S_2} \widehat{U}_{k\ell}^n(x_{3,j_3}) \Psi_k^1(x_{1,j_1}) \Psi_\ell^2(x_{2,j_2}).$$

A detailed analysis will be presented only for the pseudoparabolic problem (the parabolic problem can be solved in a similar way). Substituting these sums into (9), we obtain a sequence of independent discrete problems for spectral coefficients $\widehat{U}_{k\ell}^n$, $k \in S_1$, $\ell \in S_2$,

$$\big[\big(1 + \eta\big(\lambda_k^1 + \lambda_\ell^2\big)\big)\mathcal{I} + \mathcal{A}_{h,3}\big]\partial_{\bar{t}}\widehat{U}_{k\ell}^n + \big(\big(\lambda_k^1 + \lambda_\ell^2\big)\mathcal{I} + \mathcal{A}_{h,3}\big)\widehat{U}_{k\ell}^n = 0. \tag{12}$$

The parallel implementation of this FAFDS is done by using data parallel decomposition method. Let us assume that p processors are used in computations. Then the grid D_h is decomposed into p three-dimensional subgrids by using one-dimensional block distribution of the x_3 coordinate. Each subgrid

$$D_{h,\ell} = \left\{ X_{j_1,j_2,j_3} = (x_{\alpha,j_\alpha},\, \alpha = 1,2,3),\ 0 \leqslant x_{1,j_1}, x_{2,j_2} \leqslant 1,\ \frac{\ell}{p} < x_{3,j_3} \leqslant \frac{\ell+1}{p} \right\},$$
$$\ell = 0, \ldots, p-1,$$

has J^3/p computational points of the grid D_h and it is assigned to one processor. For such decomposition of the grid, the Fourier sums are computed by using the sequential FFT algorithm. The complexity of this part of the scheme is $\mathcal{O}(J^3 \log J)$ operations.

Now we consider the parallel algorithm for solving J^2 independent systems of linear equations (12). Modifying the method used in [9, 10], the solution $U_{k\ell}^n$ is expressed in the following form:

$$\widehat{U}_{k\ell}^n(x_{3j}) = c_{1,k\ell}^n V_{1,k\ell}^n(x_{3j}) + c_{2,k\ell}^n V_{2,k\ell}^n(x_{3j}) + W_{k\ell}^n(x_{3j}),$$

where $W_{k\ell}^n$ is a solution of the nonhomogeneous discrete boundary value problem with the Dirichlet boundary conditions

$$\begin{aligned} &\big[\big(1 + \eta\big(\lambda_k^1 + \lambda_\ell^2\big)\big)I + A_{h,3}\big]\frac{W_{k\ell}^n - \widehat{U}_{k\ell}^{n-1}}{\tau} + \big(\big(\lambda_k^1 + \lambda_\ell^2\big)I + A_{h,3}\big)W_{k\ell}^n = 0, \\ &W_{k\ell}^n(0) = 0, \qquad W_{k\ell}^n(1) = 0. \end{aligned} \tag{13}$$

Functions $V_{m,k\ell}^n$, $m = 1, 2$, are solutions of the following problems:

$$\begin{aligned} &\big[\big(1 + \eta\big(\lambda_k^1 + \lambda_\ell^2\big)\big)I + A_{h,3}\big]\frac{V_{m,k\ell}^n}{\tau} + \big(\big(\lambda_k^1 + \lambda_\ell^2\big)I + A_{h,3}\big)V_{m,k\ell}^n = 0, \\ &V_{m,k\ell}^n(0) = \delta_{m1}, \qquad V_{m,k\ell}^n(1) = \delta_{m2}, \end{aligned} \tag{14}$$

where δ_{ml} is the Kronecker delta. We note that if the discrete operator A_h does not depend on t^n, then functions $V_{m,k\ell}^n$, $m = 1, 2$, also do not depend on t^n. In this case, it is sufficient to solve problems (14) only once.

Coefficients $c^n_{1,k\ell}$, $c^n_{2,k\ell}$ are obtained by using the discrete nonlocal conditions

$$\begin{aligned}&\big(1-\gamma_1 V^n_{1,k\ell}(a)\big)c^n_{1,k\ell}-\gamma_1 V^n_{2,k\ell}(a)c^n_{2,k\ell}=\gamma_1 W^n_{k\ell}(a),\\&-\gamma_2 V^n_{1,k\ell}(b)c^n_{1,k\ell}+\big(1-\gamma_2 V^n_{2,k\ell}(b)\big)c^n_{2,k\ell}=\gamma_2 W^n_{k\ell}(b).\end{aligned}\tag{15}$$

Thus we must solve one/three blocks of independent systems of linear equations with tridiagonal matrices. It is well known that the complexity of solving one tridiagonal system of J equations by the sequential factorization algorithm is equal to $8J$ arithmetical operations. Thus the total complexity of solving problems (13) and (14) by the sequential algorithm is equal to $T_0 = cJ^3$ operations.

When J^2 systems are distributed between $p > 2$ processors, the Wang parallel factorization algorithm is used [9–11]. The main idea of this method is to reduce the given system to a new tridiagonal system of p equations, where each processor has only one equation. The obtained small system of linear equations is solved by using the sequential factorization algorithm.

Now we will present estimates of communication costs among processors. The implementation of the given parallel algorithm requires local send/receive of c_2J^2 data between neighbour processes, one global reduce operation of c_3J^2 data for the construction of the auxiliary system of linear equations by the master process and one global broadcast operation of J^2 elements to distribute the solution of this system to all processes.

At each time step two additional global broadcast operations are required to distribute $W^n_{k\ell}(a)$, $W^n_{k\ell}(b)$, which are needed to implement nonlocal boundary conditions (15). In order to minimize the influence of start-up costs, blocks of cJ^2 data are send in each message. Therefore we will neglect the start-up costs in our scalability analysis.

The total costs of the parallel algorithm (13)–(15) can be estimated as

$$T_p(J) = 17\frac{cJ^3}{p} + 8cpJ^2 + \big(\beta + R(p)\big)J^2,$$

where the factor 17 is included, since the complexity of the parallel Wang algorithm to solve a tridiagonal system of dimension J is $17J$ arithmetical operations. Here $R(p)$ depends on the algorithm used to implement the `MPI_ALLREDUCE` operation and the architecture of the computer. For different computers, this function can be estimated as

$$\gamma \log p \leqslant R(p) \leqslant \gamma p.$$

According to the definition of the isoefficiency function of a parallel algorithm, we must find the rate at which the problem size $W = 17cJ^3$ needs to grow with p for a fixed efficiency of the algorithm. Let $H(p, W) = pT_p - W$ be the total overhead of a parallel algorithm. Then the *isoefficiency* function $W = g(p)$ is defined by the implicit equation [11]

$$W = H(p, W).$$

We get the following nonlinear equation:

$$W = 8cp^2J^2 + \big(\beta + R(p)\big)pJ^2.$$

The asymptotical isoefficiency function can be obtained by analyzing the component that requires the problem size to grow at the fastest rate, thus it is sufficient to consider the nonlinear equation

$$W = \mu p^2 J^2.$$

After simple computations, taking into account that $W = \mathcal{O}(J^3)$, we get the following isoefficiency function:

$$W = \mathcal{O}\big(p^6\big).$$

Thus the number of grid points $J = \mathcal{O}(p^2)$ must grow quadratically with respect to the number of processors in order to guarantee a fixed efficiency of the parallel FAFDS algorithm. In computational experiments, a good recommendation on the maximal number processors is to determine it from the equation $J = (\beta + R(p))p/c$.

3 LOD scheme

In this section, we solve 3D parabolic problem (1) by using the following LOD scheme:

$$(\mathcal{I} + \tau \mathcal{A}_{h,k}) U^{n-1+k/3} = U^{n-1+(k-1)/3}, \quad k = 1, 2, 3. \tag{16}$$

It is well known that a simple direct definition of boundary conditions for internal vectors $U^{n-1+k/3}$ can lead to accuracy reduction. Thus some boundary correction techniques should be used. A general method to derive such corrections is to treat boundary points of the domain in the same way as the interior points [4, 12].

Let us assume that all boundary conditions are satisfied at time moment t^n, i.e.

$$\begin{aligned} &U^n = 0 \quad \text{on } \partial D_{h1}, \qquad U^n_{j_1,k,j_3} = U^n_{j_1,J+k,j_3}, \quad k = -1, 0, \quad \text{on } \partial D_{h2}, \\ &U^n_{j_1,j_2,0} = \gamma_1 U^n(x_{1,j_1}, x_{2,j_2}, a), \quad U^n_{j_1,j_2,J} = \gamma_2 U^n(x_{1,j_1}, x_{2,j_2}, b) \quad \text{on } \partial D_{h3}. \end{aligned} \tag{17}$$

Due to the definition of domains $D_{h\alpha}$, $\partial D_{h\alpha}$, $\alpha = 1, 2, 3$, and since the implicit backward Euler method is used to integrate internal one-dimensional problems, the boundary conditions should be corrected only for the first stage problem. After simple computations we get from (16) that

$$U^{n-2/3} = \big(\mathcal{I} + \tau(\mathcal{A}_{h,2} + \mathcal{A}_{h,3}) + \tau^2 \mathcal{A}_{h,2}\mathcal{A}_{h,3}\big) U^n.$$

Due to the definition of operators $\mathcal{A}_{h,\alpha}$, $\alpha = 2, 3$, this formula can be used on the whole boundary ∂D_{h1}. In the case of homogeneous boundary conditions (3), the correction is not required.

Next, we consider very briefly the stability of the LOD method. First, by using the spectral method we define the stability region of the LOD integration scheme. As a test model we consider

$$w'(t) + \lambda_1 w(t) + \lambda_2 w(t) + \lambda_3 w(t) = 0. \tag{18}$$

Applying the LOD method to (18) gives the stability factor

$$q = \frac{1}{(1+\tau\lambda_1)(1+\tau\lambda_2)(1+\tau\lambda_3)}.$$

Thus the LOD method is stable if all eigenvalues of operators $\mathcal{A}_{h,k}$ belong to the region

$$|1+\tau\lambda_k| \geqslant 1, \quad k = 1,2,3.$$

Note that these inequalities define sufficient stability conditions. For real eigenvalues λ_k, we get the well-known sufficient stability conditions $\lambda_k \geqslant 0$.

Now let us assume that $\lambda_1 > 0$ and $\lambda_2 > 0$ are real positive numbers and only $\lambda_3 = \lambda_{3R} + \mathrm{i}\lambda_{3I}$ can take complex values. Then the stability region for λ_3 is defined by

$$(1+\tau\lambda_{3R})^2 + (\tau\lambda_{3I})^2 \geqslant \frac{1}{1+\tau(\lambda_1+\lambda_2)^2}. \tag{19}$$

It is easy to get a sufficient stability condition

$$\lambda_{3R} \geqslant -1 + \frac{1}{1+\tau(\lambda_1+\lambda_2)}.$$

Now we can apply these stability results for LOD scheme (16). Again, it is assumed that operators $\mathcal{A}_{\alpha,h}$ commute, matrices can be diagonalized and eigenvalues and eigenvectors of operator $\mathcal{A}_h$ are defined by

$$\mathcal{A}_h \Psi_k^1 \Psi_\ell^2 \Psi_m^3 = \big(\lambda_k^1 + \lambda_\ell^2 + \lambda_m^3\big)\Psi_k^1\Psi_\ell^2\Psi_m^3, \quad (k,\ell,m) \in S_1 \times S_2 \times S_3.$$

Then we get from (19) that scheme (16) is stable if

$$\big(1+\tau\lambda_{mR}^3\big)^2 + \big(\tau\lambda_{mI}^3\big)^2 \geqslant \frac{1}{(1+\tau\min_{(k,\ell)\in S_1\times S_2}(\lambda_k^1+\lambda_\ell^2))^2}, \quad m \in S_3.$$

Parallel LOD algorithm. The parallel implementation of this LOD scheme is done by using data parallel decomposition method. Let p processors be distributed by using three dimensional virtual topology $p = p^{1/3} \times p^{1/3} \times p^{1/3}$, each processor has a unique label p_{m_1,m_2,m_3}, $m_\alpha = 0,\ldots,n^{1/3}-1$, $\alpha = 1,2,3$. Then the grid D_h is decomposed into p three-dimensional subgrids by using the three-dimensional block distribution technique. Each subgrid $D_{h,\ell}$, $\ell = (\ell_1,\ell_2,\ell_3)$, $\ell_\alpha = 0,\ldots,p^{1/3}-1$,

$$D_{h,\ell} = \left\{ X_{j_1,j_2,j_3} = (x_{\alpha,j_\alpha},\, \alpha = 1,2,3):\ \frac{\ell_\alpha}{p^{1/3}} < x_{\alpha,j_\alpha} \leqslant \frac{\ell_\alpha+1}{p^{1/3}} \right\}, \tag{20}$$

has J^3/p computational points of the grid D_h and it is assigned to processor p_{ℓ_1,ℓ_2,ℓ_3}. The parallel algorithm consists of three steps:

Step 1. Processors are divided into $p^{2/3}$ groups

$$P_{\ell_2,\ell_3} = \big\{p_{m,\ell_2,\ell_3},\ m = 0,\ldots,p^{1/3}-1\big\}, \quad \ell_2,\ell_3 = 0,\ldots,p^{1/3}-1.$$

Each group of processors independently and in parallel solves linear systems (16) for $k = 1$. The Wang algorithm is used to solve the blocks of tridiagonal systems. The total costs of this stage of the parallel LOD algorithm are estimated as

$$T_{p,1}(J) = 17\frac{c_1 J^3}{p} + 8c_1 p^{1/3}\left(\frac{J}{p^{1/3}}\right)^2 + \bigl(\beta + R\bigl(p^{1/3}\bigr)\bigr)\left(\frac{J}{p^{1/3}}\right)^2.$$

Step 2. Processors are divided into $p^{2/3}$ groups

$$P_{\ell_1,\ell_3} = \bigl\{p_{\ell_1,m,\ell_3},\ m = 0,\dots,p^{1/3}-1\bigr\}, \quad \ell_1,\ell_3 = 0,\dots,p^{1/3}-1.$$

Each group independently and in parallel solves linear systems (16) for $k = 2$.

Periodic boundary conditions are formulated for each subproblem. We again use a similar modification of the factorization algorithm as for the parallel FAFDS with nonlocal boundary conditions. In fact, periodic boundary conditions also can be considered as nonlocal conditions. The solution $U^{n-1/3}$ is expressed in the following form:

$$U_{j\ell}^{n-1/3}(x_{2k}) = c_{1,j\ell}^{n-1/3}V_{1,j\ell}^{n-1/3}(x_{2k}) + c_{2,j\ell}^{n-1/3}V_{2,j\ell}^{n-1/3}(x_{2k}) + W_{j\ell}^{n-1/3}(x_{2k}), \quad (21)$$

where $W_{j\ell}^{n-1/3}$ is a solution of the nonhomogeneous discrete boundary value problem with artificial Dirichlet boundary conditions

$$\begin{aligned} &(\mathcal{I} + \tau A_{h,2})W_{j\ell}^{n-1/3} = U_{j\ell}^{n-2/3},\\ &W_{j\ell}^{n-1/3}(x_{2,-1}) = 0, \qquad W_{j\ell}^{n-1/3}(x_{2,J}) = 0. \end{aligned} \quad (22)$$

Functions $V_{m,j\ell}^{n-1/3}$, $m = 1, 2$, are solutions of the following problems:

$$\begin{aligned} &\bigl(\mathcal{I} + \tau A_{h,2}\bigr)V_{m,j\ell}^{n-1/3} = 0,\\ &V_{m,j\ell}^{n-1/3}(x_{2,-1}) = \delta_{m1}, \qquad V_{m,j\ell}^{n-1/3}(x_{2,J}) = \delta_{m2}. \end{aligned} \quad (23)$$

We note that if the discrete operator $A_{h,2}$ does not depend on t^n, then functions $V_{m,j\ell}^n$, $m = 1, 2$, also do not depend on t^n. In this case, it is sufficient to solve problems (23) only once.

Coefficients $c_{1,j\ell}^{n-1/3}$, $c_{2,j\ell}^{n-1/3}$ are obtained by using the discrete periodic boundary conditions

$$\begin{aligned} &\bigl(1-V_{1,j\ell}^{n-1/3}(x_{2,J-1})\bigr)c_{1,j\ell}^{n-1/3} - V_{2,j\ell}^{n-1/3}(x_{2,J-1})c_{2,j\ell}^{n-1/3} = W_{j\ell}^{n-1/3}(x_{2,J-1}),\\ &-V_{1,j\ell}^{n-1/3}(x_{20})c_{1,j\ell}^{n-1/3} + \bigl(1 - V_{2,j\ell}^{n-1/3}(x_{20})\bigr)c_{2,j\ell}^{n-1/3} = W_{j\ell}^{n-1/3}(x_{20}). \end{aligned} \quad (24)$$

The Wang algorithm is used to solve the blocks of tridiagonal systems by $p^{1/3}$ processors of one group. The total costs of this stage of the parallel LOD algorithm can be estimated as

$$T_{p,2}(J) = 17\frac{c_2 J^3}{p} + 8c_2 p^{1/3}\left(\frac{J}{p^{1/3}}\right)^2 + \bigl(\beta + R\bigl(p^{1/3}\bigr)\bigr)\left(\frac{J}{p^{1/3}}\right)^2. \quad (25)$$

Step 3. Processors are divided into $p^{2/3}$ groups

$$P_{\ell_1,\ell_2} = \{p_{\ell_1,\ell_2,m},\ m = 0,\dots,p^{1/3}-1\}, \quad \ell_1,\ell_2 = 0,\dots,p^{1/3}-1.$$

Each group independently and in parallel solves linear systems (16) for $k = 3$.

The solution U^n is expressed in the following form:

$$U^n_{jk}(x_{3\ell}) = c^n_{1,jk}V^n_{1,jk}(x_{3\ell}) + c^n_{3,jk}V^n_{3,jk}(x_{3\ell}) + W^n_{j\ell}(x_{3\ell}), \tag{26}$$

where $W^{n-1/3}_{j\ell}$ is a solution of the nonhomogeneous discrete boundary value problem with artificial Dirichlet boundary conditions

$$\begin{aligned} &(\mathcal{I} + \tau A_{h,3})W^n_{jk} = U^{n-1/3}_{jk}, \\ &W^n_{jk}(x_{3,0}) = 0, \qquad W^n_{jk}(x_{3,J}) = 0. \end{aligned} \tag{27}$$

Functions $V^n_{m,jk}$, $m = 1, 2$, are solutions of the following problems:

$$\begin{aligned} &(\mathcal{I} + \tau A_{h,3})V^n_{m,jk} = 0, \\ &V^n_{m,jk}(x_{3,0}) = \delta_{m1}, \qquad V^n_{m,jk}(x_{3,J}) = \delta_{m2}. \end{aligned} \tag{28}$$

Coefficients $c^n_{1,jk}$, $c^n_{2,jk}$ are obtained by using nonlocal boundary conditions and solving the system (15). The costs of the third stage of the parallel LOD algorithm can be estimated similarly to the second stage, see (25).

The complexity of the full parallel LOD algorithm can be estimated as

$$T_p(J) = 17\frac{c_3J^3}{p} + 8c_3p^{1/3}\left(\frac{J}{p^{1/3}}\right)^2 + 3\big(\beta + R\big(p^{1/3}\big)\big)\left(\frac{J}{p^{1/3}}\right)^2. \tag{29}$$

From (29) the isoefficiency function $W = g(p)$ is defined by the implicit equation

$$W = 8c_3p^{2/3}J^2 + 3\big(\beta + R\big(p^{1/3}\big)\big)p^{1/3}J^2.$$

In order to find the asymptotical isoefficiency function, it is sufficient to consider the nonlinear equation

$$W = \mu p^{2/3}J^2.$$

After simple computations, taking into account that $W = \mathcal{O}(J^3)$, we get the isoefficiency function $W = \mathcal{O}(p^2)$. Thus the total number of grid points $J^3 = \mathcal{O}(p^2)$ must grow quadratically with respect to the number of processors in order to guarantee a fixed efficiency of the parallel LOD algorithm and this requirement is much weaker than the one obtained for the parallel FAFDS algorithm.

4 The Douglas method

In this section, 3D parabolic problem (1) is solved by using the Douglas ADI (DADI) method [4]

$$\begin{aligned}
&(\mathcal{I}+\tau\mathcal{A}_{h,1})U^{n-2/3} = (\mathcal{I}-\tau\mathcal{A}_{h,2}-\tau\mathcal{A}_{h,3})U^{n-1},\\
&(\mathcal{I}+\tau\mathcal{A}_{h,2})U^{n-1/3} = U^{n-2/3}+\tau\mathcal{A}_{h,2}U^{n-1},\\
&(\mathcal{I}+\tau\mathcal{A}_{h,3})U^{n} = U^{n-1/3}+\tau\mathcal{A}_{h,3}U^{n-1}.
\end{aligned} \tag{30}$$

We note that all internal vectors $U^{n-k/3}$, $k=1,2,3$, are consistent approximations of the exact solution u^{n+1}. Stages $k=2,3$ of the DADI scheme are required only to stabilize the explicit approximation at the first stage.

Let us assume that boundary conditions are satisfied at time moment t^n, i.e. equalities (17) are valid. The structure of discrete equations of the second and third stages of the algorithm is the same as for the LOD method. Thus the boundary correction is required only for the first stage problem. After simple computations we get from (30) that

$$U^{n-2/3} = U^n + \tau\big((\mathcal{A}_{h,2}+\mathcal{A}_{h,3})+\tau\mathcal{A}_{h,2}\mathcal{A}_{h,3}\big)\big(U^n-U^{n-1}\big).$$

Due to definition of operators $\mathcal{A}_{h,\alpha}$, $\alpha=2,3$, this formula can be used on the whole domain ∂D_{h1}. In the case of homogeneous boundary conditions (3), the correction is not required.

Applying the DADI method to the test model (18), gives the stability factor

$$q = \frac{1+\tau^2(\lambda_1\lambda_2+\lambda_1\lambda_3+\lambda_2\lambda_3)}{(1+\tau\lambda_1)(1+\tau\lambda_2)(1+\tau\lambda_3)}.$$

For real eigenvalues λ_k, we get the well-known sufficient stability conditions $\lambda_k \geqslant 0$, $k=1,2,3$.

Next, we will use stability results provided in [4]. It is proved that, for 3D problems, the DADI method is unconditionally stable (i.e. $|q|\leqslant 1$) if λ_1 and λ_2 are real nonnegative eigenvalues

$$\lambda_1,\lambda_2 \geqslant 0,$$

and only one term may have complex eigenvalues $\lambda_3=\lambda_{3R}+\mathrm{i}\lambda_{3I}$ with $\lambda_{3R}\geqslant 0$ and arbitrary large imaginary part λ_{3I}.

This result can be applied directly for the DADI scheme used to solve 3D parabolic problem (1). It is easy to check that operators $\mathcal{A}_{h,\alpha}$ commute, eigenvalues of operators $\mathcal{A}_{h,1}$, $\mathcal{A}_{h,2}$ are real and nonnegative. We note that such an analysis can be used only if the matrix of $\mathcal{A}_{h,3}$ can be diagonalized.

Parallel Douglas algorithm. The parallel implementation of DADI scheme is done by using data parallel decomposition method. Let p processors be distributed by using three dimensional virtual topology $p=p^{1/3}\times p^{1/3}\times p^{1/3}$. The definition of three stages of the parallel algorithm is similar to the parallel LOD algorithm. The differences arise only in formulation of the auxiliary problems for functions $W^{n-k/3}$, $k=0,1,2$. For example,

function $W^{n-1/3}$ satisfies the following discrete problem with artificial Dirichlet boundary conditions:

$$(\mathcal{I}+\tau A_{h,2})W_{j\ell}^{n-1/3} = U_{j\ell}^{n-2/3} + \tau \mathcal{A}_{h,2}U^{n-1},$$
$$W_{j\ell}^{n-1/3}(x_{2,-1}) = 0, \qquad W_{j\ell}^{n-1/3}(x_{2,J}) = 0.$$

The Wang algorithm is used to solve systems of tridiagonal linear equations. The total costs of the parallel DADI algorithm are defined by (29), therefore the scalability analysis gives the same results as for the parallel LOD algorithm.

5 Conclusions

In this paper, the three-dimensional parabolic and pseudoparabolic equations with local, periodic and nonlocal boundary conditions are approximated by the backward Euler, LOD and Douglas ADI finite difference schemes. The stability regions of all algorithms are investigated. We note that the stability of the proposed numerical algorithms can be proved only if the matrix of discrete operator can be diagonalized and eigenvectors make a complete basis system.

Parallel versions of the given algorithms are constructed and the scalability analysis is done. It is shown that the scalability of LOD and ADI methods is much better than the scalability of FAFDS, since for splitting type schemes the three-dimensional domain decomposition algorithm can be applied.

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