Performance of space-time coupled least-squares spectral element methods for parabolic problems

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Abstract. We study the performance of space-time coupled least-squares spectral element method (LSSEM) for parabolic initial boundary value problem (IBVP) for different values of element size $h$, the time step $k$, the degree $q$ in the time variable and the degree $p$ in each of the space variables. We divide the space domain into a number of shape regular quadrilaterals of size $h$ and the time step $k$ is proportional to $h^2$. Each shape regular quadrilateral will be mapped to the square $(-1,1) \times (-1,1)$. In each square the solution will be defined as a polynomial of degree $p$ for the space variables and degree $q$ for the time variable. For the $p$ version of the method $h$ remains fixed and $p$ increases, for the $h$-version of the method $p$ remains fixed and $h$ decreases but for the $hp$-version of the method $h$ decreases and at the same time $p$ also increases. In this method, $k$ is proportional to $h^2$ (say $k = ch^2$) and for the $p$-version of the method, $q$ is proportional to $p^2$ (say $q = c'p^2$). The performance of the method is discussed for different values of $c$ and $c'$. The method we discussed here is spectral in both space and time and are non-conforming.

1. Introduction

Pontaza and Reddy [8] proposed a space-time coupled spectral/hp least-squares finite element method (LSSEM) for parabolic initial boundary value problem (IBVP) for different values of element size $h$, the time step $k$, the degree $q$ in the time variable and the degree $p$ in each of the space variables. We divide the space domain into a number of shape regular quadrilaterals of size $h$ and the time step $k$ is proportional to $h^2$. Each shape regular quadrilateral will be mapped to the square $(-1,1) \times (-1,1)$. In each square the solution will be defined as a polynomial of degree $p$ for the space variables and degree $q$ for the time variable. For the $p$ version of the method $h$ remains fixed and $p$ increases, for the the $h$-version of the method $p$ remains fixed and $h$ decreases but for the $hp$-version of the method $h$ decreases and at the same time $p$ also increases. In this method, $k$ is proportional to $h^2$ (say $k = ch^2$) and for the $p$-version of the method, $q$ is proportional to $p^2$ (say $q = c'p^2$). The performance of the method is discussed for different values of $c$ and $c'$. The method we discussed here is spectral in both space and time and are non-conforming.
storing the mass and stiffness matrices. A preconditioner has been defined for the minimization problem which allows the problem to decouple [3, 4]. It has been shown that the time step \( k \) is proportional to square of the element size \( h \) (say \( k = ch^2 \)) and for the \( p \)-version of the method, \( q \) is proportional to \( p^2 \) (say \( q = c'p^2 \)). In this paper, we study the performance of space-time coupled LSSEM for parabolic IBVPs considering different values of element size \( h \), time step \( k \), the degree \( q \) in the time variable and the degree \( p \) in each of the space variables taking different values of \( c \) and \( c' \).

We now describe the organization of this paper; the problem and its discretization are introduced in Section 2, followed by a description of stability estimates in Section 3. The numerical scheme is discussed in Section 4 and error estimates is described in Section 5. Numerical results are presented in Section 6 and conclusions are drawn in Section 7.

2. The Problem and its Discretization

Let \( \Omega \) be a domain in \( \mathbb{R}^2 \) with smooth boundary \( \Gamma = \bigcup_{i=1}^{N} \Gamma_i \), where \( \Gamma_i \) are smooth closed curves. Let \( \mathcal{D} \) denote a subset of the set \( \{1, 2, 3, ..., N\} \) and \( \mathcal{N} \) denote the set \( \{1, 2, 3, ..., N\} \setminus \mathcal{D} \). We shall denote the Dirichlet part of the boundary by \( \Gamma^[0] \), where \( \Gamma^[0] = \bigcup_{i\in\mathcal{D}} \Gamma_i \) and the Neumann part of the boundary by \( \Gamma^[1] \), where \( \Gamma^[1] = \bigcup_{i\in\mathcal{N}} \Gamma_i \). The space domain \( \Omega \) is divided into a quasi-uniform mesh of \( n_e \) curvilinear rectangles \( \{\omega_l\}_{1\leq l\leq n_e} \) as described in [3].

Let
\[
Lu = u_t - \sum_{i,j=1}^{2} (A_{ij}(x,t)u_{x_j})_{x_i} - \sum_{i=1}^{2} B_i(x,t)u_{x_i} - E(x,t)u,
\]
be a strongly parabolic differential operator. Consider the initial boundary value problem
\[
Lu = F \quad \text{in} \quad \Omega \times (0, T) ,
\]
with Dirichlet boundary conditions
\[
u(\Gamma, \Omega) \times (0, T) \quad \text{for} \quad i \in \mathcal{D},
\]
and Neumann boundary conditions
\[
\left( \frac{\partial u}{\partial \nu} \right)_A = g_i \quad \text{on} \quad \Gamma_i \times (0, T) \quad \text{for} \quad i \in \mathcal{N} ,
\]
and initial condition
\[
u(\Omega \times \{0\}).
\]

Here \( (\frac{\partial u}{\partial \nu})_A \) denotes the co-normal derivative of \( u \), defined as
\[
(\frac{\partial u}{\partial \nu})_A = \sum_{i=1}^{2} \nu_i A_{ij} \frac{\partial u}{\partial x_j},
\]
where \( \nu = (\nu_1, \nu_2)^\top \) denotes the normal to the boundary of \( \Omega \).

3. Stability Estimates

We define a smooth function \( (N_l)^{-1} \) that maps each curvilinear rectangle \( \tilde{\omega}_l \) \( (1 \leq l \leq n_e) \) in \( y \)-coordinates to the unit square \( S = (0, 1) \times (0, 1) \) in the \( \xi_1\xi_2 \) plane. In the unit square \( S \), the spectral element functions \( \tilde{u}_{ij}(\xi_1, \xi_2, s) \) is defined to be a polynomial of degree \( p \) in each of the space variable \( \xi_1 \) and \( \xi_2 \) and of degree \( q \) in the time variable \( s \) as:
\[
\tilde{u}_{ij}(\xi_1, \xi_2, s) = \sum_{i=0}^{p} \sum_{j=0}^{q} \sum_{k=0}^{m} e_{i,j,k}^{(m)} \xi_1^i \xi_2^j (s - m)^k , \quad m \leq s < m + 1 ,
\]
where \( l,m \) are coefficients. Now
\[
\bar{u}_l(\xi_1, \xi_2, s) = \bar{u}_l(N_i^{-1}(y_1, y_2), s) = \bar{u}_l(y_1, y_2, s).
\]

Note that \( \bar{u}_l(\xi_1, \xi_2, s) \) can be discontinuous at the plane \( s = m \), where \( m \) is a positive integer. Henceforth the open interval \((m, m + 1)\) will be denoted by \( I_m \). Let
\[
\| \tilde{v}_l \|_{L^2}^2 = \int_{S \times \{n+\}} \| \tilde{v}_l \|^2 J_l d\xi,
\]
\[
\int_{\tilde{\omega}_l \times I_n} \| \mathcal{L} \tilde{v}_l \|^2 dy ds = \int_{S \times I_n} \| \mathcal{L} \tilde{v}_l \|^2 J_l d\xi ds,
\]
\[
\sum_{i,j=1}^2 \int_{\tilde{\omega}_l \times \{n+\}} (\bar{v}_l)_y \alpha_{ij}(\bar{v}_l)_y dy = \sum_{i,j=1}^2 \int_{S \times \{n+\}} (\bar{v}_l)_{\xi_i} (\mathcal{A}_l)_{ij}(\bar{v}_l)_{\xi_j} d\xi.
\]

Here \( \| . \|^2 \) denotes the usual \( L^2 \) norm in \( \mathbb{R}^d \), \( \mathcal{L} \) denotes the differential operator \( \mathcal{L} \) in \( \xi_1, \xi_2 \) and \( s \) coordinates and \( (\mathcal{A}_l)_{ij} \) are matrices. Moreover, \( J_l \) denotes the Jacobian of the map \( N_l \) from \( S \) to \( \tilde{\omega}_l \). Let \( \mathcal{L}_l^a \) be the differential operator whose coefficients are polynomials of degree \( p \) in each variable \( \xi_1 \) and \( \xi_2 \) and of degree \( q \) in \( s \). These coefficients of \( \mathcal{L}_l^a \) are orthogonal projections of the corresponding coefficients of the differential operator \( \mathcal{L} \) into the space of polynomials with respect to the usual norm in \( H^2(S \times I_n) \) [5, 6, 7]. Let \( \tilde{J}_l \) be the unique polynomial which is the orthogonal projection of \( J_l \) into the space of polynomials of degree \( p \) in each variable \( \xi_1 \) and \( \xi_2 \) with respect to the usual norm in \( H^2(S) \). Then
\[
\int_{\tilde{\omega}_l \times I_n} \| \mathcal{L} \tilde{v}_l \|^2 dy ds = \int_{S \times I_n} \| \mathcal{L}_l^a \tilde{v}_l \|^2 \tilde{J}_l d\xi ds
\]
up to an error term which is negligible [2, 11, 10]. The stability estimates of the method has been established in [3].

4. Numerical Scheme

Let \( F_l(\xi_1, \xi_2, s) = F(N_l(\xi_1, \xi_2) h, sk) \) and \( \hat{F}_l(\xi_1, \xi_2, s) \) be the unique polynomial which is the orthogonal projection of \( F_l(\xi_1, \xi_2, s) \) onto the space of polynomials of degree \( p \) in \( \xi_1 \) and \( \xi_2 \) and \( q \) in \( s \) with respect to the usual inner product in \( L^2(S \times I_n) \). Similarly, we can define \( \hat{f}_l(\xi_1, \xi_2) \) and \( \hat{g}_l(\xi_2, s) \).

Consider that the solution up to the \( m \)-th time step, where \( m \) is an integer, is already obtained. As in [3] in order to obtain the solution at the next time step \((m + 1)\), consider the
unique polynomials \( \{ \tilde{u}_l(\xi, s) \}_{1 \leq l \leq n_e} \) which minimizes the functional

\[
\begin{align*}
r^{(m)}(\{ \tilde{u}_l(\xi, s) \}_{1 \leq l \leq n_e}) & = \sum_{l=1}^{n_e} \left( \int_{S \times \{ m^+ \}} \| \tilde{u}_l - \tilde{u}_l(\xi, m^-) \|^2 \tilde{J}_l d\xi \right) \\
& + \sum_{i,j=1}^{2} \int_{S \times \{ m^+ \}} \left( \tilde{u}_l - \tilde{u}_l(\xi, m^-) \right) \xi \left( \xi \tilde{A} \right)_{ij} \left( \tilde{u}_l - \tilde{u}_l(\xi, m^-) \right) d\xi \\
& + \frac{c (\ln p)^2}{h^2} \left( \sum_{l=1}^{n_e} \left\| \left( \mathcal{L}_l^a \tilde{u}_l - \tilde{F}_l \right) \right\|_{S \times I_m}^2 \right) \\
& + \sum_{\gamma_n \subseteq \Omega} \left( \| \tilde{v} \|^2_{(0,3/4), \gamma_n \times I_m} + \sum_{i=1}^{2} \left( \| \tilde{v}_{yi} \|^2_{(1/2,1/4), \gamma_n \times I_m} \right) \\
& + \sum_{\gamma_m \subseteq \Gamma_{l,i} \subseteq \partial \Omega} \left( \| \tilde{v} - \tilde{g}_l \|^2_{(0,3/4), \gamma_m \times I_m} + \| \tilde{v}_{\gamma} \|^2_{(1/2,1/4), \gamma_m \times I_m} \right) \right) \\
& + \sum_{\gamma_m \subseteq \Gamma_{l,i} \subseteq \partial \Omega} \left( \| \tilde{v}_\gamma \|^2_{(1/2,1/4), \gamma_m \times I_m} \right) \quad (5)
\end{align*}
\]

over all \( \{ \tilde{u}_l \}_{1 \leq l \leq n_e} \). Here, \( c \) is a constant which needs to be chosen sufficiently large. In most of our test problems we have taken \( c=1 \). Moreover, \( h \) denotes the mesh width in the spatial direction as has been defined earlier.

The above formulation amounts to finding a solution that minimizes the sum of the squares in appropriate Sobolev norms of the residuals in the partial differential equations, initial and boundary conditions and jumps in the functions and its derivatives at inter-element boundaries. Solution to the least-squares problem can be found using the pre-conditioned conjugate gradient method (PCGM) for the normal equations.

5. Error Estimates

It has been shown in [3] that if \( \{ w_l \}_{1 \leq l \leq n_e} \) be the approximate numerical solution of the IBVP in (2) then for \( h \)-version of the method the error \( (u - w) \), between the exact solution \( u \) and the approximate numerical solution \( w \), satisfies the estimate,

\[
\left( \sum_{l=1}^{n_e} \sum_{m=1}^{M} \| (u - w_l)(x, t) \|^2_{(2,1), \omega_l \times I_m} \right)^{1/2} \leq c_1 h^{2q-1} \| u \|_{(2q+6,q+3), \Omega \times (0,T)} \quad (6)
\]

for smooth \( u \), provided \( p = 2q + 1 \) and \( k \) is proportional to \( h^2 \) and for \( p \)-version of the method it has been shown that the error \( (u - w) \) follows the estimate,

\[
\left( \sum_{l=1}^{n_e} \sum_{m=1}^{M} \| (u - w_l)(x, t) \|^2_{(2,1), \omega_l \times I_m} \right)^{1/2} \leq c_2 e^{-c_3 \phi h^{c_4 p}}, \quad (7)
\]

provided \( u \in \mathcal{D}_{2,1} \left( \Omega \times [0, T] \right) \) and \( q \) is proportional to \( p^2 \). Here \( c_1, c_2, c_3, c_4 \) are constants and \( \mathcal{D}_{2,1} \left( \Omega \times [0, T] \right) \) is the Gevrey Space defined in [9, 3]. For \( h \)-version of the method we take \( k = ch^2 \) and for \( p \)-version of the method we take \( q = \lceil c' p^2 \rceil \). Here \( \lceil x \rceil \) is the ceiling function which is the smallest integer greater than \( x \). In this paper we discuss the performance of the method for different values \( c \) and \( c' \).
6. Computational Results

We present the results of the numerical simulations to show the performance of the method for different values of $c$ and $c'$. Note that the error between the exact and numerical solution is given in the left hand side of equations (6) and (7).

**Example (1D problem with variable coefficient and Dirichlet boundary condition):**

Consider the following one dimensional IBVP with variable coefficient

$$u_t - (0.1e^{2xt}u_x)_x - 0.2\sin(3\pi(x+t))u = F \quad \text{in} \quad \Omega \times (0,T),$$  

with Dirichlet boundary condition

$$Bu = g \quad \text{in} \quad \partial\Omega \times (0,T),$$

and initial condition

$$u = f \quad \text{in} \quad \Omega \times \{0\}. $$

![Graph](image_url)

**Figure 1.** (a) Error and (b) Iterations as functions of $p$ when $q = c'r^2$ with fixed $k=ch^2$.

where the spatial domain $\Omega = (0,1)$ and the time interval $(0,T) = (0,1)$. The data $f$, $g$ and $F$ are so chosen that the exact solution is

$$u(x,t) = \cos(6\pi(x+t)).$$

The convergence of the spectral element method is examined for different values of $c'$ with fixed $h = 0.5$ and fixed $k = ch^2$ as $p$ increases from 1 to 4 when $q = c'p^2$ for the $p$-version of the method. In Figures 1(a) and 1(b), the error and total number of iterations of the PCGM are plotted against $p$ respectively for different values of $c'$. Here the vertical $y$-axis is plotted in log-scale. It is clear from the graphs that the error profiles decay exponentially in $p$. Moreover it is clear from the graph that as the value of $c'$ decreases from 1 to $\frac{1}{4}$ total number of iterations of the PCGM are also decreases but error between the exact and numerical solution remains almost same. For the $h$-version of spectral element method we analyze the convergence for different values of $c$ when $k=ch^2$ with fixed $p = 2q + 1$ as $h$ decreases from 0.5 to 0.1. Figures 2(a), 2(b) and 2(c) show the error profiles for $q = 1$, $q = 2$ and $q = 3$ respectively and Figures 3(a), 3(b) and 3(c) show the total number of iterations of the PCGM for $q = 1$, $q = 2$ and $q = 3$ respectively. It is observed that as $c$ increases from 1 to 4, the error between the exact and numerical solution also increases slowly but total number of iterations of the PCGM decreases.
that as the value of $p$ against $T$ for a time interval $(0, T)$.

Choose $\Omega = (0, 1)$.

Example 2 (1D problem with Neumann boundary condition):

Choose $\Omega = (0, 1)$. Consider the initial boundary value problem

$$u_t - u_{xx} = F \quad \text{in} \quad \Omega \times (0, T),$$

with Neumann boundary conditions

$$-\frac{\partial u}{\partial n}(0, t) = \cos(t) = g_1 \quad \text{and} \quad \frac{\partial u}{\partial n}(1, t) = e \cos(t) = g_2$$

and initial condition

$$u = f \quad \text{on} \quad \Omega \times \{0\}.$$

for a time interval $(0, T)$, where $T=1$. The data $f$, $g$ and $F$ are chosen so that the solution is

$$u(x, t) = e^x \cos(t).$$

In Figures 7(a) and 7(b), the error and total number of iterations of the PCGM are plotted against $p$ respectively for different values of $c'$ keeping $h = 0.5$ fixed. It is clear from the graphs that as the value of $c'$ decreases from 1 to $\frac{1}{2}$ total number of iterations of the PCGM are also decreases but error between the exact and numerical solution remains almost same. Figures 8(a), 8(b) and 8(c) show the error profiles for different values of $c$ when $k=ch^2$ with fixed $q = 3$, $q = 4$.
and $q = 5$ respectively as $h$ decreases from 0.5 to 0.1 and Figures 9(a), 9(b) and 9(c) show the total number of iterations of the PCGM for $q = 3$, $q = 4$ and $q = 5$ respectively. It is observed that as $c$ increases from 1 to 4, both the error, between the exact and numerical solution, and total number of iterations of the PCGM decreases.

**Figure 5.** Error as functions of $h$ when $k = ch^2$ for (a) $q = 3$, (b) $q = 4$ and (c) $q = 5$ with $p = 2q + 1$.

**Example 3 (1D problem with Robin boundary condition):**

Here we shall consider the following initial boundary value problem

$$u_t - u_{xx} = F \quad \text{in} \quad \Omega \times (0, T),$$

with Robin boundary conditions

$$u(0, t) - \frac{\partial u}{\partial n}(0, t) = g_1 \quad \text{and} \quad u(1, t) + \frac{\partial u}{\partial n}(1, t) = g_2$$

and initial condition

$$u = f \quad \text{on} \quad \Omega \times \{0\}.$$  

for a time interval $(0, 1)$. The data $f$, $g$ and $F$ are chosen so that the solution is

$$u(x, t) = e^x \cos(t).$$
Figure 6. Iterations as functions of $h$ when $k=ch^2$ for (a) $q=3$, (b) $q=4$ and (c) $q=5$ with $p = 2q + 1$.

Figure 7. (a) Error and (b) Iterations as functions of $p$ for Robin boundary condition when $q = c'p^2$ with fixed $k=ch^2$.

It is clear from Figures 7(a) and 7(b) that for the $p$-version of the method, as the value of $c'$ decreases from 1 to $\frac{1}{4}$ total number of iterations of the PCGM are also decreases but error between the exact and numerical solution remains almost same. Moreover, Figures 8(a), 8(b), 8(c), 9(a), 9(b) and 9(c) show that for the $h$-version of the method, as $c$ increases from 1 to 4, both errors, between the exact and numerical solution, and total number of iterations of the PCGM decrease.

7. Conclusion
We proved in [3] that $k$ is proportional to $h^2$ (say $k = ch^2$) and for the $p$-version of the method, $q$ is proportional to $p^2$ (say $q = c'p^2$). In this paper we have investigated the performance of LSSEM for the solution of parabolic IBVP on smooth domains using parallel computers with different values of $c$ and $c'$. It has been observed that the total number of iterations in PCGM to obtain the approximate solution decreases when the value of $c'$ decreases from 1 to $\frac{1}{4}$. Moreover for the Dirichlet boundary condition, the error between the exact and numerical solution, increases very slowly. However, for Neumann and Robin boundary conditions, the errors between the exact and numerical solution, and the total number of iterations of the PCGM decrease as the value of $c$ increases from 1 to 4.
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