A well-conditioned direct parallel-in-time (PinT) solver for evolutionary PDEs

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Outline

1. Review of two parallel-in-time (PinT) algorithms
   - Iterative: Parareal, MGRIT, Space-time Multigrid, PFASST
   - Direct: space-time solver, ParaExp, Laplace Transform

2. ParaDIAG: diagonalization-based PinT algorithms
   - As preconditioner
   - As direct solver

3. Numerical examples

4. Summary
1D Heat PDE: time-stepping with Backward Euler scheme

\[ y_t(x,t) = y_{xx}(x,t), \quad (x,t) \in (0,1) \times (0,T], \]
\[ y(0,t) = y(1,t) = 0, \quad t \in [0,T], \quad \text{(Boundary Condition)} \]
\[ y(x,0) = f(x), \quad x \in (0,1). \quad \text{(Initial Condition)} \]

Uniform space-time mesh \( \{x_i = ih, t_m = m\tau\} \) with \( h = 1/(M+1), \tau = T/N_t. \)

Let \( y_i^m \approx y(x_i,t_m) \) and \( y_i^0 = f(x_i). \)

The backward Euler scheme reads:

\[
\frac{y_i^m - y_i^{m-1}}{\tau} = \frac{y_{i-1}^m - 2y_i^m + y_{i+1}^m}{h^2},
\]

Let \( y_h^m = [y_1^m, y_2^m, \cdots, y_M^m]^T \), it gives sequential time-stepping (\( N_t \) steps \( m = 1, 2, \cdots, N_t \))

\[
\left( \frac{1}{\tau} I_h + A_h \right) y_h^m = \frac{1}{\tau} y_h^{m-1},
\]

where \( A_h = \frac{1}{h^2} \text{tridiag}(-1, 2, -1) \in \mathbb{R}^{M \times M} \) is sparse.
Goal: to compute $y(x, t)$ faster with parallel machines?

Choose the IC $f(x) = 1_{[0.4, 0.6]}(x)$ and $T = 0.5$.

Figure 1: Simulation of solving 1D heat eq by backward Euler time-stepping.
Consider the (semi-discretized) ODEs IVP over \([0, T]\):

\[
\begin{align*}
u'(t) &= f(u), & u(0) &= u_0 \in \mathbb{R}^M.
\end{align*}
\] (3)

Define two propagation (time-stepping) operators for (3):

\begin{itemize}
  \item \(G(t_2, t_1, u_1)\) is a \textbf{coarse/cheap} approx. to \(u(t_2)\) with IC \(u(t_1) = u_1\);
  \item \(F(t_2, t_1, u_1)\) is a \textbf{fine/expensive} approx. to \(u(t_2)\) with IC \(u(t_1) = u_1\);
\end{itemize}

Partition \((0, T]\) into \((T_{n-1}, T_n]\) with \(0 = T_0 < T_1 < T_2 < \cdots < T_N = T\). The parareal algorithm initializes \(U^0_n \approx u(T_n)\) by coarse time-stepping:

\[
\begin{align*}
U^0_0 &= u_0; & U^0_{n+1} &= G(T_{n+1}, T_n, U^0_n), & n = 0, 1, \ldots, N - 1,
\end{align*}
\] (4)

and then runs the \(k\)-th correction iteration (marching \(n = 0, 1, 2, \cdots\) and \(U^{k+1}_0 = u_0\))

\[
U^{k+1}_{n+1} = \underbrace{F(T_{n+1}, T_n, U^k_n)}_{\text{marching in parallel}} + \underbrace{G(T_{n+1}, T_n, U^{k+1}_n)}_{\text{marching in serial}} - \underbrace{G(T_{n+1}, T_n, U^k_n)}_{\text{already computed}}.
\] (5)
The illustration and limitation of parareal algorithm

Figure 2: The initialization and 1st iteration of parareal algorithm (red $U^k_n$ are computed in serial and blue $F$ are performed in parallel). See www.unige.ch/~gander/poly.pdf

- It always converges to the fine approximation after finite $n$ steps: $U^k_n = F(T_n, 0, u_0)$ for $k \geq n$. But no speedup if needs $k \geq n$.
- The parallel efficiency $< 1/K$ with $K$ being total iteration number.
- Fast linear convergence for parabolic eq, but poor or no convergence for hyperbolic eq. [Gander and Vandewalle, 2007] (can be improved)
A fair comparison for a 2D heat eq using hypre and XBraid [Falgout et al., 2017].

- multigrid-reduction-in-time algorithm (MGRIT) [Falgout et al., 2014]
  - a multilevel extension of the parareal algorithm (2-level).
- space-time multigrid method (STMG) 📝 fastest
  [Gander and Vandewalle, 2007, Gander and Neumüller, 2016]
- waveform relaxation multigrid (WRMG–CR) [Horton et al., 1995]
Couple all the $N_t$ time steps in (2) together:

$$-\frac{1}{\tau} y_h^{m-1} + \left( \frac{1}{\tau} I_h + A_h \right) y_h^m = 0, \quad m = 1, 2, \cdots, N_t$$

(6)

to get an all-at-once system (note IC gives $y_h^0 = f_h$)

$$
\begin{bmatrix}
\frac{1}{\tau} I_h + A_h \\
-\frac{1}{\tau} I_h \\
\vdots \\
-\frac{1}{\tau} I_h \\
\frac{1}{\tau} I_h + A_h \\
\vdots \\
-\frac{1}{\tau} I_h \\
\end{bmatrix}
\begin{bmatrix}
y_1^h \\
y_2^h \\
\vdots \\
y_n^h \\
0
\end{bmatrix}
= 
\begin{bmatrix}
\frac{1}{\tau} f_h \\
0 \\
\vdots \\
0
\end{bmatrix}
$$

(7)

By separating time and space (in Kronecker product $\otimes$), rewrite into

$$L y_h := (B \otimes I_h + I_t \otimes A_h) y_h = b_h, \quad B = \frac{1}{\tau} \begin{bmatrix} 1 & -1 & 1 \\ 1 & \ddots & \ddots \\ -1 & \ddots & 1 \\ \end{bmatrix}$$

(8)

where $I_h, I_t$ are identity matrices. Clearly, $B$ (as a Jordan block) is not diagonalizable.
A tensor-product direct PinT solver [Maday and Rønquist, 2008]

But, if all time steps sizes $\tau_j$ are all different, then it is indeed diagonalizable:

$$
\hat{B} = \begin{bmatrix}
\frac{1}{\tau_1} & 1/\tau_2 \\
-1/\tau_2 & 1/\tau_2 \\
\vdots & \ddots & \ddots \\
-1/\tau_N & 1/\tau_N 
\end{bmatrix}
\overset{\text{diagonalizable}}{\Rightarrow}
VDV^{-1},
$$

(9)

which leads to a diagonalization-based PinT direct solver by inverting

$$
\hat{L} := \left( \hat{B} \otimes I_h + I_t \otimes A_h \right) = (V \otimes I_h) \left( D \otimes I_h + I_t \otimes A_h \right) (V^{-1} \otimes I_h).
$$

(10)

Since $(D \otimes I_h + I_t \otimes A_h)$ is block-diagonal, inverting $y_h = \hat{L}^{-1} b_h$ in three steps:

\[
\begin{align*}
\begin{cases}
  g = (V^{-1} \otimes I_h) b_h, & \text{step-(a),} \\
  (\lambda_j I_h + A_h) w_j = g_j, \ j = 1, 2, \ldots, n, & \text{step-(b), parallel in time,} \\
  y_h = (V \otimes I_h) w, & \text{step-(c),}
\end{cases}
\end{align*}
\]

(11)

where $D = \text{diag}(\lambda_1, \ldots, \lambda_n)$, $w = (w_1^T, \ldots, w_n^T)^T$ and $g = (g_1^T, \ldots, g_n^T)^T$. 

The limitation of $\hat{B}$-based direct PinT solver

Key limitation:

1. The roundoff errors of $y_h$ (due to diagonalization) are proportional to

$$\text{Cond}_2(V) := \|V\|_2\|V^{-1}\|_2.$$ 

2. With optimized $\tau_j = (1 + \varepsilon)^j$, $\text{Cond}_2(V)$ shows exponential growth, which limits $N_t \lesssim 25$ for stable solutions. [Gander et al., 2016, Gander et al., 2019]

3. The restriction $N_t \lesssim 25$ implies only $\sim 25$ processors are useful, although it can still be applied to many short time windows in serial. Less efficient for large $N_t$.

Two ways to control $\text{Cond}_2(V)$:

- Iterative: preconditioning $B$ by an $\alpha$-circulant matrix $C_\alpha$ (diagonalizable by FFT)
- Direct: modify the time scheme to get a ‘normal’ $B$ with well-conditioned $V$ 

A normal matrix is diagonalizable by a unitary matrix (with condition number=1)!
A block $\alpha$-circulant PinT preconditioner [Lin and Ng, 2020]

Recall the all-at-once nonsymmetric system matrix

\[
L := B \otimes I_h + I_t \otimes (-A_h), \quad B = \frac{1}{\tau} \begin{bmatrix}
1 & 1 \\
-1 & 1 & \ddots & \ddots \ \\
& \ddots & \ddots & \ddots & \ddots \\
& & \ddots & \ddots & 1 \\
& & & -1 & 1
\end{bmatrix}.
\]  

(12)

A block $\alpha$-circulant PinT preconditioner has the form ($C_\alpha$ is diagonalizable by FFT)

\[
P_\alpha := C_\alpha \otimes I_h + I_t \otimes (-A_h), \quad C_\alpha = \frac{1}{\tau} \begin{bmatrix}
1 & 1 & & & \\
-1 & 1 & & & \\
& \ddots & \ddots & \ddots & \\
& & \ddots & \ddots & 1 \\
& & & -1 & 1
\end{bmatrix}.
\]  

(13)

where the Toeplitz matrix $B$ is replaced by $\alpha$-circulant matrix (with $\alpha \in (0, 1]$)

- For a sufficiently small $\alpha$, preconditioned GMRES or fixed-point iteration has a mesh-independent convergence rate (nontrivial to prove due to non-normality).
- To control the roundoff errors in diagonalization, $\alpha$ should not be too small.
- The similar PinT preconditioner also works for wave PDE [Liu and Wu, 2020].
Revisit a boundary value method [Axelsson and Verwer, 1985]

Consider linear ODEs IVP (e.g. from semi-discretized PDE)

\[
\begin{align*}
    u'(t) + Au(t) &= g(t), \quad u(0) = u_0 \in \mathbb{R}^M. \\
\end{align*}
\]  

(14)

Use a uniform mesh \( t_j = j \tau \) with \( \tau = T/n \). Applying centered difference for the first \( (n - 1) \) time steps and backward Euler scheme for the last step, we get

\[
\begin{align*}
    \frac{u_{j+1} - u_{j-1}}{2\tau} + Au_j &= g_j, \quad j = 1, 2, \ldots, n - 1, \\
    \frac{u_n - u_{n-1}}{\tau} + Au_n &= g_n.
\end{align*}
\]  

(15)

Couple all the \( n \) time steps in (15) to get an all-at-once system with a better \( B \):

\[
\begin{align*}
(B \otimes I_h + I_t \otimes A) \mathbf{u}_h &= \mathbf{g}_h, \\
B &= \frac{1}{\tau} \begin{bmatrix}
    0 & 1/2 & 1/2 \\
    -1/2 & 0 & 1/2 \\
    \vdots & \vdots & \ddots \\
    -1/2 & 0 & 1/2 \\
    -1 & 0 & 1 \\
\end{bmatrix}
\end{align*}
\]  

(16)

Such an all-at-once time scheme should not be solved in a time-stepping fashion.
The diagonalization of the matrix $B$: formulas for $n$ eigenpairs

Consider the tridiagonal matrix

$$B = \tau B = \begin{bmatrix}
0 & 1/2 \\
-1/2 & 0 & 1/2 \\
& \ddots & \ddots & \ddots \\
& & -1/2 & 0 & 1/2 \\
& & & -1 & 1
\end{bmatrix}.$$ 

Let $T_n(x) = \cos(n \arccos x)$ and $U_n(x) = \sin[(n + 1) \arccos x]/\sin(\arccos x)$ denotes the $n$-th degree Chebyshev polynomials of the 1st- and 2nd-kind.

**Theorem 1**

Let $i = \sqrt{-1}$. The eigenvalues of $B$ are $\lambda_j = ix_j$, with $\{x_j\}_{j=1}^n$ being the $n$ roots of $U_{n-1}(x) - iT_n(x) = 0$, and the corresponding eigenvector $p_j = [p_{j,0}, \cdots, p_{j,n-1}]^T$ with $p_{j,0} = 1$ is $p_{j,k} = i^k U_k(x_j), k = 0, \cdots, n-1$. 
The diagonalization of the matrix $B$: eigenvalues are simple

**Theorem 2**

All $n$ roots of $U_{n-1}(x) - iT_n(x) = 0$ are simple, complex with negative imaginary parts, and have modulus less than $1 + 1/\sqrt{2n}$. Moreover, if $x$ is a root, then so is $-\bar{x}$.

In particular, $n$ distinct eigenvalues implies $B$ or $B$ is indeed diagonalizable.
The diagonalization of the matrix $B$: condition number of $V$

**Theorem 3**

Let $V = [p_1, p_2, \cdots, p_n]$ be the eigenvector matrix. There holds $\text{Cond}_2(V) = O(n^2)$.

Explicitly, the eigenvector matrix $V$ has the Chebyshev-Vandermonde structure

$$V = \text{diag}(i^0, i^1, \cdots, i^{n-1})$$  \[= I \text{ unitary}\]

$$\begin{bmatrix}
U_0(x_1) & \cdots & U_0(x_n) \\
\vdots & \ddots & \vdots \\
U_{n-1}(x_1) & \cdots & U_{n-1}(x_n)
\end{bmatrix}$$  \[= \Phi\] \hspace{1cm} (17)

(i) Some fast inversion algorithms (e.g. [Gohberg and Olshevsky, 1994]) for $V^{-1}$ in the literature may be unstable, mainly due to complex nodes $\{x_i\}^n_{i=1}$.

(ii) By the Vandermonde-like structure of $V = [i^kU_k(x_j)]$, we designed a stable fast algorithm with $O(n^2)$ complexity to compute $V^{-1}$. Based on 3 terms recursion.
Extension to 2nd-order problems (e.g. wave eq): $B \rightarrow B^2$

Consider the 2nd-order nonlinear ODEs IVP:

$$u''(t) + f(u(t)) = 0, \quad u(0) = u_0, \quad u'(0) = \tilde{u}_0,$$

Rewritten into first-order ODEs (with $v = u'$) and then apply the same scheme:

$$\begin{bmatrix} u(t) \\ v(t) \end{bmatrix}' = \begin{bmatrix} v(t) \\ -f(u(t)) \end{bmatrix}, \quad \begin{bmatrix} u(0) \\ v(0) \end{bmatrix} = \begin{bmatrix} u_0 \\ \tilde{u}_0 \end{bmatrix},$$

but the system size is doubled. Luckily, we can eliminate $v$'s after discretization:

**Lemma 4 (reduced all-at-once system for (18))**

The boundary-value method for the 2nd-order problem (18) can be formulated into

$$(B^2 \otimes I_x) u + F(u) = b,$$

where $b = \left( \frac{\tilde{u}_0^T}{2\tau}, -\frac{u_0^T}{4\tau^2}, 0, \ldots, 0 \right)^T$. Hence no extra cost due to $B^2 = VD^2V^{-1}$. 
Fast diagonalization algorithms for \( B = VDV^{-1} \)

Based on Theorem 1 it holds \( \lambda_j = i \cos(\theta_j) \), where \( \theta_j \) is the \( j \)-th root of 
\[
\rho(\theta) := \sin(n\theta) - i \cos(n\theta) \sin \theta = 0.
\]
Applying 1D Newton's iteration leads to

\[
\theta_j^{(l+1)} = \theta_j^{(l)} - \rho(\theta_j^{(l)}) / \rho'(\theta_j^{(l)}), \quad l = 0, 1, 2, \ldots
\]

with \( n \) accurately estimated complex initial guesses: 
\[
\theta_j^{(0)} = \frac{1}{2} \left( \frac{j\pi}{n} + \frac{j\pi}{n+1} \right) + \frac{i}{n}.
\]

Table 1: Comparison of \texttt{eig+backslash} function and our fast diagonalization algorithm

<table>
<thead>
<tr>
<th>( n )</th>
<th>MATLAB's \texttt{eig+backslash}</th>
<th>Our fast algorithm with MATLAB codes</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>\texttt{CPU}</td>
<td>\texttt{Res}_{\texttt{eig}}</td>
</tr>
<tr>
<td>512</td>
<td>0.277</td>
<td>9.69e-13</td>
</tr>
<tr>
<td>1024</td>
<td>1.107</td>
<td>3.85e-12</td>
</tr>
<tr>
<td>2048</td>
<td>6.741</td>
<td>1.01e-11</td>
</tr>
<tr>
<td>4096</td>
<td>60.257</td>
<td>4.02e-11</td>
</tr>
<tr>
<td>8192</td>
<td>606.045</td>
<td>2.25e-10</td>
</tr>
</tbody>
</table>
Approximation accuracy and $\text{Cond}_2(V)$ comparison

\[ u_{tt} - u_{xx} = 0, \ u(x, 0) = \sin(2\pi x), \ u'(x, 0) = 0, \ (x, t) \in (-1, 1) \times (0, T), \tag{22} \]

with periodic BC $u(-1, t) = u(1, t)$. With centered difference in space it gives

\[ u''_h + A_h u_h = 0, \ u_h(0) = u_0, \ u'_h(0) = 0, \ t \in (0, T). \tag{23} \]

**Figure 3:** Left: the errors for our algorithm, the algorithm in [Gander et al., 2019] and the time-stepping TR. Right: comparison of the growing $\text{Cond}_2(V)$. 
A 2D linear heat eq: scaling results with C/MPI/PETSc

\[ u_t(x, y, t) - \Delta u(x, y, t) = r(x, y, t), \text{ in } \Omega \times (0, T), \]  
\[ (24) \]

where \( \Omega = (0, \pi)^2 \) and the exact solution reads \( u(x, y, t) = \sin(x) \sin(y) e^{-t} \).

Table 2: Error and Scaling results of example 1: a heat PDE \((T = 2 \text{ with } M = 512^2)\)

<table>
<thead>
<tr>
<th>Core#</th>
<th>( s )</th>
<th>( n )</th>
<th>Error</th>
<th>CPU</th>
<th>Speedup</th>
<th>Efficiency</th>
<th>( n )</th>
<th>Error</th>
<th>CPU</th>
<th>Efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>512</td>
<td>2.23e-06</td>
<td>1318.8</td>
<td>1.0</td>
<td>100.0%</td>
<td>2</td>
<td>7.93e-02</td>
<td>5.4</td>
<td>100.0%</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>512</td>
<td>2.23e-06</td>
<td>667.8</td>
<td>2.0</td>
<td>98.7%</td>
<td>4</td>
<td>1.19e-02</td>
<td>5.4</td>
<td>100.0%</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>512</td>
<td>2.23e-06</td>
<td>346.4</td>
<td>3.8</td>
<td>95.2%</td>
<td>8</td>
<td>3.22e-03</td>
<td>5.4</td>
<td>100.0%</td>
</tr>
<tr>
<td>8</td>
<td>1</td>
<td>512</td>
<td>2.23e-06</td>
<td>173.0</td>
<td>7.6</td>
<td>95.3%</td>
<td>16</td>
<td>8.26e-04</td>
<td>5.5</td>
<td>98.2%</td>
</tr>
<tr>
<td>16</td>
<td>1</td>
<td>512</td>
<td>2.23e-06</td>
<td>90.7</td>
<td>14.5</td>
<td>90.9%</td>
<td>32</td>
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<td>5.8</td>
<td>93.1%</td>
</tr>
<tr>
<td>32</td>
<td>1</td>
<td>512</td>
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<td>51.1</td>
<td>25.8</td>
<td>80.7%</td>
<td>64</td>
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<td>6.6</td>
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<td>1</td>
<td>512</td>
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<td>41.2</td>
<td>64.4%</td>
<td>128</td>
<td>1.37e-05</td>
<td>8.3</td>
<td>65.1%</td>
</tr>
<tr>
<td>128</td>
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<td>512</td>
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<td>23.0</td>
<td>57.3</td>
<td>44.8%</td>
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</tr>
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<td>256</td>
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<td>512</td>
<td>2.23e-06</td>
<td>19.4</td>
<td>68.0</td>
<td>26.6%</td>
<td>512</td>
<td>2.23e-06</td>
<td>19.6</td>
<td>27.6%</td>
</tr>
</tbody>
</table>

Run on SIUE Campus Cluster: 10 CPU nodes via 25 Gbps Ethernet network, each node has two 3.5GHz AMD EPYC 7F52 16-Core CPU and 256GB RAM. Slow network may affect parallel efficiency. Here \( 512^3 \approx 134 \text{ millions} \)
A 2D linear wave eq: difficult for parareal-type algorithms

\[
 u_{tt}(x, y, t) - \Delta u(x, y, t) = r(x, y, t), \quad \text{in } \Omega \times (0, T),
\]

where \( \Omega = (0, 1)^2 \) and the exact solution \( u(x, y, t) = x(x - 1)y(y - 1)\sin(2\pi t) \).

**Table 3:** Error and Scaling Results of Example 2: a wave PDE (\( T = 2 \) with \( M = 512^2 \))

<table>
<thead>
<tr>
<th>Core#</th>
<th>Strong scaling</th>
<th>Weak scaling</th>
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<tbody>
<tr>
<td></td>
<td>Error</td>
<td>CPU</td>
</tr>
<tr>
<td>1</td>
<td>512</td>
<td>7.88e-05</td>
</tr>
<tr>
<td>2</td>
<td>512</td>
<td>7.88e-05</td>
</tr>
<tr>
<td>4</td>
<td>512</td>
<td>7.88e-05</td>
</tr>
<tr>
<td>8</td>
<td>512</td>
<td>7.88e-05</td>
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<tr>
<td>16</td>
<td>512</td>
<td>7.88e-05</td>
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<td>32</td>
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<td>64</td>
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<td>7.88e-05</td>
</tr>
<tr>
<td>256</td>
<td>512</td>
<td>7.88e-05</td>
</tr>
</tbody>
</table>

▶ The parallel efficiency is **the same** as heat eq, without any extra treatments;

**Fast Direct Solvers 2021 (Oct 24) A well-conditioned direct PinT solver for PDEs**
Consider the nonlinear ODEs IVP: \( u'(t) + f(u) = 0, \ u(0) = u_0 \). The scheme reads

\[
\begin{align*}
\frac{u_{j+1} - u_{j-1}}{2\tau} &+ f(u_j) = 0, \quad j = 1, 2, \ldots, n - 1, \\
\frac{u_n - u_{n-1}}{\tau} &+ f(u_n) = 0,
\end{align*}
\]

(26)

Rewrite (26) into all-at-once form (with \( F(u) = [f^T(u_1), f^T(u_2), \ldots, f^T(u_n)]^T \))

\[
(B \otimes I_x)u + F(u) = b.
\]

The Newton’s iteration (with \( \nabla F(u^k) = \text{blkdiag}(\nabla f(u^k_1), \ldots, \nabla f(u^k_n)) \)) reads

\[
(B \otimes I_x + \nabla F(u^k))u^{k+1} = b + \left( \nabla F(u^k)u^k - F(u^k) \right).
\]

(27)

Following the idea [Gander and Halpern, 2017] of averaging Jacobian matrix

\[
\nabla F(u^k) \approx I_t \otimes A_k, \quad A_k = \frac{1}{n} \left( \sum_{j=1}^{n} \nabla f(u^k_j) \right),
\]

(28)

which gives a simplified Newton iteration (SNI) can be solved PinT again:

\[
(B \otimes I_x + I_t \otimes A_k)u^{k+1} = b + \left( (I_t \otimes A_k)u^k - F(u^k) \right).
\]

(29)
A semi-linear parabolic equation: with \( f(u) = u^3 - u \)

\[
\begin{align*}
  u_t(x,y,t) - \Delta u(x,y,t) + f(u) &= r(x,y,t), & \text{in } \Omega \times (0, T), \\
  u(x,y,t) &= (x^2 - 1)(y^2 - 1)e^{-t}.
\end{align*}
\]  

where \( \Omega = (-1, 1)^2 \) and the exact solution reads \( u(x,y,t) = (x^2 - 1)(y^2 - 1)e^{-t} \).

Table 4: Error and Scaling Results of Example 3: a semi-linear PDE \((T = 2 \text{ with } M = 256^2)\)

<table>
<thead>
<tr>
<th>Core#</th>
<th>( n )</th>
<th>Error</th>
<th>SNI</th>
<th>CPU</th>
<th>Speedup</th>
<th>Efficiency</th>
<th>( n )</th>
<th>Error</th>
<th>SNI</th>
<th>CPU</th>
<th>Efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>512</td>
<td>6.36e-07</td>
<td>9</td>
<td>1514.0</td>
<td>1.0</td>
<td>100.0%</td>
<td>2</td>
<td>4.40e-01</td>
<td>11</td>
<td>6.6</td>
<td>100.0%</td>
</tr>
<tr>
<td>2</td>
<td>512</td>
<td>6.36e-07</td>
<td>9</td>
<td>770.4</td>
<td>2.0</td>
<td>98.3%</td>
<td>4</td>
<td>7.64e-03</td>
<td>9</td>
<td>5.4</td>
<td>122.2%</td>
</tr>
<tr>
<td>4</td>
<td>512</td>
<td>6.36e-07</td>
<td>9</td>
<td>400.6</td>
<td>3.8</td>
<td>94.5%</td>
<td>8</td>
<td>2.33e-03</td>
<td>11</td>
<td>6.8</td>
<td>97.1%</td>
</tr>
<tr>
<td>8</td>
<td>512</td>
<td>6.36e-07</td>
<td>9</td>
<td>217.2</td>
<td>7.0</td>
<td>87.1%</td>
<td>16</td>
<td>6.38e-04</td>
<td>9</td>
<td>5.9</td>
<td>111.9%</td>
</tr>
<tr>
<td>16</td>
<td>512</td>
<td>6.36e-07</td>
<td>9</td>
<td>126.9</td>
<td>11.9</td>
<td>74.6%</td>
<td>32</td>
<td>1.63e-04</td>
<td>9</td>
<td>7.0</td>
<td>94.3%</td>
</tr>
<tr>
<td>32</td>
<td>512</td>
<td>6.36e-07</td>
<td>9</td>
<td>84.7</td>
<td>17.9</td>
<td>55.9%</td>
<td>64</td>
<td>4.07e-05</td>
<td>9</td>
<td>9.4</td>
<td>70.2%</td>
</tr>
<tr>
<td>64</td>
<td>512</td>
<td>6.36e-07</td>
<td>9</td>
<td>67.6</td>
<td>22.4</td>
<td>35.0%</td>
<td>128</td>
<td>1.02e-05</td>
<td>9</td>
<td>28.8</td>
<td>22.9%</td>
</tr>
<tr>
<td>128</td>
<td>512</td>
<td>6.36e-07</td>
<td>9</td>
<td>60.6</td>
<td>25.0</td>
<td>19.5%</td>
<td>256</td>
<td>2.55e-06</td>
<td>9</td>
<td>29.8</td>
<td>22.1%</td>
</tr>
<tr>
<td>256</td>
<td>512</td>
<td>6.36e-07</td>
<td>9</td>
<td>60.8</td>
<td>24.9</td>
<td>9.7%</td>
<td>512</td>
<td>6.36e-07</td>
<td>9</td>
<td>61.6</td>
<td>10.7%</td>
</tr>
</tbody>
</table>

- The SNI shows a mesh-independent linear convergence rate
- A clear drop in efficiency when across computer nodes (32 cores per node), but over 20 times speedup is still higher than the parareal (< 10 times).
The summarized strong/weak scaling results

The nonlinear case’s parallel efficiency is much lower, which is expected due to the extra communication cost in (i) distributing the averaged Jacobian matrices and (ii) dispatching the residuals during the sequential SNI iterations.

The current weak scaling results is less satisfactory; no MPI coding experience.
Summary

Major contribution:

- New direct PinT solver works equally well for parabolic and hyperbolic eqs
- The condition number of eigenvector matrix $V$ can be controlled ($O(n^2)$)
- Fast $O(n^2)$ diagonalization (i.e. $D, V^{-1}$) algorithms of $B$ are designed

Some open problems:

- The convergence (rate) analysis for nonlinear problems is still missing?
- How to efficiently solve $n$ independent complex-shifted systems in step-(b)? multigrid, model order reduction [Liu and Wang, 2020]
- Which time scheme leads to a diagonalizable $B$ with minimal $\text{Cond}(V)$? optimize parametric time scheme for better conditioned $V$
- Use adaptive time step sizes for improved accuracy e.g., adaptive parareal algorithm [Maday and Mula, 2020]
Iterative and Direct ParaDIAG related algorithms with C/MPI codes:

github.com/wushulin/ParaDIAG

Main reference:


References II


A "parareal" in time discretization of PDE's.

A rom-accelerated parallel-in-time preconditioner for solving all-at-once systems from evolutionary pdes.

A fast block $\alpha$-circulant preconditoner for all-at-once systems from wave equations.

An adaptive parareal algorithm.
*Journal of computational and applied mathematics*, 377:112915.

Parallelization in time through tensor-product space-time solvers.