Time-parallel iterative solvers for parabolic evolution equations: an inf-sup theoretic approach

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joint work with

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Parallel-in-time methods

Motivations for parallel-in-time:

- Potential for faster total time to solution than sequential approach on parallel computers, and can complement spatial parallelism.

- Some problems have forward/backward structure (e.g. control problems) that cannot be solved sequentially like initial value problems.

- Many methods (parareal, space-time multigrid, PFASST, MGRIT...) Nievergelt 64, Hackbusch 84, Womble 90, Horton 92, Horton Vandewalle 95, Lions Maday & Turinici 01, Bal 05, Gander & Vandewalle 07, Emmett & Minion 12, Falgout et al. 14, Gander & Neumüller 16 ...
Parallel-in-time methods

Another reason to be interested in PinT

- Available theory and understanding of iterative methods for nonsymmetric systems is much less developed than for symmetric problems.

- Time-global formulation of evolution problems leads to nonsymmetric systems that are not “perturbations” of symmetric ones (e.g. non-diagonalizability)

\[
y' + ay = 0 \rightarrow \begin{bmatrix} 1 + \tau a & 1 + \tau a \\ -1 & 1 + \tau a \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} y_0 \\ 0 \end{bmatrix}
\]

- Suggests understanding of PinT methods is relevant in the broader context of iterative methods for nonsymmetric systems.

Can we develop a (reasonably) systematic approach to preconditioning nonsymmetric linear systems?
Approach based on inf-sup theory

Key motivation: sufficient and necessary conditions for well-posedness for linear problems (Nečas 62, Babuška 72, Brezzi 74)

Applications of inf-sup theory in numerical analysis of time-dependent problems are diverse:

- A priori error analysis, e.g. Tantardini & Veeser ’16
- A posteriori error analysis, e.g. Ern, S. & Vohralik ’17
- Reduced basis methods, e.g. Urban & Patera ’14

In the context of iterative methods for solving discrete systems:

I. Inf-sup theory
Reminder

**Inf-sup theorem** *(quoted here from Schwab 98)*

Let $X$ and $Y$ real reflexive Banach spaces with norms $\| \cdot \|_X$ and $\| \cdot \|_Y$ respectively. Let $Y^*$ be the dual of $Y$.

Let further $B : X \to Y^*$ be a bounded linear operator. Then the conditions

\[
\inf_{u \in X \setminus \{0\}} \sup_{v \in Y \setminus \{0\}} \frac{\langle Bu, v \rangle_{Y^* \times Y}}{\|u\|_X \|v\|_Y} \geq \beta > 0, \quad (*)
\]

\[
\sup_{u \in X} \langle Bu, v \rangle_{Y^* \times Y} > 0 \quad \forall \ v \in Y \setminus \{0\}, \quad (**)
\]

are necessary and sufficient for **well-posedness**: 

\[
\forall f \in Y^*, \exists! \ u \in X \text{ such that } Bu = f \text{ and } \|u\|_X \leq \beta^{-1} \|f\|_{Y^*}.
\]

Remark: can be equivalently formulated in terms of bilinear forms with

\[
b(u, v) = \langle Bu, v \rangle_{Y^* \times Y}.
\]
Inf-sup theory

Inf-sup theory for an abstract parabolic problem

\[ \partial_t u + A(t) u = f \quad \text{in } (0, T), \quad u(0) = u_0 \in \mathcal{H} \] (1)

with separable Hilbert spaces \( \mathcal{V} \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{V}^* \) (densely and compactly)
and \( A(t): \mathcal{V} \to \mathcal{V}^* \),

\[
\|A(t)\|_{\mathcal{V} \to \mathcal{V}^*} \leq C \quad \text{bounded}
\]

\[
\langle A(t)u, v \rangle_{\mathcal{V}^* \times \mathcal{V}} = \langle A(t)v, u \rangle_{\mathcal{V}^* \times \mathcal{V}}, \quad \text{self-adjoint}
\]

\[
\alpha \|u\|_{\mathcal{V}}^2 \leq \langle A(t)u, u \rangle_{\mathcal{V}^* \times \mathcal{V}}, \quad \text{coercive}
\]

for all \( u, v \in \mathcal{V} \), with \( C \) and \( \alpha > 0 \) independent of \( t \).
Suppose also that \( f \in L^2(0, T; \mathcal{V}^*) \).
Inf-sup theory

Let $\langle \cdot, \cdot \rangle$ be the duality pairing on $\mathcal{V}^* \times \mathcal{V}$ from now on.

**Well-posed weak formulation**

Find $u \in S := L^2(0, T; \mathcal{V}) \cap H^1(0, T; \mathcal{V}^*)$ s.t. $u(0) = u_0$ and

$$
\int_0^T \langle \partial_t u + A(t)u, \nu \rangle dt = \int_0^T \langle f, \nu \rangle dt \quad \forall \nu \in L^2(0, T; \mathcal{V}),
$$

Full details of theory in many standard references, see e.g. Wloka 87, Zeidler 90 (II/A).

Extension to many nonlinear problems in Roubíček 05.

Remark: $\int_0^T \langle \cdot, \cdot \rangle dt$ is equivalent to the duality pairing on $L^2(0, T; \mathcal{V}^*)$ and $L^2(0, T; \mathcal{V})$. 
Inf-sup theory

Key identity: For all \( u \in S := L^2(0, T; \mathcal{V}) \cap H^1(0, T; \mathcal{V}^*) \)

\[
\|u\|_S^2 = \left[ \sup_{v \in X \setminus \{0\}} \frac{\int_0^T \langle \partial_t u + A(t)u, v \rangle \, dt}{\|v\|_A} \right]^2 + \|u(0)\|^2_\mathcal{H} \tag{†}
\]

where the norms are defined by

\[
\|u\|_S^2 := \int_0^T \|\partial_t u\|_{*, t}^2 + \|u\|_{A(t)}^2 \, dt + \|u(T)\|_\mathcal{H}^2
\]

\[
\|v\|_A^2 := \int_0^T \|v\|_{A(t)}^2 \, dt
\]

with \( \|\cdot\|_{A(t)}^2 = \langle A(t)\cdot, \cdot \rangle_{\mathcal{V}^* \times \mathcal{V}} \), and with \( \|\cdot\|_{*, t} \) the dual-norm on \( \mathcal{V}^* \) wrt \( \|\cdot\|_{A(t)} \), i.e. \( \|\phi\|_{*, t}^2 = \langle \phi, A^{-1}(t)\phi \rangle \) for \( \phi \in \mathcal{V}^* \).

The identity implies that inf-sup condition (†) holds here with constant \( \beta = 1 \).
Proof

For all $u \in S := L^2(0, T; \mathcal{V}) \cap H^1(0, T; \mathcal{V}^*)$

$$
\|u\|_S^2 = \left[ \sup_{v \in \mathcal{X} \setminus \{0\}} \frac{\int_0^T \langle \partial_t u + A(t)u, v \rangle \, dt}{\|v\|_A} \right]^2 + \|u_0\|_\mathcal{H}^2
$$

Proof. Let $w_* = A^{-1}(t)\partial_t u$, then $\langle \partial_t u + A(t)u, v \rangle = \langle A(t)(w_* + u), v \rangle$ and

$$
\left[ \sup_{v \in L^2(0,T;\mathcal{V}) \setminus \{0\}} \frac{\int_0^T \langle A(t)(w_* + u), v \rangle \, dt}{\|v\|_A} \right]^2 = \int_0^T \|w_* + u\|^2_{A(t)} \, dt \text{ (equality with } v = w_* + u) \\
= \int_0^T \|w_*\|^2_{A(t)} + 2\langle A(t)w_*, u \rangle + \|u\|^2_{A(t)} \, dt \\
= \int_0^T \|\partial_t u\|^2_{*,t} + 2\langle \partial_t u, u \rangle + \|u\|^2_{A(t)} \, dt \\
= \int_0^T \|\partial_t u\|^2_{*,t} + \|u\|^2_{A(t)} \, dt + \|u(T)\|^2_{\mathcal{H}} - \|u(0)\|^2_{\mathcal{H}} \\
= \|u\|_S^2
$$
Proof

For all $u \in S := L^2(0, T; \mathcal{V}) \cap H^1(0, T; \mathcal{V}^*)$

$$\|u\|_S^2 = \left[ \sup_{v \in \mathcal{X} \setminus \{0\}} \frac{\int_0^T \langle \partial_t u + A(t)u, v \rangle \, dt}{\|v\|_A} \right]^2 + \|u_0\|^2_H$$

Proof. Let $w_* = A^{-1}(t) \partial_t u$, then $\langle \partial_t u + A(t)u, v \rangle = \langle A(t)(w_* + u), v \rangle$ and

$$\left[ \sup_{v \in L^2(0, T; \mathcal{V}) \setminus \{0\}} \frac{\int_0^T \langle A(t)(w_* + u), v \rangle \, dt}{\|v\|_A} \right]^2 = \int_0^T \|w_* + u\|^2_{A(t)} \, dt \quad \text{(equality with } v = w_* + u)$$

$$= \int_0^T \|w_*\|^2_{A(t)} + 2 \langle A(t)w_*, u \rangle + \|u\|^2_{A(t)} \, dt$$

$$= \int_0^T \|\partial_t u\|^2_{*,t} + 2 \langle \partial_t u, u \rangle + \|u\|^2_{A(t)} \, dt$$

$$= \int_0^T \|\partial_t u\|^2_{*,t} + \|u\|^2_{A(t)} \, dt + \|u(T)\|^2_{\mathcal{H}} - \|u(0)\|^2_{\mathcal{H}}$$

$$= \|u\|^2_S$$
Implicit Euler discretization of abstract time-dependent equation: find \( u_n \in V \)
\[
M(u_n - u_{n-1}) + \tau_n A_n u_n = \tau_n f_n, \quad n = 1, \ldots, N
\]
where \( M \) and \( \{A_n\}_{n=1}^N \) are SPD matrices, and \( u_0 \) is given.

No assumption on time-regularity/continuity of \( A_n \) or \( f_n \).

No assumption on connection between \( M \) and \( A_n \) (so no assumption on \( \tau \) and \( h^2 \))
Discrete inf-sup theory of Implicit Euler

\[ M(u_n - u_{n-1}) + \tau_n A_n u_n = \tau_n f_n, \quad n = 1, \ldots, N \]

The link between analysis of continuous and discrete settings: equivalent variational formulation (DG0): piecewise-constant approximation on intervals \( I_n = (t_{n-1}, t_n] \):

Find \( u_\tau \) s.t. \( b(u_\tau, v_\tau) = \ell(v_\tau) \quad \forall v_\tau \in V_\tau := \bigoplus_{n=1}^{N} \mathcal{P}_0(I_n; V) \).

where \( b(u_\tau, v_\tau) := \sum_{n=1}^{N} \int_{I_n} (\partial_t \mathcal{I} u_\tau, v_\tau)_M + (u_\tau, v_\tau)_{A_n} \, dt, \)

\[ \ell(v_\tau) := (u_0, v_1)_M + \sum_{n=1}^{N} \int_{I_n} (f_n, v_\tau)_M \, dt, \]

where \( \mathcal{I} u_\tau \) is P1 interpolatory reconstruction.
Discrete inf-sup theory of Implicit Euler

Discrete inf-sup condition

\[\|u_\tau\|_S = \sup_{v \in V_\tau \setminus \{0\}} \frac{b(u_\tau, v_\tau)}{\|v_\tau\|_A} \quad \forall u_\tau \in V_\tau \quad (2)\]

where

\[\|u_\tau\|^2_S := \sum_{n=1}^{N} \int_{I_n} \|\partial_t I u_\tau\|^2_{MA_n^{-1}M} + \|u_\tau\|^2_{A_n} \, dt + \|u_N\|^2_M + \sum_{n=1}^{N} \|(u_\tau)_{n-1}\|^2_M,\]

\[\|v_\tau\|^2_A := \sum_{n=1}^{N} \int_{I_n} \|v_\tau\|^2_{A_n} \, dt,\]

Full details of proof in Neumüller & S. '18, arxiv:1802.08126.

Extends to higher-order DG, see S. 17.

NB: Dual norm

\[\|v\|_{MA_n^{-1}M} = \sup_{w \in V \setminus \{0\}} \frac{(v, w)_M}{\|w\|_{A_n}} = \sqrt{v^\top MA_n^{-1}Mv}\]
Relation to other norms

<table>
<thead>
<tr>
<th>Relation to maximum norm</th>
</tr>
</thead>
<tbody>
<tr>
<td>For any $u \in S$,</td>
</tr>
<tr>
<td>$|u|_{L^\infty(0,T;H)} \leq |u|_S$.</td>
</tr>
<tr>
<td>For any $u_T \in V_T$,</td>
</tr>
<tr>
<td>$\max_{t \in [0,T]} |u_T(t)|_M \leq |u_T|_S$.</td>
</tr>
</tbody>
</table>

Constant is 1 for any $T$, any spaces $V$, $H$, and operator $A(t)$ (and in discrete case any $\{A_n\}$, any $M$, and $N, \ldots$)
II. Symmetric reformulations & inexact Uzawa iterations
Symmetric reformulations

**Matrix form**

Function \( u_\tau \in \mathbb{V}_\tau \iff u = [u_1, \ldots, u_N] \in \mathbb{V}^N := \mathbb{V} \times \cdots \times \mathbb{V} \),

\[
    b(u_\tau, v_\tau) = \ell(v_\tau)
\]

in matrix form

\[
    \begin{bmatrix}
        M + \tau_1 A_1 \\
        -M \\
        M + \tau_2 A_2 \\
        \vdots \\
        -M \\
        \vdots \\
        M + \tau_n A_n \\
    \end{bmatrix}
    \begin{bmatrix}
        u_1 \\
        \vdots \\
        u_N \\
    \end{bmatrix}
    =
    \begin{bmatrix}
        \tau_1 f_1 + Mu_0 \\
        \tau_2 f_2 \\
        \vdots \\
    \end{bmatrix}
    \]

Can write

\[
    B = K \otimes M + \text{diag}\{\tau_n A_n\}_{n=1}^N = K + A
\]

where \( K = \begin{pmatrix}
    1 & 1 \\
    -1 & 1 \\
    \cdots & \cdots \\
\end{pmatrix} \in \mathbb{R}^{N \times N} \)
Symmetric reformulations

Matrix form of inf-sup:

\[ u_\tau \in \mathbb{V}_\tau \iff u \in \mathbb{V}^N, \quad \| \cdot \|_S \iff \| \cdot \|_S, \]

with SPD matrix \( S \) defined by

\[
S := \begin{align*}
&K^T A^{-1} K \\
&\int \| \partial_t \mathcal{I} u_\tau \|_{M A_n^{-1} M}^2 \, dt \quad + \quad \text{jump terms} \quad + \quad A \\
&\int u_\tau^T u_\tau \|_{A_n}^2 \, dt
\end{align*}
\]

Matrix form of inf-sup stability of implicit Euler

\[
\| u \|_S = \sup_{v \in \mathbb{V}^N \setminus \{0\}} \frac{v^T Bu}{\|v\|_A} \quad \forall \ u \in \mathbb{V}^N,
\]

where the norm \( \| \cdot \|_S \iff \| \cdot \|_S \) with SPD matrix \( S \).

Optimal test function in inf-sup is \( v = (A^{-1} K + I)u \).
Symmetric reformulations

We can think of the mapping \( u \mapsto (A^{-1}K + I)u \) the optimal test function as a left-preconditioner of the system

\[
P = A^{-1}K + I
\]

Then

\[
S = P^\top B
\]

In theory, could solve \( Su = g \) with, e.g., Precond. Conjugate Gradients.

Not always realistic: requires exact \( A^{-1} \) since \( S := K^\top A^{-1}K + K + K^\top + A \).
Symmetric reformulations

We can think of the mapping $u \mapsto (A^{-1}K + I)u$ the optimal test function as a left-preconditioner of the system

$$P = A^{-1}K + I$$

Then

$$S = P^\top B$$

Symmetric reformulation I

So $u$ is equivalently solution of SPD problem

$$Su = g, \quad g := P^\top f.$$  

In theory, could solve $Su = g$ with, e.g., Precond. Conjugate Gradients.

Not always realistic: requires exact $A^{-1}$ since $S := K^\top A^{-1}K + K + K^\top + A$. 
Symmetric reformulations

To allow for inexact approximations of $A^{-1}$, introduce auxiliary variables

\[ Ap = Ku - f, \]
\[ Su = g \iff K^T p + (K + K^T + A)u = f. \]

Symmetric reformulation II

\[
\begin{bmatrix}
A & -K \\
-K^T & -(K + K^T + A)
\end{bmatrix}
\begin{bmatrix}
p \\ u
\end{bmatrix}
= \begin{bmatrix}
-f \\ -f
\end{bmatrix}. 
\]

$\mathcal{A}$ is a symmetric saddle-point matrix.

$S$ is the Schur complement of $\mathcal{A}$.  

- Advantage: new formulation no longer explicitly requires $A^{-1}$. 

Symmetric reformulations

\[ A = \begin{bmatrix} A & -K \\ -K^\top & -(K + K^\top + A) \end{bmatrix}, \quad Au = g, \]

**Proposition: Stability of symmetric reformulation**

\[ c_1 \|u\|_* \leq \sup_{v \in \mathbb{V}^N \times \mathbb{V}^N \setminus \{0\}} \frac{v^\top A u}{\|v\|_*} \leq c_2 \|u\|_*. \]

with \( c_1 = \frac{1}{2} (\sqrt{5} - 1) \) and \( c_2 = \frac{1}{2} (\sqrt{5} + 1) \), where

\[ \|v\|^2_* := \|q\|^2_A + \|v\|^2_S, \quad v = [q, v] \in \mathbb{V}^N \times \mathbb{V}^N. \]

- stability distinguishes this from “classical” symmetric formulations, e.g. \( B^\top Bu = B^\top f \).
- In fact, stable symmetric reformulation generalises straightforwardly to arbitrary order dG-in-time.
III. Convergent iterative method with parallel-in-time preconditioners
Inexact Uzawa method

**Inexact Uzawa method**

Sequence \( \mathbf{u}_j = [\mathbf{p}_j, \mathbf{u}_j] \) where

\[
\begin{align*}
\mathbf{p}_{j+1} &= \mathbf{p}_j + \tilde{\mathbf{A}}^{-1} (\mathbf{Ku}_j - \mathbf{Ap}_j - \mathbf{f}), \\
\mathbf{u}_{j+1} &= \mathbf{u}_j + \omega \tilde{\mathbf{H}}^{-1} (\mathbf{f} - \mathbf{K}^\top \mathbf{p}_{j+1} - [\mathbf{K} + \mathbf{K}^\top + \mathbf{A}] \mathbf{u}_j),
\end{align*}
\]

where \( \tilde{\mathbf{A}} \) and \( \tilde{\mathbf{H}} \) are respectively preconditioners for \( \mathbf{A} \) and \( \mathbf{S} \), \( \omega > 0 \) a damping parameter.

Recall \( \mathbf{A} = \text{diag}\{\tau_n A_n\}_{n=1}^N \), so \( \tilde{\mathbf{A}} \) can be built from standard elliptic solvers, trivially parallel in time.

We will specify a suitable time-parallel \( \tilde{\mathbf{H}} \) in next few slides.
Interpretation of inexact Uzawa as using inexact left-preconditioner

Inexact Uzawa

\[ p_{j+1} = p_j + \tilde{A}^{-1} (Ku_j - Ap_j - f), \]
\[ u_{j+1} = u_j + \omega \tilde{H}^{-1} (f - K^T p_{j+1} - [K + K^T + A] u_j), \]

Recall the ideal left preconditioner \( P = A^{-1}K + I \) and \( S = P^T B \).

Suppose we choose initial guess \( p_0 = -u_0 \) (consistent with exact solution).

Then doing 1 step of the Inexact Uzawa on \( u_0 = [p_0, u_0] \) is equivalent to

\[ u_1 = u_0 + \omega \tilde{H}^{-1} \tilde{P}^T (f - Bu_0) \]

with \( \tilde{P} = \tilde{A}^{-1}K + I \).

Advantage of saddle point formulation is established convergence theory.

**NB:** it is not necessary to require \( p_0 = -u_0 \) for the inexact Uzawa method to converge (see following).
General convergence theory of Uzawa

Inexact Uzawa

\[
\begin{align*}
\mathbf{p}_{j+1} &= \mathbf{p}_j + \tilde{\mathbf{A}}^{-1} (\mathbf{Ku}_j - \mathbf{Ap}_j - \mathbf{f}), \\
\mathbf{u}_{j+1} &= \mathbf{u}_j + \omega \tilde{\mathbf{H}}^{-1} (\mathbf{f} - \mathbf{K}^\top \mathbf{p}_{j+1} - [\mathbf{K} + \mathbf{K}^\top + \mathbf{A}] \mathbf{u}_j),
\end{align*}
\]

Convergence theory of inexact Uzawa requires:

\[
\|I - \tilde{\mathbf{A}}^{-1} \mathbf{A}\|_{\tilde{\mathbf{A}}} \leq \rho_\mathbf{A} < 1 \quad \text{(Contraction)}
\]

\[
\lambda_{\min} \tilde{\mathbf{H}} \leq \mathbf{S} \leq \lambda_{\max} \tilde{\mathbf{H}} \quad \text{(Spectral equivalence)}
\]

with \(\lambda_{\max} \geq \lambda_{\min} > 0\).
## General convergence theory of Uzawa

**Theorem: Convergence of inexact Uzawa**

Define the norm

\[
\|v\|_{\mathcal{D}}^2 := \omega \rho_A \|q\|_{\mathcal{A}}^2 + \|v\|_{\mathcal{H}}^2 \quad \forall v = [q, v].
\]

Then

\[
\|u - u_{j+1}\|_{\mathcal{D}} \leq \rho U \|u - u_j\|_{\mathcal{D}}
\]

where \(\rho U := \max\{\sigma_-, \sigma_+\}:\)

\[
\sigma_- := \frac{1}{2} \left[ (1 - \rho_A)(1 - \omega \lambda_{\min}) + \sqrt{4 \rho_A + (1 - \rho_A)^2 (1 - \omega \lambda_{\min})^2} \right],
\]

\[
\sigma_+ := \frac{1}{2} \left[ (1 + \rho_A)(1 + \omega \lambda_{\max}) - 2 + \sqrt{4 \rho_A + [(1 + \rho_A)(1 + \omega \lambda_{\max}) - 2]^2} \right].
\]

Convergent under damping condition:

\[
\omega \lambda_{\max} < 2 \frac{1 - \rho_A}{1 + \rho_A} \implies \rho U < 1.
\]

Proof based on Zulehner 02
Preconditioners for the Schur complement

We need to find \( \tilde{H} \) such that

\[
\lambda_{\text{min}} \tilde{H} \leq S \leq \lambda_{\text{max}} \tilde{H}
\]

Motivation by following example:

Example: Constant operators with uniform time-steps

In special case \( \tau_n = \tau \) and \( A_n = A \):

\[
S = \frac{1}{\tau} K^T K \otimes MA^{-1} M + (K + K^T) \otimes M + \text{Id}_N \otimes \tau A.
\]

\[
K^T K = \begin{pmatrix}
2 & -1 & \cdot & \cdot & \cdot \\
-1 & 2 & -1 & \cdot & \cdot \\
\cdot & \cdot & \ldots & \cdot & \cdot \\
-1 & -1 & 1 & \cdot & \cdot \\
\end{pmatrix}, \quad K + K^T = \begin{pmatrix}
2 & -1 & \cdot & \cdot & \cdot \\
-1 & 2 & -1 & \cdot & \cdot \\
\cdot & \cdot & \ldots & \cdot & \cdot \\
-1 & -1 & 1 & \cdot & \cdot \\
\end{pmatrix}.
\]
Preconditioners for the Schur complement

So far, \( \{A_n\}_{n=1}^N \) are SPD but otherwise general.

**Main assumption:** quasi-uniform spectral equivalence of \( \tau_n A_n \)

Assume \( \exists \) SPD matrix \( A \), \( \tau > 0 \), and \( \alpha \geq 1 \) s.t.

\[
\frac{1}{\alpha} \tau A \leq \tau_n A_n \leq \alpha \tau A \quad \forall n = 1, \ldots, N,
\]

- Weaker than assuming quasi-unif. of \( \{A_n\}_{n=1}^N \) and of \( \{\tau_n\}_{n=1}^N \) separately.
- Rules out degeneracy.
- User can choose \( A \) and \( \tau \), but these are required in the computation.
- Does not require any time-regularity/continuity of the operators \( \{A_n\} \).
- Does not require any relation between \( M \) and \( \tau_n A_n \): no mesh-size/time-step restriction.
Preconditioners for the Schur complement

So far, \( \{A_n\}_{n=1}^{N} \) are SPD but otherwise general.

**Main assumption:** quasi-uniform spectral equivalence of \( \tau_n A_n \)

Assume \( \exists \) SPD matrix \( A, \tau > 0, \text{ and } \alpha \geq 1 \) s.t.

\[
\frac{1}{\alpha} \tau A \leq \tau_n A_n \leq \alpha \tau A \quad \forall \ n = 1, \ldots, N,
\]

**Consequence**

Then \( S \) is spectrally equivalent to a simpler matrix \( \tilde{S} \):

\[
\frac{1}{\alpha} \tilde{S} \leq S \leq 3\alpha \tilde{S},
\]

\[
\tilde{S} := \frac{1}{\tau} K^\top K \otimes MA^{-1} M + \tilde{I}_d \otimes \tau A, \quad \tilde{I}_d = \begin{pmatrix} 1 \\ \vdots \\ 1/2 \end{pmatrix}
\]
Preconditioners for the Schur complement

**Idea:** Block-diagonalise the simpler matrix \( \tilde{S} \) by a Discrete Sine Transform (DST)

Define (Type-II/III) DST

\[
\hat{u} = \Phi u, \quad \hat{u}_k = \frac{2}{N} \sum_{n=1}^{N} \frac{1}{1 + \delta_{nN}} u_n \sin \left( \frac{(2k - 1)n\pi}{2N} \right), \quad k = 1, \ldots, N.
\]

\[
u = \Phi^{-1} \hat{u}, \quad u_n = \sum_{k=1}^{N} \hat{u}_k \sin \left( \frac{(2k - 1)n\pi}{2N} \right), \quad n = 1, \ldots, N.
\]

**Parallelization:** implemented via Fast Fourier Transform: \( O(\log N) \) parallel complexity (and trivially parallel wrt space).

\[
\tilde{S} = \Phi^T \hat{D} \Phi, \quad \hat{D} := \frac{N}{2} \text{diag} \left\{ \frac{\mu_k^2}{\tau} MA^{-1} M + \tau A \right\}_{k=1}^N
\]

with \( \mu_k := 2 \sin \left( \frac{(2k-1)\pi}{4N} \right) > 0 \) for \( k = 1, \ldots, N \).
Preconditioners for the Schur complement

\[ \tilde{S} = \Phi^\top \hat{D} \Phi, \quad \hat{D} := \frac{N}{2} \text{diag} \left\{ \frac{\mu_k^2}{\tau} MA^{-1} M + \tau A \right\}_{k=1}^N, \]

Idea from Pearson & Wathen 2014:

\[ \frac{\mu_k^2}{\tau} MA^{-1} M + \tau A \approx \frac{1}{\tau} H_k A^{-1} H_k, \quad H_k := \mu_k M + \tau A \]

So we propose “ideal” (exact spatial inverses) preconditioner

\[ H := \Phi^\top \hat{H} \Phi, \quad \hat{H} := \frac{N}{2} \text{diag} \left\{ \frac{1}{\tau} H_k A^{-1} H_k \right\}_{k=1}^N, \]

Main spectral equivalence result

\[ \frac{1}{2\alpha} H \leq \tilde{S} \leq 3\alpha H. \]

Proof: \[ \frac{1}{2} H \leq \tilde{S} \leq H \text{ and } \frac{1}{\alpha} \tilde{S} \leq S \leq 3\alpha \tilde{S}. \]
Preconditioners for the Schur complement

In practice, we approximate $\mathbf{H} \approx \tilde{\mathbf{H}}$ where $H_k^{-1} = (\mu_k \mathbf{M} + \tau \mathbf{A})^{-1}$ is approximated by a spatial solver, e.g. multigrid V-cycle.

We shall assume that there are fixed positive constants $\gamma$ and $\Gamma$ such that

$$\gamma \tilde{\mathbf{H}} \leq \mathbf{H} \leq \Gamma \tilde{\mathbf{H}}$$

Then

$$\frac{\gamma}{2\alpha} \tilde{\mathbf{H}} \leq \mathbf{S} \leq 3\alpha \Gamma \tilde{\mathbf{H}}.$$ 

So we can take $\lambda_{\text{min}} = \gamma/2\alpha$ and $\lambda_{\text{max}} = 3\alpha \Gamma$ in the convergence theorem of inexact Uzawa.
Preconditioners for the Schur complement

Summary of convergence theory

If \( \| I - \tilde{A}^{-1} A \| \tilde{A} \leq \rho_A < 1, \gamma \tilde{H} \leq H \leq \Gamma \tilde{H} \), and if \( \omega < \frac{2}{3\alpha \Gamma} \frac{1-\rho_A}{1+\rho_A} \),
then \( \exists \rho_U \in (0, 1) \) such that

\[
\| u - u_{j+1} \|_D \leq \rho_U \| u - u_j \|_D.
\]

- Rigorous proof of convergence provided availability of spatial solvers, which is robust wrt number of time-steps \( N \), time-length \( T \), mesh size and spatial operators (for fixed \( \omega, \alpha, \rho_A, \gamma \) and \( \Gamma \)).
- Only a small number of quantities determine \( \rho_U \): \( \rho_A, \gamma, \Gamma, \alpha, \omega \).
Parallel complexity

Cost of different spatial operations treated abstractly:

- \( C_{\text{add}}^V \) cost of additions and subtractions of vectors in \( V \);
- \( C_{\text{mult}}^V \) cost of performing a matrix vector product with \( M, A \) or \( A_n, n = 1, \ldots, N \);
- \( C_{\text{prec}}^V \) cost of performing the action of the spatial preconditioners \( \tilde{A}_{n-1} \) or \( \tilde{H}_{k-1} \).

Parallel complexity (assuming \( \Omega(N) \) processors)

\[
\text{Parallel complexity} = O \left( C_{\text{add}}^V (\log N + 1) + C_{\text{mult}}^V + C_{\text{prec}}^V \right),
\]

where constant is independent of \( V \) and of \( N \).
Theory summary

• existing theory of iterative methods for symmetric systems to solve nonsymmetric $Bu = f$.
• allows for minimal regularity of data, operators & solutions
• allows inexact solves of spatial problems
• convergence robust wrt timesteps $N$, mesh & time-steps sizes
• no restrictions between time-steps/spatial meshes
• optimal time-parallel complexity of order $\log N$ (cf Worley 91)
V. Numerical experiments

Model problem: heat equation in one, two, and three space dimensions

• Condition numbers (1D)
• Influence of spatial preconditioners (2D)
• Time-parallel (3D)
• Space-time parallel (3D)
Numerical experiments: condition numbers $H^{-1}S$

1D heat equation (for accuracy of computations)

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<th>$N = 8$</th>
<th>$N = 16$</th>
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<th>$N = 1024$</th>
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<td>0.8099</td>
<td>0.7080</td>
<td>0.6270</td>
<td>0.5728</td>
<td>0.5402</td>
<td>0.5223</td>
<td>0.5129</td>
<td>0.5081</td>
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<td>2.8248</td>
<td>3.1893</td>
<td>3.4906</td>
<td>3.6994</td>
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<td>0.5081</td>
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<td>3.4916</td>
<td>3.7014</td>
<td>3.8278</td>
<td>3.8967</td>
<td>3.9310</td>
<td>3.9445</td>
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</table>

Theoretical bound: $\kappa(H^{-1}S) \leq 6$

In practice: $\kappa(H^{-1}S) \leq 4$

Eigenvalue $\lambda_{\max} \approx 2$ suggest that damping parameter $\omega < 1$ is enough for $\rho_A$ reasonably small: e.g. we can take $\omega = 0.9$. 

Numerical experiments

Effect of spatial approximations in $\tilde{A}_n \approx A_n$ and $\tilde{H}_k \approx H_k$ on convergence

- Direct solvers
- 1 multigrid V-cycle
- 2 multigrid V-cycles

2D computation with 4,064,256 DOFs
Numerical experiments

Robustness with respect to mesh size $h$, time-steps $N$

2D problem, using 1 multigrid V-cycle for spatial inverses:

<table>
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<tr>
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<th>$h = 1/8$</th>
<th>$h = 1/16$</th>
<th>$h = 1/32$</th>
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<tr>
<td>1024</td>
<td>22</td>
<td>22</td>
<td>22</td>
<td>22</td>
</tr>
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</table>

Iterations to reach $\|u - u_j\|_S < 10^{-6}\|u\|_S$. 
Parallel computations

Setup

- 3D Heat equation on uniform meshes
- *Vulcan* BlueGene Q at Lawrence Livermore
- Computations up to 131,072 processors and 2,249,728,000 DOFs
- Time-parallelism in FFT using FFTW3 library
- Spatial problems using MFEM and *hype*re AMG solvers
- We used GMRES as an acceleration method for Uzawa
Time-parallel results

Weak scaling tests for time-parallel results

- Fixed spatial mesh
- Assign 16 time-steps per processor, and increase $N$
- Iterations and timings to reach a residual tolerance of $10^{-8}$

<table>
<thead>
<tr>
<th>procs</th>
<th>$N$</th>
<th>dofs</th>
<th>iter</th>
<th>time/iter</th>
<th>total time</th>
<th>time FFT (%)</th>
<th>time AMG (%)</th>
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<td>1 257 728</td>
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<td>26.60</td>
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<td>82.4%</td>
</tr>
<tr>
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<td>256</td>
<td>2 515 456</td>
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<tr>
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<td>76.4%</td>
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</table>

Weak scaling. Computational times in seconds.

Notice that time/iter is essentially constant.
Strong scaling results

- Fix $N = 65\,356$ and increase number of processors
- Iterations and timings to reach a residual tolerance of $10^{-8}$

<table>
<thead>
<tr>
<th>proc</th>
<th>$N$</th>
<th>dofs</th>
<th>iter</th>
<th>time/iter</th>
<th>total time</th>
<th>time FFT (%)</th>
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<td>1.87</td>
<td>41.09</td>
<td>7.4%</td>
<td>76.4%</td>
</tr>
</tbody>
</table>

Strong scaling. Computational times in seconds.

- Very good strong scaling
- Costs of time-parallelism for FFTs is much smaller than cost of solving spatial problems.
Space-time parallelism

- 3D heat equation in unit cube with 262,144 elements, and $N = 4096$ time-steps. Total 2,249,728,000 DOFs.
- $p_x$ processors in space, $p_t$ in time: total $p_xp_t$ processors (up to 131,072).
- Spatial parallelism in AMG provided by hypre (default settings).
- Timings to solution

<table>
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<tr>
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<th>16</th>
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Summary

- Parabolic problems
  - general time-dependent self-adjoint operators and right-hand sides,
  - No regularity/continuity assumptions on the data/operators
- Equivalent inf-sup stable saddle-point symmetric formulations
- Robust convergence rates for inexact Uzawa
  - Time-parallel & spectrally equivalent preconditioners for $S$
  - Easy implementation: FFT and black-box spatial preconditioners.
  - Parallel complexity $O(\log N)$.
  - No restrictions on spatial mesh & time-step sizes
- Good weak and strong scaling in parallel computations

Full details in Neumüller & S. 18, arxiv:1802.08126

Inf-sup approach for more general nonsymmetric linear systems?

Thank you!