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)

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

- 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:

- Andreev, SIAM J. Numer. Anal. 16: wavelet-in-time method, multigrid in space, based on continuous inf-sup stability of problem
- S., IMA J. Numer. Anal. 17: high-order DG time-stepping, based on discrete inf-sup stability of the method, considered system of a single time-step, robust with respect to space, time, & poly degree.

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

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

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

are necessary and sufficient for **well-posedness:**
$\forall f \in Y^*$, $\exists!\, u \in X$ such that $Bu = f$ 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 for an abstract parabolic problem

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

with separable Hilbert spaces $\mathcal{V} \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{V}^*$ (densely and compactly)

and $\mathcal{A}(t) \colon \mathcal{V} \to \mathcal{V}^*$,

$$\begin{aligned} \|\mathcal{A}(t)\|_{\mathcal{V}\to\mathcal{V}^*} &\leq C && \text{bounded} \\ \langle \mathcal{A}(t)\, u, v\rangle_{\mathcal{V}^*\times\mathcal{V}} &= \langle \mathcal{A}(t)\, v, u\rangle_{\mathcal{V}^*\times\mathcal{V}}, && \text{self-adjoint} \\ \alpha\|u\|_{\mathcal{V}}^2 &\leq \langle \mathcal{A}(t) u, u\rangle_{\mathcal{V}^*\times\mathcal{V}}, && \text{coercive} \end{aligned}$$

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

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

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: $\int_0^T \langle \cdot, \cdot \rangle \mathrm{d}t$ 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 $u \in S := L^2(0,T;\mathcal{V}) \cap H^1(0,T;\mathcal{V}^*)$

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

where the norms are defined by

$$\|u\|_S^2 := \int_0^T \|\partial_t u\|_{*,t}^2 + \|u\|_{\mathcal{A}(t)}^2 \mathrm{d}t + \|u(T)\|_{\mathcal{H}}^2$$

$$\|v\|_A^2 := \int_0^T \|v\|_{\mathcal{A}(t)}^2 \mathrm{d}t$$

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

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

Proof

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

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

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

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

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

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

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

Proof

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

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

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

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

Discrete inf-sup theory of Implicit Euler

Implicit Euler discretization of abstract time-dependent equation: find $u_n \in \mathbb{V}$

$$M(u_n - u_{n-1}) + \tau_n A_n u_n = \tau_n f_n, \qquad n = 1, \ldots, N$$

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 τ and h^2)

Discrete inf-sup theory of Implicit Euler

$$M(u_n - u_{n-1}) + \tau_n A_n u_n = \tau_n f_n, \qquad n = 1, \dots, N$$

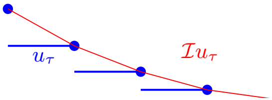
The link between analysis of continuous and discrete settings: equivalent variational formulation (DG0): piecewise-constant approximation on intervals $I_n = (t_{n-1}, t_n]$:

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

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

$$\ell(v_\tau) := (u_0, v_1)_M + \sum_{n=1}^{N} \int_{I_n} (f_n, v_\tau)_M \, \mathrm{d}t,$$

where $\mathcal{I} u_\tau$ is P1 interpolatory reconstruction.



Discrete inf-sup theory of Implicit Euler

Discrete inf-sup condition

$$\|u_\tau\|_{\mathbb{S}} = \sup_{v \in \mathbb{V}_\tau \setminus \{0\}} \frac{b(u_\tau, v_\tau)}{\|v_\tau\|_{\mathbb{A}}} \quad \forall\, u_\tau \in \mathbb{V}_\tau \qquad (2)$$

where

$$\|u_\tau\|_{\mathbb{S}}^2 := \sum_{n=1}^{N} \int_{I_n} \|\partial_t \mathcal{I} u_\tau\|_{MA_n^{-1}M}^2 + \|u_\tau\|_{A_n}^2 \,\mathrm{d}t + \|u_N\|_M^2 + \sum_{n=1}^{N} \underbrace{\|(\!|u_\tau|\!)_{n-1}\|_M^2}_{\text{jump terms}},$$

$$\|v_\tau\|_{\mathbb{A}}^2 := \sum_{n=1}^{N} \int_{I_n} \|v_\tau\|_{A_n}^2 \,\mathrm{d}t,$$

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

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

NB: Dual norm

$$\|v\|_{MA_n^{-1}M} = \sup_{w \in \mathbb{V} \setminus \{0\}} \frac{(v, w)_M}{\|w\|_{A_n}} = \sqrt{v^\top M A_n^{-1} M v}$$

Relation to other norms

Relation to maximum norm

For any $u \in S$,

$$\|u\|_{L^\infty(0,T;\mathcal{H})} \leq \|u\|_S.$$

For any $u_\tau \in \mathbb{V}_\tau$,

$$\max_{t\in[0,T]} \|u_\tau(t)\|_M \leq \|u_\tau\|_{\mathbb{S}}.$$

Constant is 1 for any T, any spaces $\mathcal{V}$, $\mathcal{H}$, and operator $\mathcal{A}(t)$ (and in discrete case any $\{A_n\}$, any M, and N, ...)

II. Symmetric reformulations & inexact Uzawa iterations

Symmetric reformulations

Matrix form

Function $u_\tau \in \mathbb{V}_\tau \iff \mathbf{u} = [u_1, \dots, u_N] \in \mathbb{V}^N := \mathbb{V} \times \cdots \times \mathbb{V}$,

$$b(u_\tau, v_\tau) = \ell(v_\tau)$$

in matrix form

$$\underbrace{\begin{bmatrix} M + \tau_1 A_1 & & \\ -M & M + \tau_2 A_2 & \\ & & \ddots \end{bmatrix}}_{\mathbf{B}} \underbrace{\begin{bmatrix} u_1 \\ \vdots \\ u_N \end{bmatrix}}_{\mathbf{u}} = \underbrace{\begin{bmatrix} \tau_1 f_1 + M u_0 \\ \tau_2 f_2 \\ \dots \end{bmatrix}}_{\mathbf{f}}$$

Can write

$$\mathbf{B} = K \otimes M + \operatorname{diag}\{\tau_n A_n\}_{n=1}^N = \mathbf{K} + \mathbf{A}$$

where $K = \begin{pmatrix} 1 & & \\ -1 & 1 & \\ & & \ddots \end{pmatrix} \in \mathbb{R}^{N \times N}$

Symmetric reformulations

Matrix form of inf-sup:

$$u_\tau \in \mathbb{V}_\tau \iff \mathbf{u} \in \mathbb{V}^N, \quad \|\cdot\|_{\mathbb{S}} \iff \|\cdot\|_{\mathbf{S}},$$

with SPD matrix $\mathbf{S}$ defined by defined by

$$\mathbf{S} := \underbrace{\mathbf{K}^\top \mathbf{A}^{-1} \mathbf{K}}_{\int \|\partial_t \mathcal{I} u_\tau\|^2_{MA_n^{-1}M} \mathrm{d}t} + \underbrace{\mathbf{K} + \mathbf{K}^\top}_{\text{jump terms}} + \underbrace{\mathbf{A}}_{\int \|u_\tau\|^2_{A_n} \mathrm{d}t}$$

Matrix form of inf-sup stability of implicit Euler

$$\|\mathbf{u}\|_{\mathbf{S}} = \sup_{\mathbf{v} \in \mathbb{V}^N \setminus \{0\}} \frac{\mathbf{v}^\top \mathbf{B} \mathbf{u}}{\|\mathbf{v}\|_{\mathbf{A}}} \quad \forall \mathbf{u} \in \mathbb{V}^N,$$

where the norm $\|\cdot\|_{\mathbf{S}} \iff \|\cdot\|_{\mathbb{S}}$ with SPD matrix $\mathbf{S}$.

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

Symmetric reformulations

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

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

Then

$$\mathbf{S} = \mathbf{P}^{\top}\mathbf{B}$$

Symmetric reformulation I

So $\mathbf{u}$ is equivalently solution of SPD problem

$$\mathbf{S}\mathbf{u} = \mathbf{g}, \quad \mathbf{g} := \mathbf{P}^{\top}\mathbf{f}.$$

In theory, could solve $\mathbf{S}\mathbf{u} = \mathbf{g}$ with, e.g., Precond. Conjugate Gradients.

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

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Symmetric reformulations

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

$$\begin{aligned} \mathbf{A}\mathbf{p} &= \mathbf{K}\mathbf{u} - \mathbf{f}, \\ \mathbf{S}\mathbf{u} = \mathbf{g} \iff \mathbf{K}^\top \mathbf{p} &+ (\mathbf{K} + \mathbf{K}^\top + \mathbf{A})\mathbf{u} = \mathbf{f}. \end{aligned}$$

Symmetric reformulation II

$$\underbrace{\begin{bmatrix} \mathbf{A} & -\mathbf{K} \\ -\mathbf{K}^\top & -\left(\mathbf{K} + \mathbf{K}^\top + \mathbf{A}\right) \end{bmatrix}}_{\boldsymbol{\mathcal{A}}} \underbrace{\begin{bmatrix} \mathbf{p} \\ \mathbf{u} \end{bmatrix}}_{\boldsymbol{u}} = \underbrace{\begin{bmatrix} -\mathbf{f} \\ -\mathbf{f} \end{bmatrix}}_{\boldsymbol{g}}.$$

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

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

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

Symmetric reformulations

$$\boldsymbol{\mathcal{A}} = \begin{bmatrix} \mathbf{A} & -\mathbf{K} \\ -\mathbf{K}^\top & -\left(\mathbf{K} + \mathbf{K}^\top + \mathbf{A}\right) \end{bmatrix}, \qquad \boldsymbol{\mathcal{A}} \boldsymbol{u} = \boldsymbol{g},$$

Proposition: Stability of symmetric reformulation

$$c_1 \|\boldsymbol{u}\|_* \le \sup_{\boldsymbol{v} \in \mathbb{V}^N \times \mathbb{V}^N \setminus \{0\}} \frac{\boldsymbol{v}^\top \boldsymbol{\mathcal{A}} \boldsymbol{u}}{\|\boldsymbol{v}\|_*} \le c_2 \|\boldsymbol{u}\|_*.$$

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

$$\|\boldsymbol{v}\|_*^2 := \|\mathbf{q}\|_{\mathbf{A}}^2 + \|\mathbf{v}\|_{\mathbf{S}}^2, \quad \boldsymbol{v} = [\mathbf{q}, \mathbf{v}] \in \mathbb{V}^N \times \mathbb{V}^N.$$

- stability distinguishes this from “classical” symmetric formulations, e.g. $\mathbf{B}^\top \mathbf{B} \mathbf{u} = \mathbf{B}^\top \mathbf{f}$.
- 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 $\boldsymbol{u}_j = [\mathbf{p}_j, \mathbf{u}_j]$ where

$$\mathbf{p}_{j+1} = \mathbf{p}_j + \widetilde{\mathbf{A}}^{-1} \left(\mathbf{K}\mathbf{u}_j - \mathbf{A}\mathbf{p}_j - \mathbf{f} \right),$$
$$\mathbf{u}_{j+1} = \mathbf{u}_j + \omega \widetilde{\mathbf{H}}^{-1} \left(\mathbf{f} - \mathbf{K}^\top \mathbf{p}_{j+1} - \left[\mathbf{K} + \mathbf{K}^\top + \mathbf{A} \right] \mathbf{u}_j \right),$$

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

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

We will specify a suitable time-parallel $\widetilde{\mathbf{H}}$ in next few slides.

Interpretation of inexact Uzawa as using inexact left-preconditioner

Inexact Uzawa

$$\mathbf{p}_{j+1} = \mathbf{p}_j + \widetilde{\mathbf{A}}^{-1} \left(\mathbf{K}\mathbf{u}_j - \mathbf{A}\mathbf{p}_j - \mathbf{f} \right),$$
$$\mathbf{u}_{j+1} = \mathbf{u}_j + \omega \widetilde{\mathbf{H}}^{-1} \left(\mathbf{f} - \mathbf{K}^\top \mathbf{p}_{j+1} - \left[\mathbf{K} + \mathbf{K}^\top + \mathbf{A} \right] \mathbf{u}_j \right),$$

Recall the ideal left preconditioner $\mathbf{P} = \mathbf{A}^{-1}\mathbf{K} + \mathbf{I}$ and $\mathbf{S} = \mathbf{P}^\top \mathbf{B}$.

Suppose we choose initial guess $\mathbf{p}_0 = -\mathbf{u}_0$ (consistent with exact solution)

Then doing 1 step of the Inexact Uzawa on $\boldsymbol{u_0} = [\mathbf{p}_0, \mathbf{u}_0]$ is equivalent to

$$\mathbf{u}_1 = \mathbf{u}_0 + \omega \widetilde{\mathbf{H}}^{-1} \widetilde{\mathbf{P}}^\top \left(\mathbf{f} - \mathbf{B}\mathbf{u}_0 \right)$$

with $\widetilde{\mathbf{P}} = \widetilde{\mathbf{A}}^{-1}\mathbf{K} + \mathbf{I}$.

Advantage of saddle point formulation is established convergence theory.

NB: it is not necessary to require $\mathbf{p}_0 = -\mathbf{u}_0$ for the inexact Uzawa method to converge (see following).

General convergence theory of Uzawa

Inexact Uzawa

$$\mathbf{p}_{j+1} = \mathbf{p}_j + \widetilde{\mathbf{A}}^{-1}\left(\mathbf{K}\mathbf{u}_j - \mathbf{A}\mathbf{p}_j - \mathbf{f}\right),$$
$$\mathbf{u}_{j+1} = \mathbf{u}_j + \omega\widetilde{\mathbf{H}}^{-1}\left(\mathbf{f} - \mathbf{K}^\top\mathbf{p}_{j+1} - \left[\mathbf{K} + \mathbf{K}^\top + \mathbf{A}\right]\mathbf{u}_j\right),$$

Convergence theory of inexact Uzawa requires:

$$\|\mathbf{I} - \widetilde{\mathbf{A}}^{-1}\mathbf{A}\|_{\widetilde{\mathbf{A}}} \leq \rho_{\mathbf{A}} < 1 \qquad \text{(Contraction)}$$
$$\lambda_{\min}\widetilde{\mathbf{H}} \leq \mathbf{S} \leq \lambda_{\max}\widetilde{\mathbf{H}} \qquad \text{(Spectral equivalence)}$$

with $\lambda_{\max} \geq \lambda_{\min} > 0$.

General convergence theory of Uzawa

Theorem: Convergence of inexact Uzawa

Define the norm

$$\|\boldsymbol{v}\|_{\boldsymbol{\mathcal{D}}}^2 := \omega\rho_{\mathbf{A}}\|\mathbf{q}\|_{\widetilde{\mathbf{A}}}^2 + \|\mathbf{v}\|_{\widetilde{\mathbf{H}}}^2 \quad \forall \boldsymbol{v} = [\mathbf{q}, \mathbf{v}].$$

Then

$$\|\boldsymbol{u} - \boldsymbol{u}_{j+1}\|_{\boldsymbol{\mathcal{D}}} \leq \rho_U \|\boldsymbol{u} - \boldsymbol{u}_j\|_{\boldsymbol{\mathcal{D}}}$$

where $\rho_U := \max\{\sigma_-, \sigma_+\}$:

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

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

Convergent under damping condition:

$$\omega\,\lambda_{\max} < 2\,\frac{1-\rho_{\mathbf{A}}}{1+\rho_{\mathbf{A}}} \implies \rho_U < 1.$$

Proof based on Zulehner 02

Preconditioners for the Schur complement

We need to find $\widetilde{\mathbf{H}}$ such that

$$\lambda_{\min}\widetilde{\mathbf{H}} \leq \mathbf{S} \leq \lambda_{\max}\widetilde{\mathbf{H}}$$

Motivation by following example:

Example: Constant operators with uniform time-steps

In special case $\tau_n = \tau$ and $A_n = A$:

$$\mathbf{S} = \frac{1}{\tau} K^\top K \otimes M A^{-1} M + (K + K^\top) \otimes M + \mathrm{Id}_N \otimes \tau A.$$

$$K^\top K = \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & & \ddots & -1 \\ & & -1 & 1 \end{pmatrix}, \quad K + K^\top = \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & & \ddots & -1 \\ & & -1 & 2 \end{pmatrix}.$$

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 τ, 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.

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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.

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

Consequence

Then $\mathbf{S}$ is spectrally equivalent to a simpler matrix $\widetilde{\mathbf{S}}$:

$$\frac{1}{\alpha}\widetilde{\mathbf{S}} \leq \mathbf{S} \leq 3\alpha\widetilde{\mathbf{S}},$$

$$\widetilde{\mathbf{S}} := \frac{1}{\tau} K^\top K \otimes M A^{-1} M + \widetilde{\mathrm{Id}}_N \otimes \tau A, \qquad \widetilde{\mathrm{Id}}_N = \begin{pmatrix} 1 & & \\ & \ddots & \\ & & 1/2 \end{pmatrix}$$

Preconditioners for the Schur complement

Idea: *Block-diagonalise the simpler matrix* $\widetilde{\mathbf{S}}$ *by a Discrete Sine Transform (DST)*
Define (Type-II/III) DST

$$\hat{\mathbf{u}} = \mathbf{\Phi}\,\mathbf{u}, \qquad \hat{u}_k = \frac{2}{N}\sum_{n=1}^{N}\frac{1}{1+\delta_{nN}}u_n \sin\left(\frac{(2k-1)n\pi}{2N}\right), k = 1,\dots,N.$$

$$\mathbf{u} = \mathbf{\Phi}^{-1}\hat{\mathbf{u}}, \qquad u_n = \sum_{k=1}^{N}\hat{u}_k \sin\left(\frac{(2k-1)n\pi}{2N}\right), \quad n = 1,\dots,N.$$

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

$$\widetilde{\mathbf{S}} = \mathbf{\Phi}^\top \hat{\mathbf{D}}\,\mathbf{\Phi}, \qquad \hat{\mathbf{D}} := \frac{N}{2}\,\mathrm{diag}\left\{\frac{\mu_k^2}{\tau}MA^{-1}M + \tau A\right\}_{k=1}^{N},$$

with $\mu_k := 2\sin\left(\frac{(2k-1)\pi}{4N}\right) > 0$ for $k = 1,\dots,N$.

Preconditioners for the Schur complement

$$\widetilde{\mathbf{S}} = \mathbf{\Phi}^\top \hat{\mathbf{D}}\, \mathbf{\Phi}, \qquad \hat{\mathbf{D}} := \frac{N}{2}\,\mathrm{diag}\left\{ \frac{\mu_k^2}{\tau} M A^{-1} M + \tau A \right\}_{k=1}^{N},$$

Idea from Pearson & Wathen 2014:

$$\frac{\mu_k^2}{\tau} M A^{-1} M + \tau A \approx \frac{1}{\tau} H_k A^{-1} H_k, \qquad H_k := \mu_k M + \tau A$$

So we propose "ideal" (exact spatial inverses) preconditioner

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

Main spectral equivalence result

$$\frac{1}{2\alpha}\mathbf{H} \leq \mathbf{S} \leq 3\alpha \mathbf{H}.$$

Proof: $\frac{1}{2}\mathbf{H} \leq \widetilde{\mathbf{S}} \leq \mathbf{H}$ and $\frac{1}{\alpha}\widetilde{\mathbf{S}} \leq \mathbf{S} \leq 3\alpha\widetilde{\mathbf{S}}$.

Preconditioners for the Schur complement

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

We shall assume that there are fixed positive constants γ and Γ such that

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

Then

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

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

Preconditioners for the Schur complement

Summary of convergence theory

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

$$\|\boldsymbol{u} - \boldsymbol{u}_{j+1}\|_{\boldsymbol{\mathcal{D}}} \leq \rho_U \|\boldsymbol{u} - \boldsymbol{u}_j\|_{\boldsymbol{\mathcal{D}}}.$$

- 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 ω, α, $\rho_{\mathbf{A}}$, γ and Γ).
- Only a small number of quantities determine ρ_U: $\rho_{\mathbf{A}}$, γ, Γ, α, ω.

Parallel complexity

Cost of different spatial operations treated abstractly:

- $C_{\mathbb{V}}^{\mathrm{add}}$ cost of additions and subtractions of vectors in $\mathbb{V}$;
- $C_{\mathbb{V}}^{\mathrm{mult}}$ cost of performing a matrix vector product with M, A or A_n, $n = 1, \ldots, N$;
- $C_{\mathbb{V}}^{\mathrm{prec}}$ cost of performing the action of the spatial preconditioners $\widetilde{A_n}^{-1}$ or $\widetilde{H_k}^{-1}$.

Parallel complexity (assuming O(N) processors)

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

where constant is independent of $\mathbb{V}$ and of N.

Theory summary

- existing theory of iterative methods for symmetric systems to solve nonsymmetric $\mathbf{Bu} = \mathbf{f}$.
- 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 $\mathbf{H}^{-1}\mathbf{S}$

1D heat equation (for accuracy of computations)

$h = 1/64$	$N = 4$	$N = 8$	$N = 16$	$N = 32$	$N = 64$	$N = 128$	$N = 256$	$N = 512$	$N = 1024$
$\lambda_{\min}$	0.8099	0.7080	0.6270	0.5728	0.5402	0.5223	0.5129	0.5081	0.5056
$\lambda_{\max}$	1.9999	1.9998	1.9996	1.9993	1.9986	1.9972	1.9944	1.9888	1.9780
$\kappa(\mathbf{H}^{-1}\mathbf{S})$	2.4693	2.8248	3.1893	3.4906	3.6994	3.8237	3.8885	3.9145	3.9122

$h = 1/128$	$N = 4$	$N = 8$	$N = 16$	$N = 32$	$N = 64$	$N = 128$	$N = 256$	$N = 512$	$N = 1024$
$\lambda_{\min}$	0.8099	0.7079	0.6270	0.5728	0.5402	0.5223	0.5129	0.5081	0.5056
$\lambda_{\max}$	2.0000	2.0000	1.9999	1.9998	1.9996	1.9993	1.9986	1.9972	1.9944
$\kappa(\mathbf{H}^{-1}\mathbf{S})$	2.4694	2.8250	3.1897	3.4916	3.7014	3.8278	3.8967	3.9310	3.9445

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

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

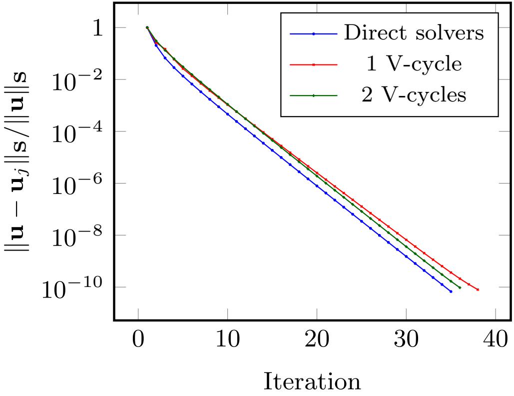
Eigenvalue $\lambda_{\max} \approx 2$ suggest that damping parameter $\omega < 1$ is enough for $\rho_{\mathbf{A}}$ reasonably small: e.g. we can take $\omega = 0.9$.

Numerical experiments

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

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

2D computation with 4 064 256 DOFs



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

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

	$h = 1/8$	$h = 1/16$	$h = 1/32$	$h = 1/64$
$N = 128$	20	21	21	21
$N = 256$	21	22	22	22
$N = 512$	22	22	22	22
$N = 1024$	22	22	22	22

Iterations to reach $\|\mathbf{u} - \mathbf{u}_j\|_{\mathsf{S}} < 10^{-6}\|\mathbf{u}\|_{\mathsf{S}}$.

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 *hypre* 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}

procs	N	dofs	iter	time/iter	total time	time FFT (%)	time AMG (%)
1	16	157 216	15	1.87	28.00	0.9%	84.5%
2	32	314 432	15	1.85	27.75	1.5%	83.4%
4	64	628 864	15	1.81	27.16	1.7%	82.8%
8	128	1 257 728	15	1.77	26.60	1.9%	82.4%
16	256	2 515 456	15	1.78	26.72	2.1%	82.1%
32	512	5 030 912	15	1.79	26.78	2.3%	82.0%
64	1 024	10 061 824	16	1.79	28.66	3.0%	81.3%
128	2 048	20 123 648	19	1.81	34.35	4.1%	79.8%
256	4 096	40 247 296	20	1.81	36.11	4.2%	79.5%
512	8 192	80 494 592	21	1.80	37.88	4.2%	79.3%
1 024	16 384	160 989 184	22	1.81	39.77	4.4%	79.0%
2 048	32 768	321 978 368	22	1.82	40.10	5.3%	78.3%
4 096	65 536	643 956 736	22	1.87	41.09	7.4%	76.4%

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}

procs	N	dofs	iter	time/iter	total time	time FFT (%)	time AMG (%)
16	65 536	643 956 736	22	310.18	6823.88	3.9%	72.9%
32	65 536	643 956 736	22	155.68	3425.04	4.1%	72.9%
64	65 536	643 956 736	22	78.66	1730.53	4.8%	72.4%
128	65 536	643 956 736	22	39.98	879.52	5.5%	72.0%
256	65 536	643 956 736	22	20.89	459.60	7.1%	70.5%
512	65 536	643 956 736	22	10.76	236.82	7.3%	70.9%
1024	65 536	643 956 736	22	5.65	124.22	6.8%	72.3%
2048	65 536	643 956 736	22	3.13	68.79	7.0%	74.1%
4096	65 536	643 956 736	22	1.87	41.09	7.4%	76.4%

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 $p_x p_t$ processors (up to 131 072)
- Spatial parallelism in AMG provided by *hypre* (default settings).
- Timings to solution

		procs w.r.t. space p_x					
		16	32	64	128	256	512
procs w.r.t. time p_t	4	12 158.70	7 000.47	4 381.72	2 925.62	2 132.41	2 107.73
	8	6 721.02	3 911.30	2 437.63	1 654.01	1 219.39	1 170.38
	16	4 016.91	3 522.05	1 459.71	1 007.60	728.52	703.79
	32	2 203.77	1 946.12	822.15	565.93	421.31	418.68
	64	1 212.84	9 04.27	429.03	304.47	238.31	245.17
	128	667.20	468.11	220.43	162.00	130.97	135.74
	256	341.14	232.08	117.75	85.76	70.97	74.36
	512	172.21	119.18	59.54	44.76	37.58	
	1 024	84.94	60.44	30.12	23.07		
	2 048	44.92	31.73	15.96			
	4 096	27.94	21.29				

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 $\mathbf{S}$
  - 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!