

Preconditioning for parallel-in-time

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ODE IVP

$$y' = ay + f, \quad y(t_0) = y_0$$

discretise: e.g.

$$\frac{y^{k+1} - y^k}{\tau} = \theta ay^{k+1} + (1 - \theta)ay^k + f^k, \quad y^0 = y_0,$$

$k = 0, 1, \dots, \ell$ with $\ell\tau = T$ gives

$$B \underbrace{\begin{bmatrix} y^1 \\ y^2 \\ y^3 \\ \vdots \\ y^\ell \end{bmatrix}}_y = \underbrace{\begin{bmatrix} \tau f^1 + (1 + a(1 - \theta)\tau)y^0 \\ \tau f^2 \\ \tau f^3 \\ \vdots \\ \tau f^\ell \end{bmatrix}}_f,$$

where the $\ell \times \ell$ coefficient matrix B is

$$\begin{bmatrix} b & & & & & \\ c & b & & & & \\ & c & b & & & \\ & & \ddots & \ddots & & \\ & & & c & b & \end{bmatrix},$$

$$b = 1 - a\theta\tau, \quad c = -1 - a(1 - \theta)\tau.$$

i.e. B is a bidiagonal Toeplitz (constant diagonal) matrix.

- forward substitution \rightarrow sequential—*causality*

Iterative methods for $\mathbf{B}\mathbf{x} = \mathbf{c}$, $\mathbf{B} \in \mathbb{R}^{n \times n}$:

From $\mathbf{x}_0 = \mathbf{0}$ (typically) generate $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k, \dots\}$ using one matrix \times vector product at each iteration:

$$\mathbf{B}\mathbf{c}, \mathbf{B}(\mathbf{B}\mathbf{c}), \dots, \mathbf{B}^k\mathbf{c}, \dots \quad \text{so that}$$

$$\mathbf{x}_1 \in \text{span}\{\mathbf{c}\}, \mathbf{x}_2 \in \text{span}\{\mathbf{c}, \mathbf{B}\mathbf{c}\}, \dots, \mathbf{x}_k \in \text{span}\{\mathbf{c}, \mathbf{B}\mathbf{c}, \dots, \mathbf{B}^{k-1}\mathbf{c}\}, \dots$$

\Rightarrow Krylov subspace methods generally described by:

$$\mathbf{r}_k = \mathbf{p}_k(\mathbf{B})\mathbf{r}_0, \quad \mathbf{r}_k = \mathbf{c} - \mathbf{B}\mathbf{x}_k, \quad \mathbf{p}_k \in \Pi_k, \mathbf{p}_k(\mathbf{0}) = \mathbf{1}$$

so if $\mathbf{B} = \mathbf{X}\mathbf{\Lambda}\mathbf{X}^{-1}$ then

$$\|\mathbf{r}_k\| \leq \|\mathbf{X}\| \|\mathbf{p}_k(\mathbf{\Lambda})\| \|\mathbf{X}^{-1}\| \|\mathbf{r}_0\|$$

and if $\mathbf{B} = \mathbf{B}^T$ so that $\mathbf{X}^{-1} = \mathbf{X}^T$ then this bound on convergence in $\|\cdot\|_2$ depends only on eigenvalues

Well distributed (clustered) eigenvalues \Rightarrow fast convergence for symmetric matrices.

All-at-once system

Consider $y' = ay$, $y(0) = y_0$ i.e. $f = 0 \Rightarrow$ all-at-once system

$$By = \begin{bmatrix} b & & & & & \\ c & b & & & & \\ & c & b & & & \\ & & & \ddots & & \\ & & & & \ddots & \\ & & & & & c & b \end{bmatrix} \begin{bmatrix} y^1 \\ y^2 \\ y^3 \\ \vdots \\ y^\ell \end{bmatrix} = \begin{bmatrix} \tau f^0 - cy^0 \\ \tau f^1 \\ \tau f^2 \\ \vdots \\ \tau f^{\ell-1} \end{bmatrix} = \mathbf{f},$$

All-at-once system

But consider $y' = ay$, $y(0) = y_0$ i.e. $f = 0 \Rightarrow$
all-at-once system

$$By = \begin{bmatrix} b & & & & & \\ c & b & & & & \\ & c & b & & & \\ & & \ddots & \ddots & & \\ & & & c & b & \end{bmatrix} \begin{bmatrix} y^1 \\ y^2 \\ y^3 \\ \vdots \\ y^\ell \end{bmatrix} = \begin{bmatrix} 0 - cy^0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \mathbf{f},$$

i.e. \mathbf{f} only its first entry non-zero \Rightarrow with zero initial guess

$$y_1 \in \text{span} \left\{ \begin{bmatrix} \times \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \right\}, y_2 \in \text{span} \left\{ \begin{bmatrix} \times \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \begin{bmatrix} \times \\ \times \\ 0 \\ \vdots \\ 0 \end{bmatrix} \right\}, \dots$$

$$y_k \in \text{span} \left\{ \begin{bmatrix} \times \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \begin{bmatrix} \times \\ \times \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \dots, \begin{bmatrix} \times \\ \vdots \\ \times \\ 0 \\ \vdots \\ 0 \end{bmatrix} \right\}, \quad k = 1, 2, \dots$$

but solution is an exponential (non-zero for every time step) \Rightarrow need ℓ iterations.

Precisely: exact solution up to $k\tau$ at k^{th} iteration, zero for all other time steps: **causality**

thus solution for all ℓ time-steps only at ℓ^{th} iteration

NOT a parallel-in-time method!!

Iterative methods for linear systems

This is true for any of the available iterative methods:

(For self-adjoint problems/symmetric matrices, iterative methods of choice exist: conjugate gradients for Symmetric Positive Definite matrices, MINRES otherwise)

and any of the many possible methods for non-self-adjoint problems/nonsymmetric matrices: GMRES , BICGSTAB , LSQR , QMR , IDR , ...

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But it is well known that for almost all systems we need *preconditioning*

Preconditioner \mathbf{P} such that

$$“\mathbf{P}^{-1}\mathbf{B}\mathbf{x} = \mathbf{P}^{-1}\mathbf{b}”$$

has much faster convergence with the appropriate iterative method than $\mathbf{B}\mathbf{x} = \mathbf{b}$.

All-at-once system

A practical and guaranteed preconditioning approach: use
Pestana & W, 2015:

If \mathbf{B} is a real Toeplitz matrix then

$$\underbrace{\begin{bmatrix} a_0 & a_{-1} & \cdot & \cdot & a_{1-n} \\ a_1 & a_0 & a_{-1} & \cdot & \cdot \\ \cdot & a_1 & a_0 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & a_{-1} \\ a_{n-1} & \cdot & \cdot & a_1 & a_0 \end{bmatrix}}_{\mathbf{B}} \quad \underbrace{\begin{bmatrix} 0 & 0 & \cdot & 0 & 1 \\ 0 & \cdot & 0 & 1 & 0 \\ \cdot & 0 & 1 & 0 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & 0 & \cdot & 0 & 0 \end{bmatrix}}_{\mathbf{Y}}$$

is the real *symmetric* (Hankel) matrix

$$\begin{bmatrix} a_{1-n} & \cdot & \cdot & a_{-1} & a_0 \\ \cdot & \cdot & a_{-1} & a_0 & a_1 \\ \cdot & \cdot & a_0 & a_1 & \cdot \\ a_{-1} & \cdot & \cdot & \cdot & \cdot \\ a_0 & a_1 & \cdot & \cdot & a_{n-1} \end{bmatrix}$$

Thus MINRES can be robustly applied to \mathbf{BY} — it is symmetric but generally indefinite — and its convergence will depend only on eigenvalues.

BUT preconditioning? – needs to be symmetric and positive definite for MINRES

Fortunately it is well known that many Toeplitz matrices are well approximated by related circulant matrices, \mathbf{C} (*Strang, 1986, Chan, 1988, Chan, 1989, Tyrtyshnikov, 1996/7*) which are diagonalised by an FFT in $O(n \log n)$ work: $\mathbf{C} = \mathbf{F}^* \mathbf{\Lambda} \mathbf{F}$,

For many symmetric Toeplitz matrices we have that the Strang or Optimal (Chan) circulant \mathbf{C} satisfy

$$\mathbf{C}^{-1} \mathbf{B} = \mathbf{I} + \mathbf{R} + \mathbf{E}$$

where \mathbf{R} is of small rank and \mathbf{E} is of small norm

⇒ eigenvalues clustered around 1 except for a few outliers

For example, the Strang circulant for the standard Toeplitz matrix (as above) is

$$\underbrace{\begin{bmatrix}
 a_0 & a_{-1} & \dots & a_{-\lfloor \frac{n}{2} \rfloor} & a_{\lfloor \frac{n-1}{2} \rfloor} & \dots & a_2 & a_1 \\
 a_1 & a_0 & a_{-1} & \dots & a_{-\lfloor \frac{n}{2} \rfloor} & a_{\lfloor \frac{n-1}{2} \rfloor} & \dots & a_2 \\
 \dots & a_1 & a_0 & \ddots & \dots & a_{-\lfloor \frac{n}{2} \rfloor} & \ddots & \vdots \\
 a_{\lfloor \frac{n}{2} \rfloor} & \dots & \ddots & \ddots & \ddots & \dots & \ddots & a_{\lfloor \frac{n-1}{2} \rfloor} \\
 a_{-\lfloor \frac{n-1}{2} \rfloor} & \ddots & \dots & \ddots & \ddots & \ddots & \dots & a_{-\lfloor \frac{n}{2} \rfloor} \\
 \vdots & \ddots & a_{\lfloor \frac{n}{2} \rfloor} & \dots & \ddots & a_0 & a_{-1} & \dots \\
 a_{-2} & \dots & a_{-\lfloor \frac{n-1}{2} \rfloor} & a_{\lfloor \frac{n}{2} \rfloor} & \dots & a_1 & a_0 & a_1 \\
 a_{-1} & a_{-2} & \dots & a_{-\lfloor \frac{n-1}{2} \rfloor} & a_{\lfloor \frac{n}{2} \rfloor} & \dots & a_1 & a_0
 \end{bmatrix}}_C$$

To ensure a symmetric and positive definite preconditioner for **BY** just use

$$|\mathbf{C}| = \mathbf{F}^* |\mathbf{\Lambda}| \mathbf{F}$$

which is real symmetric and positive definite

To ensure a symmetric and positive definite preconditioner for $\mathbf{B}\mathbf{Y}$ just use

$$|\mathbf{C}| = \mathbf{F}^* |\mathbf{\Lambda}| \mathbf{F}$$

which is real symmetric and positive definite

Theorem (*Pestana & W, 2015*)

$$|\mathbf{C}|^{-1} \mathbf{B}\mathbf{Y} = \mathbf{J} + \mathbf{R} + \mathbf{E}$$

where \mathbf{J} is real symmetric and orthogonal with eigenvalues ± 1 , \mathbf{R} is of small rank and \mathbf{E} is of small norm

\Rightarrow guaranteed fast convergence because MINRES convergence only depends on eigenvalues which are clustered around ± 1 except for few outliers!

To ensure a symmetric and positive definite preconditioner for $\mathbf{B}\mathbf{Y}$ just use

$$|\mathbf{C}| = \mathbf{F}^* |\mathbf{\Lambda}| \mathbf{F}$$

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Theorem (*Pestana & W, 2015*)

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where \mathbf{J} is real symmetric and orthogonal with eigenvalues ± 1 , \mathbf{R} is of small rank and \mathbf{E} is of small norm

For the ODE problem ($\tau = 0.2$, $a = -0.3$, $\theta = 0.8$):

ℓ	$\kappa(B)$	Iterations
10	10.474	4
100	30.852	4
1000	33.887	4

Multistep method: BDF2

$$\frac{y^{k+1} - \frac{4}{3}y^k + \frac{1}{3}y^{k-1}}{\tau} = \frac{2}{3}ay^{k+1} + \frac{2}{3}f^{k+1},$$

with $y^0 = y_0$ and $y^{-1} = y_{-1}$ leads to the monolithic or all-at-once system

$$B \underbrace{\begin{bmatrix} y^1 \\ y^2 \\ y^3 \\ \vdots \\ y^\ell \end{bmatrix}}_y = \underbrace{\begin{bmatrix} \frac{2}{3}\tau f^1 + \frac{4}{3}y^0 - \frac{1}{3}y^{-1} \\ \frac{2}{3}\tau f^2 - \frac{1}{3}y^0 \\ \frac{2}{3}\tau f^3 \\ \vdots \\ \frac{2}{3}\tau f^\ell \end{bmatrix}}_f$$

This gives a *parallel-in-time* method if all components are efficiently implemented in parallel.

Moreover we *observe* that GMRES with just \mathbf{C} as preconditioner gives even better convergence (but no proof!)

Preconditioning

Note that the circulant preconditioner here simply represents preconditioning the Initial Value Problem

$$y' = ay + f, \quad y(0) = y_0$$

with the *nearby* periodic problem

$$y' = ay + f, \quad y(0) = y(T)$$

for which Fourier technology gives rapid (and parallel) application

This approach also applies for systems of ODEs and for time-dependent PDEs \Rightarrow block Toeplitz/block circulant matrices for which standard parallel technologies can be applied in space and the periodic preconditioning only applied in time

PDEs: diffusion problem

$$\begin{aligned}u_t &= \Delta u + f && \text{in } \Omega \times (0, T], \quad \Omega \subset \mathbb{R}^2 \text{ or } \mathbb{R}^3, \\u &= g && \text{on } \partial\Omega, \\u(x, 0) &= u_0(x) && \text{at } t = 0\end{aligned}$$

Discretize - finite elements, mesh size h , and n spatial dofs:

$$M \frac{u_k - u_{k-1}}{\tau} + K u_k = f_k, \quad k = 1, \dots, \ell,$$

or

$$\mathcal{A}_{BEX} := \begin{bmatrix} A_0 & & & & \\ A_1 & A_0 & & & \\ & \ddots & \ddots & & \\ & & & A_1 & A_0 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_\ell \end{bmatrix} = \begin{bmatrix} M u_0 + \tau f_1 \\ \tau f_2 \\ \vdots \\ \tau f_\ell \end{bmatrix},$$

where $A_0 = M + \tau K$ is symmetric positive definite and $A_1 = -M$ is symmetric.

We use the block circulant preconditioner

$$\mathcal{P}_{BE} := \begin{bmatrix} A_0 & & & A_1 \\ A_1 & A_0 & & \\ & \ddots & \ddots & \\ & & A_1 & A_0 \end{bmatrix} \cdot$$

Theorem (*McDonald, Pestana & W, 2018*)

$\mathcal{P}_{BE}^{-1} \mathcal{A}_{BE}$ is diagonalisable, has $(\ell - 1)n$ eigenvalues of 1 and n eigenvalues which cluster around 1 for small h .

\Rightarrow fast and ℓ -independent convergence (with flip to be guaranteed) of the appropriate iterative methods

2nd part of talk: Incompressible Navier-Stokes

$$\left\{ \begin{array}{l} \frac{\partial \mathbf{u}}{\partial t}(\mathbf{x}, t) + (\mathbf{w}(\mathbf{x}, t) \cdot \nabla) \mathbf{u}(\mathbf{x}, t) \\ \quad - \mu \nabla^2 \mathbf{u}(\mathbf{x}, t) + \nabla p(\mathbf{x}, t) = \mathbf{f}(\mathbf{x}, t) \\ \quad \quad \quad \nabla \cdot \mathbf{u}(\mathbf{x}, t) = 0 \end{array} \right.$$

\mathbf{u} : velocity, p : pressure, \mathbf{w} : wind (= \mathbf{u} for full N-S)

Linearisation is time-dependent Stokes equations:

$$\left\{ \begin{array}{l} \frac{\partial \mathbf{u}}{\partial t}(\mathbf{x}, t) - \mu \nabla^2 \mathbf{u}(\mathbf{x}, t) + \nabla p(\mathbf{x}, t) = \mathbf{f}(\mathbf{x}, t) \\ \quad \quad \quad \nabla \cdot \mathbf{u}(\mathbf{x}, t) = 0 \end{array} \right.$$

Discretize: Galerkin finite elements in space, Backwards Euler in time, constant time-step Δt

$$\begin{cases} \frac{1}{\Delta t} \mathcal{M}_u (u^k - u^{k-1}) + \mu \mathcal{A}_u u^k + \mathcal{W}_{u,k} u^k + \mathcal{B}^T p^k = f^k \\ \mathcal{B} u^k = 0 \end{cases},$$

$k = 1, \dots, \ell$ with $\ell \Delta t = T$.

To simplify notation define the time-dependent advection-diffusion operator

$$\mathcal{F}_{u,k} = \frac{\mathcal{M}_u}{\Delta t} + \mathcal{W}_{u,k} + \mu \mathcal{A}_u, \quad k = 1, \dots, \ell.$$

This is thus the system

$$\begin{bmatrix} \mathcal{F}_{u,1} & \mathcal{B}^T \\ \mathcal{B} \\ -\frac{\mathcal{M}_u}{\Delta t} \\ \vdots \\ \mathcal{F}_{u,l} & \mathcal{B}^T \\ \mathcal{B} \\ \vdots \end{bmatrix} \begin{bmatrix} u^1 \\ p^1 \\ \vdots \\ u^l \\ p^l \end{bmatrix} = \begin{bmatrix} f^1 \\ 0 \\ \vdots \\ f^l \\ 0 \end{bmatrix} .$$

Reorder to

$$\underbrace{\begin{bmatrix} \mathcal{F}_{u,1} & & & \mathcal{B}^T \\ -\frac{\mathcal{M}_u}{\Delta t} & \ddots & & \ddots \\ & \ddots & \mathcal{F}_{u,l} & \mathcal{B}^T \\ \hline \mathcal{B} & & & \\ & \ddots & & \\ & & \mathcal{B} & \end{bmatrix}}_{A = \begin{bmatrix} F & B^T \\ B & \end{bmatrix}} \underbrace{\begin{bmatrix} u^1 \\ \vdots \\ u^l \\ \hline p^1 \\ \vdots \\ p^l \end{bmatrix}}_{\begin{bmatrix} u \\ \hline p \end{bmatrix}} = \begin{bmatrix} f^1 \\ \vdots \\ f^l \\ \hline 0 \\ \vdots \\ 0 \end{bmatrix} ;$$

Important point: Saddle-point system: F is now a time-dependent (advection-)diffusion operator; something we might have excellent PinT methods for!!

Block preconditioning for Saddle-point systems

based on the observation (*Murphy, Golub, W (2000)*)

$$\begin{bmatrix} F & B^T \\ B & 0 \end{bmatrix}$$

preconditioned by

- $\begin{bmatrix} F & 0 \\ 0 & S \end{bmatrix}$ has 3 distinct eigenvalues
- $\begin{bmatrix} F & B^T \\ 0 & S \end{bmatrix}$ has 2 distinct eigenvalues

where $S = BF^{-1}B^T$ (Schur Complement)

⇒ MINRES /GMRES terminates in 3 / 2 iterations

⇒ want approximations \hat{F} , \hat{S} ⇒ 3 / 2 clusters

⇒ fast convergence

Preconditioning the All-at-once system

use PinT method for F and Schur complement approximation

$$S^{-1} \approx M_p^{-1} F_p A_p^{-1}$$

where

- M_p is a block diagonal matrix of pressure mass matrices
- F_p represents time-integration on the pressure space analogous to F_u
- A_p represents a block diagonal matrix of discrete pressure Laplacians

which is essentially an identical approach to the highly successful PCD approach for the steady-state problem

Elman, Silvester, W (2014)

Number of GMRES iterations: driven cavity problem for $t \in [0, 1]$ (thus $T = 1$)

$\Delta x \Delta t$	2^{-3}		2^{-4}		2^{-5}		2^{-6}		2^{-7}	
2^{-4}	25	(25)	25	(26)	24	(25)	24	(31)	23	(28)
2^{-5}	23	(25)	23	(24)	22	(24)	23	(32)	22	(24)
2^{-6}	22	(26)	21	(26)	21	(26)	22	(28)	21	(28)
2^{-7}	21	(28)	20	(28)	21	(31)	21	(32)	20	(33)
2^{-8}	20	(28)	19	(30)	20	(32)	19	(32)	19	(34)

exact subsystem solves (iterative subsystem solves)

- F_u^{-1} : AIR
- M_p^{-1} : Chebyshev (semi-)iteration
- F_p : matrix multiply
- A_p^{-1} : AMG (BoomerAMG)

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