On the usage of spectral information about matrices arising from parallel-in-time integration

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MATHEMATICAL MODELLING, ANALYSIS AND COMPUTATIONAL MATHEMATICS



BERGISCHE UNIVERSITÄT WUPPERTAL

# Outline

#### Introduction

## Approximation of the spectrum

Local Fourier Analysis Semi-algebraic mode analysis Momentary symbol

#### Usage of the spectral information

Analysis of stationary iterative methods Analysis of Krylov subspace methods

#### Conclusion



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## Analysis of all-at-once systems

Consider

$$u_t = u_x x, \quad x \in \mathbb{R}/\mathbb{Z}, t \in [0, T].$$

Parallel-in-time integration using backward Euler yields linear system

$$A_{\mathbf{n}}x=b,\quad A_{\mathbf{n}}=J_{N_t}\otimes\mathbb{I}_{N_x}+\mathbb{I}_{N_t}\otimes Q_{N_x}\in\mathbb{R}^{N\times N},\quad x,b\in\mathbb{R}^N,$$
 with

$$J_{N_t} = \frac{1}{h_t} \begin{bmatrix} 1 & & & \\ -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{bmatrix}, \quad Q_{N_x} = \frac{1}{h_x^2} \begin{bmatrix} 2 & -1 & & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & & & -1 & 2 \end{bmatrix}$$

We want to compute the spectrum of these systems in order to analyze and design iterative methods for their solution.

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## **Toeplitz matrices**

▶ Toeplitz matrices  $\{T_n\}_{n=0}^\infty \in \mathbb{C}^{n \times n}$  given by

$$T_n = \begin{pmatrix} t_0 & t_{-1} & t_{-2} & \cdots & t_{-n+1} \\ t_1 & t_0 & t_{-1} & \ddots & \vdots \\ t_2 & t_1 & t_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ t_{n-1} & t_{n-2} & t_{n-3} & \cdots & t_0 \end{pmatrix}$$

Diagonal entries given by Fourier coefficients of generating symbol f:

$$t_j = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-2\pi \mathrm{i} j x} dx$$

Classical result from Szegö:

Theorem

If  $f \in L_{\infty}$  is real-valued, then the eigenvalues of the Hermitian Toeplitz matrices  $A_n$  are distributed as f(x).



## Circulant matrices

Circulant matrices are "periodic cousins" of Toeplitz matrices
 Given a vector c = (c<sub>0</sub>, c<sub>1</sub>, c<sub>2</sub>, ..., c<sub>n-1</sub>)<sup>T</sup> it is defined as

$$C_{n}(\mathbf{c}) := \begin{pmatrix} c_{0} & c_{1} & c_{2} & \cdots & c_{n-1} \\ c_{n-1} & c_{0} & c_{1} & \cdots & c_{n-2} \\ c_{n-2} & c_{n-1} & c_{0} & \cdots & c_{n-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_{1} & c_{2} & c_{3} & \cdots & c_{0} \end{pmatrix} \in \mathbb{R}^{n \times n}.$$

• Can be defined using the generating symbol f by

$$C_n(f) = F_n \operatorname{diag}_{i=0,\dots,n-1} (f(\theta_i^{(n)}) F_n^H),$$

where 
$$F_n = \frac{1}{\sqrt{n}} \left[ e^{-ij\theta_i^{(n)}} \right]_{i,j=0}^{n-1}$$
 and  $\theta_i^{(n)} = \frac{2\pi i}{n}$ .



# All-at-once matrix and it's Toeplitz and circulant symbols

►  $J_{N_t}$  has unilevel scalar Toeplitz structure with  $f_J(\theta) = 1 - e^{i\theta}$ :

$$J_{N_t} = \frac{1}{h_t} \begin{bmatrix} 1 & & & \\ -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{bmatrix} = \frac{1}{h_t} T_{N_t}(f_J)$$

•  $Q_{N_x}$  is a circulant matrix with  $f_Q(\xi) = 2 - 2\cos\xi$ :

$$Q_{N_x} = \frac{1}{h_x^2} \begin{bmatrix} 2 & -1 & & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & & & -1 & 2 \end{bmatrix} = \frac{1}{h_x^2} C_{N_x}(f_Q)$$

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#### Local Fourier Analysis (LFA) e.g., Wienands, Joppich (2005)

#### Error Propagation Operator

$$e_{j+1} = Ee_j$$

$$||E|| = \max_{\|e\|=1} ||Ee|| \qquad E_{\rm J} = I - \omega D^{-1} A$$
  

$$\rho(E) = \lim_{n \to \infty} ||E^n||^{1/n} \qquad E_{\rm TG} = S(I - PA_2^{-1}RA_1)S$$





# Local Fourier Analysis - Simplifications



$$[Lu](C) = -1u(N) - 1u(W) + 4u(C) - 1u(E) - 1u(S)$$



## Local Fourier Analysis – Simplifications





# Local Fourier Analysis - DTFT of constant stencils



#### Theorem

Let  $\hat{a} \in L^{\infty}(\Theta_h)$  be the Fourier symbol of A. Then,  $\|A\|_{\ell_2} = \operatorname{ess-sup}_{\vartheta} |\hat{a}(\vartheta)|$  and  $\rho(A) = \operatorname{ess-sup}_{\vartheta} |\hat{a}(\vartheta)|$ 





#### Local Fourier Analysis – DTFT of periodic stencils B. , Rittich (2018)

$$\begin{aligned} [\mathcal{R}_{\mathbf{n}} : L_{2}(\Theta_{\mathbf{h}}) &\to L_{2}(\Theta_{\mathbf{n} \cdot \mathbf{h}}) \\ [\mathcal{R}_{\mathbf{n}} \hat{u}]_{\mathbf{j}}(\theta) &= \hat{u} \left( \theta + \frac{2\pi}{\mathbf{hn}} \mathbf{j} \right) \end{aligned}$$

$$\hat{A} \hat{u} &= \mathcal{F}_{\mathbf{h}'} A \mathcal{F}_{\mathbf{h}}^{-1} \hat{u} \qquad u \xrightarrow{\mathcal{F}_{\mathbf{h}}} \hat{u} \xrightarrow{\mathcal{R}_{\mathbf{n}}} \hat{u} \\ \mathcal{R}_{\mathbf{m}} \hat{A} \mathcal{R}_{\mathbf{n}}^{-1} \hat{u} &= \hat{a} \cdot \hat{u} \\ \hat{a} \in L_{\infty}(\Theta_{\mathbf{n} \cdot \mathbf{h}})^{\mathbf{m} \times \mathbf{n}} \qquad A \downarrow \qquad \downarrow \hat{A} \qquad \downarrow \hat{f} = \hat{a} \cdot \vec{u} \\ f \xrightarrow{\mathcal{F}_{\mathbf{h}'}} \hat{f} \xrightarrow{\mathcal{R}_{\mathbf{m}'}} \hat{f} \xrightarrow{\mathcal{R}_{\mathbf{m}'}} \vec{f} \end{aligned}$$

 $\mathcal{D} \to L(\Omega) \to L(\Omega)^n$ 

#### Theorem

$$||A|| = \operatorname{ess-sup}_{\vartheta} ||\hat{a}(\vartheta)||_{2}$$
  

$$\rho(A) = \operatorname{ess-sup}_{\vartheta} \rho(\hat{a}(\vartheta))$$

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https://hrittich.github.io/lfa-lab/

- Versatile; based on combination of Fourier matrix symbols.
- Uses two-pass evaluation strategy.

1st Determine proper settings for evaluation.

2nd Evaluate formula.



# Spectra of backward Euler via direct computation and LFA



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#### Semi-algebraic mode analysis (SAMA) (1/2)Friedhoff, MacLachlan (2015)

- To account for non-normality of the matrix in the time-direction SAMA permutes system matrix, s.t. time-direction is the innermost
- For our example application of this permutation P yields

$$\tilde{A}_{\mathbf{n}} := P^{-1}A_{\mathbf{n}}P = P^{-1} \left( J_{N_t} \otimes \mathbb{I}_{N_x} + \mathbb{I}_{N_t} \otimes Q_{N_x} \right) P$$
$$= \mathbb{I}_{N_x} \otimes J_{N_t} + Q_{N_x} \otimes \mathbb{I}_{N_t}$$

Block-Fourier transformation yields

$$(F_{N_x} \otimes \mathbb{I}_{N_t})^H \tilde{A}_{\mathbf{n}}(F_{N_x} \otimes \mathbb{I}_{N_t}) = \begin{bmatrix} B_1^{(A)} & 0 & \cdots & 0\\ 0 & B_2^{(A)} & & 0\\ & \ddots & \ddots & \vdots\\ 0 & \cdots & 0 & B_{N_x}^{(A)} \end{bmatrix}$$

with lower triangular blocks  $B_k^A$ ,  $k = 1, \ldots, N_x$ .



#### Semi-algebraic mode analysis (SAMA) (2/2)Friedhoff, MacLachlan (2015)

• Blocks  $B_k^A$  have the structure

$$B_k^A = \begin{bmatrix} 1 + \lambda_k & 0 & \cdots & 0 \\ -1 & 1 + \lambda_k & & 0 \\ & \ddots & \ddots & \vdots \\ & & -1 & 1 + \lambda_k \end{bmatrix}$$

- Problem of approximating spectrum boils down to solving N<sub>x</sub> (small) eigenvalue problems
- More complicated structure for higher order schemes, SDC,...
- Allows for two-level (three-level,...) analyis in the usual (LFA) manner
- Can be carried out using LFA Lab



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## Approximating classes of sequences (a.c.s.)

Let  $\{A_n\}_n$  be a matrix sequence and  $\{\{B_{n,m}\}_n\}_m$  be sequence of matrix sequences.  $\{\{B_{n,m}\}_n\}_m$  is an a.c.s. if for every m there exists  $n_m$  s.t. for  $n \ge n_m$ ,

$$A_n = B_{n,m} + R_{n,m} + N_{n,m}, \operatorname{rank}(R_{n,m}) \le c(m)n, ||N_{n,m}|| \le \omega(m),$$

where  $\lim_{m\to\infty} c(m) = \lim_{m\to\infty} \omega(m) = 0.$ 

$$\begin{aligned} & \mathsf{ACS1} \ \{A_n\}_n \sim_{\sigma} f \text{ iff there exist } \{B_{n,m}\} \sim_{\sigma} f_m \text{ s.t.} \\ & \{B_{n,m}\}_n \xrightarrow{a.c.s.} \{A_n\}_n \text{ and } f_m \to f \text{ in measure.} \\ & \mathsf{ACS2} \ \mathsf{Let} \ A_n^H = A_n. \ \{A_n\}_n \sim_{\lambda} f \text{ iff there exist } \{B_{n,m}\} \sim_{\lambda} f_m \text{ s.t.} \\ & \{B_{n,m}\}_n \xrightarrow{a.c.s.} \{A_n\}_n \text{ and } f_m \to f \text{ in measure.} \\ & \mathsf{ACS3} \ \mathsf{Let} \ p \in [1,\infty] \text{ and assume that for every } m \text{ there exists an } n_m \text{ s.t.}, \\ & \text{ for } n \geq n_m, \ \|A_n - B_{n,m}\|_p \leq \epsilon(m,n)n^{1/p}, \text{ where} \\ & \lim_{m \to \infty} \limsup_{n \to \infty} \epsilon(n,m) = 0. \ \text{Then} \ \{B_{n,m}\}_n \xrightarrow{a.c.s.} \{A_n\}_n. \end{aligned}$$

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# Generalized locally Toeplitz (GLT) sequences e.g., Garoni, Serra-Capizzano (2017,2018)

Based on the a.c.s. we can define GLT sequences, fulfilling:

- GLT1 Each GLT sequence has a unique GLT symbol  $\mathbf{f}(\boldsymbol{\theta})$  with  $\boldsymbol{\theta} \in [-\pi, \pi]^d$ , i.e.,  $\{A_n\}_n \sim_{\text{GLT}} \mathbf{f}(\boldsymbol{\theta})$ . The GLT symbol is singular value symbol, if  $A_n = A_n^H$  for all n it is also eigenvalue symbol.
- GLT2 The set of GLT sequences forms \*-algebra, i.e., it is closed under linear combinations, products, inversion and conjugation.
- GLT3 Every Toeplitz sequence  $\{T_n(\mathbf{f})\}_n$  generated by a function  $\mathbf{f} \in L^1([-pi, pi]^d)$  is a GLT-sequence and its GLT symbol is  $\mathbf{f}$ . Each diagonal sampling sequence  $\{D_n(\mathbf{a})\}_n$  with a Riemann-integrable over  $[0, 1]^d$  is a GLT sequence with GLT symbol  $\mathbf{a}$ .
- GLT4 Every sequence distributed as constant zero in singular value sense is GLT sequence with symbol 0.



# Advantages and limitations of analysis of Toeplitz matrices and GLT

- + Technique covers single- and multilevel (i.e., one- and multi-dimensional), scalar and block cases
- + Analysis of multigrid methods using Toeplitz matrices or GLT allows for multigrid convergence results by analyzing full multigrid hierarchy
- + GLT provides asymptotic results for non-constant coefficient PDEs
- + GLT has proven to be efficient tool for analysis of complicated discretizations (e.g. IGA)
- Toeplitz matrices and GLT do not cover presence of different powers of h properly
- No tool support similar to LFA Lab available



#### Toeplitz momentary symbol B., Ekström, Furci, Serra-Capizzano (2022)

Presence of different powers of h can be overcome using the following:

#### Definition (Toeplitz momentary symbol)

Let  $\{X_n\}_n$  be a matrix sequence, assume that there exist matrix sequences  $\{A_n^{(j)}\}_n$ ,  $\{R_n\}_n$ , zero-distributed, scalar sequences  $\{c_n^{(j)}\}$  and Lebesgue integrable functions  $f_j$  defined over  $[-\pi, \pi]$ ,  $j = 0, \ldots, t$ , s.t.

$$c_n^{(0)} = 1, \quad c_n^{(s)} = o(c_n^{(r)}), \quad t \ge s > r,$$
  
 $\{X_n\}_n = \{A_n^{(0)}\}_n + \sum_{j=1}^t \{A_n^{(j)}\}_n + \{R_n\}_n.$ 

Then  $f_n = f_0 + \sum_{j=1}^t c_n^{(j)} f_j$  is the Toeplitz momentary symbol for  $X_n$  and  $\{f_n\}_n$  the sequence of Toeplitz momentary symbols for  $\{X_n\}_n$ .

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#### Analysis of PFASST B., Moser, Speck (2017)

Iteration matrix:

$$\mathbf{T}_{\mathsf{PFASST}} = \mathbf{I} - \left(\mathbf{I}_{2h}^{h} \tilde{\mathbf{P}}_{\mathsf{aGS}}^{-1} \mathbf{I}_{h}^{2h} + \mathbf{P}_{\mathsf{aJac}}^{-1} - \mathbf{P}_{\mathsf{aJac}}^{-1} \mathbf{M}_{\mathsf{lcp}} \mathbf{I}_{2h}^{h} \tilde{\mathbf{P}}_{\mathsf{aJac}}^{-1} \mathbf{I}_{h}^{2h}\right) \mathbf{M}_{\mathsf{lcp}}$$



Iteration matrix:

$$\mathbf{T}_{\mathsf{PFASST}} = \mathbf{I} - \left(\mathbf{I}_{2h}^{h} \tilde{\mathbf{P}}_{\mathsf{aGS}}^{-1} \mathbf{I}_{h}^{2h} + \mathbf{P}_{\mathsf{aJac}}^{-1} - \mathbf{P}_{\mathsf{aJac}}^{-1} \mathbf{M}_{\mathsf{lcp}} \mathbf{I}_{2h}^{h} \tilde{\mathbf{P}}_{\mathsf{aJac}}^{-1} \mathbf{I}_{h}^{2h}\right) \mathbf{M}_{\mathsf{lcp}}$$
$$= \underbrace{\left(\mathbf{I} - \mathbf{P}_{\mathsf{aJac}}^{-1} \mathbf{M}_{\mathsf{lcp}}\right)}_{\mathsf{Post-Smoother}} \underbrace{\left(\mathbf{I} - \mathbf{I}_{2h}^{h} \tilde{\mathbf{P}}_{\mathsf{aGS}}^{-1} \mathbf{I}_{h}^{2h} \mathbf{M}_{\mathsf{lcp}}\right)}_{\mathsf{ecG-Correction}} \underbrace{\mathbf{I}_{\mathsf{cp}}^{-1} \mathbf{I}_{\mathsf{cp}}^{2h} \mathbf{I}_{\mathsf{cp}}^{2h} \mathbf{I}_{\mathsf{cp}}^{2h}}_{\mathsf{ecg}} \mathbf{I}_{\mathsf{cp}}^{2h} \mathbf{I}_$$



Iteration matrix:

$$\begin{split} \mathbf{T}_{\mathsf{PFASST}} &= \mathbf{I} - \left( \mathbf{I}_{2h}^{h} \tilde{\mathbf{P}}_{\mathsf{aGS}}^{-1} \mathbf{I}_{h}^{2h} + \mathbf{P}_{\mathsf{aJac}}^{-1} - \mathbf{P}_{\mathsf{aJac}}^{-1} \mathbf{M}_{\mathsf{lcp}} \mathbf{I}_{2h}^{h} \tilde{\mathbf{P}}_{\mathsf{aJac}}^{-1} \mathbf{I}_{h}^{2h} \right) \mathbf{M}_{\mathsf{lcp}} \\ &= \underbrace{\left( \mathbf{I} - \mathbf{P}_{\mathsf{aJac}}^{-1} \mathbf{M}_{\mathsf{lcp}} \right)}_{\mathsf{Post-Smoother}} \underbrace{\left( \mathbf{I} - \mathbf{I}_{2h}^{h} \tilde{\mathbf{P}}_{\mathsf{aGS}}^{-1} \mathbf{I}_{h}^{2h} \mathbf{M}_{\mathsf{lcp}} \right)}_{\mathsf{Pre-Smoother}} \underbrace{\mathbf{I}}_{\mathsf{Pre-Smoother}} \end{split}$$

Decomposable into 3 layers:



Iteration matrix:

$$\begin{split} \mathbf{T}_{\mathsf{PFASST}} &= \mathbf{I} - \left( \mathbf{I}_{2h}^{h} \tilde{\mathbf{P}}_{\mathsf{aGS}}^{-1} \mathbf{I}_{h}^{2h} + \mathbf{P}_{\mathsf{aJac}}^{-1} - \mathbf{P}_{\mathsf{aJac}}^{-1} \mathbf{M}_{\mathsf{lcp}} \mathbf{I}_{2h}^{h} \tilde{\mathbf{P}}_{\mathsf{aJac}}^{-1} \mathbf{I}_{h}^{2h} \right) \mathbf{M}_{\mathsf{lcp}} \\ &= \underbrace{\left( \mathbf{I} - \mathbf{P}_{\mathsf{aJac}}^{-1} \mathbf{M}_{\mathsf{lcp}} \right)}_{\mathsf{Post-Smoother}} \underbrace{\left( \mathbf{I} - \mathbf{I}_{2h}^{h} \tilde{\mathbf{P}}_{\mathsf{aGS}}^{-1} \mathbf{I}_{h}^{2h} \mathbf{M}_{\mathsf{lcp}} \right)}_{\mathsf{Pre-Smoother}} \underbrace{\mathbf{I}}_{\mathsf{Pre-Smoother}} \end{split}$$

Decomposable into 3 layers:

 $\mathbf{T}_{\mathsf{PFASST}} \simeq \mathbf{T}_{\mathsf{space}} \otimes \mathbf{T}_{\mathsf{time}} \otimes \mathbf{T}_{\mathsf{colloc}}$ dof e.g. 10000 10 5



 $\mathcal{F}^{-1}\mathbf{T}_{\mathsf{PFASST}}\mathcal{F} \simeq$ 



# $\mathcal{F}^{-1}\mathbf{T}_{\mathsf{PFASST}}\mathcal{F} \simeq \psi^{-1}\mathbf{T}_{\mathsf{space}}\psi \otimes \mathbf{T}_{\mathsf{time}} \otimes \mathbf{T}_{\mathsf{colloc}}$









Small blocks  $\mathcal{B}_l$  allow for easy calculation of:

• Spectral radius:  $\rho(\mathbf{T}) = \max_l \rho(\mathcal{B}_l)$ 

$$\blacktriangleright \text{ Norm: } \|\mathbf{T}\|_2 = \max_l \|\mathcal{B}_l\|_2$$

▶ Power:  $\mathbf{T}^k = \mathcal{F} \operatorname{diag} \left( \mathcal{B}_1^k, \mathcal{B}_2^k, \dots, \mathcal{B}_N^k \right) \mathcal{F}^{-1}$ 



Use second order difference method to discretize the heat equation



Use second order difference method to discretize the heat equation

$$\mathbf{u}_{t}(t) = \mathbf{A}\mathbf{u}(t)$$

$$\mathbf{A} = \frac{\mu}{(\Delta x)^{2}} \begin{pmatrix} 2 & -1 & 0 & \cdots & -1 \\ -1 & 2 & -1 & & \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & -1 & 2 & -1 \\ -1 & 0 & \cdots & -1 & 2 \end{pmatrix}$$

$$\nu = \mu \Delta t / (\Delta x)^{2}$$



Use second order difference method to discretize the heat equation

$$\mathbf{u}_{t}(t) = \mathbf{A}\mathbf{u}(t)$$

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$$\nu = \mu \Delta t / (\Delta x)^{2}$$

Space problem is decomposable into the modes  $\mathbf{m}_k = \left[\exp\left(i \cdot \frac{kn}{N}\right)\right]_{n=1,\dots,N}$ .



# Model problem

1.0 Use second order difference method to discretize 0.8 the heat equation 0.6 04  $\mathbf{u}_t(t) = \mathbf{A}\mathbf{u}(t)$ 02  $\mathbf{A} = \frac{\mu}{\left(\Delta x\right)^2} \begin{pmatrix} 2 & -1 & 0 & \cdots & -1\\ -1 & 2 & -1 & & \\ 0 & \ddots & \ddots & \ddots & 0\\ \vdots & & -1 & 2 & -1\\ -1 & 0 & \cdots & -1 & 2 \end{pmatrix}$ t 0.5 0.0 -0.2- -0.4 - -0.6 -0.8 -1.0 $\nu = \mu \Delta t / (\Delta x)^2$ 0 π  $2\pi$ x

Figure: Numerical solution for the initial value  $u_0 = \sin(x)$ .

Space problem is decomposable into the modes  $\mathbf{m}_k = \left[\exp\left(i \cdot \frac{kn}{N}\right)\right]_{n=1,\dots,N}$ .

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## First convergence tests

#### 8 time steps



32 spatial nodes, 5 quadrature nodes and  $\mu = 0.01$ .

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## First convergence tests



32 spatial nodes, 5 quadrature nodes and  $\mu=0.01.$ 







- Works great with a few time steps.
- Is awfully wrong for many time steps



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Not ideal, so what about  $\|\mathbf{T}\|_2 = \max_l \|\mathcal{B}_l\|_2$ ?

Matrix matrix multiplication for each iteration.



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Not ideal, so what about  $\|\mathbf{T}\|_2 = \max_l \|\mathcal{B}_l\|_2$ ?

- Matrix matrix multiplication for each iteration.
- $\Rightarrow$  Analysis of mode-wise behavior provides additional insight



1. Decompose spatial problem into modes  $\mathbf{m}_j$ 

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- 1. Decompose spatial problem into modes  $\mathbf{m}_j$
- 2. Spread *j*-th mode across all collocation points and time steps to get initial error mode:

$$\mathbf{e}_{j}^{0}=\mathbf{m}_{j}\otimes\mathbf{1}_{L}\otimes\mathbf{1}_{M}$$



- 1. Decompose spatial problem into modes  $\mathbf{m}_j$
- 2. Spread *j*-th mode across all collocation points and time steps to get initial error mode:

$$\mathbf{e}_j^0 = \mathbf{m}_j \otimes \mathbf{1}_L \otimes \mathbf{1}_M$$

3. Use block Fourier transformation to track *j*-th error mode over iterations:

$$\|\mathcal{F}\mathbf{e}_{j}^{k}\| = \|\mathcal{F}\mathbf{T}^{k}\mathbf{e}_{j}^{0}\| = \left\|\operatorname{diag}(\mathcal{B}_{l}^{k})\mathcal{F}\mathbf{e}_{j}^{0}\right\| = \left\|\mathcal{B}_{j}^{k}\mathbf{1}_{LM}\right\|.$$



- 1. Decompose spatial problem into modes  $\mathbf{m}_j$
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4. Estimate number of iterations  $K_{\text{PFASST}}$  to achieve a certain error reduction for this mode



# Convergence of PFASST for another setup



128 spatial nodes, 5 quadrature nodes, 10 time steps and  $\nu = 0.01$ 



# Convergence of PFASST for another setup



128 spatial nodes, 5 quadrature nodes, 10 time steps and  $\nu = 1.0$ 



## How to estimate the speedup



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## How to estimate the speedup



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## How to estimate the speedup



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# How SDC performs



128 spatial nodes, 5 quadrature nodes, 128 time steps and  $\nu = 0.01$ .





128 spatial nodes, 5 quadrature nodes, 128 time steps and  $\nu = 1.0$ .



## Estimated speedup



128 spatial nodes, 5 quadrature nodes, 128 time steps and  $\nu = 0.01$ .

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## Estimated speedup



128 spatial nodes, 5 quadrature nodes, 128 time steps and  $\nu = 1.0$ .



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#### MINRES for nonsymmetric Toeplitz matrices Pestana, Wathen (2015)

Using the flip matrix

$$Y_n = \begin{bmatrix} & & 1 \\ & \ddots & \\ 1 & & \end{bmatrix}$$

the system  $A_n x = b$  can be preconditioned as

$$Y_n A_n x = Y_n b.$$

The resulting system matrix is a Hankel matrix and the system can be solved using MINRES. Further, an optimal circulant preconditioner  $C_n$  can be used. To obtain a symmetric preconditioner like required by MINRES the absolute value of  $C_N$  is used, c.f. Andy's talk on Monday:

$$|C_n| = (C_n^T C_n)^{\frac{1}{2}} = (C_n C_n^T)^{\frac{1}{2}} = U_n^* |\Lambda_n| U_n.$$



For nonsymmetric systems other solvers have to be used, GMRES is one of the most widely used and best understood variant.

One alternative for analyzing is the ideal GMRES analysis, considering the "ideal" polynomial  $p_{\rm ideal}(A)$ :

$$p_{\text{ideal}}(A) = \arg \min_{\substack{p(A) \in \pi_k \\ p(0) = 1}} \|p(A)\|_2,$$
$$\|r^{(k+1)}\|_2 = \min_{\substack{p(A) \in \pi_k \\ p(0) = 1}} \frac{\|p(A)r^{(0)}\|}{\|r^{(0)}\|_2} \le \|p_{\text{ideal}}(A)\|_2.$$

Minimizes the 2-norm of p(A), not of  $p(A)r^{(0)}$  and can be approx. using randomized normalized vectors  $\xi$  by  $p_{\text{rand}}$ .



# Speedup of ideal GMRES analysis using SAMA

- Coefficients of GMRES polynomial can be computed as described in Nachtigal, Reichel and Trefethen (1992)
- Ideal GMRES analysis requires computation of spectral radius of matrix polynomial for each iteration
- Polynomial evaluation can be carried out approximately using SAMA
- Test case:
  - ▶ 1d advection on  $[-\pi,\pi] \times [0,T]$  with periodic boundary conditions in space discretized using BDF1
  - Preconditioned using MGRIT
  - ▶  $N_x = 8, 16, N_t = 16, 32$
  - usage of variable-precision floating point arithmetic
- Speedup by using SAMA in comparison to naïve implementation: up to 88.87 times faster



# Results of ideal GMRES analysis using SAMA (1/2)



On the usage of spectral information about matrices arising from parallel-in-time integration Matthias Bolten



# Results of ideal GMRES analysis using SAMA (2/2)



One-dimensional advection, Nx=16, Nt=32



# Outline

#### Introduction

#### Approximation of the spectrum

Local Fourier Analysis Semi-algebraic mode analysis Momentary symbol

#### Usage of the spectral information

Analysis of stationary iterative methods Analysis of Krylov subspace methods

#### Conclusion



## Conclusion

#### Analysis of all-at-once matrices difficult due to

- lack of symmetry
- non-normality
- ► Analysis based on Toeplitz structure possible nevertheless:
  - SAMA as extension of LFA
  - Generalization of Toeplitz theory possible, as well
- Techniques allow for analysis and development of advanced stationary solvers (PFASST) as well as of Krylov subspace methods (preconditioned MINRES, MGRIT-preconditioned GMRES)



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#### Thank you for your attention!