A multigrid perspective on PFASST

November 28, 2016 | Dieter Moser, Robert Speck, Matthias Bolten
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Motivation

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Motivation

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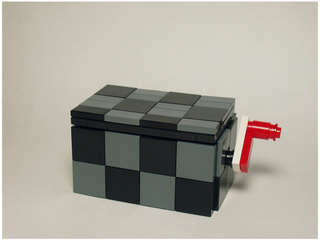
Embedding PFASST into multigrid theory



- PFASST looks complicated
- PFASST shows similarities to multigrid
- multigrid is extensively studied

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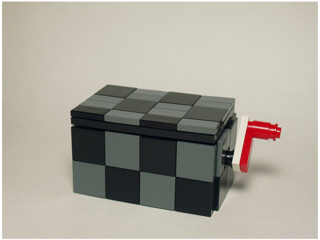
Embedding PFASST into multigrid theory



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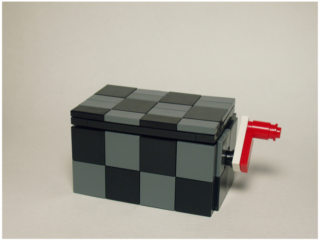

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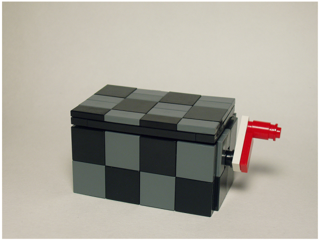

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- PFASST shows similarities to multigrid
- multigrid is extensively studied

Now let's show that PFASST actually is a multigrid algorithm, under certain assumptions and use this to analyze the parallel performance.

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Collocation formulation on a single time-step

Consider the Picard form of an initial value problem on $[T_l, T_{l+1}]$

$$u(t) = u_l + \int_{T_l}^{t} \mathbf{A} \cdot u(s) ds,$$

discretized using spectral quadrature rules with nodes τ_m:

$$(\mathbf{I} - \Delta t \mathbf{Q} \otimes \mathbf{A})(\mathbf{u}) = \mathbf{u}_l$$

This corresponds to a fully implicit Runge-Kutta method on $[T_l, T_{l+1}]$, which we solve iteratively.

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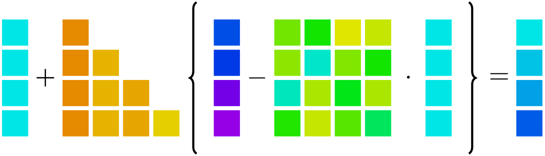

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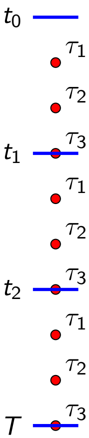
Linked collocation problem



We now link L time-steps together, using $\mathbf{N}$ to transfer information from step l to step $l+1$. We get:

$$\begin{pmatrix} \mathbf{I} - \Delta t \mathbf{Q} \otimes \mathbf{A} & & & \\ -\mathbf{N} & \mathbf{I} - \Delta t \mathbf{Q} \otimes \mathbf{A} & & \\ & \ddots & \ddots & \\ & & -\mathbf{N} & \mathbf{I} - \Delta t \mathbf{Q} \otimes \mathbf{A} \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \vdots \\ \mathbf{u}_L \end{pmatrix} = \begin{pmatrix} \mathbf{u}_0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

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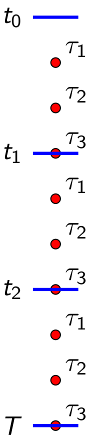
Linked collocation problem



We now link L time-steps together, using $\mathbf{N}$ to transfer information from step l to step $l+1$. We get:

$$\mathbf{M}_{\mathrm{lcp}}\mathbf{U} = \mathbf{U}_0$$

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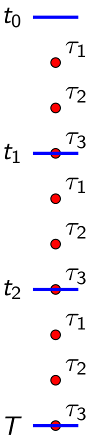
Linked collocation problem



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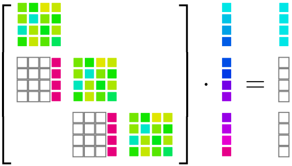

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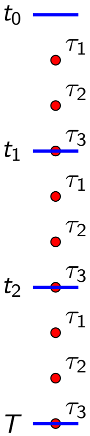

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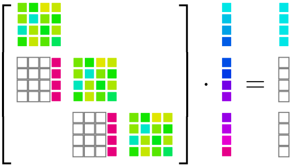

- use (linear/FAS) multigrid to solve this system iteratively
- exploit cheapest coarse level to quickly propagate information forward in time
- smoother: block Jacobi + block Gauß-Seidel

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Approximative Block-Gauß-Seidel

t_0

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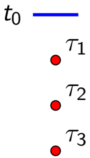
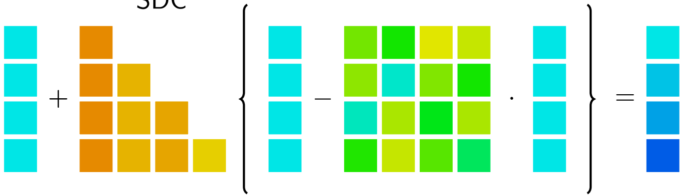
Approximative Block-Gauß-Seidel

… on the first subinterval



$$\mathbf{u}^0 + \mathbf{P}_{\mathrm{SDC}}^{-1} \left(\mathbf{u}_0 - \mathbf{M} \cdot \mathbf{u}^0 \right) = \mathbf{u}^1$$



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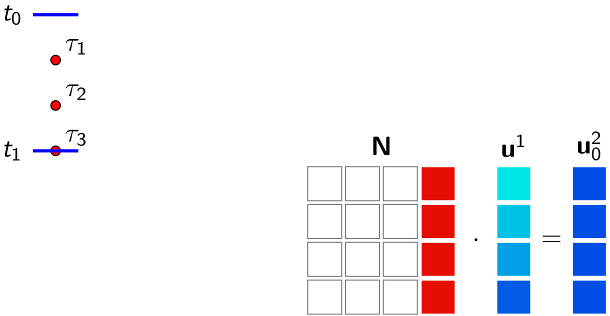
Approximative Block-Gauß-Seidel

… passing end value to the next subinterval



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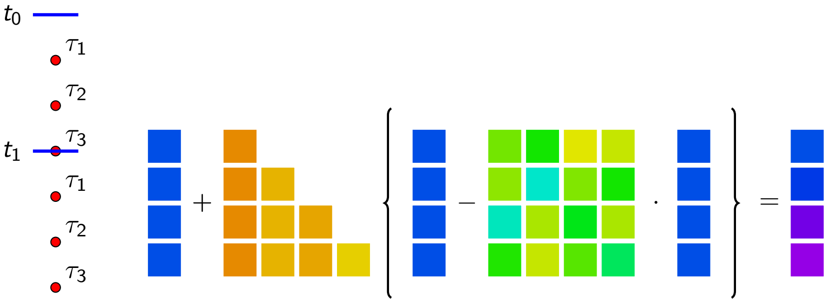
Approximative Block-Gauß-Seidel

... on the second subinterval



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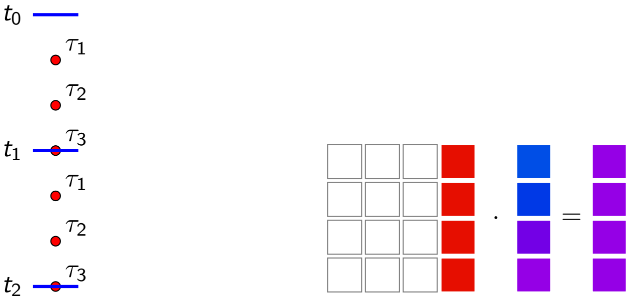

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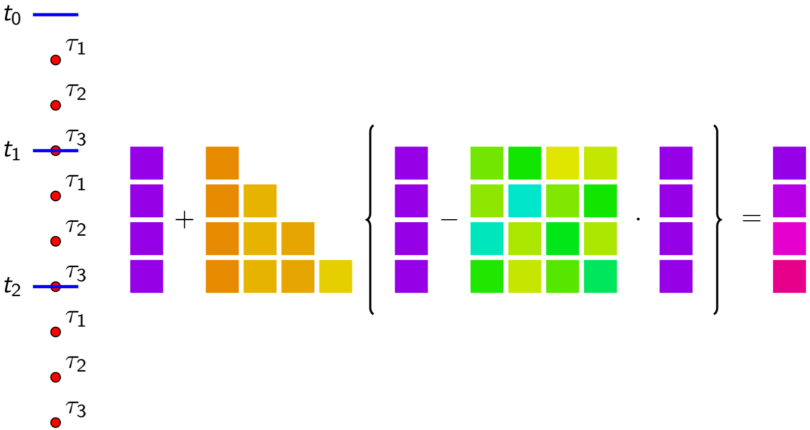
Approximative Block-Gauß-Seidel

… on the last subinterval



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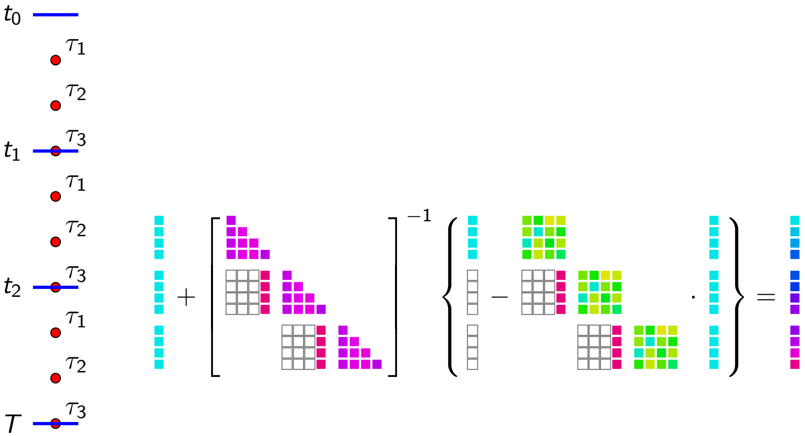
Approximative Block-Gauß-Seidel

… all in one



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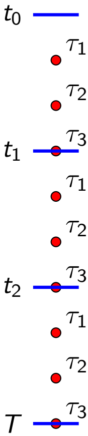
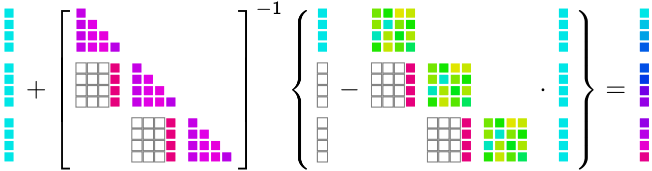
Approximative Block-Gauß-Seidel



$$\mathbf{U}^0 + \mathbf{P}_{\text{aGS}}^{-1} \quad \mathbf{U}_0 - \mathbf{M}_{\text{lcp}} \cdot \mathbf{U}^0 = \mathbf{U}^1$$



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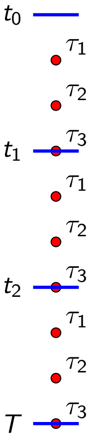
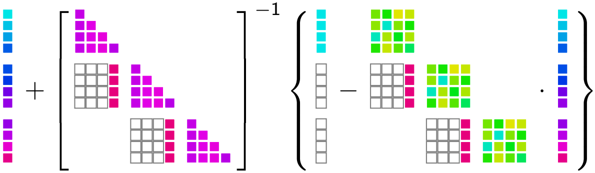
Approximative Block-Jacobi

... starting from the approximative Gauß-Seidel





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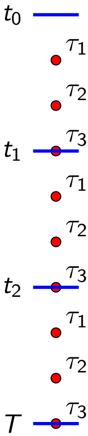
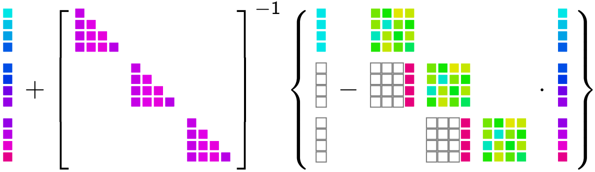
Approximative Block-Jacobi

... one little adjustment



$$\mathbf{P}_{\text{aJac}}^{-1}$$



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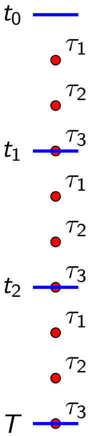
Approximative Block-Jacobi

… another little manipulation



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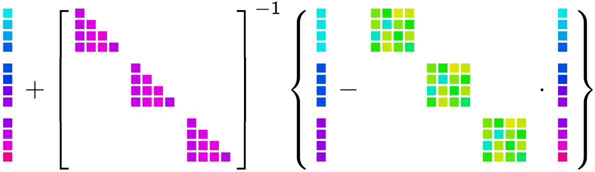

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Coarse Grid Correction

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Coarse Grid Correction

Do a **block Jacobi step**

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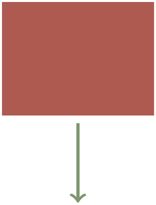

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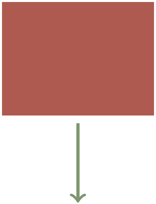

Do a **block Jacobi step**

Compute $\tau_k = \tilde{\mathbf{M}}_{\mathrm{lcp}} \mathbf{I}_h^{2h} \mathbf{U}^k - \mathbf{I}_h^{2h} \mathbf{M}_{\mathrm{lcp}} \mathbf{U}^k$

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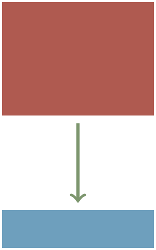

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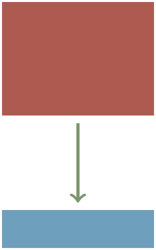

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Do a **block Gauß-Seidel step** with $\tilde{\mathbf{U}}_0^k + \tau_k$

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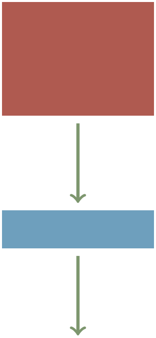
Coarse Grid Correction



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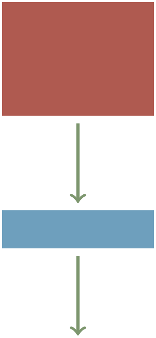

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Do a **block Gauß-Seidel step** with $\tilde{\mathbf{U}}_0^k + \tau_k$

Correct $\mathbf{U}^{k+1} = \mathbf{U}^k + \mathbf{I}_{2h}^h \left(\tilde{\mathbf{U}}^{k+1/2} - \mathbf{I}_h^{2h} \mathbf{U}^k \right)$

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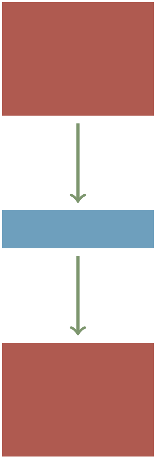
Coarse Grid Correction



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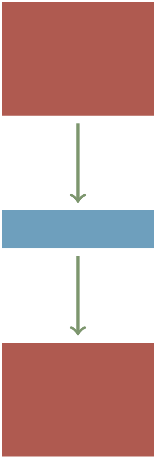

Do a **block Jacobi step**

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Do a **block Gauß-Seidel step** with $\tilde{\mathbf{U}}_0^k + \tau_k$

Correct $\mathbf{U}^{k+1} = \mathbf{U}^k + \mathbf{I}_{2h}^h \left(\tilde{\mathbf{U}}^{k+1/2} - \mathbf{I}_h^{2h} \mathbf{U}^k \right)$

Do next **block Jacobi step**

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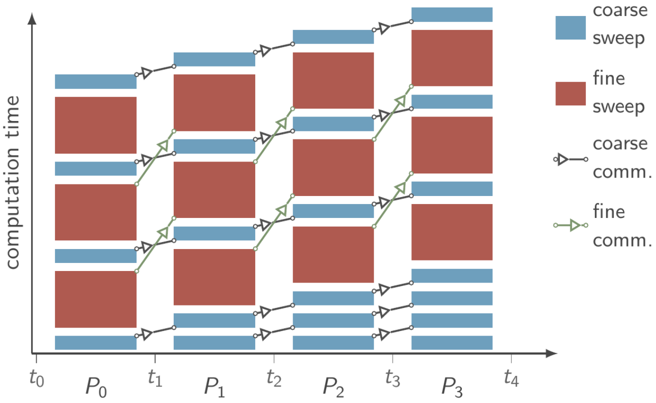
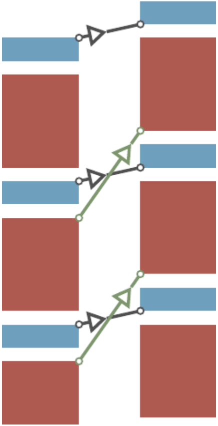
PFASST overview



Putting the pieces together



This can easily be written as

$$\mathbf{U}^{k+\frac{1}{2}} = \mathbf{U}^{k} + \mathbf{I}_{2h}^{h}\tilde{\mathbf{P}}_{\mathrm{aGS}}^{-1}\mathbf{I}_{h}^{2h}\left(\mathbf{U}_0 - \mathbf{M}_{\mathrm{lcp}}\mathbf{U}^{k}\right)$$

$$\mathbf{U}^{k+1} = \mathbf{U}^{k+\frac{1}{2}} + \mathbf{P}_{\mathrm{aJac}}^{-1}\left(\mathbf{U}_0 - \mathbf{M}_{\mathrm{lcp}}\mathbf{U}^{k+\frac{1}{2}}\right),$$

which is a two-level multigrid scheme, with an approximative **Block-Gauß-Seidel** on the coarse level and an approximative **Block-Jacobi** on the fine level.

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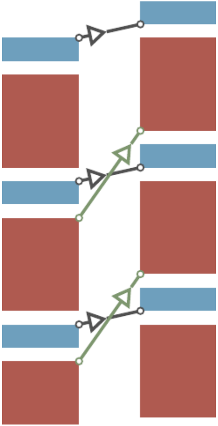
Putting the pieces together



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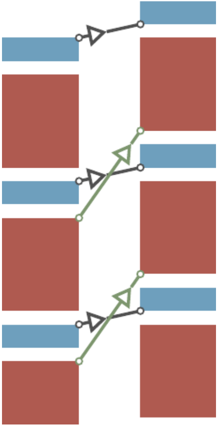

This can easily be written as

$$\mathbf{U}^{k+\frac{1}{2}} = \mathbf{U}^{k} + \mathbf{I}^{h}_{2h}\tilde{\mathbf{P}}^{-1}_{\mathrm{aGS}}\mathbf{I}^{2h}_{h}\left(\mathbf{U}_0 - \mathbf{M}_{\mathrm{lcp}}\mathbf{U}^{k}\right)$$
$$\mathbf{U}^{k+1} = \mathbf{U}^{k+\frac{1}{2}} + \mathbf{P}^{-1}_{\mathrm{aJac}}\left(\mathbf{U}_0 - \mathbf{M}_{\mathrm{lcp}}\mathbf{U}^{k+\frac{1}{2}}\right),$$

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Analysis of PFASST - a modest try

The center of attention is the **iteration matrix of PFASST**

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

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$$= \underbrace{\left(\mathbf{I} - \mathbf{P}_{\text{aJac}}^{-1}\mathbf{M}_{\text{lcp}}\right)}_{\text{Post-Smoother}}\underbrace{\left(\mathbf{I} - \mathbf{I}_{2h}^{h}\tilde{\mathbf{P}}_{\text{aGS}}^{-1}\mathbf{I}_{h}^{2h}\mathbf{M}_{\text{lcp}}\right)}_{\approx\text{CG-Correction}}\underbrace{\mathbf{I}}_{\text{Pre-Smoother}},$$

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

which is decomposable into 3 layers.

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$$= \underbrace{\left(\mathbf{I} - \mathbf{P}_{\text{aJac}}^{-1}\mathbf{M}_{\text{lcp}}\right)}_{\text{Post-Smoother}}\underbrace{\left(\mathbf{I} - \mathbf{I}_{2h}^{h}\tilde{\mathbf{P}}_{\text{aGS}}^{-1}\mathbf{I}_{h}^{2h}\mathbf{M}_{\text{lcp}}\right)}_{\approx\text{CG-Correction}}\underbrace{\mathbf{I}}_{\text{Pre-Smoother}},$$

which is decomposable into 3 layers.

dof e.g.	over 9000	10	5

$$\mathbf{T}_{\text{PFASST}} \simeq \mathbf{T}_{\text{space}} \otimes \mathbf{T}_{\text{time}} \otimes \mathbf{T}_{\text{colloc}}$$

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Analysis of PFASST - a modest try

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☺ (under $\mathbf{T}_{\text{space}}$) ☹ (under $\mathbf{T}_{\text{colloc}}$)

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Local Fourier Analysis from a matrix point of view

just transformation

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

$$= \begin{bmatrix} \mathcal{B}_1 & & & \\ & \mathcal{B}_2 & & \\ & & \ddots & \\ & & & \mathcal{B}_k \end{bmatrix}$$

Now we have e.g. 4500 "time collocation" blocks $\mathcal{B}_k$ of size $2 \cdot 10 \cdot 5$ instead of **one** matrix of size $4.5 \cdot 10^5$.

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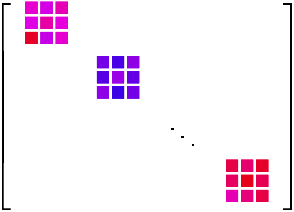

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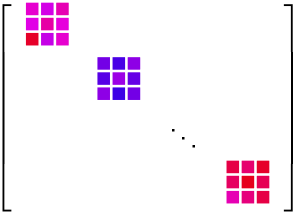

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The convenience of blocks

spectral radii

$$\rho(\mathbf{T}) = \max_{l} \rho(\mathcal{B}_l)$$

norms

$$\|\mathbf{T}\|_2 = \max_{l} \|\mathcal{B}_l\|_2$$

power

$$\mathbf{T}^k = \mathcal{F}\,\mathrm{diag}\left(\mathcal{B}_1^k, \mathcal{B}_2^k, \ldots, \mathcal{B}_N^k\right)\,\mathcal{F}^{-1}$$

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A model problem

Use second order difference method to discretize the heat equation

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

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

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

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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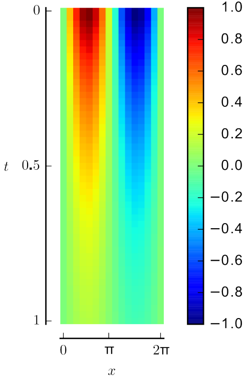

Figure: Numerical solution for the initial value $u_0 = \sin(x)$.

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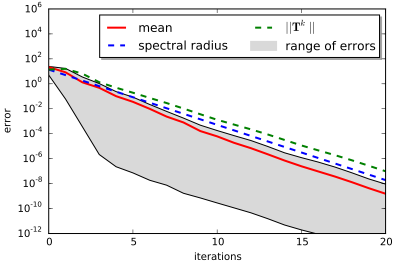
First convergence tests

8 time steps



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

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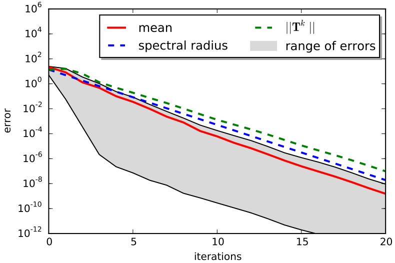
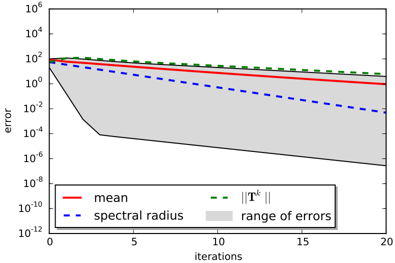


128 time steps



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Estimating iterations

Use the spectral radius

- Works great with a few time steps.
- Is awfully wrong for many time steps
- Only a worst case estimation

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

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$\Rightarrow$ **back to the roots, back to counting!**

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Block structure and space modes

. . . how to count

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:

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

4. Estimate number of iterations K_{PFASST} to achieve a certain error reduction for this mode

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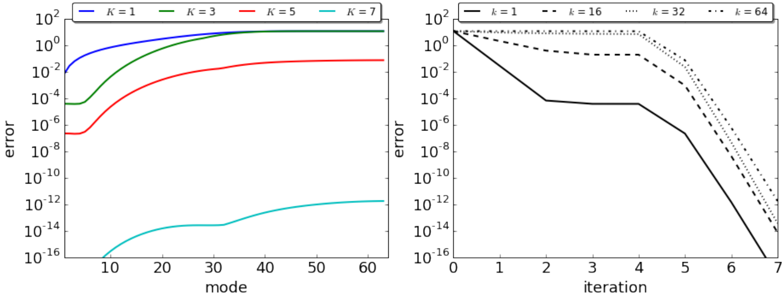
Convergence of PFASST for another setup



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

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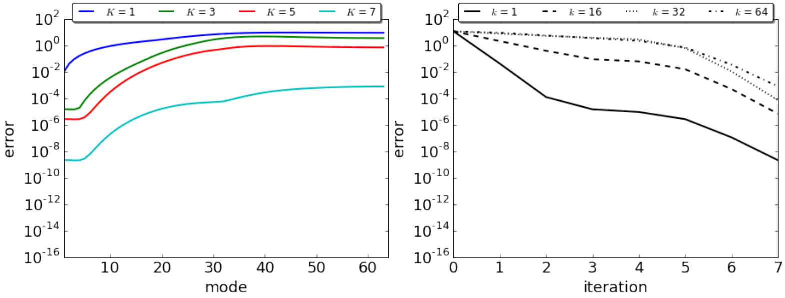

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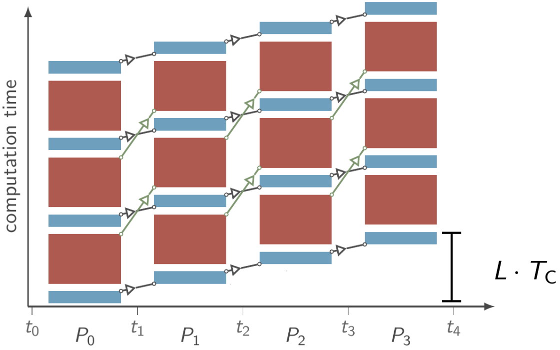
How to estimate the speedup



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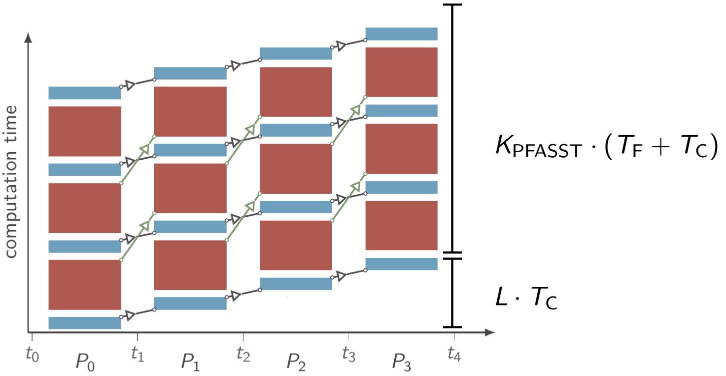

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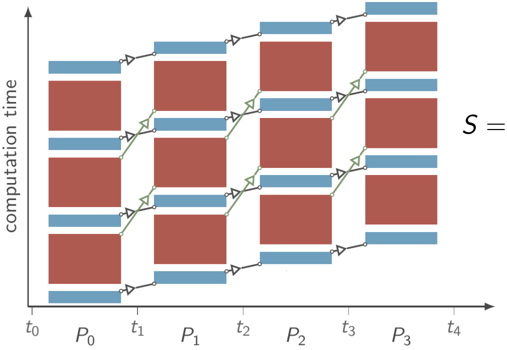

$$S = \frac{\sum_{l=1}^{L} K_{\mathrm{SDC},l} \cdot T_{\mathrm{F}}}{L \cdot T_{\mathrm{C}} + K_{\mathrm{PFASST}} \cdot (T_{\mathrm{F}} + T_{\mathrm{C}})}$$

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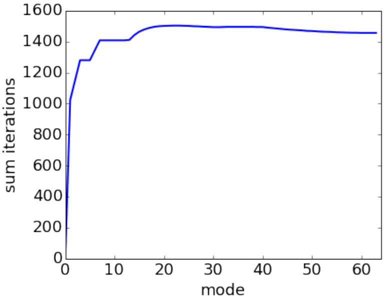
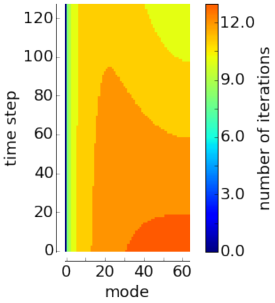
How SDC performs





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JÜLICH
FORSCHUNGSZENTRUM

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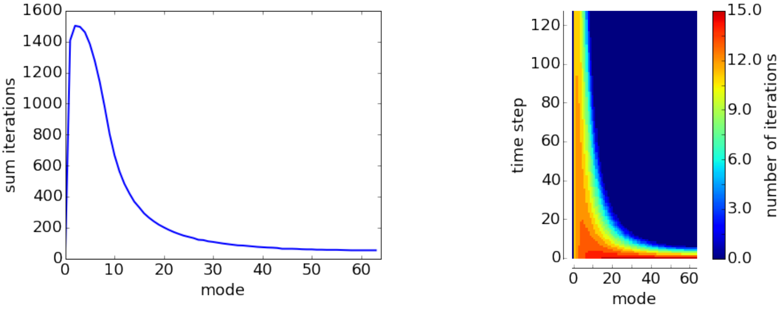

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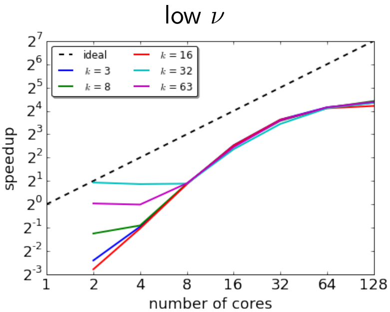
Estimated speedup



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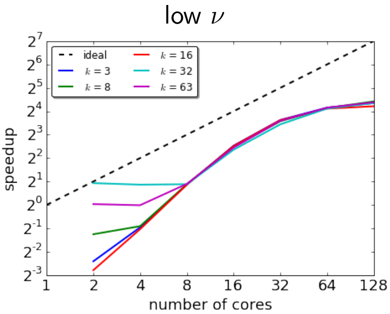

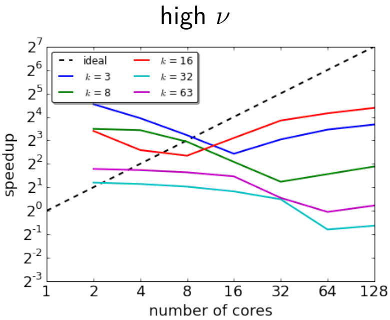

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What's next?

Achievments until now

- A multigrid view on PFASST
- Iteration matrix in a nice form
- Plug&Play framework
- First insights in the parallel performance

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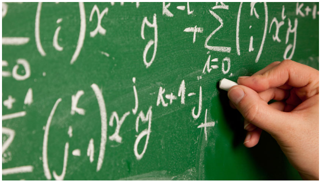
Upcoming challenges

- Local Fourier analysis
- Time coarsening
- Compare to other space time MGs
- Writing the PhD thesis



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Thank you for your attention!

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