PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Fime Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacobi

Numerical Experiments Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method

MGR

・ロト ・ 同ト ・ ヨト ・ ヨー・ つへぐ

PFASST

ntegral Deferred Correction Classical Parallel IDC

Time Parallel Time Integration Chapter 4: Space-Time Multigrid Methods

Martin J. Gander martin.gander@unige.ch

University of Geneva

Michigan, August 4th, 2022

Space-Time Multigrid Methods

1960 < small scale large scale	small scale Martin _	J. Gander
ITERATIVE DI	RECT	
Picard Lindeloef 1893/4 Nievergelt 1964	Parabolic	: Multigrid
Mirank	er Liniger 1967 Smoother	
1970 Sham	Dine Watts 1969	
1970	Early Remed	iles
	Dahlquist Ed	uation
	FLA	
1980	Results	
Lelarasmee Ruehli Sangiovanni–Vincentelli 1982	Space-Ti	
Hackbusch 1984 Axelson Verwe		
Lubich Ostermann 1987 Gear 1988 Ja	ckson Norsett 1986 Block Jacob	
	FLA	
	1991 Numerical E	
	ett Wanner 1992 Scalings	
Horton Vandewalle 1995 Burrage 1995		
Saha Stadel Tremaine 1996 Gander 1996	Multigrid	
Chase Class That	nee 1999	
2000 Gander Halpern Nataf 1999 Steen Stoan Thor Lions Maday Turinici 2001	Parareal	
	Parareal as a multigrid me	
Gander, Vandewalle 2007	AMG	
Gander, Hairer 2007 Maday	Ronquist 2008	
2010 Emmett-Minion-2010/2012 Christlieb Macd		
Gander Kwok Mandal 2013 Gander Guettel 20	13 PFASST	
Gander Neumueller 2014	Integral Defe	erred Correction
Falgout, Friedhoff, Kolev, MacLachlan, Schroder 2014 Gander 2015 Conden	Classical	
Gander,	Halpern, Ryan 2016 Parallel IDC	
2020		
V		
	▶ ▲ 唐 ▶ 目 ● 9 € ●	

PinT Summer

Parabolic Multigrid

Wolfgang Hackbusch (1984): Parabolic Multi-Grid Methods

"A multi-grid iteration for solving parabolic partial differential equations is presented. It is characterized by the simultaneous computation of several time steps in one step to the computational process."

One dimensional heat equation as the model problem:

$$\begin{array}{rcl} \partial_t u(x,t) &=& \partial_{xx} u(x,t) + f(x,t) & \mbox{in } \Omega \times (0,T], \ \Omega := (0,L), \\ u(x,0) &=& u_0(x) & \mbox{in } \Omega, \\ u(0,t) &=& g_0(t) & \mbox{in } (0,T], \\ u(L,t) &=& g_L(t) & \mbox{in } (0,T]. \end{array}$$

Centered differences in space and Backward Euler in time:

$$\frac{\boldsymbol{u}_{n+1} - \boldsymbol{u}_n}{\Delta t} = L \boldsymbol{u}_{n+1} + \boldsymbol{f}_{n+1},$$

where $L := \frac{1}{\Delta x^2} \begin{bmatrix} 1 & -2 & 1 \end{bmatrix} \in \mathbb{R}^{J \times J}.$

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid Block Jacobi FLA Numerical Experiments Scalings

Multigrid nterpretations

Parareal Parareal as a geometric multigrid method AMG MGRIT

PFASST

Hackbusch's Idea for a Smoother

"The conventional approach is to solve time step by time step; \mathbf{u}_{n+1} is computed from \mathbf{u}_n , then \mathbf{u}_{n+2} from \mathbf{u}_{n+1} etc. The following process will be different. Assume that \mathbf{u}_n is already computed or given as an initial state. Simultaneously, we shall solve for $\mathbf{u}_{n+1}, \mathbf{u}_{n+2}, \ldots, \mathbf{u}_{n+k}$ in one step of the algorithm."

$$\underbrace{(I-\Delta tL)}_{\mathsf{A}}\boldsymbol{u}_{n+1}=\underbrace{\boldsymbol{u}_n+\Delta t\boldsymbol{f}_{n+1}}_{\boldsymbol{b}}.$$

A = L + D + U, D := diag(A), damped Jacobi for $k = 0, 1, \dots, \nu$

$$\boldsymbol{u}_{n+1}^{k+1} = \boldsymbol{u}_{n+1}^{k} + \alpha D^{-1} (\boldsymbol{b} - A \boldsymbol{u}_{n+1}^{k})$$

= $\boldsymbol{u}_{n+1}^{k} + \frac{\alpha}{1 + \frac{2\Delta t}{\Delta x^{2}}} (\boldsymbol{u}_{n}^{\nu} + \Delta t \boldsymbol{f}_{n+1} - (I - \Delta t L) \boldsymbol{u}_{n+1}^{k})$

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother

Coarse Correction Early Remedies

Fime Multigrid

Dahlquist Equation FLA Results

Space-Tim Multigrid

Block Jacobi

FLA

Numerical Experiments Scalings

Multigrid Interpretations

arareal arareal as a geometric uultigrid method MG

MGRI

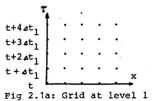
PFASST

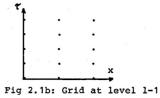
Integral Deferred Correction Classical Parallel IDC

▲□▶ ▲御▶ ▲臣▶ ▲臣▶ ―臣 – のへで

Hackbusch's Idea for Coarsening

Now use this sequential Jacobi procedure in time as a smoother, and use a coarse correction in space:





Hackbusch observes:

- Very fast multigrid convergence when coarsening in space
- Much less good convergence when coarsening in time as well

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother

Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid Block Jacobi FLA Numerical Experimen Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method AMG

MGRI

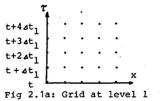
PFASST

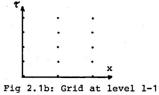
ntegral Deferred Correction Classical Parallel IDC

<□▶ <□▶ < □▶ < □▶ < □▶ < □ > ○ < ○

Hackbusch's Idea for Coarsening

Now use this sequential Jacobi procedure in time as a smoother, and use a coarse correction in space:





Hackbusch observes:

- Very fast multigrid convergence when coarsening in space
- Much less good convergence when coarsening in time as well

Lubich and Ostermann (1987): Multigrid WR

"For the case when the same step-size is used at all the nodes of a level, we regain the method proposed by Hackbusch to which our results will apply in particular."

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother

Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

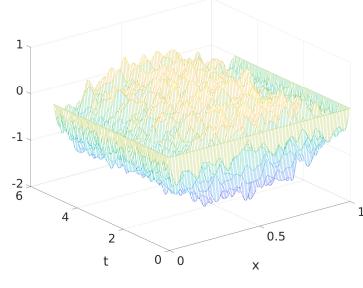
Space-Time Multigrid Block Jacobi FLA Numerical Experiment Scalings

Multigrid Interpretations

Parareal Parareal as a geometric multigrid method AMG MGRIT

PFASST

Error after 5 presmoothing steps, iteration k=1



PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother

Coarse Correction

Time Multigrid

Dahlquist Equatior FLA Results

Space-Time Multigrid

FLA Numerical Experime Scalings

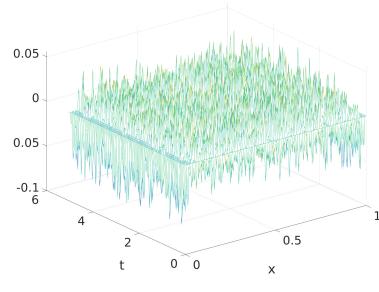
Multigrid Interpretations

Parareal Parareal as a geometric nultigrid method AMG MGRIT

PFASST

ntegral Deferred Correctior Classical Parallel IDC

Error after coarse correction, iteration k=1



PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother

Coarse Correction

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid Block Jacobi FLA Numerical Experimer Scalings

Multigrid Interpretations

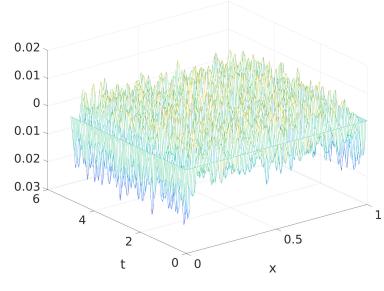
Parareal Parareal as a geometric nultigrid method AMG MGRIT

PFASST

ntegral Deferred Correction Classical Parallel IDC

▲□▶ ▲□▶ ▲□▶ ▲□▶ = 三 のへ

Error after 5 postsmoothing steps, iteration k=1



PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother

Coarse Correction

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid ^{Block Jacobi} FLA

Numerical Experiments Scalings

Multigrid Interpretations

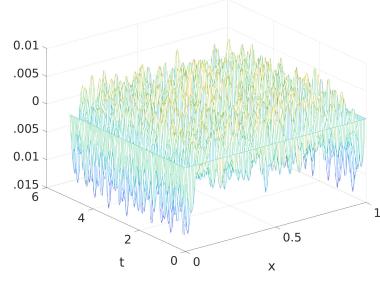
Parareal Parareal as a geometric multigrid method AMG MGRIT

PFASST

ntegral Deferred Correctior Classical Parallel IDC

▲□▶ ▲□▶ ▲□▶ ▲□▶ = 三 のへ

Error after 5 presmoothing steps, iteration k=2



PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother

Coarse Correction

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid ^{Block} Jacobi FLA

Numerical Experiments Scalings

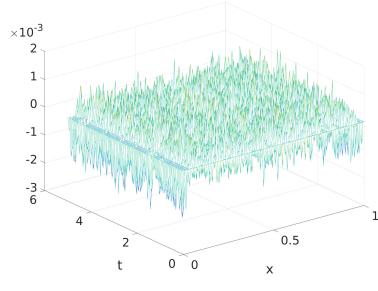
Multigrid Interpretations

arareal arareal as a geometric nultigrid method MG IGRIT

PFASST

ntegral Deferred Correction Classical Parallel IDC

Error after coarse correction, iteration k=2



PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother

Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid Block Jacobi FLA Numerical Experimen

Aultigrid

Interpretations

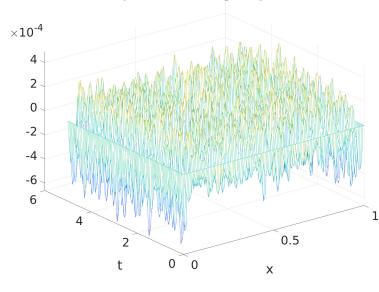
Parareal Parareal as a geometric multigrid method AMG MGRIT

PFASST

ntegral Deferred Correctior Classical Parallel IDC

▲□▶ ▲□▶ ▲□▶ ▲□▶ = 三 のへ

Error after 5 postsmoothing steps, iteration k=2



PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother

Coarse Correction

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid Block Jacobi FLA Numerical Experime

Scalings

Multigrid Interpretations

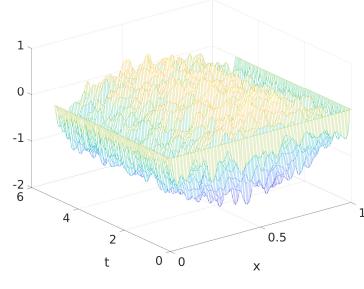
Parareal Parareal as a geometric nultigrid method AMG MGRIT

PFASST

ntegral Deferred Correction Classical Parallel IDC

▲□▶ ▲□▶ ▲□▶ ▲□▶ ▲□ ● のへ

Error after 5 presmoothing steps, iteration k=1



PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother

Coarse Correction

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

FLA Numerical Experimer

Multigrid Interpretations

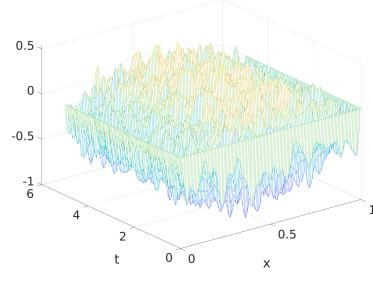
Parareal Parareal as a geometric multigrid method AMG MGRIT

PFASST

ntegral Deferred Correctior Classical Parallel IDC

▲□▶ ▲□▶ ▲□▶ ▲□▶ ▲□ ● のの

Error after coarse correction, iteration k=1



PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother

Coarse Correction

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid Block Jacobi FLA

Numerical Experiments Scalings

Multigrid Interpretations

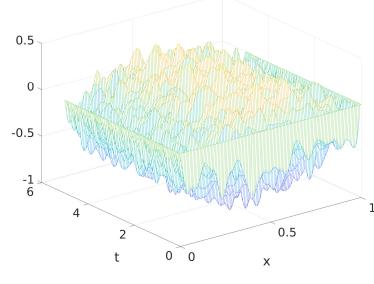
Parareal Parareal as a geometric multigrid method AMG MGRIT

PFASST

ntegral Deferred Correction Classical Parallel IDC

▲□▶ ▲□▶ ▲□▶ ▲□▶ = 三 のの

Error after 5 postsmoothing steps, iteration k=1



PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother

Coarse Correction

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid Block Jacobi FLA

Numerical Experiments Scalings

Multigrid Interpretations

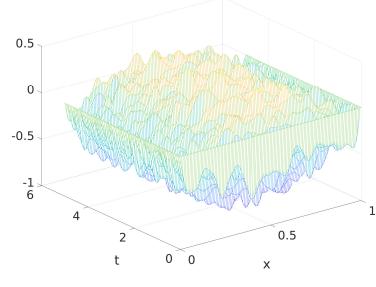
Parareal Parareal as a geometric multigrid method AMG MGRIT

PFASST

ntegral Deferred Correction Classical Parallel IDC

▲□▶ ▲□▶ ▲□▶ ▲□▶ = 三 のへ

Error after 5 presmoothing steps, iteration k=2



PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother

Coarse Correction

Time Multigrid

Dahlquist Equatior FLA Results

Space-Time Multigrid

FLA Numerical Experimen Scalings

Multigrid Interpretations

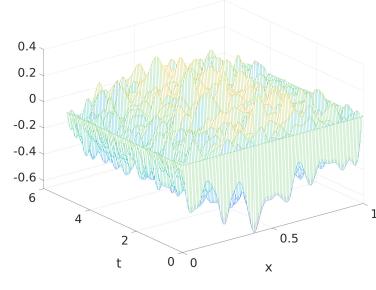
Parareal Parareal as a geometric nultigrid method AMG AGRIT

PFASST

ntegral Deferred Correctior Classical Parallel IDC

▲□▶ ▲□▶ ▲□▶ ▲□▶ ▲□ ● のの

Error after coarse correction, iteration k=2



PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother

Coarse Correction

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid Block Jacobi FLA

Numerical Experiments Scalings

Multigrid Interpretations

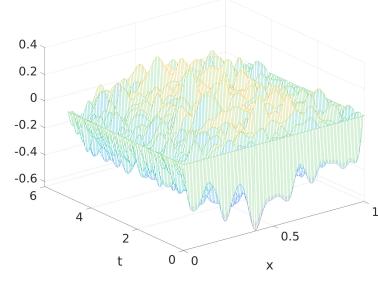
Parareal Parareal as a geometric multigrid method AMG MGRIT

PFASST

ntegral Deferred Correction Classical Parallel IDC

▲□▶ ▲□▶ ▲□▶ ▲□▶ = 三 のの

Error after 5 postsmoothing steps, iteration k=2



PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother

Coarse Correction

Time Multigrid

- Dahlquist Equation FLA Results
- Space-Time Multigrid Block Jacobi

FLA Numerical Experiments Scalings

Multigrid Interpretations

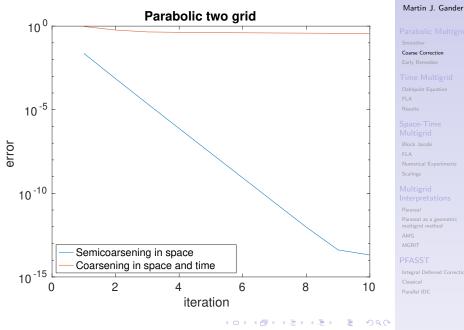
Parareal Parareal as a geometric nultigrid method AMG MGRIT

PFASST

ntegral Deferred Correctior Classical Parallel IDC

▲□▶▲舂▶▲差▶▲差▶ 差 のの

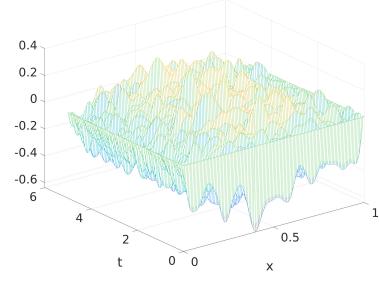
Convergence Comparison



PinT Summer

What goes wrong with space-time coarsening?

Error after 5 postsmoothing steps, iteration k=2



<ロト 4個ト 4 注ト 4 注ト 注目の Q</p>

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother

Coarse Correction

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

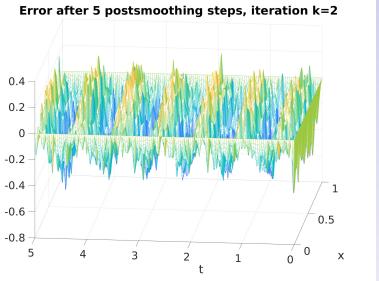
FLA Numerical Experiments Scalings

Multigrid Interpretations

'arareal 'arareal as a geometric nultigrid method MGRIT

PFASST

There is no smoothing in time!



<□> <@> < E> < E> E の Q

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother

Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacobi

Numerical Experiments Scalings

Multigrid Interpretations

Parareal Parareal as a geometric nultigrid method AMG

PFASST

Early Remedies

Horton and Vandewalle (1995): A Space-Time Multigrid Method for Parabolic Partial Differential Equations

"The fully discrete PDE is a strongly anisotropic problem. Pointwise smoothing combined with standard coarsening is a notoriously slow procedure for such problems."

Proposed Remedies:

- 1. Adaptive semi-coarsening in space or time depending on the anisotropy
- 2. Prolongation operators only forward in time

"Numerical results [...] for the one- and two-dimensional heat equations for both first- and second-order discretizations of the time derivative [...] proved to converge quickly, although at present the F-cycle seems to be necessary to achieve grid-independent rates."

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correctior

Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid Block Jacobi FLA Numerical Experiment Scalings

Multigrid Interpretations

Parareal Parareal as a geometric multigrid method AMG MGRIT

PFASST

◆□▶ ◆□▶ ◆□▶ ◆□▶ ○□ のQ@

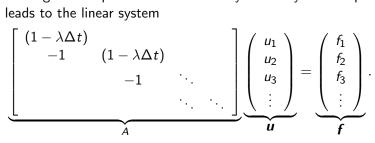
Time Multigrid for Dahlquist's Equation

$$\partial_t u = \lambda u, \quad u(0) = 0, \quad \lambda \in \mathbb{C}$$

Applying Backward Euler in time, we obtain

$$\frac{u_{n+1}-u_n}{\Delta t}=\lambda u_{n+1}\quad\Longleftrightarrow\quad (1-\lambda\Delta t)u_{n+1}-u_n=0.$$

Writing these equations simultaneously for many time steps leads to the linear system



Using a Jacobi smoother for this linear system $A\mathbf{u} = \mathbf{f}$ with damping parameter α gives

$$\boldsymbol{u}^{k+1} = \boldsymbol{u}^k + \alpha D^{-1} (\boldsymbol{f} - A \boldsymbol{u}^k) = \boldsymbol{u}^k - \frac{\alpha}{1 - \lambda \Delta t} A \boldsymbol{u}^k.$$

PinT Summer School

Martin J. Gander

Dahlguist Equation

Local Fouriermode Analysis (LFA)

Insert a Fourier mode in time,

$$u_n^k := C_\omega^k e^{i\omega n\Delta t},$$

into the Jacobi smoother

$$\boldsymbol{u}_n^{k+1} = \boldsymbol{u}_n^k - \frac{\alpha}{1-\lambda\Delta t}((1-\lambda\Delta t)\boldsymbol{u}_n^k - \boldsymbol{u}_{n-1}^k),$$

on one line (LFA does not see initial conditions)

$$\begin{array}{lll} \mathcal{C}^{k+1}_{\omega} &=& \mathcal{C}^{k}_{\omega} - \frac{\alpha}{1-\lambda\Delta t} \left((1-\lambda\Delta t) \mathcal{C}^{k}_{\omega} - \mathcal{C}^{k}_{\omega} e^{-i\omega\Delta t} \right) \\ &=& \left(1 - \alpha + \frac{\alpha e^{-i\omega\Delta t}}{1-\lambda\Delta t} \right) \mathcal{C}^{k}_{\omega}. \end{array}$$

The convergence factor is thus

$$\rho(\omega, \alpha) = \left(1 - \alpha + \frac{\alpha e^{-i\omega\Delta t}}{1 - \lambda\Delta t}\right), \quad \omega\Delta t \in (-\pi, \pi).$$

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Fime Multigrid

Dahlquist Equation

FLA Results

Space-Time Multigrid

Block Jacobi

FLA

Numerical Experiments Scalings

Multigrid Interpretations

arareal arareal as a geometric sultigrid method MG

MGRI

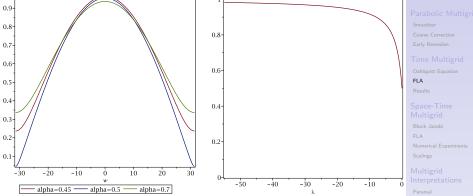
PFASST

ntegral Deferred Correction Classical Parallel IDC

▲□▶ ▲□▶ ▲□▶ ▲□▶ ▲□ ● のへで

Smoothing Properties of Jacobi in time

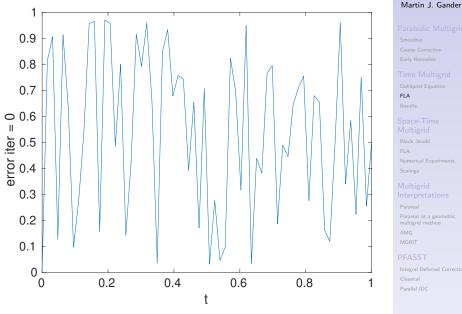
PinT Summer School Martin J. Gander



Left: Smoothing properties for the Jacobi smoother applied to the Dahlquist equation.

Right: $\alpha^* = \frac{\Delta t^2 \lambda^2 - 3\Delta t \lambda + 2}{\Delta t^2 \lambda^2 - 4\Delta t \lambda + 4}$ for best smoothing properties. Damped Jacobi is a good smoother in time !?

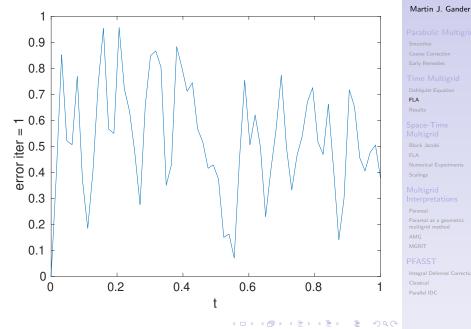
Jacobi Smoother for Dahlquist's Equation: k = 0



イロト 不得 トイヨト イヨト 三日

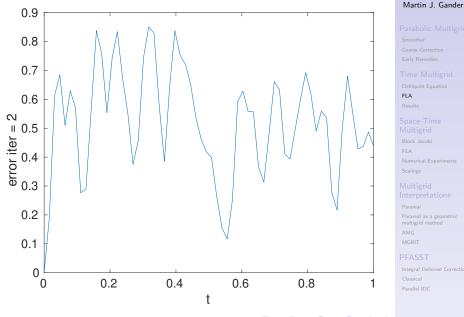
PinT Summer

Jacobi Smoother for Dahlquist's Equation: k = 1



PinT Summer School

Jacobi Smoother for Dahlquist's Equation: k = 2

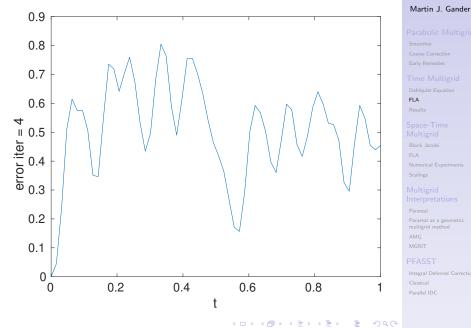


▲□▶ ▲□▶ ▲□▶ ▲□▶ = 三つへ

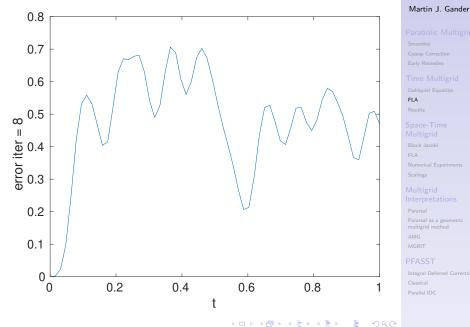
PinT Summer

Jacobi Smoother for Dahlquist's Equation: k = 4

PinT Summer



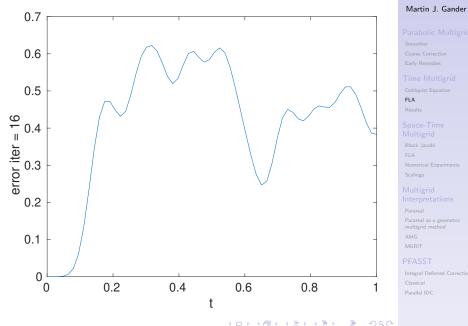
Jacobi Smoother for Dahlquist's Equation: k = 8



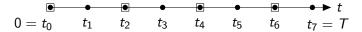
PinT Summer

Jacobi Smoother for Dahlquist's Equation: k = 16

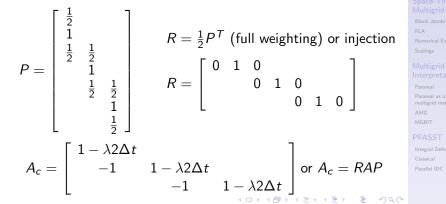
PinT Summer



Two Grid Method in Time



$$\begin{aligned} & \boldsymbol{u}^{k+\frac{1}{3}} = S(\boldsymbol{f}, \boldsymbol{u}^{k}, \nu_{1}); & \% \text{ presmoothing} \\ & \boldsymbol{u}^{k+\frac{2}{3}} = \boldsymbol{u}^{k+\frac{1}{3}} + PA_{c}^{-1}R(\boldsymbol{f} - A\boldsymbol{u}^{k+\frac{1}{3}}) & \% \text{ coarse correction} \\ & \boldsymbol{u}^{k+1} = S(\boldsymbol{f}, \boldsymbol{u}^{k+\frac{2}{3}}, \nu_{2}); & \% \text{ postsmoothing} \end{aligned}$$



PinT Summer School

Martin J. Gander

EL A

Convergence, and best choice of $\boldsymbol{\alpha}$

10⁰

10-2



Martin J. Gander



Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA

Results

Space-Time Multigrid Block Jacobi FLA Numerical Experime Scalings

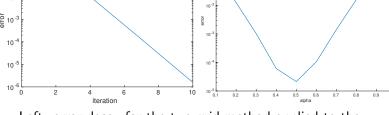
Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method AMG MGRIT

PFASST

ntegral Deferred Correction Classical Parallel IDC



10

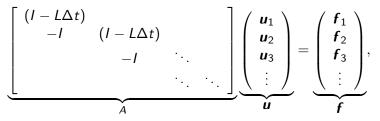
Left: error decay for the two grid method applied to the Dahlquist equation.

Right: dependence on the choice of the relaxation parameter α of the error after k = 30 iterations

error after 30 2-grid iterations, 1 Jacobi smoothing step

Space-Time Multigrid

All at once system for the heat equation in space-time:



Key idea: need to divide by the diagonal block $I - L\Delta t$, as we divided by $1 - \lambda\Delta t$ in Jacobi for the Dahlquist equation, i.e. use a block Jacobi smoother.

Insert a Fourier mode in space and time

$$u_{n,j}^k := C_{\omega,\xi}^k e^{i\omega n\Delta t} e^{i\xi j\Delta x}$$

into the block Jacobi smoother

$$\boldsymbol{u}_n^{k+1} = \boldsymbol{u}_n^k - \alpha (I - L\Delta t)^{-1} ((I - \lambda L\Delta t) \boldsymbol{u}_n^k - \boldsymbol{u}_{n-1}^k)$$

= $(1 - \alpha) \boldsymbol{u}_n^k + \alpha (I - L\Delta t)^{-1} \boldsymbol{u}_{n-1}^k$

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacobi

Numerical Experiments Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method

AM

MGRI

PFASST

Smoothing Analysis

For the term $L \boldsymbol{u}_{n-1}^k$ we get with $u_{n,j}^k := C_{\omega,\xi}^k e^{i\omega n\Delta t} e^{i\xi j\Delta x}$

$$\frac{1}{\Delta x^2} (u_{n-1,j+1} - 2u_{n-1,j} + u_{n-1,j-1})$$

$$= e^{-i\omega\Delta t} \frac{1}{\Delta x^2} \left(e^{i\xi\Delta x} - 2 + e^{-i\xi\Delta x} \right) C^k_{\omega,\xi} e^{i\omega n\Delta t} e^{i\xi j\Delta x}$$

$$= e^{-i\omega\Delta t} \frac{2(\cos\xi\Delta x - 1)}{\Delta x^2} C^k_{\omega,\xi} e^{i\omega n\Delta t} e^{i\xi j\Delta x}.$$

The symbol of the block Jacobi smoother

$$(1-\alpha)\boldsymbol{u}_n^k + \alpha(\boldsymbol{I} - \boldsymbol{L}\Delta t)^{-1}\boldsymbol{u}_{n-1}^k$$

is thus for $\omega \Delta t \in (-\pi,\pi)$, $\xi \Delta x \in (-\pi,\pi)$

$$\rho(\omega,\xi,\alpha) = 1 - \alpha \left(1 - \frac{e^{i\omega\Delta t}}{1 + 2\frac{\Delta t}{\Delta x^2}(1 - \cos\xi\Delta x)} \right)$$

G, Neumüller (2016): Analysis of a New Space-Time Parallel Multigrid Algorithm for Parabolic Problems

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacobi

FLA Numerical Experiments Scalings

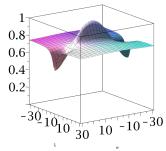
Multigrid Interpretations

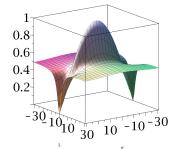
arareal arareal as a geometric ultigrid method MG

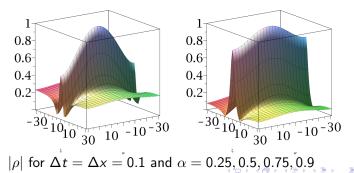
MGR

PFASST

Fourier Local Mode Analysis Results







PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacob

FLA

Numerical Experiments Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method

AM

MGR

PFASST

Time and Space Smoothing Lemmas Lemma (Optimal parameter for smoothing in time) The best choice for α to obtain smoothing in time is

$$\alpha^* = \frac{1}{2}.$$

Then all high frequencies in time, $\omega \in \pm(\frac{\pi}{2\Delta t}, \frac{\pi}{\Delta t})$ are multiplied by at least the factor $\frac{1}{\sqrt{2}}$. Proof. The derivative w.r.t ω ,

$$\partial_{\omega} |\rho(\omega,\xi,\alpha)|^2 = -2\alpha(1-\alpha) \frac{\Delta x^2 \Delta t \sin(\omega \Delta t)}{2\Delta t (1-\cos(\xi \Delta x)) + \Delta x^2}$$

is negative for positive ω , and positive for negative ω . Thus the maximum for $\omega \in \left(\frac{\pi}{2\Delta t}, \frac{\pi}{\Delta t}\right)$ is attained at $\omega = \frac{\pi}{2\Delta t}$, and similarly for negative ω at $\omega = -\frac{\pi}{2\Delta t}$. The derivative with respect to ξ at $\omega = \frac{\pi}{2\Delta t}$ is

$$\partial_{\xi} |
ho(rac{\pi}{2\Delta t},\xi,lpha)|^2 = -rac{4lpha^2\Delta x^5\Delta t\sin(\xi\Delta x)}{(2\Delta t(1-\cos(\xi\Delta x))+\Delta x^2)^3},$$

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacob

FLA

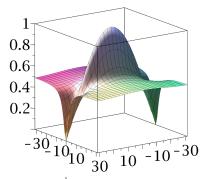
Numerical Experiments Scalings

Multigrid Interpretations

Parareal Parareal as a geometric multigrid method AMG MGRIT

PFASST

Proof continued



which shows that the maximum is attained at $\xi = 0$. The worst smoothing in time is thus at $(\omega, \xi) = (\pm \frac{\pi}{2\Delta t}, 0)$, and the convergence factor value in modulus at this location is

$$|\rho(\pm \frac{\pi}{2\Delta t}, 0, \alpha)|^2 = (1 - \alpha)^2 \alpha^2$$

and this value is minimized for $\alpha = \alpha^* = \frac{1}{2}$, for which $|\rho(\pm \frac{\pi}{2\Delta t}, 0, \frac{1}{2})| = \frac{1}{\sqrt{2}}$.

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacob

FLA

Numerical Experiments Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method AMG

MGRI

PFASST

Lemma (Condition for smoothing in space)

With $\alpha = \alpha^* = \frac{1}{2}$, high frequencies in space $\xi \in \pm(\frac{\pi}{2\Delta x}, \frac{\pi}{\Delta x})$ are at least damped by the factor $\frac{1}{\sqrt{2}}$ if

$$\mu := \frac{\Delta t}{\Delta x^2} \ge \frac{1}{\sqrt{2}}$$

Proof.

By the derivatives from the previous Lemma, the least damping is at $\omega = 0$ and $\xi = \pm \frac{\pi}{2\Delta x}$, namely

$$|\rho(\mathbf{0},\frac{\pi}{2\Delta x},\alpha^*)|=\frac{\mu+1}{2\mu+1}$$

and

$$\frac{\mu+1}{2\mu+1} \le \frac{1}{\sqrt{2}} \iff \sqrt{2}(\mu+1) \le 2\mu+1$$
$$\iff \sqrt{2}-1 \le (2-\sqrt{2})\mu \iff \mu \ge \frac{1}{\sqrt{2}}$$

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacob

FLA

Numerical Experiments Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method

AM

MGRI

PFASST

Theorem (Space-time multigrid coarsening)

In the Space-Time Multi-Grid (STMG) method with block Jacobi smoother applied to the all at once space time system of the one dimensional heat equation discretized by Backward Euler in time and centered finite differences in space, and the best choice of the relaxation parameter for time smoothing $\alpha^* = \frac{1}{2}$, one can always perform coarsening in time, and in space one can also use coarsening provided the condition $\frac{\Delta t}{\Delta x^2} \geq \frac{1}{\sqrt{2}}$ holds on the current level.

Proof.

For the two level method, this is a direct consequence of the two Lemmas, and the extension to the multilevel case follows by the fact that for the multigrid method, the two grid correction is simply applied recursively, with the bounds not depending on the levels.

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Fime Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacob

FLA

Numerical Experiments Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method AMG MGRIT

PFASST

Multigrid Iterations 3D Heat Equation

One V-cycle in space to invert the diagonal blocks

space	time levels									
levels	1	2	3	4	5	5	7	8	9	10
0	7	8	8	8	7	7	7	8	8	8
1	7	8	8	8	7	7	7	8	8	8
2	8	8	8	8	8	7	8	8	8	8
3	8	9	8	8	8	8	8	8	8	8
4	10	9	9	9	8	8	8	8	8	8
5	10	10	10	9	9	8	8	8	8	8

Solution times in seconds:

dof	forward substitution	multigrid
2 304	3.30	0.06
23 296	3.69	1.02
218 880	9.80	13.19
1 912 576	95.27	136.99
16 015 104	1031.43	1155.12
131 120 896	9970.89	10416.90

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correctior Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacobi

FLA

Numerical Experiments

Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method

AMG

MGRI

PFASST

ntegral Deferred Correction Classical Parallel IDC

590

3

3D Heat Equation Weak Scaling Results

dof

cores | time steps |

PinT Summer School

Wartin J. G	IWU. SUD.		itei	401	time steps	COLES
	19.0	28.8	7	59 768	2	1
Smoother	37.9	29.8	7	119 536	4	2
Coarse Correction	75.9	29.8	7	239 072	8	4
Early Remedies	152.2	29.9	7	478 144	16	8
	305.4	29.9	7	956 288	32	16
FLA	613.6	29.9	7	1 912 576	64	32
Results	1 220.7	29.9	7	3 825 152	128	64
Space-Time Multigrid	2 448.4	29.9	7	7 650 304	256	128
Block Jacobi	4 882.4	30.0	7	15 300 608	512	256
FLA Numerical Experir	9 744.2	29.9	7	30 601 216	1 024	512
Scalings	19 636.9	30.0	7	61 202 432	2 048	1 024
Multigrid	38 993.1	29.9	7	122 404 864	4 096	2 048
Interpretation Parareal	81 219.6	30.0	7	244 809 728	8 192	4 096
Parareal as a geor multigrid method	162 551.0	30.0	7	489 619 456	16 384	8 192
AMG	313 122.0	30.0	7	979 238 912	32 768	16 384
MGRIT	625 686.0	30.0	7	1 958 477 824	65 536	32 768
PFASST	1 250 210.0	30.0	7	3 916 955 648	131 072	65 536
Integral Deferred Classical	2 500 350.0	30.0	7	7 833 911 296	262 144	131 072
Parallel IDC	4 988 060.0	30.0	7	15 667 822 592	524 288	262 144
			,			

iter itime

fwd sub

Vulcan BlueGene/Q Supercomputer in Livermore (by M. Neumüller)

3D Heat E	Equation St	rong Scaling	Results	5	School
cores	time steps	dof	iter	time	Martin J. Gander
1	512	15 300 608	7	7 635.2	
2	512	15 300 608	7	3 821.7	Parabolic Multigrid
4	512	15 300 608	7	1 909.9	Coarse Correction
8	512	15 300 608	7	954.2	Early Remedies
16	512	15 300 608	7	477.2	Time Multigrid
32	512	15 300 608	7	238.9	FLA
64	512	15 300 608	7	119.5	Results
128	512	15 300 608	7	59.7	Space-Time Multigrid
256	512	15 300 608	7	30.0	Block Jacobi FLA
512	524 288	15 667 822 592	7	15 205.9	FLA Numerical Experiments
1 024	524 288	15 667 822 592	7	7 651.5	Scalings
2 048	524 288	15 667 822 592	7	3 825.3	Multigrid Interpretations
4 096	524 288	15 667 822 592	7	1 913.4	Parareal
8 192	524 288	15 667 822 592	7	956.6	Parareal as a geometric multigrid method
16 384	524 288	15 667 822 592	7	478.1	AMG MGRIT
32 768	524 288	15 667 822 592	7	239.3	PFASST
65 536	524 288	15 667 822 592	7	119.6	Integral Deferred Correction
131 072	524 288	15 667 822 592	7	59.8	Classical Parallel IDC
262 144	524 288	15 667 822 592	7	30.0	

PinT Summer

Vulcan BlueGene/Q Supercomputer in Livermore (by M. Neumüller)

Parareal as a Geometric Multigrid Method

Consider the Dahlquist equation

$$\frac{du}{dt} = \lambda u \quad \text{in } (0, T), \quad u(0) = u_0$$

N coarse time intervals and M fine time steps in every coarse time interval, $0 = t_0 < t_1 < t_2 < \ldots < t_{MN} = T$, $t_m - t_{m-1} = \Delta t$, forward Euler

$$A\boldsymbol{u} := \begin{pmatrix} 1 & & \\ -\phi & 1 & & \\ & \ddots & \ddots & \\ & & -\phi & 1 \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ u_{MN} \end{pmatrix} = \begin{pmatrix} u_0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} =: \boldsymbol{f},$$

where $\phi := 1 + \lambda \Delta t$. Eliminate every second unknown

$$\begin{pmatrix} 1 & & \\ -\phi^2 & 1 & \\ & \ddots & \ddots & \\ & & -\phi^2 & 1 \end{pmatrix} \begin{pmatrix} u_0 \\ u_2 \\ \vdots \\ u_{MN} \end{pmatrix} = \begin{pmatrix} u_0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid Block Jacobi

Numerical Experiments Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method AMG MGRIT

PFASST

Eliminate more unknowns, keeping only every M-th one,

$$\tilde{A}\tilde{\boldsymbol{U}} := \begin{pmatrix} 1 & & & \\ -\tilde{F} & 1 & & \\ & \ddots & \ddots & \\ & & -\tilde{F} & 1 \end{pmatrix} \begin{pmatrix} \tilde{U}_0 \\ \tilde{U}_1 \\ \vdots \\ \tilde{U}_N \end{pmatrix} = \begin{pmatrix} u_0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} =: \tilde{\boldsymbol{f}},$$

where $\tilde{F} := (1 + \lambda \Delta t)^M$. Note that at the coarse nodes $T_n := nM\Delta t$ we have $\tilde{U}_n = u_{nM}$. Now approximate

with $\tilde{G} := 1 + \lambda \Delta T$ one forward Euler step, and consider the preconditioned stationary iteration

$$\tilde{\boldsymbol{U}}^{k+1} = \tilde{\boldsymbol{U}}^k + \tilde{M}^{-1}(\boldsymbol{f} - \tilde{A}\tilde{\boldsymbol{U}}^k).$$

・ロト ・ 同 ト ・ ヨ ト ・ ヨ ・ つ へ ()

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacobi

FLA

Numerical Experiments Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method AMG MGRIT

PFASST

Theorem

The stationary iteration is equal to Parareal, $\tilde{U}_n^k = U_n^k$ for k = 1, 2, ... and n = 0, 1, ..., N, provided initially we have $\tilde{U}_n^0 = U_n^0$ for n = 0, 1, ..., N.

Proof. The preconditioned stationary iteration computes

$$\begin{pmatrix} 1 & & \\ -\tilde{G} & 1 & & \\ & \ddots & \ddots & \\ & & -\tilde{G} & 1 \end{pmatrix} \begin{pmatrix} \begin{pmatrix} \tilde{U}_0^{k+1} \\ \tilde{U}_1^{k+1} \\ \vdots \\ \tilde{U}_N^{k+1} \end{pmatrix} - \begin{pmatrix} \tilde{U}_0^k \\ \tilde{U}_1^k \\ \vdots \\ \tilde{U}_N^k \end{pmatrix} \end{pmatrix}$$
$$= \begin{pmatrix} u_0 - \tilde{U}_0^k \\ \tilde{F} \tilde{U}_0^k - \tilde{U}_1^k \\ \vdots \\ \tilde{F} \tilde{U}_{N-1}^k - \tilde{U}_N^k \end{pmatrix}$$

The *n*-th line in this iteration reads

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Fime Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid Block Jacobi FLA Numerical Experime

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method AMG MGRIT

PFASST

ntegral Deferred Correction Classical Parallel IDC

▲□▶ ▲□▶ ▲□▶ ▲□▶ ▲□ ● のへで

Proof continued

$$-\tilde{G}\tilde{U}_{n-1}^{k+1}+\tilde{G}\tilde{U}_{n-1}^{k}+\tilde{U}_{n}^{k+1}-\tilde{U}_{n}^{k}=\tilde{F}\tilde{U}_{n-1}^{k}-\tilde{U}_{n}^{k},$$

and we obtain after simplification

$$\tilde{U}_n^{k+1} = \tilde{F}\tilde{U}_{n-1}^k + \tilde{G}\tilde{U}_{n-1}^{k+1} - \tilde{G}\tilde{U}_{n-1}^k.$$

Applying parareal to the Dahlquist problem using forward Euler, we get for the parareal fine integrator

$$F(T_{n+1}, T_n, v) := (1 + \lambda \Delta t)^M v \equiv \tilde{F} v$$

and for the coarse integrator

$$G(T_{n+1}, T_n, v) := (1 + \lambda \Delta T) v \equiv \tilde{G} v,$$

and thus the updating formula coincides with Parareal.

Remark: This result also holds for any other integrator since we never used the precise form of Forward Euler, e.g. for Backward Euler $\phi = (1 - \lambda \Delta t)^{-1}$, $\tilde{F} = (1 - \lambda \Delta t)^{-M}$, $\tilde{G} = (1 - \lambda \Delta T)^{-1}$.

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacobi

Numerical Experiments Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method AMG MGRIT

PFASST

Parareal as a geometric multigrid method

For solving approximately the linear system

$$A\mathbf{u}=\mathbf{f},$$

a geometric two grid method would, starting with the initial guess \boldsymbol{u}^0 , compute for k = 0, 1, 2, ...

$$\begin{aligned} \tilde{\boldsymbol{u}}^k &:= \operatorname{Smooth}(A, \boldsymbol{f}, \boldsymbol{u}^k); \\ \boldsymbol{e} &:= A_c^{-1} R(\boldsymbol{f} - A \tilde{\boldsymbol{u}}^k); \\ \boldsymbol{u}^{k+1} &:= \tilde{\boldsymbol{u}}^k + P \boldsymbol{e}; \end{aligned}$$

To identify parareal with geometric multigrid, we need a block Jacobi splitting

$$A=\tilde{M}_J-\tilde{N}_J,$$

where \tilde{M}_J is a block diagonal matrix with diagonal blocks of size $M \times M$, except for the first block which is one bigger because of the initial condition of the problem.

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Fime Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid Block Jacobi FLA Numerical Experiment

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method

AMG

MGRI

PFASST

Theorem (Parareal=Multigrid+Agressive Coarsening)

Using one presmoothing step with the modified block Jacobi smoother

$$\boldsymbol{u}^{\ell} = \boldsymbol{u}^{\ell-1} + E\tilde{M}_J^{-1}(\boldsymbol{f} - A\boldsymbol{u}^{\ell-1}),$$

where E is the identity, except with zeros at the coarse nodes, injection for P and $R := P^T$, and $A_c = \tilde{M}$, then the two grid algorithm produces the parareal iterates at the coarse nodes, $U_n^k = u_{nM}^k$, provided one starts with an initial approximation \mathbf{u}^0 that satisfies $U_n^0 = u_{nM}^0$.

Proof. By induction on k: statement holds trivially for k = 0 by assumption.

We thus assume that for k, $u_{nM}^k = U_n^k$ for n = 0, 1, ..., N, and prove this for k + 1. After one step with the modified block Jacobi smoother, $\tilde{\boldsymbol{u}}^k$ contains the fine solutions starting at each initial condition U_n^k ,

$$\tilde{u}_{nM+j}^{k} = (1 + \lambda \Delta t)^{j} U_{n}^{k}, \quad j = 0, 1, \dots, M-1,$$

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid Block Jacobi FLA Numerical Experime

Multigrid

Parareal

Parareal as a geometric multigrid method

AMG

MGRI

PFASST

except for the coarse variables which have not changed because of E, we still have $\tilde{u}_{nM}^k = U_n^k$ for n = 0, 1, ..., N. Now with the coarse operator $A_c = \tilde{M}$ we need to solve

$$\tilde{M}\boldsymbol{e}=R(\boldsymbol{f}-A\tilde{\boldsymbol{u}}^{k}).$$

Looking at any line n > 0, with R the transpose of injection, the definition of A and \tilde{M} , and that f is zero except in the first component

$$\boldsymbol{e}_n - G(\boldsymbol{e}_{n-1}) = -U_n^k + (1 + \lambda \Delta t)(\tilde{u}_{nM-1}^k).$$

Now from the Jacobi smoother, we have

$$\tilde{u}_{nM-1}^{k} = (1 + \lambda \Delta t)^{M-1} u_{(n-1)M}^{k} = (1 + \lambda \Delta t)^{M-1} U_{n-1}^{k},$$

and thus with the definition of F

$$\boldsymbol{e}_n = -U_n^k + F(U_{n-1}^k) + G(\boldsymbol{e}_{n-1}),$$

Now performing the last of the 3 multigrid steps, with P injection, and $\tilde{u}_{nM}^k = U_n^k$, we get on the lines nM

$$u_{nM}^{k+1} = F(U_{n-1}^k) + G(e_{n-1}).$$
 (*)

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Fime Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid Block Jacobi FLA Numerical Experimen Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method

AMG

MGRI

PFASST

We next note that at step n-1 can be written as

$$\boldsymbol{e}_{n-1} = -U_{n-1}^k + F(U_{n-2}^k) + G(\boldsymbol{e}_{n-2}) = -U_{n-1}^k + u_{(n-1)M}^{k+1},$$

where we used (*) for the last step, and inserting this into (*) and using linearity gives

$$u_{nM}^{k+1} = F(U_{n-1}^k) + G(u_{(n-1)M}^{k+1}) - G(U_{n-1}^k),$$

which concludes the proof by induction, since this is the recurrence formula for the parareal algorithm, and $u_0^{k+1} = U_0^{k+1} = u_0$.

Remarks:

- This Theorem also holds in the non-linear context [G, Vandewalle 2007]
- The special block Jacobi smoother is only modifying the fine nodes, and is thus not convergent, and the second iteration will not produce any modification.
- Multilevel Parareal by recursion on \tilde{M}

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

FLA Numerical Experimen Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method

AMG

MGRI

PFASST

Algebraic Multigrid (AMG)

Ruge, Stüben (1987): Algebraic multigrid

"Thus, the set of variables on level h can be split into two disjoint subsets: the first one contains the variables also represented in the coarser level (Cvariables), and the second one is just the complementary set (F-variables)."

Reordering the system matrix accordingly yields

$$A\boldsymbol{u} = \begin{bmatrix} A_{\rm ff} & A_{\rm fc} \\ A_{\rm cf} & A_{\rm cc} \end{bmatrix} \begin{pmatrix} \boldsymbol{u}_f \\ \boldsymbol{u}_c \end{pmatrix} = \begin{pmatrix} \boldsymbol{f}_f \\ \boldsymbol{f}_c \end{pmatrix} = \boldsymbol{f}.$$

A block-LU factorization is given by

$$\left[\begin{array}{cc} A_{\rm ff} & A_{\rm fc} \\ A_{\rm cf} & A_{\rm cc} \end{array} \right] = \left[\begin{array}{cc} I \\ A_{\rm cf} A_{\rm ff}^{-1} & I \end{array} \right] \left[\begin{array}{cc} A_{\rm ff} \\ S_{\rm cc} \end{array} \right] \left[\begin{array}{cc} I & A_{\rm ff}^{-1} A_{\rm fc} \\ I \end{array} \right],$$

with the Schur complement $S_{cc} := A_{cc} - A_{cf}A_{ff}^{-1}A_{fc}$.

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Fime Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacobi

FLA Numerical Experimen

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method

AMG

・ロト ・ 同 ト ・ ヨ ト ・ ヨ ・ う へ や

MGRIT

PFASST

One can express then the inverse of A explicitly,

$$A^{-1} = \begin{bmatrix} I & -A_{\rm ff}^{-1}A_{\rm fc} \\ I \end{bmatrix} \begin{bmatrix} A_{\rm ff}^{-1} & \\ S_{\rm cc}^{-1} \end{bmatrix} \begin{bmatrix} I \\ -A_{\rm cf}A_{\rm ff}^{-1} & I \end{bmatrix}$$

Defining the coarse restriction and extension matrices by

$$R_c := \begin{bmatrix} -A_{\rm cf} A_{\rm ff}^{-1} I \end{bmatrix}, \quad P_c := \begin{bmatrix} -A_{\rm ff}^{-1} A_{\rm fc} \\ I \end{bmatrix},$$

and the more simple fine restriction and extension matrices by

$$R_f := \begin{bmatrix} I & 0 \end{bmatrix}, \quad P_f := R_f^T,$$

one can obtain the following surprising result

Lemma

The inverse A^{-1} of the reordered system matrix A can be expressed as a sum of an inverse just acting on the fine variables, and a complementary inverse,

$$A^{-1} = P_c (R_c A P_c)^{-1} R_c + P_f (R_f A P_f)^{-1} R_f.$$

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

pace-Time Aultigrid Block Jacobi

Numerical Experiments Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method

AMG

MGRI

PFASST

ntegral Deferred Correction Classical Parallel IDC

・ロト ・ 四ト ・ ヨト ・ ヨト ・ りゃく

Proof.

By a direct calculation: we first compute for the coarse nodes

$$R_{c}AP_{c} = \begin{bmatrix} -A_{cf}A_{ff}^{-1} I \end{bmatrix} \begin{bmatrix} A_{ff} & A_{fc} \\ A_{cf} & A_{cc} \end{bmatrix} \begin{bmatrix} -A_{ff}^{-1}A_{fc} \\ I \end{bmatrix}$$
$$= \begin{bmatrix} -A_{cf}A_{ff}^{-1} I \end{bmatrix} \begin{bmatrix} 0 \\ A_{cc} - A_{cf}A_{ff}^{-1}A_{fc} \end{bmatrix} = S_{cc}.$$

For the fine nodes, we get with the simple P_f and R_f

$$R_f A P_f = A_{\rm ff}.$$

We thus get

$$P_{c}(R_{c}AP_{c})^{-1}R_{c} + P_{f}(R_{f}AP_{f})^{-1}R_{f}$$

$$= \begin{bmatrix} -A_{\text{ff}}^{-1}A_{\text{fc}} \\ I \end{bmatrix} S_{\text{cc}}^{-1}[-A_{\text{cf}}A_{\text{ff}}^{-1}I] + \begin{bmatrix} I \\ 0 \end{bmatrix} A_{\text{ff}}^{-1}[I \quad 0]$$

$$= \begin{bmatrix} I & -A_{\text{ff}}^{-1}A_{\text{fc}} \\ I \end{bmatrix} \begin{bmatrix} A_{\text{ff}}^{-1} \\ S_{\text{cc}}^{-1} \end{bmatrix} \begin{bmatrix} I \\ -A_{\text{cf}}A_{\text{ff}}^{-1} \\ I \end{bmatrix}$$

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

- Dahlquist Equation FLA Results
- Space-Time Multigrid
- Block Jacobi
- FLA
- Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method

AMG

MGRIT

.

PFASST

This result is interesting when we look at a classical stationary iterative method with preconditioner $M \approx A$,

$$\boldsymbol{u}^{k+1} = \boldsymbol{u}^k + M^{-1}(\boldsymbol{f} - A\boldsymbol{u}^k)$$

The error $\boldsymbol{e}^k := \boldsymbol{u} - \boldsymbol{u}^k$ satisfies

$$\boldsymbol{e}^{k+1} = (I - M^{-1}A)\boldsymbol{e}^k$$

Using for $M^{-1} = A^{-1}$, the error propagator $(I - M^{-1}A)$ vanishes identically, but writing it down explicitly gives

$$0 = (I - A^{-1}A)$$

= $I - P_c(R_cAP_c)^{-1}R_cA - P_f(R_fAP_f)^{-1}R_fA$,

which is an optimal additive correction scheme between fine and coarse nodes, it converges in one iteration (nilpotent). For a multiplicative correction scheme, we compute

$$(I - P_c(R_cAP_c)^{-1}R_cA) (I - P_f(R_fAP_f)^{-1}R_fA) = I - P_c(R_cAP_c)^{-1}R_cA - P_f(R_fAP_f)^{-1}R_fA + P_c(R_cAP_c)^{-1}R_cAP_f(R_fAP_f)^{-1}R_fA,$$

and the last term cancels, because the middle term = >

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacobi FLA Numerical Experin

Multigrid nterpretations

Parareal

Parareal as a geometric multigrid method

AMG

MGRIT

PFASST

$$egin{aligned} \mathcal{R}_{c}\mathcal{A}\mathcal{P}_{f} &= \left[-\mathcal{A}_{\mathrm{cf}}\mathcal{A}_{\mathrm{ff}}^{-1} \ \mathcal{I}
ight] \left[egin{aligned} \mathcal{A}_{\mathrm{ff}} & \mathcal{A}_{\mathrm{fc}} \ \mathcal{A}_{\mathrm{cc}} \end{array}
ight] \left[egin{aligned} \mathcal{I} \ \mathcal{O} \end{array}
ight] \ &= \left[-\mathcal{A}_{\mathrm{cf}}\mathcal{A}_{\mathrm{ff}}^{-1} \ \mathcal{I}
ight] \left[egin{aligned} \mathcal{A}_{\mathrm{ff}} \ \mathcal{A}_{\mathrm{cf}} \end{array}
ight] = \mathbf{0}. \end{aligned}$$

Therefore, the multiplicative correction scheme in this exact setting coincides with the additive one.

AMG idea:

approximate the operators

$$R_c = [-A_{\mathrm{cf}}A_{\mathrm{ff}}^{-1} I], \quad P_c := \left[egin{array}{c} -A_{\mathrm{ff}}^{-1}A_{\mathrm{fc}} \\ I \end{array}
ight]$$

in these exact correction schemes, i.e. A_{ff}^{-1}

very different from geometric multigrid based on smoothing and coarse correction.

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacobi

FLA

Numerical Experiments Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method

AMG

MGRIT

PFASST

ntegral Deferred Correction Classical Parallel IDC

・ロト ・ 四ト ・ ヨト ・ ヨト ・ りゃく

MGRIT (Multigrid Reduction in Time)

Friedhoff, Falgout, Kolev, MacLachlan, Schroder (2013): A multigrid-in-time algorithm for solving evolution equations in parallel

"Our algorithm is based on interpreting the parareal time integration method as a two level reduction scheme, and developing a multilevel algorithm from this viewpoint"

Theorem

In the parareal algorithm, the error propagation operator is

 $(I-P_c\tilde{M}^{-1}R_cA)(I-P_f(R_fAP_f)^{-1}R_fA),$

where \tilde{M} is the coarse time stepping matrix.

The only approximation is therefore $\tilde{M} \approx R_c A P_c$ in the AMG setting of Parareal.

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacobi

Numerical Experiments Scalings

Multigrid nterpretations

Parareal

Parareal as a geometric multigrid method

MGRIT

PFASST

ntegral Deferred Correction Classical Parallel IDC

・ロト ・ 四ト ・ ヨト ・ ヨト ・ りゃく

Proof.

The error propagation operator of Parareal on the coarse variables is

$$(I - \tilde{M}^{-1}\tilde{A}).$$

To write this for all variables, we need $R := [0 \ I]$ selecting the coarse nodes. Noting that

$$\mathbf{P}_{c} = \begin{bmatrix} -A_{\mathrm{ff}}^{-1}A_{\mathrm{fc}} \\ I \end{bmatrix},$$

leaves coarse nodes invariant, and extends to fine by fine solves the error propagation operator of Parareal for all variables is

$$P_c(I-\tilde{M}^{-1}\tilde{A})R$$

Now $\tilde{A} = R_c A P_c = S_{cc}$ is the Schur complement in the proof of the Lemma, since \tilde{A} was obtained by elimination of the fine unknowns. Thus the error propagation operator becomes

$$P_c(I - \tilde{M}^{-1}\tilde{A})R = P_c(I - \tilde{M}^{-1}R_cAP_c)R$$
$$= (I - P_c\tilde{M}^{-1}R_cA)P_cR,$$

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Fime Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacobi

FLA Numerical Expe

calings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method

MGRIT

PFASST

Proof continued

and since

$$P_{c}R = \begin{bmatrix} -A_{\rm ff}^{-1}A_{\rm fc} \\ I \end{bmatrix} \begin{bmatrix} 0 & I \end{bmatrix} = \begin{bmatrix} 0 & -A_{\rm ff}^{-1}A_{\rm fc} \\ 0 & I \end{bmatrix}$$

is identical to

$$\begin{split} I - P_f (R_f A P_f)^{-1} R_f A &= I - \begin{bmatrix} A_{\rm ff}^{-1} \\ 0 \end{bmatrix} \begin{bmatrix} A_{\rm ff} & A_{\rm fc} \end{bmatrix} \\ &= \begin{bmatrix} 0 & -A_{\rm ff}^{-1} A_{\rm fc} \\ 0 & I \end{bmatrix}, \end{split}$$

the error propagation operator of parareal is indeed

$$(I-P_c\tilde{M}^{-1}R_cA)(I-P_f(R_fAP_f)^{-1}R_fA),$$

which concludes the proof.

Remark: Multilevel Parareal by recursion on \tilde{M} .

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

- Dahlquist Equation FLA Results
- Space-Time Multigrid
- Block Jacobi
- Numerical Experiments Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method

AM

ъ.

MGRIT

PFASST

MGRIT and FCF relaxation

Idea of MGRIT: replace the *F*-relaxation, the second term in the error propagation operator, by

 $(I - P_f(R_f A P_f)^{-1} R_f A)(I - R^T (RAR^T)^{-1} RA)(I - P_f(R_f A P_f)^{-1} R_f A)$

The C-relaxation term $(I - R^T (RAR^T)^{-1}RA)$ closes precisely the gap left by the F-relaxation to make a second F-relaxation useful (cf the *E* matrix in the geometric setting)

Theorem

The two level MGRIT algorithm with FCF-smoother computes the same iterations as the parareal algorithm with overlap of one coarse time interval,

$$U_0^{k+1} = u_0, \quad U_1^{k+1} = \tilde{F} u_0, U_n^{k+1} = \tilde{F} \tilde{F} U_{n-2}^k + \tilde{G} U_{n-1}^{k+1} - \tilde{G} \tilde{F} U_{n-2}^k.$$

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equatior FLA Results

```
Space-Time
Multigrid
Block Jacobi
FLA
Numerical Experime
```

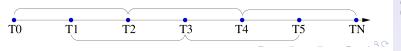
Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method

MGRIT

PFASST



Proof.

Need an interpretation of the added CF-relaxation in MGRIT in terms of the parareal algorithm. For the C-part, we obtain

$$I - R^{T} (RAR^{T})^{-1} RA = I - \begin{bmatrix} 0 & 0 \\ 0 & A_{cc}^{-1} \end{bmatrix} \begin{bmatrix} A_{ff} & A_{fc} \\ A_{cf} & A_{cc} \end{bmatrix}$$
$$= \begin{bmatrix} I & 0 \\ -A_{cc}^{-1} A_{cf} & 0 \end{bmatrix},$$

and multiplying with the F-part leads to

$$\begin{bmatrix} I & 0 \\ -A_{\rm cc}^{-1}A_{\rm cf} & 0 \end{bmatrix} \begin{bmatrix} 0 & -A_{\rm ff}^{-1}A_{\rm fc} \\ 0 & I \end{bmatrix} = \begin{bmatrix} 0 & -A_{\rm ff}^{-1}A_{\rm fc} \\ 0 & A_{\rm cc}^{-1}A_{\rm cf}A_{\rm ff}^{-1}A_{\rm fc} \end{bmatrix}$$

Now this is multiplied from the left by the parareal error propagation operator $P_c(I - \tilde{M}^{-1}\tilde{A})R$, and we get

$$P_{c}(I - \tilde{M}^{-1}\tilde{A})R\begin{bmatrix} 0 & -A_{\rm ff}^{-1}A_{\rm fc} \\ 0 & A_{\rm cc}^{-1}A_{\rm cf}A_{\rm ff}^{-1}A_{\rm fc} \end{bmatrix} = P_{c}(I - \tilde{M}^{-1}\tilde{A})[0 & A_{\rm cc}^{-1}A_{\rm cf}A_{\rm ff}^{-1}A_{\rm fc}].$$

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid Block Jacobi FLA Numerical Experimer Scalings

Multigrid nterpretations

Parareal

.

Parareal as a geometric multigrid method

MGRIT

PFASST

Proof continued

Now parareal is only operating on the coarse variables, so we obtain for them the error propagation operator of MGRIT to be

$$(I - \tilde{M}^{-1}\tilde{A})A_{\mathrm{cc}}^{-1}A_{\mathrm{cf}}A_{\mathrm{ff}}^{-1}A_{\mathrm{fc}}.$$
 (*)

Now recall the Schur complement

$$S_{\rm cc} = A_{\rm cc} - A_{\rm cf} A_{\rm ff}^{-1} A_{\rm fc},$$

which equals \tilde{A} , and since in parareal $A_{cc} = I$, because the original matrix only contains ones on the diagonal, we get

$$I - \tilde{A} = I - (A_{\rm cc} - A_{\rm cf}A_{\rm ff}^{-1}A_{\rm fc}) = A_{\rm cc}^{-1}A_{\rm cf}A_{\rm ff}^{-1}A_{\rm fc},$$

and inserting this into (*) we see that the error propagation operator of MGRIT on the coarse variables is simply

$$(I - \tilde{M}^{-1}\tilde{A})(I - \tilde{A}).$$

This corresponds to the two step iterative procedure

$$\begin{array}{rcl} \boldsymbol{Y}^{k} &=& \boldsymbol{U}^{k} + \boldsymbol{f} - \tilde{A} \boldsymbol{U}^{k}, \\ \tilde{M} \boldsymbol{U}^{k+1} &=& \tilde{M} \boldsymbol{Y}^{k} + \boldsymbol{f} - \tilde{A} \boldsymbol{Y}^{k}, \\ \end{array}$$

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacobi

FLA

Numerical Experiments Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method

AM

MGRIT

PFASST

Proof continued

Writing this componentwise, we obtain

$$Y_0^k = u_0, \quad Y_n^k = \tilde{F} U_{n-1}^k$$
$$U_0^k = u_0, \quad U_n^{k+1} = \tilde{F} Y_{n-1}^k + \tilde{G} U_{n-1}^{k+1} - \tilde{G} Y_{n-1}^k.$$

Substituting the values of Y_n^k into the equation for U_n^{k+1} then yields the result.

Corollary

The two level MGRIT algorithm with the $F(CF)^{\nu}$ -smoother computes the same iterations as the parareal algorithm using $\nu\Delta T$ overlap.

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correctior Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacobi

Numerical Experiment

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method

AM

MGRIT

PFASST

ntegral Deferred Correction Classical Parallel IDC

▲□▶ ▲□▶ ▲□▶ ▲□▶ ▲□ ● のへで

PFASST

PFASST stands for Parallel Full Approximation Scheme in Space-Time, and there are several steps in the development PFASST:

Minion (2010): A hybrid parareal spectral deferred corrections method

"This paper investigates a variant of the parareal algorithm first outlined by Minion and Williams in 2008 that utilizes a deferred correction strategy within the parareal iterations."

Deferred correction: consider the initial value problem

$$u'=f(u),\quad u(0)=u_0.$$

We can rewrite this problem in integral form

$$u(t) = u(0) + \int_0^t f(u(\tau)) d\tau.$$

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacobi

FLA Numerical Experiments Scalings

Multigrid Interpretations

Parareal

Parareal as a geometric multigrid method AMG

MGRI

PFASST

Integral Deferred Correction

Let $\tilde{u}(t)$ be an approximation with error $e(t) := u(t) - \tilde{u}(t)$. Inserting $u(t) = \tilde{u}(t) + e(t)$ into the integral form, we get

$$\tilde{u}(t) + e(t) = u(0) + \int_0^t f(\tilde{u}(\tau) + e(\tau))d\tau.$$
 (*)

Let $F(u) := u(0) + \int_0^t f(u(\tau))d\tau - u(t)$ from the integral form, the residual r(t) of the approximate solution $\tilde{u}(t)$ is

$$r(t) := F(\widetilde{u}) = \widetilde{u}(0) + \int_0^t f(\widetilde{u}(\tau))d\tau - \widetilde{u}(t),$$

and thus from (*) the error satisfies the equation

$$\begin{aligned} e(t) &= u(0) + \int_0^t f(\tilde{u}(\tau) + e(\tau))d\tau - \tilde{u}(t) \\ &= r(t) + \int_0^t f(\tilde{u}(\tau) + e(\tau)) - f(\tilde{u}(\tau))d\tau, \end{aligned}$$

or written as a differential equation

$$e'(t) = r'(t) + f(\tilde{u}(t) + e(t)) - f(\tilde{u}(t)).$$

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacob

FLA

Numerical Experiments Scalings

Multigrid Interpretations

Parareal

multigrid method

AIVIC

MGRI

PFASST

Integral Deferred Correction

Idea of integral deferred correction:

1. use e.g. Forward Euler to get a first approximate solution of the ODE,

 $\tilde{u}_{m+1} = \tilde{u}_m + \Delta t f(\tilde{u}_m), \quad \text{for } m = 0, 1, \dots, M-1.$

- 2. With these values, compute the residual at the points t_m , m = 0, 1, ..., M using a high order quadrature formula.
- 3. Solve the error equation in differential form again with Forward Euler,

$$e_{m+1} = e_m + r_{m+1} - r_m + \Delta t (f(\tilde{u}_m + e_m) - f(\tilde{u}_m)).$$

4. Add this correction to obtain a new approximation

$$\tilde{u}_m + e_m$$

One can show that the order has increased by one, and one can continue this process to increase the order up to the order of the quadrature used.

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Fime Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid Block Jacobi FLA Numerical Experime

Multigrid Interpretations

Parareal Parareal as a geometric multigrid method AMG MGRIT

PFASST

tegral Deferred Correction

Classical Parallel IDC

Integral Deferred Correction as Iteration

This is an iterative method to compute the Runge-Kutta method corresponding to the quadrature rule used to approximate the integral: with u^0 obtained by forward Euler, we have the non-linear fixed point iteration

$$\boldsymbol{u}^{k}=F(\boldsymbol{u}^{k-1},u_{0}).$$

Classical Use of Integral Deferred Correction: partition the time interval [0, T] into subintervals $[T_{j-1}, T_j]$ j = 1, 2, ..., J, and then perform K iterations on each: $u_{0,M}^K = u_0;$ for j = 1 : Jcompute u_j^0 as Euler approximation on $[T_{j-1}, T_j];$ for k = 1 : K $u_j^k = F(u_j^{k-1}, u_{j-1,M}^K);$ end; end;

This is purely sequential, like a time stepping scheme,

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equation FLA Results

Space-Time Multigrid

Block Jacobi FLA Numerical Experim

Multigrid Interpretations

Parareal Parareal as a geometric multigrid method AMG MGRIT

PFASST

ntegral Deferred Correction

Classical

Parallel ID

Idea Proposed by Minion (2010)

Replace the inner updating formula by (see Womble later)

$$oldsymbol{u}_j^k = oldsymbol{F}(oldsymbol{u}_j^{k-1}, u_{j-1,M}^k), \hspace{1em} (ext{note the lower case } k \; !).$$

Can now perform spectral deferred corrections in parallel.

Minion (2010) combines this with a coarse correction from parareal, thus using a more and more accurate fine integrator.

PFASST Emmett, Minion (2012) uses this as a smoother in a FAS scheme in space-time:

"The method is iterative with each iteration consisting of deferred correction sweeps performed alternately on fine and coarse space-time discretizations. The coarse grid problems are formulated using a space-time analog of the full approximation scheme popular in multigrid methods for nonlinear equations."

PinT Summer School

Martin J. Gander

Parabolic Multigrid

Smoother Coarse Correction Early Remedies

Time Multigrid

Dahlquist Equatior FLA Results

Space-Time Multigrid Block Jacobi FLA Numerical Experiment Scalings

Multigrid Interpretations

Parareal Parareal as a geometric multigrid method AMG

MGRIT

PFASST