PinT

Martin J. Gander

Introduction

Causality Principl Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Conclusion

Why Parallel in Time (PinT) methods are different for Parabolic and Hyperbolic Problems

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University of Geneva

Pisa, Italy, April 3rd, 2024

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, Euler: $\frac{du}{dt} \approx \frac{u(t_{n+1}) - u(t_n)}{\Delta t}$
 $u_1 = u_0 + \Delta t f(u_0)$
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PinT

Martin J. Gander

Introduction

Causality Principle

Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Conclusion

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 $u_2 = u_1 + \Delta t f(u_1)$
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PinT

Martin J. Gander

Introduction

Causality Principle

Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Conclusion

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PinT

Martin J. Gander

Introduction

Causality Principle

Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Conclusion

t

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 $u_4 = u_3 + \Delta t f(u_3)$
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PinT

Martin J. Gander

Introduction

Causality Principle

Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Conclusion

t

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 $u_5 = u_4 + \Delta t f(u_4)$
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PinT

Martin J. Gander

Introduction

Causality Principle

Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Conclusion

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 $u_6 = u_5 + \Delta t f(u_5)$
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PinT

Martin J. Gander

Introduction

Causality Principle

Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Conclusion

t

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 $u_{n+1} = u_n + \Delta t f(u_n)$
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$$t_{0} \quad t_{1} \quad t_{2} \quad t_{3} \quad t_{4} \quad t_{5} \quad t_{6} \quad t_{7} \quad t_{8} \quad t_{9} \quad t_{10} \quad t_{11} \quad t_{12} \quad t_{11} \quad t_{12}$$

PinT

Martin J. Gander

Introduction

Causality Principle

Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Conclusion



Transport Equation: Dirichlet and Periodic $u_t + u_x = f$, u(0, t) = 0 and u(0, t) = u(1, t)



PinT

Martin J. Gander

Introduction

Causality Principle Parabolic

Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Parabolic PinT: the Parareal Algorithm

For solving the evolution problem

$$\begin{aligned} \partial_t \boldsymbol{u}(t) &= \boldsymbol{f}(t, \boldsymbol{u}(t)) \quad t \in (0, T], \\ \boldsymbol{u}(0) &= \boldsymbol{u}^0, \end{aligned}$$

Parareal needs two propagation operators:

- 1. $G(t_2, t_1, u_1)$ is a coarse approximation to the solution $u(t_2)$ with initial condition $u(t_1) = u_1$,
- 2. $F(t_2, t_1, u_1)$ is a more accurate approximation of the solution $u(t_2)$ with initial condition $u(t_1) = u_1$.

The time interval (0, T] is partitioned into subintervals $(T_{n-1}, T_n]$. Parareal then starts with an initial coarse approximation U_n^0 at T_0, T_1, \ldots, T_N , and then computes

$$U_0^{k+1} := u^0, U_{n+1}^{k+1} := F(T_{n+1}, T_n, U_n^k) + G(T_{n+1}, T_n, U_n^{k+1}) - G(T_{n+1}, T_n, U_n^k)$$

Lions, Maday, Turinici (2001): Résolution d'EDP par un schéma en temps "pararéel"

PinT

Martin J. Gander

Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm

Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolid

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Theorem (Heat Equation (G, Vandewalle 2007)) Let F be exact, G have stability function R_G with $\rho_s := sup_{x<0}|e^x - R_G(x)|$ finite. Then

$$\max_{1 \le n \le N} ||u(t_n) - U_n^k||_2 \le \frac{\rho_s^k}{k!} \prod_{\ell=1}^k (N-\ell) C_0^N,$$

$$C_0^N := \sqrt{\sum_{\omega=1}^\infty \max_{1 \le n \le N} |\hat{u}(T_n, \omega) - \hat{U}_n^0(\omega)|^2}.$$

If the negative real axis is in the region of absolute stability of G and $\lim_{x\to-\infty} |R_G(x)| < 1$ (A₀-stability), then

$$\sup_{n>0}||u(t_n)-U_n^k||_2\leq \rho_l^k C_0^\infty,$$

$$\rho_I := \sup_{\omega \in \mathbb{R}} \frac{|e^{-\omega^2 \Delta T} - R_G(-\omega^2 \Delta T)|}{1 - |R_G(-\omega^2 \Delta T)|}, \quad T_n - T_{n-1} \equiv \Delta T.$$

2

PinT

Martin J. Gander

Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm

Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag





PinT

Martin J. Gander

Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm

Heat equation example

Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag





PinT

Martin J. Gander

Causality Principle
Parabolic
Hyperbolic
The Parareal Algorithm
Heat equation example
Advection example
Parareal no Coarse
STMG
PinT for Hyperbolic
Mapped Tent Pitching
Red-Black SWR
Unmapped Tent Pitching
ParaExp





PinT

Martin J. Gander



ParaDiag





PinT

Martin J. Gander

Causality Principle
Parabolic
Hyperbolic
The Parareal Algorithm
Heat equation example
Advection example
Parareal no Coarse
STMG
PinT for
Hyperbolic
Mapped Tent Pitching
Red-Black SWR
Unmapped Tent Pitching
ParaExp
ParaDiag





PinT

Martin J. Gander

Causality Principle
Parabolic
Hyperbolic
The Parareal Algorithm
Heat equation example
Advection example
Parareal no Coarse
STMG
PinT for
Hyperbolic
Mapped Tent Pitching
Red-Black SWR
Unmapped Tent Pitching
ParaExp
ParaDiag





PinT

Martin J. Gander







PinT

Martin J. Gander

Causality Principle
Parabolic
Hyperbolic
The Parareal Algorithm
Heat equation example
Advection example
Parareal no Coarse
STMG
PinT for
Hyperbolic
Mapped Tent Pitching
Red-Black SWR
Unmapped Tent Pitching
ParaExp
ParaDiag





PinT

Martin J. Gander

Causality Principle
Parabolic
Hyperbolic
The Parareal Algorithm
Heat equation example
Advection example
Parareal no Coarse
STMG
PinT for
Hyperbolic
Mapped Tent Pitching
Red-Black SWR
Unmapped Tent Pitching
ParaExp
ParaDiag





PinT

Martin J. Gander

Parabolic
Hyperbolic
The Parareal Algorithm
Heat equation example
Advection example
Parareal no Coarse
STMG
PinT for
Hyperbolic
Mapped Tent Pitching
Red-Black SWR
Unmapped Tent Pitching
ParaExp
ParaDiag





PinT

Martin J. Gander

Causality Principle
Parabolic
Hyperbolic
The Parareal Algorithm
Heat equation example
Advection example
Parareal no Coarse
STMG
PinT for
Hyperbolic
Mapped Tent Pitching
Red-Black SWR
Unmapped Tent Pitching
ParaExp
ParaDiag

What about Parareal without coarse for the heat equation,

$$\boldsymbol{U}_{n+1}^{k+1} := \boldsymbol{F}(T_{n+1}, T_n, \boldsymbol{U}_n^k)$$

instead of the original Parareal algorithm

$$\boldsymbol{U}_{n+1}^{k+1} := \boldsymbol{F}(T_{n+1}, T_n, \boldsymbol{U}_n^k) + \boldsymbol{G}(T_{n+1}, T_n, \boldsymbol{U}_n^{k+1}) - \boldsymbol{G}(T_{n+1}, T_n, \boldsymbol{U}_n^k)$$



PinT

Martin J. Gander

Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

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PinT

Martin J. Gander

Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

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PinT

Martin J. Gander

Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

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PinT

Martin J. Gander

Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Convergence Result for a Special Case

Dirichlet BC: Spectral fine propagator F using m_F modes:

$$F(U_n^k, T_n, T_{n+1}) = \sum_{m=1}^{m_F} \left(\hat{U}_{m,n}^k e^{-m^2 \Delta T} + \int_{T_n}^{T_{n+1}} \hat{f}_m(\tau) e^{-m^2(t-\tau)} d\tau \right) \sin m\tau$$

Spectral coarse propagator G using m_G modes:

$$G(U_n^k, T_n, T_{n+1}) = \sum_{m=1}^{m_G} \left(\hat{U}_{m,n}^k e^{-m^2 \Delta T} + \int_{T_n}^{T_{n+1}} \hat{f}_m(\tau) e^{-m^2(t-\tau)} d\tau \right) \sin m \lambda$$

Theorem (G, Ohlberger, Rave (2024))

This parareal algorithm for the heat equation on $(0, \pi) \times (0, T)$ with Dirichlet boundary conditions satisfies for any initial guess U_n^0 the convergence estimate

$$\sup_{n} ||U_{n}^{k}(\cdot)-u(\cdot, T_{n})||_{2} \leq e^{-(m_{g}+1)^{2}k\Delta T} \sup_{n} ||U_{n}^{0}(\cdot)-u(\cdot, T_{n})||_{2},$$

and this estimate also holds if the coarse propagator does not contain any modes, $m_G = 0$.

PinT

Martin J. Gander

Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse

PinT for Hyperbolid

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Comparison of the Convergence Estimates



PinT

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Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse

Parareal no Coa STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Remarks

- Scalability: for ΔT constant, convergence does not depend on the number of time subdomains even without G! Equivalent to DD result in space:
 - Maday, Stamm et al (2013-2014): Domain decomposition for implicit solvation models
 - G, Ciaramella (2017, 2018) Analysis of the parallel Schwarz method for growing chains of fixed-sized subdomains I, II, III
- Similar estimate for Neumann boundary conditions, but need at least the constant mode in G for contraction.
- The same estimate holds in full generality for a more general parabolic equation in arbitrary spatial dimensions, the convergence factor then becomes

$$e^{-\lambda_{m_G+1}\Delta T},$$

where λ_{m_G+1} is the m_G plus first eigenvalue of the corresponding spatial operator.

PinT

Martin J. Gander

Introduction

Causality Principl Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Much better: Space-Time Multigrid

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

$$\underbrace{\begin{bmatrix} (I-L\Delta t) & & \\ & -I & (I-L\Delta t) & \\ & & \ddots & \ddots \end{bmatrix}}_{A} \underbrace{\begin{pmatrix} \mathbf{u}_{1} \\ \mathbf{u}_{2} \\ \vdots \\ \mathbf{u} \end{pmatrix}}_{\mathbf{u}} = \underbrace{\begin{pmatrix} \mathbf{f}_{1} \\ \mathbf{f}_{2} \\ \vdots \\ \mathbf{f} \end{bmatrix}}_{\mathbf{f}}$$

- Parabolic Multigrid (Hackbusch 1984)
- Multigrid Waveform Relaxation (Lubich and Ostermann 1987)
- Space-Time Multigrid (Horton and Vandewalle (1995)

G, Neumüller (2016): Analysis of a New Space-Time Parallel Multigrid Algorithm for Parabolic Problems **Key idea:** use block Jacobi smoother with optimal damping!

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PinT

Martin J. Gander

Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

3D Heat Equation Weak Scaling Results 1 :.... | ||| ----- | +:---- -+---- |

-1 - 5

PinT

Martin J. Gander

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16	32	956 288	7	29.9	305.4
32	64	1 912 576	7	29.9	613.6
64	128	3 825 152	7	29.9	1 220.7
128	256	7 650 304	7	29.9	2 448.4
256	512	15 300 608	7	30.0	4 882.4
512	1 024	30 601 216	7	29.9	9 744.2
1 024	2 048	61 202 432	7	30.0	19 636.9
2 048	4 096	122 404 864	7	29.9	38 993.1
4 096	8 192	244 809 728	7	30.0	81 219.6
8 192	16 384	489 619 456	7	30.0	162 551.0
16 384	32 768	979 238 912	7	30.0	313 122.0
32 768	65 536	1 958 477 824	7	30.0	625 686.0
65 536	131 072	3 916 955 648	7	30.0	1 250 210.0
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Vulcan BlueGene/Q Supercomputer in Livermore (by M. Neumüller) Sac

3D Heat Equation Strong Scaling Results

PinT

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	Causality Principle
4	512	15 300 608	7	1 909.9	Parabolic Hyperbolic
8	512	15 300 608	7	954.2	
16	512	15 300 608	7	477.2	The Parareal Algorithm
32	512	15 300 608	7	238.9	Heat equation example Advection example
64	512	15 300 608	7	119.5	Parareal no Coarse
128	512	15 300 608	7	59.7	SIMG DinT for
256	512	15 300 608	7	30.0	Hyperbolic
512	524 288	15 667 822 592	7	15 205.9	Mapped Tent Pitching Red-Black SWR
1 024	524 288	15 667 822 592	7	7 651.5	Unmapped Tent Pitching
2 048	524 288	15 667 822 592	7	3 825.3	ParaExp ParaDiag
4 096	524 288	15 667 822 592	7	1 913.4	
8 192	524 288	15 667 822 592	7	956.6	
16 384	524 288	15 667 822 592	7	478.1	
32 768	524 288	15 667 822 592	7	239.3	
65 536	524 288	15 667 822 592	7	119.6	
131 072	524 288	15 667 822 592	7	59.8	
262 144	524 288	15 667 822 592	7	30.0	

Hard for hyperbolic problems (MGRIT, Falgout et al 2017-2024)

Hyperbolic PinT: Mapped Tent Pitching (MTP)

Gopalakrishnan, Schöberl, Wintersteiger (2017): Mapped Tent Pitching Schemes for Hyperbolic Systems

"This paper explores a technique by which standard discretizations, including explicit time stepping, can be used within tent-shaped spacetime domains. The technique transforms the equations within a spacetime tent to a domain where space and time are separable."



(a) Initial tents forming layer 1.



(b) Layer 2 tents in gray (and layer 1 tents in blue).



PinT

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Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Key new idea for MTP

Tent shaped subdomains are mapped to tensor shaped subdomains and then solved by any classical time stepping method, before being mapped back:



FIG. 2. Tent mapped from a tensor product domain.

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Introduction

Causality Principl Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp

Conclusion

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Application to Maxwell's Equations

Gopalakrishnan, Hochteger, Schöberl, Wintersteiger (2020): An Explicit Mapped Tent Pitching Scheme for Maxwell Equations

"This method is highly parallel, since many tents can be solved independently."



	p = 2	p = 3
Number of spatial dof	2.938×10^7	5.875×10^{7}
Number of spacetime dof per slab	1.908×10^{9}	7.632×10^{9}
Simulation time per slab	4.6 s	49.2 s
Total simulation time	20 min	3 h 33 min

This data was generated using a shared memory server with 4 E7-8867 CPUs with 16 cores each

Probably the best PinT Maxwell solver currently available!

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PinT

Martin J. Gander

Introduction

Causality Principl Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Red-Black Schwarz Waveform Relaxation

Nievergelt (1964): "... much wider class of numerical procedures in which parallelism is introduced at the expense of redundancy of computation."

Following this approach, we use Red-Black Schwarz Waveform Relaxation (RBSWR). 1D example:

Wave equation, decomposition of $\Omega = (x_0, x_N)$ into N subdomains $\Omega_j = (x_j, x_{j+2})$, $j = 0, \ldots, N-1$ (decomposition with generous overlap). Let $\mathcal{R} = \{0, 2, 4, \ldots\}$ and $\mathcal{B} = \{1, 3, 5, \ldots\}$:

$$\begin{array}{ll} \partial_{tt} u_j^k(x,t) = c^2 \partial_{xx} u_j^k(x,t) & \quad \text{in } I_j \times (0,T), \\ u_j^k(x_j,t) = u_{j-1}^{k-1}(x_j,t) & \quad \text{for } t \in [0,T], \\ u_j^k(x_{j+2},t) = u_{j+1}^{k-1}(x_{j+2},t) & \quad \text{for } t \in [0,T], \end{array}$$

where k is the iteration index, and $j \in \mathcal{R}$ for k odd and $j \in \mathcal{B}$ for k even.

PinT

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Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching

Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Choosing Tentpole Time Intervals in RBSWR



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Second Iteration of RBSWR



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Third Iteration of RBSWR



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Fourth Iteration of RBSWR



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Tent mapping is replaced by redundancy!

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Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR

Unmapped Tent Pitching ParaExp ParaDiag

Conclusion

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Example: wave equation



Red iteration 1 error



Black iteration 1 error



Red iteration 2 error



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Black iteration 2 error



Red iteration 3 error



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Black iteration 3 error



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Red iteration 4 error



Black iteration 4 error



Red iteration 5 error



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Unmapped Tent Pitching

Black iteration 5 error



Red iteration 6 error



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Causality Principle
Parabolic
Hyperbolic
The Parareal Algorithm
Heat equation example
Advection example
Parareal no Coarse
STMG
PinT for
Hyperbolic
Mapped Tent Pitching
Red-Black SWR
Unmapped Tent Pitching
ParaExp
ParaDiag

ParaExp

Consider the linear system of evolution equations

$$u'(t) = Au(t) + g(t), \quad t \in [0, T], \quad u(0) = u_0.$$

ParaExp is based on a completely overlapping decomposition of the time interval [0, T] into subintervals, e.g. $[0, T_4 := T]$, $[T_1, T_4]$, $[T_2, T_4]$, and $[T_3, T_4]$.



G., Güttel (2013): ParaExp: a Parallel Integrator for Linear Initial-Value Problems

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Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp

ParaDiag

Direct parallel solve in two steps

1. solve the non-overlapping inhomogeneous red problems

$$m{v}_j'(t) = Am{v}_j(t) + m{g}(t), \quad m{v}_j(T_{j-1}) = 0, \quad t \in [T_{j-1}, T_j]$$

2. solve the overlapping homogeneous blue problems

$$m{w}_j'(t) = Am{w}_j(t), \quad m{w}_j(T_{j-1}) = m{v}_{j-1}(T_{j-1}), \ t \in [T_{j-1}, T]$$

By linearity, the solution is then obtained by summation,

$$\boldsymbol{u}(t) = \boldsymbol{v}_k(t) + \sum_{j=1}^k \boldsymbol{w}_j(t)$$
 with k s.t. $t \in [T_{k-1}, T_k]$.

Blue problems even over long time are very cheap:

1. Approximate $a_n(t) \approx exp(tA)v$ from a Krylov space built with $S := (I - A/\sigma)^{-1}A$

2. $\exp(tA)\mathbf{v} \approx \sum_{j=0}^{n-1} \beta_j(t) p_j(A)\mathbf{v}$, where p_j are polynomials or rational functions.

PinT

Martin J. Gander

Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp

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ParaExp for the Wave Equation

$$\begin{array}{rcl} \partial_{tt}u(t,x) &=& \alpha^2\partial_{xx}u(t,x) + \mathsf{hat}(x)\sin(2\pi ft), & x,t \in (0,1) \\ u(t,0) &=& u(t,1) = u(0,x) = u'(0,x) = 0 \end{array}$$

		serial		parallel			effi-	F
$ \alpha^2 $	f	$ au_0$	error	$\max(au_1)$	$\max(\tau_2)$	error	ciency	
0.1	1	2.54e-01	3.64e-04	4.04e-02	1.48e-02	2.64e-04	58 %	
0.1	5	1.20e+00	1.31e-04	1.99e-01	1.39e-02	1.47e-04	71%	F
0.1	25	6.03e+00	4.70e-05	9.83e-01	1.38e-02	7.61e-05	76 %	ŀ
1	1	7.30e-01	1.56e-04	1.19e-01	2.70e-02	1.02e-04	63 %	
1	5	1.21e+00	4.09e-04	1.97e-01	2.70e-02	3.33e-04	68 %	
1	25	6.08e+00	1.76e-04	9.85e-01	2.68e-02	1.15e-04	75 %	F
10	1	2.34e+00	6.12e-05	3.75e-01	6.31e-02	2.57e-05	67 %	
10	5	2.31e+00	4.27e-04	3.73e-01	6.29e-02	2.40e-04	66 %	
10	25	6.09e+00	4.98e-04	9.82e-01	6.22e-02	3.01e-04	73%	

Finite differences and RK45 for the red problems, Chebyshev exponential integrator for the blue ones, 8 processors

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Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching **ParaExp** ParaDiag

ParaDiag

Model Problem: discretize a linear evolution problem $u_t = Lu + f$ using Backward Euler,

$$\begin{pmatrix} \frac{1}{\Delta t} - L & & \\ -\frac{1}{\Delta t} & \frac{1}{\Delta t} - L & \\ & \ddots & \ddots & \\ & & -\frac{1}{\Delta t} & \frac{1}{\Delta t} - L \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{pmatrix} = \begin{pmatrix} f_1 + \frac{1}{\Delta t} u_0 \\ f_2 \\ \vdots \\ f_N \end{pmatrix}$$

Using the Kronecker symbol, this linear system can be written in compact form as

$$(B\otimes I_x-I_t\otimes L)\boldsymbol{u}=\boldsymbol{f},$$

 I_x and I_t identity matrices and B is the time stepping matrix

Maday, Rønquist (2008): Parallelization in time through tensor-product space-time solvers Brugnano, Trigiante (1996-): Boundary value methods for ODEs

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Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

ParaDiag-I for diagonalizable B

$$B := \begin{pmatrix} \frac{1}{\Delta t_1} & & & \\ -\frac{1}{\Delta t_2} & \frac{1}{\Delta t_2} & & \\ & \ddots & \ddots & \\ & & -\frac{1}{\Delta t_N} & \frac{1}{\Delta t_N} \end{pmatrix}.$$

With $B = SDS^{-1}$, one can rewrite the system in factored form, namely

$$(S \otimes I_x)(\operatorname{diag}(D-L))(S^{-1} \otimes I_x)\boldsymbol{u} = \boldsymbol{f},$$

and we can hence solve it in 3 steps:

$$\begin{array}{rcl} (a) & (S \otimes I_{x})\mathbf{g} &=& \mathbf{f}, \\ (b) & (\frac{1}{\Delta t_{n}} - L)\mathbf{w}^{n} &=& \mathbf{g}^{n}, \quad 1 \leq n \leq N, \\ (c) & (S^{-1} \otimes I_{x})\mathbf{u} &=& \mathbf{w}. \end{array}$$

The expensive step (b) solving with the system matrix *L* can be done entirely in parallel for all time levels $t_{n_{2}}$, t_{2} , t_{3} , $t_{$

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Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Industrial Elasticity Example

Response of a carbon/epoxy laminated composite panel to an impact-like loading, modeled by the elasticity equations

$$\rho \ddot{\boldsymbol{u}} = \operatorname{div}(\sigma) + \boldsymbol{f}, \quad \epsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right).$$



152607 dofs, 2000 time steps over the 10ms simulation range

G, Halpern, Rannou, Ryan (2019): A Direct Time Parallel Solver by Diagonalization for the Wave Equation

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Strong Scaling Results



Computing times (in seconds) for the industrial elasticity problem (all computations performed by J. Rannou 2017)

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ParaDiag-II: non-diagonalizable B

Can one make B with equal time steps diagonalizabe ?

$$\tilde{B} = \begin{bmatrix} \frac{1}{\Delta t} & & -\frac{\alpha}{\Delta t} \\ -\frac{1}{\Delta t} & \frac{1}{\Delta t} & & \\ & \ddots & \ddots & \\ & & -\frac{1}{\Delta t} & \frac{1}{\Delta t} \end{bmatrix}$$

But then we solve the wrong problem, need to iterate:

$$A = (B \otimes I_x - I_t \otimes L), \quad \tilde{A} = (\tilde{B} \otimes I_x - I_t \otimes L),$$
$$u^{k+1} = u^k + \tilde{A}^{-1}(f - Au^k).$$

Independently discovered:

- α = 1: McDonald, Pestana, Wathen (2018): Preconditioning and iterative solution of all-at-once systems for evolution partial differential equations.
- Optimized α: Shulin Wu (2018): Toward parallel coarse grid correction for the parareal algorithm (2018)

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Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

ParaDiag II on advection: Initial Guess





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Introduction

Causality Principle Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

ParaDiag II on advection: Iteration 1





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Conclusion

ParaDiag II on advection: Iteration 2





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ParaDiag II on advection: Iteration 3





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Causality Principle Parabolic Hyperbolic PinT for Parabolic The Parateal Algorithm Heat equation example Advection example Parareal no Coarse STMG PinT for Hyperbolic Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

Conclusions

Parabolic problems are natural for PinT, hyperbolic problems are not!

- There are many good PinT methods for parabolic problems: Parareal and variants (PITA, PFASST, MGRIT), Space-Time Multigrid (STMG), Domain Decomposition Waveform relaxation (Schwarz WR, Dirichlet-Neumann WR, Neumann-Neumann WR)
- Domain Decomposition Waveform relaxation methods are also suitable for hyperbolic problems
 Mapped and Unmapped Tent Pitching.
- ParaExp and ParaDiag methods are also suitable for hyperbolic problems (see also G, Palitta 2024).

New PinT book (2024): Time Parallel Time Integration

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Introduction

Causality Principl Parabolic Hyperbolic

PinT for Parabolic

The Parareal Algorithm Heat equation example Advection example Parareal no Coarse STMG

PinT for Hyperbolic

Mapped Tent Pitching Red-Black SWR Unmapped Tent Pitching ParaExp ParaDiag

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Conclusion