# An Introduction to Parallel-in-time methods 

Ausra Pogozelskyte<br>University of Geneva<br>Paris, 16th of May 2023

## Motivation

What is a Parallel-in-Time method?
Methods that compute solutions at a further time step before that the solution at a closer time step has been computed.

- Usually iterative methods
- Usually comes at the expense of additional work

Why are Parallel-in-Time methods interesting?

- Problems that need a solution by a certain deadline
- Problems that are very long in time


## Outline

Traditionally, Parallel-in-Time methods are classified in the following categories:
(1) Shooting type methods

- Parareal
(2) Multigrid methods
- Multigrid Reduction-in-Time
- Space-Time Multigrid
(3) Domain Decomposition methods
- Schwarz Waveform Relaxation

4 Direct methods

- ParaExp

Space-time decomposition in ...


## References

- 50 Years of Time Parallel Time Integration (2015)
M. J. Gander
- Applications of time parallelization (2020)
B. W. Ong and J. B. Schroder
- Multigrid methods with space-time concurrency (2017)
R. D. Falgout, S. Friedhoff, Tz. V. Kolev, S. P. MacLachlan, J. B. Schroder, S. Vandewalle


## Setting

We will solve the 1 d heat equation $(c=1)$

$$
\begin{cases}u_{t}(x, t)=u_{x x}(x, t), & (x, t) \in(0, L) \times(0, T), \\ u(0, t)=u(L, t)=0, & t \in(0, T), \\ u(x, 0)=u_{0}(x), & x \in(0, L)\end{cases}
$$

We will discretize it using finite differences in space,

$$
\left\{\begin{array}{l}
v_{t}(t)=\frac{1}{\Delta x^{2}} L v(t), \quad t \in(0, T) \\
v(0)=u_{0}
\end{array}\right.
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$$

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$$
L=\left(\begin{array}{cccc}
-2 & 1 & & \\
1 & -2 & \ddots & \\
& \ddots & \ddots & 1 \\
& & 1 & -2
\end{array}\right)
$$

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$$
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v_{t}(t)=\frac{1}{\Delta x^{2}} L v(t), \quad t \in(0, T) \\
v(0)=u_{0} \in \mathbb{R}^{n_{x}}
\end{array}\right.
$$

We discretize in time using a Runge-Kutta scheme

$$
u_{n+1}=\Phi u_{n}, \quad u_{0}=v(0) \in \mathbb{R}^{n_{x}}, \quad n=0,1, \ldots, N_{t}
$$

Example: If we use Backward Euler $\Phi=\left(I-\frac{\Delta t}{\Delta x^{2}} L\right)^{-1}$.


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## Parareal

## First step: Nievergelt's method (1964)

Method introduced in a 3-page paper in 1964 by J. Nievergelt.


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## Developments of the method

1989 Bellen and Zenaro: solve $u_{n+1}=\Phi u_{n}$ using (a variant of) Newton's method.

$$
\begin{gathered}
\boldsymbol{u}^{k+1}=\varphi\left(\boldsymbol{u}^{k}\right)+\Delta \varphi\left(\boldsymbol{u}^{k}\right)\left(\boldsymbol{u}^{k+1}-\boldsymbol{u}^{k}\right) \\
\text { where } \varphi(\boldsymbol{u})=\left(\begin{array}{c}
u_{0}-v(0) \\
u_{1}-\Phi u_{0} \\
\vdots \\
u_{N}-\Phi u_{N-1}
\end{array}\right) \text { and } \boldsymbol{u}=\left(\begin{array}{c}
u_{0} \\
u_{1} \\
\vdots \\
u_{N}
\end{array}\right) .
\end{gathered}
$$

- Quadratic convergence
- Finite-time convergence

1993 Chartier and Philippe: Noticed that it isn't effective for all kinds of problems.

## Parareal ${ }^{1}$

Consider a coarsening factor of $m$ (fine/coarse grid). Let $F=\Phi^{m}$ and $G$ a cheap approximation of $F$.
Idea: Approximate $\Delta \varphi$ by the finite difference $\left(G U_{n}^{k+1}-G U_{n}^{k}\right) /\left(U_{n}^{k+1}-U_{n}^{k}\right)$.

Initialization:

$$
\left\{\begin{array}{l}
U_{0}^{0}=u_{0} \\
U_{n+1}^{0}=G U_{n}^{0}, \quad n=0, \ldots, N_{t}-1
\end{array}\right.
$$

Parareal iteration: for $k=0, \ldots, K-1$

$$
\left\{\begin{array}{l}
U_{0}^{k+1}=u_{0}, \\
U_{n+1}^{k+1}=F U_{n}^{k}+G U_{n}^{k+1}-G U_{n}^{k}, \quad n=0, \ldots, N_{t}-1
\end{array}\right.
$$

## Illustration of Parareal

## Initialization:

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## Summary

- Nievergelt's method is too expensive for large problems
- Parallelism in Parareal is achieved though additional work of a coarse operator
- For Parareal to be effective, the coarse operator needs to:
- be a good approximation of the fine
- be much cheaper to compute


## References

- Résolution d'EDP par un schéma en temps "pararéel" (2001) J.-L. Lions, Y. Maday, G. Turinici
- A Micro-Macro Parareal Algorithm: Application to Singularly Perturbed Ordinary Differential Equations (2013)
F. Legoll, T. Lelièvre, G. Samaey
- PARAOPT: A Parareal Algorithm for Optimality Systems (2020) M. J. Gander, F. Kwok, J. Salomon
- Low-rank Parareal: a low-rank parallel-in-time integrator (2023)
B. Carrel, M. J. Gander, B. Vandereycken


## Multigrid Reduction-in-Time

## All-at-once system

We are interested in solving the time stepping scheme

$$
u_{n+1}=\Phi u_{n}, \quad u_{0}=u_{0}, \quad n=0,1, \ldots, N_{t}-1
$$

This can be written as the following system to solve

$$
\underbrace{\left(\begin{array}{cccc}
I & & & \\
-\Phi & I & & \\
& \ddots & \ddots & \\
& & -\Phi & I
\end{array}\right)}_{=: A} \underbrace{\left(\begin{array}{c}
u_{0} \\
u_{1} \\
\vdots \\
u_{N_{t}}
\end{array}\right)}_{=: \boldsymbol{u}}=\underbrace{\left(\begin{array}{c}
0 \\
0 \\
\vdots \\
0
\end{array}\right)}_{=: \boldsymbol{b}}
$$

$\rightarrow$ It can be solved using Multigrid!

## Multigrid Reduction-in-Time

The Multigrid Reduction-in-Time algorithm ${ }^{2}$ (MGRIT) follows the same steps as a traditional Multigrid algorithm:
(1) Pre-smoothing: FCF-relaxation
(2) Computation of the residual and restriction: Injection
(3) Coarse grid solve
(9) Prolongation and correction: Ideal prolongation
(5) Post-smoothing: None

[^0]
## Smoothing: What is FCF-relaxation?

fine grid

coarse grid


C-points points that belong both to the coarse and fine grids
F-points the others
C-relaxation update C-points
F-relaxation update F-points

## Smoothing: What is FCF-relaxation?

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## Smoothing: What is FCF-relaxation?

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C-points points that belong both to the coarse and fine grids
F-points the others
C-relaxation update C-points
F-relaxation update F-points
Link to Parareal: $F=\Phi^{m}$

## Transfer operators in MGRIT

fine grid
coarse grid


Restriction by injection


Ideal prolongation

## Parareal and MGRIT are related

Recall (Parareal)

$$
\begin{cases}U_{0}^{k+1}=u_{0} & k=0, \ldots, K, \\ U_{n+1}^{k+1}=F U_{n}^{k}+G U_{n}^{k+1}-G U_{n}^{k} & n=0, \ldots, N_{t}-1, \quad k=0, \ldots, K .\end{cases}
$$

## Theorem (Gander, Kwok, Zhang, 2018)

The two-level MGRIT algorithm with FCF-relaxation computes the same iterations as the Parareal algorithm using generous overlap of one coarse time interval

$$
\begin{cases}U_{0}^{k+1}=u_{0} & k=0, \ldots, K, \\ U_{1}^{k+1}=F u_{0} & k=0, \ldots, K, \\ U_{n+1}^{k+1}=F F U_{n-1}^{k}+G U_{n}^{k+1}-G F U_{n-1}^{k} & n=0, \ldots, N_{t}-1, \quad k=0, \ldots, K .\end{cases}
$$

## Parareal and MGRIT are related

## Parareal (MGRIT with F-relaxation)



MGRIT with FCF-relaxation


## How do Parareal and MGRIT converge?

The convergence of Parareal: from the iteration

$$
U_{n+1}^{k+1}=F U_{n}^{k}+G U_{n}^{k+1}-G U_{n}^{k}, \quad n=1, \ldots, n_{t}
$$

the error, $\epsilon_{n}^{k}:=u_{n}-U_{n}^{k}$, can be computed as

$$
\epsilon_{n+1}^{k+1}=F \epsilon_{n}^{k}+G \epsilon_{n}^{k+1}-G \epsilon_{n}^{k} .
$$

In turn, it can be bounded as


## We thus only need to solve the iteration

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$$
\epsilon_{n+1}^{k+1}=F \epsilon_{n}^{k}+G \epsilon_{n}^{k+1}-G \epsilon_{n}^{k} .
$$

In turn, it can be bounded as

$$
\left\|\epsilon_{n+1}^{k+1}\right\|=: e_{n+1}^{k+1} \leq \underbrace{\|F-G\|}_{=\alpha} e_{n}^{k}+\underbrace{\|G\|}_{=\beta} e_{n}^{k+1} .
$$

We thus only need to solve the iteration

$$
e_{n+1}^{k+1}=\alpha e_{n}^{k}+\beta e_{n}^{k+1}
$$

## How do Parareal and MGRIT converge?

The iteration $e_{n+1}^{k}=\alpha e_{n}^{k-1}+\beta e_{n}^{k}$ can be written in matrix form as

$$
\left(\begin{array}{cccc}
I & & & \\
-\beta & I & & \\
& \ddots & \ddots & \\
& & -\beta & 1
\end{array}\right)\left(\begin{array}{c}
e_{0}^{k} \\
e_{1}^{k} \\
\vdots \\
e_{n_{t}}^{k}
\end{array}\right)=\left(\begin{array}{cccc}
0 & & & \\
\alpha & 0 & & \\
& \ddots & \ddots & \\
& & \alpha & 0
\end{array}\right)\left(\begin{array}{c}
e_{0}^{k-1} \\
e_{1}^{k-1} \\
\vdots \\
e_{n_{t}}^{k-1}
\end{array}\right) .
$$

## Lemma (Recurrence solving)

Assuming that $\alpha$ and $\beta$ are scalars, the error at step $k$ is given by

$$
\boldsymbol{e}^{k}=M(\beta)\left(I_{n_{t}} \otimes \alpha\right) \boldsymbol{e}^{k-1}=\ldots=M(\beta)^{k}\left(I_{n_{t}} \otimes \alpha^{k}\right) \boldsymbol{e}^{0}
$$

## How do Parareal and MGRIT converge?

We then want to bound

$$
\boldsymbol{e}^{k}=M(\beta)^{k}\left(I_{n_{t}} \otimes \alpha^{k}\right) \boldsymbol{e}^{0}
$$

## Linear Bound [Lemma 4.4, Gander, Vandewalle, 2007]

$$
\left\|M(\beta)^{k}\right\|_{\infty} \leq\|M(\beta)\|_{\infty}^{k}=\left(\frac{1-|\beta|^{n_{t}}}{1-|\beta|}\right)^{k}
$$

## Superlinear Bound [Lemma 4.3, Gander, Vandewalle, 2007]

$$
\left\|M(\beta)^{k}\right\|_{\infty}=\sum_{i=0}^{n_{t}-k}\binom{i+k-1}{k-1}|\beta|^{i}=\frac{1}{(k-1)!} \sum_{i=0}^{n_{t}-k}\left[\prod_{l=1}^{k-1}(i+l)\right]|\beta|^{i}
$$

M. J. Gander, S. Vandewalle. "Analysis of the Parareal Time-Parallel Time-Integration Method", 2007.

## How do Parareal and MGRIT converge?

We then want to bound

$$
\boldsymbol{e}^{k}=M(\beta)^{k}\left(I_{n_{t}} \otimes \alpha^{k}\right) \boldsymbol{e}^{0}
$$

## Linear Bound [Lemma 4.4, Gander, Vandewalle, 2007]

$$
\left\|M(\beta)^{k}\right\|_{\infty} \leq\|M(\beta)\|_{\infty}^{k}=\left(\frac{1-|\beta|^{n_{t}}}{1-|\beta|}\right)^{k}
$$

## Explicit Superlinear Bound [Lemma 4.4, Gander, Vandewalle, 2007]

If $|\beta|<1$, then

$$
\left\|M(\beta)^{k}\right\|_{\infty} \leq\binom{ n_{t}}{k}=\frac{1}{k!} \prod_{l=0}^{k-1}\left(n_{t}-l\right)
$$

M. J. Gander, S. Vandewalle. "Analysis of the Parareal Time-Parallel Time-Integration Method", 2007.

## Bound on the eigenvalues ${ }^{3}$

Assume $\lambda_{F}$ and $\lambda_{G}$ are the eigenvalues of $F$ and $G$.
Let $\alpha=\lambda_{F}-\lambda_{G}$ and $\beta=\lambda_{G}$, then

$$
\left\|M(\beta)\left(I_{n_{t}} \otimes \alpha\right)\right\|_{\infty} \leq\left|\lambda_{F}-\lambda_{G}\right| \frac{1-\left|\lambda_{G}\right|^{n_{t}}}{1-\left|\lambda_{G}\right|}
$$




[^1]
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\left\|M(\beta)\left(I_{n_{t}} \otimes \alpha\right)\right\|_{\infty} \leq\left|\lambda_{F}-\lambda_{G}\right| \frac{1-\left|\lambda_{G}\right|^{n_{t}}}{1-\left|\lambda_{G}\right|}
$$




[^2]
## Convergence of Parareal and MGRIT

Initial guess: $u_{0}(x)=\sin (\pi x), x \in[0,1] . n_{x}=100, n_{t}=256, T=0.02$ for heat and $T=1$ for advection. SDIRK2 in time and second order centered for heat and upwind for advection.



## Convergence of Parareal and MGRIT

$$
\text { Efficiency }=\frac{\text { Speedup }}{\# \text { processors }}=\frac{T_{\text {seq }}}{T_{\text {para }} \cdot \# \text { processors }}
$$




## Summary

- MGRIT is a multilevel version of Parareal
- MGRIT usually uses FCF-relaxation, whereas Parareal uses F-relaxation
- From superlinear bound: superlinear + finite time convergence
- From linear bound: eigenvalues that are close to unity need to be well approximated.


## References

- Analysis of the Parareal Time-Parallel Time-Integration Method (2007) M. J. Gander, S. Vandewalle
- Parallel Time Integration with Multigrid (2014)
R. D. Falgout, S. Friedhoff, Tz. V. Kolev, S. P. MacLachlan, J. B. Schroder
- Two-Level Convergence Theory for Multigrid Reduction in Time (MGRIT) (2017)
V. A. Dobrev, Tz. V. Kolev, N. A. Petersson, J. B. Schroder
- Scheduling of tasks in the Parareal algorithm (2011)
E. Aubanel
- A Unified Analysis Framework for Iterative Parallel-in-Time Algorithms (2022) M. J. Gander, T. Lunet, D. Ruprecht, R. Speck


## Space-Time Multigrid

## All-at-once system

The time-stepping procedure

$$
u_{n+1}=\Phi u_{n}, \quad u_{0}=u_{0}, \quad n=0,1, \ldots, N_{t}-1
$$

was formulated as a all-at-once system for MGRIT. For the Space-Time algorithm, we consider a different formulation.

Separate the operator $\Phi=Q^{-1} P$ where $Q$ and $P$ are the implicit and explicit parts of $\Phi$. In turn, it can be written as the all-at-once system,

$$
\underbrace{\left(\begin{array}{cccc}
Q & & & \\
-P & Q & & \\
& \ddots & \ddots & \\
& & -P & Q
\end{array}\right)}_{=: A} \underbrace{\left(\begin{array}{c}
u_{1} \\
u_{2} \\
\vdots \\
u_{N_{t}}
\end{array}\right)}_{=: \boldsymbol{u}}=\underbrace{\left(\begin{array}{c}
P u_{0} \\
0 \\
\vdots \\
0
\end{array}\right)}_{=: \boldsymbol{b}} .
$$

## Space-Time Multigrid with point-wise smoother ${ }^{4}$

Idea: Apply Multigrid on the space-time problem.
(1) Pre-smoothing: $\nu_{1}$ damped Jacobi iterations
(2) Computation of the residual and restriction: Full-weighting
(3) Coarse grid solve
(9) Prolongation and correction: Linear interpolation
(3) Post-smoothing: $\nu_{2}$ damped Jacobi iterations

Reminder: The point-wise recall the damped Jacobi smoother is given by

$$
\boldsymbol{v}^{k+1}=\boldsymbol{v}^{k}+\omega D^{-1}\left[\boldsymbol{b}-A \boldsymbol{v}^{k}\right]
$$

where $D$ is the diagonal matrix such that $D_{i i}=A_{i j}$.

## Transfer operators in STMG

fine grid
coarse grid


Restriction by full-weighting


Linear interpolation

$$
\longrightarrow \quad \times 1 \quad \longrightarrow \quad \times 0.5 \quad \longrightarrow \times 0.25
$$

## Space-Time Multigrid with point-wise smoother



Figure: Convergence factor of STMG with point-wise smoother from Horton, Vandewalle (1995)

## STMG with block Jacobi smoother ${ }^{5}$

Goal: Be able to always smooth in the time dimension.

Consider the damped block-Jacobi smoother

$$
\boldsymbol{v}^{k+1}=\boldsymbol{v}^{k}+\omega D^{-1}\left[\boldsymbol{b}-A \boldsymbol{v}^{k}\right],
$$

with $D$ a block diagonal matrix with blocks $Q$ and $\omega \in[0,2]$ a damping parameter.
$\rightarrow$ Always allows for coarsening in time

[^3]
## STMG has good scaling properties

Weak and Strong scaling results: 3D Heat Equation

|  | Weak scaling |  |  |  |  | Strong scaling |  |  |  |
| ---: | ---: | ---: | :---: | :---: | ---: | ---: | ---: | ---: | ---: |
| cores | $n_{t}$ | dof | iter | time | fwd. subs. | $n_{t}$ | dof | iter | time |
| 1 | 2 | 59,768 | 7 | 28.8 | 19.0 | 512 | $15,300,608$ | 7 | $7,635.2$ |
| 2 | 4 | 119,536 | 7 | 29.8 | 37.9 | 512 | $15,300,608$ | 7 | $3,821.7$ |
| 4 | 8 | 239,072 | 7 | 29.8 | 75.9 | 512 | $15,300,608$ | 7 | $1,909.9$ |
| 8 | 16 | 478,144 | 7 | 29.9 | 152.2 | 512 | $15,300,608$ | 7 | 954.2 |
| 16 | 32 | 956,288 | 7 | 29.9 | 305.4 | 512 | $15,300,608$ | 7 | 477.2 |
| 32 | 64 | $1,912,576$ | 7 | 29.9 | 613.6 | 512 | $15,300,608$ | 7 | 238.9 |
| 64 | 128 | $3,825,152$ | 7 | 29.9 | $1,220.7$ | 512 | $15,300,608$ | 7 | 119.5 |
| 128 | 256 | $7,650,304$ | 7 | 29.9 | $2,448.4$ | 512 | $15,300,608$ | 7 | 59.7 |
| 256 | 512 | $15,300,608$ | 7 | 30.0 | $4,882.4$ | 512 | $15,300,608$ | 7 | 30.0 |

Table: Vulcan BlueGene /Q Supercomputer in Livermore (Martin Neumüller)

## STMG has good scaling properties

Weak and Strong scaling results: 3D Heat Equation

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| cores | $n_{t}$ | dof | iter | time | fwd. subs. | $n_{t}$ | dof | iter | time |
| 1 | 2 | 59,768 | 7 | 28.8 | 19.0 | 512 | $15,300,608$ | 7 | $7,635.2$ |
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| 2 | 4 | 119,536 | 7 | 29.8 | 37.9 | 512 | $15,300,608$ | 7 | $3,821.7$ |
| 4 | 8 | 239,072 | 7 | 29.8 | 75.9 | 512 | $15,300,608$ | 7 | $1,909.9$ |
| 8 | 16 | 478,144 | 7 | 29.9 | 152.2 | 512 | $15,300,608$ | 7 | 954.2 |
| 16 | 32 | 956,288 | 7 | 29.9 | 305.4 | 512 | $15,300,608$ | 7 | 477.2 |
| 32 | 64 | $1,912,576$ | 7 | 29.9 | 613.6 | 512 | $15,300,608$ | 7 | 238.9 |
| 64 | 128 | $3,825,152$ | 7 | 29.9 | $1,220.7$ | 512 | $15,300,608$ | 7 | 119.5 |
| 128 | 256 | $7,650,304$ | 7 | 29.9 | $2,448.4$ | 512 | $15,300,608$ | 7 | 59.7 |
| 256 | 512 | $15,300,608$ | 7 | 30.0 | $4,882.4$ | 512 | $15,300,608$ | 7 | 30.0 |

Table: Vulcan BlueGene /Q Supercomputer in Livermore (Martin Neumüller)

## The convergence of STMG depends on the ratio $\sigma=\Delta t / \Delta x^{2}$

Let $\mu$ be the smoothing factor associated to the block-Jacobi smoother obtained by Local Fourier Analysis (LFA),


## Summary

- STMG has very good scaling properties
- The convergence of STMG depends on the ratio $\Delta t / \Delta x^{2}$
- STMG with block-smoothing allows to always coarsen in time


## References

- A Space-Time Multigrid for Parabolic Partial Differential Equations (1995) G. Horton, S. Vandewalle
- Analysis of a New Space-Time Parallel Multigrid Algorithm for Parabolic Problems (2016) M. J. Gander, M. Neumüller
- An Optimized Space-Time Multigrid Algorithm for Parabolic PDEs (2023, in review) B. Chaudet-Dumas, M. J. Gander, A. P.


## Schwarz Waveform Relaxation

## Schwarz Waveform Relaxation

We will solve the 1D heat equation

$$
\begin{cases}u_{t}(x, t)=u_{x x}(x, t), & (x, t) \in \Omega \times(0, T), \\ u(x, t)=0, & x \in \partial \Omega, t \in(0, T), \\ u(x, 0)=u_{0}(x), & x \in \Omega\end{cases}
$$

## Partition the domain $\Omega=\Omega_{1} \cup \Omega_{2}$.

 Define for $i \in\{0,1\}$,

## Schwarz Waveform Relaxation

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Partition the domain $\Omega=\Omega_{1} \cup \Omega_{2}$.
Define for $i \in\{0,1\}$,

$$
\begin{cases}\partial_{t} u_{i}^{k+1}(x, t)=\partial_{x x} u_{i}^{k+1}(x, t) & (x, t) \in \Omega_{1} \times(0, T] \\ u_{i}^{k+1}(x, 0)=u_{0}(x) & x \in \Omega_{i} \\ u_{i}^{k+1}(x, t)=0 & x \in \partial \Omega, t \in(0, T] \\ u_{i}^{k+1}\left(\Gamma_{i}, t\right)=u_{1-i}^{k}\left(\Gamma_{i}, t\right) & t \in(0, T]\end{cases}
$$



## Convergence of SWR

Goal: Compute the solution for the 1D heat equation with Dirichlet boundary conditions with $u_{0}=20$ and initial guess $u_{0}=0$.

On the right, first 6 iterations of SWR at time $T=0.5$.


## Convergence is superlinear ${ }^{6}$



[^4]
## Optimized Schwarz Waveform Relaxation

Recall: Schwarz wave relaxation is given for $i \in\{0,1\}$ by

$$
\begin{cases}\partial_{t} u_{i}^{k+1}(x, t)=\partial_{x x} u_{i}^{k+1}(x, t) & (x, t) \in \Omega_{1} \times(0, T] \\ u_{i}^{k+1}(x, 0)=u_{0}(x) & x \in \Omega_{i} \\ u_{i}^{k+1}(x, t)=0 & x \in \partial \Omega, t \in(0, T] \\ u_{i}^{k+1}\left(\Gamma_{i}, t\right)=u_{1-i}^{k}\left(\Gamma_{i}, t\right) & t \in(0, T]\end{cases}
$$

Goal: Do SWR without overlap.

$$
\begin{cases}\partial_{t} u_{i}^{k+1}(x, t)=\partial_{x x} u_{i}^{k+1}(x, t) & (x, t) \in \Omega_{1} \times(0, T] \\ u_{i}^{k+1}(x, 0)=u_{0}(x) & x \in \Omega_{i} \\ u_{i}^{k+1}(x, t)=0 & x \in \partial \Omega, t \in(0, T] \\ \left(\partial_{x}+p\right) u_{i}^{k+1}\left(\Gamma_{i}, t\right)=\left(\partial_{x}+p\right) u_{1-i}^{k}\left(\Gamma_{i}, t\right) & t \in(0, T]\end{cases}
$$

Solution: Change transmission conditions to Robin type and optimize for $p_{\text {s }}$

## Optimizing Optimized Schwarz Waveform Relaxation



## Summary

- Schwarz Wave Relaxation allows parallelism in time by cutting the spatial domain in two (or more) subdomains
- Schwarz Wave Relaxation has superlinear convergence
- Optimized Schwarz Waveform Relaxation allows to have no overlap between domains.


## References

- The waveform relaxation method for time-domain analysis of large scale integrated circuits (1983)
E. Lelarasmee, A. E. Ruehli, and A. L. Sangiovanni-Vincentelli.
- Overlapping Schwarz of linear and non-linear Parabolic problems (1996) M. J. Gander
- Dirichlet-Neumann and Neumann-Neumann waveform relaxation algorithms for parabolic problems (2013)
M. J. Gander, F. Kwok, B. C. Mandal
- Work by M. Gander, L. Halpern, V. Martin, F. Nataf.


## ParaExp

## ParaExp

Introduced by Gander and Güttel in 2013. Let $A \in \mathbb{R}^{n \times n}$ and $f$ a non-linear function.

$$
u^{\prime}(t)=A u(t)+f(t), \quad t \in(0, T), \quad u(0)=u_{0}
$$

## Observation

A homogenous problem can be integrated much faster than an inhomogenous problem.
Separate $u=v+w$, where

$$
\begin{gathered}
v^{\prime}(t)=A v(t), \quad v(0)=u_{0} \\
w^{\prime}(t)=A w(t)+f(t), \quad w(0)=0
\end{gathered}
$$

## ParaExp - illustration



Figure: Illustration of ParaExp from the original article (Gander, Güttel, 2013)
(1) On $\left[T_{n}, T_{n+1}\right]$ : Solve with serial integrator
(2) On $\left[T_{n}, T\right]$ : Solve with near optimal exponential integrator
(3) Get the final solution by superposition of solutions

## Fast computation of matrix exponentials

Question: If $A$ is very big, how to compute efficiently $\exp (t A)$ ?
Idea: Compute $\exp (t A) v$ directly for some initial condition $v$ using Krylov methods.
(1) Generate the Krylov space $\mathcal{K}_{m}=\operatorname{span}\left\{v, A v, \ldots, A^{m-1} v\right\}$.

- Use the Arnoldi method.
(2) Get an orthonormal basis $V_{m}$ of $\mathcal{K}_{m}$.
- Use a modified Gram-Schmidt process.
(3) Compute $H_{m}$ the projection of $A$ on the space $\mathcal{K}_{m}$ with respect to the basis $V_{m}$.
(9) Get the approximation $e^{t A} \approx \beta V_{m} e^{t H_{m}} e_{1}$ (good even for small $m$ )
- Apply traditional techniques to compute $e^{t H_{m}} e_{1}$.


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- Use a modified Gram-Schmidt process.
(3) Compute $H_{m}$ the projection of $A$ on the space $\mathcal{K}_{m}$ with respect to the basis $V_{m}$.
- The matrix $H_{m}$ is upper Hessenberg and verifies $H_{m}=V_{m}^{\top} A V_{m}$.
(9) Get the approximation $e^{t A} \approx \beta V_{m} e^{t H_{m}} e_{1}$ (good even for small $m$ )
- Apply traditional techniques to compute $e^{t H_{m}} e_{1}$.


## What about non-linear problems?

Consider the non-linear problem, with $B: \mathbb{R}^{n} \rightarrow \mathbb{R}^{n}$ a non-linear application,

$$
u^{\prime}(t)=A u(t)+B(u(t))+f(t), t \in[0, T], \quad u(0)=u_{0}
$$

Problem: Applying the splitting $u=v+w$ does not verify the original equation.

$$
\begin{array}{ll}
v^{\prime}(t)=A v(t), & v(0)=u_{0} \\
w^{\prime}(t)=A w(t)+B(w(t))+f(t), & w(0)=0
\end{array}
$$

## Non-linear ParaExp

Consider the following iterative method: for $k=0$ initialize

$$
u_{n}^{0}=w_{n}^{0}=0, \quad n=0, \ldots, N_{t}-1
$$

For $k=1,2, \ldots$ solve the homogenous problems

$$
\begin{array}{ll}
\left(w_{n}^{k}\right)^{\prime}(t)=A w_{n}^{k}(t) & t \in\left[T_{n-1}, T_{n}\right] \\
w_{1}^{k}\left(T_{0}\right)=u_{0}, w_{n}^{k}(0)=u_{n-1}^{k-1}(0)-\sum_{j=1}^{n-1} w_{j}^{k-1}(0) &
\end{array}
$$

and then solve the non-homogenous problem

$$
\begin{aligned}
\left(u_{n}^{k}\right)^{\prime}(t) & =A u_{n}^{k}(t)+B\left(u_{n}^{k}(t)\right)+f(t), & t \in\left[T_{n-1}, T_{n}\right] \\
u_{n}^{k}(0) & =\sum_{j=1}^{n} w_{j}^{k}\left(T_{n-1}\right) &
\end{aligned}
$$

## Non-linear ParaExp equivalence with Parareal

## Theorem [Theorem 2, Gander, Güttel, Petcu, 2018]

Let the coarse propagator $G\left(U_{n}\right)$ solve the linear problem

$$
u^{\prime}(t)=A u(t), \quad t \in\left(T_{n}, T_{n+1}\right), \quad u(0)=U_{n}
$$

and the fine propagator $F\left(U_{n}\right)$ solve the non-linear problem

$$
u^{\prime}(t)=A u(t)+B(u(t))+f(t), \quad t \in\left(T_{n}, T_{n+1}\right), \quad u(0)=U_{n}
$$

Then the Parareal iteration computed with those operators is equivalent to the non-linear ParaExp algorithm.

## Summary

- Direct method for linear problems
- Acceleration of computation of the exponential using Krylov methods
- Iterative method for non-linear problems
- Equivalence of non-linear ParaExp with Parareal


## References

- ParaExp: a Parallel Integrator for Linear Initial-Value Problems (2013) M. J. Gander, S. Güttel
- A Nonlinear ParaExp Algorithm (2018) M. J. Gander, S. Güttel, M. Petcu
- Analysis of Some Krylov Subspace Approximations to the Matrix Exponential (1992) Y. Saad


[^0]:    ${ }^{2}$ Falgout, Friedhoff, Kolev, MacLachlan, Schroder (2014)

[^1]:    ${ }^{3}$ Dobrev, Kolev, Petersson, Schroder (2017)

[^2]:    ${ }^{3}$ Dobrev, Kolev, Petersson, Schroder (2017)

[^3]:    ${ }^{5}$ Gander, Neumüller (2016)

[^4]:    ${ }^{6}$ M. J. Gander (1997, PhD thesis)

