MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC
COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

Solving Differential Matrix Equations using Parareal

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joint work with

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Partners:

TECHNISCHE UNIVERSITÄT
CHEMNITZ

Differential Riccati Equations

Consider the linear quadratic optimal control problem:

$$\min_u \mathcal{J}(y,u) = \frac{1}{2}\left(\int_0^{t_f} y^T y + u^T u \,\mathrm{d}t \; + y_{t_f}^T Q y_{t_f}\right),$$

$$\text{subject to} \quad E\dot{x}(t) = Ax(t) + Bu(t),$$
$$y(t) = Cx(t)$$

where A, E, B, and C may depend on t as well and the states $x(t) \in \mathbb{R}^n$, inputs $u(t) \in \mathbb{R}^m$, and outputs $y(t) \in \mathbb{R}^q$.

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$$u(t) = -B^T X(t) E x(t),$$

where $X(t)$ is the solution of the Differential Riccati Equation (DRE)

$$E^T \dot{X}(t) E = C^T C + A^T X(t) E + E^T X(t) A - E^T X(t) B B^T X(t) E := \mathcal{R}(X(t)),$$
$$X(t = t_f) := Q.$$

Differential Lyapunov Equation

Simplification of the DRE

By setting $B = 0$ in the DRE we get the Differential Lyapunov Equation (DLE):

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Application in Model Order Reduction:

$\rightarrow$ used for *Linear Time-Variant (LTV)* Balanced Truncation.

Time integration methods

- The **DLE** is a matrix-valued ordinary differential equation.
- The **DRE** is a non-linear, matrix-valued, and highly stiff ordinary differential equation.

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Implicit time integrators [Mena '07, Benner/Mena '12]

- Backward differentiation formula (BDF)
- Linear implicit Runge-Kutta (Rosenbrock) methods
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Numerical issues

- Methods are fairly time and storage consuming for large-scale problems.
- High accuracy requires small time steps or high order methods.
- At every time step a number of algebraic matrix equations needs to be solved.

Rosenbrock Methods

Restriction by Parareal:

Only single-step integrators are well suited.

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General Rosenbrock Scheme

The s-stage Rosenbrock method applied to a matrix differential equation of the form $\dot{X} = F(X)$ is given as

$$X_{k+1} = X_k + \tau_k \sum_{\ell=1}^{s} b_\ell K_\ell^{(k)},$$

$$K_i^{(k)} = F(X_k + \tau_k \sum_{\ell=1}^{i-1} \alpha_{i,\ell} K_\ell^{(k)}) + \tau_k \mathcal{J}_k \sum_{\ell=1}^{i} \gamma_{i,\ell} K_\ell^{(k)}, \quad \forall i = 1, \ldots, s.$$

- s : order of the method
- τ_k : time step
- $\mathcal{J}_k$: Fréchet derivative of F at X_k
- $\alpha_{i,\ell}, \gamma_{i,\ell}, \mu_\ell$: determining coefficients

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Fréchet derivative of $\mathcal{R}(X)$ is a Lyapunov operator.

Rosenbrock Methods

[Mena '07, Benner/Mena '12]

We only consider the DRE, where $E^T \dot{X} E = \mathcal{R}(X)$:

1st order Rosenbrock scheme (Ros1)

$$X_{k+1} = X_k + \tau_k K_1^{(k)}$$

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$$E^T K_1^{(k)} E - \tau_k \mathcal{R}'|_{X_k}(K_1^{(k)}) = \mathcal{R}(X)$$

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$$X_{k+1} = X_k + \tau_k K_1^{(k)}$$

$$E^T K_1^{(k)} E - \tau_k (A - BB^T X_k E)^T K_1^{(k)} E - \tau_k E^T K_1^{(k)} (A - BB^T X_k E) = \mathcal{R}(X)$$

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$$(\tau_k(A - BB^T X_k E) - \frac{1}{2}E)^T K_1^{(k)} E + E^T K_1^{(k)} (\tau_k(A - BB^T X_k E) - \frac{1}{2}E) = -\mathcal{R}(X)$$

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$$\tilde{A} := \tau_k (A - BB^T X_k E) - \frac{1}{2} E$$

Solve one Algebraic Lyapunov Equation (ALE) inside the 1-stage Rosenbrock method.

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2nd order Rosenbrock scheme (Ros2) [Dekker/Verwer '84]

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Solve two ALEs inside the 2-stage Rosenbrock method.

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Higher Order Schemes:

- 3rd order scheme based on `ode23s` (numerically unstable)
- 3rd order scheme based on `Ros3P` [Lang, Verwer '01]
- 4th order scheme [Shampine '82]

Optimize before Parallelize

High Computational Cost

- Need the solution of s algebraic Lyapunov equations per time step.
  $\rightarrow$ Bartels-Stewart algorithm requires a QZ decomposition.
- Mostly matrix-matrix products.

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Redundant Information

- Each right hand side of the Lyapunov equation includes $\mathcal{R}(X_k)$.
- Redundant information in the linear part of $\mathcal{R}(X_k + \tau_k K_j + \ldots)$.
- Solutions of the Lyapunov equations K_j are symmetric.

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Strategies

- Computational Cost: Use level-3 BLAS enabled algorithms.
- Redundant Information: Reformulation of the right hand sides.

Level-3 BLAS enabled Algorithms

Matrix-Matrix Products

Use Intel® MKL, AMD ACML, BLIS, OpenBLAS or ATLAS.

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Generalized Bartels-Stewart algorithm available in SLICOT: [Penzl '97]

- All stages have the same coefficient matrices.
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- Matrix Sign Function Iteration [Quintana-Ortí/ Benner '99]
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- Reuse of the QZ decomposition and level-3 BLAS block generalized Bartels-Stewart algorithm. [GLYAP3: K./Saak '14 '15]

Right-Hand-Side Rearrangement

Consider the stages of the 2nd order Rosenbrock scheme:

$$\tilde{A}_k^T K_1 E + E^T K_1 \tilde{A}_k = -\mathcal{R}(X_k)$$

and

$$\tilde{A}_k^T K_2 E + E^T K_2 \tilde{A}_k = -\mathcal{R}(X_k + \tau_k K_1) + 2E^T K_1 E$$

with $\tilde{A} := \gamma\tau_k(A - BB^T X_k E) - \frac{1}{2}E$.

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&= -\mathcal{R}(X_k) - \tau_k \left((A^T - BB^T X_k E)^T K_1 E + E^T K_1 (A^T - BB^T X_k E) \right) \\
&\quad + \tau_k^2 E^T K_1 BB^T K_1 E + 2E^T K_1 E \\
&= -\mathcal{R}(X_k) - \frac{1}{\gamma} \left(\tilde{A}_k^T K_1 E + E^T K_1 \tilde{A}_k \right) - \frac{1}{\gamma} E^T K_1 E \\
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&\quad + \tau_k^2 E^T K_1 BB^T K_1 E + 2E^T K_1 E \\
&= -(1 - \frac{1}{\gamma})\mathcal{R}(X_k) + \tau_k^2 E^T K_1 BB^T K_1 E + (2 - \frac{1}{\gamma}) E^T K_1 E.
\end{aligned}$$

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Using the linearity of the Lyapunov-Equation we reformulate the 2nd order Rosenbrock scheme as:

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\begin{aligned}
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- The 3rd and 4th order scheme can be rearranged in the same way.
- Symmetric terms are computed like

$$
E^T K_j B B^T K_j E = K_E^{(j)^T} K_E^{(j)} \quad \text{with} \quad K_E^{(j)} := B^T K_j E.
$$

Parareal Implementation

Following [Maday/Lions/Turinici '01] we use

$$X_0^{(k+1)} := X(t = t_f),$$
$$X_p^{(k+1)} := F(t_{p-1}, t_p, X_{p-1}^{(k)}) + G(t_{p-1}, t_p, X_{p-1}^{(k+1)}) - G(t_{p-1}, t_p, X_{p-1}^{(k)})$$

as parareal-scheme, where $F(t_p, t_{p+1}, X_s)$ and $G(t_p, t_{p+1}, X_s)$ integrate the DRE from t_p to t_{p+1} with the initial value X_s.

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Coarse and Fine Solvers

Use our four Rosenbrock methods as coarse and the fine solvers:

- The coarse solver G performs one time step from t_p to t_{p+1}.
- The fine solver F performs f time steps from t_p to t_{p+1}.

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We obtain 16 combinations for Parareal setup.

Parareal Implementation

Classical Pipeline Implementation: Stage-Code

```
for it:=1 to maxit do
    Receive X_s^(it) from ProcessID-1
    X_G^(it) = G(X_s^(it))
    if it = 1 then
        Send X_G^(it) to ProcessID+1
    else
        X^(it) := X_G^(it) + X_F^(it-1) - X_G^(it-1)
    end if
    X_F^(it) = F(X_s^(it-1))
    if ||X^(it) - X^(it-1)|| < δ||X^(it)|| then
        Stop.
    end if
end for
```

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    end if
    X_F^(it) = F(X_s^(it-1))
    if ||X^(it) - X^(it-1)|| < δ||X^(it)|| then
        Stop.
    end if
end for
```

Can be easily implemented on

- distributed systems using MPI,
- shared memory systems using OpenMP or PThreads.

Large Scale Problems

For large scale problems $n \geq 1\,000$ we approximate $X(t) \approx L(t)D(t)L(t)^T$, where $L(t) \in \mathbb{R}^{n \times p}$ and $D \in \mathbb{R}^{p \times p}$ diagonal with $p \lll n$.

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$$X^{(i)} := X_G^{(i)} + X_F^{(i-1)} - X_G^{(i-1)}$$

by

$$L^{(i)} D^{(i)} {L^{(i)}}^T = L_G^{(i)} D_G^{(i)} {L_G^{(i)}}^T + L_F^{(i-1)} D_F^{(i-1)} {L_F^{(i-1)}}^T - L_G^{(i-1)} D_G^{(i-1)} {L_G^{(i-1)}}^T$$

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$$\begin{aligned} L^{(i)}D^{(i)}L^{(i)^T} &= L_G^{(i)}D_G^{(i)}L_G^{(i)^T} + L_F^{(i-1)}D_F^{(i-1)}L_F^{(i-1)^T} - L_G^{(i-1)}D_G^{(i-1)}L_G^{(i-1)^T} \\ &= \underbrace{\begin{bmatrix} L_G^{(i)} & L_F^{(i-1)} & L_G^{(i-1)} \end{bmatrix}}_{L^{(i)}} \underbrace{\begin{bmatrix} D_G^{(i)} & & \\ & D_F^{(i-1)} & \\ & & -D_G^{(i-1)} \end{bmatrix}}_{D^{(i)}} \underbrace{\begin{bmatrix} L_G^{(i)} \\ L_F^{(i-1)} \\ L_G^{(i-1)} \end{bmatrix}^T}_{L^{(i)^T}}. \end{aligned}$$

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&= \tilde{L}^{(i)} \tilde{D}^{(i)} {\tilde{L}^{(i)}}^T
\end{aligned}
$$

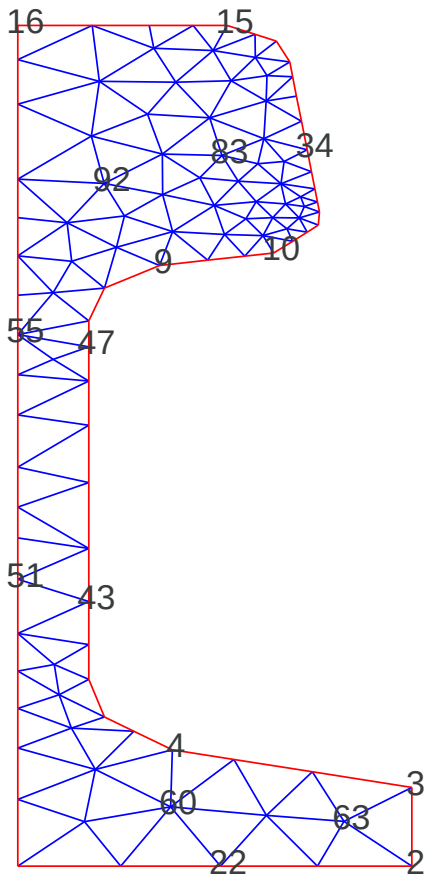
$\rightarrow$ Only proof of concept due to bad load balancing in the pipeline parallelism.

Model Problem

[Oberwolfach Rail]

- Mathematical model: boundary control for linearized 2D heat equation:

$$
\begin{aligned}
c \cdot \rho \frac{\partial}{\partial t} x &= \lambda \Delta x, && x \in \Omega \\
\lambda \frac{\partial}{\partial n} x &= \kappa(u_k - x), && x \in \Gamma_k,\ 1 \leq k \leq 7, \\
\frac{\partial}{\partial n} x &= 0, && x \in \Gamma_7.
\end{aligned}
$$



- FEM discretization with $n = 371$ states, $m = 7$ inputs, and $q = 6$ outputs
- computations with $\tau = 0.1ms$ on $[0, 45]s$
- evaluations for one component of the feedback $K(t) = -B^T X(t) E$

Experimental Results

Hardware Environment

HPC-Cluster `otto`

- 450 Intel® Xeon® Westmere-EP cores @ 2.66GHz with 4 GB RAM each
- QDR-Infiniband interconnect

Software

- Intel® Parallel Studio 2015 XE
- OpenMPI 1.8.1 with threading support
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Reference Result

- 450 000 steps with $\tau = 0.1$ms with Ros4 in **3.46 days**
- Memory requirements for the trajectory: $X(t)$ – **1.4 TB**, $K(t)$ – **9 GB**

Experimental Results

Sequential Runtimes

Rosenbrock Order	SLICOT	GLYAP 3	ratio
1	4.40 d	2.87 d	1.53
2	6.15 d	3.06 d	2.01
3	7.84 d	3.27 d	2.40
4	9.55 d	3.46 d	2.75

Table: Sequential Runtime of the Rosenbrock methods with different Lyapunov solvers.

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Table: Sequential Runtime of the Rosenbrock methods with different Lyapunov solvers.

First observations

- A fast solver for the Lyapunov equations is a key ingredient,
- Choosing the correct Lyapunov solver already gains a speed up of 2.75,
- But 3.46 days are still too long for a accurate solution of such a small problem.

Experimental Results

Distributed Parallel Execution

Parareal Setup

- 450 coarse steps, $\tau_{coarse} = 100\text{ms}$
- 1000 fine steps per coarse step, $\tau = 0.1\text{ms}$
- Maximum number of iterations: 10
- Stopping criteria: $\delta = 10^{-6}$

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Fine \ Coarse	Ros1		Ros2		Ros3		Ros4	
	Time	Iter	Time	Iter	Time	Iter	Time	Iter
Ros1	3.30 h	9	2.97 h	8	3.29 h	9	1.74 h	4
Ros2	3.59 h	9	3.27 h	8	3.61 h	9	1.89 h	4
Ros3	3.87 h	9	3.51 h	8	3.88 h	9	2.02 h	4
Ros4	4.17 h	9	3.78 h	8	4.18 h	9	2.19 h	4

Table: Runtime and maximum iteration number.

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Fine \ Coarse	Ros1	Ros2	Ros3	Ros4
Ros1	2.01e-05	2.01e-05	2.01e-05	2.01e-05
Ros2	2.07e-05	2.07e-05	2.07e-05	2.07e-05
Ros3	2.07e-05	2.07e-05	2.07e-05	2.07e-05
Ros4	**1.27e-09**	**3.00e-10**	**9.71e-08**	**6.10e-14**

Table: Relative 1-norm error between the Parareal solution and the reference.

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Fine \ Coarse	Ros1	Ros2	Ros3	Ros4
Ros1	*	7.69e-05	7.68e-05	7.68e-05
Ros2	*	7.81e-05	7.80e-05	7.80e-05
Ros3	*	7.81e-05	7.80e-05	7.80e-05
Ros4	*	**3.14e-11**	**5.76e-09**	**1.14e-14**

Table: Relative 1-norm error between the Parareal solution and the reference for $K(t)_{1,77}$.

Conclusions and Open Problems

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We have seen that:

- "optimize before parallelize" already gains nearly a factor of up to 3,
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Thank you for your attention! Questions?