In-Time-Parallelization of Atmospheric Chemical Kinetics

4th Workshop on Parallel-in-Time Integration, Dresden
Teresa Beck, Vincent Heuveline, 28/05/2015
Outline

In-Time-Parallelization of Atmospheric Chemical Kinetics

1) Motivation
2) In-Time Parallelization of Chemistry
   1. Internal Parallelization
   2. External Parallelization
3) Conclusions
4) Outlook
Atmospheric Chemical Kinetics are a very time-consuming component within an Air Quality Model.
Motivation

Atmospheric Chemical Kinetics in Air Quality Models

- chemical mechanisms (e.g. RADM2): 50-100 species, 100-200 reactions
- wide range of time-scales: \( \text{CH}_4 \) (years), radicals like OH (10^{-4} sec)
- temporal evolution described by stiff ODEs \( \frac{\partial t}{\partial t} c = f(c) \)
- quickly adjusting step sizes → adaptive Rosenbrock solvers

![Graph](image-url)

- small \( \Delta t \) at initial time to capture transient species
- fast processes in equilibrium allows using big \( \Delta t \)
Motivation
Parallelization of Air Quality Models

1st Level of Parallelization

- numerical solution of PDEs → discretization in space + time
- parallelization → domain decomposition in space
- decoupling of adv./diff./react./etc. → operator splitting
Motivation
Parallelization of Air Quality Models

2nd Level of Parallelization
- N *decoupled* ODE systems $\rightarrow$ trivial parallelization
- potential speed-up = N
- ... what if #procs > N?

3rd Level of Parallelization
- across the method: implicit, multi-stage method $\rightarrow$ Limited.
- across the system: high degree of couplings $\rightarrow$ Limited.
- across time:

  $\rightarrow$ Parareal.
In-Time-Parallelization
Two Concepts

1. Internal Parallelization within one splitting interval

2. External Parallelization across splitting intervals
1. Internal Parallelization

The Challenge: Stiffness

1. Internal Parallelization within one splitting interval

- F = adaptive Rosenbrock solver (rtol=10^{-4})
- load-imbalances when executing F on equidistant time-slabs:

\[ \text{Adapted Timesteps } \mathcal{F} (\text{rtol}_F=10^{-4}) \]
Internal Parallelization
Solution Strategy I: Double Adaptive Parareal

Naive Idea...

- $(F, G) = \text{adaptive Rosenbrock solvers (rtol}=10^{-4}, \text{rtol}=10^0)$
- initial adaptive decomposition: let $G$ suggest the decomposition into time-slabs

Convergence: 1 – 3 iterations

Performance: Best performance with $N = 1$.
- $G$ is always initiated with small $\Delta t$
- number of acc. timesteps over all $N$ time-slabs grows with $N$
  $\rightarrow$ Overhead in coarse update.

  $\rightarrow$ No performance gains.
Another Naive Idea...: Use a reduced model for G.

Popular Model Reduction Approaches in Atmospheric Chemistry:

- **Removal** of redundant species or reactions

- **Lumping** describe similar species by means of one surrogate spc in the mechanism
  
  \[ \text{smaller sets of ODEs, not necessarily less stiff} \]

- **Time Scale Separation**: separate fast from slow processes, e.g. QSSA, ILDM
  
  \[ \text{smaller, less stiff system of ODEs + algebraic constraints} \]

- **Repro-Modelling** construct functional representation of input-output relationship of
  
  \[ c(t + \Delta t) := h(c(t)) \]
  
  \[ \text{→ None really promising in this context...} \]
In-Time-Parallelization
Two Concepts

1. Internal Parallelization within the splitting interval

2. External Parallelization across splitting intervals
2. External Parallelization of subsequent splitting intervals

- operator splitting decouples chemistry from other external effects
- in fact: two-way feedbacks between chemistry ← → meteorology

1. How to incorporate feedbacks?

- meteorology → chemistry: very sensitive to photolysis, \((T, p)\)
- chemistry → meteorology: radiation budget, cloud physics

- If incorporating all effects: solution is discontinuous over the timeslabs

2. How do we measure convergence for discontinuous solution?

→ for now: only update photolysis → continuous solution
**External Parallelization**  
**Solution Strategy II: Adaptive Reduced-Model Parareal**

**G = High Dimensional Model Representation** (Rabitz et al. [1998])

**Idea:** functional representation of input-output relationship

\[ c(t + \Delta t) := h(c(t)) \]

**Construction:**
- define input space, that covers a realistic range for parameter species
- define a reference point
- carry out learning runs with parameter spc. varied within input space
- evaluate input-output responses and tabulate correlated effects
External Parallelization
Solution Strategy II: Adaptive Reduced-Model Parareal

G = High Dimensional Model Representation (Rabitz et al. [1998])

Performance: up to 1000x faster than adaptive scheme
(e.g. Wang et al., [2001], [2005])

Scalability: linearly with N...

Drawback: Not generic!
- only valid, if c(t) is in the defined input range
- fixed timestep size → adaptivity ↯

→ „coarse propagation“ = calculate output from a given input state by interpolation from HDMR
Test-Bed:

- RADM2 mechanism: 63-species, 157 reactions
- simulation over 24 hours with N = 24
- F = adaptive Rosenbrock (rtol=10^{-4})
- G = 24: 1^{st} order HDMR expansions, each with different photolysis conditions, two parametrizing variables, varied over 11 points
- initial values = reference point +/- 10% used for construction of HDMR
External Parallelization
Numerical Results

Convergence

![Graph showing convergence](image)

- Relative error at $T_{\text{end}}$ vs. iteration
External Parallelization

Numerical Results – 1\textsuperscript{st} order HDMR, n=2, s=11

\begin{align*}
\text{k}=1 & \quad \text{NO}_2 \quad \text{H}_2\text{O}_2 \\
\text{k}=3 & \quad \text{NO}_2 \quad \text{H}_2\text{O}_2 \\
\text{k}=5 & \quad \text{NO}_2 \quad \text{H}_2\text{O}_2 \\
\end{align*}

\begin{align*}
\text{O}_3 & \quad \text{sequential} \quad \text{parareal} \\
\text{sequential} \quad \text{parareal} \\
\end{align*}
External Parallelization
Numerical Results

Speed-Up

- none so far....
- HDMR expansion was ~10x faster than F → in literature up to 1000x
- CPU time to evaluate an HDMR expansion grows with
  - #(parameter species) → here: 2
  - #(parametrizing points) → here: 11
  - #(degree of HDMR) → here: 1st order
  - incompetence of the programmer....
Conclusions

- parareal for stiff atmospheric chemistry embedded in air quality models
- two fields of application: internal and external parallelization
- internal parallelization within a splitting interval → dismissed.
- external parallelization across splitting intervals poses problems
  - necessity of a reduced model
  - functional representation (HDMR) as coarse propagator
  - very high potential
  - construction of an HDMR far from obvious...
Outlook

Current Work:

- find an optimal HDMR expansion
- verify assumption, that only photolysis needs to be considered
- test with real air quality model

Future Work:

- operator splitting approach in fact is a sequentialisation of parallel processes → parareal operator splitting?
Thank's for your attention!
Appendix
High Dimensional Model Representation (Rabitz et al. [1998])

Construction of an HDMR expansion:

- define $n$ parameter species with $n \leq \#\text{species}$
- define input variable space $\mathcal{I} \subset \mathbb{R}^n$, covering a realistic range for parameter species
- carry out $\#\text{runs}$ learning runs with $n$ parameters varied over $s$ discrete values within
  
  1st order HDMR: $\#\text{runs} = 1 + ns$
  
  2nd order HDMR: $\#\text{runs} = 1 + ns + \frac{n(n-1)s^2}{2}$

- evaluate input-output responses over the desired domain of the input variable space
- construct HDMR: tables with correlated effects

Drawback:

- not generic $\rightarrow$ only gives a valid approximation, if $c(t) \in \mathcal{I}$
Appendix
Air Quality Models and Parallelization

3rd Level of Parallelization?!?

1) Load-imbalances in global simulations
   - photolytic reactions activated with sun
   - short lived, transient species are created/destroyed with sunlight
   - very small $\Delta t$ at day/night transitions

2) Typical AQM chemical mechanisms = subsets of huge reactions systems
   - derived for computational convenience
   - computing the full system is too expensive and takes too much time
Appendix

Atmospheric Chemical Kinetics

**Stiff problems** are “exceedingly difficult to solve by ordinary numerical procedures” [Curtis and Hirschfelder (1951)]

- classified typically via range of eigenvalues \( \lambda_1, \ldots, \lambda_n \) of \( J := \partial f / \partial c \)
- in atmospheric chemistry ~ \((|\lambda_{min}|, |\lambda_{max}|) = (10^8, 10^{-8})\)
- quickly adjusting step sizes → adaptive Rosenbrock solvers