EFFICIENT NUMERICAL METHODS IN AIR POLLUTION TRANSPORT MODELLING: OPERATOR SPLITTING AND RICHARDSON EXTRAPOLATION

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Outline

- The transport-chemistry system
- Operator splitting
- Richardson extrapolation
- Stability issues
- Computational efficiency
- Numerical experiments

The transport-chemistry system

$$\frac{\partial c_i}{\partial t} = -\nabla(uc_i) + \nabla(K\nabla c_i) - \sigma_i c_i + R_i(c_1,\ldots,c_m) + E_i(x,t) \qquad (1)$$

$$i = 1,2,\ldots,q$$

- Coupled nonlinear system
- Direct discretization by *M* grid points → large nonlinear system of ODE's with $M \cdot q$ unknowns

→ Off-the-shelf solvers are not applicable

Operator splitting

Note: the rhs of (1) is a sum of simpler terms

Idea: decompose (split) system (1) into a sequence of simpler problems.

- Divide the time interval into sub-intervals of length τ
- Solve each sub-problem successively at each time step τ
- Always use the solution of the previous sub-problem as initial condition

Advantages

- Problem (1) is decomposed into several simpler problems.
- Apart from term R_i, independent linear scalar equations are obtained for each species (M unknowns instead of Mq unknowns).
- Each sub-problem can be solved in a mathematically correct way.

Disadvantages

- Local splitting error

Splitting techniques with smaller splitting error:

- Marchuk-Strang splitting
- SWS splitting

But these are more costly!

- Difficulties with the boundary conditions

Problems of the accuracy

p: order of the splitting method

r: order of the applied numerical method

$\longrightarrow$ The whole approximation will have order min{p,r}

$\Longrightarrow$ It is not worth using a higher order numerical method for the sub-problems, unless the splitting method is of higher order, too. But they are expensive.

Question: How to enhance the accuracy in a cost-effective way?

Richardson extrapolation (RE)

Task: $$\frac{dy}{dt} = f(t, y), \quad t \in [a, b], \quad y(a) = y_0,$$

Idea: apply the same p-th order numerical method by two different step sizes, and combine the solutions by some weights

Denote the numerical solution at time t_{n-1} by y_{n-1} .

1. Perform one time step τ to calculate the approximation z_n of $y(t_n)$
2. Perform two time steps $\tau/2$ to calculate the approximation w_n of $y(t_n)$
3. Combine them as $$y_n := \frac{2^p w_n - z_n}{2^p - 1}$$
4. Then $$y(t_n) - y_n = O(\tau^{p+1})$$

Passive RE

$$
\begin{tikzcd}
 & z_1 \arrow[r] & z_2 \arrow[r] & \cdots \\
y_0 \arrow[ur] \arrow[dr] & & & \\
 & w_1 \arrow[r] \arrow[d] & w_2 \arrow[r] \arrow[d] & \cdots \\
 & y_1 & y_2 &
\end{tikzcd}
$$

Active RE

$$
\begin{array}{ccccccccc}
 & & z_1 & & & & z_2 & & \\
 & \nearrow & & \searrow & & \nearrow & & \searrow & \\
y_0 & & & & y_1 & & & & y_2 \cdots \\
 & \searrow & & \nearrow & & \searrow & & \nearrow & \\
 & & w_1 & & & & w_2 & &
\end{array}
$$

Stability issues

- The passive RE preserves the stability properties of the underlying method
- This is not necessarily true for the active RE:

- Trapezoidal rule + RE: not A-stable
- BE + RE: L-stable
- General θ-method + RE: A-stable for $\theta \in [2/3, 1]$
- For two implicit RK methods very large stability regions were found.

Computational efficiency

Let $T = N\tau$. Then by time step $\tau/2$, $2N$ steps are needed.

- Both RE's require ~1.5 times more computations than performing $2N$ steps with the underlying method.
- If we have the solution with time step τ (N steps), then the passive RE hardly requires more time than performing $2N$ steps with the underlying method
- When parallelized, the active RE does not require much more time than performing $2N$ steps with the underlying method

Numerical experiments

We applied RE in the chemical module of UNI-DEM

- Chemical scheme of EMEP with 56 species
- Nonlinear system of ODEs
- Strongly stiff
- 24-hour time interval
- Reference solution: 4-step, fifth-order L-stable implicit RK solver
- Errors measured in the maximum norm

Errors obtained by the backward Euler method + RE

N	BE	BE+ active RE	BE+ passive RE
1344	3.063E-1	7.708E-3	6.727E-3
2688	1.516E-1 (2.02)	1.960E-3 (3.93)	1.739E-3 (3.87)
5376	7.536E-2 (2.01)	5.453E-4 (3.59)	4.417E-4 (3.94)
10752	3.757E-2 (2.01)	1.455E-4 (3.75)	1.113E-4 (3.97)
21504	1.876E-2 (2.00)	3.765E-5 (3.86)	2.793E-5 (3.98)
43008	9.371E-3 (2.00)	9.583E-6 (3.93)	6.997E-6 (3.99)
86016	4.684E-3 (2.00)	2.418E-6 (3.96)	1.751E-6 (4.00)
172032	2.341E-3 (2.00)	6.072E-7 (3.98)	4.379E-7 (4.00)
344064	1.171E-3 (2.00)	1.522E-7 (3.99)	1.095E-7 (4.00)

CPU times (seq) and numbers of time steps (BE method) needed for prescribed accuracy

Global error	BE		BE + RE	
	CPU time	No.of steps	CPU time	No.of steps
[1E-1, 1E-2]	274	5376	304	672
[1E-2, 1E-3]	862	43008	374	1344
[1E-3, 1E-4]	7144	688128	661	5376
[1E-4, 1E-5]	42384	5505024	1428	21504
[1E-5, 1E-6]	265421	44040192	2240	43008

Errors obtained by the sequential splitting (+BE) without and with RE

N	Seq. splitting	Seq. spl. + RE
1344	2.154e-1	1.799e-2
2688	1.093e-1 (1.97)	5.862e-3 (3.07)
5376	5.509e-2 (1.99)	1.698e-3 (3.45)
10752	2.764e-2 (1.99)	4.598e-4 (3.69)
21504	1.384e-3 (2.00)	1.199e-4 (3.84)
43008	6.926e-3 (2.00)	3.062e-5 (3.92)
86016	3.464e-3 (2.00)	7.740e-6 (3.96)
172032	1.733e-3 (2.00)	1.946e-6 (3.98)

Further plans

- Extending our theoretical results to further underlying methods (general RK method)
- Stability analysis of the RE when combined with different splittings
- Investigating the possibilities of the RE for solving PDEs