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

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Abstract: The mathematical modelling of air pollution processes is usually based on a system of nonlinear partial differential equations called transport-chemistry system. The numerical integration of this system is a rather difficult computational task, especially in large-scale and global models, where the number of grid-points can range from a few thousand to a few hundred thousand, and the number of chemical species is typically between 20 and 200. We present two robust techniques that can significantly enhance the efficiency of the numerical solution and the computer realization. During operator splitting the different sub-processes of the described phenomenon are treated separately, by coupling the corresponding mathematical problems through their initial conditions. Richardson extrapolation is based on a combination of two numerical solutions obtained by different discretization parameters. We present the basics of these methods and illustrate their benefits in different environmental models.

Key words: *Transport-chemistry system, Danish Eulerian Model, splitting methods, passive and active Richardson extrapolation.*

INTRODUCTION

The spatial and temporal changes of pollutant concentrations in the atmosphere are typically described by a system of nonlinear partial differential equations called transport-chemistry system. This system is rather complex in its original form, since the right-hand sides of the equations contain several terms with different mathematical properties. These terms describe advection, diffusion, deposition, chemical reactions and emissions in the general case. Due to the complicated structure and the large size, the solution of this system imposes a very challenging task for environmental modellers.

In this contribution we introduce the general form of the transport-chemistry system and outline the problems of its numerical solution. Then we present two approaches that – applied separately or together – can provide a sufficiently accurate numerical solution of the transport-chemistry system within reasonable computational time: operator splitting and Richardson extrapolation. The achievable efficiency is illustrated by numerical experiments.

THE TRANSPORT-CHEMISTRY SYSTEM

In the centre of deterministic air pollution models one finds the system of partial differential equations

$$\frac{\partial c_i}{\partial t} = -\nabla(uc_i) + \nabla(K\nabla c_i) - \sigma_i c_i + R_i(c_1,...,c_m) + E_i(x,t)\,,\ i = 1,2,...,m \qquad (1)$$

called transport-chemistry system (Zlatev, 1995). Here m denotes the number of chemical species, $c_i = c_i(x, t)$ denotes the concentration of the i-th species, u is the three-dimensional wind field, K is the turbulent diffusion matrix, σ_i denotes the (dry and/or wet) deposition velocity, R_i describes the chemical reactions and radioactive decay (in case of radionuclides), while E_i involves the emission sources.
The direct numerical treatment of this system is rather difficult for the following reasons.

- Due the term R_i , we have a coupled system of nonlinear partial differential equations.
- The direct discretisation of this system would result in a large nonlinear system of ordinary differential equations, where in case of M grid points for each time layer mM unknown values are to be computed.
- The numerical method is expected to satisfy certain properties, such as consistency, stability, convergence and other qualitative properties. However, if some off-the-shelf numerical method is applied directly to such a complicated system, these properties cannot be guaranteed.

In the following we present two powerful techniques which make the above system tractable for numerical integration.

OPERATOR SPLITTING

During this procedure the right-hand side of the system to be solved is divided into a few simpler terms, and the corresponding sub-systems – which are connected to each other through the initial conditions – are solved one after the other in each time step of the numerical integration. In this manner, we replace the original model with one in which the different sub-processes take place successively in time. For example, in the Danish Eulerian Model the five sub-systems describe 1) the horizontal advection, 2) the horizontal diffusion, 3) the chemical reactions to which also emissions are added, 4) the deposition and 5) the vertical exchange (Zlatev, 1995). Assume that some approximation to the concentration vector (c_1, . . . , c_m) at the beginning of the time step has been found. The first system is solved by using this vector as a starting vector. The obtained solution will serve as the initial vector in the treatment of the second system and so on. The solution of the fifth system is accepted as an approximation to the concentration vector at the end of the time step. So, this so-called DEM splitting is based on a separation of the different physical processes of the air pollution transport and a separation of the vertical and horizontal directions for advection and diffusion. The distinction of the vertical and horizontal directions is natural in shallow atmospheres, and makes it easier to switch on to the 2-D version of the model. An alternative of the DEM splitting is the so-called physical splitting, where the sub-operators belong to the five basic air pollution processes, and there is no directional separation.

The application of any of the above splitting methods has the following advantages:

- The original problem is decomposed into several simpler problems.
- Apart from the reaction problem, we obtain independent linear scalar equations for the different species. Therefore, instead of a complicated problem with mM unknowns in each time step, we practically obtain discrete models with only M unknowns.
- When operator splitting is applied, each sub-problem is solved by using a numerical method that is tailored to the given sub-problem, and so the sub-problems can be treated in a mathematically correct way.

Operator splitting has the disadvantage that even if the sub-problems are solved exactly, the application of splitting gives rise to the local splitting error, defined as the difference of the exact model and the split model by assuming exact solution of the sub-problems after one splitting time step. There are certain splitting techniques which have smaller local splitting error, but these are more costly (Strang-Marchuk splitting (Strang, 1968 and Marchuk, 1968), symmetrically weighted sequential (SWS) splitting (Strang, 1963, Csomós et al., 2005). The treatment of the boundary conditions (in case they exist) are not trivial, either, when operator splitting is applied.

RICHARDSON EXTRAPOLATION

It can be shown that if the local splitting error has order p and each sub-problem is solved by a p-th order numerical method, then the whole numerical method will also have order p. When the order of the local splitting error and the order of the applied numerical methods are different, the whole approximation will be determined by the lowest error order. This means that it is not worth using higher order methods for the sub-problems, unless the splitting method is also of higher order. However, the application of a higher order splitting method and higher order numerical methods for the sub-problems would often be too expensive. So the question arises how we can enhance the accuracy in a cost-effective way. A possible approach to this problem is Richardson extrapolation.

The Richardson extrapolation can be applied for the increase of the order of convergence (and so efficiency) of any convergent time integration method (Richardson, 1911 and Richardson, 1927). The key to this procedure is to apply the same *p*-th order method by two different choices of the time-step size, and combine the two solutions by appropriately chosen weights as follows.

Assume that we apply a numerical method of order *p* for the solution of a system of ordinary differential equations, and denote the numerical solution at time layer t_{n-1} by y_{n-1}. Then we calculate the approximation y_n in three steps:

1. Perform one time step of size τ to calculate the approximation z_n of $y(t_n)$.
2. Perform two small time steps with step-size $\tau/2$ to calculate another approximation w_n of $y(t_n)$.
3. Calculate an improved approximation y_n by applying the formula

$$y_n = \frac{2^p w_n - z_n}{2^p - 1} \tag{2}$$

The order of accuracy of the improved approximation y_n given by (2) is $p+1$.
The Richardson Extrapolation can be implemented in two different ways. One can apply the improved approximation y_n in step $n+1$ to z_{n+1} and w_{n+1} or one can alternatively use the approximations z_n and w_n in the calculation of z_{n+1} and w_{n+1}, respectively. The first implementation is called active, while the name passive is used for the second one.

Assume that the computations have been performed with the larger time-step τ, and denote by *N* the number of time-steps. Obviously, during the computation with the halved time-step $\tau/2$, 2*N* time-steps are to be taken. It is easy to see that both the passive and active Richardson extrapolations require approximately 1.5 times more computations than the integration with the underlying method in 2*N* time-steps. Moreover, if the computation has been performed with the time step τ (which means *N* steps), then applying the passive Richardson extrapolation hardly requires more computations than performing 2*N* steps with the underlying method. In case parallel computers are available, then even applying the active Richardson extrapolation does not require significantly more computational time than performing 2*N* steps with the underlying method. This clearly shows the efficiency of the Richardson extrapolation.

The implementation of the Richardson Extrapolation is relatively simple. It is nearly obvious that the stability properties of the combined method obtained when the passive implementation is used are the same as those of the underlying numerical method. However, the requirement for stability of the computational process may cause serious difficulties when the active Richardson extrapolation is used. Through the investigation of the stability function of the combined method separately in each case the following results have been obtained (Zlatev et al., 2010):

- The combination of the trapezoidal rule and the active Richardson extrapolation is not A-stable.
- The combination of backward Euler method and the active Richardson extrapolation is L-stable.
- The combination of the general θ-method and the active Richardson extrapolation is A-stable for $\theta \in [2/3,1]$.
- In case of two implicit Runge-Kutta methods (three-stage fifth-order fully implicit Runge-Kutta method and two-stage third-order diagonally implicit Runge-Kutta method) we could not prove A-stability, strong A-stability and L-stability, but found very large stability regions (Zlatev et al. 2015).

NUMERICAL EXPERIMENTS

We successfully applied Richardson extrapolation in some simplified environmental models, see Brajnovits, 2010 and Mona et al., 2015. Here we will show some results that have been obtained when we applied passive and active Richardson extrapolation in the chemistry module of UNI-DEM. This module is based on the chemical scheme of the EMEP model with 56 chemical species. The computations were performed on the computers of the Centre for Scientific Computing at the Technical University of Denmark (http://www.hpc.dtu.dk) and at the Department of Environmental Science at the Aarhus University. The equations describing the chemical transformations between these species form a nonlinear system of ordinary differential equations. Due to the fact that the reaction rates have very

different magnitudes, some species transform slowly, while others very rapidly, which results in a strongly stiff system. During the experiments the time interval of the computations was 24 hours long (from noon to the noon of the next day). The reference solution was computed by a four-step, fifth-order L-stable implicit Runge-Kutta method. The errors were measured in the maximum norm.

Table 1. Errors obtained by the backward Euler method and the combinations of the backward Euler method with passive/active Richardson extrapolation (RE) in the chemical module of UNI-DEM. *N* denotes the number of time-steps that were taken during the time integration. The numbers in parentheses give the ratio of the given error and the error obtained by using the previous time-step size.

N	Backward Euler	Backward Euler + active RE	Backward Euler + 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)

The backward Euler method is a first-order numerical method, which is reflected by the fact that the errors are roughly halved when the time-step size is halved during the direct implementation of this method. Both Richardson extrapolations increase the order to 2, which is shown by error ratios around 4. Note that for the achievement of the same accuracy much fewer time-steps are needed when the Richardson extrapolation is used. This is even clearer from Table 2, which shows how many time integration steps were needed in order to achieve some given accuracy. One can see that the Richardson extrapolation considerably enhances the efficiency.

Table 2. CPU times in seconds and numbers of time-steps needed for the global errors to fall into given intervals. The results are the same for both the active and passive Richardson extrapolations.

Global error	Backward Euler		Backward Euler + RE	
	CPU time / Number of time-steps		CPU time / Number of time-steps	
[1e-2,1e-1]	274	5376	304	672
[1e-3,1e-2]	862	43008	374	1344
[1e-4,1e-3]	7144	688128	661	5376
[1e-5,1e-4]	42384	5505024	1428	21504
[1e-6,1e-5]	265421	44040192	2240	43008

Table 3. Errors obtained when the chemical scheme of UNI-DEM was solved by sequential splitting and the combination of sequential splitting and Richardson extrapolation. The sub-problems were solved by the backward Euler method. *N* denotes the number of time-steps that were taken during the time integration. The numbers in parentheses give the ratio of the given error and the error obtained by using the previous time-step size.

N	Sequential splitting	Sequential splitting + 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)

Finally we illustrate that the Richardson extrapolation can be successfully applied in combination with operator splitting as well. The above chemical scheme was split into two parts: The first part contained mainly the chemical reactions in which ozone participates. The second part contained all the other chemical reactions. The backward Euler method was run in combination with (a) only the sequential

splitting procedure and (b) both the sequential splitting procedure and Richardson Extrapolation. Results are given in Table 3. It is clearly seen that the application of Richardson Extrapolation together with the backward Euler method and the sequential splitting procedure results in a second-order numerical method and, thus, in significantly more accurate results. For more details see Zlatev et al., 2012.

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