CHALLENGES IN USING SPLITTING TECHNIQUES FOR LARGE-SCALE ENVIRONMENTAL MODELLING

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The splitting idea

$$\left.\begin{aligned} \frac{du(t)}{dt} &= Au(t), \quad t \in (0,T] \\ u(0) &= u_0, \end{aligned}\right\}$$

and assume that $A = A_1 + A_2$. Let us divide the time interval $[0,T]$ into n subintervals of length $\tau = T/n$.

$$\left.\begin{aligned} \frac{du_k^{(1)}(t)}{dt} &= A_1 u_k^{(1)}(t), \quad t \in ((k-1)\tau, k\tau] \\ u_k^{(1)}((k-1)\tau) &= u_{k-1}^{(2)}((k-1)\tau) \end{aligned}\right\}$$

$$\left.\begin{aligned} \frac{du_k^{(2)}(t)}{dt} &= A_2 u_k^{(2)}(t), \quad t \in ((k-1)\tau, k\tau] \\ u_k^{(2)}((k-1)\tau) &= u_k^{(1)}(k\tau) \end{aligned}\right\}$$

for $k = 1, 2, \ldots, n$, where $u_0^{(2)}(0) = u_0$.

A brief historical overview

- **1957** - A simple splitting procedure for partial differential equations was proposed by Bagrinovskii and Godunov
  - *Difference schemes for multidimensional problems*. Dokl. Akad. Nauk USSR, 115: 431-433.

- Different splitting procedures have been developed and/or studied
  - **1962** - Dyakonov, E. G., *Difference schemes with splitting operators for multidimensional stationary problems*. Journal of Computational Mathematics and Mathematical Physics, 2(4): 57-79 (in Russian).
  - **1962** - Yanenko, N. N., *On convergence of the splitting method for heat equation with variable coefficients*. Journal of Computational Mathematics and Mathematical Physics, 2(5): 933-937 (in Russian).
  - **1968** - Marchuk, G. I., *Some application of splitting-up methods to the solution of mathematical physics problems*. Applik. Mat., 13(2).

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- **1982** - McRae, G. J., Goodin, W. R. and Seinfeld, J. H., *Numerical solution of the atmospheric diffusion equations for chemically reacting flows*. Journal of Computational Physics, 45: 1-42.
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- **1999** - Lanser, D. and Verwer, J. G., *Analysis of operators splitting in advection-diffusion-reaction problems in air pollution modelling*. Journal of Computational and Applied Mathematics, 111: 201-216.

- **2003** - Csomos, P., Faragó, I. and Havasi, Á., *Weighted sequential splitting and their analysis.* Comput. Math. Appl. (to appear).

- A detailed theoretical study and analysis of some splitting procedures can be found in

  - **1980** - Marchuk, G. I., *Methods of computational mathematics.* Nauka, Moscow, 1980.
  - **1982** - McRae, G. J., Goodin, W. R. and Seinfeld, J. H., *Numerical solution of the atmospheric diffusion equations for chemically reacting flows.* Journal of Computational Physics, 45: 1-42.
  - **1988** - Marchuk, G. I., *Methods of Splitting.* Nauka, Moscow, (in Russian).
  - **1999** - Dimov, I., Faragó, I. and Zlatev, Z., *Commutativity of the operators in splitting methods for air pollution models.* Report 04/99, Central Laboratory for Parallel Processing, Bulgarian Academy of Sciences, Acad. G. Bonchev, Bl. 25A, 1113 Sofia, Bulgaria.
  - **2001** - Dimov, I., Faragó, I., Havasi, Á. and Zlatev, Z., *Commutativity of the operators in splitting methods for air pollution models.* Annalles Univ. Sci. Budapest., 44: 129-150.
  - **2002** - Faragó, I. and Havasi, Á., *The mathematical background of operator splitting and the effect of non-commutativity.* In: Large Scale Scientific Computations III (Margenov, S., Yalamov P. and Wasniewski, J. eds.), pp. 264-271. Springer, Berlin.

– **2002** - Faragó, I., Havasi Á. and Korotov, S., *Mathematical analysis of the weighted splitting*. Technical Report, University of Jyväskylä.
– **2003** - Faragó, I. and Havasi Á., *On the accuracy of the Strang and weighted Strang splitting methods*. submitted to Comp. Appl. Math.
– **2003** - Faragó, I. and Havasi, Á., *On the convergence and local splitting error of different splitting schemes*. Internal report, Eötvös Loránd University.
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General description of splitting procedures

$$\frac{\partial \mathbf{c}(\mathbf{x},t)}{\partial t} = A(\mathbf{c}(\mathbf{x},t)),$$

where $t \in [0,T]$, $\mathbf{x} \in D$ and A is a differential operator.

We shall assume that operator $A(\mathbf{c})$ can be represented as a sum of m operators, which are in some sense "$simpler$" than the original operator $A(\mathbf{c})$:

$$A(\mathbf{c}) = \sum_{i=1}^{m} A^{[i]}(\mathbf{c}).$$

It should be noted here that the division of the operator $A(\mathbf{c})$ to a sum of "$simpler$" operators is in general not unique.

This means that the original problem can be split into the following m sub-problems:

$$\frac{\partial \mathbf{c}^{[i]}(\mathbf{x},t)}{\partial t} = A^{[i]}(\mathbf{c}^{[i]}), \quad i = 1, 2, \ldots, m.$$

Moreover, the time-interval $[0, T]$ is divided to $n = T/\tau$ *"small"* sub-intervals, where τ is called the splitting time-stepsize.

The particular splitting procedure depends

- on the way in which the operator $A(\mathbf{c})$ is represented as a sum of *simpler* operators and

- on the ordering in which the *smaller* problems are treated.

Assume that the representation of the original operator $A(\mathbf{c})$ as a sum of *simpler* operators $A^{[i]}(\mathbf{c})$ is fixed. Then four types of splitting procedures can be constructed by ordering the *simpler* operators from in different way:

- sequential splitting procedures,
- symmetric splitting procedures,
- weighted sequential splitting procedures,
- weighted symmetric splitting procedures.

DEM - the Danish Eulerian Model

$$
\begin{aligned}
\frac{\partial \mathbf{c}(\mathbf{x},t)}{\partial t} \quad = \quad & -\frac{\partial(u\mathbf{c})}{\partial x} - \frac{\partial(v\mathbf{c})}{\partial y} - \frac{\partial(w\mathbf{c})}{\partial z} \\
& + \frac{\partial}{\partial x}\left(K_x \frac{\partial \mathbf{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial \mathbf{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial \mathbf{c}}{\partial z}\right) \\
& + E + Q(\mathbf{c}) \\
& - \mathbf{c}\ \kappa^T,
\end{aligned}
$$

where $\mathbf{x} = (x, y, z)$, $\mathbf{c} = (c_1, c_2, \ldots, c_{N_s})^T$, $E = (E_1, E_2, \ldots, E_{N_s})^T$, $Q = (Q_1, Q_2, \ldots, Q_{N_s})^T$ and $\kappa = (\kappa_{11} + \kappa_{21}, \kappa_{12} + \kappa_{22}, \ldots, \kappa_{1N_s} + \kappa_{2N_s})^T$

Sequential splitting procedures

The traditional DEM splitting

$$\frac{\partial \mathbf{c}^{[1]}(\mathbf{x},t)}{\partial t} = -\frac{\partial(u\mathbf{c}^{[1]})}{\partial x} - \frac{\partial(v\mathbf{c}^{[1]})}{\partial y} \tag{1}$$

$$\frac{\partial \mathbf{c}^{[2]}(\mathbf{x},t)}{\partial t} = \frac{\partial}{\partial x}\left(K_x \frac{\partial \mathbf{c}^{[2]}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial \mathbf{c}^{[2]}}{\partial y}\right) \tag{2}$$

$$\frac{\partial \mathbf{c}^{[3]}(\mathbf{x},t)}{\partial t} = E + Q(\mathbf{c}^{[3]}) \tag{3}$$

$$\frac{\partial \mathbf{c}^{[4]}(\mathbf{x},t)}{\partial t} = -\mathbf{c}^{[4]}\ \kappa^T \tag{4}$$

$$\frac{\partial \mathbf{c}^{[5]}(\mathbf{x},t)}{\partial t} = -\frac{\partial (w\mathbf{c}^{[5]})}{\partial z} + \frac{\partial}{\partial z}\left(K_z \frac{\partial \mathbf{c}^{[5]}}{\partial z}\right). \tag{5}$$

- the solution $\mathbf{c}^{[i]}$ at $t = t_{n+1}$ is used as initial value when solving (i) at time-step $n+1$ (i.e. when $\mathbf{c}^{[i+1]}$ is computed at $t = t_{n+1}$), i= 1,. . . ,4.

The solution $\mathbf{c}^{[5]}$ of the last sub-model at $t = t_{n+1} = t_n + \tau$ is accepted as an approximation of the solution $\mathbf{c}$ of the original system at time-step $n+1$. This means that the splitting time-step $n+1$ is completed and everything is ready to carry out the same kind of computations at splitting time-step $n+2$.

The new DEM splitting

$$
\begin{aligned}
\frac{\partial \mathbf{c}^{[1]}(\mathbf{x},t)}{\partial t} &= -\frac{\partial (w\mathbf{c}^{[1]})}{\partial z} + \frac{\partial}{\partial z}\left(K_z \frac{\partial \mathbf{c}^{[1]}}{\partial z}\right) \\
\frac{\partial \mathbf{c}^{[2]}(\mathbf{x},t)}{\partial t} &= -\frac{\partial (u\mathbf{c}^{[2]})}{\partial x} - \frac{\partial (v\mathbf{c}^{[2]})}{\partial y} \\
&\quad + \frac{\partial}{\partial x}\left(K_x \frac{\partial \mathbf{c}^{[2]}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial \mathbf{c}^{[2]}}{\partial y}\right) \\
\frac{\partial \mathbf{c}^{[3]}(\mathbf{x},t)}{\partial t} &= E + Q(\mathbf{c}^{[3]}) - \mathbf{c}^{[3]}\ \kappa^T.
\end{aligned}
$$

PhP sequential splitting procedure

$$\begin{aligned}
\frac{\partial \mathbf{c}^{[1]}(\mathbf{x},t)}{\partial t} &= -\frac{\partial (u\mathbf{c}^{[1]})}{\partial x} - \frac{\partial (v\mathbf{c}^{[1]})}{\partial y} - \frac{\partial (w\mathbf{c}^{[1]})}{\partial z} \\
\frac{\partial \mathbf{c}^{[2]}(\mathbf{x},t)}{\partial t} &= \frac{\partial}{\partial x}\left(K_x \frac{\partial \mathbf{c}^{[2]}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial \mathbf{c}^{[2]}}{\partial y}\right) + \frac{\partial}{\partial y}\left(K_z \frac{\partial \mathbf{c}^{[2]}}{\partial z}\right) \\
\frac{\partial \mathbf{c}^{[3]}(\mathbf{x},t)}{\partial t} &= -\mathbf{c}^{[3]}\ \kappa^T \\
\frac{\partial \mathbf{c}^{[3]}(\mathbf{x},t)}{\partial t} &= E \\
\frac{\partial \mathbf{c}^{[5]}(\mathbf{x},t)}{\partial t} &= Q(\mathbf{c}^{[5]})
\end{aligned}$$

Symmetric splitting procedures

$$(A^{[1]})_{\tau/2}(A^{[2]})_{\tau/2}\ldots(A^{[m-1]})_{\tau/2}(A^{[m]})_{\tau}(A^{[m-1]})_{\tau/2}\ldots(A^{[2]})_{\tau/2}(A^{[1]})_{\tau/2}.$$

Weighted sequential splitting procedures

$$(A^{[1]})_\tau (A^{[2]})_\tau \dots (A^{[m-1]})_\tau (A^{[m]})_\tau$$

and

$$(A^{[m]})_\tau (A^{[m-1]})_\tau \dots (A^{[2]})_\tau (A^{[1]})_\tau.$$

Denote by $\mathbf{c}_{forward}$ and $\mathbf{c}_{backward}$ the results obtained when the first and the second sequence of operators are applied at a given splitting time-step. Then an approximation:

$$\mathbf{c} = \theta \; \mathbf{c}_{forward} + (1-\theta) \; \mathbf{c}_{backward}, \quad 0 < \theta < 1$$

is used.

Weighted symmetric splitting procedures

$$(A^{[1]})_{\tau/2}(A^{[2]})_{\tau/2}\ldots(A^{[m-1]})_{\tau/2}(A^{[m]})_{\tau}(A^{[m-1]})_{\tau/2}\ldots(A^{[2]})_{\tau/2}(A^{[1]})_{\tau/2}.$$

and

$$(A^{[m]})_{\tau/2}(A^{[m-1]})_{\tau/2}\ldots(A^{[2]})_{\tau/2}(A^{[1]})_{\tau}(A^{[2]})_{\tau/2}\ldots(A^{[m-1]})_{\tau/2}(A^{[m]})_{\tau/2}.$$

$$\mathbf{c} = \theta\ \mathbf{c}_{forward} + (1-\theta)\ \mathbf{c}_{backward}, \quad 0 < \theta < 1$$

Advantages and disadvantages of the splitting procedures

- It is in general much easier to find optimal (or, at least, good) numerical methods for the $simpler$ systems than for the big system arising after the direct discretization of operator $A(\mathbf{c}(\mathbf{x}, t))$.

- It is easy to change numerical algorithms and physical mechanisms used in the different sub-problems arising as a results of the implementation of the splitting procedure chosen. Thus, improvements of the code can easily be achieved.

- The application of splitting procedure facilitates the preparation of efficient codes for different parallel computers. In many cases, the splitting procedure is leading directly to parallel tasks.

Comparison of different splitting procedures

An attempt to give some recommendations about the choice of a suitable splitting procedure according to two important criteria:

- the computational cost

and

- the accuracy of the results

Comparing the computational cost

- The sequential splitting procedures have the cheapest computational cost (among the four types of splitting procedures) when the number of simple operators m is fixed.

- If a symmetric splitting procedure is to be selected, then it is best to put the most expensive operator in the middle. In this way the total computational cost of the symmetric splitting procedure is reduced, but this cost will always be higher than the cost of the corresponding sequential procedure.

- The computational cost of a weighted sequential splitting procedure is higher, by a factor approximately equal to two, than that of the corresponding sequential procedure.

- Similar conclusions (as those for the relationship between weighted sequential splitting procedures and sequential splitting procedures) are valid for the relationship between weighted symmetric splitting procedures and symmetric splitting procedures.

Comparing the accuracy properties

- All sequential splitting procedures are of first order, i.e. of order $O(\tau)$. This means that the errors due to these splitting procedures are proportional to the splitting time-stepsize τ.

- Some symmetric splitting procedures are of second order, i.e. $O(\tau^2)$. This means that if the splitting time-stepsize τ is sufficiently small and if the error due to the use of the splitting procedure chosen is dominant, then one should expect the errors caused by the splitting procedure to be reduced by a factor of four when the splitting time-stepsize is reduced from τ to $\tau/2$.

- Weighted sequential and symmetric splitting procedure of order higher than two can be constructed.

Structure of the splitting error

Theorem *Consider the PhP splitting. Assume that*

$$\left.\begin{array}{c} \dfrac{\partial u}{\partial x} + \dfrac{\partial v}{\partial y} + \dfrac{\partial w}{\partial z} = 0 \\ \dfrac{\partial K_x}{\partial x} + \dfrac{\partial K_y}{\partial y} + \dfrac{\partial K_z}{\partial z} = 0 \\ \dfrac{\partial \kappa}{\partial x} + \dfrac{\partial \kappa}{\partial y} + \dfrac{\partial \kappa}{\partial z} = 0 \\ \dfrac{\partial E}{\partial x} + \dfrac{\partial E}{\partial y} + \dfrac{\partial E}{\partial z} = 0 \end{array}\right\}$$

Under these assumptions the operators in any pair formed from the first four operators L-commute except the operators in the pair $(A^{[3]}, A^{[4]})$*. If, moreover, the fifth operator* $A^{[5]}$ *is independent of the spatial variables, then it L-commutes with the first three operators.*

Numerical experiments

Three important cases were studied by this experiments:

- The behaviour of the results in the case where only splitting errors appear in the computations.

- The behaviour of the results in the case where the splitting errors are appearing together with errors due to the spatial discretization and the errors due to the time integration.

- The behaviour of the results in the case where there are no splitting errors (i.e. all pairs of the involved operators are L-commuting).

Only splitting errors appear in the computations

Table 1: The values of $ERRMAX$ obtained when the problem is solved without splitting and with splitting (the number of time-steps is 1500 for all grids, but the values of $ERRMAX$ are rather insensitive to variations of the number of the time-steps when no splitting is used). The values of $ERRMAX$ are close to the machine precision when no splitting is used. The values of $ERRMAX$ are of order $O(10^{-4})$ for all grids when the splitting procedure is applied.

Grid	Without splitting	With splitting
8×8	3.34E-14	1.70E-4
16×16	3.79E-14	1.80E-4
32×32	3.99E-14	1.80E-4
96×96	7.21E-14	1.97E-4
288×288	4.57E-14	1.99E-4
480×480	4.28E-14	1.99E-4

Only splitting errors appear in the computations

Table 2: The values of $ERRMAX$ obtained when the problem is solved by using different numbers of time-steps without splitting and with splitting. The 16×16 grid is used in the discretization of the spatial derivatives. The experiment shows that the values of $ERRMAX$ does not depend on the number of time-steps when no splitting is used, while in the case where splitting is applied, the values of $ERRMAX$ are reduced when the number of steps is increased, because as stated in the text $\triangle t = \tau$.

Steps	Stepsize	Without splitting	With splitting
10	0.1	4.35E-14	2.42E-2
100	0.01	4.36E-15	2.39E-3
1000	0.001	5.76E-14	2.39E-4
10000	0.0001	7.24E-13	2.39E-5

Splitting errors versus other numerical errors

Table 3: Values of $ERRMAX$ obtained when the problem is solved with the splitting procedure by using different numbers of time-steps and different spatial grids ($\tau = \Delta t$).

Time-step Δt	16x16x16	32x32x32	64x64x64	128x128x128
8.0E-3	1.58E-2	1.92E-2	unstable	unstable
4.0E-3	7.99E-3	9.03E-3	unstable	unstable
2.0E-3	4.03E-3	4.55E-3	5.07E-3	unstable
1.0E-3	2.22E-3	2.33E-3	2.53E-3	unstable
5.0E-4	1.32E-3	1.22E-3	1.28E-3	1.35E-3
2.5E-4	1.00E-3	6.73E-4	6.58E-4	6.74E-4
1.25E-4	1.02E-3	4.02E-4	3.47E-4	3.43E-4
6.25E-5	1.03E-3	2.96E-4	1.91E-4	1.77E-4
3.125E-5	1.03E-3	2.95E-4	1.14E-4	9.32E-5
1.5625E-5	1.03E-3	2.94E-4	8.11E-5	5.15E-5
7.8125E-6	1.03E-3	2.94E-4	8.09E-5	3.07E-5
3.90625E-6	1.03E-3	2.94E-4	8.08E-5	2.15E-5

Vanishing splitting errors

Table 4: The values of $ERRMAX$ obtained when the problem is solved without splitting and with splitting (the values for the same grid are equal when rounded to three digits). The same time-stepsize $\triangle t = \tau = 1.5625 \times 10^{-5}$ has been used in the runs on different grids.

Grid	Without splitting	With splitting
16×16	1.47E-3	1.47E-3
32×32	3.97E-4	3.97E-4
96×96	4.67E-5	4.67E-5
288×288	5.35E-6	5.35E-6
480×480	1.94E-6	1.94E-6

Table 5: The values of $ERRMAX$ obtained when the problem is solved by using different time-steps Δt without splitting and with splitting. The 16×16 grid is used in the discretization of the spatial derivatives. The experiment shows that the values of $ERRMAX$ does not depend on the length of time-steps. As in the previous table, these values remain the same both when no splitting is used and when splitting is applied.

$\Delta t = \tau$	Without splitting	With splitting
$3.33E-3$	1.47E-3	1.47E-3
$6.67E-3$	1.47E-3	1.47E-3
$6.67E-4$	1.47E-3	1.47E-3

Results: SO2 concentrations in air for 1998 ($96 \times 96 \times 1$ grid) compared to the measurements of 35 stations in Europe									
Month	Concentration [mol/l]				||Discrepancy %||			Correlation		
	Obs.	**Sq.**	**W.**	**M-S**	**Sq.**	**W.**	**M-S**	**Sq.**	**W.**	**M-S**
Jan.	1.36	2.70	2.72	2.49	50	50	46	0.83	0.83	0.83
Feb.	1.41	2.02	2.04	1.91	30	31	26	0.61	0.61	0.69
March	1.11	1.49	1.51	1.41	26	26	22	0.64	0.64	0.64
April	0.80	1.06	1.07	1.01	25	25	21	0.60	0.60	0.64
May	0.73	1.13	1.14	1.12	35	36	35	0.71	0.71	0.72
June	0.51	0.72	0.72	0.72	29	30	30	0.72	0.72	0.70
July	0.49	0.63	0.64	0.62	22	23	20	0.82	0.83	0.83
Aug.	0.56	0.73	0.74	0.75	23	24	25	0.63	0.63	0.71
Sept.	0.60	0.85	0.88	0.86	29	29	30	0.82	0.82	0.81
Oct.	0.58	0.68	0.69	0.67	16	17	15	0.75	0.75	0.81
Nov.	1.32	1.59	1.60	1.58	17	18	17	0.29	0.28	0.45
Dec.	1.41	2.89	2.91	2.64	51	52	47	0.39	0.39	0.52
mean	0.91	1.38	1.39	1.32	34	34	31	0.71	0.71	0.77

Table 6: Sulfur dioxide in the air in 1998:
Obs. - observed by the measurement stations; **Sq.** - computed by DEM with sequential splitting; **W.** - computed by DEM with weighted sequential splitting; **M-S** - computed by DEM with Marchuk - Strang splitting.

Results: NH3+NH4 concentrations in air for 1998 ($96 \times 96 \times 1$ grid) compared to the measurements of 24 stations in Europe										
Month	Concentration [mol/l]				$\|\|$Discrepancy %$\|\|$			Correlation		
	Obs.	**Sq.**	**W.**	**M-S**	**Sq.**	**W.**	**M-S**	**Sq.**	**W.**	**M-S**
Jan.	1.02	1.27	1.37	1.04	20	26	2	0.78	0.78	0.80
Feb.	1.51	1.43	1.51	1.18	5	0	28	0.79	0.79	0.79
March	1.19	1.42	1.52	1.17	16	22	2	0.67	0.64	0.67
April	1.36	1.29	1.35	1.13	6	0	21	0.65	0.64	0.63
May	1.46	1.67	1.75	1.32	12	17	11	0.76	0.75	0.69
June	1.20	0.99	1.02	0.93	21	18	29	0.74	0.74	0.74
July	1.09	1.00	1.03	0.97	9	6	12	0.72	0.72	0.68
Aug.	1.01	1.67	1.18	1.05	13	15	4	0.83	0.83	0.82
Sept.	1.39	1.86	1.96	1.53	25	29	9	0.78	0.77	0.80
Oct.	0.73	0.89	0.93	0.76	18	21	4	0.65	0.64	0.67
Nov.	1.19	1.82	1.95	1.59	34	39	25	0.65	0.64	0.66
Dec.	1.13	1.70	1.83	1.46	33	38	22	0.76	0.73	0.77
mean	1.19	1.38	1.45	1.18	13	17	1	0.77	0.77	0.77

Table 7: Ammonia in the air in 1998:

Obs. - observed by the measurement stations; **Sq.** - computed by DEM with sequential splitting; **W.** - computed by DEM with weighted sequential splitting; **M-S** - computed by DEM with Marchuk - Strang splitting.

Observations:

- In most cases the results, obtained with the weighted sequential splitting, are quite similar to those of the sequential splitting. This could be an indication for a small commutator of the two operators.

- For some species (NO2, ammonia) the Marchuk-Strang scheme gives results, closer to the measurements than the other two splitting methods. More experiments are needed in order to investigate the consistency of such behaviour.

- Although the weighted and the Marchuk-Strang schemes are of higher order with respect to the splitting error, this cannot be clearly confirmed by the experimental results because of the influence of other sources of error as well as the uncertainty of the measurements.

One year experiment with 2-D UNI-DEM					
Splitting scheme	**Time [sec.] (*Speed-up*)**				
	1 pr.	2 proc.	4 proc.	8 proc.	16 proc.
Sequential	37893	18570 (*2.04*)	8406 (*4.51*)	4588 (*8.26*)	2362 (*16.0*)
Marchuck - Strang	45864	23116 (*1.98*)	11780 (*3.89*)	5684 (*8.07*)	2942 (*15.6*)
Weighted sequenial	68746	33465 (*2.05*)	16227 (*4.24*)	7700 (*8.93*)	4127 (*16.7*)

Table 8: Time in seconds and speed-up (in brackets) of the three splitting schemes for an one-year experiment with the 2-D version of UNI-DEM on a $(96 \times 96 \times 1)$ grid. The results are obtained on SUN SunFire 6800 machines in DTU, Lyngby, Denmark. The chemistry-deposition stage is perfectly parallelized as it is independently executed for each grid point. Moreover, it shows superlinear speed-up because of the cache utilization of the processors. The superlinear speed-up of the chemistry-deposition stage has stronger influence on the total speed-up in the sequential and weighted sequential schemes, where this stage takes more than 70% of the total time. In the Marchuk - Strang scheme it is put in the middle and is surrounded by 2 advection-diffusion stages with a half time-step, so its relative weight decreases as well as the total speed-up.

Conclusions and plans for future research

Even in very simple cases the splitting procedure will in general cause splitting errors. Therefore, it is worthwhile to carry out work in three important directions:

- to attempt to avoid the use of splitting procedures when this is possible

- to study the structure of the splitting error

and

- to find reliable and robust methods for evaluating the splitting errors,

All three problems are still open when general large-scale air pollution problems are to be handled. Success in the solution of any of these two problems is a very desirable, but also a very challenging task.