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Implementation of sparse matrix algorithms in an advection–diffusion–chemistry module

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ABSTRACT

A two-dimensional advection–diffusion–chemistry module of a large-scale environmental model is taken. The module is described mathematically by a system of partial differential equations. Sequential splitting is used in the numerical treatment. The non-linear chemistry is most time-consuming part and it is handled by six implicit algorithms for solving ordinary differential equations. This leads to the solution of very long sequences of systems of linear algebraic equations. It is crucial to solve these systems efficiently. This is achieved by applying four different algorithms. The numerical results indicate that the algorithms based on a preconditioned sparse matrix technique and on a specially designed algorithm for the particular problem under consideration perform best.

1. The problem solved

Long-range transport air pollution is usually studied by a system of partial differential equations (PDEs), which can be written as follows (it should be mentioned that similar systems are also used in other environmental models):

$$\begin{aligned}
\frac{\partial c_i}{\partial t} = & -u\frac{\partial c_i}{\partial x} - v\frac{\partial c_i}{\partial y} && \text{horizontal advection}\\
& + \frac{\partial}{\partial x}\left(K_x\frac{\partial c_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial c_i}{\partial y}\right) && \text{horizontal diffusion}\\
& + Q_i\left(t, x, y, z, c_1, c_2, \ldots, c_q\right) && \text{chemical reactions}\\
& + E_i\left(t, x, y, z\right) && \text{emissions}\\
& + \left(k_{1i} + k_{2i}\right) c_i && \text{dry and wet deposition}\\
& - w\frac{\partial c_i}{\partial z} + \frac{\partial}{\partial z}\left(K_z\frac{\partial c_i}{\partial z}\right) && \text{vertical exchange}\\
i = 1, 2, \ldots, q & && q\text{— number of chemical species}
\end{aligned} \tag{1}$$

where

- $c_i = c_i\left(t, x, y, z\right)$ is the concentration of the chemical species i at point (x, y, z) of the space domain and at time t of the time-interval,

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- $u = u(t, x, y, z)$, $v = v(t, x, y, z)$ and $w = w(t, x, y, z)$ are wind velocities along the Ox, Oy and Oz directions respectively at point (x, y, z) and time t,
- $K_x = K_x(t, x, y, z)$, $K_y = K_y(t, x, y, z)$ and $K_z = K_z(t, x, y, z)$ are diffusivity coefficients at point (x, y, z) and time t (it is often assumed that K_x and K_y are non-negative constants, while the calculation of K_z is normally rather complicated),
- $k_{1i} = k_{1i}(t, x, y, z)$ and $k_{2i} = k_{2i}(t, x, y, z)$ are deposition coefficients (dry and wet deposition respectively) of chemical species i at point (x, y, z) and time t of the time-interval (for some species these coefficients are non-negative constants and furthermore the wet deposition coefficients k_{2i} are equal to zero when it is not raining).

It is convenient to use the following two-dimensional module when different numerical methods are to be tested:

$$\frac{\partial c_i}{\partial t} = -\mu(y - y_1)\frac{\partial c_i}{\partial x} + -\mu(x_1 - x)\frac{\partial c_i}{\partial y} + K\left(\frac{\partial^2 c_i}{\partial x^2} + \frac{\partial^2 c_i}{\partial y^2}\right) + E_i(t, x, y) + Q_i\left(t, x, y, c_1, c_2, \ldots, c_q\right), \tag{2}$$

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

$$x \in [a_1, b_1], \qquad y \in [a_2, b_2], \qquad t \in [a, b], \qquad x_1 = \frac{b_1 - a_1}{2}, \qquad y_1 = \frac{b_2 - a_2}{2}, \qquad \mu = \frac{2\pi}{b - a}. \tag{3}$$

In the computations the following values of the parameters involved in (2) will be used:

$$a_1 = a_2 = 0, \qquad b_1 = b_2 = 500 \text{ km}, \qquad a = 21\,600 \text{ s}, \qquad b = 108\,000 \text{ s}, \qquad q = 56, \tag{4}$$

which means that (i) the space domain is square, (ii) (x_1, y_1) is the centre of the space domain and (iii) the length of the time-interval is 86 400 s (24 h; the starting point being 6 o'clock in the morning and the end-point being 6 o'clock on the next day).

Problem (2) has to be considered together with a given initial value vector $c(x, y, a)$ and with some boundary conditions. It will be assumed that Dirichlet boundary conditions are used.

The problem defined by (2)–(4) can be considered as a special, and simplified, case of UNI-DEM (the Unified Danish Eulerian Model, [1,2]), which is often used to study air pollution levels in Europe. The most essential difference is the special definition of the wind velocity field. It is defined by the coefficients of the first-order spatial derivatives. The trajectories of the wind are concentric circles with centre (x_1, y_1) and particles are rotated along these trajectories with a constant angular velocity. Such values of the wind velocity field were first defined in [3,4].

In the air pollution processes, the advection (described mathematically by the terms containing first-order derivatives) is dominating over the diffusion (described by the terms containing second-order derivatives). Therefore, (2) was run by using a very small constant K.

The non-linear terms Q_i, $i = 1, 2, \ldots, q$, describe the chemical reactions (these are precisely the same as those in one of the chemical schemes used in UNI-DEM). Some of these reactions are photo-chemical. The photo-chemical reactions are deactivated during the night and activated during the day. Therefore, the length of the time-interval should be at least 24 h in order to study the performance during the changes from day-time to night-time and from night-time to day-time when some of the concentrations are very rapidly changing.

Problem (2) was run in two typical cases: (a) when all emissions E_i set equal to zero (puff) and (b) when there are some non-zero emissions (plume). In the latter case we have: (i) all non-zero emissions are specified in a circle with centre $(x_0, y_0) = (0.25(b_1 - a_1), 0.5(b_2 - a_2))$ and radius $r = 0.125(b_1 - a_1)$, the emissions outside this circle are equal to zero, (iii) the emissions form cone, the highest emissions being in the centre (x_0, y_0) of the circle.

As mentioned above, the test in which only the first two terms in the right-hand-side of (2) are kept (the pure advection test) was introduced in 1968 simultaneously by Crowley and Molenkampf ([3,4]). Chemical reactions were included to the Crowley–Molenkampf test by Hov et al. [5]. The module defined in this paper by (2) is a further extension of the original Crowley–Molenkampf test. It is worthwhile to study this module because it is much closer to the real environmental model than the previous two modules. By setting some of the coefficients to zero or keeping all of them different from zero, six situations can be studied by (2):

- *No non-zero emissions are specified (puff; $E_i = 0$ for all values of i)*:
  - (A) Pure advection–diffusion process (only the terms containing the spatial derivatives are kept).
  - (B) Pure chemical process (only the non-linear functions Q_i are kept).
  - (C) Combining the advection–diffusion process with the chemistry process (all terms except the emissions are kept).
- *Some emissions are not equal to zero (plume; $E_i \neq 0$ for some values of i)*:
  - (D) Pure advection–diffusion process (only the terms containing the spatial derivatives and the emissions are kept).
  - (E) Pure chemical process (only the non-linear functions Q_i and the emissions are kept).
  - (F) Combining the advection–diffusion process with the chemistry process (all terms are kept).