SPLITTING TECHNIQUES

Major questions related to the use of splitting techniques

1. Is it **worthwhile** to use splitting techniques?
2. Are there **drawbacks** when splitting techniques are used?

Major drawback: splitting errors

1. Could we **avoid** the splitting errors?
2. Could we **evaluate** the splitting errors?

Some kind of splitting is used in all large-scale environmental models I know

Air Pollution Models

$$\frac{\partial c_s}{\partial t} = -\frac{\partial (uc_s)}{\partial x} - \frac{\partial (vc_s)}{\partial y}$$ hor. transport

$$+\frac{\partial}{\partial x}\left(K_x \frac{\partial c_s}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial c_s}{\partial y}\right)$$ hor. diffusion

$$- \quad (k_{1s} + k_{2s})c_s$$ deposition

$$+ E_s + Q_s(c_1, c_2, \ldots, c_q)$$ chemistry

$$-\frac{\partial (wc_s)}{\partial z} + \frac{\partial}{\partial z}\left(K_z \frac{\partial c_s}{\partial z}\right)$$ vert. exchange

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

$$\frac{dg}{dt} = A_1(t)g + A_2 g + A_3(t)g + A_4(t, g) + A_5(t)g$$

Air Pollution Models-continuation

$$\frac{dg}{dt} = A_1(t)g + A_2 g + A_3(t)g + A_4(t,g) + A_5(t)g$$

$$f(t,y) = A_1(t)g + A_2 g + A_3(t)g + A_4(t,g) + A_5(t)g$$

$$g = y$$

$$\frac{dy}{dt} = f(t,y) \qquad \text{stiff system of ODEs}$$

$$y \in \Re^N, \quad N = (N_x \times N_y \times N_z) \times N_{species} \quad ; \quad N > 80 \text{ mill.}$$

Implications from the stiffness of the system of ODEs:

1. Implicit time-integration methods are to be used.
2. Huge systems of linear algebraic equations are to be treated (at many time-steps and at many iterations)

Air Pollution Models-continuation

Use of (Quasi) Newton Iterative process

$$\frac{dy}{dt} = f(t, y)$$

$$y_{n+1} = y_n + \Delta t \ f_{n+1}, \qquad y_n \approx y(t_n), \quad f_n = f(t_n, y_n)$$

$$F(y_{n+1}) = 0, \qquad F(y_{n+1}) = y_{n+1} - y_n - \Delta t \ f_{n+1}$$

$$J_{n+1} = \frac{\partial f(t, y)}{\partial y}, \qquad for \qquad t = t_{n+1}, \quad y = y_{n+1}$$

$$\frac{\partial F(y_{n+1})}{\partial y_{n+1}} = I - \Delta t \, J_{n+1}$$

Air Pollution Models-continuation

$$\left(I - \Delta t J_{n+1}^{[i-1]}\right)\Delta y_{n+1}^{[i]} = - y_{n+1}^{[i-1]} + y_n + \Delta t\, f\,(t_{n+1}, y_{n+1}^{[i-1]})$$

$$y_{n+1}^{[i]} = y_{n+1}^{[i-1]} + \Delta y_{n+1}^{[i]}$$

$$y_{n+1}^{[0]} = y_n \qquad or \qquad y_{n+1}^{[0]} = y_n + \frac{\Delta t_{n+1}}{\Delta t_n}\left(y_n - y_{n-1}\right)$$

At each iteration the following operations must be carried out:

1. Function evaluation

2. Jacobian evaluation

3. Form a system of linear algebraic equations

4. Solve the system of linear algebraic equations

5. Update the solution

Air Pollution Models-continuation

$$\left(I-\Delta t J_{n+1}^{[i-1]}\right)\Delta y_{n+1}^{[i]} = -y_{n+1}^{[i-1]} + y_n + \Delta t\, f(t_{n+1}, y_{n+1}^{[i-1]})$$

$$\frac{dy}{dt} = A_1(t)y + A_2 y + A_3(t)y + A_4(t,y) + A_5(t)y$$

$$\frac{dy^1}{dt} = A_1(t)y^1 \qquad \frac{dy^3}{dt} = A_3(t)y^3 \qquad \frac{dy^5}{dt} = A_5(t)y^5$$

$$\frac{dy^2}{dt} = A_2 y^2 \qquad \frac{dy^4}{dt} = A_4(t, y^4)$$

Advantages of the splitting procedures

- Easy to exploit the special properties of the involved operators
- Many small problems are to be solved instead of one very big problem
- Parallel computations can be introduced in a natural way

Need for splitting

- Bagrinowskii and Godunov 1957
- Strang 1968
- Marchuk 1968, 1982
- McRay, Goodin and Seinfeld 1982
- Lancer and Verwer 1999
- Dimov, Farago and Zlatev 1999

- Zlatev 1995

Criteria for choosing the splitting procedure

- **Accuracy**
- **Efficiency**
- **Preservation of the properties of the involved operators**

No splitting errors

$$A_1(c) = -\nabla(uc), \quad A_2(c) = \nabla(K\nabla c), \quad A_3(c) = \kappa\, c,$$
$$A_4(c) = E, \quad A_5(c) = Q(c)$$

If $\nabla u = 0, \quad \nabla K = 0, \quad \nabla \kappa = 0, \quad \nabla E = 0$

then any pair of the first four operators L-commutes except the third and the fourth.
If the fifth operator is independent of the spatial variables, then it L-commutes with the first three operators

The conditions of this theorem are unfortunately never satisfied in practice

Order of the splitting error

- **Sequential splitting: it can be proved that the order is one**
- **Symmetric splitting: second order can be achieved**

Marchuk (1968)

Strang (1968)

If the accuracy is the important issue, then symmetric splitting is to be chosen

If the cost of computations is the crucial factor, then sequential splitting might be chosen

Numerical example

Test 6 - The numerical methods are not causing errors (excepting rounding errors)

$$\frac{\partial c}{\partial t} = y\frac{\partial c}{\partial x} - x\frac{\partial c}{\partial y} + (1 + x - y)\frac{\partial c}{\partial z}$$

$$c(x, y, z, 0) = x + y + z$$

$$x \in [0,1], \quad y \in [0,1], \quad z \in [0,1], \quad t \in [0,1]$$

$$c(x, y, z, t) = x + y + z + t$$

$$\frac{\partial c^1}{\partial t} = y\frac{\partial c^1}{\partial x} - x\frac{\partial c^1}{\partial y}$$

$$\frac{\partial c^2}{\partial t} = (1 + x - y)\frac{\partial c^2}{\partial z}$$

Numerical example - results

Time-steps	Error	Decreasing factor
125	1.90E-3	-
250	9.50E-4	2.00
500	4.75E-4	2.00
1000	2.37E-4	2.00
2000	1.19E-4	1.99
4000	5.94E-5	2.00
8000	2.97E-5	2.00
16000	1.48E-5	2.01
32000	7.42E-6	1.99

Rotation test + chemistry

Hov et al. (1988)

$$\frac{\partial c_s}{\partial t} = (1-y)\frac{\partial c_s}{\partial x} + (x-1)\frac{\partial c_s}{\partial y} + Q_s(c_1, c_2, \ldots, c_q)$$

$$x \in [0,2], \quad y \in [0,2], \quad t \in [0,2\pi]$$

$$x_0 = 0.5, \quad y_0 = 1.0, \quad r = 0.25, \quad r^* = \sqrt{(x-x_0)^2 + (y-y_0)^2}$$

$$c_s(x,y,0) = c_{s0} + 99c_{s0}\left(1 - \frac{r^*}{r}\right) \quad for \quad r^* < r$$

$$c_s(x,y,0) = c_{s0} \qquad\qquad for \quad r^* \geq r$$