Computer treatment of the horizontal advection in air pollution models

1. *The horizontal advection problem*
2. *Spatial discretization*
3. *Predictor-corrector (PC) schemes*
4. *VSVFMs*
5. *Absolute stability*
6. *Choice of particular PC schemes*
7. *Unresolved problems*

1. Horizontal advection

$$\frac{\partial c}{\partial t} = -\frac{\partial (u c)}{\partial x} - \frac{\partial (v c)}{\partial y}$$

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

$$u = u(x, y, t), \qquad v = v(x, y, t)$$

c - concentration (unknown function)
u and v - wind velocities (known functions)

2. Numerical treatment

- **Parallel tasks (shared memory)**

  The calculations for a given compound

- **Numerical methods**

  Pseudo-spectral discretization (Zlatev, 1984)

  Finite elements (Pepper et al., 1979)

  Finite differences (up-wind)

  “Positive” methods (Bott, 1989; Holm, 1994)

  Semi-Lagrangian algorithms (Neta, 1995)

  Wavelets (not tried yet)

3. Pseudo-spectral (PS) method

$$f(x) \in \Re, \quad x \in [0, 2\pi], \quad f(x + 2\pi) = f(x)$$

$$X_N = \left\{ x_n / \; x_n = \frac{2n\pi}{2N+1}, \quad n = 0(1)2N \right\}$$

$$F_N = \{ f(x_0), f(x_1), \dots, f(x_{2N}) \}$$

$$G_N = \left\{ \frac{df(x_0)}{dx}, \frac{df(x_1)}{dx}, \dots, \frac{df(x_{2N})}{dx} \right\}$$

3a. PS method - continuation

$$T_N(x) = A + \sum_{k=1}^{N} \left[a_k \cos(kx) + b_k \sin(kx) \right]$$

Truncated Fourier series

$$A = \frac{1}{2N+1} \sum_{m=0}^{2N} f(x_m)$$

$$a_k = \frac{1}{2N+1} \sum_{m=0}^{2N} f(x_m) \cos(k x_m)$$

$$b_k = \frac{1}{2N+1} \sum_{m=0}^{2N} f(x_m) \sin(k x_m)$$

Fourier coefficients

Use the derivative of the interpolation polynomial to get approximations of the derivatives of function f

3b. PS method - convergence

If $f(x)$ is continuous and periodic and if $f'(x)$ is piece-wise continuous, then the Fourier series of $f(x)$ converges uniformly and absolutely to $f(x)$.

Davis (1963)

3c. PS method - accuracy

It can be proved (Davis, 1963) that

$$|a_k| \leq \frac{M}{k^{\mu+1}} \quad \text{and} \quad |b_k| \leq \frac{M}{k^{\mu+1}}, \quad M \text{ is a constant,}$$

if

$$f^{(\nu)}(0) = f^{(\nu)}(2\pi), \ \nu = 0, 1, \ldots, \mu$$

3d. PS method - drawbacks

Drawback	Removing	Reference
Equidistant grids	?	
Periodicity for convergence	Yes	Lyness, 1974
Periodicity for accuracy	Yes	Roache, 1971, 1978

4. Finite elements

The application of finite elements in the advection module leads to an ODE system:

$$P\frac{dg}{dt} = Hg$$

Choice of method

P is a constant matrix,
H depends on the wind

$$P^{-1}, \quad (P - \Delta t \beta H)^{-1}$$

5. Predictor-corrector schemes

$$\frac{dg}{dt} = f, \qquad f, g \in \Re^N, \qquad f = P^{-1}Hg$$

$$g_k^{[0]} = \sum_{i=1}^{\mu_j^{[0]}} \alpha_{ji}^{[0]} g_{k-i} + \Delta t \sum_{i=1}^{\nu_j^{[0]}} \beta_{ji}^{[0]} f_{k-i}$$

$$g_k^{[r]} = \sum_{i=1}^{\mu_j^{[r]}} \alpha_{ji}^{[r]} g_{k-i} + \Delta t \beta_{j0}^{[r]} f_k^{[r-1]}$$

$$+ \Delta t \sum_{i=1}^{\nu_j^{[r]}} \beta_{ji}^{[r]} f_{k-i}, \qquad r = 1, 2, \ldots, q_j$$

$$F = \{F_1, F_2, \ldots, F_j \ldots, F_m\}$$

6. Variation of the stepsize

$$G_K^* = \{t_k \mid t_0 = a, \Delta t_k = t_k - t_{k-1} > 0, k = 1(1)K, t_K = b\}$$

$$\Delta t_{kj}^* = \left\{ \frac{\Delta t_{k-1}}{\Delta t_k}, \frac{\Delta t_{k-2}}{\Delta t_k}, \ldots, \frac{\Delta t_{k-s_j+1}}{\Delta t_k} \right\}$$

$$s_j = \max(\mu_j^{[0]}, \nu_j^{[0]}, \mu_j^{[1]}, \nu_j^{[1]}, \ldots, \mu_j^{q_j}, \nu_j^{q_j})$$

Δt_{kj}^* *is associated with* F_j

7. VSVFMs

$$g_k^{[0]} = \sum_{i=1}^{\mu_j^{[0]}} \alpha_{ji}^{[0]}(\Delta t_{kj}^{*}) g_{k-i} + \sum_{i=1}^{\nu_j^{[0]}} \Delta t_{k-i} \beta_{ji}^{[0]}(\Delta t_{kj}^{*}) f_{k-i}$$

$$g_k^{[r]} = \sum_{i=1}^{\mu_j^{[r]}} \alpha_{ji}^{[r]}(\Delta t_{kj}^{*}) g_{k-i} + \Delta t_k \beta_{j0}^{[r]}(\Delta t_{kj}^{*}) f_k^{[r-1]}$$

$$+ \sum_{i=1}^{\nu_j^{[r]}} \Delta t_{k-i} \beta_{ji}^{[r]}(\Delta t_{kj}^{*}) f_{k-i}$$

Constant stepsizes

Advantages and disadvantages

8. Convergence - 1

$$\Delta t = \max_{1<k<K} (\Delta t_k), \quad \Delta t K \le \tau < \infty \quad for \quad \forall K$$

$$K \to \infty \quad \Rightarrow \quad \forall \Delta t_k \to 0$$

$$0 < \overline{\alpha} \le \frac{\Delta t_k}{\Delta t_{k-1}} \le \overline{\beta} \le \infty \quad for \quad \forall k$$

$$\alpha_{j1}^{[r]}(\Delta_{kj}^{*}) = \alpha_{j1}^{[r]} = \alpha_{j}^{[r]}, \quad \alpha_{j2}^{[r]}(\Delta_{kj}^{*}) = \alpha_{j2}^{[r]} = 1 - \alpha_{j}^{[r]},$$

$$\alpha_{js}^{[r]}(\Delta_{kj}^{*}) = \alpha_{js}^{[r]} = 0, \quad s = 3(1)\mu_j, \quad r = 0(1)q_j, \quad \forall k, \quad \forall j.$$

$$s_j \le k \quad for \quad \forall k$$

selfstarting VSVFM

8a. Convergence - 2

Theorem 1

If a selfstarting VSVFM that is based on two-ordinate PC schemes corresponding to two-ordinate basic PC schemes is applied on a grid which determines a stable stepsize selection strategy, then the VSVFM is consistent, zero-stable and convergent when

$$0 \le \alpha_j^{[q_j]} < 2 \quad for \quad \forall j$$

9. Absolute stability

Theorem 2

The length h_{imag} of the absolute stability interval on the positive part of the imaginary axis cannot exceed $q_j + 1$ when a basic PC scheme with q_j correctors is used

10. Restrictions on the stepsize

$$\frac{dg}{dt} = P^{-1} Hg$$

Assumptions: 1. $P^{-1}H = Q \Lambda Q^{T}$

2. $\lambda_{ii} \quad imaginary \quad for \quad \forall i$

3. $\lambda = \max(|\lambda_{ìi}|)$

Then: $\lambda \Delta t \leq h_{imag}$

11. Preserving the stability

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x}, \qquad u \quad \text{being a constant}$$

$$\lambda \approx \frac{1.73u}{\Delta x} \quad \Rightarrow \quad \frac{\lambda_1 u \Delta t}{\Delta x} < h_{imag} \qquad (\lambda_1 \approx 1.73)$$

General <u>1-D</u> case:

$$\Delta t < \alpha \frac{h_{imag}}{\lambda_1 U} \Delta x$$

General <u>2-D</u> case:

$$\Delta t < \alpha \frac{h_{imag}}{\lambda_1 (U + V)} \Delta x$$

12. Choice of good PC schemes

$PC-scheme$	$Number\ of\ formulae$	h_{imag}
F_1	4	3.26
F_2	3	2.51
F_3	2	1.62

Avoiding reductions of the time-stepsize

Stability control

$$\Delta t < \alpha \frac{h_{imag}}{\lambda_1 (U+V)} \Delta x$$

13. PLANS FOR FUTURE WORK

- Accuracy control
- Moving to fully VSVFM mode
- Object-oriented code
- Using 3-D refined resolution codes
- Selection of higher order methods
- Better coupling of the advection process with the other physical processes
- Evaluation the splitting errors