Models and Numerical Methods for Environmental Problems. Part I: A Multilayer Convection-Diffusion Model

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Abstract

In this lecture first we review the general theory of splitting algoritmhs and thus we apply this concept to the construction of a multilayer convection-diffusion model and its numerical approximation based on a combination of the Adaptive Finite Element Method with characteristics in the horizontal directions and Finite Differences in the vertical direction.

1 General splitting algoritms of evolution equations

For a complete study of these methods see [1]. For a brief introduction see [2]. Let consider equations of evolution of the following general form

$$M\frac{du}{dt} + A(u) = f \tag{1.1}$$

$$u(0) = u_0 \tag{1.2}$$

where u is a $d-$dimensional vector, M is a positive definite symmetric matrix and A is a function (non necessary linear) from R^d into R^d. In the following we endow R^d with the following energy inner product (Mu, v) for every $u, v \in R^d$, with its associated norm $||u|| = (Mu, u)^{1/2}$.

An unconditionally stable algorithm for equation (1.1)-(1.2) is given by a family of functions $F(\tau) : R^d \to R^d, \quad \tau > 0$, satisfying

1. consistency:

$$\lim_{\tau\to 0} M\frac{F(\tau)u-u}{\tau} = -Au \quad \text{for every} \quad u \in R^d\,. \tag{1.3}$$

We will consider in the following methods of at least order one, that is, verifying

$$F(\tau)u = u + \tau M^{-1}(-A(u)+f) + O(\tau^2) \tag{1.4}$$

2. unconditional stability:

$$||F(\tau)u - F(\tau)v|| \le ||u-v|| \quad \text{for every} \quad u,v \in R^d, \quad \tau > 0\,. \tag{1.5}$$

When the mapping $F(\tau)$ is linear, the stability condition (1.5) reduces to

$$||F(\tau)u|| \le ||u|| \quad \text{for every} \quad u \in R^d\,. \tag{1.6}$$

Examples

1. The Euler implicit algorithm is

$$M\frac{u^{n+1}-u^n}{\tau} + Au^{n+1} = f^{n+1} \tag{1.7}$$

$$u^0 = u_0\,; \tag{1.8}$$

in that case

$$F(\tau)u = (M+\tau A)^{-1}u \tag{1.9}$$

and the solution at time step $n+1$ is given as a function of u^n by

$$u^{n+1} = (M+\tau A)^{-1}u^n + \tau(M+\tau A)^{-1}f^{n+1}\,. \tag{1.10}$$

The Euler method is consistent of order one as it is easy to verify.

2. The Crank-Nicolson scheme is

$$M\frac{u^{n+1}-u^n}{\tau} + \frac{1}{2}(Au^{n+1}+Au^n) = \frac{1}{2}(f^{n+1}+f^n) \tag{1.11}$$

$$u^0 = u_0\,; \tag{1.12}$$

we have

$$F(\tau)u = (M+\frac{1}{2}\tau A)^{-1}(M-\frac{1}{2}\tau A)u \tag{1.13}$$

which is a second order algorithm.

In a variety of environmental problems and continuous mechanics the operator A and the source term f admit an additive decomposition

$$A = \Sigma_i^N A_i, \qquad f = \Sigma_{i=1}^N f_i \,. \tag{1.14}$$

We are concerned with algorithms that exploit the additive form of A and f. Let $F_i, i = 1, ..., N$ denote stable algorithms consistent with M and A_i. The corresponding splitting algorithm then takes the form

$$F(\tau) = F_N(\tau)F_{N-1}(\tau)...F_1(\tau) = \Pi_{i=1}^N F_i(\tau)\,. \tag{1.15}$$

In other words, the algorithm $F(\tau)$ amounts to applying the individual algorithms $F_i(\tau)$ consecutively to the solution vector, taking the result from each one as the initial conditions for the next algorithm. We have,

Proposition

The algorithm (1.15) is consistent with M and A and is unconditionally stable if the individual algorithms are.

Proof: The consistency of the individuals operators $F_i(\tau)$ implies

$$F_i(\tau)u = u + \tau M^{-1}(-A_i(u) + f_i) + O(\tau^2), \qquad i = 1, ..., N.$$

Taken the product of $F_1(\tau)$ and $F_2(\tau)$ and retaining terms up to second order we obtain

$$\begin{aligned} F_2(\tau)F_1(\tau)u &= F_2(\tau)(F_1(\tau)u) \\ &= F_1(\tau)u - \tau M^{-1}A_2(F_1(\tau)u) + \tau M^{-1}f_2 + O(\tau^2) \\ &= u - \tau M^{-1}(A_1 + A_2)(u) + \tau M^{-1}(f_1 + f_2) + O(\tau^2)\,. \end{aligned}$$

Proceeding by induction it is readily shown that

$$\begin{aligned} F(\tau)u &= (\Pi_{i=1}^N F_i(\tau))u = u - \tau M^{-1}(\Sigma_{i=1}^N A_i)u + \tau M^{-1}(\Sigma_{i=1}^N f_i) + O(\tau^2) \\ &= u - \tau M^{-1}A(u) + \tau M^{-1}f + O(\tau^2)\,. \end{aligned}$$

■

Proposition: The algorithm (1.15) is unconditionally stable if all the individual algorithms are.

Proof: It follows from the definition of unconditional stability (1.6) that for every $u, v \in R^d$ and $\tau > 0$

$$\begin{aligned} ||F(\tau)u - F(\tau)v|| &= ||(\Pi_{i=1}^N F_i(\tau))u - (\Pi_{i=1}^N F_i(\tau))v|| \\ &= ||F_N(\tau)(\Pi_{i=1}^{N-1} F_i(\tau))u - F_N(\tau)(\Pi_{i=1}^{N-1} F_i(\tau))v|| \\ &\leq ||(\Pi_{i=1}^{N-1} F_i(\tau))u - (\Pi_{i=1}^{N-1} F_i(\tau))v||\,. \end{aligned}$$

Proceeding by induction one finds

$$||F(\tau)u - F(\tau)v|| \leq ||u - v|| \,. \tag{1.16}$$

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Remark: Although the algortihms corresponding to $F_i(\tau)$ are second order accurate, the splitting algorithm (1.15) is not ([2]). Using a a double pass procedure the second order accuracy can be recovered, i.e.,

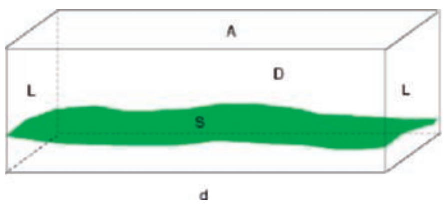
$$F(\tau)u = (\Pi^1_{i=N} F_i(\frac{1}{2}\tau))(\Pi^N_{i=1} F_i(\frac{1}{2}\tau))u \,. \tag{1.17}$$

2 A Multilayer Convection-Diffusion Model: Preliminaries

In the following we deal with the mathematical model of a convection-diffusion process in a three dimensional domain characterized as corresponding to a zone where the surface is not necessarily flat. Let $\omega \subset \mathbb{R}^2$ be a two–dimensional normalized bounded and connected domain representing the projection of the three–dimensional ground surface, $x = (x_1, x_2)$ be any of its points and τ be the time. We use small letters for the two–dimensional problem, and capital letters for the three dimensional problem.

Let us consider the three dimensional domain $\Omega = \{(x, z) : x \in \omega, \; h(x) < z < \delta\}$ representing the studied air layer. Let δ be the height of the domain Ω and assume that the height $h(x)$ of the surface at point x is smaller than δ. In this section, we denote by an index $_{xy}$ the bi-dimensional operators and by the index $_z$ the operators concerning the vertical component. We note the air velocity $U = (U_1, U_2, U_3)$. We distinguish the vertical velocity from the horizontal one denoting $W = U_3$, $V = (U_1, U_2)$.

3 The convection-diffusion model



The convection diffusion equation governing the dispersion of pollutant in the atmosphere is

$$\frac{\partial u}{\partial t} + V.\nabla_{xy} u + W \frac{\partial u}{\partial z} - \nabla(k_{xy} \nabla_{xy} u) - \frac{\partial}{\partial z}(k_z \frac{\partial u}{\partial z}) = f \,. \tag{3.1}$$

In order the problem to be well defined we have to add boundary and initial condition. We assume that the air is initially clean, that is $u = 0$ at time $t = 0$. The following boundary conditions will be assumed

$$-k_{xy}\nabla u.\nu = [V.\nu]^{+} u\,. \tag{3.2}$$

3.1 Change of coordinates

We make a change of coordinates in order to transform the domain into a cuboid. The new coordinates will be

$$\begin{aligned}\tau &= t\\ \xi &= x\\ \eta &= y\\ \zeta &= z - h(x,y)\,.\end{aligned}$$

By straightforward computations for any function $\phi = \phi(t,x,y,z)$ we have

$$\begin{aligned}\frac{\partial\phi}{\partial t} &= \frac{\partial\phi}{\partial\tau}\\ \frac{\partial\phi}{\partial x} &= \frac{\partial\phi}{\partial\xi} - \frac{\partial h}{\partial x}\frac{\partial\phi}{\partial\zeta}\\ \frac{\partial\phi}{\partial y} &= \frac{\partial\phi}{\partial\eta} - \frac{\partial h}{\partial y}\frac{\partial\phi}{\partial\zeta}\\ \frac{\partial\phi}{\partial z} &= \frac{\partial\phi}{\partial\zeta}\,.\end{aligned}$$

Then the convection term becomes

$$U\nabla u = V\nabla_{\xi\eta}u + (W - V_1\frac{\partial h}{\partial x} - V_2\frac{\partial h}{\partial y})\frac{\partial u}{\partial\varsigma}\,,$$

and the diffusion term is

$$\begin{aligned}-\nabla(k\nabla u) = &- \nabla_{\xi\eta}(k_{\xi\eta}\nabla_{\xi\eta}u)\\ &- \frac{\partial}{\partial\zeta}\Big(\big(k_{\zeta} + k_{\xi\eta}(\frac{\partial h}{\partial x})^2 + k_{\xi\eta}(\frac{\partial h}{\partial y})^2\big)\frac{\partial u}{\partial\zeta}\Big)\\ &+ \frac{\partial}{\partial\xi}(k_{\xi\eta}\frac{\partial h}{\partial x}\frac{\partial u}{\partial\zeta}) + \frac{\partial}{\partial\zeta}(k_{\xi\eta}\frac{\partial h}{\partial x}\frac{\partial u}{\partial\xi})\\ &+ \frac{\partial}{\partial\eta}(k_{\xi\eta}\frac{\partial h}{\partial y}\frac{\partial u}{\partial\zeta}) + \frac{\partial}{\partial\zeta}(k_{\xi\eta}\frac{\partial h}{\partial y}\frac{\partial u}{\partial\eta})\,.\end{aligned} \tag{3.3}$$

Consequently the equations in the transformed domain are analogous to (3.1) and (3.2) replacing W by $W - V_1\frac{\partial h}{\partial x} - V_2\frac{\partial h}{\partial y}$ and k_z by $\big(k_{\zeta} + k_{\xi\eta}(\frac{\partial h}{\partial x})^2 + k_{\xi\eta}(\frac{\partial h}{\partial y})^2\big)$ plus the terms with crossed derivatives in (3.3). In the following we use the notation x, y and z for the new coordinates instead of ξ, η, ς.

4 Numerical Method

4.1 A Finite Element - Characteristic - Finite Difference method

Let A_l^n be a Finite Element approximation of the operator $-\nabla(k_{xy}\nabla)$ in the layer l and at the time t_n and we note u_l^n the solution in this level at this time. We use a two dimensional Finite Element method in each level combined with the Characteristic method. In the vertical direction we approximate the convection term with an upwind first order scheme and the diffusion term with a secod order Finite Differences scheme. The crossed derivatives are approximated using prisms with triangular section, which is equivalent to use triangular finite elements in the horizontal direction and finite differences in the vertical direction. Let $\bar{\omega}$ be any of the horizontal sections of the cuboid. We denote B_l and C_l the matrices defined by the coefficients

$$(B_l)_{ij} = \int_{\bar{\omega}} k_{xy}(\frac{\partial h}{\partial x}\frac{\partial \varphi_j}{\partial x} + \frac{\partial h}{\partial y}\frac{\partial \varphi_j}{\partial y})\varphi_i)\,, \tag{4.1}$$

$$(C_l)_{ij} = \int_{\bar{\omega}} k_{xy}(\frac{\partial h}{\partial x}\frac{\partial \varphi_i}{\partial x} + \frac{\partial h}{\partial y}\frac{\partial \varphi_i}{\partial y})\varphi_j)\,. \tag{4.2}$$

A one step Euler implicit method

Given a time step Δt, and an interval length Δz in the vertical direction,

For each layer $l = 1, ..., L$

$$\begin{aligned} \frac{u_l^{n+1} - \bar{u}_l^n}{\Delta t} &+ \frac{W_l^+}{\Delta z}(u_l^{n+1} - u_{l-1}^{n+1}) - \frac{W_l^-}{\Delta z}(u_{l+1}^{n+1} - u_l^{n+1}) \\ &+ A_l u_l^{n+1} + k_z \frac{-u_{l-1}^{n+1} + 2u_l^{n+1} - u_{l+1}^{n+1}}{(\Delta z)^2} \\ &+ \frac{1}{2\Delta z} B_l(u_{l+1}^{n+1} - u_{l-1}^{n+1}) + \frac{1}{2\Delta z} C_l(u_{l+1}^{n+1} - u_{l-1}^{n+1}) \\ &\quad \{if(l == 1) + \lambda u^{n+1}\} = f^{n+1} \end{aligned} \tag{4.3}$$

where $W_l^+ = \max\{0, W_l\}$ and $W_l^- = \max\{0, -W_l\}$, and $\bar{u}_l^n$ is given by $\bar{u}_l^n = u_l^n \circ X^n$ where $X^n(x) = X(x; t^n)$ is the solution at time t^n of the final value problem

$$\frac{dX}{dt} = V \tag{4.4}$$

$$X(x, t^{n+1}) = x\,. \tag{4.5}$$

In the former scheme all the levels are coupled, in consequence it is not very suitable from a practical point of view. Next we consider a splitting method where the problem can be solved at each level separately.

Splitting Method

For $l = 1, ..., L$

$$\frac{u_l^{n+1/4} - \bar{u}_l^n}{\Delta t/2} = 0 \tag{4.6}$$

$$\begin{aligned} \frac{u_l^{n+1/2} - u_l^{n+1/4}}{\Delta t} &+ \frac{W_l^+}{\Delta z}(u_l^{n+1/2} - u_{l-1}^{n+1/2}) \\ &+ \frac{1}{2}A_l u_l^{n+1/2} + k_z \frac{-u_{l-1}^{n+1/2} + u_l^{n+1/2}}{(\Delta z)^2} \\ &+ \frac{1}{2\Delta z}(-B_l u_{l-1}^{n+1/2}) + \frac{1}{2\Delta z}(-C_l u_{l-1}^{n+1/2}) \\ &\{if\,(l == 1) + \lambda u^{n+1/2}\} = \frac{1}{2} f^{n+1/2}. \end{aligned} \tag{4.7}$$

For $l = L, ..., 1$

$$\begin{aligned} \frac{u_l^{n+3/4} - u_l^{n+1/2}}{\Delta t} &- \frac{W_l^-}{\Delta z}(u_l^{n+3/4} - u_{l-1}^{n+3/4}) \\ &+ \frac{1}{2}A_l u_l^{n+3/4} + k_z \frac{u_l^{n+3/4} - u_{l+1}^{n+3/4}}{(\Delta z)^2} \\ &+ \frac{1}{2\Delta z}(B_l u_{l+1}^{n+3/4}) + \frac{1}{2\Delta z}(C_l u_{l+1}^{n+3/4}) \\ &\{if(l == 1) + \lambda u^{n+3/4}\} = \frac{1}{2} f^{n+3/4} \end{aligned} \tag{4.8}$$

$$\frac{u_l^{n+1} - \bar{u}_l^{n+3/4}}{\Delta t/2} = 0\,. \tag{4.9}$$

Remark The term $(l == 1)\lambda u^{n+1}$ represents the eventual absorption by the terrain and it appears only in the surface level $(l = 1)$.

Justification of the splitting method

In order to simplify, we consider the former problem without convection terms and without crossed derivatives. The discrete equations can be written using matricial notation as follows:

$$\frac{du}{dt} + Au + Tu = f\,, \tag{4.10}$$

where

$$u = \begin{bmatrix} u_1 \\ ... \\ u_l \\ ... \\ u_L \end{bmatrix}$$

$$A = \begin{bmatrix} A_1 & ... & 0 \\ & ... & \\ 0 & A_l & 0 \\ & ... & \\ 0 & ... & A_L \end{bmatrix}$$

$$T = \frac{1}{(\Delta z)^2} \begin{pmatrix} 2 & -1 & 0 & \dots & 0 \\ -1 & 2 & -1 & \dots & \vdots \\ & \ddots & \ddots & \ddots & \\ & & & & -1 \\ 0 & 0 & \dots & -1 & 2 \end{pmatrix} . \tag{4.11}$$

We split the tridiagonal matrix T, $T = U + L$ where

$$L = \frac{1}{(\Delta z)^2} \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ -1 & 1 & 0 & \dots & \vdots \\ & \ddots & \ddots & \ddots & \\ & & & & 0 \\ 0 & 0 & \dots & -1 & 1 \end{pmatrix} \tag{4.12}$$

and

$$U = \frac{1}{(\Delta z)^2} \begin{pmatrix} 1 & -1 & 0 & \dots & 0 \\ 0 & 1 & -1 & \dots & \vdots \\ & \ddots & \ddots & \ddots & \\ & & & & -1 \\ 0 & 0 & \dots & 0 & 1 \end{pmatrix} . \tag{4.13}$$

Finally the splitting algorithm is

$$\frac{u^{n+1/2} - u^n}{\Delta t} + \frac{1}{2} A u^{n+1/2} + L u^{n+1/2} = \frac{1}{2} f^{n+1/2} \tag{4.14}$$

$$\frac{u^{n+1} - u^{n+1/2}}{\Delta t} + \frac{1}{2} A u^{n+1} + U u^{n+1} = \frac{1}{2} f^{n+1} . \tag{4.15}$$

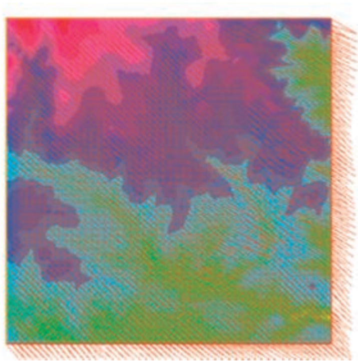


Figure 1: velocity field

5 Numerical results

The following results correspond to the orography in an area near Cofrentes (a small town in central Spain) and a typical wind field shown in Figure 1. The wind field has been computed at five different levels. The wind field in the figure corresponds to the wind field at the surface level. The wind model and its numerical solution is described in [3], [4] and [5].

We assume that at a given time a certain amount of pollutant is released to the atmosphere taking place at the ground surface, according to the expression (gaussian emission)

$$f(t,x) = ae^{-(\frac{\log(2)}{c}t)}e^{-((X[0]-x[0])^2+(X[1]-x[1])^2)/(2b^2))},$$

where

- t is the time in seconds
- $a = 100$ is a pre-exponential factor.
- $b = 100$ is the standar deviation of the gaussian distribution
- $c = 300$ is the half life time of the emision in seconds
- $X = [500, 4500]^t$ is the point where the emision takes place.

The other physical values are:

- Horizontal diffusion coefficient, $k_{xy} = 10^{-1}$
- Vertical diffusion coefficient, $k_z = 10^{-3}$

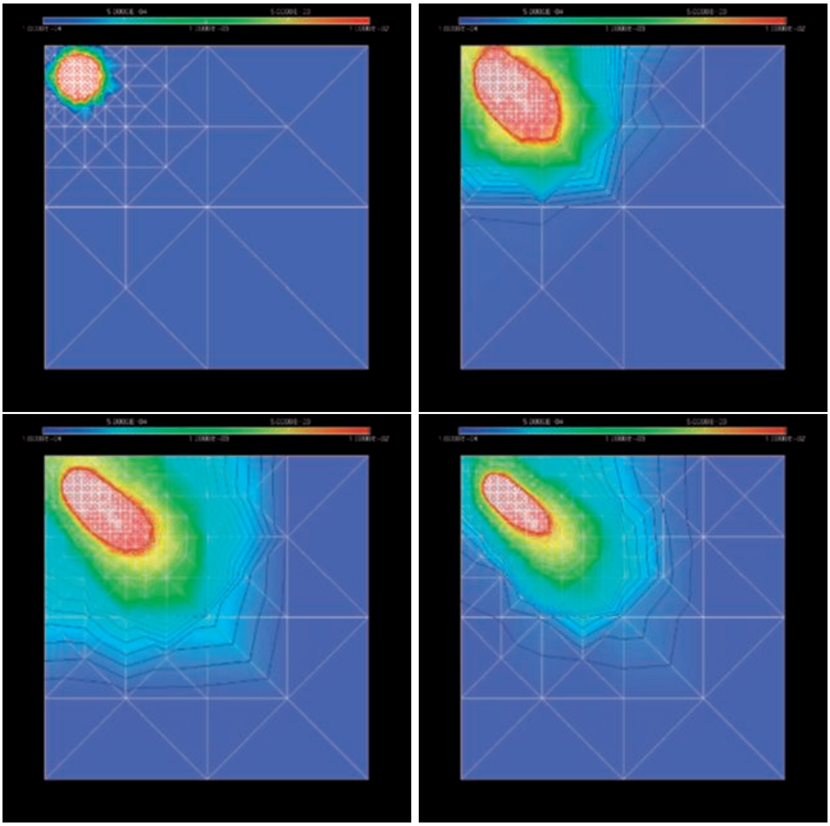


Figure 2: Concentration in the first level at different time steps

- Absorption coefficient in the surface level, $\lambda = 0.001$.

Figure 2 shows the concentration at the first level at the initial time then after 10, 20 and 30 time steps respectively.

Figure 3 shows the concentration at the third level after 10, 20, 30 and 40 time steps respectively.

Figure 4 shows the concentration at the fifth level after 10, 20, 30 and 40 time steps respectively.

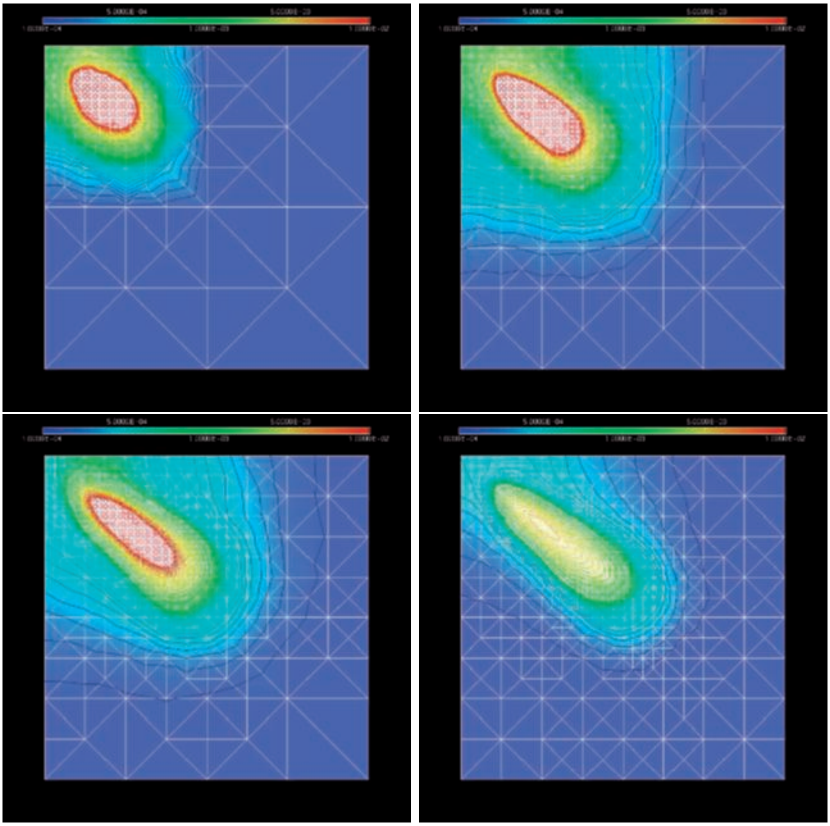


Figure 3: Concentration in the third level at different time steps

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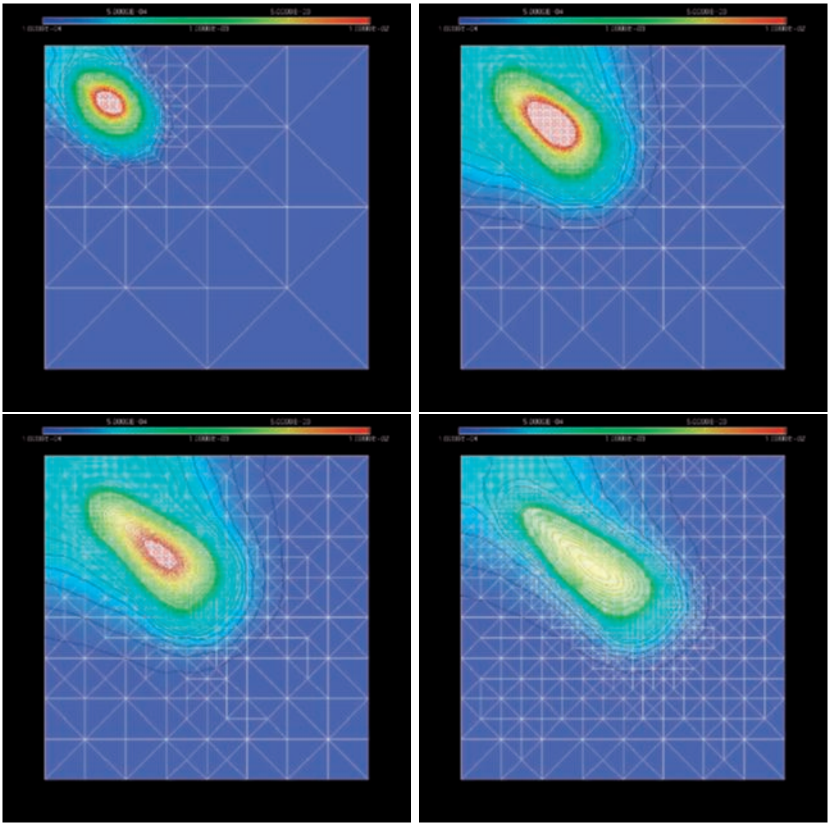

Figure 4: Concentration in the fifth level at different time steps

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