Comparison of Finite Element and Finite Box Discretization for Three-Dimensional Diffusion Modeling Using AMIGOS

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Abstract

The occurrence of unphysical negative concentrations in solutions to diffusion equations is a well known and severe problem. Especially in three dimensions finite element discretizations give qualitatively very poor results, while finite volume discretizations are much more stable. We investigate the cause of these instabilities and trace them back to constraints on the mesh. It turns out that in three dimensions conventional (i.e. Delaunay) meshes are only suitable for the finite box method, while Delaunay is an invalid constraint in the case of finite elements.

1. Introduction

The maximum principle is the most important property of solutions to convection-diffusion equations. In its simplest form it states that both the maximum and the minimum concentrations occur on the boundary or at the initial time. This implies that if the boundary and initial values are positive, then the solution is positive everywhere and the concentration never reaches negative values. It is desirable that the employed discretization also satisfies a maximum principle. As is well known, this is guaranteed, if the system matrix resulting from the discretization is an M-matrix [1].

2. Discretization using AMIGOS

We compare the results of two different spatial discretizations for diffusion in three dimensions using AMIGOS [2] which is especially designed for simple but efficient model development. Through its powerful analytical model interface (AMI) it was possible to implement the Finite Volume (FV) as well as the Finite Element (FE) method. This allows the comparison of the solutions on identical meshes with the same linear solver in a very simple and straightforward manner.

Both for FV and FE we use the well known standard approaches with backwards Euler time discretization.

For FV (see e.g. [3]) we calculate the Voronoi boxes and the corresponding interface areas for each element. In the case of FE we use the Galerkin weighted residual approach with linear form functions.

Then the system matrix K is of the form

$$K = \frac{M}{\triangle t} + \alpha S$$

where M denotes the mass matrix, S is the stiffness matrix, and α denotes the diffusion constant (homogeneous case). To make K an M-matrix, the mass matrix has to be lumped, and S also has to be an M-matrix. Since S depends on the mesh, this condition translates to a constraint on the mesh.

In two dimensions Delaunay meshes guarantee that the maximum principle is satisfied for FV as well as for FE. In three dimensions Delaunay meshes are still sufficient and necessary for FV, as shown in [4].

However, for FE this does not hold anymore [5]: When applying FE on a Delaunay mesh in three dimensions negative concentrations emerge, which implies that the M-matrix property is lost. Until recently this phenomenon was not fully understood. But by using results from [4] and [6] it is possible to grasp what is going on: The constraints on the mesh for FE and FV are two different purely geometric notions which are equivalent only in two dimensions. Each of them generalizes naturally to higher dimensions, and it can be proved that neither of them implies the other any more. This is an essential discovery with heavy impact on the development of meshing strategies.

3. Numerical Experiments

To illustrate some of the consequences we solve the pure diffusion equation on one and the same three dimensional Delaunay mesh using FE and FV. We used an ortho-product point distribution on the cubic simulation domain. Every sub-cube was tetrahedralized into six tetrahedra. [1]

In both cases a Gaussian profile (offset 10^{12}) is used as the initial three-dimensional distribution. As expected FV gives qualitatively correct results. Fig. 1 is a one-dimensional cut, showing the initial distribution and the FE and the FV solution after 120 time-steps. Even for this simple test problem the FE solution strongly violates the maximum principle.

Fig. 2 gives a two-dimensional cut and shows the bad quality of the FE solution. On the black areas the solution becomes negative. Note that the mesh has translational symmetries, which spoil the rotational symmetry of the initial distribution. These areas spread out in time, as shown in Fig. 3. The absolute value of the emerging negative concentrations is much larger than the minimal initial concentration. Finally, Fig. 4 depicts the corresponding relative error between the FE and the FV solution. The error oscillates strongly and is large on the regions, where the concentration is negative. But since mass is conserved the negative concentrations are compensated by additional erroneous mass in the positive areas.

The negative concentrations are a particularly serious problem in diffusion in process simulation, because in typical applications the concentration varies in many orders of magnitude within a small area. For a more complicated transient problem like the pair diffusion model the negative concentrations lead to severe instabilities.

[1]Note that in this simple case the usage of a T5 tessellation for the sub-cubes will result in a Delaunay mesh which fulfills the newly introduced criterion by Xu and Zikatanov.

4. Impact on Meshing Strategies

The obvious cure for these FE-troubles would be to use a mesh which gives an M-Matrix. However, as long as the available meshing tools concentrate on the Delaunay criterion, there is little hope of achieving this.

We want to stress that from a Delaunay point of view these meshes can look really bad, but they are especially tuned to the FE-discretization and give qualitatively correct results.

Otherwise mesh refinement has to be employed. In practice this greatly increases the computational costs and only mitigates the observed effects. It will depend on the application, if one can live with negative concentrations and unphysical flows. As alternative one must decide for FV.

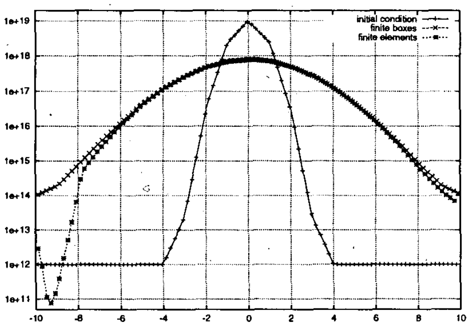

Figure 1: Comparison FE versus FV. FE violates the maximum principle.

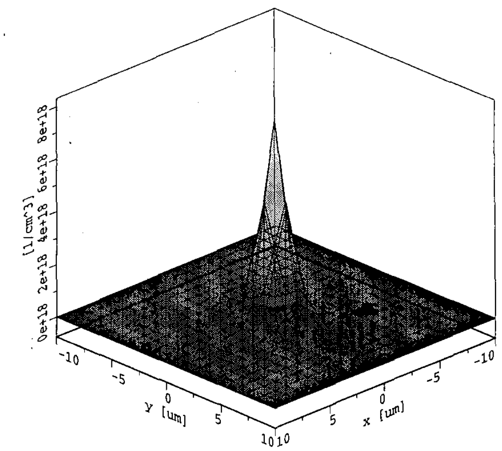

Figure 2: 2D-cut after 5500 seconds. Concentration is negative on black areas.

5. Conclusion

Using AMIGOS, we investigated the constraints which must be imposed on the mesh to avoid the occurrence of negative concentrations in diffusion simulation.

1. In two dimensions a Delaunay triangulation will result in an M-Matrix both for the FE and the FV discretization.

2. In three dimensions Delaunay is the proper constraint on the mesh for FV. But for FE we get a constraint which may be fulfilled by non-Delaunay grids and not fulfilled by Delaunay triangulations. In short: Delaunay is the wrong criterion (neither necessary nor sufficient) for FE grids in three dimensions.

3. Using currently available meshing tools the preferable approach to diffusion modeling is finite volumes.

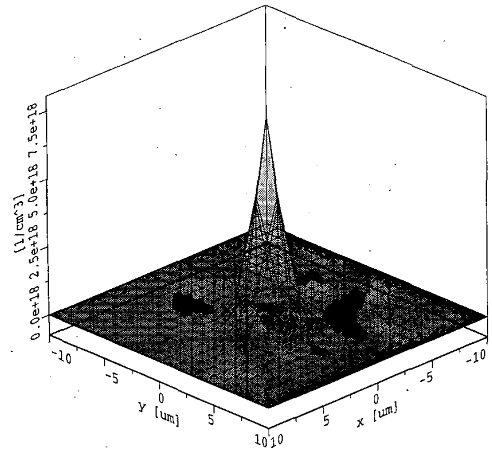

Figure 3: 2D-cut after 8500 seconds. Negative concentrations spread out.

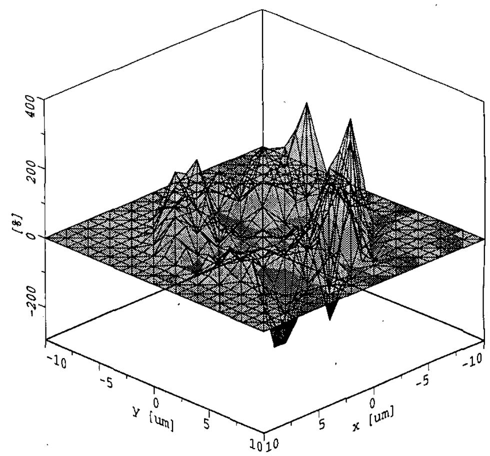

Figure 4: Relative error between FE and FV.

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