Coupling of Lattice-Gas- and Finite Element-Methods

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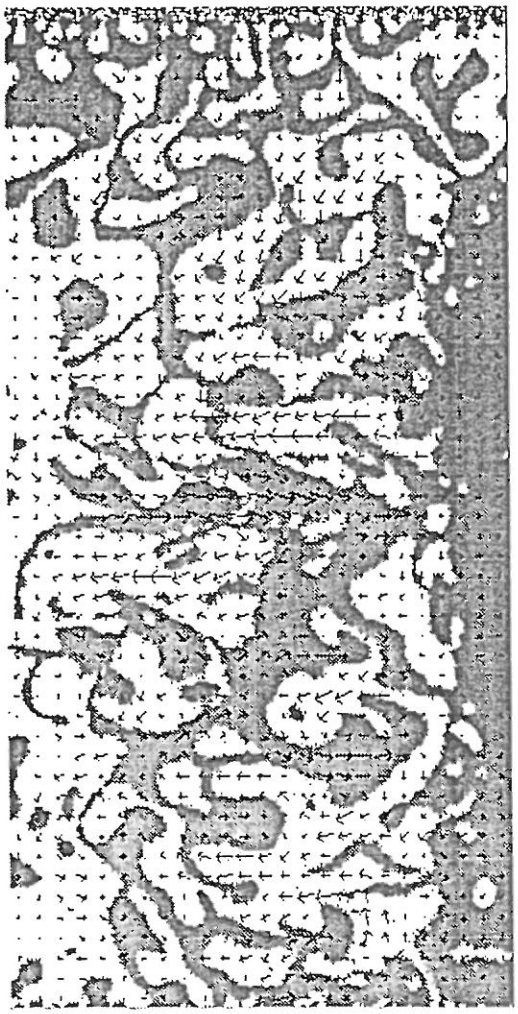

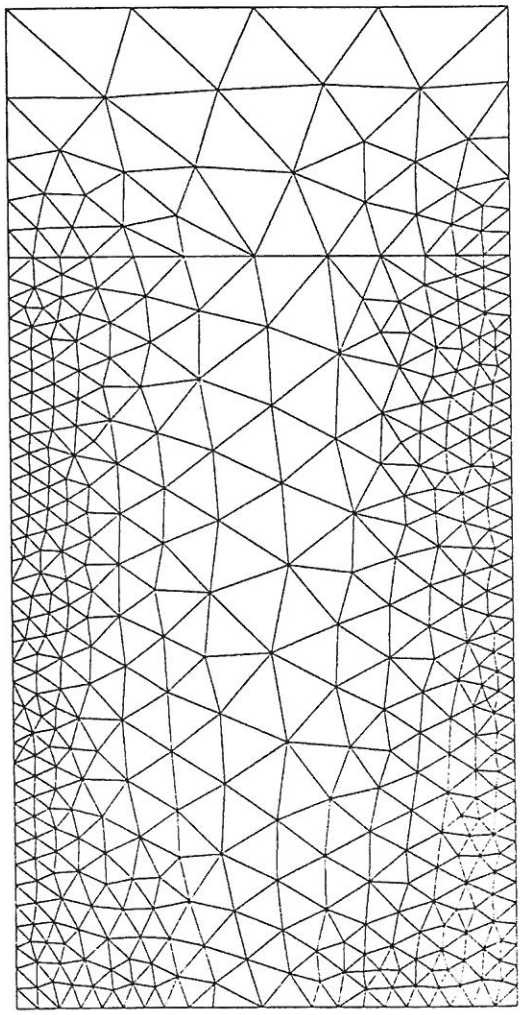

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1 Abstract

During the last decade there has been a very successful development of Lattice Gas (LG) algorithms for simulation of flow-problems and related topics parallel to the refinement of classical methods like Finite Differences, Finite Elements (FE) and spectral methods.[1-5]
Due to their inherent structural differences LG- and FE-algorithms show specific advantages and disadvantages when being applied to specific parts of e.g. multiphase-flow-problems governed by the incompressible Navier-Stokes-equations. The main difference can be recognized in the fact that LG-methods are strictly local algorithms while FE-methods proceed (typically) in a non-local way.
Analysing problems where both local and non-local interactions are equally important, it is evidently desirable to couple the two algorithms in order to gain the advantages of both formalisms.
In order to demonstrate the power and efficiency of a mixed algorithm we implemented the so-called Immiscible Lattice Gas [6] in its Galilean invariant form and coupled it with a FE-program for field computations. As a preliminary example we calculate the qualitative dynamics of a two-phase charged fluid which is accelerated by the electric field of a capacitor, changing the field by its own charge. The increase in computational time for the coupled program turns out to be small compared to the stand-alone CA-implementation. The principal coupling algorithm is the same for all LG and FE-variants and might serve as a valuable algorithmic help for the simulation of a variety of complex coupled problems.

References

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(4) P. Clavin, P. Lallemand, Y. Pomeau, G. Searby, J. Fluid Mech. 188, 437-464 (1988)
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2 The problem

Consider a two fluid mixture flowing through a channel. At the upper boundary particles of both colours enter with a predefined average speed and flow downwards. The influence of surface tension generates a steadily increasing decomposition of the mixture. Both fluids carry a certain amount of charge per particle of a sign according to their colour. The electric field of these charged particles is small enough, so that decomposition is still possible, but weakened. A capacitor located at the lower part of the channel (fig.1) produces an electric field which accelerates particles according to their charge, but large bubbles of particles of common colour decrease the electric field of the capacitor plate towards which they move. This is a 'non-local' field-effect which can not be efficiently treated by local CA-algorithms alone.

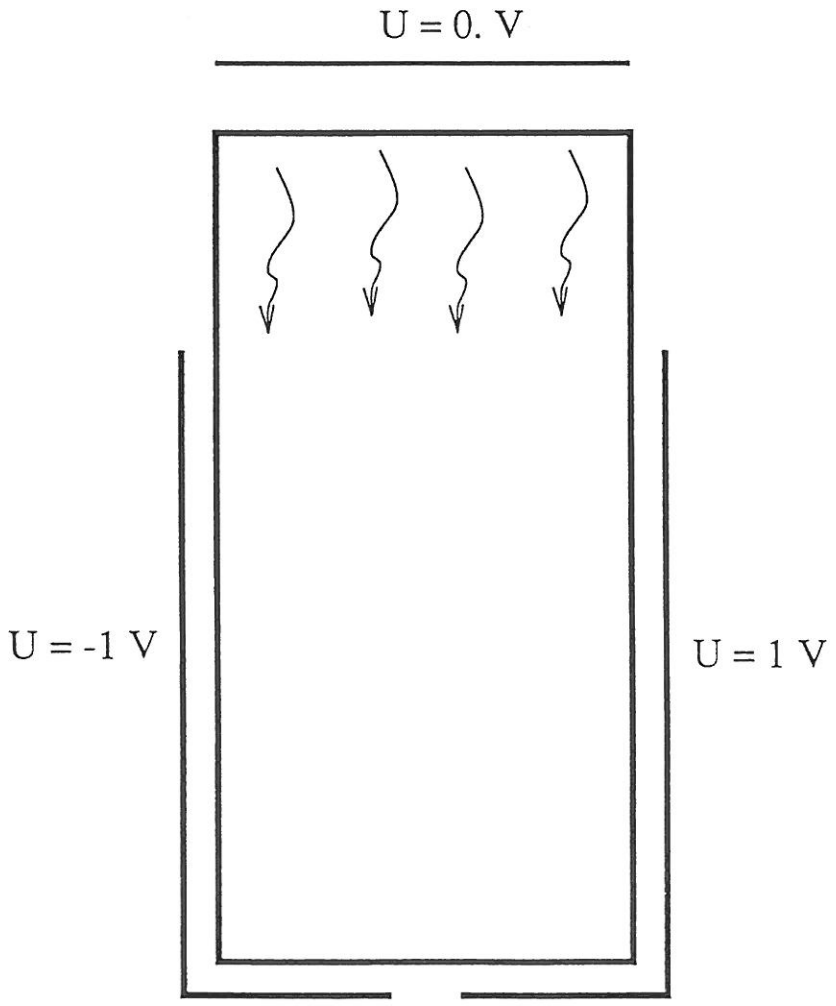


Figure 1: Flow channel with capacitor

3 The Lattice Gas Model

We use the socalled immiscible lattice gas (ILG) algorithm of Rothmann et al. (1-3) which allows to simulate two-phase flow while producing surface-tension-effects with a $g(\varrho) = 1$ condition to ensure Galilean invariance of interface - flow. The automaton particles move on a hexagonal grid, there is a maximum of 16 rest-particles (more are possible but not used in the following example) and 6 moving particles per site. The look-up-table for the collisions is quasi-deterministic because the individual post-collision-state on a site is chosen from all possible ones according to its probability of existence in order to obtain balanced collisions.
For each site a 'colour'-field is computed at each time-step from the neighbour-sites in order to send particles of a certain colour into the direction of neighbours with a majority of particles of the same colour. The influence of the electric field on the redistribution of particles on a site is precomputed in an additional look-up-table. The direction of the electric field is quantized so that there are 32 directions left to serve as an entry for this look-up-table. For every possible combination of moving particles at a site we precomputed the distribution that maximizes the scalar product of site velocity and electric field . These new states differ in their new momentum (i.e. acceleration) and so an additional look-up-table is created with weights antiproportional to the change of momentum in the new site distribution. This ensures that later the average acceleration at a site is equal for all possible distributions on that site and so a quantitative scaling of the field-strength is easier to achieve. Multiple alternatives with equal weights are randomly chosen.
The ILG-automaton currently runs on a HP-9000-735 workstation with a speed of about 150.000 sites per second, but there is still a variety of technical possibilities left to improve performance.
For simplicity the vertical boundary-conditions are set to be periodical although this might be unsatisfying in a quantitative simulation. The horizontal boundary conditions are so called 'slip-conditions'.

4 The finite element formulation

The quasistationary equation for the electrical potential u in our model problem is give by

$$\nabla(\epsilon(\mathbf{x})\nabla u) = -q(\mathbf{x}) \quad in \quad \Omega \tag{1}$$

with appropriate boundary conditions, a space dependant dielectricity constant ϵ and a distributed charge density q. Multiplication of the differential equation by an arbitrary 'test function v' and integration over the domain Ω yields the following 'weak form' of the differentioal equation :

Find the function u in an appropriate solution space satisfying the potential boundary conditions so that for every test function v of an appropriate test space V

$$\int_\Omega \epsilon(\mathbf{x})\nabla u \nabla v d\Omega = \int_\Omega q(\mathbf{x}) v d\Omega \tag{2}$$

After triangulation of the domain of computation an 'ansatz' of the form

$$U = \sum_{i=1}^{n} a_i N_i(\mathbf{x}) \tag{3}$$

is made . a_i are unknown coefficients and N_i are 'shape functions' having support only on neighboring elements. Using the same set $N_i, i = 1, ..., n$ as test functions, a linear equation system can be formulated to define the coefficients a_i .For more details, see e.g. Zienkiewicz)7].

Usually shape functions are used being only continuous, but not continuously differentiable across element edges. So the coupling field to the CA, the flux ∇U is discontinous as obtained directly from the finite element solution U. Yet a simple postprocessing, averaging nodal values and using the shape functions N_i to interpolate these nodal values, yields a continuous electrical field $\vec{E} = \epsilon\nabla\tilde{U}$.

5 The Coupling - Algorithm

The main task of the coupling algorithm is to pass and transform information of physical properties between the sites of the ILG and the elements (here: triangles) of the FE-domain. In our case the sites of the ILG carry a little charge depending on the number of particles of a certain colour at a distinct timestep. The charge-density of an element is the sum over the charge of all sites within its area divided by this area:

$$q_e(e(i)) = \frac{1}{area(e(i))} \sum_{j=1}^{J} q_s(site(x,y)) \quad \wedge site(x,y) \in e(i) \tag{4}$$

After generation of a finite element mesh a list K(x,y) is computed containing the index of the FE-element that site(x,y) belongs to. Another triple of lists L(1,x,y), L(2,x,y) and L(3,x,y) is computed containing the three *natural coordinates* of a site with respect to its element. These lists are needed to compute efficiently the *local electric field for every site* at a certain timestep. The natural or *area coordinates* of a point P in a triangle with nodes 1,2 and 3 (see figure 2) are defined as

$$L(1,P) = \frac{area(P23)}{area(123)} \quad , \quad L(2,P), L(3,P) \quad analoguously \tag{5}$$

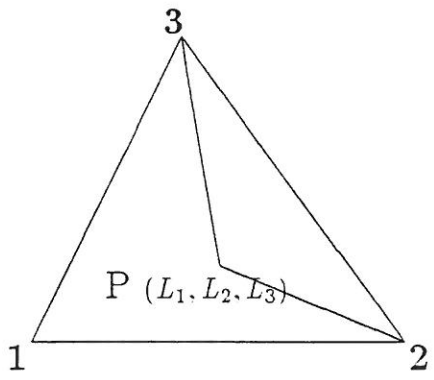


Figure 2 : Natural coordinates in a triangle

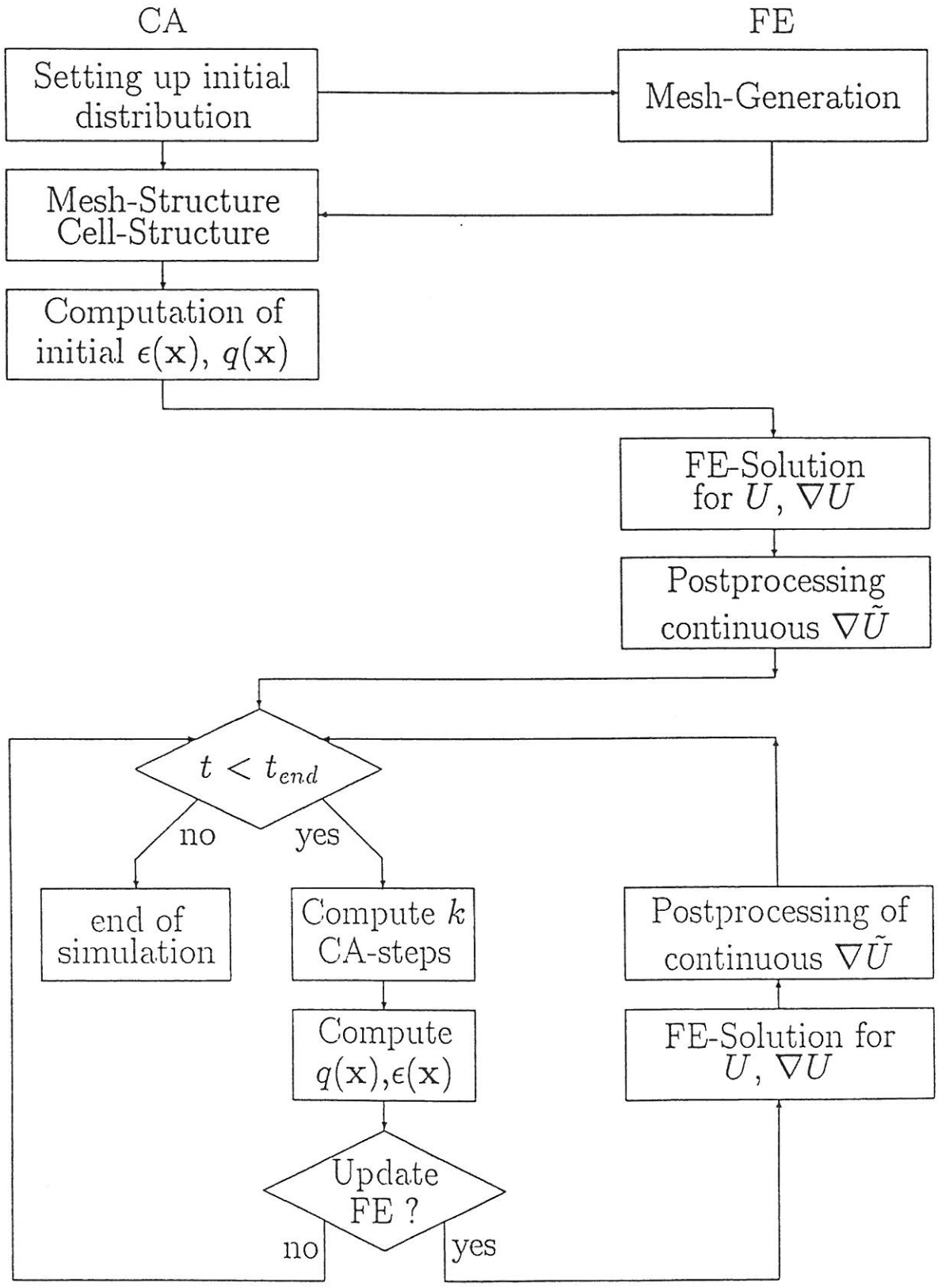
Note that L(i,x,y) $\in [0,1]$ for a point P(x,y) inside the element.

The advantage of these natural coordinates is the fact that they can directly be used as weights for the computation of the electric field at a site, being is a function of the field at the nodes of the element:

$$\vec{E}(site(x,y)) = \sum_{i=1}^{3} \vec{E}(node(i)) \cdot L(i,x,y) \tag{6}$$

Combined with appropriate pointer structures which guarantees fast access to every part of the FE-data this results in a very fast computation of the local field at a site. The structure of the simulation algorithm is shown in the following flow-diagram. After an initial cycle the automaton computes k-1 timesteps with a constant local electric field. After k timesteps the change of charge in all elements is computed, k depending on the average element-size. If this change is higher than a defined threshold (here 10 per cent) in any element, new charge densities and dielectricities are computed and the FE-program is called to compute a new electric field from the charge distributions in the system.

$$\delta_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + \nu(\rho)\Delta \mathbf{v} + f(\nabla u) \qquad \nabla(\epsilon \nabla u) = -q(\mathbf{v})$$



6 Numerical Example

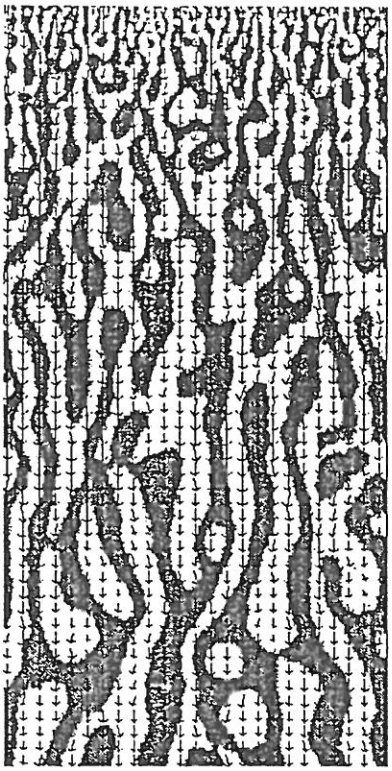


Figure 3a : Initial two-phase flow

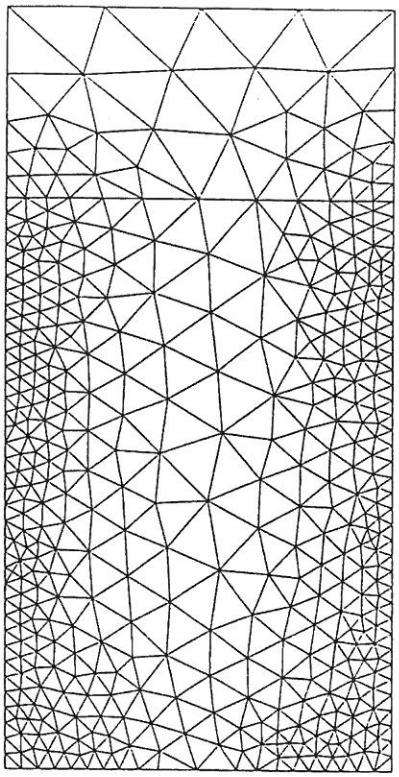


Figure 3b : Finite element mesh

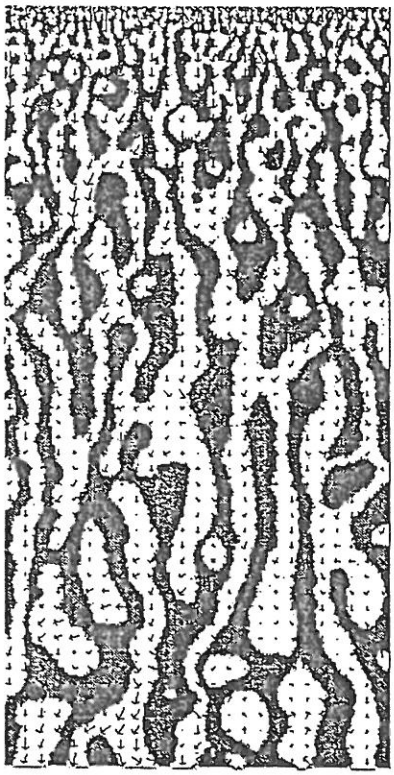


Figure 4a : Flow after 100 timesteps

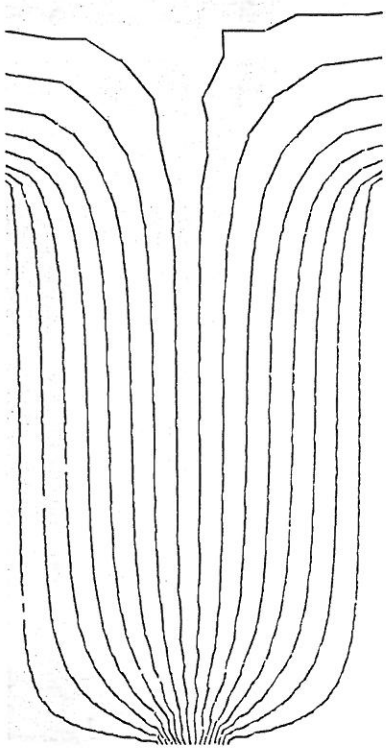


Figure 4b : Electrical field

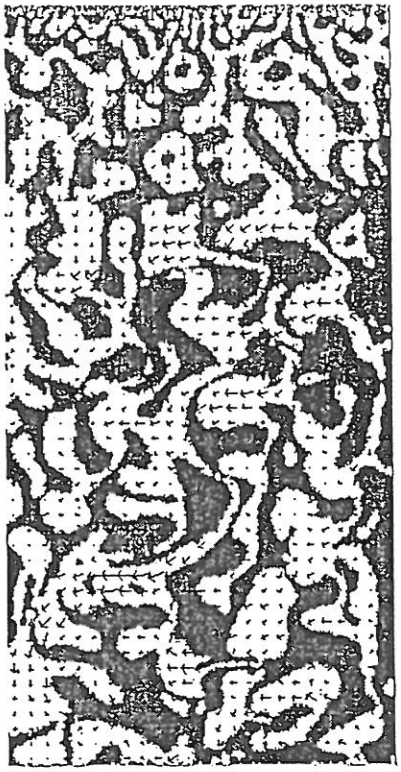


Figure 5 : Flow field after 500 timesteps

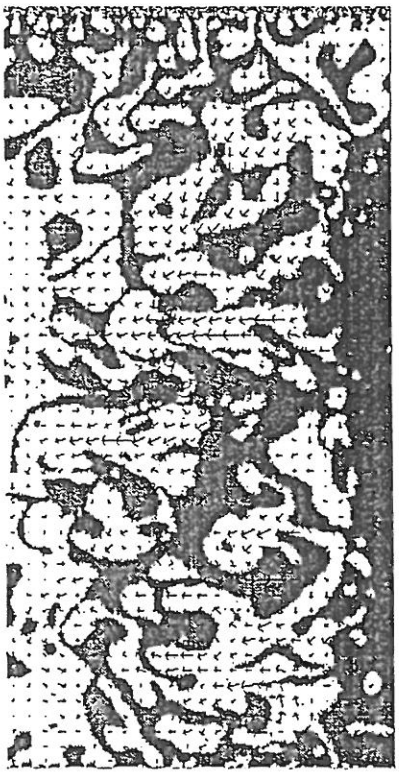


Figure 6 : Flow field after 1000 timesteps

Figure 3 shows the initial two-phase flow without influence of the capacitor and the finite element mesh for the computation of the electrical field. In figure 4 the flow after 100 timesteps and contour lines of the corresponding electrical potential are plotted. Figures 5 and 6 show the continuing process, where the positively charged fluid flows to the left and the negatively charged one to the right. After 3000 timesteps (figure 7) the main part of the fluids has already seperated, modifying the source term q on the righthand side of the potential equation significantly. The influence of this separation on the electrical field can be seen in figure 6b. In the middle of the channel the field has decreased, allowing a nearly undisturbed vertical flow of the fluids.
The lattice consists of 250x500 sites, the finite element mesh has 467 nodes and 823 triangles. The total computation time for 4000 ILG timesteps and 16 Finite Element updates was about 2 hours on a HP9000/735.

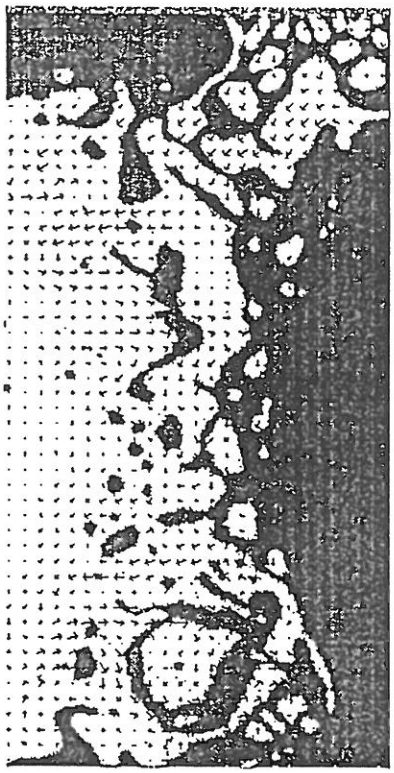


Figure 7a : Flow field after 3000 timesteps

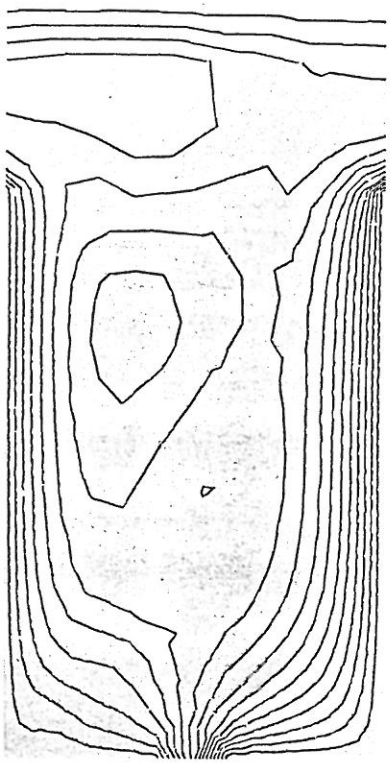


Figure 7b : Electrical field