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AN INTRODUCTION TO FRONT TRACKING

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Abstract. In fluid flows one can often identify surfaces that correspond to special features of the flow. Examples are boundaries between different phases of a fluid or between two different fluids, slip surfaces, and shock waves in compressible gas dynamics. These prominent features of fluid dynamics present formidable challenges to numerical simulations of their mathematical models. The essentially nonlinear nature of these waves calls for nonlinear methods. Here we present one such method which attempts to explicitly follow (track) the dynamic evolution of these waves (fronts). Most of this exposition will concentrate on one particular implementation of such a front tracking algorithm for two space, where the fronts are one-dimensional curves. This is the code associated with J. Glimm and many co-workers.

Introduction. In fluid flows one can often identify surfaces of co-dimension one that correspond to prominent features in the flow. Examples are boundaries between different phases of a fluid or between two different fluids, slip surfaces, shock curves in compressible gasdynamics. All such surfaces are characterized by significant changes in the flow variables over length scales small compared to the flow scale. For example in oil reservoirs the oil banks have a size of 10 meters compared to an average length scale of 10 kilometers; or in compressible gas dynamics shock waves have a width of 10^{-5} cm compared to a length scale of 10 cm. The dynamics of such waves may be influenced by their internal structures. Whereas for shock waves the speed depends on the asymptotic states to the left and right, for two dimensional detonation waves the speed depends also on the chemistry and curvature, [B], [J]. There are situations where it is necessary to take these physical aspects of the flow into account when doing a numerical simulation.

A simple model for nonlinear wave propagation is Burger's equation

$$u_t + uu_x = \nu u_{xx} \ ,$$

where the state variable u is convected with characteristic speed u and diffused with viscosity ν. Because of the dependence of the characteristic speed on the state variable one obtains a focusing effect that leads to the formation of shock waves. Consider initially a wave of length L (see Fig. 1). The monotone decreasing part of the wave will steepen such that in a thin layer the solution rapidly decreases from a value u_l to u_r. The width w of this layer is about $\dfrac{\nu}{|u_l - u_r|}$, and this layer moves with speed $s = \dfrac{1}{2}\,(u_l - u_r)$. If $w \ll L$, we may approximate the layer by a jump from u_l to u_r and consider the inviscid limit by neglecting ν to obtain the inviscid Burger's equation

$$u_t + \left(\frac{u^2}{2}\right) x = 0 \ .$$

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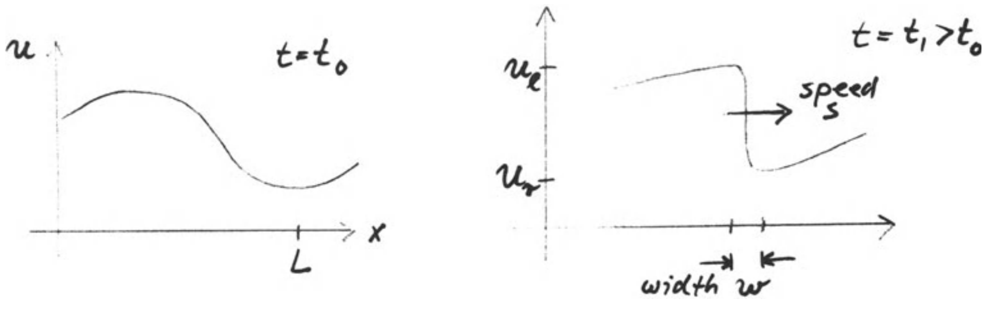

Fig. 1 The evolution of the initial data (left) under

$$u_t + uu_x = \nu u_{xx}$$

is given on the right.

Now data as in Fig. 1 leads to jumps in the solution, where the Rankine–Hugoniot conditions govern the relationship between the speed of the jump and its left and right asymptotic states.

When computing such a flow with very small viscosity ν, suppose we represent the state variables associated with points on a fixed underlying grid with spacing Δx. In this framework we would like to contrast two numerical methodologies: shock capturing and shock tracking. In the shock capturing methods ν is replaced by a numerical viscosity $\nu_{\text{num}} \gg \nu$. The width of a shock layer $w_{\text{num}} = \dfrac{\nu_{\text{num}}}{|u_l - u_r|} \sim 3\Delta x$, so that these waves are most accurate for weak waves. In a shock tracking method an additional moving grid point is introduced which serves as a marker for the shock position. The algorithm has to update its position and the asymptotic left and right states on the underlying fixed grid. For the moving of the shock point analytic information about it is necessary. Shock tracking corresponds to replacing ν by zero, so it is best for strong waves and gives a high resolution on relatively coarse grids.

The front tracking principle, which is not limited to conservation laws or to shocks, is that a lower dimensional grid gets fit to and follows the significant features in the flow. This is coupled with a high quality interior scheme to capture the waves that are not tracked.

In the following we talk only about front tracking in two space dimensions. First we describe tracking of a single wave and mathematical issues arising from this. Next we discuss tracking wave interactions and its mathematical issues. Then follows a section describing the data structure of a front tracking code. After a few numerical examples we give a conclusion.

Front tracking applied to a singe wave. Suppose we consider an expanding cylindrical shock wave for a certain time interval. Say this is modeled by the two dimensional Euler equations for polytropic gas dynamics where the outstanding feature of the flow is a shockwave with smooth flow in front and behind it. If the numerical simulation requires a high level of resolution on a moderate size grid, front tracking lends itself to this problem. To this end a one dimensional grid is fitted to the shock wave and follows its dynamic evolution. The smooth flow is captured using an underlying two dimensional grid, where in each time step an initial-boundary value problem is solved in each smooth component of the flow field.

The front is represented by a finite number of points along the curve, which carry with them physical data, in this case the left and right states and the fact that it is a hydrodynamic shock wave. Say the underlying grid is cartesian, which carries the associated state variables at each grid point. Each timestep consists of a front propagation and an interior update.

THE CURVE PROPAGATION is achieved by locally at each curve point rewriting the equation in a rotated coordinate system, normal and tangential to the front:

$$u_t + \hat{n}\big((\hat{n}\cdot\nabla)f(u)\big) + \hat{s}\cdot\big((\hat{s}\cdot\nabla)f(u)\big) = 0.$$

This then gets solved through dimensional splitting. The normal step reduces to a one dimensional Riemann problem, if one approximates the data to the left and right of the shock by constants.

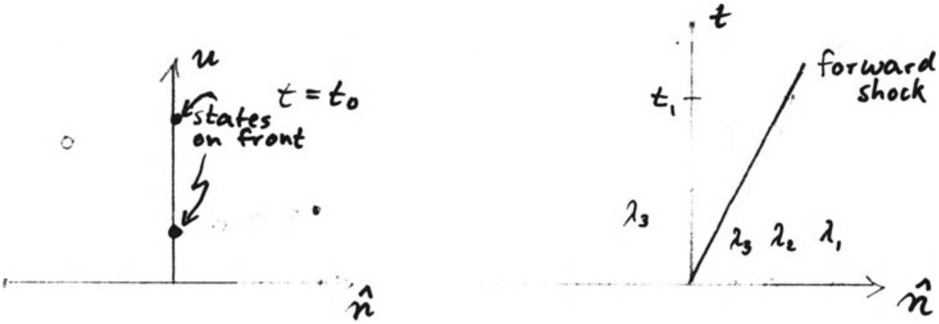

Fig. 2 A second order scheme for the normal propagation of a hydrodynamic shock wave, [CG].

This normal step can be made into a second order scheme in the following way [CG], see Fig. 2:

- first solve Riemann problem to obtain speed and approximate states at $t = t_1$,
- follow the characteristics from the left and right states at $t = t_1$ back to $t = t_0$ and use the data at the foot of them to obtain updated left and right states at $t = t_1$

– finally solve a Riemann problem at $t = t_1$ to improve states and speed there.

After the normal step has been implemented at all points representing the shock curve, the tangential step, which propagates surface waves, is done by a one dimensional finite difference scheme on each side of the front.

Because points on the front may move too far apart (or too close together) during propagation, a routine which redistributes the points along the curve is sometimes useful. One has to be cautious though, because this routine stabilizes the curve which may tend to become unstable due to physical or numerical effects.

THE INTERIOR SCHEME. The underlying principle is to solve an initial-boundary value problem on both sides of the front (the front is a moving boundary), and to never use states on the opposite side of the front. Away from the front this is readily achieved by using any finite difference scheme compatible with the resolution one needs in the interior. Near the front an algorithm which is consistent with the underlying partial differential equation has yet to be worked out. The following recipe has been implemented successfully (see Fig. 3): suppose the stencil gets cut off by the front. Use the states at the nearest crossing point (obtained through linear interpolation from the front states) and place them at the missing stencil points.

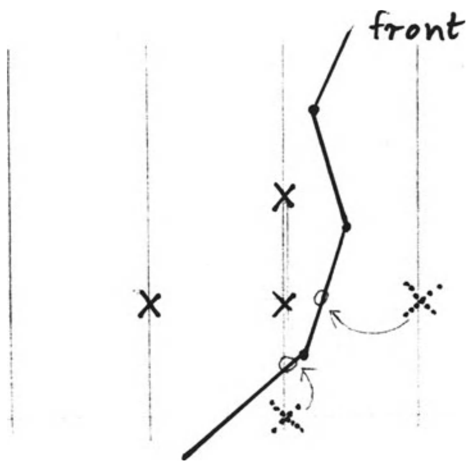

Fig. 3 A five point centered stencil near the front, where the states on the front are assigned to the two grid points on the opposite side of the front.

So far two papers have addressed the front-interior coupling problem in two space dimensions: [CC] suggest and implement a coupling which is conservative for gas dynamics. [KZ] have formulated a class of front tracking schemes for which they show stability.

Mathematical issues related to this. In the previous section we saw that this approach leads to the study of one dimensional Riemann problems. This is a special Cauchy problem of the type

$$u_t + f(u)_x = 0$$
$$u(0,) = \begin{cases} u_L, x < 0 \\ u_R, x > 0 \end{cases}$$

Since the equation and initial data are scale invariant

$$(x,t) \longrightarrow (\alpha x, \alpha t)\ ,\ \alpha > 0$$

we may expect scale invariant solutions. These are well understood e.g. for the scalar equation and for gas dynamics.

There is a considerable research effort trying to understand the Riemann solutions of more complicated models. One example are the 2×2 systems with quadratic flux functions studied by various authors, e.g. [IM], [IT]. New interesting mathematical phenomena arise:

– non-classical waves

– non-contractible discontinuous waves, i.e. it is not possible to decrease the wave strength to zero while following a connected brach of the wave curve

– open existence and uniqueness questions.

Another example are Riemann solvers for equations describing conservation of mass, momentum and energy in real materials. Their effects on the wave structure has been studied , [MP]. In another approach the equation of state is tabulated (SESAME code at Los Alamos). Scheuermann used this for a Riemann solver by preprocessing the data.

Finally we mention certain waves where the internal structure of the waves play a role. Whereas say for shock waves of isentropic gas dynamics the two jump equations plus the three pieces of information given by the impinging characteristics determine the four state variables on both sides of the shock with its speed, for transitional shock waves not enough information impinges through the characteristics and one needs information from the internal structure in order to determine speed and states. The structure depends sensitively on the viscosity used in the parabolic approximation. These waves thus present a danger for finite difference schemes, which introduce their own brand of viscosity which is different for different schemes. Here a tracking algorithm which mimicks the structure with a Riemann solver lends itself naturally to this problem.

The front tracking method described so far could also be applied to more complex flow patterns than the expanding spherical shock wave by simply tracking a single front and capturing all other phenomena using a high quality interior scheme. An example are the Euler equations coupled with complex chemistry used to model the flow around a hypersonic projectile [Zhu]. Here the hydrodynamic bowshock is tracked and the flow with most of the chemistry concentrated right behind this shock is captured. This is an example where a tracking of the bowshock is necessary.

Wave interaction. One can also track interacting waves. To illustrate this consider a planar shock wave impinging on a curved ramp (Fig. 4), giving rise first to a regular and then to a Mach reflection. This is an example on how new curves may arise. For hydrodynamic shock waves this bifurcation may arise through the intersection of shocks with each other or with other "curves", or through compressive waves ("blow up" of the smooth solution). If one wants to incorporate these phenomena into a front tracking algorithm it is necessary to understand them mathematically. For example in the case of the planar shock impinging onto the wedge, one needs a criterion which gives for given shock strength the ramp-angle when a bifurcation from regular to Mach reflection occurs. If one wants to track all the waves, the algorithm needs to have this criterion built in.

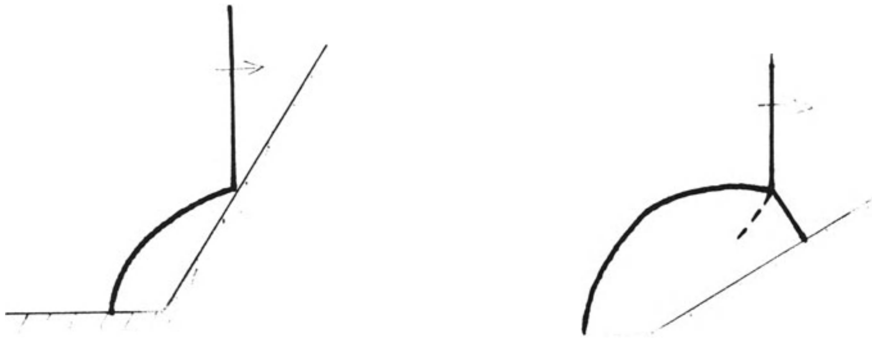

Fig. 4 A planar shock impinges onto a wedge, and, depending on the shock strength and wedge angle, give rise either to a regular reflection (left) or a Mach reflection (right). In the latter the reflected point has lifted off the wall to become a "triple point" from which a "Mach stem" connects to the wall.

This is an example of a two dimensional Riemann problem. In general, at the meeting point of more than two curves, if one approximates the curves by rays and the states nearby by constant states, these nodes are examples of two dimensional Riemann problems. As in one dimensional case, this is scale invariant Cauchy data $(x, y, t \longrightarrow \alpha, \alpha y, \alpha t\ ,\ \alpha > 0)$ giving rise to a self similar solution $u = u\left(\frac{x}{t}\ , \frac{y}{t}\right)$. Thus front tracking may lead to two dimensional Riemann problems.

Mathematical issues related to this. There has been some progress on studying the qualitative behavior of two dimensional Riemann problems. For the equations of compressible inviscid, polytropic gas dynamics, in analogy to the one dimensional Riemann problem which is resolved by elementary waves, one expects that the two dimensional Riemann problem will evolve into a configuration containing several two dimensional elementary waves. This this end these elementary waves were completely classified [GK], some of them can already be found in [L].

For the scalar two dimensional conservation law the two dimensional Riemann problem could be solved much further. For

$$u_t + f(u)_x + g(u)_y = 0$$

with $f = g$ it was solved in [W] (f convex), [L1], [L2] (f one inflection point), [KO] (f any number of inflection points). For $f \neq g$ [W] (f close to g, f convex) and [KO], [CH] (f convex, g one inflection point) gave solutions.

Numerical implementation. This knowledge of two dimensional Riemann problems has been used in front tracking codes to some extent. The classification of elementary waves for gas dynamics gave a list of the generic node one can expect there, that is all generic meeting points of shock waves, contact discontinuities and centered rarefaction waves. The tracking of a node is the numerical solution of a subcase of the full Riemann problem, one has to determine the velocity and states associated with one specific elementary wave. for gas dynamics this has been done [GK], G1], [G2].

For the scalar two dimensional conservation law the resolution of the two dimensional Riemann problem caused by the crossing of two shocks has been implemented. Whereas in [K] the point is to solve the interaction of two scalar waves quite accurately, in [GG] the emphasis is on following scalar wave interaction within a complicated topology of curves in a robust fashion without an unacceptable proliferation of subcases. An approximate numerical solution to a general two dimensional Riemann problem was implemented by approximating the flux functions by piecewise linear functions [R].

Computer science issues related to front tracking. Here we briefly describe a package of subroutines which provides facilities for defining, building and modifying decompositions of the plane into disjoint components separated by curves. It is worth noting that ideas from conceptual mathematics, symbolic computation and computer science have been utilized, thereby going beyond the usual numerical analysis framework, see [GM].

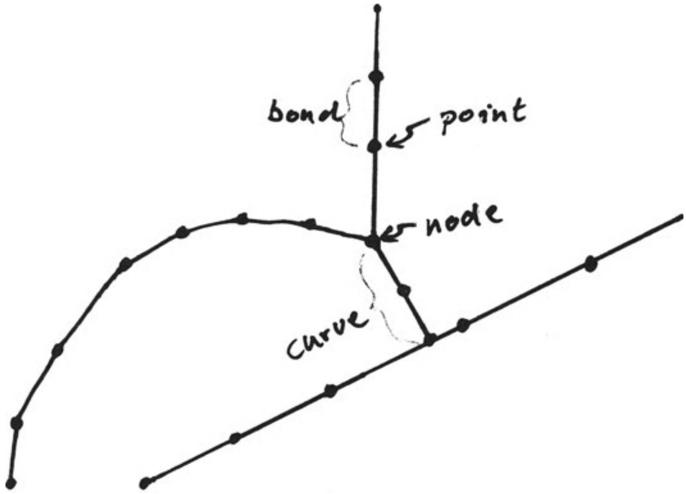

Fig. 5 The front tracking representation of a Mach reflection.

Taking the Mach reflection example (Fig. 4), we illustrate in Fig. 5 the representation of this particular flow. The front consists of piecewise linear curves at the endpoints of each linear piece we have associated quantities like states and wave types. Given this interface, the plane is decomposed into disjoint components. An integer component value is associated with each such component. Given any point x, y in the plane, the component value can be recovered. The underlying grid and possible interpolating grids near the front allow the definition of associated state variables in the interior.

There is a recursive data structure. It consists of

POINT:	which denotes the position of the grid points on the curve
BOND:	which denotes the piece of the curve between two adjacent points and previous bond by giving a start and an end point and having a pointer to the next
CURVE:	denoting usually a pice of the interface homotopic to an interval. A curve is a doubly-linked list of bonds given by a start and node (see below). It has a point to the first and last band.
NODE:	which is the position of a point on the interface where more than two curves meet. Its position is given with a list in and out curves.
INTERFACE:	is a list of nodes and curves

Then there are routines that operate on the interface structure. There are routines that allocate and delete the above structures, then those which add these to the interface, routines that split and join bonds and curves, all needed for example when there is a change in topology. Also one can traverse a list of the above structures.

The code has purposely been set up in such a way that this interface data structure can be dressed with the physics of a given problem containing curves. For gas dynamics one would associate with each point a left and right state, with each curve the wave type and at the node the state in each sector in order to have the set up for the Riemann problem.

This whole structure now needs routines which allows the interface to propagate from one timestep to the next. This is done by first moving the interface. This means moving bonds and nodes. Next the interior is updated. Then one has to handle possible interactions and bifurcations. These have to be detected, classified (they could be tangler of curves or two dimensional Riemann problems and then resolved. There is also a routine which redistribute points on the interface, in case they become to close together or too far apart.

Numerical examples. We shall give four examples out of many that have been calculated over the years with the code. Fig. 6 shows regular and Mach reflection, [GK]. Fig. 7 show an underwater explosion [G2]. Fig. 8 shows Rayleigh–Taylor instability [FG]. Fig. 9 shows an example from oil reservoir modelling [GG].

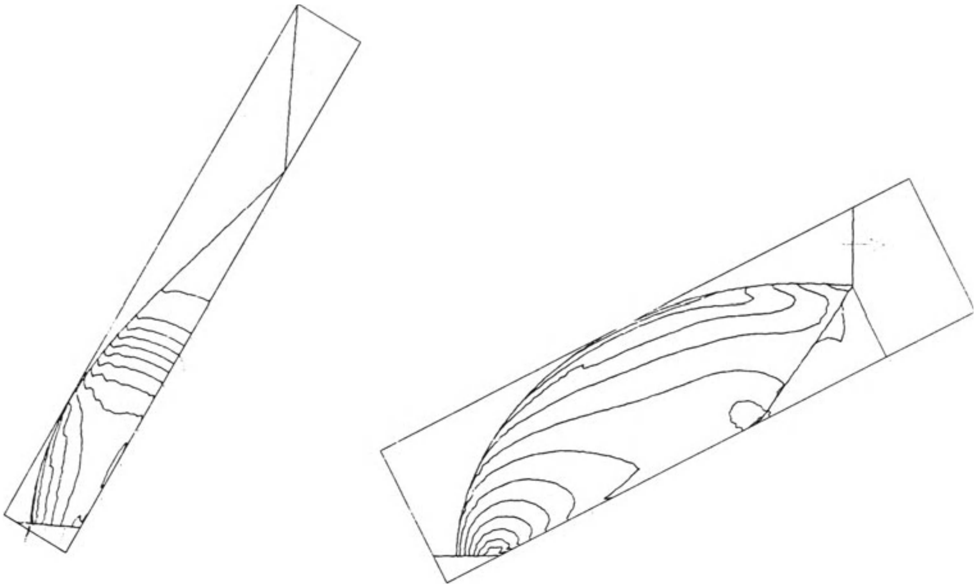

Fig. 6 On the left the numerical simulation of regular reflection, where the incident shock has Mach number 2.05 and the wedge angle is 63.4°. The calculation was performed on a 80 by 20 grid. The picture shows lines of constant density inside the bubble formed by the reflected shock.

On the right the numerical simulation of a Mach reflection, where the incident shock has Mach number 2.03 and the wedge is 27°. Inside the bubble formed by the reflected shock the calculated lines of constant density are shown. The calculations we performed on a 60 by 40 grid.

In both cases there is excellent agreement with experiments, [GK].

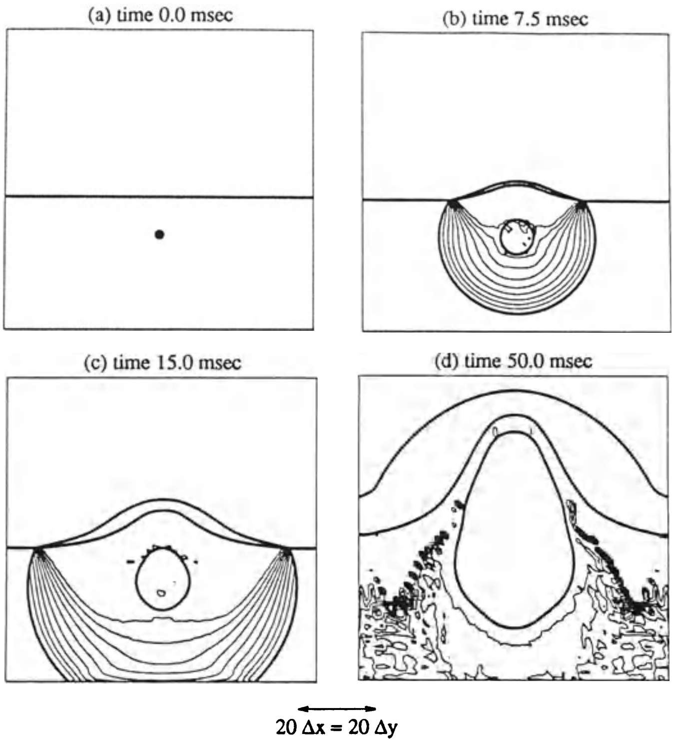

Fig. 7 An underwater expanding shock wave diffracting through the water's surface. The internal pressure is 100 kbans and initial radius of 1 meter installed 10 meters below the water's surface. The tracked front in dark lines is super imposed over lines of constant pressure. The grid is 60 by 120.

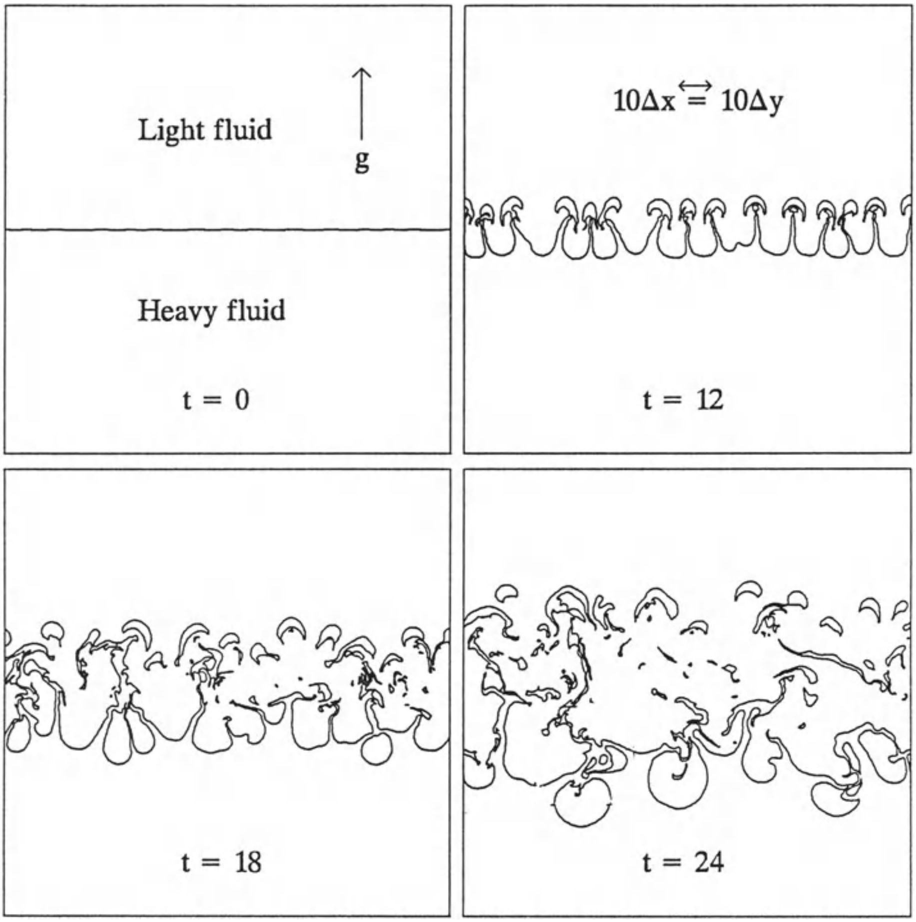

Fig. 8 Two compressible fluids of different densities, with gravitational forces (here positing upward) pushing lighter fluid into heavy one. The interface is initialized by 14 bubbles with different wave length and initial amplitude of 0.01. The density ratio is 10. The interface between these fluids is unstable and leads to a mixing layer, with bubbles of light fluid rising in the heavy fluid.

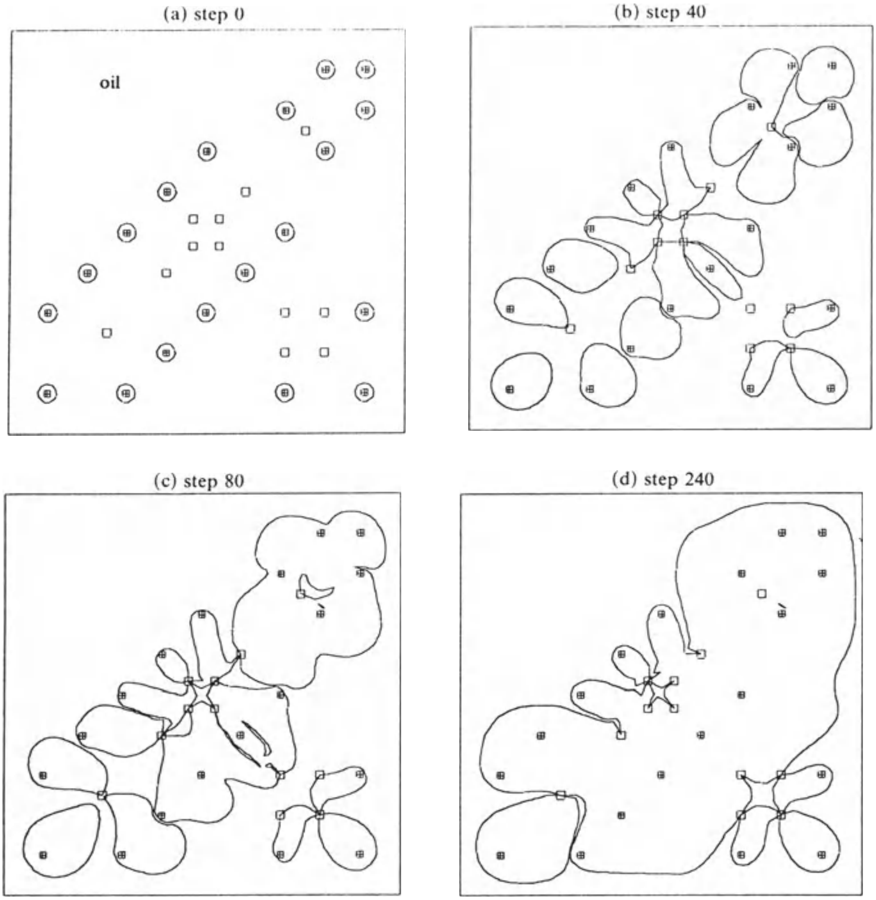

Fig. 9 A horizontal cross section of an oil reservoir modeled by the Buckley–Leverett equations. Water gets injected at 19 injection wells (cross squares), displacing the oil in the porous media, and oil get extracted at 12 producing wells (open squares). Plots of the fronts between water and oil are shown. The frontal mobility ratio for water displacing oil is 1.33.

Conclusion. It should have become clear that this numerical approach forces one to think hard about underlying physics and mathematics. If one is successful at penetrating the problem at hand, front tracking can give the correct simulation with very high resolution.

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