The Early Days of Lagrangian Hydrodynamics at Lawrence Livermore Laboratory*

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ABSTRACT

Reminiscences about the earliest 2-dimensional hydrodynamic calculations and their impact on later colliding black hole calculations.

I first arrived at Livermore on September 1, 1952 and was placed in what they called the "leper colony" for two or three months, waiting for my clearance to come through. I was given two books and told to read them. One was Chandrasekhar's Radiative Transfer, the other was Courant and Friedrichs' Supersonic Flow and Shockwaves. I couldn't understand Chandrasekhar's book, but I did enjoy Courant and Friedrichs. The day finally arrived when my clearance came through (this was a little before Jim arrived at the Lab), and I was shown to my office, right across the hall from Edward Teller. The first thing that happened was that Teller took me into his office and told me how bombs were made, with diagrams. I guess he wanted me to lose my virginity immediately. Then I was asked to study how to calculate problems in neutron diffusion when there are very rapidly changing parameters. So I learned about energy groups and diffusion equations, about matrices and operators which are not Hermitian and which don't

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have complete sets of eigenvectors. I remember seeing some papers of Dirac and Wigner that were still classified, on rather straightforward mathematical problems.

I had an officemate whose name I have forgotten (Jim can't remember it either). Bob Jastrow, who had arranged for me to come to the Lab (the deal was made at the APS Washington meeting, the previous May), was trying to get a two-dimensional hydrodynamic code operating. The réason for this effort had something to do with NATO, which I suppose I mustn't discuss. (But gosh, after 30 years!) At any rate my officemate was involved in it. I, too, began to think about hydrodynamical problems occasionally, particularly after Jim's arrival in the spring of '53. The kind of practical hydrodynamics the Lab had been involved with was spherical, one-dimensional. One used Lagrangian coordinates because they were generally the most accurate. Similar accuracy was needed in the two-dimensional effort, but everyone was afraid of using Lagrangian coordinates because they would inevitably become curvilinear and require the introduction of Jacobians! Being a relativist, I never could understand why people were so worried. I always thought that curvilinear coordinates were as good as any other. Well, you must understand that computers were a little slower in those days than they are now, and it was the Jacobians that really had everyone scared.

I was still working on neutron diffusion, but every once in a while I would talk to my officemate, or he would talk to me, giving me an account of the two-dimensional code. They had decided to try to model the fluid by means of individual mass points and to introduce forces between nearest neighbors. In the end that code just never flew. One evening, breaking the rules of the lab, I decided to work on the problem at home, actually writing things down on paper. I took the hydrodynamic equations in two dimensions and differenced them.

The basic equations are:

$$\dot{U} = -\frac{1}{\rho}\,\partial(P + Q)/\partial X \quad ,$$

$$\dot{V} = -\frac{1}{\rho}\,\partial(P + Q)/\partial Y \quad ,$$

$$\dot{X} = U \quad , \qquad \dot{Y} = V \quad ,$$

$$\dot{\rho} = -\rho(\partial U/\partial X + \partial V/\partial Y) \quad , \quad \text{and}$$

$$d(P/\rho^{\gamma}) = (\gamma - 1)Q\, d\rho/\rho^{\gamma+1} \quad .$$

The variables X and Y are the Eulerian coordinates of a fluid element, U and V are its velocity components, P is the pressure, Q (we already called it Q in those days) is the artificial viscosity, and ρ is the density. The first four equations are the hydrodynamic equations, the dots denoting total or Lagrangian time derivatives. I've also written down a γ-law equation of state and introduced a particular form for the artificial viscosity. This form will only give you bulk viscosity and won't be very good if you have slippage or severe shear in the fluid. These defects were removed later.

Now if you want to do Lagrangian hydrodynamics these derivatives with respect to the Eulerian coordinates have to be converted to derivatives with respect to Lagrangian coordinates x and y. It turns out that it's very convenient to introduce something like a Poisson bracket. If A and B are functions of x and y, their Poisson bracket is defined to be $[A,B] \equiv \frac{\partial A}{\partial x}\frac{\partial B}{\partial y} - \frac{\partial B}{\partial x}\frac{\partial A}{\partial y}$. Let ρ_0 be the density relative to the Lagrangian coordinates and ρ the Eulerian density. There is a simple relation between ρ and ρ_0 involving the Jacobian J, which is just the Poisson bracket of the Eulerian coordinates with respect to the Lagrangian coordinates:

$$J = \begin{vmatrix} \frac{\partial X}{\partial x} & \frac{\partial x}{\partial y} \\ \frac{\partial Y}{\partial x} & \frac{\partial Y}{\partial y} \end{vmatrix} \quad , \quad \text{and}$$

$$\rho_0 = \rho[X,Y] \quad .$$

Now the dynamical equations involve partial derivatives with respect to the Eulerian coordinates, but in the Lagrangian system, and hence

in the code, you actually compute Lagrangian derivatives. The problem is to convert from Eulerian to Lagrangian, and this involves $1/J$ and the Poisson bracket with the variable conjugate to whatever you're differentiating with respect to. If you put this into the dynamical equations, you'll notice that on the right hand side of the $\dot{U}$ and $\dot{V}$ equations ρ^{-1} appears together with a gradient. The gradient introduces a $1/J$ which gets together with the $1/\rho$ to give you a $1/\rho_0$:

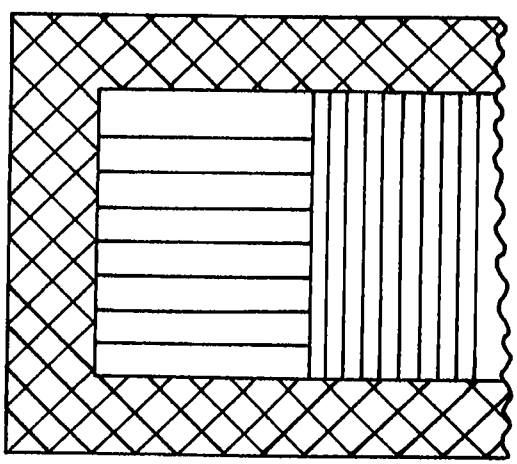
$$\dot{U} = -\frac{1}{\rho_0}\,[P + Q,\ Y] \quad ,$$

$$\dot{V} = +\frac{1}{\rho_0}\,[P + Q,\ X] \quad .$$

The Jacobians simply drop out and you're left with very simple equations. At least they seemed simple to me. So the next morning I went to Teller and said, "I must be missing something. I don't really understand what the difficulty is," and showed him these equations. That afternoon he called a meeting of the whole lab, and I stood up and went through essentially what I've just done for you here and was the overnight expert on two-dimensional hydrodynamics! I was told that I had to have a program coded and run before a certain date in June. There was going to be a test shot and the lab wanted some numbers. Well, it's one thing to have these simple-looking equations and another to apply them. I had to sit down and think about things that had never occurred to me before.

The first problem was the perennial one of what to do at the edge of the mesh. But things were even worse than that, as you can see in the accompanying sketch. Shown is a representation of a small portion of a certain "device". The crosshatched region represents a certain material that surrounds things, the horizontal lines represent some high explosive, and the vertical lines represent something else. The worrisome thing was that there was obviously going to be some strong slippage at the interfaces between different materials. I

thought at first that maybe I could just treat it as all one fluid with the density simply changing abruptly at the interfaces and allowing the mesh to stretch. But it was clear that the mesh was going to stretch far too much to be reliable, so I had to figure out how to tell the programmer (we didn't do the actual programming ourselves in those days) to make tests so that the various mesh points at the edge of one material would know which mesh points at the edge of the other material they were near to.



Sketch

I had never done a hydrodynamic calculation before, so I figured I had better do at least one 1-dimensional calculation. Of course I went to Jim for guidance, particularly on the artificial viscosity. I had seen the paper by Richtmeyer and von Neumann on the stability condition. Now it was all very nice to read that paper, which was done in terms of Fourier transforms, but it lacked a certain gut feeling. Jim pointed out the simple explanation of the stability condition: when you difference the differential equations you only hook neighboring mesh points together, and if you make the time step

too large the pressure wave simply can't get out as fast as the sound velocity, so the program blows up in your face. It's a little harder to understand the physical basis of the stability criterion for the parabolic heat equation, but even that you can sort of absorb.

After reasonable success with one-dimensional problems I tackled the two-dimensional problem in earnest. What I finally sent to the programmer must have been a sheaf of 20 or 30 pages. Of course, I was worried. When you have to come up with a number by a certain date, well, it focusses the mind! I had tried very carefully to think out every single step, to give correct sequences of commands like $\rho_{k\ell n} = \rho_{k\ell n-1} + \ldots$, or something like that, repeated with k and ℓ ranging over certain values, and with occasional iterations. Then there were all the special commands at the interfaces. Incidentally, there were no textbooks in numerical analysis, but I don't think they would have helped. We had all attended a course in which we learned a little bit of machine language, and I remember there were commands like BOOM... and ZOOM... One had to tell the machine every step. Our instructors were great; full of enthusiasm. They prayed to our computer every night, I believe. For them it was God. They were fascinated by being so close to such a great machine, which, of course, was just a piddling little machine by present standards.

Anyway, to get back to my story, I gave my sheets of paper to the programmer. I don't know what his own personal debugging problems were, but he didn't come back to me before the program actually ran. They got a number out after two or three hundred hours of computer time, before the test shot! Then I was told to prepare another program. Not until then did the programmer come to see me again. He didn't know what the computation was all about. He had previously just taken my instructions and done what I had indicated. He now thought it might be a good idea if he knew a little bit about the problem. So I spent two or three days going step by step and explaining everything. Then he pointed out to me that one could greatly improve the data input scheme and the way the computations were organized. This gave birth to a new program, but I don't know what ever happened to it. I left the lab before the next test shot came up. All I know is that it was a much more efficient code and ran more rapidly.

When I left Livermore, I went to the University of North Carolina and all these hydrodynamical problems were put out of my mind for years. But in 1970 I had begun to think about the gravitational two-body problem. I thought it was a scandal that nobody had ever tackled this problem. The three-body problem had been the great challenge in Newtonian mechanics. The two-body problem was the analogous challenge in general relativity. I discovered that my time at Livermore hadn't been wasted. (Nothing you learn is ever wasted.) All the lore of differencing partial differential equations came back to me, and I guided my student Andrej Cadez on the first colliding-black-hole computation. Then I moved to Texas, and Larry Smarr was induced to continue the work. By that time, textbooks on numerical analysis were available. Students nowadays seem to be afraid to get into big computations before they've checked what the textbooks say. I would tell Larry: "Listen, Jim Wilson doesn't operate that way. Just take the damned equations and difference them" I think my having referred to Jim so often, as a kind of model for how to attack big problems, led Larry to seek Jim out later. Well, to me at any rate, it seemed that you should just use common sense. Don't be afraid to try something. If there are physical constraints that can help you choose how to do the differencing, fine, but don't be afraid to go ahead anyway. Larry proved to me later that, occasionally, it is good to use fancy techniques. He pointed out that in the case of the diffusion equation there was a method that had been developed in the years since 1952 known as overrelaxation. He was all fired up about it, and I said "Yeah, okay, I'm glad."

Just this last summer, I had a student working on a problem in which we needed to compute the world function (which is one-half the square of the geodetic distance between two space-time points) in a Robertson-Walker universe. The world function satisfies a certain partial differential equation, which is basically a Hamilton-Jacobi equation, so I said, "It seems to me that the simplest thing to do would be to use this Hamilton-Jacobi equation." So he put it on the computer and got bad results no matter what he tried. I said, "Gosh, I don't know. Maybe you should give it a stability analysis," that is, look at the Fourier transform. We discovered that this is an equation which is unconditionally unstable no matter how you differ-

ence it. So sometimes it does pay to do a little analytical work ahead of time.

Let me end by showing you what the hydrodynamic equations look like in 3-D:

$$\dot{U} = -\frac{1}{\rho_0}\,[P + Q,\ Y,\ Z] \quad ,$$

$$\dot{V} = -\frac{1}{\rho_0}\,[P + Q,\ Z,\ X] \quad ,$$

$$\dot{W} = -\frac{1}{\rho_0}\,[P + Q,\ X,\ Y] \quad ,$$

$$\dot{X} = U \quad , \qquad \dot{Y} = V \quad , \qquad \dot{Z} = W \quad ,$$

$$\rho_0 = \rho[X,\ Y,\ Z] \quad , \quad \text{and}$$

$$[A,B,C] \equiv \frac{\partial A}{\partial x}\frac{\partial B}{\partial y}\frac{\partial C}{\partial z} + \frac{\partial A}{\partial y}\frac{\partial B}{\partial z}\frac{\partial C}{\partial x} + \frac{\partial A}{\partial z}\frac{\partial B}{\partial x}\frac{\partial C}{\partial y} - \frac{\partial A}{\partial x}\frac{\partial B}{\partial z}\frac{\partial C}{\partial y} - \frac{\partial A}{\partial z}\frac{\partial B}{\partial y}\frac{\partial C}{\partial x} - \frac{\partial A}{\partial y}\frac{\partial B}{\partial x}\frac{\partial C}{\partial y} \quad .$$

They have the same form as in 2-D, only a triple bracket appears instead of a Poisson bracket. I had shown these equations to Teller that day, too. He once came to me later saying that we must get <u>them</u> on the computer because they are what is needed for the attack on the turbulence problem! As far as I know, that problem still stands.

Warmest birthday greetings, Jim, and thanks for giving me this chance to reminisce.