

Sod's Shock Tube Problem

A simple one dimensional model of a gas was introduced by G.A. Sod, *J. Computational Physics* **27**, 1 (1978), to test the ability of various algorithms in solving fluid dynamics problems with shock wave behavior.

The equations of gas dynamics

The equations of fluid dynamics are mathematical statements of three fundamental physical principles:

- Mass is conserved
- $\mathbf{F} = m\mathbf{a}$, i.e., Newton's second law
- Energy is conserved

The one-dimensional equations for the fluid dynamics of a gas can be written in *conservation form* as follows:

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} &= 0 \\ \frac{\partial(\rho u)}{\partial t} + \frac{\partial}{\partial x}(\rho u^2 + p) &= 0 \\ \frac{\partial e}{\partial t} + \frac{\partial}{\partial x}(u(e + p)) &= 0\end{aligned}$$

where ρ is the density of the fluid, u is the fluid velocity, e is the energy per unit volume (length), and p is the pressure. We need one more equation to close the system. This is the equation of state

$$p = (\gamma - 1) \left(e - \frac{1}{2} \rho u^2 \right),$$

where γ is the adiabatic gas index. For an ideal gas $\gamma = 1.4$.

These equations can be written in vector form

$$\frac{\partial}{\partial t} \mathbf{U} + \frac{\partial}{\partial x} \mathbf{F}(\mathbf{U}) = 0,$$

where

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ e \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ u(e + p) \end{pmatrix}.$$

The shock tube problem

Sod considered a one-dimensional tube of unit length $0 \leq x \leq 1$ and the following initial conditions at $t = 0$:

$$\begin{aligned} \rho(x, 0) &= \begin{cases} 1.0 & \text{for } x \leq \frac{1}{2} \\ 0.125 & \text{for } x > \frac{1}{2} \end{cases}, \\ p(x, 0) &= \begin{cases} 1.0 & \text{for } x \leq \frac{1}{2} \\ 0.1 & \text{for } x > \frac{1}{2} \end{cases}, \\ u(x, 0) &= 0. \end{aligned}$$

This initial state can be produced by having a diaphragm in the middle of the tube. The gas to the left and right of the diaphragm is initially at rest. The pressure and density are discontinuous across the diaphragm. At $t = 0$, the diaphragm is broken. Two types of singularities then propagate through the gas:

- **Contact discontinuities:** The pressure p and velocity u are continuous, but the density ρ and energy per unit volume e are discontinuous.
- **Shock waves:** All quantities p, u, ρ and e are in general discontinuous across the shock front.

To simulate a closed tube, reflection boundary conditions can be applied at $x = 0, 1$. The shock tube then exhibits interesting behavior with shock waves and contact discontinuities bouncing back and forth in the tube and interacting with one another.

Direct Simulation Monte Carlo

Direct Simulation Monte Carlo (DSMC) was introduced by G.A. Bird in the 1960's to study the dynamics of dilute gases for which the continuum Navier-Stokes equations are no longer valid. This method uses ideas from Molecular Dynamics, Monte Carlo, and Fluid Dynamics; and it is reminiscent of cellular automaton rules. Thus it is a nice example to end this course.

The Navier-Stokes equations assume the fluid is a continuum, while the DSMC method takes into account the discrete nature of the molecules making up the fluid. If the fluid is contained in a region of typical size L (for example the diameter of a pipe), and if λ is the mean free path of a fluid molecule, then the dimensionless *Knudsen number*

$$\text{Kn} = \frac{\lambda}{L},$$

determines whether the continuum or particle description is appropriate. Generally, if $\text{Kn} > 0.1$ the continuum description breaks down and the discrete nature of the fluid particles becomes important.

In air at atmospheric pressure, $\lambda \sim 50$ nm which is comparable to the wavelength of light, so for most applications the atmosphere can be described using the Navier-Stokes equations. The gap between the head and platter of a disk drive is ≈ 50 nm which means that $\text{Kn} \approx 1$ and a particle description must be used. The mean free path of air molecules increases with height above the surface of the Earth. When the space shuttle enters the atmosphere at an altitude of ~ 120 km a bow shock develops in front of its nose cone: at this altitude the mean free path of an air molecule is a few meters, and the continuum approach is not sufficient to model the shock wave.

Under such conditions, Molecular Dynamics methods are practical only for simulations that last a few nanoseconds of real time. To speed up the calculations, the DSMC method makes the following approximations:

- The number of particles is greatly reduced by replacing N_{eff} real molecules by a single simulation particle. N_{eff} is chosen such that there are at least 20 simulational particles per λ^3 . In MD, all molecules must be simulated.
- The system volume V is divided into cells whose linear dimension L_c is no larger than the mean free path λ . Collisions take place only between particle pairs that are in the same spatial cell. In MD there is a force between every pair of particles, although simplifying approximations can be made if the forces are short ranged.

- A Monte Carlo time step τ is chosen such that it takes a few time steps for a particle to move through a cell

$$\tau = \frac{aL_c}{\langle v \rangle} ,$$

where a is a fraction, e.g., 0.2. In MD the time step must be chosen small enough to solve Newton's equations to the required accuracy. This time step is usually much smaller than that required in DSMC.

- The positions and velocities of particles are updated by
 - moving each particle ignoring possible collisions

$$\vec{r}_i(t + \tau) = \vec{r}_i(t) + \vec{v}_i(t)\tau ,$$

- updating the velocities by colliding all pairs of particles in a cell according to a stochastic formula:

Repeat sufficiently many times so that the total number of collisions in the cell is approximately the same as the total number of collisions in the real gas:

- A pair of particles in a cell is selected at random.
- The pair is collided only if the relative speed v_r is large enough: this decision made stochastically by generating a random deviate r and colliding the pair only if $v_r > rv_r^{\max}$ where $v_r^{\max}$ is the maximum relative velocity of all pairs in the cell.
- If a pair passes this “ v_r large enough” test the velocities of the two particles are changed randomly, usually by choosing a randomly from all possible final states in a realistic collision.

In MD, the positions and velocities are updated simultaneously by constructing actual trajectories.

Note the similarity of DSMC algorithm to the Lattice Gas Cellular Automaton: there is an advection step to move the particles, followed by a collision step to update their velocities.