Title: Gas Dynamics Equations: Computation

Name: Gui-Qiang G. Chen

Affil./Addr.: Mathematical Institute, University of Oxford

24–29 St Giles, Oxford, OX1 3LB, United Kingdom

Homepage: http://people.maths.ox.ac.uk/chengq/

Email: chengq@maths.ox.ac.uk

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Shock waves, vorticity waves, and entropy waves are fundamental discontinuity waves in nature and arise in supersonic or transonic gas flow, or from a very sudden release (explosion) of chemical, nuclear, electrical, radiation, or mechanical energy in a limited space. Tracking these discontinuities and their interactions, especially when and where new waves arise and interact in the motion of gases, is one of the main motivations for numerical computation for the gas dynamics equations.

The fundamental equations governing the dynamics of gases are the compressible Euler equations, consisting of conservation laws of mass, momentum, and energy:

$$\begin{cases} \partial_t \rho + \nabla \cdot \mathbf{m} = 0, \\ \partial_t \mathbf{m} + \nabla \cdot \left(\frac{\mathbf{m}\otimes\mathbf{m}}{\rho}\right) + \nabla p = 0, \\ \partial_t(\rho E) + \nabla \cdot \left(\mathbf{m}(E + \frac{p}{\rho})\right) = 0, \end{cases} \tag{1}$$

where ∇ is the gradient with respect to the space variable $\mathbf{x} \in \boldsymbol{R}^d$, ρ is the density, $\mathbf{v} \in \boldsymbol{R}^d$ is the gas velocity with $\rho\mathbf{v} = \mathbf{m}$ the momentum vector, p is the scalar pressure, and $E = \frac{1}{2}|\mathbf{v}|^2 + e(\tau, p)$ is the total energy with e the internal energy, a given function of (ρ, p) defined through thermodynamical relations. The notation $\mathbf{a} \otimes \mathbf{b}$ denotes the tensor product of two vectors. The other two thermodynamic variables are the temperature θ and the entropy S. If (ρ, S) are chosen as the independent variables, then the constitutive relations $(e, p, \theta) = (e(\rho, S), p(\rho, S), \theta(\rho, S))$ are governed by

$$\theta dS = de + p\, d(\frac{1}{\rho}).$$

For a polytropic gas, $p = R\rho\theta, e = c_v\theta, \gamma = 1 + \frac{R}{c_v}$, and

$$p = p(\rho, S) = \kappa\rho^{\gamma} e^{S/c_v}, \qquad e = \frac{\kappa}{\gamma - 1}\rho^{\gamma-1} e^{S/c_v} = \frac{R\theta}{\gamma - 1}, \tag{2}$$

where R, c_v, and κ are positive constants, respectively. System (1) is complemented by the Clausius inequality:

$$\partial_t(\rho a(S)) + \nabla \cdot (\mathbf{m} a(S)) \geq 0$$

in the sense of distributions for any $a(S) \in C^1, a'(S) \geq 0$, to identify physical shocks.

The Euler equations for an isentropic gas take the simpler form:

$$\begin{cases} \partial_t \rho + \nabla \cdot \mathbf{m} = 0, \\ \partial_t \mathbf{m} + \nabla \cdot \left(\frac{\mathbf{m} \otimes \mathbf{m}}{\rho}\right) + \nabla p = 0, \end{cases} \tag{3}$$

where $p(\rho) = \kappa_0 \rho^{\gamma}$ with constants $\gamma > 1$ and $\kappa_0 > 0$.

These systems fit into the general form of hyperbolic conservation laws:

$$\partial_t \mathbf{u} + \nabla \cdot \mathbf{f}(\mathbf{u}) = 0, \qquad \mathbf{u} \in \boldsymbol{R}^m,\ \mathbf{x} \in \boldsymbol{R}^d, \tag{4}$$

where $\mathbf{f} : \boldsymbol{R}^m \to (\boldsymbol{R}^m)^d$ is a nonlinear mapping. Besides (1) and (3), most of partial differential equations arising from physical or engineering science can be also formulated into form (4), or its variants, for example, with additional source terms or equations modeling physical effects such as dissipation, relaxation, memory, damping, dispersion, and magnetization. Hyperbolicity of system (4) requires that, for all $\xi \in S^{d-1}$, the matrix $(\xi \cdot \nabla \mathbf{f}(\mathbf{u}))_{m \times m}$ have m real eigenvalues $\lambda_j(\mathbf{u}, \xi), j = 1, 2, \cdots, m$, and be diagonalizable.

The main difficulty in calculating fluid flows with discontinuities is that it is very hard to predict, even in the process of a flow calculation, when and where new discontinuities arise and interact. Moreover, tracking the discontinuities, especially their interactions, is numerically burdensome (see [1, 6, 12, 16]).

An efficient numerical approach is shock capturing algorithms. Modern numerical ideas of shock capturing for computational fluid dynamics can date back to 1944 when von Neumann first proposed a new numerical method, a centered difference scheme, to treat the hydrodynamical shock problem, for which numerical calculations showed oscillations on mesh scale (see Lax [15]). von Neumann's dream of capturing shocks was first realized when von Neumann and Richtmyer [27] in 1950 introduced the ingenious idea of adding a numerical viscous term of the same size as the truncation error into the hydrodynamic equations. Their numerical viscosity guarantees that the scheme is consistent with the Clausius inequality, i.e., the entropy inequality. The shock jump conditions, the Rankine-Hugoniot jump conditions, are satisfied, provided that the Euler equations of gas dynamics are discretized in conservation form. Then oscillations were eliminated by the judicious use of the artificial viscosity; solutions constructed by this method converge uniformly, except in a neighborhood of shocks where they remain bounded and are spread out over a few mesh intervals.

Related analytical ideas of shock capturing, vanishing viscosity methods, are quite old. For example, there are some hints about the idea of regarding inviscid gases as viscous gases with vanishingly small viscosity in the seminal paper [23] by Stokes (1848), as well as the important contributions of Rankine [20] , Hugoniot [13], and Rayleigh [21].

The main challenge in designing shock capturing numerical algorithms is that weak solutions are not unique; and the numerical schemes should be consistent with the Clausius inequality, the entropy inequality. Excellent numerical schemes should also be numerically simple, robust, fast, and low cost, and have sharp oscillation-free resolutions and high accuracy in the domains where the solution is smooth. It is also desirable that the schemes capture vortex sheets, vorticity waves, and entropy waves, and are coordinate invariant, among others.

For the one-dimensional case, examples of success include the Lax-Friedrichs scheme (1954), the Glimm scheme (1965), the Godunov scheme (1959) and related high order schemes; for example, van Leer's MUSCL (1981), Colella-Wooward's PPM (1984), Harten-Engquist-Osher-Chakravarthy's ENO (1987), the more recent WENO (1994, 1996), and the Lax-Wendroff scheme (1960) and its two-step version, the Richtmyer scheme (1967) and the MacCormick scheme (1969). See [3, 4, 6, 8, 11, 17, 24, 25] and the references cited therein.

For the multi-dimensional case, one direct approach is to generalize directly the one-dimensional methods to solve multi-dimensional problems; such an approach has led several useful numerical methods including semi-discrete methods and Strang's dimension-dimension splitting methods.

Observe that multi-dimensional effects do play a significant role in the behavior of the solution locally, and the approach that only solves one-dimensional Riemann problems in the coordinate directions clearly lacks the use of all the multi-dimensional information. The development of fully multi-dimensional methods requires a good mathematical theory to understand the multi-dimensional behavior of entropy solutions; current efforts in this direction include using more information about the multi-dimensional behavior of solutions, determining the direction of primary wave propagation and employing wave propagation in other directions, and using transport techniques, upwind techniques, finite volume techniques, relaxation techniques, and kinetic techniques from the microscopic level. See [2, 14, 18, 24]. Also see [8, 10, 11, 17, 25] and the references cited therein.

Other useful methods to calculate sharp fronts for gas dynamics equations include front-tracking algorithms [5, 9], level set methods [19, 22], among others.

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