Artificial viscosity—then and now

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Abstract In this paper, we recount the history of artificial viscosity, beginning with its origin in previously unpublished and unavailable documents, continuing on to current research and ending with recent work describing its physical basis that suggests new directions for improvement. This review is mainly about finite volume methods and the finite scale theory, We focus on the underlying ideas that recognize the finiteness of scale and measurement.

Keywords Shocks · Artificial viscosity · Finite scale theory

1 Preface

We don’t see things as they are; we see them as we are. (Anonymous)

We celebrate the centennial anniversary of Richard Becker’s seminal paper on shock structure [4]. Becker’s paper is most often cited for his clever solution of the Navier–Stokes equations for the planar shock. However Becker’s main purpose was to cast doubt on the ability of the Navier–Stokes equations to model shock structure. Becker concluded from his solution that a shock would be about one molecular mean free path wide, violating the assumptions under which the Navier–Stokes equations are derived from the Boltzmann equation [23]. It would be more than 50 years before computer simulation [5] and laboratory experiments [3, 57] would show that physical shocks are measured to be twice the width predicted by theory, validating Becker’s assertion that something beyond the Navier–Stokes description is needed.

While the inaccuracy of Navier–Stokes as a model for shocks is generally accepted, a more accurate continuum model is still not at hand. Recently, the finite scale equations [30] have achieved some success in predicting the width and the shape of shocks as measured in the laboratory [35, 36]. The finite scale theory is designed to be a differential model of the discrete equations used in numerical simulation. One key development of the theory is the derivation of the artificial viscosity, showing that it has a physical origin in addition to its numerical benefits [31].

The focus in this paper is on the ideas that underlie artificial viscosity, both as a numerical strategy and as a physical phenomenon. We review those underlying ideas which lie mainly in finite volume methods.
and the finite scale theory and provide copious references where mathematical details can be found. We build on Becker’s original work that emphasizes the role of dissipation in accurately modeling finite shock structure, and offer the speculative conclusion that on length scales much larger than the molecular mean free path, it is in the discrete equations that an improved description of nature may be found.

2 Introduction

What we observe is not nature itself, but nature exposed to our method of questioning. (Werner Heisenberg [19])

Artificial viscosity is one of the oldest and most enduring concepts in computational fluid dynamics (CFD). The earliest computer simulations of shocks by Los Alamos staff showed unphysical oscillations (wiggles) behind the shock front. The first remedy was based on shock tracking, a cumbersome process that required continuous human interaction with the computer [47]. Artificial dissipation as it was first termed represented an effective automatic solution to eliminate the wiggles. In Sect. 3 we will describe this early history. Some of this history is newly recorded due to the recent release of formerly classified documents by Los Alamos National Laboratory.

The early simulations of shocks were done in Lagrangian codes in which the computational mesh moves with the local fluid velocity and so adapts to the large compressions within the shock profile. Explicit artificial viscosity proved overly diffusive when implemented in Eulerian codes which operate on a fixed mesh. The development of nonoscillatory methods for Eulerian codes in the early 1970s represented a revolution in CFD. In Sect. 4 we will detour to discuss the ideas that underlie this seemingly independent solution to eliminating unphysical oscillations.

In Sect. 5 we describe some current work designed to improve the application of artificial viscosity. These focus on two areas: 1) incorporating the ideas of nonoscillatory differencing to Lagrangian codes to minimize the effect of the artificial dissipation on smooth parts of the flow; 2) developing a tensor artificial viscosity to better preserve the geometric symmetries of the flow.

The finite scale theory [30] was formulated to provide a theoretical basis for implicit large eddy simulation (ILES) [17], then a controversial methodology for simulating turbulent flows. However, the derivation of the finite scale equations does not refer either to turbulence nor to numerical simulation. In Sect. 6 we review the derivation of the finite scale equations and its application to the theory of shocks. The finite scale equations provide new insights into the interpretation of artificial viscosity, which we detail in Sect. 7, and its implementation which we discuss in 8.

We conclude the paper in Sect. 9 with a brief summary and thoughts for future development.

3 The heroes of artificial viscosity

Now it can be told (Gen. Leslie Groves, [18])

Here we describe the early contributions of five heroes of artificial viscosity, Rudolf Peierls, Robert Richtmyer, John von Neumann, Rolf Landshoff and William Noh.

Rudolf Peierls

The need for artificial dissipation to smear shocks was recognized by von Neumann even before the ENIAC (the first electronic computer) was operational. von Neumann had proposed several ideas to Peierls, who responded in a letter dated March, 1944. In the last paragraph of that letter, Peierls wrote:

Incidentally, have you thought at all about the following alternative way of avoiding discontinuity. In actual fact, the shock front has a finite width because of the viscosity and thermal conductivity of the medium. But artificially, assuming a viscosity very much larger than the actual, you can obtain instead of the discontinuity a front of a finite width. [49]

The idea that important features of a shock, in particular the shock velocity and the Rankine–Hugoniot relations, (the jump conditions), are independent of the physical viscosity had been known since the 1870 paper of Rankine [56]. The application of that independence has proved a fundamental insight for CFD.

1 Numerical programs for solving hydrodynamic problems are typically called codes.
Robert Richtmyer In the open literature of numerical shocks, the name Richtmyer is invariably associated with von Neumann by virtue of their landmark paper of 1950 [65]. However, the release of several formerly classified Los Alamos reports tells a more detailed story making it clear that, in the case of artificial viscosity, it was Richtmyer alone who did the heavy lifting. In an effort to give proper credit, we will discuss the reports written solely by Richtmyer [53, 54] separately here. The scope and breadth of Richtmyer’s report is nicely captured in the abstract to [53].

This report gives a method of handling the finite difference equations of hydrodynamics of compressible fluids. Shocks are automatically taken care of by the expedient of introducing a (real or fictitious) dissipation term . . . The effect of this term is to “smear” the shock somewhat, but the Hugoniot–Rankine conditions are satisfied and the entropy increase is correct; [53]

Among the insights of this first report, Richtmyer discusses the source of the observed post-shock oscillations, the importance of conservation and the associated issues of numerical stability.

Perhaps the most important (and unexpected) contribution is the form of the dissipative term, which is quadratic in the velocity gradient as contrasted with physical viscous dissipation which is linear. Richtmyer derives the quadratic form by requiring that shocks of varying strengths, i.e, Mach number, should all have approximately the same width when measured in units of the grid spacing $\Delta x$. Richtmyer’s insight was driven by stability considerations; however it is interesting that the width of physical shocks is also relatively constant when measured in terms of the molecular mean free path [3, 57]. But Richtmyer could not have known that fact as those measurements were first made more than 20 years after his report.

The first report [53] was written in March of 1948 and quickly followed by a second report [54] in August of 1948. The main purpose of that report was to demonstrate that the artificial viscosity would be stable with the proper choice of the dimensionless coefficient. It is not explicitly stated how the numerical calculations were performed, but it appears they were done by hand rather than on an electronic computer. Richtmyer notes that the calculations were performed by Irene Stegun, who is better known as co-author of the Handbook of Mathematical Functions (Abramowitz & Stegun). In any case, those calculations which comprised less than 20 computational cycles were compelling.

Richtmyer gives explicit credit to von Neumann and Peierls for the idea of shock capturing. He also references Becker [4] for the importance of dissipation in producing a finite shock width. Curiously, the possibility of including an artificial thermal conduction is not mentioned even though the simultaneous consideration of viscosity and thermal conduction is a principal new result of Becker’s derivation of shock profile.

John von Neumann The 1950 journal article by von Neumann and Richtmyer can be seen to contain a subset of the results of Richtmyer’s report [53]. In particular, the quadratic form of the artificial viscosity is not derived in the paper, but rather is postulated and shown to satisfy certain numerical and physical requirements. Further, no simulations are presented to illustrate the effectiveness of artificial viscosity. However the importance of this paper’s appearance in the open literature cannot be overstated. The modern reader may not appreciate the challenges of computing in this period, the lack of capability and lack of access [16]. We note that Becker’s paper [4] is also cited here, though no reference is made to Peierl’s insight.

In addition to the artificial dissipation and the linearized stability analysis, the idea of the staggered mesh for Lagrangian simulations was openly introduced in this landmark paper.

Rolf Landshoff Landhoff’s singular contribution to artificial viscosity lies in an unpublished report [24] in 1955 in which the modern form of artificial viscosity, referred to as linear plus quadratic $Q$ was first formulated.

Landhoff is a curious choice for a hero of artificial viscosity. He was neither primarily a hydrodynamics nor a computational fluids physicist. Further, the theoretical development in his report is substantially incorrect. Nevertheless, his intuition has proved correct and enduring [11]. Although the quadratic viscosity of Richtmyer controlled the unphysical post-shock oscillations, it did not totally eliminate them nor the troublesome overshoot that typically appeared at the head of the numerical shock.

Landhoff’s idea was to add a second term to the artificial dissipation that is linear in the velocity
gradient. Landshoff apparently understood that the overshoot was a result of numerical (truncation) error, but still attempted to justify the linear viscosity in a more theoretical calculation. His calculation included integrating a characteristic through the shock, which effectively implies that entropy is conserved through the shock. Ironically, this is the same error made by Stokes more than 100 years earlier, only to be corrected in Rankine’s 1870 paper [56]. That entropy is not conserved in a shock but must increase was explicitly noted in Richtmyer’s report [53]. Landshoff also makes several errors in his truncation analysis of the discrete equations.

Despite these criticisms, Landshoff’s numerical simulations are more than adequate to justify the linear plus quadratic $Q$ formulation. It is unfortunate that Landshoff’s report was not submitted for publication in the open literature where a competent review might have led to a more correct exposition.

In a curious historical side note, Harwood Kolsky wrote an internal Los Alamos report [22] just a few months before Landshoff. That report describes one of the first two-dimensional hydrodynamic simulations. Kolsky discusses in detail his artificial viscosity, which employs only the Richtmyer–von Neumann quadratic term. He explicitly notes that entropy must be created in a shock and goes on to suggest the magnitude of the artificial viscosity is a good indicator of the location and movement of a shock on the mesh.

William Noh Bill Noh spent his career at Lawrence Livermore Laboratory, making fundamental contributions to CFD. These included the first method to represent multimaterial cells (SLIC) and an early effort to combine the Lagrangian and the Eulerian methodologies (the CEL code). However Bill’s lifelong passion was the study of artificial viscosity and its potential pitfalls.

Noh is most well-known for a test problem he devised to illustrate a pitfall termed wall-heating [48, 55]. His self-similar problem is designed to focus on the excess heating that occurs when a shock is reflected off a wall in plane symmetry or from a point on the excess heating that occurs when a shock is reflected off a wall in plane symmetry or from a point of convergence in cylindrical or spherical symmetry. The Noh problem is widely used for code verification [51, 64].

Noh’s 1978 paper [48] is widely cited, but most of those citations are concerned with the test problem, missing what we believe is Noh’s main point. In his own words, we want to demonstrate that the wall heating $Q$ error is unavoidable and is already an error in the solution of the differential equations with $Q$. [48]

Here, Noh is saying that the source of the wall heating lies in the model itself rather than in the process of discretization. Noh also proposed a solution to wall-heating, advocating the additional dissipation associated with an artificial heat conduction and showing it effectively mitigated the excess heating. However, artificial heat conduction is not widely used today. We will expand on this point in Sect. 8.

In [48], Noh also describes a separate problem when one wants to propagate a shock on a nonuniform mesh. Conservation is not a sufficient condition to ensure the Rankine–Hugoniot jump conditions; it is also necessary that the shock be steady. The coefficients of artificial viscosity depend on the mesh spacing rather than physical length scale. Most implementations of artificial viscosity are designed to maintain shock width of 3–4 cells. If the mesh spacing is not constant, then the shock will not be steady. For more discussion on this problem, see [40].

Equations In modern notation, the Richtmyer–von Neumann artificial viscosity is written:

$$q_{RvN} = \rho c_Q \Delta x^2 \left( \frac{du}{dx} \right)^2$$

Here, $\rho$ is fluid density, $\Delta x$ is the width of the computational cell, and $u$ is the material velocity. $c_Q$ is a dimensionless constant that is set by the user; it is usually chosen $c_Q \sim 2$ which serves to spread the shock over 3 or 4 cells. For implementation, the artificial viscosity $q$ is added to the physical pressure in the momentum and energy equations.

The linear plus quadratic viscosity suggested by Landshoff has the form

$$q_{LQ} = \rho \left[ c_Q \Delta x^2 \left( \frac{du}{dx} \right)^2 - c_L c_e \Delta x \frac{du}{dx} \right]$$

Here, $c_L$ is another dimensionless constant set by the user. $c_e$ is the fluid sound speed ahead of the shock. The linear term is sometimes only turned on when the flow is compressive [11], i.e., when $\frac{du}{ds} < 0$

Summary Flows with shocks represent many of the earliest applications of electronic computers
driven by the mission needs of Los Alamos and Livermore Laboratories. The lack of resolution of the dissipative length scales of physical viscosity and heat conduction led to the need for artificial dissipation to avoid unphysical oscillations in the solution, i.e., artificial viscosity. Even today, it is not practical to fully resolve shock structure in multidimensional problems of engineering interest. However, given the utility and the effectiveness of adding an artificial viscosity, one might ask whether it is necessary or even desirable to fully resolve shocks, and—if so—what equations should be discretized? It is well known that the Navier–Stokes equations do not accurately predict the details of shock structure as can now be measured in experiments, nor is there an accepted alternative at the level of continuum theory [35].

Remark 1 We note that there is no “correct” shape for the numerical shock profile. There is a sustained desire among code users to calculate the narrowest possible shocks that are free of unphysical oscillations. However, these are competing requirements and in the end, shock profile is determined by the user’s choice of $c_Q$ and $c_L$.

4 Nonoscillatory Eulerian simulation

The story of nonoscillatory differencing begins with the Barrier Theorem proved in Godunov’s 1954 Ph.D. thesis.

Linear numerical schemes for solving partial differential equations having the property of not generating new extrema (monotonicity preserving schemes), can be at most first-order accurate. [15]

Here, linear means that the numerical discretizations are the same at every grid point, independent of the flow conditions. In the case of artificial viscosity, linear means that the parameters $c_L$ and $c_Q$ are the same at every mesh point. Accuracy refers to the dependence of discretization error on $\Delta x$; error in a first-order scheme is directly proportional to $\Delta x$. Preserving monotonicity and high-order (or at least second-order) accuracy are both desirable properties. Donor cell approximations, also termed upwind differencing schemes, take into account the direction of fluid flow, but are only first-order accurate and are too diffusive for most applications. For the next 18 years after Godunov, Eulerian methods chose accuracy while allowing unphysical oscillations.

The strategy to bypass the Barrier Theorem was first recognized by Jay Boris and is surprisingly simple, namely to give up linearity. In the flux-corrected transport (FCT) algorithm [7] Boris and Book mix first and second-order methods locally so as to preserve monotonicity by construction. FCT uses flow dependent coefficients to approximate the advective terms and so is not linear in the sense defined above. It is also not quite second-order accurate by standard measures, but can be made very high-order in smooth regions of the flow. A fuller history of FCT can be found in [6]. Jay Boris is truly the first hero of nonoscillatory methods.

The strategy for avoiding Godunov’s barrier was quickly accepted by the computational fluid dynamics community and many new methods based on flux limiting evolved. Those are generally referred to as nonoscillatory finite volume (NFV) methods. Some elements of the similarity of these many schemes are described in [61]. All NFV schemes are nonlinearly stable under appropriate time step restrictions$^2$, enforce exact conservation of mass, momentum and energy, and do not allow unphysical oscillations. NFV schemes are free of parameters so being more automatic and perhaps less flexible than explicit artificial viscosity schemes. Most NFV schemes are built on the concept of preserving monotonicity and are generally easy to implement in a spatially split format on a structured grid.

Remark 2 Monotonicity is a mathematical property of a solution and is a one-dimensional idea. One expects enforcement of monotonicity is related to the second law [43]; however, this is open to question. We note the well-known result of Morduchow and Libby [44] that the velocity increases monotonically in Becker’s solution of the shock profile, but the thermodynamic entropy has a peak inside the profile. This counter-intuitive result is due to an entropy flux associated with heat conduction, and has been shown

\[ \text{nonlinear stability cannot be evaluated using von Neumann’s linearized analysis and must be addressed by more general methods; see e.g., [60].} \]
to be consistent with the Clausius–Duhem inequality, which is a local expression of the second-law [63].

Summary The NFV algorithms appear to offer a second, distinct methodology for controlling unphysical oscillations. Where the artificial viscosity methods alter the model equations, the NFV methods work more directly by modifying the solutions. In the next section, we will describe current research in which flux-limiting is used to replace the artificial dissipation in Lagrangian codes.

However, the connection between artificial viscosity and NFV methods is closer than one might expect. Modified equation analysis (MEA) [20] is a technique to construct a PDE that more closely represents the discretized equations solved within the code. A consistent MEA would consist of the Euler equations plus additional truncation terms depending on the discretization parameters $\Delta x$ (the computational cell size) and $\Delta t$ (the computational timestep). In [39] it was shown that the NFV method MPDATA [59] contains quadratic artificial viscosity as a truncation term. In chapter 5 of [17], the analysis is extended to several additional NFV schemes with the same result.

Remark 3 Truncation terms are not necessarily truncation error.

5 New ideas in artificial viscosity

Despite 70 years of effort and the inarguable success of the concept of artificial dissipation, several practical issues continue to occupy the attention of code developers with respect to artificial viscosity. Two of these are:

1. How to choose the optimal values of $c_L$ and $c_Q$ for a particular simulation. Those parameters are typically user input and their selection often determined by trial and error.
2. How to formulate the artificial viscosity for multidimensional problems to best preserve the physical flow symmetries and to avoid mesh dependence.

Choosing the viscosity parameters The more sensitive issue here concerns the choice of the linear coefficient $c_L$. As pointed out by Landshoff, the quadratic viscosity is not large enough to control the overshoot and postshock oscillations where the velocity gradient is small. However, use of the linear artificial viscosity is effectively adding a first-order error (i.e. $O(\Delta x)$) which can affect the smooth area of the flow, away from any shocks and where no viscosity is required [45].

An obvious solution lies in the NFV flux-limiting algorithms, which enforce monotonicity by adding a flow-dependent amount of donor cell, i.e., first-order dissipation; effectively these methods introduce a variable coefficient of linear viscosity automatically. Kuropatenkov made an early attempt to predict the “optimal” values of $c_L$ and $c_Q$ from the solutions of the Riemann problem for a perfect gas [66]. The principal result is shown in Eq. (11) of [66] (reproduced below as eq (3)), an equation that predicts the jump in pressure across a shock as a function of the jump in velocity; this equation goes back to Hugoniot [21],

$$P_1 = P_o + \Gamma \rho_o (\Delta U)^2 + \rho_o |\Delta U| [(\Gamma \Delta U)^2 + a_o^2]^{\frac{1}{2}}. \quad (3)$$

Here, $\Gamma = \frac{\gamma + 1}{4}$, where $\gamma$ is the perfect gas constant equal to the ratio of specific heats. Also $a_o$ and $\rho_o$ are the sound speed and the density in the fluid ahead of the shock.

However, Kuropatenkov’s interpretation of this equation is erroneous; if $\Delta U \approx \frac{dU}{dx} \Delta x$, then $\Delta P \approx P_1 - P_o \approx \frac{dP}{dx} \Delta x$; i.e., this is an equation for the pressure gradient, not the pressure. Further, the prediction for $c_L$ is not constant, but depends on the shock strength, e.g., Mach number, which as a practical matter is not known within the code. It is recognized that the Kuropatenkov form overly damps weak shocks [2].

Kuropatenkov’s analysis has led to numerous attempts to adapt the flux-limiting concept to a staggered mesh Lagrangian code. The earliest experiment appeared in an unpublished Livermore Laboratory report by Christiansen [12] in 1990. The Christensen limiter compares the velocity divergence in a cell (which is a scalar) with the divergences in the neighboring cells. This limiter functions as a shock detector that identifies cells where limiting should be applied; see Sect. 3 of this paper.

Subsequent work [11, 27, 46] has attempted to improve on Christiansen’s strategy by localizing the flux-limiting within the computational cell and by
providing a more multidimensional estimate of the direction of the shock. In [46], a subcell decomposition [11] is employed to integrate the momentum equation by implementing Riemann solutions at the subcell boundaries. Multidimensionality is introduced by rotating the calculation into the estimated direction of the shock. More details can be found in [46].

A different and complementary idea to choose the viscous coefficients was introduced in [52]. In the so-called C-method, an additional reaction–diffusion equation and variable is introduced. The new variable \( C(x, t) \) is used to

determine the location, localization, and strength of the artificial viscosity. Near shock discontinuities, \( C(x, t) \) is large and localized, and transitions smoothly in space-time to zero away from discontinuities. [52]

The C-equation is postulated rather than derived and oddly does not contain an advective term. We note that the C-methodology includes an artificial heat conduction (as suggested by Noh) whose coefficient is similarly limited by \( C(x, t) \). The overall C methodology does not require linear artificial viscosity nor linear artificial heat conduction.

Still another approach to generating spatially dependent viscosities is proposed in [2]. Here, a reference set of optimal values for the coefficients \( c_L \) and \( c_Q \) is pre-computed as a function of shock strength. Then for an arbitrary flow, one first estimates the shock strength and then interpolates the appropriate coefficients from the reference set. The reference set is constructed based on modifying the coefficients of the previously mentioned Kuroptenko Eq. (3). As noted at the end of Sect. 3 there is no correct profile for the numerical shock and in principle each user can weight the relative importance of a steep shock versus the lack of overshoot based on the purpose of the individual calculation. There is a detailed discussion of the construction of the reference set in [2].

Artificial tensor viscosity The early hydro codes were written in 1D, limited by the capabilities of the available computers. By the early 1960s, however, 2D codes were becoming common [1]. Multidimensional Lagrangian codes are prone to tangling the mesh, and it was quickly realized that a tensor artificial viscosity was more robust than a simpler scalar artificial pressure. There are two principal formulations, edge viscosity and cell-centered viscosity. One can think of the edge viscosity of Schulz [1] as nonlinear springs connecting the cell vertices. The cell-centered viscosity of Wilkins [66] is proportional to the velocity gradient within the cell. These are described and compared in [28] including the important modification to the edge viscosity made by Barton.

Detailed comparisons between the edge and cell-centered viscosities are presented in [10]. The edge viscosities exhibit large mesh sensitivity when the symmetries of the mesh and of the flow are discordant. In particular, the authors of [10] suggest that the edge viscosity is not a proper discretization of a continuum tensor and lacks the invariance properties of a true tensor. This opens the question about what constitutes a proper discrete calculus for the staggered mesh. Here we present a short diversion to another relevant idea in CFD, namely mimetic differencing [41].

The general idea of mimetic differencing is to identify and embed certain properties of the continuum model into the discrete equations. An early example is the development of finite volume methods by Lax [25]. Whereas finite difference methods provide conservation, e.g., of energy, to the level of truncation error, the finite volume methods ensure conservation to the level of roundoff error. The underlying idea is that of a detailed balance in which the flux of energy out of a cell is exactly the flux into its neighbor. We note that detailed balance does not ensure the flux of energy is accurate, only that the energy is conserved.

In the case of a discrete calculus, mimetic ideas were first used to ensure the discrete gradient operator is adjoint to the discrete divergence operator. This construction was described in another unpublished Los Alamos report [32] and was termed compatible differencing at the time. A simultaneous and independent presentation was published in the Soviet Union and was termed support operator theory [58].

The mimetic approach to defining the discrete differential operators is based on preserving integral identities. For example, for any scalar field \( p \) and vector field \( \mathbf{v} \), the continuous divergence operator \( \text{div} \) and the continuous gradient operator \( \text{grad} \) are related by

\[
\int_{\mathcal{V}(t)} p \text{ div}(\mathbf{v}) \, d\mathcal{V} + \int_{\mathcal{V}(t)} (\text{grad} p) \cdot \mathbf{v} \, d\mathcal{V} = 0 \tag{4}
\]

Here, \( \mathcal{V} \) is a time-dependent finite volume; \( p \) and \( \mathbf{v} \) are smooth functions assumed to vanish on the boundary.
In the mimetic formulation, we assume one of the discrete operators is known, and identify its compatible adjoint term by term. Typically, the discrete divergence is chosen as the known operator, since the volume of a computational cell is established by Pappus theorem and the divergence of the velocity is related to the time rate of change of volume. Details of that straightforward calculation can be found in [41].

For the tensor artificial viscosity, one needs both the gradient of a vector and the divergence of a tensor evaluated on a nonuniform computational mesh. Those operators are formulated in [10]. They are complicated; however the improvement in preserving symmetry is also substantial as can be seen by comparing figures 8 and 10 of that paper.

Another important idea that was unveiled in [28] concerned the model form of the tensor viscosity. There it is shown that the artificial tensor viscosity \( Q_{ij} \) should be taken to be directly proportional to the velocity gradient

\[
Q_{ij} \sim \frac{\partial u_i}{\partial x_j},
\]

(5)

rather than to the symmetrized gradient. This choice ensures that there is no mode conversion; i.e., that in a shear flow in which all velocities are parallel, the artificial viscosity will not generate velocity components perpendicular to the flow. The importance of suppressing mode conversion was illustrated in the Saltzman test problem in which a one-dimensional shock propagates through a two-dimensional mesh. The same choice of using Eq. (5) is made in [10]. We will discuss this choice further in Sect. 8.

6 The physics of finite volumes

The Finite Volume Method (FVM) [26] is a popular methodology in CFD. In FVM, the discrete variables represent volume averages over the computational cells rather than values at a particular point within the cell. FVM methods are exactly conservative of mass, momentum and total energy at the level of round off error as contrasted with finite difference methods, which are conservative only at the level of the truncation error. FVM originated at Los Alamos in an unpublished report by Peter Lax [25].

In [39] Margolin and Rider posed the following question:

If every point of a finite volume of fluid is governed by the Navier-Stokes equations, what equations describe the evolution of the volume averages of the state variables?

Answering this question led to the finite scale theory. Although [39] is ostensibly concerned with rationalizing the methodology of implicit large eddy simulation, its two principal results are more general. These are:

1. A general derivation of the evolution equations, termed the Finite Scale equations (FSE) for the volume-averaged variables of compressible fluid flow;
2. An analysis showing that a particular NFV, i.e., MPDATA, solves the FSE in the sense of modified equation analysis [20].

The FSE have the form of augmented Navier–Stokes equations. New terms appear proportional to the constant \( A \), which has the dimensions of length squared. In one spatial dimension when the equation of state is a perfect (\( \gamma \)-law) gas, the FSE are written:

\[
\begin{align*}
\frac{\partial \bar{p}}{\partial t} + \frac{\partial \bar{p} \bar{u}}{\partial x} &= 0 & (6) \\
\frac{\partial \bar{p} \bar{u}}{\partial t} + \frac{\partial}{\partial x} (\bar{p} (\bar{u})^2 + P) &= 0 & (7) \\
\frac{\partial}{\partial t} \left( \bar{I} + \frac{1}{2} \bar{p} (\bar{u})^2 \right) + \frac{\partial}{\partial x} \left( \bar{I} \bar{u} + \frac{1}{2} \bar{p} (\bar{u})^3 + P \bar{u} + Q \right) &= 0 & (8) \\
P &= (\gamma - 1) \bar{p} \bar{I} - \mu \frac{\partial \bar{u}}{\partial x} + A \bar{p} \left( \frac{\partial \bar{u}}{\partial x} \right)^2 & (9) \\
Q &= -\kappa \frac{\partial \bar{T}}{\partial x} + \gamma A \bar{p} \left( \frac{\partial \bar{I}}{\partial x} \right) \left( \frac{\partial \bar{T}}{\partial x} \right) & (10)
\end{align*}
\]

Here, the overbar signifies a volume-averaged quantity.

\[
\bar{\rho}(x) \equiv \frac{1}{\Delta x} \int_{x-\Delta x/2}^{x+\Delta x/2} \rho(x') \, dx'
\]

(11)
The length scale $\Delta x$ is assumed constant. The tilde indicates a Favre-averaged quantity. For example,

$$\tilde{I}(x) \equiv \frac{1}{\rho(x)\Delta x} \int_{x-\Delta x/2}^{x+\Delta x/2} \rho(x') I(x') \, dx'$$  \hspace{1cm} (12)$$

where $I$ is specific internal energy. Also, $\mu$ and $\kappa$ are the coefficients of physical viscosity and heat conduction. These coefficients represent processes on the length scale of the molecular mean free path $\lambda$ and the associated terms are negligible when $\Delta x \gg \lambda$.

Note that FSE is a PDE theory of volume-averaged variables rather than an integral theory of differential variables.

The constant $A \equiv \left( \frac{\Delta x}{\lambda} \right)^2$ where $\Delta x$ is the length of the (1D) finite volume. In the case of numerical simulation, $\Delta x$ is the size of a computational cell. However, the FSE are analytic equations and $\Delta x$ may be chosen arbitrarily to resolve the process or perhaps the measuring instrument of interest. With reference to the Heisenberg quote in the introduction, we refer to $\Delta x$ as the observer, so quantifying the “we” in the quote.

**Remark 4** In principle the derivation of the FSE leads to an infinite series of terms in even powers of $\Delta x$. Equations (6)–(10) are a truncation of the equations at $O(\Delta x^2)$.

Note that a quadratic viscosity term analogous to the Richtmyer–von Neumann term appears in Eq. (7) and a nonlinear heat conduction term analogous to that proposed by Noh appears in Eq. (8). By analogous, we mean that in addition to the functional form, the coefficient $A$ of the new terms is *inviscid*, i.e., is not property of the fluid. However, the analogy does not extend to include a linear inviscid viscosity; such a term is generally ruled out by the isotropy of space.

The derivation of the FSE begins at a small length scale $\Delta x$, such that all gradients of the flow variables are well-resolved. At such a scale, it is assumed that the Navier–Stokes equations are germane and that the dependent field variables can be expanded in a convergent Taylor series. The steps of the calculation can be summarized as follows.

1. Insert the Taylor series expansions into the Navier–Stokes equations and integrate the equations over $x \in [x - \Delta x/2, x + \Delta x/2]$. Carefully commute the order of operations integration and multiplication, then truncate the results to $O(\Delta x^2)$. This leads to the FSE at scale $\Delta x$.

2. Assume the form of the equations holds for arbitrary $\Delta x$ and derive the equation for $2\Delta x$. Show that the form is unchanged under that renormalization, proving form invariance of the FSE.

Details of both steps can be found in [34, 39]. Here, we discuss four further salient features of the calculation. First, there is a theorem of closure. We note that multiplication and integration do not commute, i.e., $\tilde{u}^2 \neq \tilde{u}^2$. It is that lack of commutativity due to the *nonlinearity* of advection that leads to the inviscid dissipative terms of the FSE. In general, the calculation leads to a closure theorem for finite scale variables:

**Closure theorem** For any continuum fields $A$ and $B$ that are sufficiently smooth at small scales,

$$\overline{BC} = \tilde{B} \tilde{C} + \frac{1}{3} \left( \frac{\Delta x}{2} \right)^2 \frac{\partial B}{\partial x} \frac{\partial C}{\partial x} + O(\Delta x^4)$$ \hspace{1cm} (13)$$

A similar theorem applies to Favre averaging.

Second, we observe that at every length scale $\Delta x$, there are 3 contributions to the momentum flux; these are the advective flux, the viscous diffusive flux and the inviscid diffusive flux. As one considers progressively larger averaging scales, the inviscid flux grows while the advective flux decreases. This happens so as to ensure the total momentum flux is conserved. There is an analogous result for the energy flux. Details can be found in [34].

Third, the form of the FSE has the interesting interpretation that many features of the large scales of the flow do not depend on the details of the small scale processes. For example, in a shock, the velocity and jump conditions are independent of the viscosity; only the detailed shape of a shock depends on the fluid viscosity [62]. In turbulent flow, the energy dissipated is determined by the large scales of the flow; viscosity only determines the size of the smallest eddies at which dissipation occurs; see the discussion of Kolmogorov’s $4/5$th theorem in [14]. In the theory of nonlinear PDEs, this property indicates the existence of an inertial manifold [13]. One might say that small-scale variables are only needed to predict the small-scale features of a flow, and it is
the large-scale dynamics that determine how the overall flow behaves. Or, in other words, when describing the large-scale evolution of a flow, the details often do not matter.

Fourth, we comment further on the lack of a linear inviscid term in the FSE. In [42] analytic solutions of equations with both linear and quadratic artificial viscosity were compared to solutions with only quadratic viscosity. In the case with linear artificial viscosity, the solutions were not compact, indicating the unphysical property that information can travel with “infinite” speed. However, solutions of equations with only quadratic viscosity have compact support. Although this is a positive feature for FSE, it indicates a potentially larger issue, namely that the derivation of the FSE begins at the smallest scales with Navier–Stokes and so inherits some of the issues of that continuum model.

7 A physical interpretation

The presence of inviscid fluxes in the mathematical derivation is suggestive, but a physical interpretation of those fluxes would be even more compelling. Such an interpretation was first offered in [29]. We reiterate that the FSE are not integral equations for continuous fields, they are PDEs for volume-averaged fields. Inviscid fluxes Consider integrating a 3D extension of Eq. (6) over a volume \( \Omega \). Here we have replaced the 1D partial derivative with the 3D divergence. Invoking Reynolds transport theory and using the divergence theorem,

\[
\frac{d}{dt} \left( \int_{\Omega} \bar{\rho} \, dV \right) = \int_{\partial \Omega} \bar{\rho} (\bar{u} - w) \cdot n \, dS \tag{14}
\]

where \( w \) is the velocity of the surface and \( n \) is a unit normal to the surface. The term on the left is the time rate of change of the mass of \( \Omega \). When we choose a Lagrangian volume whose surface moves with the local fluid tilde velocity, the term on the right vanishes indicating that the mass of \( \Omega \) is constant. From the kinetic point of view, this does not mean that every fluid particle initially in the cell remains in the cell for the duration of a calculation. Rather, we infer the weaker statement that the net flux of mass integrated around the total surface of the volume vanishes.

Now we note that the vanishing of the mass flux does not imply the vanishing of the momentum flux nor of the energy flux. In [29], estimates support the interpretation that these exchange fluxes are the source of the inviscid fluxes in the FSE. This interpretation gives substance to Bill Noh’s assertion that wall heating results from an inconsistent model rather than its numerical implementation. A system with artificial viscosity in the momentum equation, but without artificial heat conduction in the energy equation is simultaneously open and insulated, which is a thermodynamic inconsistency.

Discrete thermodynamics As noted in the previous section, the inviscid fluxes originate in the non-linearity of advection. There is another important nonlinearity in the FSE for a perfect gas, namely in the equation of state.

\[
\bar{p} = (\gamma - 1)(\bar{\rho} \bar{I}) \tag{15}
\]

Mathematically, the averaged term on the RHS can be resolved by the closure theorem. However, in the physics there are deeper issues that can only be resolved within the perspective of kinetic theory.

In [33], the nonequilibrium of finite volumes was discussed. Here, nonequilibrium implies the presence of macroscopic gradients, e.g., of velocity or internal energy or density. There it is demonstrated that, in the context of finite volumes, temperature and internal energy are not equivalent. Temperature is a purely equilibrium concept while the internal energy also contains the unresolved kinetic energy. The latter is an independent partition of the total energy, which is fed by inviscid fluxes and which decays into internal energy on flow-dependent time scales. We note the similarity of this result to the models of turbulent kinetic energy (TKE) commonly used in atmospheric flows [50].

Finally, the existence of significant unresolved kinetic energy implies that the assumption of local thermodynamic equilibrium (LTE) is not justifiable [38]. LTE is a basic assumption in the derivation of the Navier–Stokes equation from the Boltzmann equation via the Chapman–Enskog approximation; its failure is another reason to seek a derivation of the finite scale equations beginning at the level of gas kinetic theory.
8 Discussion

The finite scale theory provides an understanding and theoretical basis for traditional viscosity as well as for many of the ideas introduced more intuitively in Sect. 5. Here we expand on several topics:

Formulation The quadratic form of viscosity ala Richtmyer and von Neumann, shown in Eq. (1), is predicted by the FSE in Eq. (9). Its inviscid character reflects its origin in the nonlinearity of advection rather than in dissipative processes of collisions, i.e., the inviscid coefficient is geometric and independent of the molecular mean free path. The quadratic viscosity should be viewed as a flux of momentum rather than as an addition to the pressure.

The derivation of the FSE precludes a physical basis for Landshoff’s linear artificial viscosity. Furthermore, analytic solutions of the FSE show that the shock profile is monotonically increasing in velocity, density, internal energy, etc. [42] This indicates that truncation error is the source of overshoots and unphysical oscillations. Careful truncation analysis in [37] shows the error term causing the oscillations is $O(\Delta x^2)$; the linear artificial viscosity is a heavy-handed mitigation that unnecessarily alters the smooth areas of the flow.

In Eq. (10) the FSE also predicts a quadratic artificial heat conduction, similar to the form suggested by Noh in Eq. (2.4) of [48]. However, the linear analog of artificial heat conduction is also precluded in the FSE. It is interesting to note that the inviscid Prandtl number, i.e., the ratio of the inviscid momentum diffusivity to the inviscid internal energy diffusivity is predicted to be $1/\gamma$. This is exactly the value of the viscous Prandtl number assumed by Becker [4] that enables his analytic solution. See footnote #1 in [38] for more details.

Bi-velocity hydrodynamics The inviscid fluxes of Sect. 7 are transported with a velocity relative to $\vec{u}$. Indeed, there are two velocities that appear in the FSE, the average material velocity $\bar{u}$ and the Favre material velocity $\bar{u}$. A relation between these is derived in [29] using the closure theorem:

$$\bar{u} = \bar{u} + \frac{1}{3} \left( \frac{\Delta x}{2} \right)^2 \bar{u} \bar{\rho}_x \frac{\partial \bar{\rho}}{\partial \bar{x}},$$

where $\bar{\rho}_x = \frac{\partial \bar{\rho}}{\partial \bar{x}}$, etc. The FSE are written in terms of $\bar{u}$, which is the momentum velocity. $\bar{u}$ is the advective velocity. It is the relative velocity ($\bar{u} - \bar{u}$) that transports the inviscid fluxes.

The subject of bi-velocity hydrodynamics was first introduced by Howard Brenner in [8] and its consequences were explored in the context of continuum dynamics.

Acceptance of the Navier–Stokes–Fourier equations as the fundamental equations of continuum fluid mechanics for liquids and gases is noted to be inseparably linked to Euler’s implicit, but unproved, hypothesis that but a single-velocity field is required to characterize the four physically different velocities appearing in the mass, momentum, and energy equations. [9]

Brenner proposes a constitutive relation that in our notation in 1D is:

$$\bar{u} = \bar{u} + \alpha_v \frac{1}{\bar{\rho}} \frac{\partial \bar{\rho}}{\partial x}$$

where $\alpha_v$ is a constant termed the “volume diffusivity”. This is consistent with the FSE relation (16) if instead of a constant we take

$$\alpha_v = -\frac{1}{3} \left( \frac{\Delta x}{2} \right)^2 \bar{u}.$$ 

Brenner terms the velocity difference ($\bar{u} - \bar{u}$) the diffusive volume flux density.

Angular momentum In simulations in multiple spatial dimensions, concern for accuracy must be supplemented by a concomitant concern for the preservation of the geometric flow symmetries. Unlike the exact conservation of mass, momentum and energy in the FVM, angular momentum is only approximately conserved. The advection interpretation of artificial viscosity in multiple dimensions justifies the tensor form of Eq. (5).

Consider again the situation of Sect. 7. In the process by which there is no net exchange of mass, one cannot expect that all particle velocities are normal to the surface. In general, the particle exchange will generate a tangential force on the boundaries between cells. However, a cell is not an isolated rigid body and the net deformation of all the cells must be compatible, i.e., the displacements of all the cells must be continuous and single-valued. Solving the compatibility equations would be a nonlocal problem to be avoided in an explicit hydrocode.

In [28] a different approach is followed. It is suggested that the edge viscosity leads to a
better approximation of a compatible solution since the forces are shared by both cells adjacent to the boundary. Then a cell-centered (true) tensor viscosity is derived that most closely reproduces the forces of the edge viscosity. That tensor turns out to have the form of Eq. (5), a nonsymmetric tensor. It is perhaps ironic that Schulz recognized that his edge viscosity was not a symmetric tensor and considered that a weakness.

9 Conclusions

From combustion engines to the collision of gases in giant galaxy clusters, shock waves are ubiquitous in our universe. However, as first pointed out by Becker in 1922, the continuum models we use to describe them do not accurately predict the experimentally measured shapes or widths of the shock profile. The use of electronic computers has further exacerbated the situation as the dissipative process of viscosity and heat conduction are not resolved in typical engineering calculations.

In this paper we have attempted to summarize the historical development of modeling shocks on the computer, celebrating its early pioneers, giving a modern perspective of its theoretical essence, as well as offering insights for future improvements. The underlying idea of shock capturing, first elucidated by Rudolf Peierls [49] preceded the advent of the first electronic computer [16, 47] and is based on the fundamental results of Rankine [36]. The importance of dissipation in regularizing the theoretical shock structure is attributed to Becker in both [53, 65]. The importance of heat conduction in shock structure is also emphasized by Becker. This is a key idea in Bill Noh’s work [48] though no attribution is made. Nonetheless, all of these works have underlined the utility and necessity of artificial dissipation schemes when modeling shocks.

There is a broad theme woven into this paper, namely the close connection between theory and successful numerical algorithms. The flow of ideas from physics to methods is termed mimetic differencing, described in Sect. 5. However, the quadratic viscosity has followed the opposite path, originating in numerical methods and finding a realization in the theory of finite scales. That the Finite Scale Equations—contain new inviscid dissipative terms with an underlying physical interpretation suggests that the "observer" (Δx) plays a key role in consistently describing physical processes across a range of scales [30]. Further, inviscid dissipation implies that the large scales “control” the small scales, indicating that in many situations the details of the dissipative processes don’t matter. This point of view was clearly expressed in the landmark paper of von Neumann and Richtmyer [65].

Artificial viscosity is one of the oldest and most enduring concepts in computational fluid dynamics. In particular, the quadratic dependence of the artificial viscosity on the velocity gradient is now appearing in many different venues, e.g., models [34], nonoscillatory differencing [39] and theoretical physics [35, 36]. We are especially pleased to reveal the origin of this almost magical term in the unpublished work of Bob Richtmyer [53, 54].

The continued success of artificial viscosity suggests that other concepts from numerical methodology may have physical relevance in theoretical fluid dynamics. Just as role of the observer reminds one of the emphasis on measurement in quantum theory, the Courant–Friedrichs–Lewy (CFL) condition for numerical stability has a causal flavor limiting the speed with which information can be propagated across the mesh in explicit simulations. Generalizations of monotonicity preservation may be related to the dynamics of irreversible processes.

The main point of Becker’s paper was to point out the inadequacy of Navier–Stokes theory in predicting shock structure. So far, no continuum model has risen to that challenge. Perhaps it would be beneficial to look to successful numerical methodology for further improvements and a more fundamental insight to shock theory and perhaps more generally to fluid dynamics.

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Declarations

Conflict of interest  The authors declare that they have no conflict of interest.

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