LA-UR- 08-6460

Approved for public release;
distribution is unlimited.

Title:	Finite scale equations for compressible fluid flow
Author(s):	Len Margolin X-3
Intended for:	Invited Talk Royal Society of London London, England 10/27/08

Los Alamos
NATIONAL LABORATORY
EST. 1943

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Form 836 (7/06)

LA-UR-08-04911

Finite scale equations for compressible fluid flow

By L.G. Margolin

Los Alamos National Laboratory, Los Alamos, NM 87544 USA

Finite scale equations (FSE) describe the evolution of finite volumes of fluid over finite intervals of time. We discuss the FSE for a one-dimensional compressible fluid whose every point is governed by the Navier-Stokes Equations. The FSE contain new momentum and internal energy transport terms. These are similar to terms added in numerical simulation for high-speed flows (e.g., artificial viscosity) and for turbulent flows (e.g., subgrid scale models). These similarities suggest the FSE may provide a more rigorous basis for computational fluid dynamics. Our analysis of the finite scale continuity equation leads to a physical interpretation of the new transport terms and indicates the need to carefully distinguish between volume-averaged and mass-averaged velocities in numerical simulation. We make preliminary connections to the recent work of Brenner on the kinematics of volume transport.

Finite scale equations for compressible fluid flow

By L.G. Margolin

Los Alamos National Laboratory, Los Alamos, NM, USA

Finite scale equations (FSE) describe the evolution of finite volumes of fluid over time. We discuss the FSE for a one-dimensional compressible fluid whose every point is governed by the Navier-Stokes equations. The FSE contain new momentum and internal energy transport terms. These are similar to terms added in numerical simulation for high-speed flows (e.g., artificial viscosity) and for turbulent flows (e.g., subgrid scale models). These similarities suggest the FSE may provide a more rigorous basis for computational fluid dynamics. Our analysis of the finite scale continuity equation leads to a physical interpretation of the new transport terms and indicates the need to carefully distinguish between volume-averaged and mass-averaged velocities in numerical simulation. We make preliminary connections to the other recent work reformulating Navier-Stokes equations.

Keywords: Place keywords here

1. Introduction

Finite scale equations (FSE) describe the evolution of finite volumes of fluid over time. Here we introduce the FSE for parcels of fluid whose every point is governed by the compressible Navier-Stokes equations. This reformulation of classical fluid dynamics offers useful insights, especially in the context of numerical simulations of fluid flow.

In previous work, Margolin & Rider 2002; Margolin et al. 2006 (hereafter, MR 2002 and MRG 2006), we described the derivation of FSE that are based on Burgers' equation and on incompressible Navier-Stokes equations. In both cases, the FSE consist of the underlying equations augmented (at lowest order) by new terms quadratic in the length scales over which the averaging is performed. In those papers, the analysis was used as a rationale to justify the numerical technique of Implicit Large Eddy Simulation (ILES); see Grinstein, et al. 2007 for a detailed description and applications of this technique. However, here we would emphasize that the FSE themselves are an analytic result, independent of numerical considerations; in particular, the FSE are continuous equations, not discrete.

Our principal result in considering the incompressible flow equations was the appearance of a new momentum transport term. This term arises directly from the nonlinearity of the advective term after averaging in space and time. In MR 2002, we discussed the similarity of that term to truncation terms that are inherent in nonoscillatory finite volume (NFV) approximations widely used in numerical simulations in an Eulerian framework, and to the artificial viscosity that is added explicitly to simulations in a Lagrangian framework. This led to the suggestion that these terms have a physical, rather than a numerical origin. In MRG 2006, we

discussed the further similarity of the new momentum transport term in multiple spatial dimensions to a class of subgrid scale models used in large eddy simulation (LES). Similar terms will arise in our consideration of the momentum and energy equations for compressible flow.

In this paper, we are primarily concerned with the analysis of the FSE as a model for the numerical simulation of compressible flows with high Reynolds' number – e.g., flows with turbulence and/or shocks. In §2, we give a brief summary of the derivation and then present the averaged equations. In §3 we focus on the terms that arise from the nonlinearity of the advective terms. Consideration of the finite-scale (FS) continuity equation will require us to generalize the concept of Lagrangian volumes and will lead to a physical explanation of the new transport terms for momentum and energy that consequently arise. In §4, we focus on the terms that arise from the nonlinearity of the pressure-velocity work terms. We also discuss the role of unresolved kinetic energy and its relation to thermodynamics. In §5, we summarize the overlap between the FSE and the current state-of-the-art of finite volume Lagrangian/ALE and Eulerian methodologies.

Many of the new terms in our FSE have their origin in distinguishing between two velocities that naturally appear in our analysis – the average or advective velocity and the momentum or Favre averaged velocity. This distinction is also made in other recent reformulations of Navier-Stokes equations. In the appendix, we briefly discuss two of these – the volume transport concept and the Navier-Stokes α model. We do not suggest the equivalence of these theories to FSE, but merely point out the similarity of consequences that follow from the existence of these two velocities.

2. Coarse-graining

We begin this section by offering a concise statement of the theme of this paper. We consider a fluid in one dimension whose every point is described by the compressible Navier-Stokes equation. In conservative form, these are:

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= -\frac{\partial u\rho}{\partial x} \\ \frac{\partial u\rho}{\partial t} &= -\frac{\partial u^2\rho}{\partial x} - \frac{\partial p}{\partial x} \\ \frac{\partial E\rho}{\partial t} &= -\frac{\partial u^2 E}{\partial x} - \frac{\partial pu}{\partial x} - \frac{\partial q}{\partial x}. \end{aligned} \tag{2.1}$$

Here, ρ, u, E have their usual meanings of density, velocity, and specific total energy. The pressure, p, is the sum of the thermodynamic pressure plus the viscous pressure, $\eta\frac{\partial u}{\partial x}$, where η is the dynamic viscosity. Also, q is the heat flux. At this point, we make no particular assumptions about the equation of state, but we will return to this point in some detail in §4.

We define an averaging operator $\widehat{\chi}$ for any variable $\chi(x,t)$:

$$\widehat{\chi}(x,t) \equiv \frac{1}{L}\int_{x-\frac{L}{2}}^{x+\frac{L}{2}} dx'\,\chi(x',t) \tag{2.2}$$

and pose the question: *What equations govern the evolution of* $\widehat{\rho}$, $\widehat{\rho u}$ *and* $\widehat{\rho E}$*?* An answer to this question was given in MR 2002 for Burgers' equation in one dimension

and also in MRG 2006 for incompressible Navier-Stokes in two dimensions. We termed these finite scale equations. Each of these derivations followed a similar path, which we outline here.

The derivation begins by considering scales of length (L_o) for which the flow is smooth, by which we mean the dependent variables can be expanded in a convergent Taylor series. Such scales always exist, due to the presence of molecular viscosity. In this case, the integrals over the variables, including nonlinear terms, can be evaluated directly, leading to the equations for $\widehat{\rho}(x,t;L_o)$, etc.; here we explicitly indicate dependence on the averaging scale.

This derivation is ultimately not justified for large enough scales in the case of a flow with shocks or turbulence. To proceed, we note that the averaging process itself produces smoother fields. We quantify this by *assuming* that the variables averaged over any scale of (L), are smooth enough to be expanded in convergent Taylor series on scales of ($2L$). Next, we proceed by induction. We assume that the equations written for variables averaged over (L_o) continue to hold for variables averaged over (L) when $L_o \rightarrow L$, and then we prove that this implies that the equations for the variables averaged over ($2L$) have the same form when $L \rightarrow 2L$.

The net result of this derivation is that for any quantities A and B,

$$\widehat{AB} = \widehat{A}\,\widehat{B} + \frac{1}{3}\left(\frac{L}{2}\right)^2 \widehat{A}_x \widehat{B}_x + HOT\,, \tag{2.3}$$

where $A_x \equiv \frac{\partial A}{\partial x}$ and HOT are higher-order terms, e.g., $\mathcal{O}(L^4, T^4)$, etc.

We choose as our fundamental variables averaged density $\widehat{\rho}$, momentum density $\widehat{\mathcal{M}} = \widehat{\rho u}$ and the energy density $\widehat{\mathcal{E}} = \widehat{\rho E}$ and pressure $\widehat{p}$. The FSE to order (L^2, T^2) are;

$$\frac{\partial \widehat{\rho}}{\partial t} = -\frac{\partial}{\partial x}\left\{\widehat{\rho u} + \frac{1}{3}\left(\frac{L}{2}\right)^2 \widehat{u}_x \widehat{\rho}_x\right\} \tag{2.4}$$

$$\frac{\partial \widehat{\mathcal{M}}}{\partial t} = -\frac{\partial}{\partial x}\left\{\widehat{\mathcal{M}}\widehat{u} + \frac{1}{3}\left(\frac{L}{2}\right)^2 \widehat{u}_x \widehat{\mathcal{M}}_x + \widehat{p}\right\} \tag{2.5}$$

$$\frac{\partial \widehat{\mathcal{E}}}{\partial t} = -\frac{\partial}{\partial x}\left\{\widehat{\mathcal{E}}\widehat{u} + \widehat{pu} + \widehat{q} + \frac{1}{3}\left(\frac{L}{2}\right)^2 \widehat{\mathcal{E}}_x \widehat{u}_x\right\} \tag{2.6}$$

(From this point on, we refrain from writing HOT, implicitly recognizing that all of our equations are a second-order truncation of an infinite set of terms.) In these equations, we recognize the appearance of new terms of order $\mathcal{O}(L^2)$ that describe the transport of mass, momentum and energy. These terms originate specifically due to the difference of u and $\widehat{u}$.

We close with the observation that the FSE are equivalent in physical content to Navier-Stokes; they are derived from Navier-Stokes and, conversely, Navier-Stokes can be recovered in the limit $L \rightarrow 0$.

3. Analysis of the FSE

(a) *The continuity equation*

We begin our analysis with the continuity equation (2.4) and recognize an immediate issue – the appearance of $\widehat{u}$ and its derivatives. Because we have chosen momentum as our fundamental variable, $\widehat{u}$ cannot be a prognostic variable. However, we note that by equation (2.3)

$$\widehat{\mathcal{M}} = \widehat{\rho u} = \widehat{\rho}\,\widehat{u} + \frac{1}{3}\left(\frac{L}{2}\right)^2 \widehat{\rho}_x \widehat{u}_x \tag{3.1}$$

We define a "momentum" velocity $\widetilde{u}$:

$$\widetilde{u} \equiv \widehat{u} + \frac{1}{3}\left(\frac{L}{2}\right)^2 \frac{\widehat{u}_x \widehat{\rho}_x}{\widehat{\rho}} = \frac{\widehat{\mathcal{M}}}{\widehat{\rho}}, \tag{3.2}$$

and rewrite the continuity equation in more familiar form

$$\frac{\partial \widehat{\rho}}{\partial t} = -\frac{\partial}{\partial x}(\widehat{\rho}\,\widetilde{u}) \tag{3.3}$$

The meaning of this equation is as follows: When the boundaries of a parcel of fluid are moved with the momentum velocity $\widetilde{u}$, then the total mass within the parcel remains constant. This does *not* preclude the flux of mass across the boundary, but rather means that the integral of the flux around the boundary is zero. It is simple to estimate the exchange mass flux in one dimension as $\frac{1}{3}\left(\frac{L}{2}\right)^2 \widehat{\rho}\,\widetilde{u}_x$. The flux of mass implies a concomitant flux of momentum and energy, and *the integrals of these fluxes do not in general vanish.* That is, the exchange of mass by a volume with its neighbors will lead to a nonzero exchange of momentum and energy.

(b) *The momentum and total energy equations*

We now rewrite the momentum equation (2.5) in terms of $\widetilde{u}$:

$$\frac{\partial \widehat{\mathcal{M}}}{\partial t} = -\frac{\partial}{\partial x}\left\{\widehat{\mathcal{M}}\widetilde{u} + \widehat{p} + \frac{1}{3}\left(\frac{L}{2}\right)^2 \widehat{\rho}\widetilde{u}_x^2\right\} \tag{3.4}$$

where we have used $\widehat{\mathcal{M}} \approx \widehat{\rho}\,\widetilde{u}$ in collecting the second-order terms. The new term, proportional to L^2, is the net exchange of momentum referred to in the previous subsection. Its origin lies in two sources, the first being the difference between the "true" advective velocity u and the averaged advective velocity $\widehat{u}$, and the second being the difference between advective velocity $\widehat{u}$ and the momentum velocity $\widetilde{u}$. We note that the first differrence is present in both compressible and incompressible flows. However, the second difference, from equation (3.2), is proportional to the gradient of density and so vanishes in incompressible flow.

Similarly, we rewrite the energy equation in terms of $\widetilde{u}$:

$$\frac{\partial \widehat{\mathcal{E}}}{\partial t} = -\frac{\partial}{\partial x}\left\{\widehat{\mathcal{E}}\widetilde{u} + \widehat{pu} + \frac{1}{3}\left(\frac{L}{2}\right)^2 \left(\widehat{\rho}\,\widetilde{u}_x \widetilde{E}_x\right)\right\} \tag{3.5}$$

where $\widetilde{E} \equiv \widehat{\mathcal{E}}/\widehat{\rho} \neq \widehat{E}$. † Here also we identify a new term representing energy transport (kinetic and internal) associated with the exchange of mass within the volume with its neighbors. The fact that it is the same exchange mass flux that transports both momentum and energy leads to a simple relation between the respective coefficients of $\widetilde{u}_x$ and $\widetilde{E}_x$ – they are the same! This relationship is a special case of an Onsager reciprocity relation.

In this section, we have analyzed the properties of the FSE from the point of view of conservation and the convective fluxes. Next, we turn our attention to thermodynamic issues.

4. Energetics

(a) *The internal energy equation*

In continuum Navier-Stokes theory, one constructs an equation for internal energy in two steps: one manipulates the momentum equation to form an equation for kinetic energy, which one then subtracts from the total energy equation. The internal energy equation is redundant; i.e., internal energy can always be found as the difference of the total and kinetic energies. However, in many numerical algorithms for simulating high-speed flow, there are advantages to solving the internal energy equation instead of the total energy equation (Margolin & Shashkov 2004).

Directly averaging the internal energy equation for $\widehat{\mathcal{I}} \equiv \widehat{\rho \mathrm{I}}$ yields:

$$\frac{\partial \widehat{\mathcal{I}}}{\partial t} = -\frac{\partial}{\partial x}\left\{\widehat{\mathcal{I}}\widetilde{u} + \widehat{q} + \frac{1}{3}\left(\frac{L}{2}\right)^2 \widehat{\rho}\,\widetilde{u}_x \widehat{\mathrm{I}}_x\right\} - \widehat{p u_x} \tag{4.1}$$

where $\widetilde{\mathrm{I}} \equiv \widehat{\mathcal{I}}/\widehat{\rho} \neq \widehat{\mathrm{I}}$.

We derive a FS equation for macroscopic kinetic energy $\widetilde{\mathcal{K}}$ by multiplying the momentum equation (3.4) by $\widetilde{u}$. Using the identity: $\frac{\partial \widehat{\rho}\widetilde{u}^2}{\partial t} = 2\widetilde{u}\frac{\partial \widehat{\rho}\widetilde{u}}{\partial t} - \widetilde{u}^2\frac{\partial \widehat{\rho}}{\partial t}$, we find

$$\frac{\partial \widetilde{\mathcal{K}}}{\partial t} \equiv \frac{1}{2}\frac{\partial \widehat{\rho}\,\widetilde{u}^2}{\partial t} = -\frac{1}{2}\frac{\partial\, \widehat{\rho}\widetilde{u}^3}{\partial x} - \widetilde{u}\widehat{p}_x - \frac{1}{3}\left(\frac{L}{2}\right)^2 \widetilde{u}\frac{\partial \widehat{\rho}\widetilde{u}_x^2}{\partial x} \tag{4.2}$$

From equations (3.5), (4.1) and (4.2, we see $\widehat{\mathcal{I}} \neq \widehat{\mathcal{E}} - \widetilde{\mathcal{K}}$. Since at the continuum level, $\mathcal{E} = \mathcal{K} + \mathcal{I}$, we must have $\widehat{\mathcal{E}} = \widehat{\mathcal{K}} + \widehat{\mathcal{I}}$. The issue is that $\widetilde{\mathcal{K}} \neq \widehat{\mathcal{K}}$.

(b) *Resolved and unresolved kinetic energy*

From a macroscopic point of view (that is, from the point of view of an observer whose instruments can only resolve motion on scales greater than L), the cascade of fluid motions to scales smaller than L in the FSE appears to dissipate macroscopic kinetic energy. However, from the continuum viewpoint, this unresolved kinetic energy must continue its cascade down in scale until it is small enough to be dissipated by viscosity, and so does not affect the thermodynamic pressure immediately. This situation has been long recognized in the turbulence simulation community where an additional partition of the total energy, turbulence kinetic energy or TKE, is

† We endeavor to write our equations in terms of the fundamental variables chosen in §2. Note also that it is $\widetilde{u}$ and $\widetilde{\mathcal{E}}$ that are calculated in finite volume numerical codes, not $\widehat{u}$ and $\widehat{\mathcal{E}}$.

recognized and a transport equation for turbulent kinetic energy is often used to represent its evolution; see, e.g., the discussion in Pope 2000, pages 124-128.

To proceed, we formally recognize the existence of an additional partition $\mathcal{S}$ of the total energy, writing $\widehat{\mathcal{E}} = \widehat{\mathcal{K}} + \widehat{\mathcal{I}} + \widehat{\mathcal{S}}$. (We write $\mathcal{S}$ to emphasize that our discussion is not restricted to turbulent flows.) We can form the equation for the unresolved kinetic energy $\mathcal{S}$ by subtracting the sum of equations (4.1) and (4.2) from equation (3.5):

$$\frac{\partial \widehat{\mathcal{S}}}{\partial t} = -\frac{\partial \widehat{\mathcal{S}}\widetilde{u}}{\partial x} - \frac{1}{3}\left(\frac{L}{2}\right)^2 \widehat{\rho}\widetilde{u}_x^3 - (\widehat{p_x u} - \widehat{p}_x\,\widetilde{u}) \tag{4.3}$$

In equation (4.3), the work term associated with the new momentum transport is seen to be a source term to the unresolved kinetic energy partition.

From its definition, $\mathcal{S}$ is a quantity of $\mathcal{O}(L^2)$ and in fact

$$\mathcal{S} \equiv \frac{1}{2}\left(\widehat{\rho u^2} - \widehat{\rho}\,\widetilde{u}^2\right) \approx \frac{1}{6}\left(\frac{L}{2}\right)^2 \widehat{\rho}\,\widetilde{u}_x^2 \tag{4.4}$$

The significance of equation (4.4) is that it is *not necessary* to solve an additional prognostic equation for $\mathcal{S}$, in contrast to the practice in the turbulence transport theory.

(c) *Enhanced momentum and heat fluxes*

If we consider the density, momentum and total energy equations as fundamental, we see that an alternative interpretation of the new momentum exchange term is as a nonthermodynamic contribution to the pressure. That is, in the momentum equation (3.4) we could define an enhanced pressure

$$\mathcal{P} \equiv p + \frac{1}{3}\left(\frac{L}{2}\right)^2 \widetilde{\rho u_x^2} \quad ; \quad \frac{\partial \widehat{\mathcal{M}}}{\partial t} = -\frac{\partial}{\partial x}\left\{\widehat{\mathcal{M}}\widetilde{u} + \widehat{\mathcal{P}}\right\}. \tag{4.5}$$

In the energy equation, we substitute $\widetilde{E}_x = \frac{1}{2}\widetilde{u}\widetilde{u}_x + \widetilde{\mathrm{I}}_x$ (ignoring $\mathcal{S}_x$ as higher order)

$$\frac{\partial \widehat{\mathcal{E}}}{\partial t} = -\frac{\partial}{\partial x}\left\{\widehat{\mathcal{E}}\widetilde{u} + \widehat{\mathcal{P}u} + \widehat{q} + \frac{1}{3}\left(\frac{L}{2}\right)^2 (\widehat{\rho}\,\widetilde{u}_x\widetilde{\mathrm{I}}_x)\right\} \tag{4.6}$$

Indeed, this is exactly how the artificial viscosity is implemented in high-speed flow codes. This reformulation simplifies the appearance of the FS momentum and energy equations, but does not simplify the internal energy equation. Instead, we propose to define a new variable $\mathcal{U} \equiv \mathcal{I} + \mathcal{S}$. It is readily seen that $\mathcal{U}$ obeys the equation

$$\frac{\partial \widehat{\mathcal{U}}}{\partial t} = -\frac{\partial}{\partial x}\left\{\widehat{\mathcal{U}}\widetilde{u} + \widehat{q} + \frac{1}{3}\left(\frac{L}{2}\right)^2 \widehat{\rho}\,\widetilde{u}_x\widehat{\mathrm{I}}_x\right\} - \widehat{\mathcal{P}u_x} \tag{4.7}$$

In other words, in high-speed flow codes, it is $\mathcal{U}$ that is actually calculated, not $\mathcal{I}$. This has potentially new implications for how the thermodynamic equation of state is evaluated in those codes.

Before proceeding to our final step of defining an enhanced heat flux, we consider the nature of the pressure-velocity average $\widehat{p\,u}$ invoking the assumption of a specific thermodynamic equation of state, the ideal gas. Here,

$$p = (\gamma - 1)\rho \mathrm{I} \quad \Longrightarrow \quad \widehat{p} = (\gamma - 1)\widehat{\rho}\widetilde{\mathcal{I}}$$

It is straightforward to show

$$\widehat{p\,u} = \widehat{p}\widetilde{u} + (\gamma - 1)\left\{\frac{1}{3}\left(\frac{L}{2}\right)^2 (\widehat{\rho}\,\widetilde{\mathrm{I}}_x \widetilde{u}_x)\right\} \tag{4.8}$$

That is, the average of the product of pressure and velocity is the product of the averages plus a term identical to the heat exchange term except for dimensionless coefficient. This specific result for an ideal gas leads us to interpret $(\widehat{p\,u} - \widehat{p}\widetilde{u})$ more generally as another contribution to the heat flux.†

We define an enhanced heat flux by

$$\mathcal{Q} \equiv q + \frac{1}{3}\left(\frac{L}{2}\right)^2 \widehat{\rho}\widetilde{u}\widetilde{\mathrm{I}}_x + (\widehat{p\,u} - \widehat{p}\widetilde{u}) \tag{4.9}$$

to derive our final result for the FS energy and $\mathcal{U}$:

$$\frac{\partial \widehat{\mathcal{E}}}{\partial t} = -\frac{\partial}{\partial x}\left\{\widehat{\mathcal{E}}\widetilde{u} + \widehat{\mathcal{P}}\widetilde{u} + \widehat{\mathcal{Q}}\right\} \tag{4.10}$$

$$\frac{\partial \widehat{\mathcal{U}}}{\partial t} = -\frac{\partial}{\partial x}\left\{\widehat{\mathcal{U}}\widetilde{u} + \widehat{\mathcal{Q}}\right\} - \widehat{\mathcal{P}}\widetilde{u}_x \tag{4.11}$$

5. Discussion

(*a*) *FSE results*

Here, we summarize the major differences between the continuum Navier-Stokes equations and their FS counterparts. The principal difference lies in the presence of new transport terms for momentum and energy. Some of the new transport terms arise from the nonlinearity of the advective terms, as was the case in the incompressible equations (MRG 2006). However, additional terms also arise from the nonlinearity of the pressure-velocity terms (thermodynamic work). Further, the FSE predict definite relations among all these transport coefficients analogous to Onsager reciprocity relations. The FSE also allow an estimate of the unresolved kinetic energy in terms of the volume-averaged variables. This energy, dissipated from the resolved kinetic energy field, does not contribute to the thermodynamic pressure immediately; this effect is probably not important in shocks, but is important in turbulent flows.

† This would appear to be a result of dimensional analysis, not of similarity of the underlying physical origins of these terms.

(*b*) *Numerical simulation*

As stated in the introduction, we are interested in the FSE as an alternative model for numerical simulation. Here, we discuss the overlap of two modern approaches to simulating compressible flow with the FSE.

For compressible flow, especially for high Reynolds number flows with shocks and/or turbulence, most simulation codes are based on finite volume approximations; this has dictated our choice of the fundamental variables for the FSE as the densities of the conserved variables – $\widehat{\rho}$, $\widehat{\mathcal{M}}$ and $\widehat{\mathcal{E}}$. For flows with multiple materials and strong shocks, and when vorticity does not play an important role, a Lagrangian or arbitrary Lagrangian-Eulerian (ALE) formulation has considerable advantages (Margolin 1997). When vorticity becomes important, e.g., when the flow becomes turbulent, Lagrangian meshes tangle and an Eulerian formulation becomes preferable. Simulation codes may also be distinguished by the data structures of the computational variables. Lagrangian/ALE codes and many Eulerian codes are based on a staggered mesh where thermodynamic variables are placed at cell centers, but velocity is placed at the cell vertices. Other Eulerian codes, principally those based on Godunov type methods, have all variables colocated at the cell centers. See chapter 4 of Grinstein et al. 2007 for a detailed discussion of these.

Most modern Eulerian and ALE codes use nonoscillatory differencing to approximate the advective terms. Nonoscillatory approximation invokes mathematical notions such as the preservation of sign or of monotonicity to modify (limit) the advective fluxes. In MRG 2006, modified equation analysis was used to show that the combination of nonoscillatory differencing and finite volume approximation (NFV) in advection schemes effectively solves the FS momentum equation rather than the Navier-Stokes' momentum equation. This "implicit" appearance of the FS momentum exchange terms was offered as a rationale for the modeling technique of implicit large eddy simulation (ILES). We expect the NFV differencing of the energy equation will produce similar terms to the FS energy equation (3.5). However, as noted above, not all of the new FSE transport terms of energy arise from the advective terms. Further, there are still open questions in NFV methods as to the relation of the limiting process in the separate conservation equations (Schar & Smolarkiewicz 1996), which our reciprocity relations may help to clarify.

The situation in Lagrangian/ALE codes is more complicated. It was recognized from the earliest days of computing high speed flows that an artificial viscosity was required to produce the requisite entropy production in shocks. von Neumann & Richtmyer's (1950) viscosity is the momentum exchange term in the FS momentum equation (3.4), although it is typically only employed in compression. This basic viscosity with some generalization for multiple space dimensions is still in wide use today. Similarly, an artificial heat conduction was proposed by Noh (1978) to treat the numerical problem of wall heating. This term is not yet in common use. The relationship of artificial heat conduction to the artificial viscosity may be clarified by reciprocity of coefficients in the analogous terms predicted by the FSE.

The Lagrangian/ALE community has also partially confronted the thermodynamic issues discussed in §4. In these codes, velocity (more precisely, momentum velocity) is placed at the cell vertices and so the new position of a cell and its volume can be calculated geometrically. However, Reynolds' transport theorem (in integral form) offers an alternate equation to update volume. Problems associated

with the lack of consistency of the geometric volume change and the discretization of the velocity divergence led to formulation of compatible differencing techniques (Bauer et al. 2006; Margolin & Shashkov 2008). However, thermodynamic issues have continued to affect these codes (Whalen 1996). One modern approach to these problems is the technique of subcells (Bauer et al. 2006). Although the subcell technique was originally developed to control null space deformations (e.g., hourglassing), they also imply higher-order approximations to the pressure and velocity distributions within a cell and so provide a more accurate approximation to the nonlinear pressure-velocity work term.

(c) *Summary*

We have presented and analyzed the finite scale equations that describe the evolution of finite parcels of fluid whose individual points are governed by the compressible Navier-Stokes (NSE) equations. The volume-averaged variables are the fundamental variables of finite volume numerical simulation codes when one identifies the averaging scale L with the computational cell size Δx. Direct comparison of the FSE with the discretized equations shows that many of the new features of the FSE are already incorporated into the codes on a less rigorous basis, and provides guidance for future improvement.

Appendix A.

(a) *Kinematics of volume transport*

In a recent paper, Howard Brenner (2005a) discusses the kinematics of volume transport – that is, the transport and production of the extensive property of volume in a fluid (see also Brenner 2005b). Brenner's analysis has many features in common with FSE, though its derivation and context are quite different. In particular, Brenner remains in the context of the Navier-Stokes equations and does not introduce any additional length scale. All B-equation and page numbers in this subsection refer to Brenner 2005a.

Brenner begins with the recognition that the advective velocity and the momentum velocity are distinct, even in continuum Navier-Stokes theory. In contrast to our development, he chooses to maintain the framework of the advective velocity. Rewriting the continuity equation in terms of specific volume, $v = \frac{1}{\rho}$, he derives new terms representing the diffusion of v; cf. B-equation (2.11). Further, Brenner derives a relation, B-equation (3.15) between these velocities that is similar to our equation (3.2) in its dependence on the logarithmic gradient of density. Lacking any additional length scale, Brenner invokes the length scales of molecular diffusion to construct the coefficient of the gradient – B-equation (3.13).

Brenner acknowledges the redundancy of his volume transport B-equation (2.11), but emphasizes that its consideration leads to new physical insights. In particular, he discusses the possibility that volume transport will play a dynamic role in transporting energy and momentum across material surfaces (B-page 43) and derives a pressure dependent correction to the heat flux in B-equation (5.20).

Brenner's theory is focused on explaining experimental results for low-speed flows and has not yet been connected to numerical simulation.

(b) *Naver-Stokes α models*

The α-models (Holm et al. 1998) were introduced to describe the mean motion of ideal incompressible fluids. The equations are derived in an Euler-Poincaré formalism, which is the Lagrangian version of the Lie-Poisson Hamiltonian framework, and have been successfully used as a model for numerical simulation (e.g., Chen et al. 1999, Hecht et al. 2008). In the derivation of these equations, two velocities appear, the Lagrangian-averaged (momentum) velocity and the Eulerian-averaged (advection) velocity. These are related by a Helmholtz operator – compare equation (1) of Hecht et al. 2008 with our equation (3.2). Another similarity lies in the estimate of the total kinetic energy of the flow – compare equation (8) of Holm et al. 1998 with our equation (4.4).

An important difference between the α-models and the FSE is that the spatial scale α is a flow-dependent quantity representing the small scale fluctuations of the flow, whereas our L is a fixed scale representing the "observer". However, as a model for numerical simulation these may not be so dissimilar; that is, α would appear to represent the size of a cell in a Lagrangian simulation whereas L would represent the size of an Eulerian cell.

Acknowledgements: We appreciate many discussions with D.E. Burton, R.B. Lowrie, J.R. Ristorcelli and J.H. Schmidt. This work was performed under the auspices of the U.S. Department of Energy's NNSA by the Los Alamos National Laboratory operated by Los Alamos National Security, LLC under contract number DE-AC52-06NA25396.

References

Bauer, A.L., Burton, D.E., Caramana, E.J., Loubere, R., Shashkov, M.J., & Whalen, P. P. 2006 The internal consistency, stability, and accuracy of the discrete, compatible formulation of Lagrangian hydrodynamics. *J. Comput. Phys.* **218** 572–593.

Brenner, H. 2005a Kinematics of volume transport. *Physica A* **349**, 11–59.

Brenner, H. 2005b Navier-Stokes revisited. *Physica A* **349**, 60–132.

Chen, S.Y., Holm, D.D., Margolin, L.G. & Zhang, R. 1999 Direct numerical simulation of the Navier-Stokes alpha model, *Physica D* **133**, 66–83.

Grinstein, F.F., Margolin, L.G. & Rider, W.J. 2007 *Implicit large eddy simulation: computing turbulent fluid dynamics*, ch. 5, pp 195-220. Cambridge University Press, N.Y.

Hecht, M.W., Holm, D.D., Petersen, M.R., & Wingate, B.A. 2008 Implementation of the LANS-alpha turbulence model in a primitive equation ocean model. *J. Comput. Phys.* **227**, 5691–5716.

Holm, D.D., Marsden, J.E. & Ratiu, T.S. 1998 Euler-Poincaré models of ideal fluids with nonlinear dispersion. *Phys. Rev. Letters* **80** 4173-4176.

Margolin, L.G. 1997 Introduction to "An arbitrary Lagrangian-Eulerian computing method for all flow speeds." *J. Comput. Phys.* **135** 198–202.

Margolin, L.G. & Rider, W.J. 2002 A rationale for implicit turbulence modelling. *Int. J. Num. Meths. Fluids* **39**, 821–841.

Margolin, L.G. & Rider, W.J. 2005 The design and construction of implicit LES models. *Int. J. Num. Meths. Fluids* **47** 1173-1179.

Margolin, L.G., Rider, W.J. & Grinstein, F.F. 2006 Modeling turbulent flow with implicit LES. *J. Turbulence* **7**, 1–27.

Margolin, L.G. & Shashkov, M. 2004 Remapping, recovery and repair on a staggered grid. *Comput. Methods Appl. Mech. Engng* **193** 4139–4155.

Margolin, L.G. & Shashkov, M. 2008 Finite volume methods and the equations of finite scale: a mimetic approach. *Int. J. Num. Meths. Fluids* **56**, 991–1002.

Margolin, L.G., Smolarkiewicz, P.K., & Sorbjan, Z. 1999 Large-eddy simulations of convective boundary layers using nonoscillatory differencing. *Physica D* **133**, 390-397.

Noh, W.F. 1978 Errors for calculations of strong shocks using an artificial viscosity and an artificial heat flux. *J. Comput. Phys.* **72** 78–120.

Pope, Stephen B. 2000 *Turbulent flows*, Cambridge University Press, N.Y.

Schar, C. & Smolarkiewicz, P.K. 1996 A synchronous and iterative flux-correction formalism for coupled transport equations. *J. Comput. Phys.* **128** 101-120.

Smolarkiewicz, P.K. & Margolin, L.G. 1998 MPDATA: A finite-difference solver for geophysical flows. *J. Comput. Phys.* **140** 459–480.

von Neumann, J & Richtmyer, RD. 1950 A method for the numerical calculation of hydrodynamic shocks. *J. Appl. Phys.* **21** 232–237.