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Analysis into Asymptotic Convergence to Full Nonlinear Solutions and Exploration of the Implication of Numerical Operator Mutation of Differential Systems

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Objective Summary

A robust, sufficiently accurate and practical hydrodynamic simulation toolset is required as a key component of the modeling and simulation of air-gap electrostatic discharge events. This work was performed to complement these ongoing efforts. In particular, hydrodynamic simulations must be vetted to ensure they are robust and sufficiently accurate over relevant characteristic scales. Verification models were generated in order to cultivate the technical knowledge and expertise needed to properly create, implement and execute numerical simulations.

Furthermore, this effort was utilized extensively to educate students on the mathematical and numerical principles underlying hydrodynamic simulations. This education opportunity, provided in a holistic and rigorous manner, has greatly benefited developing scientists and engineers with the necessary understandings and toolsets required to excel at accomplishing the task at hand, and, more generally, it has enabled them to generate key programmatic deliverables.

This report articulates several subtleties; specifically, how perturbations, nonlinear behavior, and dissipative mechanisms influence numerical stability, how to properly structure mathematical and numerical solutions, and how to properly generate error estimation/assignment. A more rigorous discussion of the consequences of such topics can be found in the body of this report in Chapters 2 and 3 with qualitative findings discussed in Chapter 4.

Introduction

1.1. A Nexus of Numerical Methods

Myriad disciplines are involved in the analysis of *electrostatic discharges* (ESD) in ambient air arising from common triboelectric charging, *i.e.* at fixed total energy, ranging from plasma physics, chemical kinetics, atomic physics, and electrodynamics to fluid dynamics, hydrodynamics, shock physics, thermodynamics, and computational physics. The associated theoretical and mathematical complexities of such problems soon frustrate our ability to analytically solve such problems in closed form, forcing us to implement rather sophisticated numerical methods and algorithms [1]. Implementation of numerical methods and algorithms, however, is more than an exercise in mathematics or computer science, requiring a broad perspective for accuracy, efficiency, and proper interpretation of results. The distinction between model artifact and physical signature may not always be intuitively clear, including nuances between analytical and numerical formalisms.

In fluid dynamics, the *Euler equations* are a set of quasi-linear hyperbolic equations governing *adiabatic* and *inviscid* fluid flow, meaning no terms modeling the physical processes of thermal conduction or viscous flow are included in the partial differential equations (PDEs)¹. Linearization of the Navier-Stokes equations under a Maxwellian local equilibrium state also results in the Euler equations. In the case with negligible external fields, *i.e.* in the limit of high *Froude number*, the Euler equations take on what’s called the “conservation form” (also called the “Eulerian form”) when written in terms of a control volume fixed in (laboratory) space. In opposition, the “convective form” or “non-conservation form” defines a constant control mass moving with the flow and is often referred to as a “Lagrangian form”. These different forms are important when formulating analytical models for comparison with simulation results and will be discussed later.

In electrostatic shock discharge events, the electrical breakdown of ambient air creates a plasma that heats the air, generating a hydrodynamic wave propagating radially outward. The energy required to generate this time-dependent hydrodynamic wave relative to the stored initial electrostatic energy represents an essential energy budget contribution in the ESD event. The inclusion of dissipative mechanisms whereby this hydrodynamic wave energy is irreversibly lost to the fluid particles represents one important ingredient in understanding ESD events.

Dissipative mechanisms themselves can play multiple roles in practical application, *i.e.* in computational fluid dynamics. Solving fluid flow problems numerically requires discretization of the spatial and temporal coordinates associated with the governing partial differential equations (PDEs). Numerical schemes for solving **time-dependent** PDEs are conventionally referred to as being either *explicit* or *implicit*. When direct computation of the dependent variables can be made in terms of known quantities, the computation scheme is explicit. Alternatively, when the dependent variables are defined by sets of coupled equations, where matrix or iterative methods are required to obtain the solution, the numerical method is said to be implicit. Explicit methods calculate the state of a system at a later time from the state of the system at the current time, while implicit methods find a solution by solving an equation involving both the current state of the system and the later one.

The main reason for using implicit solution methods—which are more complicated to program than explicit methods and require more computational effort for each solution step—is the ability to use large time-steps, which is efficient for computing asymptotic or steady-state solutions. For modeling transient processes like ESD, explicit methods are more appropriate, but carry stability issues. *Numerical stability* has to do with the behavior of the solution as the time-step size is changed. For practical comparisons with computer simulations, our analytical analysis must use the differential form of the Euler equations, which assumes the fluid flow or governing equations are differentiable, and therefore continuous. This can be problematic whenever steep gradients or

¹Viscosity and heat conduction are examples of momentum and energy diffusion which may be present in a differential system modeling hydrodynamic flow. These processes, combined with mass diffusion, describe irreversible, entropy producing effects that are always present in reality.

shock waves occur, so whenever such circumstances are possible, *artificial* dissipative mechanisms are commonly invoked to maintain numerical stability; a typical choice is artificial viscosity.

Regardless as to their origin, dissipative effects represent irreversible thermodynamic processes. Understanding the thermodynamics of irreversible processes and mechanisms by which energy is dissipated is therefore important in the context of not only ESD events, but in numerical analysis itself and how discontinuities are treated when solving partial differential equations. This report is a preliminary assessment of some of these issues, in an attempt to understand the thermodynamic consequences of dissipation.

1.2. Organization of the Report

This report is a preliminary assessment of “dissipation” in fluid flow, and attempts to highlight some of the subtleties associated with specific numerical algorithms used to model fluid flow. Viscosity and thermal conduction represent two major dissipative mechanisms, and mathematical terms modeling these mechanisms are therefore added to the standard Euler equations such that their effects can be explored.

CHAPTER 2

Asymptotic Convergence to a Full Nonlinear Solution via Variable Expansion

2.1. Introduction

A perturbative technique is used to investigate nonlinear effects and asymptotic convergence to a fully nonlinear solution of axisymmetric flow from a source term that emanates outgoing waves in the context of the Euler equations. The physical dissipative mechanisms considered are heat conduction and viscosity¹. These cases are compared to inviscid, non conducting flows. The fully nonlinear inviscid case is compared to a robust, well-verified and validated, finite element code [4]. The finite element code solves the Lagrangian formulation of the Euler equations, see Eqs. (2.1a) to (2.1c), with the inclusion of artificial viscosity to ensure numerical stability.

$$(2.1a) \quad \frac{d}{dt}M = 0 ,$$

$$(2.1b) \quad \rho \frac{d\mathbf{v}}{dt} - \nabla \cdot \bar{\mathbf{T}} = 0 ,$$

$$(2.1c) \quad \rho \frac{de}{dt} - \bar{\mathbf{T}} : \nabla \otimes \mathbf{v} = 0$$

The structure of the chapter is as follows. Section 2.2 develops the theoretical framework that is used to derive the fully nonlinear and perturbed differential systems that are solved. Section 2.3 explains the numerical method that is used to solve the derived differential systems and provides numerical verification. Section 2.4 provides details outlining how nonlinear effects and physical dissipative mechanisms influence the solutions to perturbed and fully nonlinear differential systems. Section 2.5 discusses the results and proposes future work avenues.

2.2. Mathematical Formulation

Mathematical physics can be used as a powerful tool to describe physical phenomena, model complex processes that cannot be observed in experiment, or help verify numerical algorithms that solve problems which have no true analytical solution. In the finite element code, the full nonlinear form of the Euler equations, see Eqs. (2.1a) to (2.1c), are solved with an assumed ideal gas equation of state with artificial viscosity used for numerical stability [4]. A perturbation technique is used to asymptotically explore nonlinear effects and error with a semi-analytic solution to the Euler equations modified by viscosity and heat conduction. The Euler equations are continuity equations for mass density, momentum density, and energy density [42, 44]. They may be written as the following in an Eulerian coordinate system

$$(2.2a) \quad \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0 ,$$

$$(2.2b) \quad \frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \bar{\mathbf{T}} = 0 ,$$

$$(2.2c) \quad \frac{\partial}{\partial t}(\rho e + \tfrac{1}{2}\rho|\mathbf{v}|^2) + \nabla \cdot \left[\mathbf{v} \left(\tfrac{1}{2}\rho|\mathbf{v}|^2 + \rho e + p \right) \right] = 0 ,$$

where ρ is the mass density, $\mathbf{v}$ is the flow velocity, $\bar{\mathbf{T}}$ is the stress tensor, e is the specific internal energy, and p is the thermodynamic pressure. The Euler equations are a hyperbolic system with zero dissipation. When discontinuities or large gradients occur in the theory of the Euler equations,

¹For a physically complimentary analysis of physical dissipative mechanisms, mass diffusion would have to be included in the differential system.

at shock fronts or at material interfaces with discontinuous thermodynamic properties, non-causal, i.e. non-hyperbolic, dissipative terms must be introduced to obtain stable numerical solutions.²

2.2.1. The Inclusion of Dissipative Mechanisms. The viscous, heat conducting differential system analyzed is written as the following in one dimensional planar geometry

$$(2.3a) \quad \rho \frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x} = 0 ,$$

$$(2.3b) \quad \rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} + \frac{\partial p}{\partial x} - \overbrace{\mu \frac{\partial^2 u}{\partial x^2}}^{\text{viscous term}} = 0 ,$$

$$(2.3c) \quad \rho \frac{\partial e}{\partial t} + \rho u \frac{\partial e}{\partial x} + p \frac{\partial u}{\partial x} - \overbrace{\mu \left(\frac{\partial u}{\partial x} \right)^2}^{\text{viscous term}} + \overbrace{\frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right)}^{\text{heat conduction term}} = 0 ,$$

where u is the flow velocity in the $\hat{x}$ -direction, x is the spatial variable, t is the temporal variable, T is the thermodynamic temperature, μ is the viscosity of the fluid, and k is the thermal conductivity of the fluid. Equations (2.3a) to (2.3c) are the reduced one dimensional Euler equations modified by the addition of viscosity and heat conduction.

2.2.2. Non-dimensionalization. Typically the differential systems, shown in Eqs. (2.3a) to (2.3c) are rewritten in non-dimensional form for simplicity. For this purpose, the fundamental variables are scaled to a unitless form, which are denoted by a tilde over the variable, which is obtained by dividing the variable by a characteristic value, denoted by a subscript 0,

$$\begin{aligned} \tilde{\rho} &= \rho / \rho_0 , & \tilde{p} &= p / p_0 , \\ \tilde{u} &= u / u_0 , & \tilde{x} &= x / x_0 , \\ \tilde{e} &= e / e_0 , & \tilde{t} &= t x_0 / u_0 , \end{aligned}$$

and, after substitution into Eqs. (2.3a) to (2.3c), the desired non-dimensional differential system is obtained

$$(2.4a) \quad \frac{\partial \tilde{\rho}}{\partial \tilde{t}} + \tilde{u} \frac{\partial \tilde{\rho}}{\partial \tilde{x}} + \tilde{\rho} \frac{\partial \tilde{u}}{\partial \tilde{x}} = 0 ,$$

$$(2.4b) \quad \tilde{\rho} \frac{\partial \tilde{u}}{\partial \tilde{t}} + \tilde{\rho} \tilde{u} \frac{\partial \tilde{u}}{\partial \tilde{x}} + K_m \frac{\partial \tilde{p}}{\partial \tilde{x}} - \frac{1}{\text{Re}} \frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2} = 0 ,$$

$$(2.4c) \quad \tilde{\rho} \frac{\partial \tilde{e}}{\partial \tilde{t}} + \tilde{\rho} \tilde{u} \frac{\partial \tilde{e}}{\partial \tilde{x}} + K_e \tilde{p} \frac{\partial \tilde{u}}{\partial \tilde{x}} - \frac{1}{\text{Re}} \frac{K_e}{K_m} \left(\frac{\partial \tilde{u}}{\partial \tilde{x}} \right)^2 - \frac{1}{\text{Pe}} \frac{\partial^2 \tilde{e}}{\partial \tilde{x}^2} = 0 .$$

The non-dimensional ratios, K_m and K_e , along with the common dimensionless ratios known as the *Reynolds number* (Re) and the *Peclet number* (Pe), may be defined

$$\begin{aligned} K_m &= \frac{p_0}{\rho_0 u_0^2} , & \text{Re} &= \frac{\rho_0 u_0 x_0}{\mu} = \frac{x_0}{x_\mu} \\ K_e &= \frac{p_0}{\rho_0 e_0} , & \text{Pe} &= \frac{f k_B}{2 m} \frac{\rho_0 u_0 x_0}{k} = \frac{x_0}{x_k} , \end{aligned}$$

which characterize the physical nature of the fluid flow. An interesting thing to note is that two characteristic lengths, x_μ and x_k , may be introduced which also characterize the physical dissipative parameters of the flow. In addition to having the dimensional variables in the Re and Pe numbers, Boltzmann's constant, k_B , has also been used in addition to the mass of an individual molecule/atom in the fluid, m . As a calorically-perfect ideal gas equation of state is implemented, a constant number of internal (molecular) degrees of freedom can be incorporated into this formalism by inclusion of a single parameter indicating the number of degrees of freedom desired, denoted by the lowercase parameter f above in the Peclet ratio. Equations (2.4a) to (2.4c) is the differential system that is solved with a high order finite difference method.³ Equations (2.4a) to (2.4c) form

²Dissipation, regardless as to its origin, physical or artificial, acts to decrease or "smooth out" steep gradients or discontinuities, and thereby acts to generally improve numerical stability.

³As Galilean transforms relate reference frames that differ only by constant relative motion, spatial derivatives remain consistent between the frames or are unchanged by the transformation. This fact will be used to our advantage.

FIGURE 2.1 The above figure shows different orders of approximations to some function represented by the blue surface. The red is a linear approximation, the yellow is quadratic, and green is a cubic approximation to the blue surface which may be written as $\phi(x, t)$. Note that how the accuracy of a series approximation increases as the order of the approximation increases.

the differential system that is used in the perturbation analysis. To mathematically close the PDE system, a calorically-perfect ideal gas equation of state (EoS) is implemented⁴

$$p = (\gamma - 1)\rho e ,$$

where γ is the ratio of specific heat capacities, which at least allows for some constant internal (molecular) degrees of freedom, which will be denoted as f . The thermodynamic variables in this simple EoS can be rewritten in terms of their dimensionless counterparts, all denoted by a tilde,

$$(2.5) \quad \tilde{p} = \frac{\gamma - 1}{K_e} \tilde{\rho} \tilde{e} ,$$

along with the dimensionless ratio K_e defined above.

Equations (2.4a) to (2.4c) form one of two differential systems that has been discretized with the method of lines. (The other differential system is the perturbed differential system.) This differential system will now be referred to as the full nonlinear differential system. The isentropic version (inviscid and non conducting) has the Re and Pe numbers set to ∞ so that the second order derivatives vanish. Fortunately, the differential system that results only has first order temporal derivatives, so numerical integration such as the method of lines can be straightforwardly implemented [12, 33, 40]. The temporal discretization of the method of lines, see Fig. 2.4, was done via a Runge-Kutta 4 scheme, as given in Press et al. [28], and the spatial discretization was implemented with a fourth order central finite difference scheme. An advantage for using this central difference scheme is that it allows us to use a numerical operator that has significantly less numerical dissipation than upwinding and other numerically dissipative, stability-ensuring methods. To implement the RK4 solver, each temporal derivative in Eqs. (2.4a) to (2.4c) is isolated.

2.2.3. Nonlinear Perturbations. A perturbation expansion of arbitrary order may be performed with the non-dimensional differential system shown in Eqs. (2.4a) to (2.4c). Conventionally, an expansion approximates some function in a local neighborhood where the variables that are being expanded about do not change much⁵, which can be seen in Fig. 2.1

With the inclusion of more and more terms in an expansion, the value of the function is better approximated and the local neighborhood where the perturbation expansion is valid increases. For an expansion of infinite terms, the “local” neighborhood can be all space. This is obviously dependent on the object being expanded about. For example, a quadratic may be exactly recovered from a second order Taylor expansion. A caveat to note, however, is that a series expansion is not the same as the perturbation technique we are performing. The error in our perturbation analysis comes from the truncation of higher order terms from the differential system, *not* from terms being left out in an approximation to a variable.

Perturbation to the density, $\tilde{\rho}$, energy, $\tilde{e}$, and flow velocity, $\tilde{u}$ may be defined (the pressure is calculated from the EOS). These perturbation variables are treated as the new variables within the problem. Again, this introduction of new variables is *not* an approximation but rather a new

⁴A calorically-perfect, ideal gas, even one with a fixed number of degrees of freedom f , is not consistent with the viscous and thermal conduction terms associated with the added PDE dissipative contributions.

⁵Consider a planar approximation to a multivariate function in $\mathbb{R}^3$. If the behavior of that function is locally planar, then a plane is a good approximation for the behavior of that function in the local neighborhood.

variable definition. The error in the perturbed differential system comes from the elimination of higher order terms. The perturbation variables may be taken to any arbitrary order. These new variable definitions are

$$(2.6a) \quad \tilde{\rho} = 1 + \overbrace{\tilde{\eta} + \tilde{\eta}^2/2 + \tilde{\eta}^3/6}^{\delta\tilde{\rho}},$$

$$(2.6b) \quad \tilde{u} = 0 + \overbrace{\tilde{v} + \tilde{v}^2/2 + \tilde{v}^3/6}^{\delta\tilde{u}},$$

$$(2.6c) \quad \tilde{e} = 1 + \overbrace{\tilde{\epsilon} + \tilde{\epsilon}^2/2 + \tilde{\epsilon}^3/6}^{\delta\tilde{e}},$$

where $\tilde{\eta}$, $\tilde{v}$, and $\tilde{\epsilon}$ are the new flow variables for density, flow velocity, and specific internal energy respectively. Table 2.1 shows various values of these variables for given expansion orders and sizes of perturbations.

TABLE 2.1 Values of the size of the perturbed variables $\tilde{\eta}$, $\tilde{v}$, and $\tilde{\epsilon}$ as functions of the order of the expansion, n , and the size of the perturbation, $\delta\tilde{\phi}$.

	$\delta\tilde{\phi} = 0.01$	$\delta\tilde{\phi} = 0.1$	$\delta\tilde{\phi} = 0.55$
$n = 1$	0.01	0.1	0.55
$n = 2$	9.95049e-3	0.0954451	0.449138
$n = 3$	9.95033e-3	0.0953134	0.439351

These new variables from Eqs. (2.6a) to (2.6c) may be plugged into the non-dimensional differential system and eliminate terms of greater than the desired order. With these substitutions, with of course the help of the Eq. (2.5), the following may be written

$$(2.7a) \quad \overbrace{(1 + \delta\tilde{\rho})}_{\tilde{\rho}_{\tilde{t}}} + \overbrace{(0 + \delta\tilde{v})(1 + \delta\tilde{\rho})}_{\tilde{u}\tilde{\rho}_{\tilde{x}}} + \overbrace{(1 + \delta\tilde{\rho})(0 + \delta\tilde{v})}_{\tilde{\rho}\tilde{u}_{\tilde{x}}} = 0,$$

$$(2.7b) \quad \overbrace{(1 + \delta\tilde{\rho})(0 + \delta\tilde{v})}_{\tilde{\rho}\tilde{u}_{\tilde{t}}} + \overbrace{(1 + \delta\tilde{\rho})(0 + \delta\tilde{v})(0 + \delta\tilde{v})}_{\tilde{\rho}\tilde{u}\tilde{u}_{\tilde{x}}} + \frac{K_m}{K_e} \overbrace{(\gamma - 1)(1 + \delta\tilde{\rho} + \delta\tilde{e} + \delta\tilde{\rho}\delta\tilde{e})}_{\tilde{p}_{\tilde{x}}} - \frac{1}{\text{Re}} \overbrace{(0 + \delta\tilde{v})_{\tilde{x}\tilde{x}}}_{\tilde{u}_{\tilde{x}\tilde{x}}} = 0,$$

$$(2.7c) \quad \overbrace{(1 + \delta\tilde{\rho})(1 + \delta\tilde{\epsilon})}_{\tilde{\rho}\tilde{e}_{\tilde{t}}} + \overbrace{(1 + \delta\tilde{\rho})(0 + \delta\tilde{v})(1 + \delta\tilde{\epsilon})}_{\tilde{\rho}\tilde{u}\tilde{e}_{\tilde{x}}} + (\gamma - 1) \overbrace{(1 + \delta\tilde{\rho} + \delta\tilde{e} + \delta\tilde{\rho}\delta\tilde{e})(0 + \delta\tilde{v})}_{\tilde{p}\tilde{u}_{\tilde{x}}} - \frac{1}{\text{Re}} \frac{K_e}{K_m} \overbrace{(0 + \delta\tilde{v})_{\tilde{x}}^2}_{\tilde{v}_{\tilde{x}}^2} - \frac{1}{\text{Pe}} \overbrace{(1 + \delta\tilde{\epsilon})_{\tilde{x}\tilde{x}}}_{\tilde{e}_{\tilde{x}\tilde{x}}} = 0,$$

FIGURE 2.2 A tangent line, a linear Taylor series, that approximates some function. Note the size of the local neighborhood where the expansion is valid. If a higher order series was used, the size of the size of the local neighborhood would increase.

FIGURE 2.3 Error of Perturbation of size $\delta\tilde{\phi}$. The order of the error is $\mathcal{O}(\delta\tilde{\phi}^{n+1})$, where n is the order of the expansion, the number of terms in the expressions for the old variable see Eqs. (2.6a) to (2.6c). Here, n is plotted in a smooth, continuous manner. The quantity $\delta\tilde{\phi}$ is the size of the perturbation. The error falls off as a power law as higher order approximations are taken.

where the spatial and temporal derivatives have been replaced with subscripts for $\tilde{x}$ and $\tilde{t}$, respectively. There are now only three dependent variables in Eqs. (2.7a) to (2.7c): $\delta\tilde{\rho}$, $\delta\tilde{v}$, and $\delta\tilde{e}$.

The new definition of $\delta\tilde{\rho}$, $\delta\tilde{v}$, and $\delta\tilde{e}$ in Eqs. (2.6a) to (2.6c) may be substituted. Terms higher than an arbitrary order may be eliminated; here third order terms were chosen. This process is shown explicitly in Appendix A. This means that any variable or derivative quantity having a total combined power of 4 or greater may be dropped. The following equation are obtained

$$(2.8a) \quad \left(1 + \eta + \frac{\eta^2}{2}\right) \eta_t + \left(v + \frac{v^2}{2} + v\eta\right) \eta_x + \left(1 + v + \frac{v^2}{2} + \eta + \eta v + \frac{\eta^2}{2}\right) v_x = 0,$$

$$(2.8b) \quad \left(1 + v + \frac{v^2}{2} + \eta + \eta v + \frac{\eta^2}{2}\right) v_t + \left(v + \frac{3}{2}v^2 + \eta v\right) v_x + \frac{K_m}{K_e}(\gamma - 1) \left[\left(1 + \eta + \frac{\eta^2}{2} + \epsilon + \eta\epsilon + \frac{\epsilon^2}{2}\right) \eta_x + \left(1 + \eta + \frac{\eta^2}{2} + \epsilon + \eta\epsilon + \frac{\epsilon^2}{2}\right) \epsilon_x \right] - \frac{1}{\text{Re}} \left(\left(1 + v + \frac{v^2}{2}\right) v_{xx} + (1 + v)v_x^2 \right) = 0,$$

$$(2.8c) \quad \left(1 + \eta + \frac{\eta^2}{2} + \epsilon + \eta\epsilon + \frac{\epsilon^2}{2}\right) \epsilon_t + \left(v + v\epsilon + \frac{v^2}{2} + \eta v\right) + (\gamma - 1) \left(1 + \eta + \epsilon + v + \eta\epsilon + \eta v + \epsilon v + \frac{\eta^2}{2} + \frac{v^2}{2} + \frac{\epsilon^2}{2}\right) v_x - \frac{1}{\text{Re}} \frac{K_e}{K_m} (1 + 2v)v_x^2 - \frac{1}{\text{Pe}} \left[\left(1 + \epsilon + \frac{\epsilon^2}{2}\right) \epsilon_{xx} + (1 + \epsilon)\epsilon_x^2 \right] = 0,$$

where the tildes have been dropped for convenience. Equations (2.8a) to (2.8c) constitute the other differential system that has been discretized with the method of lines⁶. Fortunately, the differential system that results only has first order temporal derivatives, so numerical integration such as the method of lines can be implemented [12, 33, 40]. The temporal discretization of the method of lines, see Fig. 2.4, was done via a Runge-Kutta 4 scheme, as given in Press et al. [28], and the spatial discretization was implemented with a fourth order central difference scheme. To implement an RK4 solver, each temporal derivative in Eqs. (2.8a) to (2.8c) is isolated.

A key thing to note about the differential system found in Eqs. (2.8a) to (2.8c) is that error has been introduced in the truncation of higher order terms. This error is a function of both the order of the terms being truncated (linear, quadratic, cubic, etc.) and the size of the variables $\delta\rho$, δu , and δe , see Fig. 2.3. As shown in Section 2.4.2, small perturbations lead to excellent agreement

⁶The pattern of repeating terms leads to the conclusion that a generalized rule to generating a perturbed differential system of order n may be constructed.

between the perturbed differential system and the full nonlinear differential system. However, at larger perturbations, $\delta\tilde{\phi} \approx 1$, ever higher order terms are required in order to have the perturbed solution asymptotically approach the full nonlinear solution.

2.3. Numerical Methodology

As discussed in Sections 2.2.2 and 2.2.3, an RK4 solver was implemented via the method of lines [7, 12, 33, 40] for the temporal derivatives in Eqs. (2.4a) to (2.4c) and Eqs. (2.8a) to (2.8c). The spatial derivatives were approximated by a fourth order, minimally dissipative central difference scheme [7, 28]. A stencil of this numerical operator is shown in Fig. 2.4. The error that occurs within the discretized numerical solution to Eqs. (2.8a) to (2.8c) is evident in Fig. 2.5. The sources of error come from the spatial and numerical discretization of the derivatives (numerical operator), and the truncation of terms in the differential system. Recall that this truncation of terms was within the differential system and *not* in the new definition of the variables. In general, one must balance two types of errors in the perturbed differential system: error introduced by the truncation of terms in the differential system and error introduced by the numerical operator.

2.4. Results

Several simulation types were performed in order to understand how various solutions with differing physical mechanisms compared to each other within the perturbed differential system and the fully nonlinear differential system. The simulations types performed were quadratic and cubic perturbations and the full nonlinear system that were inviscid, viscous, heat conducting, and viscous-conductive. These simulation had either the Reynold number or the Péclet number set to ∞ . The inviscid case had both the Reynolds number and the Péclet number set to ∞ , while the viscous had the Péclet number set to ∞ , and the heat conducting had the Reynolds number set to ∞ . The viscous-conductive case had finite values for both the Reynolds and Péclet numbers. The initial conditions of the non-dimensional, perturbed variables:

$$\begin{aligned}\delta\rho(x, 0) &= \alpha e^{-((x-1)/\sigma)^2} , \\ \delta u(x, 0) &= \alpha e^{-((x-1)/\sigma)^2} , \\ \delta e(x, 0) &= 0 .\end{aligned}$$

The initial conditions of the simulations in non-dimensional, nonlinear variables:

$$\begin{aligned}\rho(x, 0) &= 1 + \alpha e^{-((x-1)/\sigma)^2} , \\ u(x, 0) &= \alpha e^{-((x-1)/\sigma)^2} , \\ e(x, 0) &= 1 .\end{aligned}$$

The parameters of the initial conditions, α and σ , are the amplitude of the added value, $\delta\phi$, and the Gaussian's width parameter. The simulations are characterized by $\sigma = 0.25$ and $\alpha = 0.01, 0.1, 0.55$. The results of these simulations are shown in the following subsections.

2.4.1. Numerical Convergence Studies for Inviscid Solutions (Perturbed and Fully Nonlinear). The ability to employ the use of numerical algorithms in science, and thusly decision making processes, is dependent on the validity of those models and the level of trust that may be placed in them. The verification and quantification of error that may be present in computational models is thus an important aspect of computational physics. The results from the high-order

FIGURE 2.4 A figure showing the numerical stencil that is used in the numerical method of lines. The blue box shows the possible stencil for an arbitrary grey point at some future in the spatial and temporal domain relative to a past time step in the black. The variable $\tilde{t}$ represents a non-dimensional time variable while $\tilde{x}$ represents some Galilean transformed non-dimensional spatial variable.

FIGURE 2.5 Graphic showing the relationship between the sources of error and the magnitude of those sources of error that are present in the semi-analytic solution. n is the order of the perturbation expansion, L is the length of the simulation, N is the number of points in the domain, and dt_{max} is the maximum time step specified by the adaptive Runge-Kutta scheme.

finite difference method are compared to those from a finite element code [4] to estimate accuracy and convergence rate.

Equation (2.9) shows the L_∞ error metric where z references an individual cell in the computational domain, R is the entire computational domain, c is the calculated value, a is the approximate or analytic value expected, N is the number of cells in the domain, and V_R is the volume of the mesh.

$$(2.9) \quad L_\infty = \max_{z \in R} \left(\int_z |c - a| dV \right),$$

Equation (2.9) is used to calculate the error shown in Figs. 2.6 and 2.7. Figure 2.6 shows the error from comparing the fully nonlinear differential system solution to a higher resolution, $N = 5000$, solution. Note the clean convergence of the order of the error.

Figure 2.7 shows the L_∞ error metric between a quadratic and cubic series expansion for the inviscid differential system with an α value of 0.01 and σ value of 0.25. A linear expansion was not used because the dissipative mechanisms of viscosity and heat conduction are second order phenomena. Note that the error between the simulations flatlines after the error from the numerical operator is washed out from a finely resolved spatial and temporal mesh. This flatlining shows the lower bound on the error between the cubic solution and the full nonlinear code for an α value

FIGURE 2.6 The Navier-Stokes numerical operator error for the fully nonlinear differential system as a function of the mesh resolution. The resolution taken as the analytic value had a resolution of $N = 5000$.

FIGURE 2.7 The error between the quadratic and cubic series expansions with an α value of 0.01 and σ value of 0.25 as a function of mesh resolution. The lower bound on the error $\approx 1e-6$ is the minimum error between the nonlinear solution and cubic solution. This error comes from the truncation of terms in the perturbed differential system and is of order $\mathcal{O}(\delta\phi^3) \approx 1e-6$

FIGURE 2.8 Comparison from inviscid Navier-Stokes solution at resolution of $N = 5000$ to the finite element code at the specified resolutions. Note the excellent agreement between solutions. Comparison is at a time slice of $\tilde{t} \approx 0.25$.

of 0.01 and σ value of 0.25. This error of $1e-6$ can actually be predicted from the order terms truncated from the quadratic differential system. The error is predicted to be $\mathcal{O}(\delta\phi^3)$, which for a $\delta\phi$ value of is $\approx 1e-6$. This is the value of the lower bound of the error. Figures 2.8 and 2.9 show the results of comparing the inviscid, fully nonlinear simulation to the finite element code at the specified resolutions. Note the accuracy with which the different simulations solving different differential systems with distinct numerical operators agree. The α value was 0.01 and the σ value was 0.25 for the comparison. The finite element code used as comparison is referred to as “code” in the plots. The comparison was made at a non-dimensional time of one quarter.

2.4.2. Behavior of the Perturbed Differential System’s Solutions. As with any expansion about a point, the validity of our variable expansion is determined by how well the approximate solution fits the full solution or observation. In the case of the perturbed system, small amplitude perturbations approximate the full solution well, see Figs. 2.10 and 2.11. For larger amplitude perturbations, see Figs. 2.12 and 2.13, the approximate differential system shown in Eqs. (2.8a) to (2.8c) is no longer valid and either the perturbation size must decrease or a higher order expansion and resultant differential system must be used. The consequences of Figs. 2.1 to 2.3 can now be explicitly seen in the following plots. All of the following plots had the Reynolds number or the Péclet number set to either 100 or ∞ to capture the inviscid, viscous, conductive, or viscous-conductive solutions. Note the significant modification in the solution when either viscous or conductive terms are included in the solution. Of course, as the Reynolds number and Péclet number increase, the solutions will converge to the inviscid case with zero dissipation. All plots are shown at a nondimensional time of $\tilde{t} \approx 0.25$.

FIGURE 2.9 Difference between inviscid Navier-Stokes solution at resolution of $N = 5000$ to the finite element code. The maximum difference for $N_{\text{Code}} = 100$ is not shown on the current axes. Note how the difference asymptotically approaches zero as a function of the mesh resolution.

FIGURE 2.10 Quadratic, varied purple, and cubic, varied colored, solutions compared to the full nonlinear Navier-Stokes, varied black, solutions in a simulation with $\alpha = 0.01$ and $\sigma = 0.25$. The inviscid solutions have solid curves, the viscous have dotted curves, the conductive have dot-dashed curves, and the viscous-conductive have dashed curves. The quadratic and cubic simulations have a q or c prefix to the subscript, respectively. Note the excellent agreement between all of the curves for the same physical parameters. Indeed, it is hard to distinguish the difference between each solutions for the viscous-conductive, viscous, conductive, and inviscid simulations. Comparison between solutions with different physical parameters can be made as well. Note the drastic difference between solutions with different physical parameters included.

FIGURE 2.11 Quadratic, varied purple, and cubic, varied colored, solutions compared to the full nonlinear Navier-Stokes, varied black, solutions in a simulation with $\alpha = 0.01$ and $\sigma = 0.25$. The inviscid solutions have solid curves, the viscous have dotted curves, the conductive have dot-dashed curves, and the viscous-conductive have dashed curves. The quadratic and cubic simulations have a q or c prefix to the subscript, respectively. Note the good agreement between all of the curves. The solutions are beginning to diverge slightly, as can be seen at the maximum of each rightward going wave.

FIGURE 2.12 Quadratic, varied purple, and cubic, varied colored, solutions compared to the full nonlinear Navier-Stokes, varied black, solutions in a simulation with $\alpha = 0.55$ and $\sigma = 0.25$. The viscous have dotted curves, and the viscous-conductive have dashed curves. The quadratic and cubic simulations have a q or c prefix to the subscript, respectively. Note the good agreement between all of the curves. However, the perturbed solutions have now noticeably diverged from the full nonlinear one. However, the collapsing down on the full nonlinear solutions may be observed from comparing the quadratic and cubic solutions to the full nonlinear. For larger perturbations higher order expansions would be required in order to more accurately capture nonlinearities. In addition, the conductive and inviscid solutions are not plotted due to them having “blown up” prior to the time of recording the simulation.

FIGURE 2.13 Comparison between a cubic, subscript c , a quadratic, subscript q , solution and the full Navier-Stokes for the viscous-conductive solution. Note how the quadratic and cubic solutions asymptotically converge on the the full Naiver-Stokes solution. Figure 2.12 shows a closeup view of this solutions in addition to the viscous solution.

2.5. Discussion and Conclusions

The influence of nonlinear and dissipative effects have been explored in the context of non-dimensional perturbed and fully nonlinear differential systems. These effects have large impacts on the structure, stability, and physics present in their respective differential systems as observed in Figs. 2.10 to 2.12. A fine balance between truncation error and numerical error must be struck at larger perturbations or departures away from an expanded about value.

In addition to observing the influence of dissipative terms in the differential system, asymptotic convergence to the full nonlinear solution has been observed, see Fig. 2.13. This asymptotic convergence may be predicted to have a minimum value based on error truncation terms from the perturbed differential system, see Fig. 2.7.

Future extensions of this work that could be pursued: adding other dissipative affects, for example mass diffusion; further asymptotic analysis with more terms in a perturbation and thusly truncation; and error comparison between the numerical, full nonlinear solutions and numerical, perturbed solutions to a full differential system.

Physical and Numerical Implications of Dissipative Mechanisms

3.1. Introduction

The ability to employ the use of numerical algorithms in science, and thusly decision making processes, is dependent on the validity of those models and the level of trust that may be placed in them. The verification and quantification of error that may be present in computational models is thus an important aspect of computational physics. Here, a differential system with physical dissipative mechanisms is solved using a high order finite difference method. The results of these simulations are compared to a robust, well-verified and validated, finite element code [4]. The finite element code can be implemented to have physical and numerical viscosity.

The mathematical physics implications of numerical operators are explored. Most often, mathematical physics and numerical physics are developed independently[32], and the numerical results that are produced are post priori assigned physical significance [2, 5, 15, 18, 23, 34, 35, 38]. The implications of the numerics, which approximates physical processes, are tied back to true mathematical physics. Connection has been drawn, though, that the inclusion of numerical operators does indeed approximate real physical mechanisms [20–22]. A motivation for this analysis is that the true limit of zero dissipation is never recovered due to computational and physical feasibility. The implications of the use of dissipative, and other, numerical operators and how they mutate the numerical solution to the solution of a different differential system has not been explicitly explored and compared to modified analytic equations.

Prime examples of numerical methods that ensure stability, and also mimic reality, are artificial viscosity [29, 30, 36, 41] and artificial heat conduction [5, 14, 18, 26, 27]. Mattsson and Rider [19] provide an excellent modern review of the method of artificial viscosity with historical context. Artificial heat conduction has been used since the 60s in order to ensure numerical stability [14, 26, 31]. It is not as widespread as artificial viscosity, and is often used in conjunction with artificial viscosity to ensure numerical stability and ameliorate errors. In general, since its first use artificial viscosity has been used in order to smooth hydrodynamic flows and allow numerical solutions on the length scale of a mesh, as the inclusion of real viscosity is often not computationally or physically feasible due the length scales it acts on. This overestimation of the effect of viscosity misattributes numerical artifacts with a physical phenomenon.

Physical dissipative mechanisms are functions of the thermodynamic properties of a material. Many simulations are performed treating gases as inviscid flows which ignore physical dissipative mechanisms but use numerical dissipative mechanisms to ensure numerical stability [5, 11, 14, 18, 19, 26, 27, 29–31, 36, 41]. The disparity between these simulations with numerical dissipative mechanisms and simulations with physical dissipative mechanisms is an interesting thing to explore. This exploration is done by delving into energy conservation, entropy production, and wall heating effects in the context of two problems: an ambient fluid, and a piston impinging on an ambient fluids.

Local and global entropy production and energy conservation is explored in Sections 3.2.3.1 and 3.2.3.2 and Section 3.4.4 in the context of an ambient fluid problem. It is found that local entropy production may be negative, while the overall global entropy production still remains positive. In addition, it is noted that dissipation that is created via either physical or via a numerical operator may not be fully acknowledged or understood in traditional entropy analysis due to certain terms approximating entropy producing or dissipative terms.

It is found that in the context of a wall problem, wall heating errors are recovered with a physical Re number in a viscous only simulation [26]. In addition, with the inclusion of physical heat conduction, it is found that the viscous-conductive solution corrects for the wall heating error, as was done via numerical dissipation in work done by Noh[26]. The entropy producing effects of viscosity and heat conduction are physical objects that are not always accounted for in traditional numerical schemes. A numerical coefficient is used to ensure numerical stability which may not

be physically reflective. In addition, sometimes the numerical coefficients for these dissipative mechanisms may not be explicitly implemented in the numerical algorithm, but may arise from the numerical discretization [13, 17, 25, 41, 43].

Lastly, it is shown that physical and numerical viscosity may reproduce the same solutions for sufficiently viscous mediums. However, consideration must be taken to ensure that the resolution required to capture a physical viscosity is not so finely resolved as to be too computationally expensive or require alternative physics to accurately capture. Implications of numerical algorithm verification are explored.

The structure of the chapter is as follows. Section 3.2 introduces the differential system with dissipative mechanisms whose solutions are compared to the finite element code and builds the necessary theory to observe entropy production and energy calculation. Section 3.3 and Section 3.4 explain the numerical method and results, respectively. Section 3.5 wraps up with discussion on local entropy negativity, wall heating error and correction, and implications for numerical algorithm verification.

3.2. Theoretical Background

Mathematical physics can be used as powerful tool to describe physical phenomena, model complex processes that cannot be observed in experiment, or verify numerical algorithms that solve problems that have no true analytical solution. In the finite element code, the full nonlinear form of the Euler equations are solved with an assumed ideal gas equation of state [4]. The Euler equations are continuity equations for mass density, momentum density, and energy density [42, 44]. They may be written as the following in an Eulerian coordinate system

$$(3.1a) \quad \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0 ,$$

$$(3.1b) \quad \frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \bar{\mathbf{T}} = 0 ,$$

$$(3.1c) \quad \frac{\partial}{\partial t} (\rho e + \frac{1}{2} \rho |\mathbf{v}|^2) + \nabla \cdot \left[\mathbf{v} \left(\frac{1}{2} \rho |\mathbf{v}|^2 + \rho e + p \right) \right] = 0 ,$$

where ρ is the mass density, $\mathbf{v}$ the flow velocity, $\bar{\mathbf{T}}$ the stress tensor, e the *specific* internal energy, and p the thermodynamic pressure. The conventional Euler equations are mathematically hyperbolic in form, meaning they represent *causal* behavior with zero dissipation. When fluid discontinuities or large gradients in the flow occur, such as when shock fronts form or at discrete boundaries separating materials with different physical properties, numerical instabilities or oscillatory solution behavior may arise, especially when central difference schemes are used to approximate derivatives. In such circumstances, *artificial* dissipative terms are commonly introduced to remove the instability or oscillations from the PDEs. These dissipative terms are most often artificial viscosity [29, 30, 36, 41]. Mattsson and Rider [19] provide an excellent modern review of the method of artificial viscosity with historical context. In order to illuminate the consequences of adding numerical dissipative mechanisms, the physical importance of viscosity and heat conduction are explored.

3.2.1. Explicit Dissipative Mechanisms. The viscous and heat conducting differential system that we will analyze may be written as the following in one dimensional planar geometry

$$(3.2a) \quad \frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \underbrace{\rho \frac{\partial u}{\partial x}}_{\text{viscous term}} = 0 ,$$

$$(3.2b) \quad \rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} + \frac{\partial p}{\partial x} - \underbrace{\mu \frac{\partial^2 u}{\partial x^2}}_{\text{viscous term}} = 0 ,$$

$$(3.2c) \quad \rho \frac{\partial e}{\partial t} + \rho u \frac{\partial e}{\partial x} + p \frac{\partial u}{\partial x} - \underbrace{\mu \left(\frac{\partial u}{\partial x} \right)^2}_{\text{viscous term}} + \underbrace{\frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right)}_{\text{heat conduction term}} = 0 ,$$

where u is the flow velocity in the $\hat{x}$ -direction, x the spatial variable, t the temporal variable, T the thermodynamic temperature, μ the viscosity of the fluid, and k the thermal conductivity of the fluid.

3.2.2. Non-dimensionalization . The subtle origins of dissipation even within simple, one-dimensional hydrodynamic flow are best illustrated by removing material-specific characteristic scales through non-dimensionalization. The basis of this non-dimensionalization involves scaling the (1-D) independent variables x and t ,

$$(3.3) \quad \tilde{x} \equiv \frac{x}{x_0} \quad \text{and} \quad \tilde{t} \equiv \left(\frac{u_0}{x_0} \right) t ,$$

where x_0 can be any characteristic length scale x_0 along the direction of flow, *e.g.* a finite element cell dimension, the atomic length scale, or some characteristic physical length of the problem, and u_0 is any time-independent base flow speed, for example the speed of sound. With the independent variables appropriately rescaled, the dependent hydrodynamic variables can be normalized by

$$(3.4) \quad \tilde{\rho}(\tilde{x}, \tilde{t}) \equiv \frac{\rho(\tilde{x}, \tilde{t})}{\rho_0} , \quad \tilde{u}(\tilde{x}, \tilde{t}) \equiv \frac{u(\tilde{x}, \tilde{t})}{u_0} ,$$

$$(3.5) \quad \tilde{e}(\tilde{x}, \tilde{t}) \equiv \frac{e(\tilde{x}, \tilde{t})}{e_0} , \quad \tilde{p}(\tilde{x}, \tilde{t}) \equiv \frac{p(\tilde{x}, \tilde{t})}{p_0} ,$$

which, upon substitution into Eqs. (3.2a) to (3.2c), simplifies the 1-D expanded system of Euler equations to a non-dimensional, nonlinear differential set

$$(3.6a) \quad \frac{\partial \tilde{\rho}}{\partial \tilde{t}} + \tilde{u} \frac{\partial \tilde{\rho}}{\partial \tilde{x}} + \tilde{\rho} \frac{\partial \tilde{u}}{\partial \tilde{x}} = 0 ,$$

$$(3.6b) \quad \tilde{\rho} \frac{\partial \tilde{u}}{\partial \tilde{t}} + \tilde{\rho} \tilde{u} \frac{\partial \tilde{u}}{\partial \tilde{x}} + K_m \frac{\partial \tilde{p}}{\partial \tilde{x}} - \frac{1}{\text{Re}} \frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2} = 0 ,$$

$$(3.6c) \quad \tilde{\rho} \frac{\partial \tilde{e}}{\partial \tilde{t}} + \tilde{\rho} \tilde{u} \frac{\partial \tilde{e}}{\partial \tilde{x}} + K_e \tilde{p} \frac{\partial \tilde{u}}{\partial \tilde{x}} - \frac{1}{\text{Re}} \frac{K_e}{K_m} \left(\frac{\partial \tilde{u}}{\partial \tilde{x}} \right)^2 - \frac{1}{\text{Pe}} \frac{\partial^2 \tilde{e}}{\partial \tilde{x}^2} = 0 ,$$

where the ratios

$$(3.7) \quad K_m \equiv \frac{p_0}{\rho_0 u_0^2} , \quad \text{and} \quad K_e \equiv \frac{p_0}{\rho_0 e_0}$$

are used to abbreviate static-to-dynamic pressure forces for K_m and translational versus total energy densities for K_e . The latter ratio may be close to unity depending upon the internal degrees of freedom (conventionally abbreviated as “ f ”) assumed for the fluid particles, as internal modes do not contribute to pressures p_0 . Two other ratios that arise in these modified, non-dimensional Euler equations, are the *Reynolds number* (Re) and the *Péclet number* (Pe), which describe the ratio of inertial to viscous forces for the former, and the ratio of the rate of advection to the rate of (heat) diffusion for the latter. Within this context, the Reynolds (Re) ratio is defined in terms of the ambient or unperturbed inertial fluid flow relative to the intrinsic viscous forces,

$$(3.8) \quad \text{Re} \equiv \frac{\rho_0 u_0 x_0}{\mu} = \frac{x_0}{x_\mu} ,$$

which can be thought of as a ratio of a characteristic hydrodynamic flow length x_0 versus the characteristic viscous length scale x_μ , while the heat transfer Péclet (Pe) ratio, conventionally defined by a characteristic length L , flow velocity u , and thermal diffusivity α ,

$$(3.9) \quad \text{Pe} = \frac{Lu}{\alpha} ,$$

$$(3.10) \quad = \rho_0 c_P \frac{x_0 u_0}{k} \quad \text{since} \quad \alpha = \frac{k}{\rho c_P} ,$$

which becomes

$$(3.11) \quad \text{Pe} = \rho_0 \frac{f}{2} \frac{k_B}{m} \frac{x_0 u_0}{k} = \frac{x_0}{x_k}$$

when applied to the generic 1-D flow problem, rewriting the specific heat capacity c_P in terms of the generic number of molecular degrees of freedom f and particle mass m , or $(f R_{\text{specific}})/2 = (f k_B)/(2m)$. Like the Reynolds number, the Péclet number (3.10) can also be thought of as a ratio of characteristic length scales, here the characteristic hydrodynamic scale x_0 relative to the thermal conductivity scale x_k .

Rewriting the expanded Euler equations in terms of these specific ratios, K_m , K_e , Re, and Pe, simplifies the PDEs and scales the dissipative contributions such that their influence on the solution can be examined as the Reynolds and Péclet values are changed. The replacement of the specific heat capacity with a quantity f related to the particle degrees of freedom, in moving from Eq. (3.10) to Eq. (3.11), required an assumption about the fluid heat capacity, which was

taken to be *calorically perfect*, meaning that the ratio of the heat capacities c_P/c_V is a constant, conventionally called gamma γ . This assertion is a statement about the caloric equation of state (EoS), which nominally relates the system internal energy to the temperature, and has the form $e = c_V T$ here. It is this EoS that effectively contains the molecular degrees of freedom f , allowing for the limited influence of internal energy degrees of freedom from the fluid particles.

When coupled with a *thermal* EoS, the *ideal gas law* in this case, the resulting EoS is called the *gamma-law* equation of state, and takes the form

$$(3.12) \quad p = (\gamma - 1) \rho e ,$$

where γ is the ratio of heat capacities c_P/c_V . Rewriting the gamma law in terms of non-dimensional variables gives

$$(3.13) \quad \tilde{p} = \frac{\gamma - 1}{K_e} \tilde{\rho} \tilde{e} .$$

With a non-dimensional EoS in place to mathematically close the set of Eqs. (3.6a) to (3.6c) the differential system was discretized using the method of lines. The non-dissipative version (inviscid and non-conductive flow) has Reynolds and Péclet numbers set to ∞ so that the second order derivatives vanish. Fortunately, the differential system that results only has first-order temporal derivatives, so numerical integration such as the method of lines can be implemented [12, 33, 40]. The temporal discretization of the method of lines (see Fig. 3.1) was done via a Runge-Kutta 4 scheme, as given in Press et al. [28], and the spatial discretization was implemented with fourth order (ambient fluid) central and second order (wall) finite difference scheme. An advantage for using this central difference scheme is that it allows us to use a numerical operator that has significantly less numerical dissipation than upwinding and other numerically dissipative, stability ensuring methods. To implement the RK4 solver, each temporal derivative in Eqs. (3.6a) to (3.6c) is isolated.

3.2.3. Energy & Entropy Balance Relations. The inclusion of dissipative effects in the set of partial differential equations governing fluid flow, whether to directly model physical effects or to artificially smooth out discontinuities, corresponds to irreversible thermodynamic processes, and therefore to entropy production. Thus, to understand the consequences of physical or numerical dissipative mechanisms, an analysis of the thermodynamics of irreversible processes is needed. Furthermore, some nuance exists in the comparison between an analytical treatment of these dissipative mechanisms and their numerical implementation. Energy dissipation and entropy production during the time-dependent fluid flow problem associated with ESD events therefore requires analysis of the rate of change of system energy and entropy, often referred to as balance equations. The basics of conservation laws and balance equations can be found in Glansdorff and Prigogine [8].

The mathematical form these balance equations take depends on the numerical implementation, but can generally be derived using the first and second thermodynamic laws. As comparisons here are made between an analytical analysis and a finite element code, a differential volume element fixed in space (Eulerian or “lab” frame) is considered. This element is small enough such that its thermodynamic properties may be considered as *homogeneous*, yet large enough that it contains a *statistical* number of particles with appropriate thermodynamic properties defined.

For general thermodynamic processes, the entropy change dS can be split into two contributions,

$$(3.14) \quad dS = d_i S + d_e S ,$$

where $d_i S$ is the entropy production due to changes inside the system, and $d_e S$ is the flow of entropy due to interaction with the external environment. The entropy production contribution due to changes inside the system is physically never negative,

$$(3.15) \quad d_i S \geq 0 ,$$

while the flow contribution $d_e S$ may be negative or positive, depending on the heat or mass flux across the system boundary. Note that Eq. (3.14) can be written in rate form through division by dt . Inserting the standard second law form for the $d_e S$ contribution, the classical Carnot-Claussius inequality [8] is arrived at

$$(3.16) \quad d_i S = dS - \frac{\delta Q}{T} \geq 0 .$$

Rewriting the Carnot-Claussius relation above into a form applicable for a general fluid flow with dissipative terms requires some assessment of heat and work, *i.e.* the first law of thermodynamics,

along with the Gibbs equation (or also commonly referred to as the “Euler equation” in thermodynamics.¹ While the first and second thermodynamic laws hold true even for irreversible paths, care must be taken when modeling these nonequilibrium processes. The first law embodies the concepts of work and heat,

$$(3.17) \quad dE = \delta Q - \delta W ,$$

where the infinitesimal state change dE , by energy conservation, equates to the infinitesimal heat flux δQ and work performed δW on a material parcel. In writing down the energy and entropy balance relations the notation and outline as given by Haase [9] is generally followed.

Although we are calculating many analytical results, explicitly associated with physical viscosity and thermal conductivity, these results are sought to be understood and compared with numerical implementations such as might be accomplished with finite element or finite volume calculations. For this reason, some of the purely mathematical consequences of treating finite volumes of material, small enough to be thermodynamically homogeneous but yet large enough to be statistical regarding fluid properties, are highlighted.

3.2.3.1. Total Energy and Energy Dissipation. Understanding how to modify or apply the first and second thermodynamic laws to irreversible processes begins with the first law. This is done by defining a system energy along with work and heat under open system conditions. As comparisons are to be made with numerical methods, wherein continuum mechanics applies, the analytical discussion should be appropriate for a continuum fluid element, small enough as to represent homogeneous thermodynamic properties, but large enough to be statistical so that thermodynamics applies. This will mean writing the thermodynamic balance relations in terms of intensive quantities so that they apply to any point in the parcel.

The total energy E of the fluid control volume can be split up into three contributions,

$$(3.18) \quad E = E_{\text{kin}} + E_{\text{pot}} + U ,$$

where E_{kin} is the macroscopic kinetic energy of the system, E_{pot} is the potential energy of the system in external force fields (like gravity or electromagnetic fields), and U is the internal energy of the system. For convenience, a general thermodynamic variable, Z say, will typically be written as a *density*, or Z/V , or as a *specific* quantity, Z/m , depending on the context. The kinetic energy density of the fluid is $E_{\text{kin}}/V = (\rho v^2)/2$, while the internal energy density U/V can be written in terms of the mass density ρ and *specific* energy e as $U/V = \rho e$. The potential energy density contribution is ignored in this analysis for simplicity, where conservative fields would not influence our discussion whereas non-conservative fields would lead to nonlinearities that would compete with dissipative contributions.

Expanding the first law, *i.e.* the heat supplied to the system and the work done on the system, requires some consideration. The conventional term “work” is *indeterminate* for open systems [9], although it is possible to define an expression w for that work which would be done on the region if it *were* closed. For an infinitesimal state change we have

$$(3.19) \quad \delta w = \delta w_{\ell} + \delta w_{\text{diss}} + \delta w_{\text{a}} .$$

The δw_{ℓ} contribution nominally represents the reversible deformation work (including reversible electrification or magnetization work) on a region, which conventionally is written in terms of extensive *work-coordinates* ℓ_i or displacements $d\ell_i$ and intensive conjugate *work-coefficients* L_i ,

$$\delta w_{\ell} = \sum_i L_i d\ell_i .$$

The work-coordinate and work-coefficient pairs in δw_{ℓ} generally refer to reversible deformation work, such as isotropic compression or expansion $-pdV$ work as well as anisotropic stress-strain elastic work. The δw_{a} contribution is related to the work of forces that accelerate the region or react against existing external force fields while the δw_{diss} contribution nominally represents the “dissipated” work associated with friction, turbulence, plastic flow during deformation, hysteresis phenomena, electric conduction due to external source currents, or other reversible processes. These terms have meaning in open systems, but the summation over reversible contributions within δw_{ℓ} may not.²

¹Leonhard Euler (1707–1783) was a prodigious Swiss polymath so his name adorns numerous equations. The “Euler equation” in thermodynamics, however, should not be confused with the Euler equations in fluid dynamics.

²See, for example, § 1.7 in Haase [9] for a more detailed discussion.

The “energy balance” for a continuum volume element arises from the concept of “heat” δQ absorbed by an open phase from its surroundings during an infinitesimal state change,

$$(3.20) \quad \delta Q = dE - \delta w - \sum_k H_k d_e n_k ,$$

where E is the total energy of the phase, w is the associated work for an open phase discussed above, H_k is the partial molar enthalpy of species k , and $d_e n_k$ is the infinitesimal increase of the amount n_k of substance k due to “external” driving forces, *i.e.* not by chemical reactions inside the phase but by exchange of matter with the surroundings. Defining heat in this manner, Eq. (3.20), makes it independent of the arbitrary zero point of the internal energy [9].

Rewriting the heat flux in rate form, with the kinetic energy density contribution $E_{\text{kin},V} = (\rho v^2)/2$, the change in total energy of the volume element, the work done on the volume element when it is considered closed, and the mass exchange contribution for each species k in the volume (last term in Eq. (3.20)) becomes for the control volume element

$$(3.21) \quad \frac{\partial U_V}{\partial t} = -\nabla \cdot (U_V \mathbf{v}) - \nabla \cdot \left(\mathbf{J}_Q + \sum_k H_k {}_v \mathbf{J}_k \right) - p \nabla \cdot \mathbf{v} - \sum_{i=1}^3 \sum_{j=1}^3 p_{ij} \frac{\partial v_i}{\partial x_j} + \sum_k \mathbf{K}_k {}_v \mathbf{J}_k ,$$

where the rate of change of internal energy density U_V depends on the viscous pressures p_{ij} , ($i, j = 1, 2, 3$), the three fluid velocity components v_i ($\mathbf{v}$ in Cartesian coordinates), $\mathbf{J}_Q$ the heat current density, $\mathbf{K}_k$ the molar external force for species k , and ${}_v \mathbf{J}_k$ the diffusion current density of species k . Collecting terms for easier interpretation

$$(3.22) \quad \frac{\partial U_V}{\partial t} = -\nabla \cdot (U_V \mathbf{v}) - \nabla \cdot \mathbf{J}'_U + q(U) ,$$

with the non-convective current density $\mathbf{J}'_U$

$$(3.23) \quad \mathbf{J}'_U \equiv \mathbf{J}_Q + p \mathbf{v} + \sum_k H_k {}_v \mathbf{J}_k ,$$

and the local production of internal energy

$$(3.24) \quad q(U) \equiv \mathbf{v} \nabla p - \sum_{i=1}^3 \sum_{j=1}^3 p_{ij} \frac{\partial v_i}{\partial x_j} + \sum_k \mathbf{K}_k {}_v \mathbf{J}_k .$$

3.2.3.2. Entropy & Entropy Production. Having expanded on the meaning of work and heat for open systems associated with irreversible processes in terms of the first law, we are now ready to link these changes to the entropy and other thermodynamic variables. To complement the first and second laws, we will use a variation of the Euler equation called the generalized Gibbs equation. The thermodynamic Euler equation,

$$U = TS - pV + \sum_i \mu_i N_i$$

relates all of the thermodynamic variables of interest, and can be derived from the mathematical properties of a fundamental thermodynamic relation. For open systems under irreversible processes, the differential form of Euler’s relation can also be derived using the Gibbs potential G , which is a function of the proper variables T , p , and N , or $G = G(T, P, \sum_i N_i)$. The Gibbs potential can also be defined as a Langedre transform of the internal energy U as $G = U - TS + pV + \sum \mu N$. The total differential of each form, dG can be taken, and equated, which, upon simplification, arrives at a differential form consistent with the form above. For applicability of the generalized Gibbs relation to a continuum volume element in which irreversible processes can occur, the thermodynamic differential must be written in terms of intensive variables so that it can be defined for every point in the material parcel,

$$(3.25) \quad T dS_V = dU_V - \sum_i L_i d\ell_i - \sum_k \mu_k dc_k ,$$

where the subscript “V” denotes the density versions of the variables, Z/V , and where μ_k is the chemical potential of species k , while dc_k is the concentration.

The inclusion of dissipative effects, *i.e.* irreversible processes, complicates the interpretation or application of not only the first and second thermodynamic laws, but also the classical Gibbs equation, especially for *open* systems. The term “work” becomes *indeterminate* for open systems

or regions [9], and the conventional second-law form linking entropy and heat must be expanded to quantify the energy lost due to dissipation.

The second law of thermodynamics, $dS \geq 0$, stipulates that an allowable thermodynamic process must either conserve or produce entropy³. The Euler equations are hyperbolic partial differential equations that exhibit no entropy production in contrast to the viscous, conducting flow that the Navier-Stokes equations describes, Eqs. (3.2a) to (3.2c). An interesting and advantageous quantity to compare and contrast is the entropy produced, or not produced, by these different differential systems.

An expression may be written for non-dimensional specific entropy density using Eq. (3.6c), the thermodynamic potential $Tds = de - \frac{p}{\rho^2}d\rho$, and the ideal gas equation of state, Eq. (3.13)

$$(3.26) \quad K_s K_t \tilde{\rho} \tilde{e} (\tilde{s}_{\tilde{t}} + \tilde{u} \tilde{s}_{\tilde{x}}) = \overbrace{\frac{1}{\text{Re}} \frac{K_e}{K_m} \tilde{v}_{\tilde{x}}^2}^{\text{always } \geq 0} + \overbrace{\frac{1}{\text{Pe}} \tilde{e}_{\tilde{x}\tilde{x}}}^{\text{may be } < 0},$$

$$\text{where } K_s \equiv \frac{T_0 s_0}{e_0} \quad \text{and} \quad K_t \equiv \frac{2}{f} \frac{m e_0}{k_B T_0}$$

such that the entropy balance relation, written in terms of the spatial and time derivatives of the specific entropy density s and two non-dimensional ratios K_s and K_t (defined above). An interesting thing to note is that is the specific entropy density normalization constant is set to $(k_B f)/(2m)$, both the parameters K_s and K_t are set to 1. The results shown have both K_s and K_t set to 1. The variable $\tilde{s}_{\tilde{t}}$ may be isolated and the following equation (with the tilde being dropped) may be obtained

$$(3.27) \quad s_t = \overbrace{-us_x}^{\text{flux}} + \overbrace{\frac{1}{K_s K_t \tilde{\rho} \tilde{e}} \left[\frac{1}{\text{Re}} \frac{K_e}{K_m} \tilde{v}_{\tilde{x}}^2 + \frac{1}{\text{Pe}} \tilde{e}_{\tilde{x}\tilde{x}} \right]}^{\text{production}}.$$

Equation (3.27) is the equation that is used to produce entropy plots and data. The us_x term is the amount of entropy being fluxed out of an element while the other terms with the Re and Pe numbers is the local specific entropy density being generated by dissipative effects. Note that the variable s is not a global entropy, but rather a local entropy, $s = s(x, t)$. An interesting thing to observe is that the above equation may not always locally be positive. The velocity term, v_x^2 , is always positive, but the energy term, e_{xx} is not guaranteed to be positive. This allows local specific entropy density to be negative. Results showcasing local and global entropy are in Section 3.4.4.

3.3. Numerical Methodology

As discussed in Section 3.2.2, an RK4 solver was implemented via the method of lines[7, 12, 33, 40] for the temporal derivatives in Eqs. (3.6a) to (3.6c). The spatial derivatives were approximated by a fourth (ambient fluid simulation) or second (wall simulation) order minimally dissipative central difference scheme[7, 28]. A stencil of this numerical operator is shown in Fig. 3.1.

FIGURE 3.1 A figure showing the numerical stencil that is used in the numerical method of lines. The blue box shows the stencil for an arbitrary grey point at some future in the spatial and temporal domain relative to a past time step in the black. This method is explicit so only one point in the future is being calculated. The variable $\tilde{t}$ represents a non-dimensional time variable while $\tilde{x}$ represents a non-dimensional spatial variable.

³An important caveat to this result is that it is the *global* entropy in a defined system that must increase, not a spatially varying local entropy

3.4. Numerical Results

Two different types of simulations were performed in order to explore the solution space of the non-dimensional differential system: a wall problem that may be thought of as either a piston traveling into a quiescent, ambient gas, or a wall with flow impinging upon it; a ambient fluid simulation where a Galilean transformation has been performed to a velocity where the gas is flowing at the speed of sound.

Results from both the ambient fluid and the wall problem are presented in the following sections. The initial conditions of the problems are the following in non-dimensional flow variables:

$$\begin{aligned}\rho(x, 0) &= 1 + \alpha e^{-((x-1)/\sigma)^2}, \\ u(x, 0) &= \alpha e^{-((x-1)/\sigma)^2}, \\ e(x, 0) &= 1,\end{aligned}$$

for the ambient fluid and

$$\begin{aligned}\rho(x, 0) &= 1.0 \\ u(x, 0) &= \alpha e^{-((x)/\sigma)^2} - \alpha, \\ e(x, 0) &= 1.0\end{aligned}$$

for the wall problem. The parameters of the initial conditions, α and σ , are the amplitude of the added value and Gaussian width parameter.

3.4.1. Inviscid Comparison Between Numerical Methods . In order to ensure validity we perform a self-convergence study with the finite difference method using a highly resolved calculation as reference datum, see Fig. 3.2. The error metric used is the L_∞ metric

$$(3.30) \quad L_\infty = \max_{z \in R} \left(\int_z |c - a| dV \right).$$

Equation (3.30) shows the L_∞ error metric where z references an individual cell in the computational domain, R is the entire computational domain, c is the calculated value, a is the approximate or analytic value expected, N is the number of cells in the domain, and V_R is the volume of the mesh.

FIGURE 3.2 The Navier-Stokes numerical operator error. Fifth order error is observed within the ambient fluid simulation. The resolution taken as the analytic value had a resolution of $N = 5000$. The same figure is shown in Section 2.4.1; it is shown here to have each chapter act as a standalone if required.

Figures 3.3 to 3.6 show the results of comparing the inviscid simulation for the ambient fluid and wall problems to the finite element code at the specified resolutions. Note the accuracy with which the different simulations solving different differential systems with distinct numerical operators agree. The α value for both problems was 0.01, and σ was 0.25 for the ambient fluid and wall problem.

FIGURE 3.3 Comparison from inviscid Navier-Stokes solution at a resolution of $N = 5000$ to the finite element code at the specified resolutions. Note the excellent agreement between solutions. The same figure is shown in Section 2.4.1; it is shown here to have each chapter act as a standalone if required.

FIGURE 3.4 Difference between inviscid Navier-Stokes solution at resolution of $N = 5000$ to the finite element code. The maximum difference for $N_{\text{Code}} = 100$ is not shown on the current axes. Note how the difference collapses down to zero as a function of the mesh resolution of the finite element code. The same figure is shown in Section 2.4.1; it is shown here to have each chapter act as a standalone if required.

FIGURE 3.5 Comparison from inviscid Navier-Stokes solution at a resolution of $N = 2000$ to the finite element code as the specified resolutions. Note the excellent agreement between solutions. The inviscid solution preserves the structure of the initial conditions. This structure is smeared out in the other solutions with physical dissipative mechanisms included.

FIGURE 3.6 Difference between inviscid Navier-Stokes at a resolution of $N = 2000$ to the finite element code. Note how the difference collapses down to zero as a function of the mesh resolution of the code.

3.4.2. Results $\alpha = 0.01$ for $\text{Re} = 100$ and $\text{Pe} = 100$ and fixed K_m and K_e . Figures 3.7 to 3.12 show the results of a Re number = 100 or ∞ and Pe number = 100 or ∞ parameter space mapping in the ambient fluid and wall problems. Note how the smeared out nature of the solutions' curves change as function of inclusion of specific dissipative parameters. (By setting the viscous or heat conducting terms to zero for certain simulations, we in essence set either the Re or Pe numbers to ∞ . This is shown in several graphics.) The influence of the various physical dissipative mechanisms on the solution structure cannot be understated[20–22]. Observe the drastically different amplitudes of all three variables in the domain of the ambient fluid simulations and in the overall structure of the solution. In the wall problem, note the increase in the density and the decrease in the specific internal energy at the wall in the viscous-conductive and conductive simulations. This wall heating effect, that is physical in this case, will be explored in more detail in Section 3.4.5.

Note that in many of the following plots we have defined $\delta\tilde{\phi}$ to be the difference from a non-dimensional unity or zero value depending on the variables i.e. $\delta\tilde{\phi} \equiv \tilde{\phi} - 1$ where ϕ is a placeholder variable. In addition, both the non-dimensional energy ratios K_e and K_m are fixed and equal to 0.4 and 0.714, respectively.

FIGURE 3.7 Density plots for viscous-conductive, conductive, viscous, and inviscid simulations are shown above for a Re number of 100 and Pe number of 100. The subscripts vk , k , v , and i stand for viscous-conductive, conductive, viscous, and inviscid, respectively. Note how the solution changes as dissipative mechanisms are included into the differential system. These dissipative effects combine nonlinearly to create the viscous-conductive solution.

FIGURE 3.8 Flow velocity plots for viscous-conductive, conductive, viscous, and inviscid simulations are shown above for a Re number of 100 and Pe number of 100. The same notation is used as in Fig. 3.7. Note how the solution changes as dissipative mechanisms are included into the differential system.

FIGURE 3.9 Specific internal energy plots for viscous-conductive, conductive, viscous, and inviscid simulations are shown above for a Re number of 100 and Pe number of 100. The same notation is used as in Fig. 3.7. Note how the solution changes as dissipative mechanisms are included into the differential system.

FIGURE 3.10 Density plots for viscous-conductive, conductive, viscous, and inviscid simulations are shown above for a Re number of 100 and Pe number of 100. The subscripts vk , k , v , and i stand for viscous-conductive, conductive, viscous, and inviscid, respectively. Note how the solution changes as dissipative mechanisms are included into the differential system. This dissipative effects combine nonlinearly to create the total solution.

FIGURE 3.11 Flow velocity plots for viscous-conductive, conductive, viscous, and inviscid simulations are shown above for a Re number of 100 and Pe number of 100. The same notation is used as in Fig. 3.10. Note how the solution changes as dissipative mechanisms are included into the differential system.

FIGURE 3.12 Specific internal energy plots for viscous-conductive, conductive, viscous, and inviscid simulations are shown above for Re and Pe numbers of 100. The same notation is used as in Fig. 3.10. Note how the solution changes as dissipative mechanisms are included into the differential system. Observe how the “dip” in specific internal energy here counteracts the density increase in Fig. 3.10.

3.4.3. Characteristic Propagation. Figures 3.13 to 3.16 all show calculated contours of the Riemann invariants[6,42,44] from the inviscid finite element code simulations of the ambient fluid and wall problems. Appendix C details the theory behind the Riemann invariants that were used to produce these plots. Note the information that is encoded within these plots show the rightward, leftward, and “stationary” (in the reference frame of the material) pulses propagate through the domain in the ambient fluid problem in Figs. 3.13 and 3.14. In the wall problem there is a “hump” in the profile of all variables in the inviscid simulation, see Figs. 3.10 to 3.12. This “hump” may be explained here in the characteristics of the wall simulation, seen in Figs. 3.15 and 3.16. Note how in Fig. 3.15, the information about the initial conditions is propagated in the positive x direction without any interaction from wall. In an inviscid simulation, the structure of these initial conditions is kept intact as the C_+ characteristics propagate. In the case where there is a dissipative mechanism(s), physical or numerical, at play, the structure of these initial conditions are lost. This may be seen when comparing the various solution of varying Re and Pe numbers in Figs. 3.10 to 3.12. This preservation of the initial conditions is contrasted with the solutions that have dissipative mechanisms included which smear out the initial condition. In addition to smearing out the initial condition information is propagated at a non-causal speed. This may be

observed by looking at the location of the characteristics in the following plots and the location of the propagating waves in Figs. 3.7 to 3.12.

FIGURE 3.13 C_+ characteristics from the ambient fluid. Note how they converge toward the right to match the rightward going pulse. The x coordinate is plotted in the Galilean transformed frame. The change in value to the in the opposite direction of the C_+ characteristics is numerical noise.

FIGURE 3.14 C_- characteristics from the ambient fluid. Note how they converge toward the left to match the leftward going pulse. The x coordinate is plotted in the Galilean transformed frame. The change in value to the in the opposite direction of the C_- characteristics is numerical noise.

FIGURE 3.15 C_+ characteristics from the wall problem. Note how the initial conditions are encoded in the rightward going pulse via the characteristics. Contrast the rightmost contour within this inviscid simulation with the solutions with dissipative mechanisms included.

FIGURE 3.16 C_- characteristics from the wall problem. Note how the last characteristic to interact with the piston wall at $x = 0$ is from the last point on the initial condition. This last point intersecting with the wall also coincides with the stop of any change in the profile behind the rightward going pulse, see Fig. 3.15. The change in value to the in the opposite direction of the C_- characteristics is numerical noise.

3.4.4. Results for Energy and Entropy Production for $\alpha = 0.1$ in an Ambient Fluid Problem. By the second law of thermodynamics, the global entropy of a system must increase or remain constant for a process to be thermodynamically allowable[3]. However, that does not mean that the local entropy of a point or small domain in a system may not be negative[23, 24]. If Eqs. (3.26) and (3.27) are examined, recall that these equations are derived from the conservation of energy equation and a thermodynamic potential, it is observable that the local entropy may be negative. This can occur due to the term associated with the Pe number. In Eulerian methods, numerical dissipation in the energy equation will give rise to a numerical Pe number so it is possible to have local entropy changes that are negative. Likewise, including the Noh numerical heat flux in a Lagrangian method will create a numerical Pe number. These dissipative affects can introduce decreases in entropy, consistent with solving the physical laws; the equations showing how these dissipative effects increase entropy are shown in Eqs. (3.26) and (3.27).

An example figure showing the entropy in an ambient fluid simulation for Re and Pe numbers of 100 may be seen in Figs. 3.17 and 3.18. This simulation is the same as showcased in the previous section except with $\alpha = 0.1$. Note the location where the local entropy is negative. The entropy produced as a function of which dissipative terms are turned on in the solution may be seen in

Fig. 3.18. Note how the value of entropy being produced is strongly impacted by which terms are turned on in the differential system.

FIGURE 3.17 Specific entropy produced in a viscous-conductive ambient fluid simulation calculated from Eq. (3.27). Note the dissimilar behavior associated with the leftward and rightward going pulses as seen in Figs. 3.7 to 3.9. The locally negative entropy is caused by the second term in Eq. (3.27) which is not positive definite. The global entropy, though, must by thermodynamics be globally positive. This is shown explicitly in Fig. 3.25.

FIGURE 3.18 Specific entropy produced calculated for an ambient fluid simulation from Eq. (3.27). The locally negative entropy is caused by the second term in Eq. (3.27) which is not always ≥ 0 . Note how the green, dashed line for the viscous entropy is always positive while the orange, dashed and blue, dash-dot lines are negative.

Figures 3.19 to 3.21 shows the energy as a function of space at $\tilde{t} \approx .25$ for an ambient fluid simulation. Notice how the structure of the solution impacts the overall position of the energy, but not the overall integrated amount. It was found that the overall kinetic and internal energy of the system does not change that much.

FIGURE 3.19 Kinetic energy density in ambient fluid simulation with $Re = 100$ and $Pe = 100$. The total sum of the all of the energy contained tells us that the total kinetic energy only differs by about 1%, a result that could be unexpected just by looking at the plot.

FIGURE 3.20 Internal energy density in an ambient fluid simulation with $Re = 100$ and $Pe = 100$.

FIGURE 3.21 Total energy density in an ambient fluid simulation with $Re = 100$ and $Pe = 100$.

Figures 3.22 to 3.24 show how the cross sectional energy densities, a total energy in one dimension behaves as a function of time. Note how the viscous-conductive, vk , solution has the lowest kinetic energy and highest internal energy, as expected. In contrast the inviscid solution has the highest kinetic energy and lowest internal energy, also as expected. The physical dissipative mechanisms of viscosity and heat conduction have a strong impact on both the structure and the energy contained within the solutions.

FIGURE 3.22 Total kinetic energy, of the ambient fluid simulation with $Re = 100$ and $Pe = 100$ as a function of time.

FIGURE 3.23 Total internal energy of the ambient fluid simulation with $Re = 100$ and $Pe = 100$ as a function of time. As expected, the viscous-conductive solution has the highest internal energy due to dissipative effects.

FIGURE 3.24 Total energy of the ambient fluid simulation with $Re = 100$ and $Pe = 100$ as a function of time. Note how the total energy of the system is not conserved, which is expected with this finite difference method. Once the structure of the solution has matured the inviscid solution's total energy stable.

FIGURE 3.25 Energy dissipated via viscosity and heat conduction during an ambient fluid simulation with $Re = 100$ and $Pe = 100$ as a function of time. This plot has combinations of the Re and Pe numbers set to 100 or ∞ . Note how the terms of the viscous only and conductive only entropies are not additive to the full viscous-conductive fluid. This may be seen in plots showing the shock structure of the different flows and in Eq. (3.27). In addition, note how the energy associated with irreversible entropy production in the viscous only simulation is always ≥ 0 while the conductive only simulation has negative global entropy early in time due the solution being a transient process.

Table 3.1 details the energy that goes into entropy production during the viscous-conductive ambient fluid simulation, and also kinetic and internal energies at the end of a simulation. Note that the energy that goes toward entropy production is approximately the same as the kinetic energy difference, Δ .

TABLE 3.1 A table showing the calculated values of the kinetic, internal, and total energies of the ambient fluid simulation shown in Figs. 3.19 to 3.21 evaluated at $\tilde{t} \approx .25$. The symbol vk stands for viscous-conductive, i is inviscid and non-conducting, and Δ is the absolute difference between vk and i. Note how the order of magnitude of the energy going to entropy production is on the order of the difference in energy between the vk and i simulations. The difference between the energy going toward entropy production and the Δ value in the kinetic energy is approximately the value of the total energy loss during the simulation, see Fig. 3.24.

	vk	i	Δ
$E_{kin} = \rho v^2/2$	255.39	255.44	5.28e-2
$E_{int} = \rho e$	503.45	503.42	2.90e-2
$E_{kin} + E_{int}$	758.84	758.86	2.39e-2
$K_{t\epsilon ps}$	6.16e-2		

3.4.5. Wall Heating due to Physical Dissipative Mechanisms. Here, the physical dissipative processes of viscosity and heat conduction are explored in the context of physical wall heating errors and numerical wall heating errors. Figures 3.26 and 3.27 show the density and specific internal energy wall heating errors associated with physical viscosity and heat conduction for a $\delta\tilde{u}$ value of 0.55. The inviscid solution is not shown due to spurious behavior. Note the increase in the density and decrease in the specific internal energy of the system in the conductive and viscous-conductive simulation with respect to the inviscid case. These effects are the physical analogs of the correction terms used by Noh to correct for the artificial viscosity wall heating error[26]. The combined effects of viscosity and heat conduction lead to the viscous-conductive term being between the other two solutions. The inviscid solution has been omitted due to spurious oscillations that result from the minimally dissipative numerical operator and differential system. For large gradients the inviscid solution is inherently unstable. This unstable nature of the inviscid solution necessitates the use of dissipative schemes, either physical or numerical. Here we showcase the results of physical viscosity and heat conduction which may also be recovered with a numerical dissipative scheme, acknowledged or not.

FIGURE 3.26 Density at the wall in the Wall Problem. Note how the conductive term adds an additive effect to the density. The inviscid solutions has been omitted due to spurious oscillation that result from the minimally dissipative finite difference method. Note how the less dissipative the conductive solution is. See Figs. 3.28 and 3.29 for a better look viscous wall heating.

FIGURE 3.27 Specific internal energy at the wall in the wall problem. Note how the conductive term adds an additive effect to the specific internal energy. The inviscid solutions has been omitted due to spurious oscillation that result from the minimally dissipative finite difference method. Note how the less dissipative the conductive solution is. See Figs. 3.28 and 3.29 for a better look viscous wall heating.

Figures 3.28 and 3.29 show a closeup of the density and specific internal energy at the wall for a $\delta\tilde{u}$ value of 0.55. Note the difference in the magnitude of the viscous wall heating effect. Recovery of an effect similar as that observed in the Noh paper occurs[26]. In fact, it can be seen that the conductive correction that Noh performed is also occurring with the finite difference method presently just by arbitrarily setting the Pe number. Indeed, one may exactly match the inviscid solution in this region by iteratively spanning the space parameterized by the Re and Pe numbers.

FIGURE 3.28 Closeup of the density at the wall in the wall problem for a $\delta\tilde{u} \approx 0.55$. Note the behavior of the viscous solution and how the full viscous-conductive solution corrects for the viscous solution's effect.

FIGURE 3.29 Closeup of the specific internal energy at the wall in the wall problem for a $\delta\tilde{u} \approx 0.55$. Note the behavior of the viscous solution compared to the conductive and viscous-conductive solutions.

3.4.6. Viscous Comparisons. A comparison between physical viscosity in the finite difference solution and numerical viscosity in the finite element code is implemented with two methods: an artificial viscosity coefficient which is shown to recover similar affects as physical viscosity, an implementation of physical viscosity in the same form as Eq. (3.2b). Figures 3.30 and 3.31 show the comparison between the finite difference solution and the finite element code with numerical and physical viscosity at the specified resolution.

In Fig. 3.30 an artificial viscosity coefficient is used in order to ensure numerical stability for the finite element code. The finite element code solves the viscous Navier-Stokes equations. The viscosity of the mesh dependent coefficient in the finite difference code may be written as the following

$$(3.31) \quad \mu_N = \frac{1}{2} \rho c \Delta x$$

where μ_N is the numerical viscosity, ρ the density, c the speed of sound, and Δx the distance between points in the mesh. For a Re number of 100 in the full finite difference solver, a viscosity of approximately 4 cP is calculated from the thermodynamic values. This value can be used to calculate a requisite Δx value dependent on the thermodynamic variables of the medium. This value for the physical viscosity corresponds to a mesh resolution of $N \approx 75$ based upon the thermodynamic parameters we are running in our model. Various mesh resolutions are plotted in Fig. 3.30 to showcase the result of having a numerical viscosity coefficient. It may be seen that a calculated mesh resolution of $N \approx 75$ agrees favorably with the physical solution. Note that as the mesh resolution increases the solution asymptotically approaches the theoretical inviscid solution with zero thickness. See Appendix D for explicit details. A caveat of this statement is that no matter the resolution the differential system that is being solved is an approximation to the inviscid differential system[20–22]. A true inviscid solution is never recovered, except in the limit of zero mesh size.

FIGURE 3.30 Wall problem viscous Navier-Stokes vs finite element code using a mesh dependent numerical viscosity coefficient. The structure of the solution is shown to highlight how the solution is dependent on the mesh resolution for this numerical method. Note how the finite element code asymptotically approaches the theoretical inviscid solution with zero thickness.

Not every simulation that is performed can asymptotically approach an inviscid solution, or be numerically stable with a physically appropriate viscosity coefficient. For example, the physical viscosity of the simulations that have been performed correspond to water, but what if the physical simulation was in air? The viscosity of air is on the order of one thousand times smaller than the viscosity of water. The current resolution of our simulations shown in Fig. 3.30 would not be able to recover the correct structure of the solution based upon the current dissipative mechanism as seen in Eq. (3.31). A higher resolution mesh would be required in order to have the numerical viscosity coefficient recover the physical viscosity coefficient's value. Even in 1D these resolution requirements are not always achievable. More discussion on the physical relevance of overestimating dissipative mechanics and how this may affect verification of numerical algorithms is in Section 3.5. Relevant discussions may be found in these works[2, 10, 15, 20–24, 34, 35, 37, 39].

Figures 3.31 and 3.32 show a comparison between the viscous finite difference code and the finite element code implemented with a physical viscosity coefficient. Note the excellent agreement between the solutions and how the finite element code collapses down the Navier-Stokes solution as the mesh resolution increases.

FIGURE 3.31 Wall problem full Navier-Stokes vs finite element code for a large added value and using a physical viscosity. Note how well the solutions track each other. Physics is recovered.

FIGURE 3.32 Wall problem full Navier-Stokes vs finite element code for a large added value with physical viscosity. Note how well at the wall the solutions recover each other.

3.5. Discussion and Conclusions

Dissipative affects, whether they be physical or numerical and actively understood, have large impacts on the structure, stability, and exhibited physics for solutions to differential systems. The dissipative effects of viscosity and heat conduction in the context of two sample problems have been explored within this document and two important results and one caveat have been found: entropy production can be negative within a domain, the global entropy produced is positive; wall heating and wall heating correction terms are not just effects of numerical error, but also arise from physical dissipative mechanisms; a caveat for verification of numerical algorithms has been exposed. In addition, it must be noted that the inclusion of physical dissipative mechanisms nonlinearly affects the structure of any hydrodynamic solution. In essence the inclusion of dissipative terms, either physical or numerical, mutate the differential system into another form than one without dissipation.

As shown in Section 3.4.4 with Figs. 3.17 and 3.18, the local entropy within the domain of a system may be negative due to non-positive terms in a specific entropy production equation, see Eq. (3.27). The results from these figures show what the entropy looks like when being calculated explicitly from a differential system with physical dissipative mechanisms. Numerical methods can create numerical Re and Pe number like terms that give rise to negative entropy. This effect can be unexpected and produce confusion. An example of this may be drawn to the physical mechanism of heat conduction within the context of numerical discretization of the Eulerian form of the Navier-Stokes equations. Within that discretization scheme one may reproduce a second order derivative in the specific internal energy that may replicate the locally negative entropy term in Eq. (3.27). An example of this may be observed in Appendix D. This phenomena may occur without the knowledge of a scientist/engineer if the numerical operator used is not properly understood.

Another result of using numerically dissipative effects is the case of wall heating when a numerical viscosity is used to ensure stability. As observed in the Noh problem[26], the inclusion of an artificial viscosity, Q , created a dip in the density and a jump in the specific internal energy at the wall. The result of using solely physical viscosity in a numerically integrated differential system in a wall problem recovers these affects qualitatively, see Figs. 3.26 to 3.29. In addition, the correction term, H , in Noh's paper corresponds to a numerical version of the physically dissipative effect of heat conduction. Indeed, the sole inclusion of heat conduction in the solution leads to the opposite effect of viscosity in the solution with an increase in density and decrease in specific internal energy. With both terms in the numerical solution it is observed that the inviscid case is almost recovered.

The structure of the solution of a differential system is greatly influenced by which dissipative terms are included, see Figs. 3.7 to 3.12. In addition, the local entropy produced by either physically dissipative or numerically dissipative terms may not be positive[23, 24]. This affect may not be accounted for or acknowledged if this dissipation is not an explicit function of the differential system but rather of a numerical operator. Lastly, it was shown that for certain physical systems the viscosity was sufficient to ensure numerical, smooth solutions and reproduce physical solutions, see Fig. 3.30. However, for other systems the viscosity required for numerical stability overestimates

the physical viscosity by orders of magnitude. In the example provided in Section 3.4.6, a viscosity of 4 cP, comparable to water, is recovered by the finite element code. However, the numerical algorithm would overestimate the dissipation if the physical system being modeling was air. To produce the correct solution, either an extremely fine mesh or a different numerical operator must be used. Either of these options may not always be feasible.

A caveat of using numerical dissipation is that the numerically solved differential system is irrecoverably altered from the non dissipative equations[10, 11, 20–22, 39]. Because a different differential system is being solved, different physics is demonstrated in the solution, physics which can be invalid for modeling if it is not accounted for[2, 15, 34, 35]. This fact has large impacts on verification of numerical algorithms. In the example explored in this document, mesh dependent artificial viscosity, which can replicate physical viscosity, is used in order to ensure numerical stability in the finite element code. A key repercussion of this is that even though the finite element code asymptotically approaches the theoretical inviscid solution only a truly viscous solution is actually solved.

In conclusion, the effects of both physical and numerical dissipation must be understood in order to fully grasp the full consequences of implementing a numerical operator to solve a specific differential system. Here, we have attempted to understand the consequence of the inclusion of viscosity and heat conduction in the Navier-Stokes equations and shown that local entropy need not be positive, wall heating effects and correction can occur in a differential system with physical dissipative mechanisms, and that models constructed with dissipative mechanisms can model reality inappropriately.

Concluding Remarks

The influence of perturbations, nonlinear effects, and dissipative mechanisms have been explored in the context of the hyperbolic Euler equations modified by the inclusion of momentum (momentum diffusion) and energy diffusion (heat conduction).

The use of a perturbative technique led to the observation of asymptotic convergence to a full nonlinear solution, see Fig. 2.13. This asymptotic convergence was predicted to have a minimum value based on error truncation terms from the perturbed differential system, see Fig. 2.7, which correlated the size of the perturbation used in the perturbative technique. Care must be taken, though, when applying this technique; a fine balance between truncation error and numerical error must be struck at large perturbations (departures) away from an expansion neighborhood (constructed about a particular value) to avoid large spurious oscillations or undesired deleterious effects.

Dissipative effects, whether they be physical or numerical and actively understood, have large impacts on the structure, stability, and exhibited physics for solutions to differential systems. Two important results and one caveat have been found in this study: local entropy production can be negative within a domain; wall heating and wall heating correction terms are not just effects of numerical error, but also arise from physical dissipative mechanisms; a caveat for verification of numerical algorithms has been exposed. In addition, it must be noted that the inclusion of physical dissipative mechanisms nonlinearly effects the structure of any hydrodynamic solution. In essence, the inclusion of dissipative mechanisms, either physical or numerical, mutate the non-dissipative Euler differential system into a dissipative system, with the consequence that solutions are different than the standard, “vanilla” Euler differential system. This consequence has subtle, yet sweeping implications on the verification of numerical operators.

In conclusion, the effects of both physical and numerical dissipation must be understood in order to fully grasp the broad consequences of implementing a numerical operator to solve a specific differential system. Here, we have analyzed the consequences for the inclusion of viscosity and heat conduction in the Euler equations and shown that local entropy need not be positive, wall heating effects and corrections can occur in a differential system with physical dissipative mechanisms, and that models constructed with dissipative mechanisms can simulate reality inappropriately.

APPENDIX A

Reduction of the Perturbed Differential System

The reduction of the differential system shown in Eqs. (2.7a) to (2.7c) is a process that involves much algebra, product rule, and a careful selection of terms. It is placed here in an appendix in an effort to not attempt to intercept the flow of the overall report. Rewriting the equations for convenience

$$(A.1a) \quad \tilde{\rho} = 1 + \overbrace{\tilde{\eta} + \tilde{\eta}^2/2 + \tilde{\eta}^3/6}^{\delta\tilde{\rho}},$$

$$(A.1b) \quad \tilde{u} = 0 + \overbrace{\tilde{v} + \tilde{v}^2/2 + \tilde{v}^3/6}^{\delta\tilde{u}},$$

$$(A.1c) \quad \tilde{e} = 1 + \overbrace{\tilde{\epsilon} + \tilde{\epsilon}^2/2 + \tilde{\epsilon}^3/6}^{\delta\tilde{e}},$$

for the third order perturbed variables and

$$(A.2a) \quad \overbrace{(1 + \delta\tilde{\rho})_{\tilde{t}}}^{\tilde{\rho}_{\tilde{t}}} + \overbrace{(0 + \delta\tilde{v})(1 + \delta\tilde{\rho})^{\tilde{x}}}^{\tilde{u}\tilde{\rho}_{\tilde{x}}} + \overbrace{(1 + \delta\tilde{\rho})(0 + \delta\tilde{v})_{\tilde{x}}}^{\tilde{\rho}\tilde{u}_{\tilde{x}}} = 0,$$

$$(A.2b) \quad \overbrace{(1 + \delta\tilde{\rho})(0 + \delta\tilde{v})_{\tilde{t}}}^{\tilde{\rho}\tilde{u}_{\tilde{t}}} + \overbrace{(1 + \delta\tilde{\rho})(0 + \delta\tilde{v})(0 + \delta\tilde{v})_{\tilde{x}}}^{\tilde{\rho}\tilde{u}\tilde{u}_{\tilde{x}}} + \frac{K_m}{K_e} \overbrace{(\gamma - 1)(1 + \delta\tilde{\rho} + \delta\tilde{e} + \delta\tilde{\rho}\delta\tilde{e})_{\tilde{x}}}^{\tilde{p}_{\tilde{x}}} - \frac{1}{\text{Re}} \overbrace{(0 + \delta\tilde{v})_{\tilde{x}\tilde{x}}}^{\tilde{u}_{\tilde{x}\tilde{x}}} = 0,$$

$$(A.2c) \quad \overbrace{(1 + \delta\tilde{\rho})(1 + \delta\tilde{\epsilon})_{\tilde{t}}}^{\tilde{\rho}\tilde{e}_{\tilde{t}}} + \overbrace{(1 + \delta\tilde{\rho})(0 + \delta\tilde{v})(1 + \delta\tilde{e})_{\tilde{x}}}^{\tilde{\rho}\tilde{u}\tilde{e}_{\tilde{x}}} + (\gamma - 1) \overbrace{(1 + \delta\tilde{\rho} + \delta\tilde{e} + \delta\tilde{\rho}\delta\tilde{e})(0 + \delta\tilde{v})_{\tilde{x}}}^{\tilde{p}\tilde{u}_{\tilde{x}}} - \frac{1}{\text{Re}} \frac{K_e}{K_m} \overbrace{(0 + \delta\tilde{v})_{\tilde{x}}^2}^{\tilde{u}_{\tilde{x}}^2} - \frac{1}{\text{Pe}} \overbrace{(1 + \delta\tilde{e})_{\tilde{x}\tilde{x}}}^{\tilde{e}_{\tilde{x}\tilde{x}}} = 0,$$

for the differential system we plug the perturbed variables into. Starting with Eq. (A.2a), derivatives may be taken to obtain (dropping the tilde for convenience)

$$(A.3) \quad \overbrace{\left(1 + \eta + \frac{\eta^2}{2} + \frac{\eta^3}{6}\right)_t}^{\rho_t} + \overbrace{\left(1 + \eta + \frac{\eta^2}{2} + \frac{\eta^3}{6}\right) \left(0 + v + \frac{v^2}{2} + \frac{v^3}{6}\right)_x}^{\rho u_x} + \overbrace{\left(0 + v + \frac{v^2}{2} + \frac{v^3}{6}\right) \left(1 + \eta + \frac{\eta^2}{2} + \frac{\eta^3}{6}\right)_x}^{u \rho_x} = 0$$

which is then

$$(A.4) \quad \overbrace{\eta_t + \eta\eta_t + \frac{\eta^2}{2}\eta_t}^{\rho_t} + \overbrace{\left(v + \frac{v^2}{2} + \frac{v^3}{6}\right) \left(\eta_x + \eta\eta_x + \frac{\eta^2}{2}\eta_x\right)}^{u \rho_x} + \overbrace{\left(1 + \eta + \frac{\eta^2}{2} + \frac{\eta^3}{6}\right) \left(v_x + v v_x + \frac{v^2}{2}v_x\right)}^{\rho u_x} = 0$$

when derivatives are expanded out. Multiplying terms out and canceling terms that have a higher than whatever desired order¹, the following are obtained (the highest order equation solved in the report was third.)

(A.5)

$$\begin{aligned}
 & \overbrace{\eta_t + \eta\eta_t + \frac{\eta^2}{2}\eta_t + v\eta_x + v\eta\eta_x + v\cancel{\frac{\eta^2}{2}\eta_x}^0 + \frac{v^2}{2}\eta_x + \cancel{\frac{v^2}{2}\eta\eta_x}^0 + \frac{v^2}{2}\cancel{\frac{\eta^2}{2}\eta_x}^0 + \frac{v^3}{6}\eta_x + \cancel{\frac{v^3}{6}\eta\eta_x}^0 + \frac{v^3}{6}\cancel{\frac{\eta^2}{2}\eta_x}^0}^{u\rho_x} \\
 & + \overbrace{v_x + vv_x + \frac{v^2}{2}v_x + \eta v_x + \eta vv_x + \cancel{\eta\frac{v^2}{2}v_x}^0 + \frac{\eta^2}{2}v_x + \cancel{\frac{\eta^2}{2}vv_x}^0 + \frac{\eta^2}{2}\cancel{\frac{v^2}{2}v_x}^0 + \frac{\eta^3}{6}v_x + \cancel{\frac{\eta^3}{6}vv_x}^0 + \frac{\eta^3}{6}\cancel{\frac{v^2}{2}v_x}^0}^{\rho u_x} = 0.
 \end{aligned}$$

This truncation of terms is the time when error is introduced into the differential system of the order of the truncated terms. The perturbed conservation of mass equation is then

$$(A.6) \quad \left(1 + \eta + \frac{\eta^2}{2}\right)\eta_t + \left(v + \frac{v^2}{2} + v\eta\right)\eta_x + \left(1 + v + \frac{v^2}{2} + \eta + \eta v + \frac{\eta^2}{2}\right)v_x = 0,$$

after grouping terms. Similar procedures may be performed for the other equations for conservation of momentum and energy. An expansion of second or first order could also be performed by truncating terms that had either third order or higher and second order or higher terms remaining, respectively.

¹The order of a term is the sum of all the exponents and derivatives. For example, the term $\eta v \epsilon \epsilon_{xx}$ would be fifth order.

APPENDIX B

Useful Thermodynamic Relations

Certain thermodynamic relations between variables may be written for the inviscid, non conducting case. Relationships between these variables are extremely useful for algebraic manipulation. Thermodynamic potentials, internal energy and entropy for example, may be written solely as a function of three state variables[3]. The internal energy for example may be written as

$$E = E(S, V, N)$$

where E is the internal energy of a system, S is the entropy of that system, V is the volume of that system, and N is the number of particles of that system. Furthermore, a differential dE , may be written as the sum of the differentials and derivatives

$$dE = \left(\frac{\partial E}{\partial S} \right)_{V,N} dS + \left(\frac{\partial E}{\partial V} \right)_{S,N} dV + \left(\frac{\partial E}{\partial N} \right)_{S,V} dN$$

and each derivative is itself a thermodynamic quantity that may be calculated

$$dE = TdS - pdV + \mu dN$$

where we have taken $\left(\frac{\partial E}{\partial S} \right)_{V,N}$ as the temperature, T , $\left(\frac{\partial E}{\partial V} \right)_{S,N}$ as the negative pressure, $-p$, and $\left(\frac{\partial E}{\partial N} \right)_{S,V}$ as the chemical potential, μ , of constituent particles of the system. The specific form of this system may be written as well, where all of the elements are divided by a mass density

$$de = Tds - pdv + \mu dn$$

where the lower case letters are now the specific variables of their capital counterparts. If we have an inviscid, non conducting system, we may eliminate the ds variable and if we also consider the generation of no other net particles we can also eliminate dn . Thus,

$$de = -p dv \Rightarrow de = \frac{p}{\rho^2} d\rho.$$

The above equation may be non-dimensionalized by the use of the same non-dimensional relations that were used in the previous analysis. Again thus,

$$d\tilde{e} = K_e \frac{\tilde{p}}{\tilde{\rho}^2} d\tilde{\rho},$$

and with the inclusion of the isentropic relation between non-dimensional pressure and non-dimensional density, $\tilde{p} = \tilde{\rho}^\gamma$, a relationship may be written between differential energy and density

$$(B.1) \quad d\tilde{e} = K_e \tilde{\rho}^{\gamma-2} d\tilde{\rho}.$$

A similar relationship as Eq. (B.1) between actual specific internal energy and density via Eq. (2.5) and the use of isentropic pressure-density relation may be written

$$(B.2) \quad \tilde{e} = \frac{K_e}{\gamma - 1} \tilde{\rho}^{\gamma-1}.$$

Aside from the useful of having one thermodynamic variable written solely as the function of one other as is Eq. (B.2), another thermodynamic variable that is of importance may be rewritten, the speed of sound c . The speed of sound may be written as the derivative of pressure with density at constant entropy

$$c^2 = \left(\frac{\partial p}{\partial \rho} \right)_S.$$

The non-dimensional speed of sound may be written out solely as a function of the density via the use of $\tilde{p} = \tilde{\rho}^\gamma$ and the non-dimensional variables used previously in the document. Explicitly, we have

$$(B.3) \quad \tilde{c} = \sqrt{K_m \gamma} \tilde{\rho}^{(\gamma-1)/2}.$$

APPENDIX C

Nondimensional Characteristic Calculation

The characteristics shown in Figs. 3.13 to 3.16 were all calculated using the Riemann invariants[42]. These invariants may be calculated by integrating the expression $dr^k = l_i^k du_i$ where r^k is the k 'th Riemann invariant, $\mathbf{l}^k$ is the k 'th column(left) eigenvector of a matrix defined by the coefficients multiplying the spatial derivatives in a differential system, and $d\mathbf{u}$ is a differential variable vector. The differential variable vector we shall use can be chosen by examining which variables have temporal derivatives: the density, ρ ; the flow velocity, u ; and the specific internal energy, e .

The nondimensional form of the invariants may be calculated using the methodology found in Whitham's *Linear and Nonlinear Waves*. This calculation may be begun from the inviscid, non conducting version of the nondimensional differential system in Eqs. (3.6a) to (3.6c)

$$(C.1a) \quad \frac{\partial \tilde{\rho}}{\partial \tilde{t}} + \tilde{u} \frac{\partial \tilde{\rho}}{\partial \tilde{x}} + \tilde{\rho} \frac{\partial \tilde{u}}{\partial \tilde{x}} = 0,$$

$$(C.1b) \quad \tilde{\rho} \frac{\partial \tilde{u}}{\partial \tilde{t}} + \tilde{\rho} \tilde{u} \frac{\partial \tilde{u}}{\partial \tilde{x}} + K_m \frac{\partial \tilde{p}}{\partial \tilde{x}} = 0,$$

$$(C.1c) \quad \tilde{\rho} \frac{\partial \tilde{e}}{\partial \tilde{t}} + \tilde{\rho} \tilde{u} \frac{\partial \tilde{e}}{\partial \tilde{x}} + K_e \tilde{p} \frac{\partial \tilde{u}}{\partial \tilde{x}} = 0.$$

The above expression is not in the appropriate form for the analysis described above. It must be ensured that only one temporal derivative appears in every equation. This is done by isolating each temporal derivative and substituting in for the pressure via Eq. (3.13), rewriting spatial and temporal derivatives with an $\tilde{x}$ and $\tilde{t}$, and dropping the tilde

$$(C.2a) \quad \rho_t + u\rho_x + \rho u_x = 0,$$

$$(C.2b) \quad u_t + uu_x + \frac{K_m}{K_e} \frac{\gamma - 1}{\rho} (\rho e_x + e\rho_x) = 0,$$

$$(C.2c) \quad e_t + (\gamma - 1)e u_x + u e_x = 0.$$

Equations (C.2a) to (C.2c) form the nondimensional system that we will use to calculate characteristics and invariants. From the spatial derivatives of the above equations we may construct a matrix whose eigenvalues are the characteristics velocities at which information propagates in the differential system and whose column eigenvectors can be used to calculate the Riemann invariants. This matrix is

$$(C.3) \quad a_{ij} = \begin{bmatrix} u & \rho & 0 \\ \frac{K_m}{K_e}(\gamma - 1)\frac{e}{\rho} & u & \frac{K_m}{K_e}(\gamma - 1) \\ 0 & (\gamma - 1) & u \end{bmatrix}.$$

with the three following eigenvalues (equations derived in Appendix B were used to reduce the eigenvalue expressions)

$$(C.4) \quad \lambda_0 = u \quad , \quad \lambda_{\pm} = u \pm \underbrace{\sqrt{K_m \frac{\gamma p}{\rho}}}_c$$

where each eigenvalue describes how information is propagated within the one dimensional domain. λ_0 is information propagating at the flow velocity while $\lambda_{\pm}$ is information propagating in both the positive and negative directions at the speed of sound plus the flow velocity. The left eigenvectors that correspond to each eigenvalue are

$$(C.5) \quad \mathbf{l}^{(0)} = \begin{bmatrix} -(\gamma-1)\frac{e}{\rho} \\ 0 \\ 1 \end{bmatrix} \quad \mathbf{l}^{(\pm)} = \begin{bmatrix} \frac{e}{\rho} \\ \pm \frac{\gamma e}{c} \\ 1 \end{bmatrix}.$$

These left eigenvalues are then dotted with the total differential variable $\mathbf{du} = [d\rho, du, de]^T$. Dotted $\mathbf{l}^{(0)}$ with $\mathbf{du}$ allows us to write

$$\begin{aligned} dr_0 &= \mathbf{l}^{(0)} \cdot \mathbf{du} = (\gamma-1)\frac{e}{\rho}d\rho + 0 * du + 1 * de, \\ dr_0 &= -\frac{\gamma-1}{\gamma-1} K_e \rho^{\gamma-1} d\rho + de, \end{aligned}$$

which then may be simplified with the use of the differential of Eq. (B.2)

$$\begin{aligned} dr_0 &= -K_e \rho^{\gamma-1} d\rho + \overbrace{K_e \rho^{\gamma-1} d\rho}^{de}, \\ dr_0 &= 0. \end{aligned}$$

This result states the the invariant along the characteristic λ_0 is constant throughout the domain in isentropic flow (this invariant is in fact the entropy). This is consistent with the theory of characteristics in the context of the Euler equations[16, 42, 44].

Dotting $\mathbf{l}^{\pm}$ with $\mathbf{du}$ and calculating the invariant along the other characteristics of the problem

$$\begin{aligned} dr_{(\pm)} &= \mathbf{l}^{\pm} \cdot \mathbf{du} = \frac{e}{\rho}d\rho \pm \frac{\gamma e}{c}du + de, \\ dr_{\pm} &= \frac{K_e}{\gamma-1} \rho^{\gamma-2} d\rho \pm \frac{\gamma K_e}{\gamma-1} \frac{\rho^{\gamma-1}}{c} du + K_e \rho^{\gamma-2} d\rho, \end{aligned}$$

dividing by the variable $\rho^{\gamma-2}$ and the parameter K_e we may write the following after combining the $d\rho$ term

$$\begin{aligned} dr_{\pm} &= \frac{\gamma}{\gamma-1} d\rho \pm \frac{\gamma}{\gamma-1} \frac{\rho}{c} du, \\ dr_{\pm} &= \frac{c}{\rho} d\rho - du. \end{aligned}$$

We may now integrate the expression found above to calculate the invariant. The speed of sound, c may be written solely as a function of the thermodynamic density, ρ , with the aid of Eq. (B.3).

$$\begin{aligned} \int dr_{\pm} &= \int \sqrt{K_m \gamma} \rho^{(\gamma-3)/2} d\rho \pm \int du, \\ r_{\pm} &= \frac{2}{\gamma-1} \sqrt{K_m \gamma} \rho^{(\gamma-1)/2} \pm u, \end{aligned}$$

which may also be written as

$$(C.6) \quad r_{\pm} = \frac{2}{\gamma-1} c \pm u.$$

Equation (C.6) is the value of the invariant along the $\lambda_{\pm}$ directions defined by the eigenvalues of the matrix a_{ij} . This is the expression that was evaluated and whose contours were plotted to obtain the data shown in Section 3.4.3. The invariants $r_{\pm}$ physically correspond to waves propagating sonically in the positive and negative directions. These are also the waves propagating seen propagating in Figs. 3.7 to 3.9 in Chapter 3.

APPENDIX D

The Physical Implication of Upwinding

Numerical stability and elimination of spurious data is an important aspect of numerical physics. Here, the advection diffusion equation is considered with the inclusion of a numerical viscosity that is introduced via upwinding to eliminate spurious oscillations.

Consider the one dimensional advection diffusion equation

$$(D.1) \quad \frac{\partial \phi}{\partial t} + \overbrace{u \frac{\partial \phi}{\partial x}}^{q(\phi) \text{ flux of } \phi} = \overbrace{\chi \frac{\partial^2 \phi}{\partial x^2}}^{\text{diffusion}}.$$

Equation (D.1) considers some variable ϕ being advected at some velocity $u = u(x, t)$ with diffusion being considered as a dissipative mechanism. The parameter $\chi = \chi(x, t)$ is some diffusion coefficient. The independent variables are space, x , and time, t . Equation (D.1) may be discretized with forward Euler in time, upwinding (downwinding depending on the sign of u) for the advective term, and central differencing for the diffusive term. For $u > 0$ upwinding may be used.

$$(D.2) \quad \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u_i \frac{\phi_i^n - \phi_{i-1}^n}{\Delta x} = \chi \phi_{xx}$$

where the superscript of each variable ϕ refers to temporal locations and subscript refer to spatial locations. The Δ quantities refer to discrete jumps in time and space. The diffusive term is left as is for convenience later and the xx subscript there is a spatial derivative.

The ϕ_i^n in Eq. (D.2) may be expanded for a second derivative quantity. The below equation shows what may be substituted for the ϕ_i^n in the advective term in Eq. (D.2)

$$\begin{aligned} f_{xx} &= \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} \\ f_i &= \frac{f_{i+1} + f_{i-1} - f_{xx} \Delta x^2}{2} \end{aligned}$$

and then plugging these relations into Eq. (D.2) and rearranging some terms

$$(D.3) \quad \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + \frac{u_i}{\Delta x} \left(\frac{\phi_{i+1}^n}{2} + \frac{\phi_{i-1}^n}{2} - \frac{1}{2} \phi_{xx} \Delta x^2 - \phi_{i-1}^n \right) = \chi \phi_{xx}.$$

The $1/\Delta x$ has been taken out from the advective term in combination with some rearrangement. Combining like terms and moving ϕ_{xx} over to the RHS of Eq. (D.3) we obtain

$$(D.4) \quad \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u_i \frac{\phi_{i+1}^n - \phi_{i-1}^n}{\Delta x} = \left(\chi + \overbrace{\frac{u_i \Delta x}{2}}^{\beta} \right) \phi_{xx}.$$

Equation (D.4) shows the parameter that explicitly introduces artificial dissipation into Eq. (D.1) even when the diffusive term, χ , is zero. This diffusive coefficient β is dependent upon both the mesh and the advective coefficient. For meshes whose resolution approaches infinity, this new dissipative term asymptotically approaches 0. Examples of what this β term could be physically can be made. If ϕ is a momentum variable, then β approximates artificial viscosity[29, 30, 36, 41], while if ϕ is the energy β approximates artificial heat conduction[5, 14, 18, 26, 27].

Writing out the full differential equation in analytic form

$$(D.5) \quad \phi_t + u \phi_x - (\chi + \beta) \phi_{xx} = 0$$

where now the discrete component of the differential equation shows in start contrast to the other terms of the equation. In the limit of infinity mesh resolution, computationally intractable, where $\beta \rightarrow 0$ and in the physical limit where the diffusive parameter $\chi \rightarrow 0$, the inviscid equation is recovered. Note however, that the computational limit of infinite mesh resolution is not possible, and that there is always a mutation of the underlying differential system with the inclusion of upwinding[11].

Nomenclature

a_{ij}	Jacobian matrix for spatial derivatives
c	Speed of sound
E_{int}	Internal energy
E_{kin}	Kinetic energy
e	Specific internal energy
f	Degrees of freedom within a fluid (translational, vibrational, rotational)
K_e	Nondimensional energy ratio of translational energy to total energy densities
K_m	Nondimensional energy ratio of static to dynamic pressure
K_s	Nondimensional energy ratio of energy to entropic energy
K_t	Nondimensional energy ratio of total energy to degrees of freedom energy
k	Thermal conductivity coefficient (energy diffusion)
L_∞	Error metric
M	Mass
p	Thermodynamic pressure
Pe	Péclet number, a nondimensional ratio of advection rate to heat diffusion rate
Re	Reynolds number, a nondimensional ratio of inertial to viscous forces
r_i	i'th Riemann invariant
S	Entropy
s	Specific entropy density
T	Thermodynamic temperatures
$\bar{\mathbf{T}}$	Cauchy stress tensor
t	Time (independent variable)
u	One dimensional fluid flow velocity $\hat{x}$ direction
$\mathbf{v}$	Fluid flow velocity (particle velocity)
v	Perturbed fluid flow velocity
x	1D spatial variable $\hat{x}$ direction
x_k	Characteristic length of heat conduction effects
x_μ	Characteristic length of viscous effects
α	Amplitude of normalized perturbed variable
β	Approximate dissipative coefficient from upwinding
γ	Ratio of specific heats of a material
ϵ	Perturbed specific internal energy
η	Perturbed mass density
λ_i	i'th characteristic velocity
μ	Coefficient of viscosity (momentum diffusion)
ν	Specific volume
ρ	Mass density
σ	Width of Gaussian for perturbed variable
ϕ	Placeholder variable
$\tilde{\phi}$	Nondimensional variable ($\phi = \phi_0 \tilde{\phi}$)
ϕ_0	Reference variable value (normalization factor)
χ	Dissipative coefficient
∇	Del operator

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