PH.D. DISSERTATION PROSPECTUS

ENTROPY STABLE APPROXIMATIONS OF NONLINEAR CONSERVATION LAWS

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1. Introduction

A central problem in computational fluid dynamics is the development of the numerical approximations for nonlinear hyperbolic conservation laws and related time-dependent problems governed by additional dissipative and dispersive forcing terms. Entropy stability serves as an essential guideline in the design of new computationally reliable numerical schemes.

My dissertation research involves a systematic study of the novel entropy stable approximate methods of nonlinear conservation laws and application of those methods to solve one and two dimensional systems, e.g., the Navier-Stoke equations, the shallow water equations, and more. We develop second-order difference schemes which avoid artificial numerical viscosity in the sense that their entropy dissipation is dictated *solely* by physical dissipation terms. The numerical results of 1D compressible Navier-Stokes equations equations provide us a remarkable evidence for different roles of viscosity and heat conduction in forming sharp monotone profiles in the immediate neighborhoods of shocks and contacts. Further implementation in 2D shallow water equations is realized dimension by dimension. These entropy-stable schemes also play a crucial role in the simulations of vanishing Leray-α smoothing model for Burgers equation. All the numerical experiments are implemented by a robust numerical package that offers a relatively simple, "black-box" solver for a wide variety of problems governed by nonlinear conservation laws.

2. Entropy-stable schemes for 1D Navier-Stokes equations

We consider the Navier-Stokes equations (NSE) for compressible viscous flows in one-space dimension as a system of conservation laws of density $\rho = \rho(x,t)$, momentum $m = m(x,t)$, and energy $E = E(x,t)$,

$$\frac{\partial}{\partial t}\mathbf{u} + \frac{\partial}{\partial x}\mathbf{f}(\mathbf{u}) = \epsilon\frac{\partial^2}{\partial x^2}\mathbf{d}(\mathbf{u}), \quad \mathbf{u} = \left[\rho, m, E\right]^\top \tag{2.1}$$

They are driven by the convective flux $\mathbf{f}(\mathbf{u}) = \left[m, qm + p, q(E+p)\right]^\top$, together with the dissipative flux $\epsilon\mathbf{d}(\mathbf{u}) = (\lambda+2\mu)\left[0, q, q^2/2\right]^\top + \kappa\left[0,0,\theta\right]^\top$ which stands for the combined viscous and heat fluxes. These fluxes involve the velocity $q := m/\rho$, the pressure p and temperature θ which are determined by the polytropic equation of state. Here, the viscosity λ, μ and conductivity κ are fixed.

The viscous and heat fluxes are dissipative terms in the sense that they are responsible for the dissipation of total *entropy*, $U(\mathbf{u}) = -\rho S$ with $S = \ln(p\rho^{-\gamma})$ being the specific entropy,

$$\frac{\partial}{\partial t}(-\rho S) + \frac{\partial}{\partial x}(-mS + \kappa(\ln\theta)_x) = -(\lambda+2\mu)\frac{q_x^2}{\theta} - \kappa\left(\frac{\theta_x}{\theta}\right)^2 \leq 0. \tag{2.2}$$

Spatial integration of (2.2) then yields the second law of thermodynamics,

$$\frac{d}{dt}\int_x(-\rho S)\,dx = -(\lambda+2\mu)\int_x\frac{q_x^2}{\theta}dx - \kappa\int_x\left(\frac{\theta_x}{\theta}\right)^2 dx \leq 0. \tag{2.3}$$

In fact, (2.3) specifies the precise entropy decay rate. For the Euler equations, $\lambda = \mu = \kappa = 0$, total entropy is precisely conserved, $\int_x -\rho S(x,t)\,dx = \int_x -\rho S(x,0)\,dx$.

To discretize NSE (2.1) in space, we use the conservative differences for convective flux and standard centered differences for the dissipative terms on the RHS.

$$\frac{d}{dt}\mathrm{u}_\nu(t) + \frac{1}{\Delta x}\left(\mathrm{f}^*_{\nu+\frac{1}{2}} - \mathrm{f}^*_{\nu-\frac{1}{2}}\right) = \frac{\epsilon}{(\Delta x)^2}\left(\mathrm{d}_{\nu+1} - 2\mathrm{d}_\nu + \mathrm{d}_{\nu-1}\right). \tag{2.4}$$

Here, $\mathrm{u}_\nu(t)$ denotes the discrete solution along the gridline (x_ν, t) with $x_\nu := \nu\Delta x$, Δx being the uniform meshsize, $\mathrm{d}_\nu := \mathrm{d}(\mathrm{u}_\nu)$, and $\mathrm{f}^*_{\nu+\frac{1}{2}} := \mathrm{f}(\mathrm{u}_{\nu-r+1}, \cdots, \mathrm{u}_{\nu+r})$ is a consistent numerical flux based on a stencil of $2r+1$ neighboring grid values. We seek a proper $\mathrm{f}^*_{\nu+\frac{1}{2}}$, so that the semi-discrete entropy balance statement $\frac{d}{dt}U_\nu(t) + \frac{1}{\Delta x}(F_{\nu+\frac{1}{2}} - F_{\nu-\frac{1}{2}}) \le 0$ is guaranteed with $U_\nu(t) := U(\mathrm{u}_\nu(t))$ and the consistent numerical entropy flux $F_{\nu+\frac{1}{2}}$. Instead of adding excessive amount of artificial viscosity as in many other numerical schemes, we construct a more faithful approximation of (2.1) by utilizing the 3-point entropy-conservative numerical flux $\mathrm{f}^*_{\nu+\frac{1}{2}}$, and thus recover the *precise* entropy balance dictated by viscous and heat fluxes in NSE. $\mathrm{f}^*_{\nu+\frac{1}{2}}$ is constructed along a piecewise-constant path in phase space dictated by an arbitrary set of 3 linear independent 3-vectors $\{\mathrm{r}^j\}_{j=1}^{j=3}$ and its orthogonal set $\{\ell^j\}_{j=1}^{j=3}$. Details are outlined in the following main result.

Theorem 2.1 ([TaZh2006], Theorem 3.6). *Consider the 3-point semi-discrete approximation* (2.4)*, where* $\mathrm{f}^*_{\nu+\frac{1}{2}}$ *is an entropy conservative numerical flux,*

$$\mathrm{f}^*_{\nu+\frac{1}{2}} = (\gamma - 1)\sum_{j=1}^{3}\frac{m^{j+1}_{\nu+\frac{1}{2}} - m^j_{\nu+\frac{1}{2}}}{\left\langle \ell^j_{\nu+\frac{1}{2}}, \Delta\mathrm{v}_{\nu+\frac{1}{2}}\right\rangle}\ell^j_{\nu+\frac{1}{2}}, \qquad \Delta\mathrm{v}_{\nu+\frac{1}{2}} = \mathrm{v}_{\nu+1} - \mathrm{v}_\nu. \tag{2.5}$$

Here $\mathrm{v} := U_{\mathrm{u}}(\mathrm{u})$ *are the entropy variable,* $\gamma > 1$ *is the constant specific heat ratio, and* $\{m^j_{\nu+\frac{1}{2}}\}$ *are intermediate values of momentum along the phase path. The resulting scheme* (2.5) *is entropy-dissipative in the sense that* [1]

$$\begin{aligned}\frac{d}{dt}\sum_\nu U_\nu(t)\,\Delta x &= -\sum_\nu \frac{\epsilon}{\Delta x}\left\langle \Delta\mathrm{v}_{\nu+\frac{1}{2}}, \frac{\Delta\mathrm{d}_{\nu+\frac{1}{2}}}{\Delta\mathrm{v}_{\nu+\frac{1}{2}}}\Delta\mathrm{v}_{\nu+\frac{1}{2}}\right\rangle \\ &= -(\lambda+2\mu)\sum_\nu\left(\frac{\Delta q_{\nu+\frac{1}{2}}}{\Delta x}\right)^2\left(\widehat{1/\theta}\right)_{\nu+\frac{1}{2}}\Delta x - \kappa\sum_\nu\left(\frac{\Delta\theta_{\nu+\frac{1}{2}}}{\Delta x}\right)^2\left(\widetilde{1/\theta}\right)^2_{\nu+\frac{1}{2}}\Delta x \le 0 \end{aligned} \tag{2.6}$$

This entropy balance is a discrete analogue of the entropy balance statement (2.3).

Here is our main point: we introduce no spurious, *artificial* numerical viscosity: by (2.6), the semi-discrete scheme contains the precise amount of numerical viscosity to enforce the correct entropy dissipation dictated by NSE.

To complete the computation of a semi-discrete scheme, it needs to be augmented with a proper time discretization. To enable a large time-stability region and maintain simplicity, the three-stage third-order Runge-Kutta (RK3) method is used to do the time discretization, consult [GST2001]. Discussions in detail and numerical results of these novel entropy-stable schemes for 1D compressible NSE/Euler equations can be found in [Ta2004, TaZh2006].

[1] We let $\widehat{z}_{\nu+\frac{1}{2}} = (z_\nu + z_{\nu+1})/2$ and $\widetilde{z}_{\nu+\frac{1}{2}} = \sqrt{z_\nu z_{\nu+1}}$.

The remaining challenges in developing and implementing these methods include the higher (than second) order entropy stable schemes by utilizing the finite element discretization on wider numerical stencils, and creating a object-oriented software module for these methods.

3. Entropy Stable Schemes for 2D Shallow Water equations

We extend our discussion about the entropy stable schemes to the 2D shallow water equations with no viscous and source terms as the prototype of 2D nonlinear conservation laws

$$\partial_t \mathbf{u} + \partial_x \mathbf{f}(\mathbf{u}) + \partial_y \mathbf{g}(\mathbf{u}) = 0, \tag{3.1}$$

with $\mathbf{u} = [h, uh, vh]^\top$ being the vector of conserved variables, and the flux vectors f and g given as

$$\mathbf{f} = [uh,\ u^2h + gh^2/2,\ uvh]^\top, \quad \mathbf{g} = [vh,\ uvh,\ v^2h + gh^2/2]^\top.$$

The total energy $U(\mathbf{u}) = gh^2/2 + (u^2h + v^2h)/2$ serves as the entropy function for the shallow water equations. Arguing along the same line as the above NSE dimension by dimension, we obtain the semi-discrete entropy-stable schemes without artificial viscosity for the shallow water equations

$$\frac{d}{dt}\mathbf{u}_{\nu,\mu}(t) + \frac{1}{\Delta x}(\mathbf{f}^*_{\nu+\frac{1}{2},\mu} - \mathbf{f}^*_{\nu-\frac{1}{2},\mu}) + \frac{1}{\Delta y}(\mathbf{g}^*_{\nu,\mu+\frac{1}{2}} - \mathbf{g}^*_{\nu,\mu-\frac{1}{2}}) = 0, \tag{3.2}$$

with $\mathbf{f}^*_{\nu+\frac{1}{2},\mu}$ and $\mathbf{g}^*_{\nu,\xi+\frac{1}{2}}$ constructed along the same recipe as (2.5) in x and y direction, respectively, while two sets of vectors $\{\ell^j\}$ and entropy potentials ψ are set up separately in x and y direction as well. Details of entropy stability analysis and numerical results of both inviscid and viscous cases for 2D Dam-Break problem (consult [FC1990]) have been done in [TaZh2006P].

The boundary effects are not negligible in physical realistic models. To avoid the zero-height due to the spurious numerical oscillations close to the internal boundary, more realistic treatment, like the boundary layers, remains an ongoing issue in the implementation of the entropy stable schemes for 2D shallow water equations.

4. Application to Vanishing Leray-α Smoothing Model of Burgers Equation

We prove that solutions of the vanishing $\alpha-$equation, $v^\alpha_t + [(I - (\alpha\partial_x)^2)^{-1}v^\alpha]v^\alpha_x = 0$ converge to the entropy solution of the corresponding inviscid Burgers equation $u_t + (u^2/2)_x = 0$ as $\alpha \downarrow 0$. In our numerical experiments, we compare the Leray$-\alpha$ model with R-C-E (Rosenau regularization of the Chapman-Enskog expansion) model and the usual artificial viscous model. In order to truly recover the effects of different regularization models, the entropy stable schemes with no artificial viscosity in discretizing the nonlinear flux (2.5) are employed in numerical simulations.

References

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