Structure preserving schemes for conservation laws

Well-balanced schemes for Euler equations with gravity

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Structure preserving schemes

- Usual considerations: stability and accuracy
- Accuracy is an asymptotic property: $\Delta x \to 0$
- Euler equations
  - Density, temperature must be positive
  - Smooth solutions: entropy is conserved
  - Steady solutions: enthalpy is constant along streamlines
  - Incompressible: kinetic energy is conserved
  - With gravity: non-trivial stationary solutions
- Shallow water: energy and potential enstrophy conserved
- Desirable to have numerical solutions satisfy these additional properties

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Euler equations with gravity

Flow properties

$$\rho = \text{density}, \qquad u = \text{velocity}$$

$$p = \text{pressure}, \qquad E = \text{total energy} = e + \frac{1}{2}\rho u^2$$

Gravitational potential ϕ; force per unit volume of fluid

$$-\rho \nabla \phi$$

System of conservation laws

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) &= 0 \\
\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(p + \rho u^2) &= -\rho \frac{\partial \phi}{\partial x} \\
\frac{\partial E}{\partial t} + \frac{\partial}{\partial x}(E + p)u &= -\rho u \frac{\partial \phi}{\partial x}
\end{aligned}$$

Euler equations with gravity

In compact notation

$$\frac{\partial \boldsymbol{q}}{\partial t} + \frac{\partial \boldsymbol{f}}{\partial x} = - \begin{bmatrix} 0 \\ \rho \\ \rho u \end{bmatrix} \frac{\partial \phi}{\partial x}$$

where

$$\boldsymbol{q} = \begin{bmatrix} \rho \\ \rho u \\ E \end{bmatrix}, \qquad \boldsymbol{f} = \begin{bmatrix} \rho u \\ p + \rho u^2 \\ (E + p) u \end{bmatrix}$$

Hydrostatic solutions

- Fluid at rest

$$u_e = 0$$

- Momentum equation

$$\frac{\mathrm{d}p_e}{\mathrm{d}x} = -\rho_e \frac{\mathrm{d}\phi}{\mathrm{d}x} \tag{1}$$

- Assume ideal gas and some temperature profile $T_e(x)$

$$p_e(x) = \rho_e(x) R T_e(x), \qquad R = \text{gas constant}$$

integrate (1) to obtain

$$\boxed{p_e(x) \exp\left(- \int_{x_0}^{x} \frac{\phi'(s)}{R T_e(s)} \mathrm{d}s \right) = p_0}$$

Hydrostatic solutions

- **Isothermal** hydrostatic state, i.e., $T_e(x) = T_e = \text{const}$, then

$$\boxed{p_e(x) \exp\left(\frac{\phi(x)}{RT_e}\right) = \text{const}} \tag{2}$$

$$\text{Density} \qquad \rho_e(x) = \frac{p_e(x)}{RT_e}$$

- **Polytropic** hydrostatic state

$$p_e \rho_e^{-\nu} = \text{const}, \qquad p_e T_e^{-\frac{\nu}{\nu-1}} = \text{const}, \qquad \rho_e T_e^{-\frac{1}{\nu-1}} = \text{const} \tag{3}$$

where $\nu > 1$ is some constant. From (1) and (3), we obtain

$$\boxed{\frac{\nu R T_e(x)}{\nu - 1} + \phi(x) = \text{const}}$$

E.g., pressure is

$$p_e(x) = C_1 \left[C_2 - \phi(x)\right]^{\frac{\nu-1}{\nu}}$$

Well-balanced scheme

- General evolutionary PDE

$$\frac{\partial \boldsymbol{q}}{\partial t} = R(\boldsymbol{q})$$

Stationary solution $\boldsymbol{q}_e$; scheme is well-balanced if

$$R(\boldsymbol{q}_e) = 0$$

- We are interested in computing small perturbations

$$\boldsymbol{q}(x,0) = \boldsymbol{q}_e(x) + \varepsilon \tilde{\boldsymbol{q}}(x,0), \qquad \varepsilon \ll 1$$

- Perturbations are governed by linear equation

$$\frac{\partial \tilde{\boldsymbol{q}}}{\partial t} = R'(\boldsymbol{q}_e)\tilde{\boldsymbol{q}}$$

Well-balanced scheme

- Some numerical scheme

$$\frac{\partial \boldsymbol{q}_h}{\partial t} = R_h(\boldsymbol{q}_h)$$

- $\boldsymbol{q}_{h,e} =$ interpolation of $\boldsymbol{q}_e$ onto the mesh

Scheme is well balanced if

$$R_h(\boldsymbol{q}_{h,e}) = 0$$

- Suppose scheme is not well-balanced $R_h(\boldsymbol{q}_{h,e}) \neq 0$. Solution

$$\boldsymbol{q}_h(x,t) = \boldsymbol{q}_{h,e}(x) + \varepsilon \tilde{\boldsymbol{q}}_h(x,t)$$

Well-balanced scheme

- Linearize the scheme around $\boldsymbol{q}_{h,e}$

$$\frac{\partial}{\partial t}(\boldsymbol{q}_{h,e} + \varepsilon \tilde{\boldsymbol{q}}_h) = R_h(\boldsymbol{q}_{h,e} + \varepsilon \tilde{\boldsymbol{q}}_h) = R_h(\boldsymbol{q}_{h,e}) + \varepsilon R_h'(\boldsymbol{q}_{h,e})\tilde{\boldsymbol{q}}_h$$

or

$$\frac{\partial \tilde{\boldsymbol{q}}_h}{\partial t} = \frac{1}{\varepsilon} R_h(\boldsymbol{q}_{h,e}) + R_h'(\boldsymbol{q}_{h,e})\tilde{\boldsymbol{q}}_h$$

- Scheme is consistent of order r: $R_h(\boldsymbol{q}_{h,e}) = Ch^r \|\boldsymbol{q}_{h,e}\|$

$$\frac{\partial \tilde{\boldsymbol{q}}_h}{\partial t} = \frac{1}{\varepsilon} Ch^r \|\boldsymbol{q}_{h,e}\| + R_h'(\boldsymbol{q}_{h,e})\tilde{\boldsymbol{q}}_h$$

- $\varepsilon \ll 1$ then first term may dominate the second term; need $h \ll 1$ and/or $r \gg 1$

Evolution of small perturbations

The initial condition is taken to be the following

$$\phi = \frac{1}{2}x^2, \quad u_e = 0, \quad \rho_e(x) = p_e(x) = \exp(-\phi(x))$$

Add small perturbation to equilibrium pressure

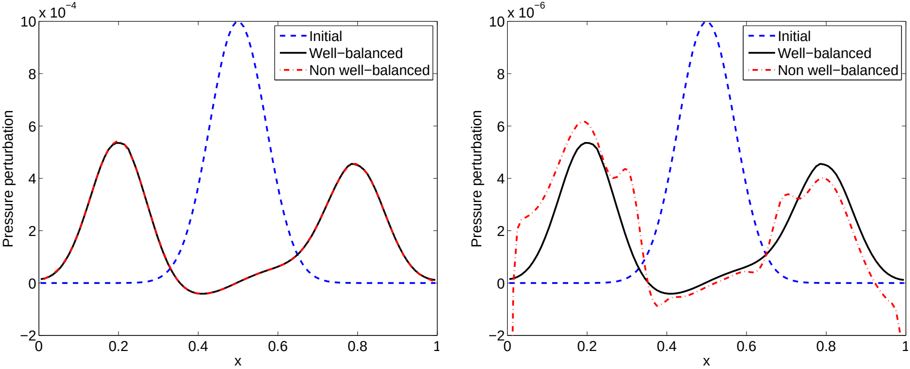
$$p(x) = \exp(-\phi(x)) + \varepsilon \exp(-100(x - 1/2)^2), \qquad 0 < \varepsilon \ll 1$$

Non-well-balanced scheme

$$\frac{\partial \phi}{\partial x}(x_i) \approx \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}, \qquad \text{reconstruct } \rho, u, p$$

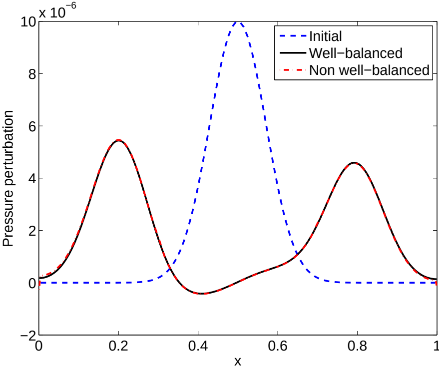
Using exact derivative of potential does not improve results. In practice, ϕ is only available at grid points.

Evolution of small perturbations

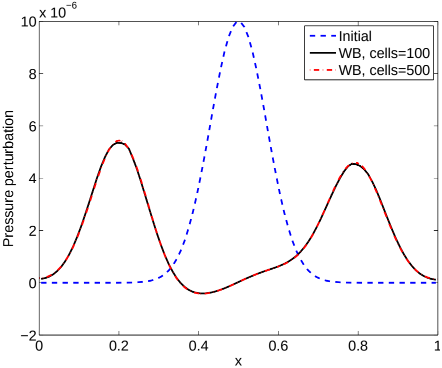


$\varepsilon = 10^{-3}$, $N = 100$ cells $\qquad$ $\varepsilon = 10^{-5}$, $N = 100$ cells

Evolution of small perturbations



$\varepsilon = 10^{-5}$, $N = 500$ cells



$\varepsilon = 10^{-5}$

1-D finite volume scheme

Define (Xing & Shu, 2013)

$$\psi(x) = -\int_{x_0}^{x} \frac{\phi'(s)}{RT(s)} \mathrm{d}s, \qquad x_0 \text{ is arbitrary}$$

Euler equations

$$\frac{\partial \boldsymbol{q}}{\partial t} + \frac{\partial \boldsymbol{f}}{\partial x} = -\begin{bmatrix} 0 \\ \rho \\ \rho u \end{bmatrix} \frac{\partial \phi}{\partial x} = \begin{bmatrix} 0 \\ p \\ pu \end{bmatrix} \exp(-\psi(x)) \frac{\partial}{\partial x} \exp(\psi(x))$$

- Divide domain into N finite volumes each of size Δx
- i'th cell $= (x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}})$

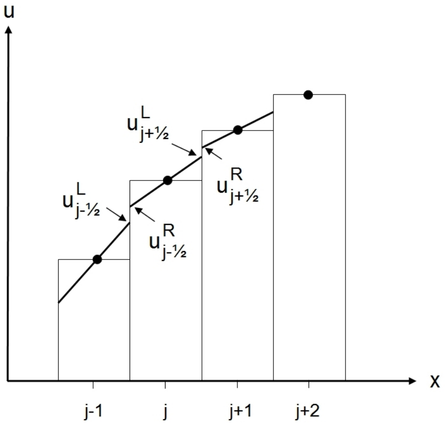
1-D finite volume scheme

- semi-discrete finite volume scheme for the i'th cell

$$\frac{\mathrm{d}\boldsymbol{q}_i}{\mathrm{d}t} + \frac{\hat{\boldsymbol{f}}_{i+\frac{1}{2}} - \hat{\boldsymbol{f}}_{i-\frac{1}{2}}}{\Delta x} = \mathrm{e}^{-\psi_i} \left(\frac{\mathrm{e}^{\psi_{i+\frac{1}{2}}} - \mathrm{e}^{\psi_{i-\frac{1}{2}}}}{\Delta x} \right) \begin{bmatrix} 0 \\ p_i \\ p_i u_i \end{bmatrix} \tag{4}$$

- ψ_i, $\psi_{i+\frac{1}{2}}$ etc. are consistent approximations to the function $\psi(x)$
- consistent numerical flux $\hat{\boldsymbol{f}}_{i+\frac{1}{2}} = \hat{\boldsymbol{f}}(\boldsymbol{q}^L_{i+\frac{1}{2}}, \boldsymbol{q}^R_{i+\frac{1}{2}})$

1-D finite volume scheme



Piecewise linear extrapolation

1-D finite volume scheme

Def: Property C

The numerical flux $\hat{\boldsymbol{f}}$ is said to satisfy Property C if for any two states

$$\boldsymbol{q}^L = [\rho^L, 0, p/(\gamma-1)] \quad \text{and} \quad \boldsymbol{q}^R = [\rho^R, 0, p/(\gamma-1)]$$

we have

$$\hat{\boldsymbol{f}}(\boldsymbol{q}^L, \boldsymbol{q}^R) = [0,\ p,\ 0]^\top$$

- New set of independent variables

$$\boldsymbol{w} = \boldsymbol{w}(\boldsymbol{q}, x) := \left[\rho \mathrm{e}^{-\psi},\ u,\ p\mathrm{e}^{-\psi}\right]^\top$$

- We can compute $\boldsymbol{q} = \boldsymbol{q}(\boldsymbol{w}, x)$
- States for computing numerical flux

$$\boldsymbol{q}^L_{i+\frac{1}{2}} = \boldsymbol{q}(\boldsymbol{w}^L_{i+\frac{1}{2}}, x_{i+\frac{1}{2}}), \qquad \boldsymbol{q}^R_{i+\frac{1}{2}} = \boldsymbol{q}(\boldsymbol{w}^R_{i+\frac{1}{2}}, x_{i+\frac{1}{2}})$$

1-D finite volume scheme

- First order scheme

$$\boldsymbol{w}^L_{i+\frac{1}{2}} = \boldsymbol{w}_i, \qquad \boldsymbol{w}^R_{i+\frac{1}{2}} = \boldsymbol{w}_{i+1}$$

- Higher order scheme: Reconstruct $\boldsymbol{w}$ variables, e.g.,

$$\boldsymbol{w}^L_{i+\frac{1}{2}} = \boldsymbol{w}_i + \frac{1}{2} m(\theta(\boldsymbol{w}_i - \boldsymbol{w}_{i-1}), (\boldsymbol{w}_{i+1} - \boldsymbol{w}_{i-1})/2, \theta(\boldsymbol{w}_{i+1} - \boldsymbol{w}_i))$$

1. Chandrashekar & Klingenberg, SIAM J. Sci. Comput., Vol. 37, No. 3, 2015

2. Dominik Zoar, Master Thesis, Dept. of Mathematics, Univ. of Würzburg

Theorem

The finite volume scheme (4) together with a numerical flux which satisfies property C and reconstruction of $\boldsymbol{w}$ variables is well-balanced in the sense that the initial condition given by

$$u_i = 0, \qquad p_i \exp(-\psi_i) = const, \qquad \forall\ i \tag{5}$$

is preserved by the numerical scheme.

$$u^L_{i+\frac{1}{2}} = u^R_{i+\frac{1}{2}} = 0, \qquad p^L_{i+\frac{1}{2}} = p^R_{i+\frac{1}{2}} = p_{i+\frac{1}{2}}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(\rho u)_i + \frac{f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}}}{\Delta x} = \mathrm{e}^{-\psi_i}\left(\frac{\mathrm{e}^{\psi_{i+\frac{1}{2}}} - \mathrm{e}^{\psi_{i-\frac{1}{2}}}}{\Delta x}\right) p_i$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(\rho u)_i + \frac{p_{i+\frac{1}{2}} - p_{i-\frac{1}{2}}}{\Delta x} = \frac{p_{i+\frac{1}{2}} - p_{i-\frac{1}{2}}}{\Delta x}$$

Approximation of source term

- How to approximate ψ_i, $\psi_{i+\frac{1}{2}}$, etc. ? Need some quadrature
- To compute the source term in i'th cell, we define

$$\psi(x) = -\int_{x_i}^{x} \frac{\phi'(s)}{RT(s)} \mathrm{d}s$$

- piecewise constant temperature

$$T(x) = \hat{T}_{i+\frac{1}{2}}, \qquad x_i < x < x_{i+1} \tag{6}$$

where $\hat{T}_{i+\frac{1}{2}}$ is the logarithmic average given by

$$\hat{T}_{i+\frac{1}{2}} = \frac{T_{i+1} - T_i}{\log T_{i+1} - \log T_i}$$

Approximation of source term

- The integrals are evaluated using the approximation of the temperature given in (6) leading to the following expressions for ψ.

$$
\begin{aligned}
\psi_i &= 0 \\
\psi_{i-\frac{1}{2}} &= -\frac{1}{R\hat{T}_{i-\frac{1}{2}}} \int_{x_i}^{x_{i-\frac{1}{2}}} \phi'(s)\mathrm{d}s = \frac{\phi_i - \phi_{i-\frac{1}{2}}}{R\hat{T}_{i-\frac{1}{2}}} \\
\psi_{i+\frac{1}{2}} &= -\frac{1}{R\hat{T}_{i+\frac{1}{2}}} \int_{x_i}^{x_{i+\frac{1}{2}}} \phi'(s)\mathrm{d}s = \frac{\phi_i - \phi_{i+\frac{1}{2}}}{R\hat{T}_{i+\frac{1}{2}}}
\end{aligned}
$$

- Gravitational potential required at faces $\phi_{i+\frac{1}{2}}$

$$
\phi_{i+\frac{1}{2}} = \phi(x_{i+\frac{1}{2}}), \qquad \phi_{i+\frac{1}{2}} = \frac{1}{2}(\phi_i + \phi_{i+1})
$$

Approximation of source term

Theorem

The source term discretization is second order accurate.

Theorem

Any hydrostatic solution which is isothermal or polytropic is exactly preserved by the finite volume scheme (4).

Isothermal examples: well-balanced test

Density and pressure are given by

$$\rho_e(x) = p_e(x) = \exp(-\phi(x))$$

$$N = 100, 1000, \qquad \text{final time} = 2$$

	Potential 1	Potential 2	Potential 3
$\phi(x)$	x	$\frac{1}{2}x^2$	$\sin(2\pi x)$

Table: Potential functions used for well-balanced tests

Isothermal examples: well-balanced test

Potential	Cells	Density	Velocity	Pressure
x	100	8.21676e-15	4.98682e-16	9.19209e-15
	1000	8.00369e-14	1.51719e-14	9.15152e-14
$\frac{1}{2}x^2$	100	1.01874e-14	2.49332e-16	1.06837e-14
	1000	1.05202e-13	4.10434e-16	1.11861e-13
$\sin(2\pi x)$	100	1.12466e-14	5.79978e-16	1.74966e-14
	1000	1.16191e-13	2.93729e-15	1.76361e-13

Table: Error in density, velocity and pressure for isothermal example

Shock tube under gravitational field

Gravitational field

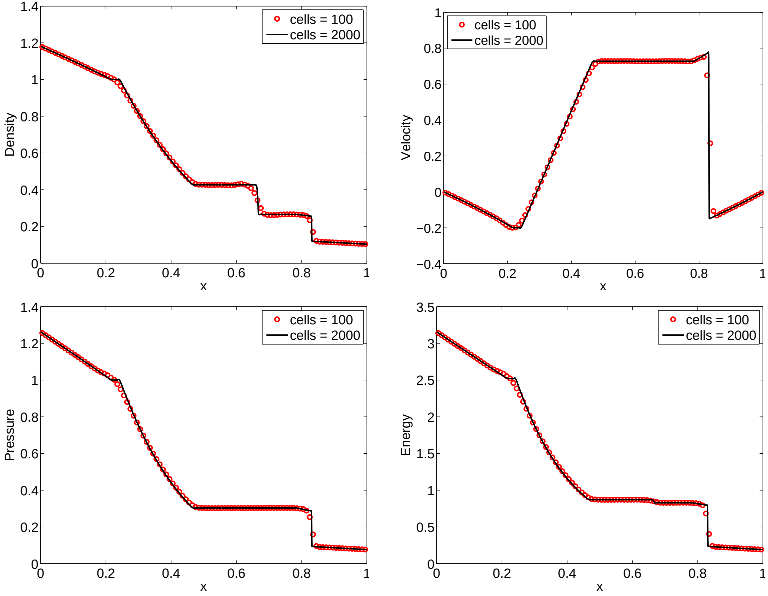
$$\phi(x) = x$$

The domain is $[0, 1]$ and the initial conditions are given by

$$(\rho, u, p) = \begin{cases} (1, 0, 1) & x < \frac{1}{2} \\ (0.125, 0, 0.1) & x > \frac{1}{2} \end{cases}$$

Solid wall boundary conditions. Final time $t = 0.2$, $N = 100, 2000$ cells

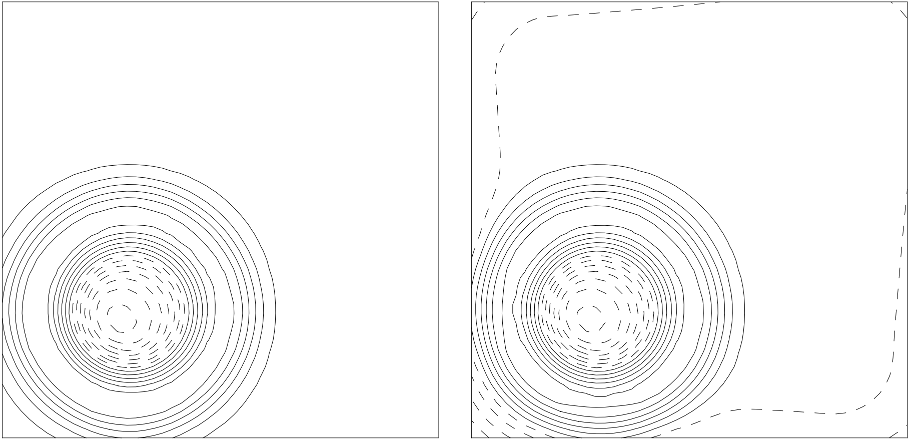
Shock tube under gravitational field



2-D Scheme

Polytropic hydrostatic solution

pressure perturbation with $\eta = 0.1$

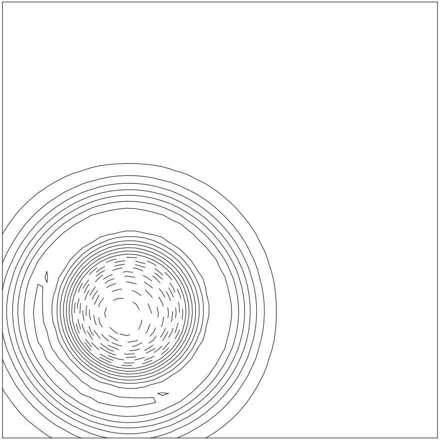


well-balanced non well-balanced

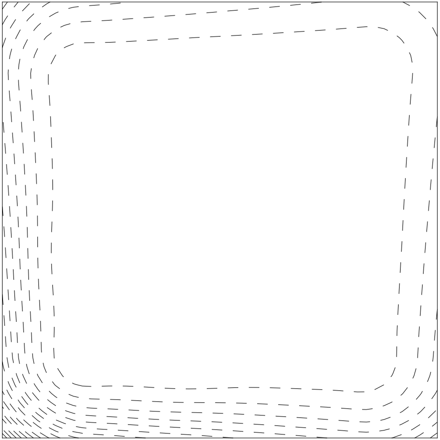
20 equally spaced contours between -0.03 and +0.03

Polytropic hydrostatic solution

pressure perturbation with $\eta = 0.001$



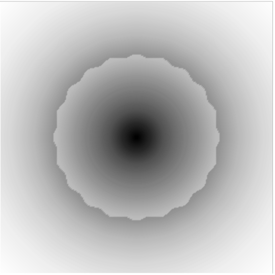
well-balanced
20 contours in [-0.00025,+0.00025]

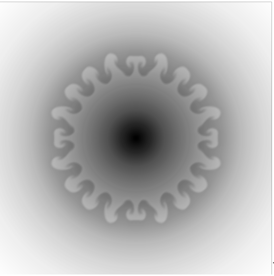


non well-balanced
20 contours in [-0.015,+0.0003]

Rayleigh-Taylor instability

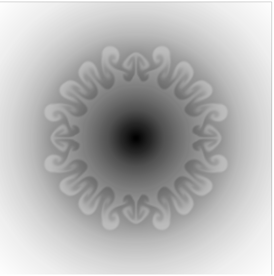
$t = 0$

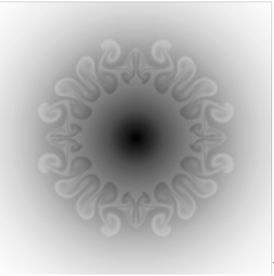




$t = 2.9$

$t = 3.8$





$t = 5.0$

More hydrostatic solutions

We will write the hydrostatic solution as

$$\rho_e(x) = \rho_0 \alpha(x), \qquad p_e(x) = p_0 \beta(x)$$

From hydrostatic condition

$$p_e'(x) = -\rho_e(x)\phi'(x), \qquad \text{i.e.,} \qquad \phi'(x) = -\frac{p_0}{\rho_0}\frac{\beta'(x)}{\alpha(x)} \tag{7}$$

Isothermal solution

$$\alpha(x) = \beta(x) = \exp\left(-\frac{\phi(x)}{RT_0}\right), \qquad \rho_0 = \frac{p_0}{RT_0}$$

Polytropic solution

$$\alpha(x) = \left[1 + \frac{\nu - 1}{s\nu\rho_0^{\nu-1}}(\phi_0 - \phi(x))\right]^{1/(\nu-1)}, \qquad \beta(x) = (\alpha(x))^\nu$$

More hydrostatic solutions

Constant potential temperature

Modeling atmosphere: Exner pressure and potential temperature

$$\pi = \left(\frac{p}{p_0}\right)^{\frac{\gamma-1}{\gamma}}, \qquad \theta = \frac{T}{\pi}$$

Taking the potential $\phi(x) = gx$, we get

$$\alpha(x) = \left[1 - \frac{(\gamma-1)gx}{\gamma R\theta_0}\right]^{\frac{1}{\gamma-1}}, \qquad \beta(x) = (\alpha(x))^\gamma$$

Specified Brunt-Väisälä frequency (N)

For potential $\phi(x) = gx$ and specified frequency N where

$$N^2 = g\frac{\mathrm{d}}{\mathrm{d}x}\ln(\theta) = \text{const} \qquad \theta = \theta_0 \exp(N^2 x/g)$$

More hydrostatic solutions

The equilibrium functions are given by

$$\alpha(x) = \exp(-N^2 x/g) \left[1 + \frac{(\gamma-1)g^2}{\gamma R \theta_0 N^2} \left\{\exp(-N^2 x/g) - 1\right\}\right]^{\frac{1}{\gamma-1}}$$

$$\beta(x) = \left[1 + \frac{(\gamma-1)g^2}{\gamma R \theta_0 N^2} \left\{\exp(-N^2 x/g) - 1\right\}\right]^{\frac{\gamma}{\gamma-1}}$$

Radiation pressure

$$p = \rho R T + \frac{1}{3} a T^4$$

Tabulated equation of state

(ρ_i, T_i, p_i), $i = 1, 2, \ldots$

1-D Finite Volume Scheme

See Berberich et al., Int. Conf. on Hyperbolic Problems, Aachen, 1-5 Aug., 2016

$$\frac{\mathrm{d}\boldsymbol{q}_i}{\mathrm{d}t} + \frac{\hat{\boldsymbol{f}}_{i+\frac{1}{2}} - \hat{\boldsymbol{f}}_{i-\frac{1}{2}}}{\Delta x} = \begin{bmatrix} 0 \\ s_i \\ u_i s_i \end{bmatrix}$$

Consistent numerical flux

$$\hat{\boldsymbol{f}}_{i+\frac{1}{2}} = \hat{\boldsymbol{f}}(\boldsymbol{q}^L_{i+\frac{1}{2}}, \boldsymbol{q}^R_{i+\frac{1}{2}})$$

Gravitational source

$$s(x,t) = \frac{p_0}{\rho_0} \frac{\beta'(x)}{\alpha(x)} \rho(x,t)$$

Central difference discretization

$$s_i = \frac{p_0}{\rho_0} \frac{\beta_{i+\frac{1}{2}} - \beta_{i-\frac{1}{2}}}{\Delta x} \frac{\rho_i}{\alpha_i}$$

1-D Finite Volume Scheme

Define new set of independent variables

$$\boldsymbol{w} = \boldsymbol{w}(\boldsymbol{q}, x) := [\rho/\alpha,\ u,\ p/\beta]^\top$$

Reconstruct $\boldsymbol{w}$ variables and compute

$$\boldsymbol{q}^L_{i+\frac{1}{2}} = \boldsymbol{q}(\boldsymbol{w}^L_{i+\frac{1}{2}}, x_{i+\frac{1}{2}}), \qquad \boldsymbol{q}^R_{i+\frac{1}{2}} = \boldsymbol{q}(\boldsymbol{w}^R_{i+\frac{1}{2}}, x_{i+\frac{1}{2}})$$

Well-balanced property

The finite volume scheme (4) together with any consistent numerical flux and reconstruction of $\boldsymbol{w}$ variables is well-balanced in the sense that the initial condition given by

$$u_i = 0, \qquad \rho_i/\alpha_i = \text{const}, \qquad p_i/\beta_i = \text{const}, \qquad \forall\ i$$

is preserved by the numerical scheme.

Remarks

- We must know a priori the hydrostatic state $(\alpha(x), \beta(x))$
- Well-balanced scheme for any equation of state
- Extended to curvilinear grids
  - Seven-League Hydro Code (`https://slh-code.org`)
- Extended to unstructured grids
  - UG3 code (`https://bitbucket.org/cpraveen/ug3/wiki/Home`)

Well-balanced DG schemes

Finite element method

Conservation law with source term

$$q_t + f(q)_x = s(q)$$

stationary solution q_e

$$f(q_e)_x = s(q_e)$$

Weak formulation: Find $q(t) \in V$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t}(q, \varphi) + a(q, \varphi) = (s(q), \varphi), \qquad \forall \varphi \in V$$

FEM with quadrature: Find $q_h(t) \in V_h$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t}(q_h, \varphi_h)_h + a_h(q_h, \varphi_h) = (s_h(q_h), \varphi_h)_h, \qquad \forall \varphi_h \in V_h$$

Finite element and well-balanced

Stationary solution is not a polynomial, $q_e \notin V_h$.

Let

$$q_{e,h} = \Pi_h(q_e), \qquad \Pi_h : V \to V_h, \text{ interpolation or projection}$$

FEM is well-balanced if

$$a_h(q_{e,h}, \varphi_h) = (s_h(q_{e,h}), \varphi_h)_h, \qquad \forall \varphi_h \in V_h$$

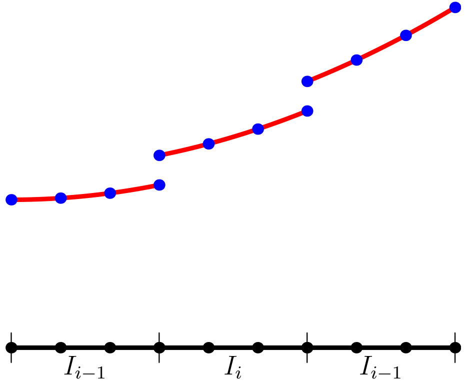
How to construct a_h, s_h to achieve well-balancing ?

Mesh and basis functions

- Partition domain into disjoint cells

$$C_i = (x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}), \qquad \Delta x_i = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$$

- Approximate solution inside each cell by a polynomial of degree N



Discontinuous Galerkin Scheme

Consider the single conservation law with source term

$$\frac{\partial q}{\partial t} + \frac{\partial f}{\partial x} = s(q, x)$$

Solution inside cell C_i is polynomial of degree N

$$q_h(x, t) = \sum_{j=0}^{N} q_j(t)\varphi_j(x), \qquad q_j(t) = q_h(x_j, t)$$

Approximate the flux

$$f(q_h) \approx f_h(x, t) = \sum_{j=0}^{N} f(q_h(x_j, t))\varphi_j(x) = \sum_{j=0}^{N} f_j(t)\varphi_j(x)$$

Discontinuous Galerkin Scheme

Gauss-Lobatto-Legendre quadrature

$$\int_{C_i} \phi(x)\psi(x)\mathrm{d}x \approx (\phi, \psi)_h = \Delta x_i \sum_{q=0}^{N} \omega_q \phi(x_q)\psi(x_q)$$

Semi-discrete DG: For $0 \leq j \leq N$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}(q_h, \varphi_j)_h + (\partial_x f_h, \varphi_j)_h &+ [\hat{f}_{i+\frac{1}{2}} - f_h(x^-_{i+\frac{1}{2}})]\varphi_j(x^-_{i+\frac{1}{2}}) \\ &- [\hat{f}_{i-\frac{1}{2}} - f_h(x^+_{i-\frac{1}{2}})]\varphi_j(x^+_{i-\frac{1}{2}}) = (s_h, \varphi_j)_h\end{aligned} \tag{1}$$

where $\hat{f}_{i+\frac{1}{2}} = \hat{f}(q^-_{i+\frac{1}{2}}, q^+_{i+\frac{1}{2}})$ is a numerical flux function. This is also called a *DG Spectral Element Method*[1].

[1] **See arXiv:1511.08739 for more details**.

Approximation of source term: isothermal case

Let

$$\bar{T}_i = \text{temperature corresponding to the cell average value in cell } C_i$$

Rewrite the source term in the momentum equation as (Xing & Shu)

$$s = -\rho \frac{\partial \Phi}{\partial x} = \rho R \bar{T}_i \exp\left(\frac{\Phi}{R\bar{T}_i}\right) \frac{\partial}{\partial x} \exp\left(-\frac{\Phi}{R\bar{T}_i}\right)$$

Source term approximation: For $x \in C_i$

$$s_h(x) = \rho_h(x) R\bar{T}_i \exp\left(\frac{\Phi(x)}{R\bar{T}_i}\right) \frac{\partial}{\partial x} \sum_{j=0}^{N} \exp\left(-\frac{\Phi(x_j)}{R\bar{T}_i}\right) \varphi_j(x) \qquad (2)$$

Source term in the energy equation

$$\frac{1}{\rho_h} (\rho u)_h s_h$$

Approximation of source term: polytropic case[2]

Define $H(x)$ inside each cell C_i as

$$H(x) = \frac{\nu}{\nu-1} \ln\left[\frac{\nu-1}{\nu\alpha_i}(\beta_i - \Phi(x))\right], \qquad x \in C_i$$

α_i, β_i: constants to be chosen. Rewrite source term

$$s(x) = -\rho\frac{\partial \Phi}{\partial x} = \frac{\nu-1}{\nu}\rho(\beta_i - \Phi(x))\exp(-H(x))\frac{\partial}{\partial x}\exp(H(x)), \quad x \in C_i$$

Source term approximation: For $x \in C_i$

$$s_h(x) = \frac{\nu-1}{\nu}\rho_h(x)(\beta_i - \Phi(x))\exp(-H(x))\frac{\partial}{\partial x}\sum_{j=0}^{N}\exp(H(x_j))\varphi_j(x)$$

$$\beta_i = \max_{0\le j\le N}\left[\frac{\nu}{\nu-1}\frac{p_j}{\rho_j} + \Phi(x_j)\right], \qquad \alpha_i = p_{j^*}\rho_{j^*}^{-\nu}$$

[2] with Markus Zenk

Well-balanced property

Well-balanced property

Let the initial condition to the DG scheme (1), (2) be obtained by interpolating the **isothermal/polytropic** hydrostatic solution corresponding to a continuous gravitational potential Φ. Then the scheme (1), (2) preserves the initial condition under any time integration scheme.

Proof: For continuous hydrostatic solution, $q_h(0)$ is continuous. By flux consistency

$$\hat{f}_{i+\frac{1}{2}} - f_h(x_{i+\frac{1}{2}}^-) = 0, \qquad \hat{f}_{i-\frac{1}{2}} - f_h(x_{i-\frac{1}{2}}^+) = 0$$

Above is true even if density is discontinuous, provided flux satisfies contact property.

$$\Longrightarrow \text{density and energy equations are well-balanced}$$

Well-balanced property

Momentum eqn: flux f_h has the form

$$f_h(x,t) = \sum_{j=0}^{N} p_j(t)\varphi_j(x), \qquad p_j = \text{pressure at the GLL point } x_j$$

Isothermal initial condition, $\bar{T}_i = T_e = \text{const}$. The source term evaluated

Well-balanced property

at any GLL node x_k is given by

$$
\begin{aligned}
s_h(x_k) &= \underbrace{\rho_h(x_k) R T_e}_{p_k} \exp\left(\frac{\Phi(x_k)}{RT_e}\right) \sum_{j=0}^{N} \exp\left(-\frac{\Phi(x_j)}{RT_e}\right) \frac{\partial}{\partial x} \varphi_j(x_k) \\
&= p_k \exp\left(\frac{\Phi(x_k)}{RT_e}\right) \sum_{j=0}^{N} \exp\left(-\frac{\Phi(x_j)}{RT_e}\right) \frac{\partial}{\partial x} \varphi_j(x_k) \\
&= \sum_{j=0}^{N} p_k \exp\left(\frac{\Phi(x_k)}{RT_e}\right) \exp\left(-\frac{\Phi(x_j)}{RT_e}\right) \frac{\partial}{\partial x} \varphi_j(x_k) \\
&= \sum_{j=0}^{N} p_j \exp\left(\frac{\Phi(x_j)}{RT_e}\right) \exp\left(-\frac{\Phi(x_j)}{RT_e}\right) \frac{\partial}{\partial x} \varphi_j(x_k) \\
&= \sum_{j=0}^{N} p_j \frac{\partial}{\partial x} \varphi_j(x_k) = \frac{\partial}{\partial x} f_h(x_k)
\end{aligned}
$$

Well-balanced property

Since

$$\partial_x f_h(x_k) = s_h(x_k) \quad \text{at all the GLL nodes } x_k$$

we can conclude that

$$(\partial_x f_h, \varphi_j)_h = (s_h, \varphi_j)_h \,, \qquad 0 \le j \le N$$

$\Longrightarrow$ scheme is well-balanced for the momentum equation

The proof for polytropic case is similar. □

2-D Euler equations with gravity

$$\frac{\partial \boldsymbol{q}}{\partial t} + \frac{\partial \boldsymbol{f}}{\partial x} + \frac{\partial \boldsymbol{g}}{\partial y} = \boldsymbol{s}$$

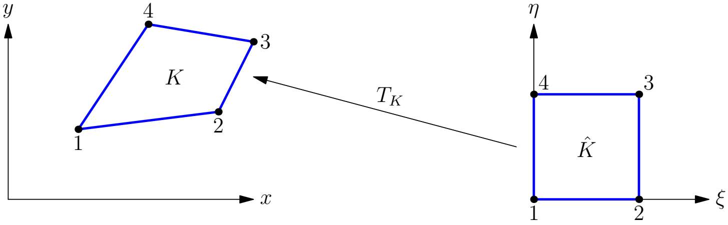
$\boldsymbol{q}$ = vector of conserved variables, $(\boldsymbol{f}, \boldsymbol{g})$ = flux vector and $\boldsymbol{s}$ = source term, given by

$$\boldsymbol{q} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ E \end{bmatrix}, \qquad \boldsymbol{f} = \begin{bmatrix} \rho u \\ p + \rho u^2 \\ \rho u v \\ (E+p)u \end{bmatrix}, \qquad \boldsymbol{g} = \begin{bmatrix} \rho v \\ \rho u v \\ p + \rho v^2 \\ (E+p)v \end{bmatrix}$$

$$\boldsymbol{s} = \begin{bmatrix} 0 \\ -\rho \frac{\partial \Phi}{\partial x} \\ -\rho \frac{\partial \Phi}{\partial y} \\ -\left(u \frac{\partial \Phi}{\partial x} + v \frac{\partial \Phi}{\partial y} \right) \end{bmatrix}$$

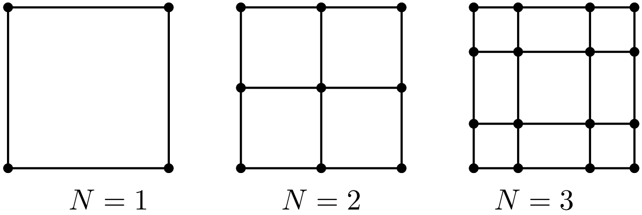
Mesh and basis functions

A quadrilateral cell K and reference cell $\hat{K} = [0,1] \times [0,1]$



1-D GLL points: $\xi_r \in [0,1], \qquad 0 \le r \le N$

Tensor product of GLL points



Numerical Results

1-D hydrostatic test: Well-balanced property

Potential

$$\Phi = x, \qquad \Phi = \sin(2\pi x)$$

Initial state

$$u = 0, \qquad \rho = p = \exp(-\Phi(x))$$

Mesh	ρu	ρ	E
25x25	1.03822e-13	2.72604e-14	9.53913e-14
50x50	1.04783e-13	2.67559e-14	9.36725e-14
100x100	1.05019e-13	2.66323e-14	9.34503e-14
200x200	1.05088e-13	2.66601e-14	9.33861e-14

Table: Well-balanced test on Cartesian mesh using Q1 and potential $\Phi = y$

1-D hydrostatic test: Well-balanced property

Mesh	ρu	ρ	E
25x25	1.04518e-13	2.7548e-14	9.64205e-14
50x50	1.04983e-13	2.69317e-14	9.43158e-14
100x100	1.05069e-13	2.69998e-14	9.39126e-14
200x200	1.05089e-13	2.68828e-14	9.462e-14

Table: Well-balanced test on Cartesian mesh using Q2 and potential $\Phi = x$

Mesh	ρu	ρ	E
25x25	9.23424e-13	2.31405e-13	8.16645e-13
50x50	9.36459e-13	2.28315e-13	8.04602e-13
100x100	9.39613e-13	2.28001e-13	8.03005e-13
200x200	9.40422e-13	2.2792e-13	8.02653e-13

Table: Well-balanced test on Cartesian mesh using Q1 and $\Phi = \sin(2\pi x)$

1-D hydrostatic test: Well-balanced property

Mesh	ρu	ρ	E
25x25	9.34536e-13	2.35173e-13	8.30316e-13
50x50	9.39556e-13	2.29908e-13	8.10055e-13
100x100	9.40442e-13	2.28538e-13	8.04638e-13
200x200	9.40668e-13	2.28051e-13	8.0357e-13

Table: Well-balanced test on Cartesian mesh using Q2 and $\Phi = \sin(2\pi x)$

1-D hydrostatic test: Evolution of perturbations

Potential

$$\Phi(x) = x$$

Initial condition

$$u = 0, \qquad \rho = \exp(-x), \qquad p = \exp(-x) + \eta \exp(-100(x - 1/2)^2)$$

1-D hydrostatic test: Evolution of perturbations

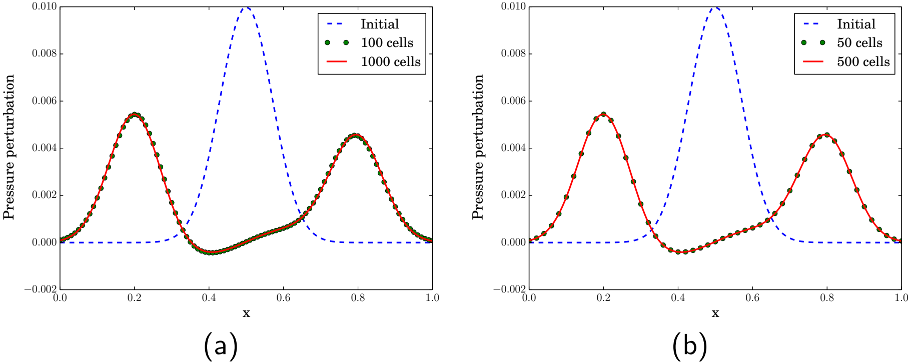


Figure: Evolution of perturbations for $\eta = 10^{-2}$: (a) Q1 (b) Q2

1-D hydrostatic test: Evolution of perturbations

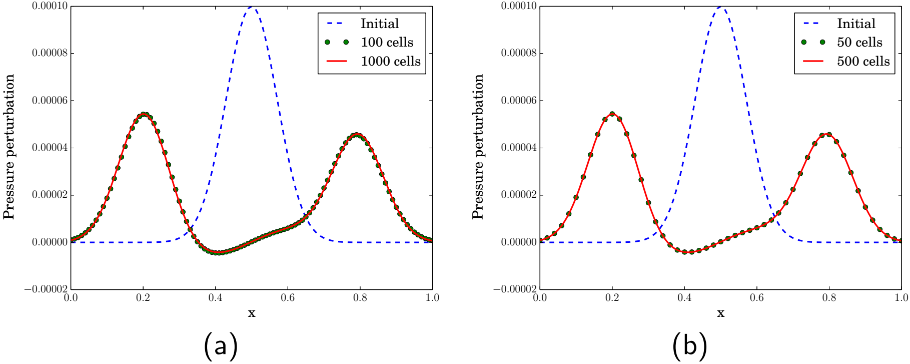
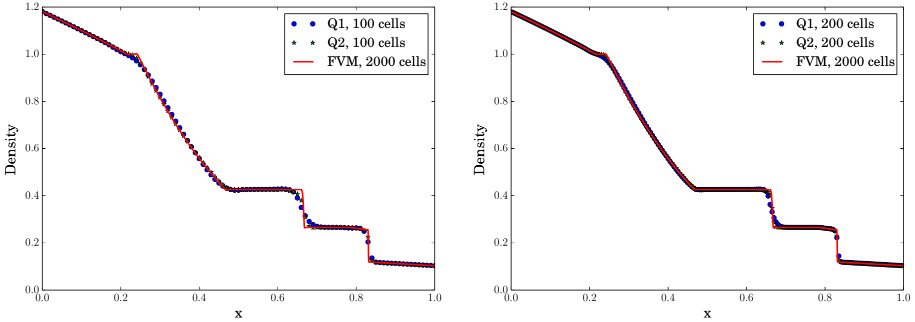


Figure: Evolution of perturbations for $\eta = 10^{-4}$: (a) Q1 (b) Q2

Shock tube problem

Potential $\Phi(x) = x$ and initial condition

$$(\rho, u, p) = \begin{cases} (1, 0, 1) & x < \frac{1}{2} \\ (0.125, 0, 0.1) & x > \frac{1}{2} \end{cases}$$



2-D hydrostatic test: Well-balanced test

Potential

$$\Phi = x + y$$

Hydrostatic solution is given by

$$\rho = \rho_0 \exp\left(-\frac{\rho_0 g}{p_0}(x+y)\right), \quad p = p_0 \exp\left(-\frac{\rho_0 g}{p_0}(x+y)\right), \quad u = v = 0$$

	ρu	ρv	ρ	E
$Q1,\ 25 \times 25$	9.85926e-14	9.85855e-14	5.32357e-14	1.55361e-13
$Q1,\ 50 \times 50$	9.94493e-14	9.94451e-14	5.37084e-14	1.56669e-13
$Q1,\ 100 \times 100$	9.96481e-14	9.96474e-14	5.38404e-14	1.57062e-13
$Q2,\ 25 \times 25$	9.9256e-14	9.92682e-14	5.39863e-14	1.57435e-13
$Q2,\ 50 \times 50$	9.961e-14	9.96538e-14	5.41091e-14	1.57521e-13
$Q2,\ 100 \times 100$	9.95889e-14	9.97907e-14	5.43145e-14	1.57728e-13

2-D hydrostatic test: Evolution of perturbation

$$p = p_0 \exp\left(-\frac{\rho_0 g}{p_0}(x+y)\right) + \eta \exp\left(-100\frac{\rho_0 g}{p_0}\left[(x-0.3)^2 + (y-0.3)^2\right]\right)$$

2-D hydrostatic test: Evolution of perturbation

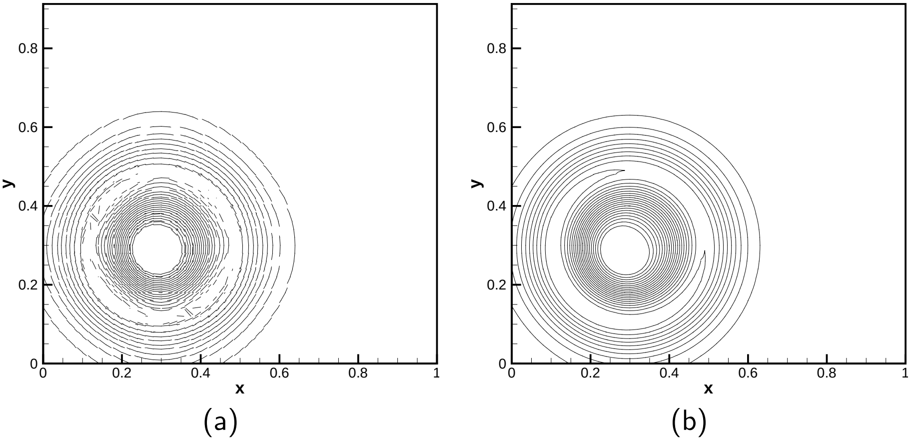


Figure: Pressure perturbation on 50×50 mesh at time $t = 0.15$ (a) Q_1 (b) Q_2. Showing 20 contours lines between -0.0002 to $+0.0002$

2-D hydrostatic test: Evolution of perturbation

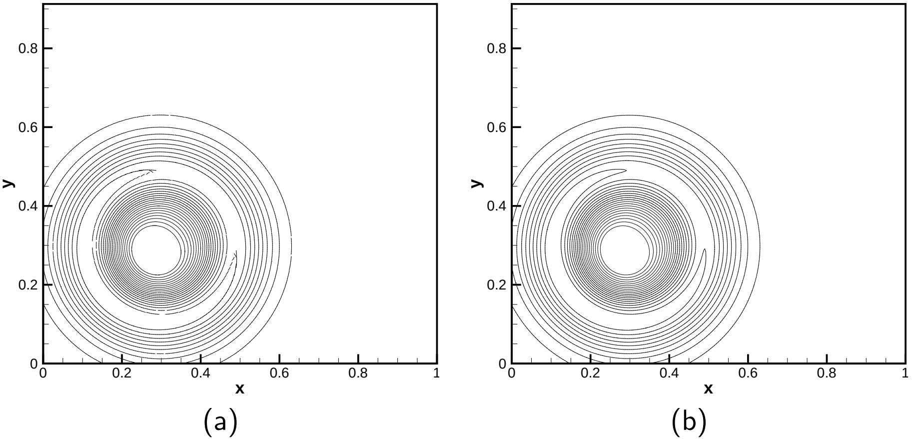
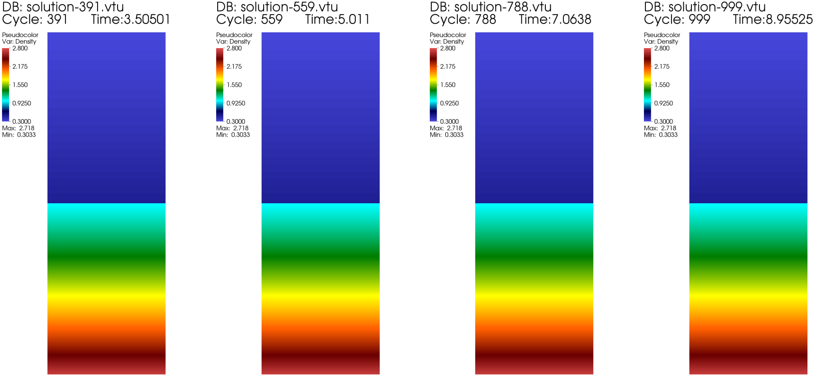


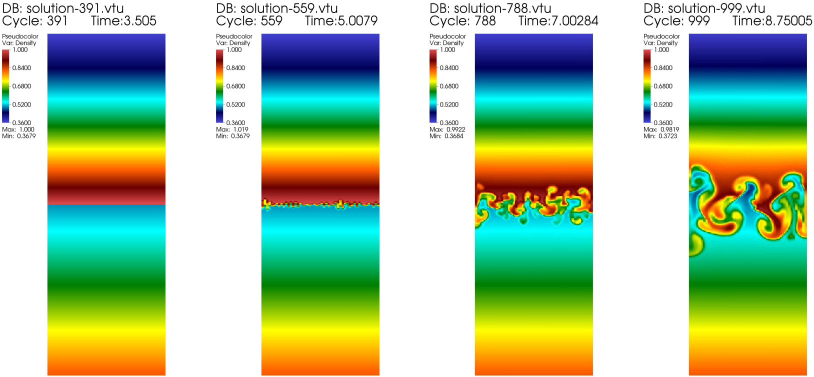
Figure: Pressure perturbation on 200×200 mesh at time $t = 0.15$ (a) Q_1 (b) Q_2. Showing 20 contours lines between -0.0002 to $+0.0002$

2-D hydrostatic test: Discontinuous density



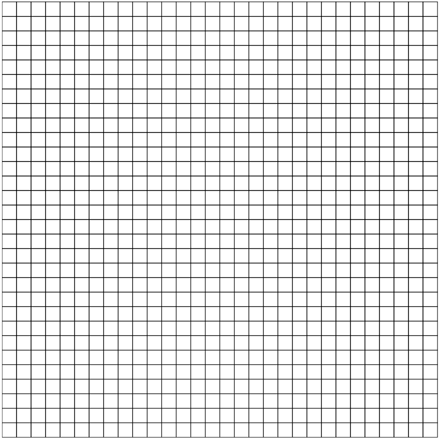
Ligther fluid on top

2-D hydrostatic test: Discontinuous density

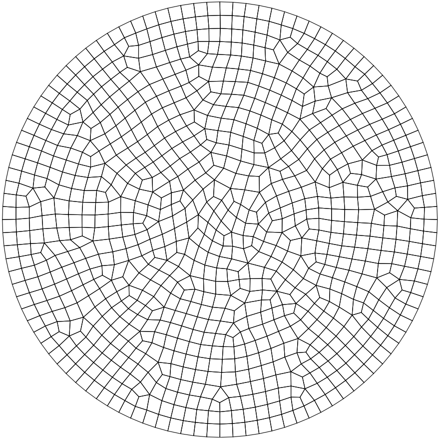


Heavier fluid on top

Radial Rayleigh-Taylor problem



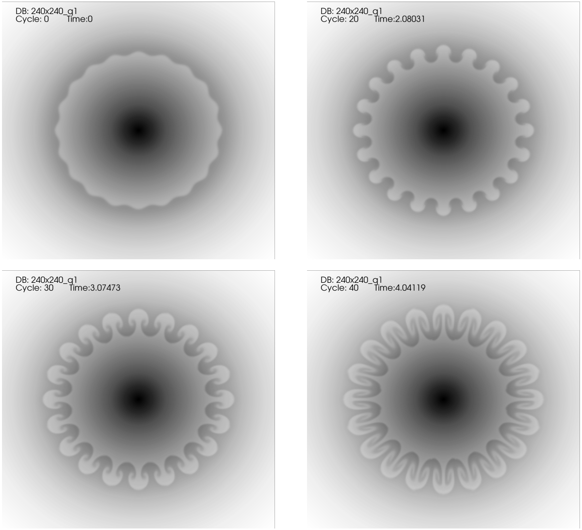
30×30 cells



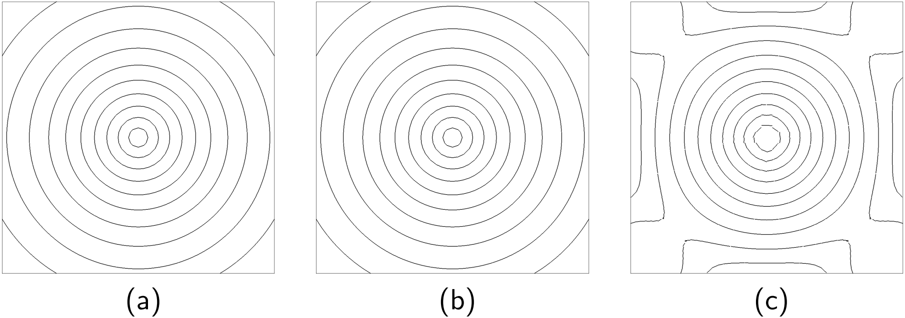
956 cells

Radial Rayleigh-Taylor problem: Perturbations

Cartesian mesh of 240×240 and Q_1 basis



Well-balanced versus non well-balanced



Well balanced test for radial Rayleigh-Taylor problem on 50×50 mesh. (a) Initial density, (b) well-balanced scheme, density at $t = 1.5$, (c) non well-balanced scheme, density at $t = 1.5$

Kinetic energy and entropy consitency

Kinetic energy

Kinetic energy per unit volume

$$K = \frac{1}{2}\rho u^2$$

satisfies the following equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega K \mathrm{d}x = \int_\Omega p\frac{\partial u}{\partial x}\mathrm{d}x - \frac{4}{3}\int_\Omega \mu\left(\frac{\partial u}{\partial x}\right)^2 \mathrm{d}x \le \int_\Omega p\frac{\partial u}{\partial x}\mathrm{d}x$$

Work done by pressure forces, absent in incompressible flows

Irreversible destruction due to molecular diffusion

Note: Convection contributes to only flux of KE across $\partial\Omega$

Entropy condition

Entropy-Entropy flux pair: $U(\mathbf{u}), F(\mathbf{u})$

$$U(\mathbf{u}) \text{ is strictly convex} \qquad \text{and} \qquad U'(\mathbf{u})\mathbf{f}'(\mathbf{u}) = F'(\mathbf{u})$$

Then, for hyperbolic problem (Euler equation)

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}}{\partial x} = 0 \quad \Longrightarrow \quad U'(\mathbf{u})\frac{\partial \mathbf{u}}{\partial t} + U'(\mathbf{u})\mathbf{f}'(\mathbf{u})\frac{\partial \mathbf{u}}{\partial x} = 0$$

$$\Downarrow$$

$$\frac{\partial U(\mathbf{u})}{\partial t} + \frac{\partial F(\mathbf{u})}{\partial x} = 0$$

For discontinuous solutions, only inequality

$$\frac{\partial U(\mathbf{u})}{\partial t} + \frac{\partial F(\mathbf{u})}{\partial x} \leq 0$$

$\int_\Omega U(\mathbf{u})\mathrm{d}x$ for an isolated system decreases with time

Second law of thermodynamics

Euler equations

- Jameson: KE consistent
- Ismail & Roe: Entropy consistent
- KEPEC: Both KE and entropy consistent
  - Ch., CICP, vol. 14, no. 5, 2013
  - Ray et al., CICP, vol. 19, no. 5, 2016

FVM for NS equation

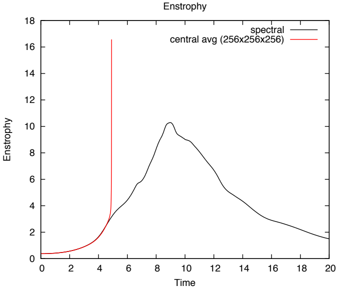
The semi-discrete finite volume method for NS equations using the centered KEP and entropy conservative flux is stable for the kinetic energy and entropy, i.e.,

$$\begin{aligned}\sum_j \Delta x \frac{\mathrm{d}K_j}{\mathrm{d}t} &= \sum_j \left[\frac{\Delta u_{j+\frac{1}{2}}}{\Delta x} \tilde{p}_{j+\frac{1}{2}} - \frac{4}{3}\mu \left(\frac{\Delta u_{j+\frac{1}{2}}}{\Delta x} \right)^2 \right] \Delta x \\ &\leq \sum_j \left[\frac{\Delta u_{j+\frac{1}{2}}}{\Delta x} \tilde{p}_{j+\frac{1}{2}} \right] \Delta x\end{aligned}$$

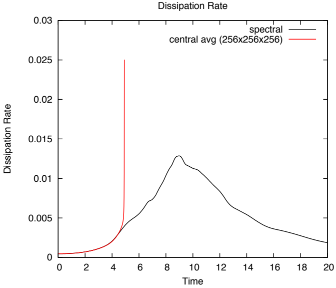
and

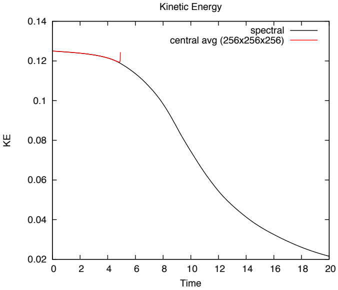
$$\sum_j \Delta x \frac{\mathrm{d}U_j}{\mathrm{d}t} = -\sum_j \left[\frac{8\mu\overline{\beta}_{j+\frac{1}{2}}}{3} \left(\frac{\Delta u_{j+\frac{1}{2}}}{\Delta x} \right)^2 + \frac{\kappa}{RT_jT_{j+1}} \left(\frac{\Delta T_{j+\frac{1}{2}}}{\Delta x} \right)^2 \right] \Delta x \leq 0$$

DNS of 3-D Taylor-Green vortex: central scheme

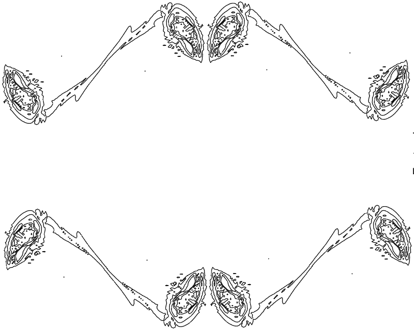


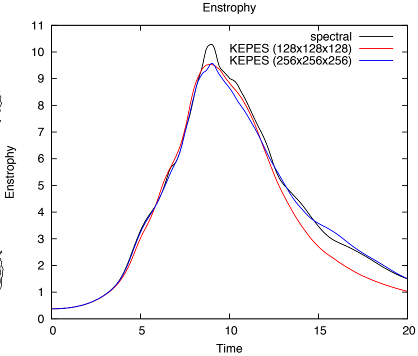
$$\mathbf{f}_{j+\frac{1}{2}} = \frac{1}{2}(\mathbf{f}_j + \mathbf{f}_{j+1})$$



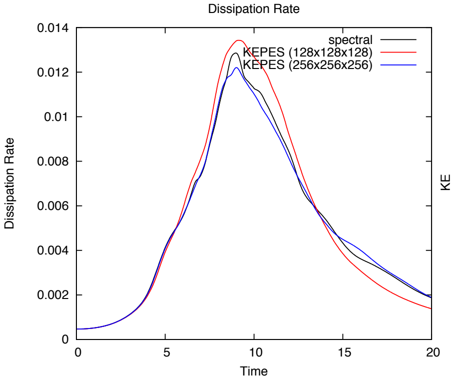


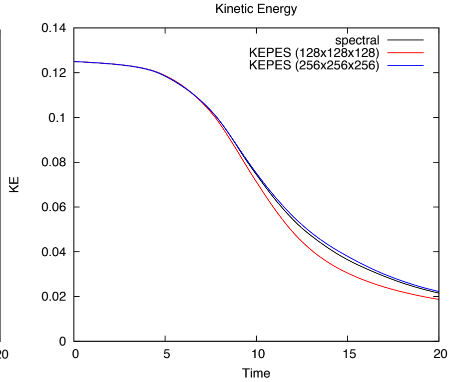
DNS of 3-D Taylor-Green vortex



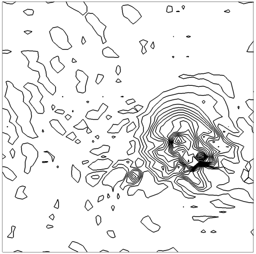


DNS of 3-D Taylor-Green vortex

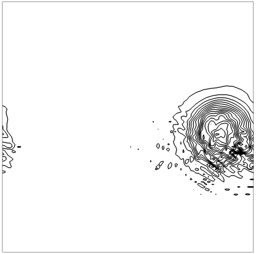




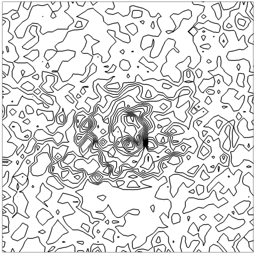
Isentropic vortex advection: Density contours



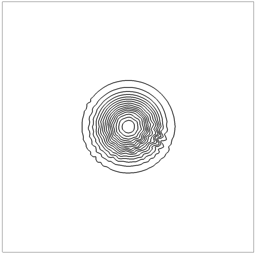
(KEP, 50×50, T=57)



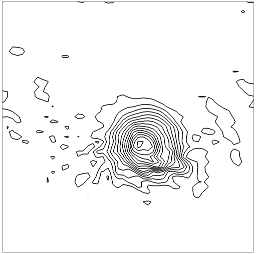
(KEP, 100×100, T=87)



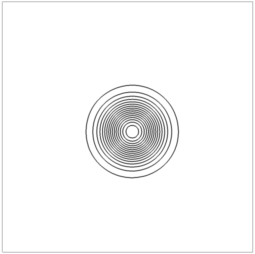
(KEP4, 50×50, T=100)



(KEP4, 100×100, T=100)



(ROE-EC, 100×100, T=100)



(Others configs, T=100)

Ideal compressible MHD

$$\boldsymbol{w} = \left[\rho,\ \rho u_1,\ \rho u_2,\ \rho u_3,\ E,\ B_1,\ B_2,\ B_3\right]^\top$$

$$\boldsymbol{f}_1 = \begin{bmatrix} \rho u_1 \\ p + \rho u_1^2 + \frac{1}{2}|\boldsymbol{B}|^2 - B_1^2 \\ \rho u_1 u_2 - B_1 B_2 \\ \rho u_1 u_3 - B_1 B_3 \\ (E + p + \frac{1}{2}|\boldsymbol{B}|^2) u_1 - (\boldsymbol{u}\cdot\boldsymbol{B}) B_1 \\ 0 \\ u_1 B_2 - u_2 B_1 \\ u_1 B_3 - u_3 B_1 \end{bmatrix}, \quad \boldsymbol{f}_2 = \begin{bmatrix} \rho u_2 \\ \rho u_1 u_2 - B_1 B_2 \\ p + \rho u_2^2 + \frac{1}{2}|\boldsymbol{B}|^2 - B_2^2 \\ \rho u_2 u_3 - B_2 B_3 \\ (E + p + \frac{1}{2}|\boldsymbol{B}|^2) u_2 - (\boldsymbol{u}\cdot\boldsymbol{B}) B_2 \\ u_2 B_1 - u_1 B_2 \\ 0 \\ u_2 B_3 - u_3 B_2 \end{bmatrix}$$

Magnetic field must be divergence free: $\nabla \cdot \boldsymbol{B} = 0$, an intrinsic property

$$\frac{\partial}{\partial t} \nabla \cdot \boldsymbol{B} = 0$$

Entropy pair

$$U = -\frac{\rho s}{\gamma - 1}, \qquad F_\alpha = -\frac{\rho s u_\alpha}{\gamma - 1}, \qquad s = \ln(p\rho^{-\gamma}) \tag{3}$$

Ch. & Klingenberg, SINUM, vol. 54, issue 2, 2016
Yee & Sjogreen, ICOSAHOM, Rio, June, 2016

Thank You