A Conservative Approach to the Multiphase Euler Equations without Spurious Pressure Oscillations

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1 Abstract

In [4], the pressure evolution equation was used to calculate smooth pressure profiles for otherwise oscillatory contact discontinuities. The nonconservative approach in [4] was modified to fully conserve mass, momentum, and energy in [1]. Both [4] and [1] construct schemes valid for a gamma law gas. In [2], we extended the work in [4] to cover general equations of state. In this paper, we extend the ideas in [1] to cover general equations of state as well. Thus, we propose a method which is conservative (conserving the total mass, momentum, and energy exactly), works for general equations of state, and avoids spurious oscillations at material interfaces.

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2 Introduction

Standard conservative schemes will admit non-physical oscillations near material interfaces, which can be avoided by the application of a nonconservative correction to the internal energy [4, 3, 2]. These modifications give rise to conservation errors in the total energy of the system, and thus yield a locally nonconservative formulation. In general, nonconservative formulations give the wrong shock speeds, although the errors in shock speeds can be reduced significantly with the addition of a special viscosity term [6].

In standard conservative schemes, the pressure is calculated from the equation of state, and we refer to this pressure as p_{eos}. While this pressure does well away from material interfaces, it may admit erroneous pressure profiles near material interfaces. In [4], the pressure was calculated from the pressure evolution equation, and we refer to this pressure as p_{eep}. This pressure is essentially non-oscillatory across material interfaces, but it does not satisfy the equation of state and hence is responsible for the loss of conservation.

In contrast to the above schemes, we propose a conservative method (conserving the total mass, momentum, and energy exactly) which is able to avoid the spurious oscillations near material interfaces common to other conservative shock capturing schemes. This new method converges to the correct weak solution under grid refinement.

We note that a scheme with similar properties was proposed in [1], although that scheme was only valid for a gamma law gas. The author in [1] observed that a general conservative method will produce a perfect contact discontinuity (constant pressure and velocity) as long as the evolution equation for the interface was advection of $\frac{1}{\gamma-1}$. In fact, this is equivalent to advecting $\frac{\rho e}{p}$ and bears some resemblance to the pressure evolution equation. While this method works well for a gamma law gas, problems can occur with more general equations of state especially when one considers that $\frac{\rho e}{p}$ is not always constant across a shock as it is in the gamma law gas. Our scheme extends the ideas in [1] to general equations of state.

Our new technique has two key ideas:

(1) The pressure is chosen to be a convex combination of p_{eos} and p_{eep}. By choosing proper weights, the combined pressure is essentially p_{eep} at the interfaces and p_{eos} away from the interfaces. One of the advantages of the convex combination is that there is no need to track the material interfaces. This is important in two or three dimensions, because it is quite difficult to track the interfaces with all possible topological changes.

(2) We use a general equation of state that reduces to the single equation of state in each different fluid region, but still applies everywhere, even at interfaces where the single equations of state breakdown. It is capable of representing any combination of different fluids such as γ-law gas, water and JWL.

We point out that this technique works in multiple dimensions and is scheme-independent, which means it should work for typical users' existing code with only minor modifications.

3 Equations

The 3D Euler Equations in conservation form are

$$\begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ E \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ (E+p)u \end{pmatrix}_x + \begin{pmatrix} \rho v \\ \rho vu \\ \rho v^2 + p \\ \rho vw \\ (E+p)v \end{pmatrix}_y + \begin{pmatrix} \rho w \\ \rho wu \\ \rho wv \\ \rho w^2 + p \\ (E+p)w \end{pmatrix}_z = 0 \tag{1}$$

where ρ is the density, $\mathbf{u} = (u, v, w)$ is the velocity, E is the total energy per unit volume, p is the pressure, $\mathbf{x} = (x, y, z)$ is the spatial location and t is the time. We define a filter function, ψ, which is initially 0 in one fluid and 1 in the other. Then ψ satisfies

$$\psi_t + \mathbf{u} \cdot \triangledown \psi = 0. \tag{2}$$

Let $p = p_1(\rho, e)$ be the equation of state for the first fluid and $p = p_2(\rho, e)$ be the equation of state for the other. The general equation of state is

$$p = \psi * p_1(\rho, e) + (1 - \psi) * p_2(\rho, e). \tag{3}$$

This system (1-3) completes the mathematical model of two phase flow.

4 Numerical Method

Given the values of ρ^n, $(\rho u)^n$, $(\rho v)^n$, $(\rho w)^n$, E^n, and ψ^n at time t^n, the pressure p^n is calculated from the general equation of state (3) i.e.

$$p^n = \psi^n * p_1(\rho^n, e^n) + (1 - \psi^n) * p_2(\rho^n, e^n) \tag{4}$$

where we assume p^n has no oscillations at material interfaces, e.g. initial data. One can solve the Euler equations (1) with any reasonable conservative scheme (such as Convex ENO [7]) to update the variables in time as ρ^{n+1}, $(\rho u)^{n+1}$, $(\rho v)^{n+1}$, $(\rho w)^{n+1}$, and E^{n+1}. We also solve the advection equation (2) for the filter function ψ_{eos}^{n+1} with any reasonable upwind scheme [2]. If we use these values to calculate the pressure from the equation of state,

$$p_{eos}^{n+1} = \psi_{eos}^{n+1} * p_1(\rho^{n+1}, e^{n+1}) + (1 - \psi_{eos}^{n+1}) * p_2(\rho^{n+1}, e^{n+1}) \tag{5}$$

we get a standard conservative scheme where oscillations in pressure may be generated near material interfaces and lead to the pollution of the rest of the solution [4, 3]. Since it is unwise to modify conservative quantities, we instead modify the filter function ψ^{n+1}.

In [4], the pressure evolution equation for a γ-law gas

$$p_t + \mathbf{u} \cdot \triangledown p + \gamma p \triangledown \cdot \mathbf{u} = 0,$$

was used to calculate the pressure obtaining smooth pressure profiles where the standard conservative schemes oscillated wildly. The pressure evolution equation can be extended [2] to cover any fluid with a general equation of state

$$p_t + \mathbf{u} \cdot \triangledown p + \rho c^2 \triangledown \cdot \mathbf{u} = 0, \tag{6}$$

and this equation will give similar results for a gamma law gas, while extending to more general fluids as well.

Remark: The $\rho c^2 \bigtriangledown \cdot \mathbf{u}$ term in the pressure evolution equation is not always well-behaved at contact discontinuities where it is needed. In general ρ, c^2, and $\bigtriangledown \cdot \mathbf{u}$ could all be discontinuous functions. In the simple case of a gamma law gas the discontinuities in ρ and c^2 blend nicely to give γp with p continuous and γ a smeared out Heaviside function. Thus there are only two discontinuous functions for a gamma law gas, and for most contact discontinuities the velocity is constant implying that $\bigtriangledown \cdot \mathbf{u}$ is not only continuous, but identically zero. The reader is warned that some of the harder problems will require special regularization of $\rho c^2 \bigtriangledown \cdot \mathbf{u}$ in order to obtain good numerical results.

Using a reasonable upwind scheme [2] to solve equation (6) we obtain the pressure evolution equation pressure, p_{eep}^{n+1}, which is smooth across material interfaces. Thus there are two candidates, p_{eos}^{n+1} and p_{eep}^{n+1}, for p^{n+1}. The new idea here is to use a convex combination of the two candidate pressures.

$$p_{new}^{n+1} = \alpha * p_{eos}^{n+1} + \beta * p_{eep}^{n+1} \qquad \alpha, \beta \geq 0 \quad \text{and} \quad \alpha + \beta = 1. \tag{7}$$

The goal is to weight the combined pressure p_{new}^{n+1} toward p_{eep}^{n+1} at material interfaces and toward p_{eos}^{n+1} away from them. Once this is done, p_{new}^{n+1} will not satisfy the general equation of state (3), that is

$$p_{new}^{n+1} \neq \psi_{eos}^{n+1} * p_1(\rho^{n+1}, e^{n+1}) + (1 - \psi_{eos}^{n+1}) * p_2(\rho^{n+1}, e^{n+1}),$$

and this situation can be remedied by modifying ψ_{eos}^{n+1}. First calculate

$$\psi_{new}^{n+1} = \frac{p_{new}^{n+1} - p_2(\rho^{n+1}, e^{n+1})}{p_1(\rho^{n+1}, e^{n+1}) - p_2(\rho^{n+1}, e^{n+1})},$$

and then invoke a straightforward limiter

$$\psi^{n+1} = \begin{cases} \psi_M & \psi_{new}^{n+1} > \psi_M \\ \psi_m & \psi_{new}^{n+1} < \psi_m \\ \psi_{new}^{n+1} & \text{otherwise,} \end{cases} \tag{8}$$

where ψ_M (ψ_m) is the maximum (minimum) of filter function at its immediate neighbors at time t^n. We then recalculate the pressure p^{n+1} as

$$p^{n+1} = \psi^{n+1} * p_1(\rho^{n+1}, e^{n+1}) + (1 - \psi^{n+1}) * p_2(\rho^{n+1}, e^{n+1}). \tag{9}$$

This pressure, p^{n+1}, is essentially non-oscillatory across material interfaces, since $p^{n+1} \simeq p_{new}^{n+1} \simeq p_{eep}^{n+1}$ there.

While this pressure construction procedure works well, it allows the interface to dissipate. Since convergence to the correct weak solution requires a sharp interface, we need to further sharpen the interface to obtain good solutions on a reasonably coarse mesh. We sharpen the interface as follows:

(1) At each grid point, calculate the pressure p_0 by enforcing $\Delta p = 0$ i.e. in 1-dimension, $p_0 = \frac{p_{j+1}^{n+1} + p_{j-1}^{n+1}}{2}$;

(2) Calculate the corresponding filter function ψ_0:

$$\psi_0 = \frac{p_0 - p_2(\rho^{n+1}, e^{n+1})}{p_1(\rho^{n+1}, e^{n+1}) - p_2(\rho^{n+1}, e^{n+1})};$$

(3) Sharpen the interface

$$\psi^{n+1} = \begin{cases} \max(\psi^{n+1}, \min(\psi_0, 1)) & \text{if } \psi^{n+1} \geq \frac{1}{2} \\ \min(\psi^{n+1}, \max(\psi_0, 0)) & \text{otherwise;} \end{cases} \tag{10}$$

(4) Recalculate the pressure

$$p^{n+1} = \psi^{n+1} * p_1(\rho^{n+1}, e^{n+1}) + (1 - \psi^{n+1}) * p_2(\rho^{n+1}, e^{n+1}). \tag{11}$$

Remark: The filter function in (10) is sharper than the one in (8) and the pressure in (11) is smoother than the one in (9).

This completes the calculation cycle from $\rho^n, (\rho u)^n, (\rho v)^n, (\rho w)^n, E^n$, and ψ^n to ρ^{n+1}, $(\rho u)^{n+1}$, $(\rho v)^{n+1}$, $(\rho w)^{n+1}$, E^{n+1} and ψ^{n+1}.

4.1 Choosing the Weights

In this section, we define the weights, α and β. The goal is to weight p^{n+1}_{new} toward p^{n+1}_{eep} at a material interface and toward p^{n+1}_{eep} elsewhere. We make two observations:

(1) The filter function, ψ, is *rapidly varying* near material interfaces and *nearly constant* away from them.

(2) The pressure, p, is *rapidly varying* near at shock and *nearly constant* at a material interface. Define δ as an undivided difference operator that gives a discrete meaning to the phrases *rapidly varying* and *nearly constant*. For example, in one dimension, we define

$$\begin{aligned}
\delta\psi_j &= \mid \psi^n_{j+1} - \psi^n_j \mid + \mid \psi^n_{j-1} - \psi^n_j \mid, \\
\delta p_j &= 128 \cdot [0.5 \mid p^n_{j+1} - p^n_j \mid / \max(p^n_{j+1}, p^n_j) + 0.5 \mid p^n_{j-1} - p^n_j \mid / \max(p^n_{j-1}, p^n_j)].
\end{aligned}$$

Then the definition of α and β is as follows,

IF ($\delta\psi == 0$) THEN

$\alpha = 1$, $\beta = 0$;

ELSEIF ($\delta p == 0$) THEN

$\alpha = 0$, $\beta = 1$;

ELSE

$\alpha = \frac{\delta p^d}{\delta p^d + \delta\psi^d}$, $\beta = 1 - \alpha$

ENDIF

where we set $d = 8$ for our numerical experiments.

Remark: (1) in constant regions of the flow $\delta\psi = 0$ and $\delta p = 0$, and we obtain $\alpha = 1$, $\beta = 0$, and $p^{n+1}_{new} = p^{n+1}_{eos}$ which is the standard conservative solution. (2) at an isolated interfaces $\delta\psi \not\simeq 0$ and $\delta p = 0$, and we obtain $\alpha = 0$, $\beta = 1$, and $p^{n+1}_{new} = p^{n+1}_{eep}$ which avoids oscillations and doesn't affect shocks since none are in the vicinity. (3) at an isolated shock $\delta\psi = 0$ and $\delta p \neq 0$, and we obtain $\alpha = 1$, $\beta = 0$, and $p^{n+1}_{new} = p^{n+1}_{eos}$ which is the standard conservative solution maintaining a good shock speed. (4) when a shock hits an interface $\delta\psi \not\simeq 0$ and $\delta p \not\simeq 0$, and we obtain $\alpha \simeq 1$ and

$\beta \simeq 0$ and hence $p_{new}^{n+1} \simeq p_{eos}^{n+1}$ which is essentially the standard conservative solution maintaining a good shock speed.

5 Numerical Experiments

We have used our new scheme to reproduce the numerical experiments from [4, 5, 10] with our conservative scheme. In the following we show our results for γ-law gas, water and JWL.

For water, we use

$$p(\rho) = \begin{cases} B\left((\rho/\rho_0)^\gamma - 1\right) + A & \text{if} \quad \rho > \rho_c \\ p_c & \text{otherwise,} \end{cases}$$

where $A = 10^6$, $b = 3.31 * 10^9$, $\gamma = 7.15$, $\rho_0 = 1$, $\rho_c = 0.99995775$ and $p_c = 220.272586$.

For a gamma law gas, we use

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

where $e = (E/\rho - 0.5(u^2 + v^2 + w^2))$ is the internal energy per unit mass.

For a JWL gas, we use

$$p(\rho, e) = A\left(1 - \frac{\omega\rho}{R_1\rho_o}\right) exp(-R_1\rho_o/\rho) + B\left(1 - \frac{\omega\rho}{R_2\rho_o}\right) exp(-R_2\rho_o/\rho) + \omega\rho e,$$

where $A = 5.484 * 10^{12}$, $B = 0.09375 * 10^{12}$, $R_1 = 4.94$, $R_2 = 1.21$, $\omega = 0.28$, and $\rho_o = 1.63$.

Example 1: In this example, we redo the numerical experiments from [4]. Refer to [4] to see the large spurious oscillations introduced when solving the following problems with a standard conservative scheme.

A tube with length one is filled with two fluids. They are separated by an interface which is located at the center ($x = 0.5$) of the tube. Except for the first case, we start with a shock at $x = 0.25$ which moves to the right and will intersect the interface at a later time. See Figure 1.

Five sets of initial data are used for $W = (\rho, u, p, \gamma)$:

data 1:	$W_1 = (1.0, 0.0, 1.0, 1.4)$	Air
	$W_2 = (1.0, 0.0, 1.0, 1.4)$	Air
	$W_3 = (0.125, 0.0, 0.1, 1.2)$	(Unknown)
data 2:	$W_1 = (1.3333, 0.3535, 1.5, 1.4)$	Air
	$W_2 = (1.0, 0.0, 1.0, 1.4)$	Air
	$W_3 = (0.1379, 0.0, 1.0, 1.67)$	Helium
data 3:	$W_1 = (1.3333, 0.3535, 1.5, 1.4)$	Air
	$W_2 = (1.0, 0.0, 1.0, 1.4)$	Air
	$W_3 = (3.1538, 0.0, 1.0, 1.249)$	R22
data 4:	$W_1 = (4.3333, 3.2817, 15.0, 1.4)$	Air
	$W_2 = (1.0, 0.0, 1.0, 1.4)$	Air
	$W_3 = (0.1379, 0.0, 1.0, 1.67)$	Helium
data 5:	$W_1 = (4.3333, 3.2817, 15.0, 1.4)$	Air
	$W_2 = (1.0, 0.0, 1.0, 1.4)$	Air
	$W_3 = (3.1538, 0.0, 1.0, 1.249)$	R22

We used the 3rd order accurate central Convex ENO scheme [7]. The results shown in Figure 2 to Figure 6 below avoid the oscillations at the interface while still conserving mass, momentum, and energy exactly.

Example 2: A tube, one unit long, contains a JWL gas and water. The left hand side of the tube, $x < 0.5$, is a JWL gas with $\rho = 1.63$, $e = 42.814 * 10^{10}$, $p = 7.81 * 10^{10}$, and $u = 0$. The right hand side of the tube, $x \geq 0.5$, is water with $\rho = 1$, $e = N/A$ (we chose $e = 10^7$ for numerical implementation), $p = 1 * 10^6$, and $u = 0$. The computation is terminated before the boundaries can be influence the solution. We used 3rd order field-by-field Convex ENO [7] for Euler equations, a 2nd order TVD upwind scheme for the filter function, and 2nd order central Convex ENO [7] for the pressure evolution equation. The results are shown in Figure 7.

Example 3: A tube, one unit long and closed at both ends, is filled with a gamma law gas with $\gamma = 1.25$ and water. The initial conditions are

$$(\rho, e, p, u) = \begin{cases} (0.00826605505, 48390677000, 10^8, 294997.131) & \gamma - \text{law gas}, \quad \text{if } \ x \leq 0.096 \\ (0.001, 4 * 10^9, 10^6, 0) & \gamma - \text{law gas}, \quad \text{if } \ 0.096 < x < 0.5 \\ (1, N/A, 10^6, 0) & \text{water}, \quad \text{if } \ 0.5 \leq x < 0.96 \\ (1.0041303, N/A, 10^8, -638.13588) & \text{water}, \quad \text{otherwise} \end{cases}$$

Reflection boundary conditions are applied at both boundaries. We used 3rd order central Convex ENO [7] for the Euler equations, a 2nd order TVD upwind scheme for the filter function, and 2nd order central Convex ENO [7] for the pressure evolution equation. The results are shown in Figure 8.

Example 4: A JWL gas fills a small bubble with a radius of $r = 16$ that is surrounded by water. The initial conditions are:

$$(\rho, e, p, u) = \begin{cases} (1.63, 4.2814 * 10^{10}, 7.8039 * 10^{10}, 0) & \text{JWL, for } \ r \leq 16 \\ (1, N/A, 10^6, 0) & \text{water, for } \ 16 \leq r \leq 1000. \end{cases}$$

The problem is cast in *spherical* coordinates. The computation is ended before the outer boundary can influence the solution. We used 3rd order central Convex ENO [7] for the Euler equations, a 2nd order TVD upwind scheme for the filter function, and 2nd order central Convex ENO [7] for the pressure evolution equation. The results are shown in Figure 9.

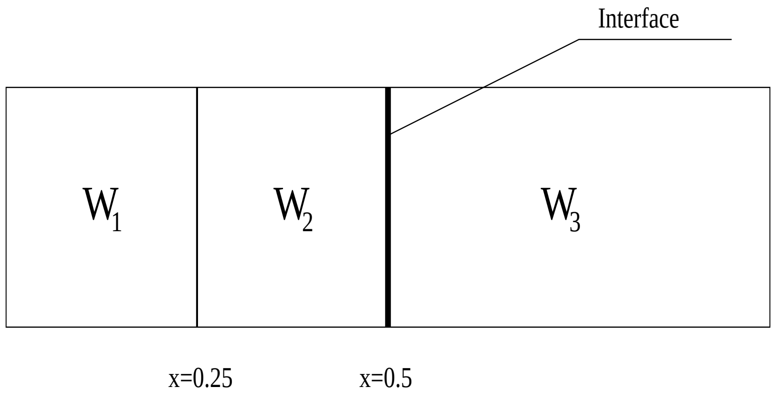


Figure 1: Tube

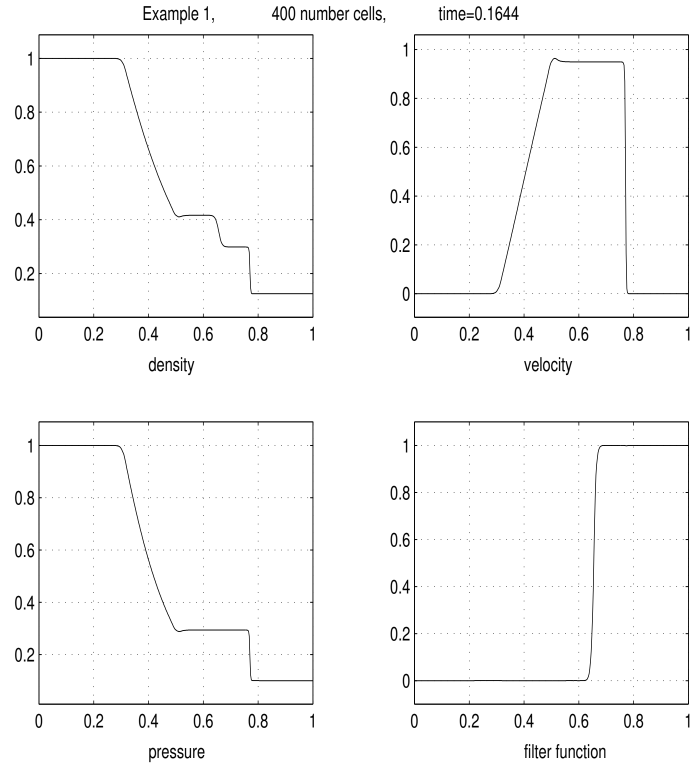
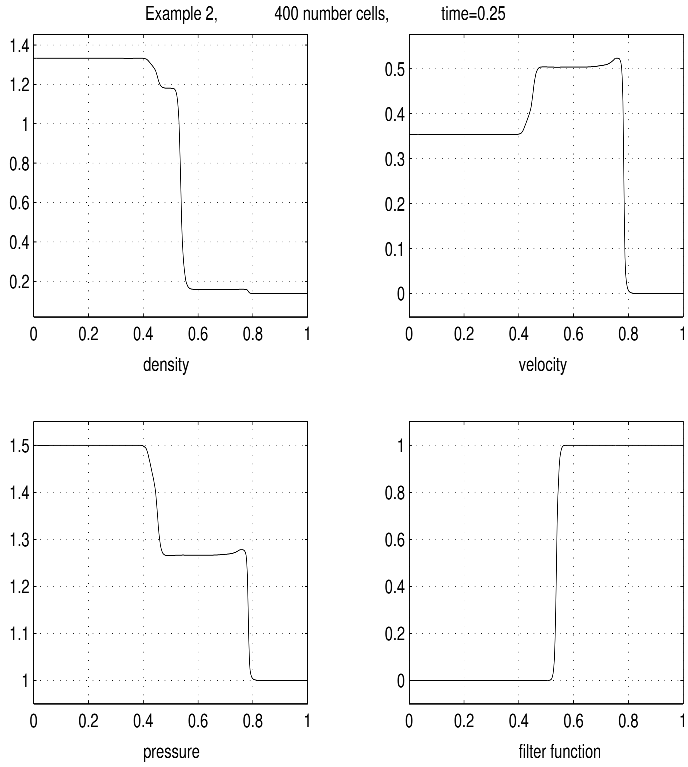
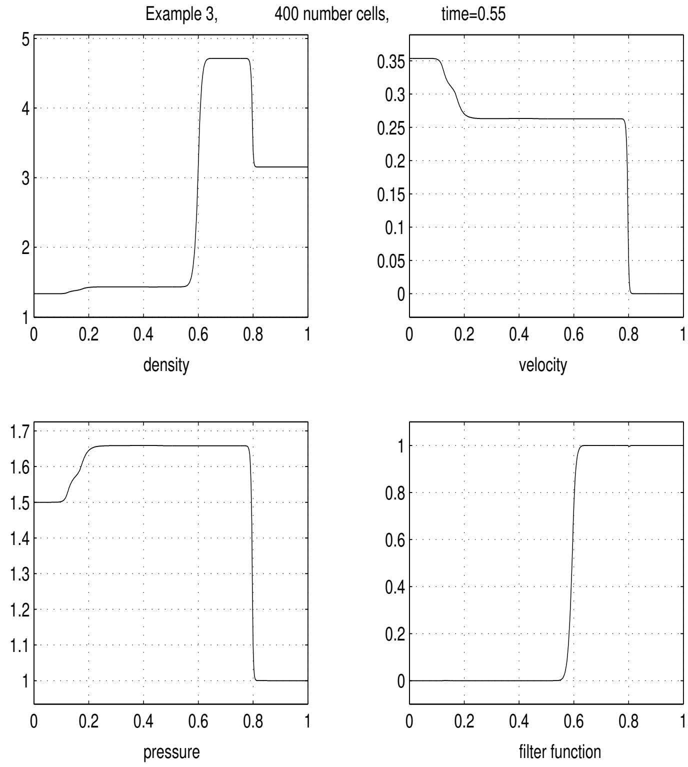

Example 1, 400 number cells, time=0.1644
density
velocity
pressure
filter function

Figure 2:



Example 2,
400 number cells,
time=0.25
density
velocity
pressure
filter function

Figure 3:



Example 3, 400 number cells, time=0.55
density
velocity
pressure
filter function

Figure 4:

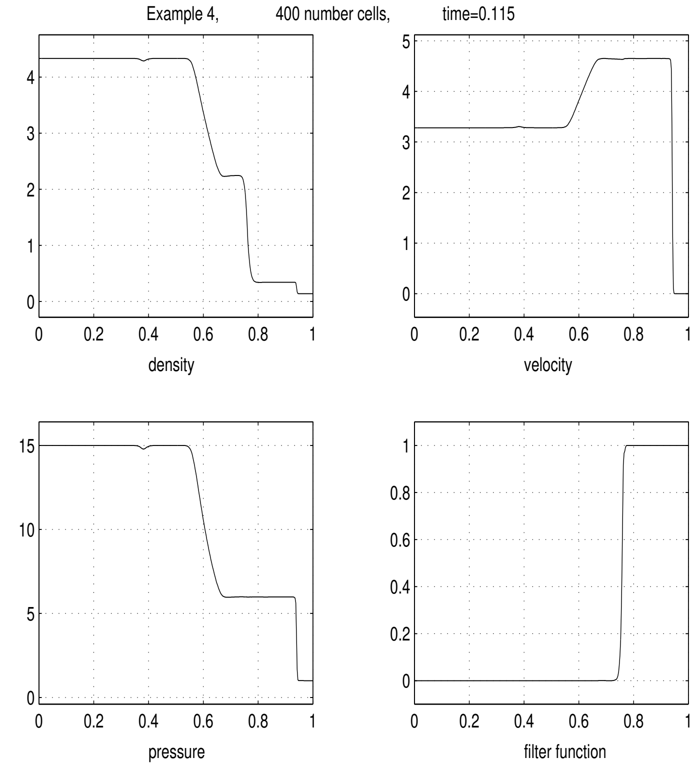

Example 4, 400 number cells, time=0.115
density
velocity
pressure
filter function

Figure 5:

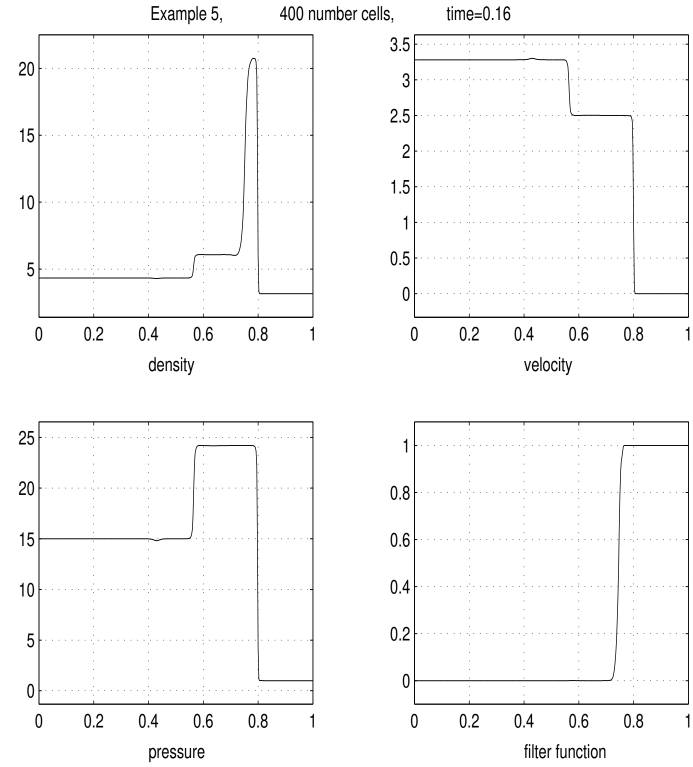

Example 5, 400 number cells, time=0.16
density
velocity
pressure
filter function

Figure 6:

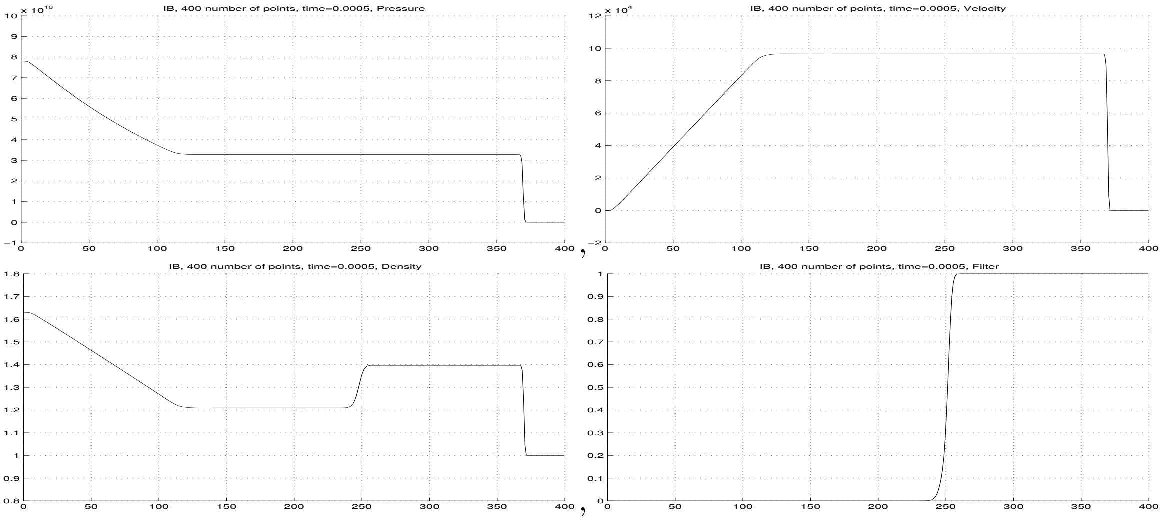

IB, 400 number of points, time=0.0005, Pressure
IB, 400 number of points, time=0.0005, Velocity
IB, 400 number of points, time=0.0005, Density
IB, 400 number of points, time=0.0005, Filter

Figure 7:

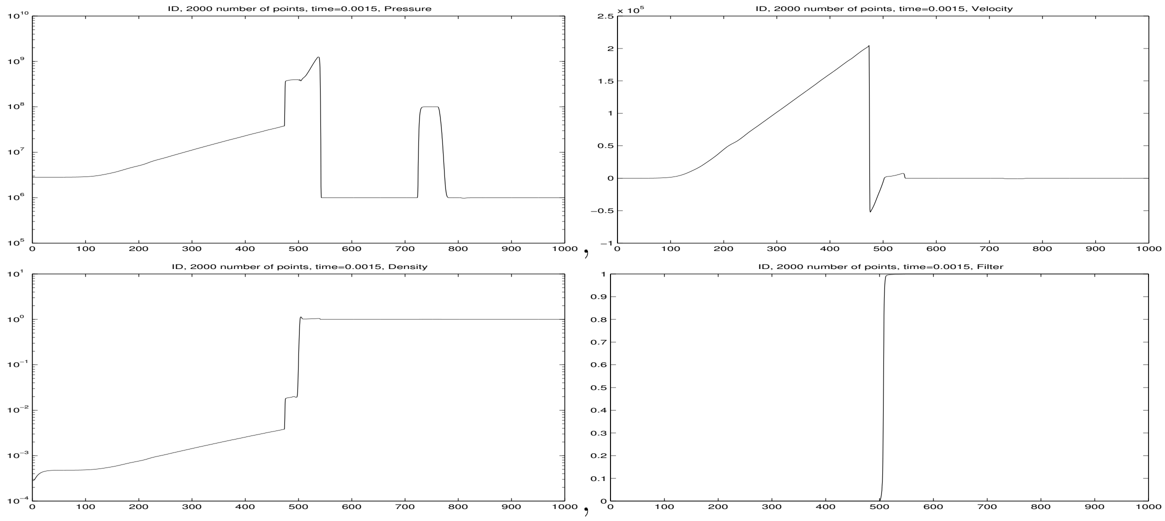
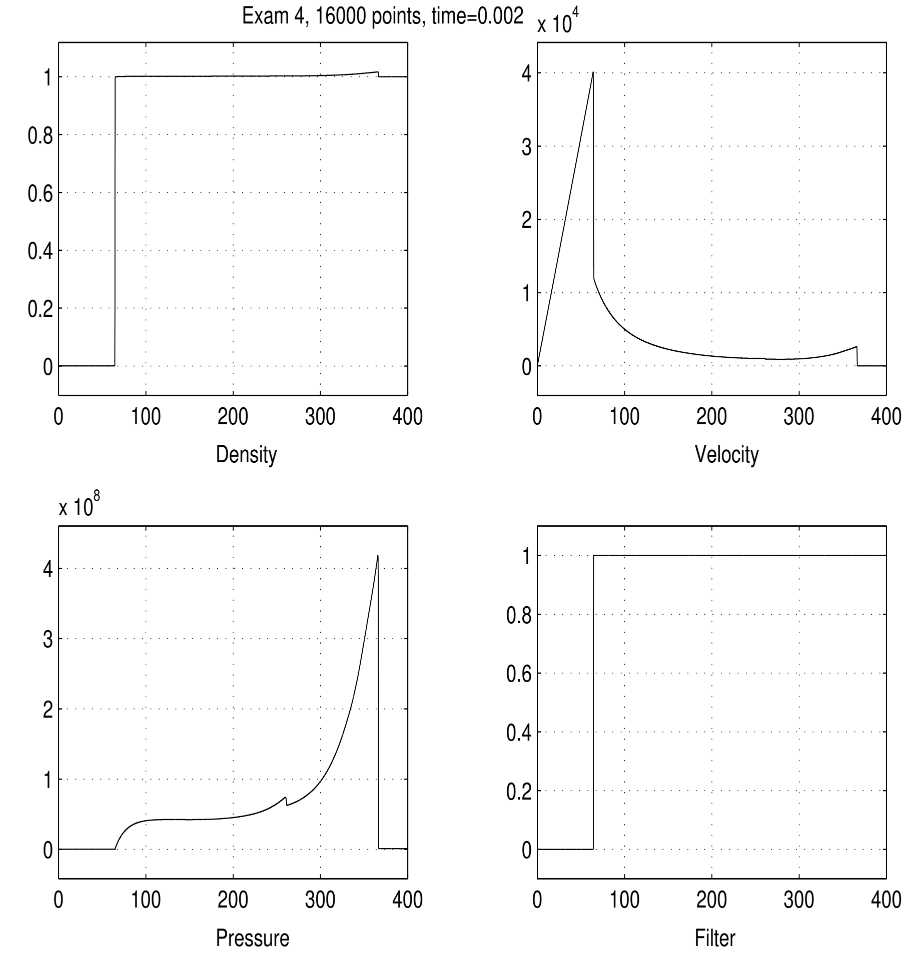

ID, 2000 number of points, time=0.0015, Pressure
ID, 2000 number of points, time=0.0015, Velocity
ID, 2000 number of points, time=0.0015, Density
ID, 2000 number of points, time=0.0015, Filter

Figure 8:



Exam 4, 16000 points, time=0.002
x 10^4
Density
Velocity
x 10^8
Pressure
Filter

Figure 9:

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