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Manufactured Solutions with Energy-only Source Terms

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• Introduction
• Energy-only MMS
  – Lagrangian Hydrodynamics
  – Eulerian Hydrodynamics
• Example Solutions
• Conclusion
Introduction

• Code Verification is the process of establishing that a physics code can correctly solve the mathematical model it implements.
  – Based on test problems
  – Often limited by available exact solutions to the mathematical model

• The method of manufactured solutions (MMS) provides a framework for code verification using more complex test problems.
  – Three-dimensional features
  – Complicated boundary conditions
  – More sophisticated mathematical models

• Although MMS has been around for many years, it has remained challenging to implement in many environments.
The challenge associated with implementing MMS verification for a physics code boils down to generating the appropriate source terms and then incorporating them into the physics code.

Generating the source terms isn’t necessarily a code-specific challenge, but incorporating into the physics code certainly is.

Often, codes may only support source terms for certain quantities, but it is our responsibility to verify what we can within these constraints.

We present a methodology for “deriving” solutions for inviscid hydrodynamics that exactly satisfy mass and momentum conservation.
Equations of Eulerian Hydrodynamics

\[
0 = \frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho u_i \\ \rho e_T \end{pmatrix} + \frac{\partial}{\partial x_j} \begin{pmatrix} \rho u_j \\ \rho u_i u_j + \delta_{ij} p \\ \rho u_j e_T + u_j p \end{pmatrix}
\]
The Lagrangian Coordinate Transformation

• A general, time-dependent coordinate transformation can be defined by introducing new coordinates $\tau, \xi, \eta, \zeta$.

• If we wish these to be lagrangian coordinates, then we require:

$$\frac{\partial t}{\partial \tau} = 1 \quad \frac{\partial t}{\partial \xi} = \frac{\partial t}{\partial \eta} = \frac{\partial t}{\partial \zeta} = 0 \quad \frac{\partial x_i}{\partial \tau} = u_i$$

• It is convenient to require that lagrangian and eulerian coordinates coincide at $t = 0$, and the remainder of the transformation may be represented as $\frac{\partial x_i}{\partial \xi^j}$.

• The transformation is singular if its jacobian, $J \equiv \left| \frac{\partial x_i}{\partial \xi^j} \right|$, vanishes.

• This is the continuum equivalent of grid lines crossing.
Equations of Lagrangian Hydrodynamics

• If we transform the Euler equations using these coordinates, we can derive conservation equations for lagrangian hydrodynamics:

\[
0 = \frac{\partial}{\partial \tau} \left( \begin{array}{c} \rho J \\
\rho J u_i \\
\rho J e_T 
\end{array} \right) + \frac{\partial}{\partial \xi^j} \left( \begin{array}{c} 0 \\
\frac{\partial \xi_j}{\partial x^i} Jp \\
\frac{\partial \xi_j}{\partial x^k} J u_k p 
\end{array} \right)
\]

\[
u_i(\tau, \xi, \eta, \zeta) = \frac{\partial}{\partial \tau} x_i(\tau, \xi, \eta, \zeta)
\]

• Solving these equations numerically is challenging, because they require nine additional evolution equations for metric components.
Equations of Lagrangian Hydrodynamics

\[ 0 = \frac{\partial}{\partial \tau} \begin{pmatrix} \rho J \\ \rho J u_i \\ \rho J e_T \end{pmatrix} + \frac{\partial}{\partial \xi_j} \begin{pmatrix} 0 \\ \frac{\partial \xi_j}{\partial x^i} J p \\ \frac{\partial \xi_j}{\partial x^k} J u_k p \end{pmatrix} \]

• We are not required to define a solution in terms of these quantities.
• Instead, define a solution using fluid particle trajectories: \( x_i(\tau, \xi, \eta, \zeta) \).
• The choice here must satisfy \( J \equiv \left| \frac{\partial x_i(\tau, \xi, \eta, \zeta)}{\partial \xi_j} \right| > 0 \) within some domain.
• Given \( x_i(\tau, \xi, \eta, \zeta) \), it is straightforward to compute \( \rho \):

\[ \rho(\tau, \xi, \eta, \zeta) = \rho_0(\xi, \eta, \zeta) \frac{J_0(\xi, \eta, \zeta)}{J(\tau, \xi, \eta, \zeta)} \]
Equations of Lagrangian Hydrodynamics

\[ 0 = \frac{\partial}{\partial \tau} (\rho J u_i) + \frac{\partial}{\partial \xi_j} \left( \frac{\partial \xi_j}{\partial x^i} J p \right) = \frac{\partial}{\partial \tau} (\rho J u_i) + \frac{\partial \xi_j}{\partial x^i} \frac{\partial}{\partial \xi_j} (J p) \]

- Having chosen \( x_i(\tau, \xi, \eta, \zeta) \), and computed \( \rho(\tau, \xi, \eta, \zeta) \), the momentum equation can be solved for \( p \):

\[
p(\tau, \xi, \eta, \zeta) = \left[ (Jp)_0(\tau) - \int_{\xi_0}^{\xi} \frac{\partial x_i}{\partial \xi_j} \frac{\partial}{\partial \tau} (\rho J u_i) d\xi_j \right] / J (\tau, \xi, \eta, \zeta)
\]

- The pressure is therefore fully determined by a time-dependent gauge value given at a single point in Lagrangian space.
Example – Constant Vortex

\[ x = \xi \cos(\omega \tau) - \eta \sin(\omega \tau) \]
\[ y = \eta \cos(\omega \tau) - \xi \sin(\omega \tau) \]
\[ z = \zeta \]
\[ \xi_0 = (0,0,0) \]
\[ \rho|_{\tau_0} = 1 \]
\[ p|_{\xi_0} = 1 \]
\[ \rho = (\cos^2(\omega \tau) - \sin^2(\omega \tau))^{-1} \]
\[ p = \frac{1}{\cos(2\omega \tau)} \left( \frac{1}{2} \omega^2 (\xi^2 + \eta^2) + \cos(2\omega \tau) - \xi \eta \omega^2 \sin(2\omega \tau) \right) \]

Assuming ideal gas, \( \gamma = \frac{7}{5} \) and \( \omega = 1 \):

\[ S_e = -\frac{1}{\cos(2\tau)} \left( (\xi^2 + \eta^2) \sin(2\tau) + \frac{5}{2} \xi \eta \cos^2(2\tau) + \frac{9}{4} \xi \eta \cos(4\tau) + \frac{7}{2} \sin(4\tau) + \frac{1}{4} \xi \eta \right) \]
Equations of Eulerian Hydrodynamics

\[
0 = \frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho u_i \\ \rho e_T \end{pmatrix} + \frac{\partial}{\partial x_j} \begin{pmatrix} \rho u_j \\ \rho u_i u_j + \delta_{ij} p \\ \rho u_j e_T + u_j p \end{pmatrix}
\]

- It is more challenging to unpack the Euler equations in the same way, because, given \( u_j \), density must be computed as a solution to a PDE.
- However, it is straightforward to transform a Lagrangian solution into Eulerian coordinates, by simply computing \( \xi_i(t, x, y, z) \).
Example – Constant Vortex

• The coordinates can be solved directly:

\[ x = \xi \cos(\omega \tau) - \eta \sin(\omega \tau) \]
\[ y = \eta \cos(\omega \tau) - \xi \sin(\omega \tau) \]

\[ \xi(t, x, y, z) = \frac{x \cos(\omega t) + y \sin(\omega t)}{\cos^2(\omega t) - \sin^2(\omega t)} \]
\[ \eta(t, x, y, z) = \frac{x \csc(\omega t) + y \csc(\omega t) \cot(\omega t)}{\cot^2(\omega t) - 1} \]

• The computation of solution fields in terms of Eulerian coordinates is straightforward, and is left as an exercise for the reader.
Conclusions

• We have demonstrated that it is indeed possible to derive energy-only source terms for inviscid hydrodynamics, provided that a smooth manufactured solution is used.

• The conservation equations of Lagrangian hydrodynamics are integral to this process, but Eulerian solutions can also be derived.

• It is unclear whether non-smooth solutions can be derived in this way.

• Use of symbolic manipulators (e.g. Mathematica, Sympy) is still recommended.
Questions?