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Dynamic Compressible Flow Verification Problems: *Oldies but Goodies*

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Overview

Verification

- Code verification *vs.* Solution Verification *vs.* Software Verification

Euler Equations of Gas Dynamics

- Foundation of coupled models involving multiple physics

Comments on Exact Solutions

- Similarity solutions & Lie group methods

Some "Workhorse" Exact Solutions

- And why they're important

Summary

"A computer lets you make more mistakes faster than any invention in human history — with the possible exceptions of handguns and tequila." Mitch Ratliffe, *Technology Review*, April, 1992.

A little bit more about verification…

"Verification is the process of evaluating if a computer code correctly implements the algorithms that were intended."

- Successful verification admits the possibility of inadequate algorithms.

Software

Testing

Algorithms

Software Verification: SQE practices including regression, unit tests, etc.

Code Verification: Are the equations represented by a code and the algorithms for the numerical solution of these equations themselves mathematically correct?

Calculation Verification: What is the error in a given calculation? This includes discretization robustness and convergence studies, formal error estimation procedures, inference from test problem suites.

"Nobody's perfect, and most people drastically underestimate their distance from that state."
Mahaffy's First Law of Human Nature

The Euler equations of gas dynamics form the base of computational mechanics.

Conservation of mass, momentum, and energy:

State

$$\frac{\partial U}{\partial t} + \mathrm{div}\, f(U) = 0 \qquad x \in \Omega \subset \Re^d, \;\; t \geq 0$$

Flux function

- The state $U(x,t)$: $\mathcal{R}^d$ ´ $\mathcal{R}$ ® $\mathcal{R}^n$ is the array of conserved quantities
- There may be additional constraints or source terms on the RHS
- Appropriate initial and boundary conditions must also be given
- For 1-D compressible, inviscid, non-heat-conducting flow, the state U and flux f are given by:

$$U = [\rho,\; \rho u,\; \rho E]^{\mathrm{T}} \qquad f = [\rho u,\; \rho u^2 + p,\; \rho E u + p u]^{\mathrm{T}}$$

where $E = e + \frac{1}{2}u^2$ $\qquad p = P(\rho, e)$

Specific internal energy (SIE) *Specific kinetic energy* *Equation of state (EOS)*

How does one find exact solutions?

Recall, one must have exact solutions for Code Verification.

- The ICs and BCs are inextricably woven into the solution.
- One must be able to specify these ICs and BCs — or some (*very*) close approximation to them — in the code being analyzed.

There are a few ways to find exact solutions to PDEs:

- "Straightforward" — the Method of Manufactured Solutions (MMS)
  - Want: $L(u) = 0$ in W, with $I(u) = 0$ at t=0 and $B(u) = 0$ on ∂W
  - Use: $L(v) = f$ in W, with $I(v) = g$ at t=0 and $B(v) = h$ on ∂W
- "Not so straightforward"
  - Lie groups (and variants) – see Coggeshall*, etc.

New exact solutions continue to be found for coupled physics.

- E.g., in conduction-hydrodynamics†, radiation-acoustics‡, and radiation-hydrodynamics§.

* S. Coggeshall, "Analytic solutions of hydrodynamics equations," *Phys. Fluids A* **3**:757–769 (1991).

† P. Reinicke, J. Meyer-ter-Vehn, "The point explosion with heat conduction", *Phys. Fluids A* **3**:1807–1818 (1991).

‡ W.G. Vincenti, B.S. Baldwin, "Effect of Thermal Radiation on the Propagation of Plane Acoustic Waves," *J. Fluid Mech.* **12**, pp. 449–477 (1962).

§ R. Lowrie, R. Rauenzahn, "Radiative shock solutions in the equilibrium diffusion limit," *Shock Waves* **16**:445–453 (2007); R. Lowrie, J. Edwards, "Radiative shock solutions with grey nonequilibrium diffusion," *Shock Waves* **18**:129–453 (2008).

What are Lie groups and how are they used?

Quick historical perspective…

- Theory proposed and worked out by Sophus Lie.
- Lie began investigations by trying to use Galois' ideas to understand differential equations.
- Modern proponents include Ovsiannikov, Ibragimov, Olver,…

M. Sophus Lie
(1842-1899)

"the genius who created the theory of transformation groups" *Élie Cartan*

Goals: (1) Find the symmetry groups of solutions to a given equation, and (2) use these groups to reduce the equations to a more tractable form.

- In practice, one hopes to reduce PDEs to ODEs.
- The reason this helps is that, in general, we can compute solutions to (many) ODEs with greater accuracy and higher precision — i.e., *with more confidence* — than solutions to (almost all) PDEs.
- There is no claim that this approach produces all solutions.
- Symmetry group methods have been applied to a wide range of equations across a broad spectrum of science.
- Can also be used to obtain new solutions from a given, known solution.

"Das Ziel der Wissenschaft ist einerseits, neue Tatsachen zu erobern, andrerseits, bekannte unter höheren Gesichtspunkten zusammenzufassen."
Sophus Lie, *Gesammelte Abhandlungen*, B.G.Teubner, Leipzig, 1934.

A quick-and-dirty overview of Lie group methods applied to the Euler equations…

Start with the conservation laws, written as Eulerian-frame PDEs:

$$\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial r} + \rho\left(\frac{\partial u}{\partial r} + \frac{\nu u}{r}\right) = 0$$

$$\rho\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial r}\right) + \frac{\partial p}{\partial r} = 0$$

$$\frac{\partial p}{\partial t} + u\frac{\partial p}{\partial r} + \frac{\gamma p}{\rho}\left(\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial t}\right) = 0$$

- A non-trivial analysis shows that these equations are invariant under the following transformations:

$$t^* = a_1 t + a_2$$

$$r^* = (a_2 + a_3) r$$

$$u^* = a_3 u$$

$$p^* = a_4 p$$

$$\rho^* = \frac{a_4}{a_3^2}\rho$$

- The collection of invariance properties can be written in terms of a "group generator" operator:

$$\hat{U} = (a_2 + a_3)\, r\frac{\partial}{\partial r} + (a_1 + a_2 t)\frac{\partial}{\partial t} + a_3\, u\frac{\partial}{\partial u} + a_4\frac{\partial}{\partial P} + (a_4 - 2a_3)\,\rho\frac{\partial}{\partial \rho}$$

"Mathematics is an interesting intellectual sport but it should not be allowed to stand in the way of obtaining sensible information about physical processes." Richard Hamming

The group generator is used to complete the Lie group analysis.

1. Operate on the Euler equations

- The operator $\hat{U}$ must first be "extended" to include terms with partial derivatives with respect to the partial derivatives of variables.
- This extension results in additional terms involving operators such as:

$$\frac{\partial}{\partial u_t}, \frac{\partial}{\partial \rho_r}, \frac{\partial}{\partial P_r}, \ldots$$

- Operating on the Euler equations with the *extended* generator returns zero identically.
  - This confirms the validity of the underlying symmetries and subsequent analysis.

2. Operate on an arbitrary function F

- Solving the equation

$$\hat{U}F = 0$$

with the method of characteristics gives *new dimensionless variables* with which to reduce the Euler equations to ODEs:

$$\xi = \frac{r}{t^\alpha} \qquad V(\xi) = \frac{t}{r}u$$

$$D(\xi) = \frac{\rho}{\rho_0} \qquad C(\xi) = \gamma \frac{t^2}{r^2}\frac{P}{\rho}$$

- This is a codified procedure by which to obtain similarity variables for PDEs.

Substitute the new variables into the Euler equations to obtain a system of ODEs.

The final result of this analysis for the Euler equations is:

$$\frac{1}{C}\frac{dC}{dV} = F_1(C,V)$$

$$\frac{1}{D}\frac{dD}{dV} = F_2(C,V)$$

$$\frac{1}{\xi}\frac{d\xi}{dV} = F_3(C,V)$$

- F_1, F_2, and F_3 are nonlinear functions of C and V.
- Once the function $C(V)$ is known, the remaining two equations reduce to quadratures.
- The solution of this system is transformed back to physical variables using the dimensionless variable definitions.

Important note: the above analysis is valid only if all associated initial conditions, boundary conditions, and constraints are also invariant under the identified symmetries.

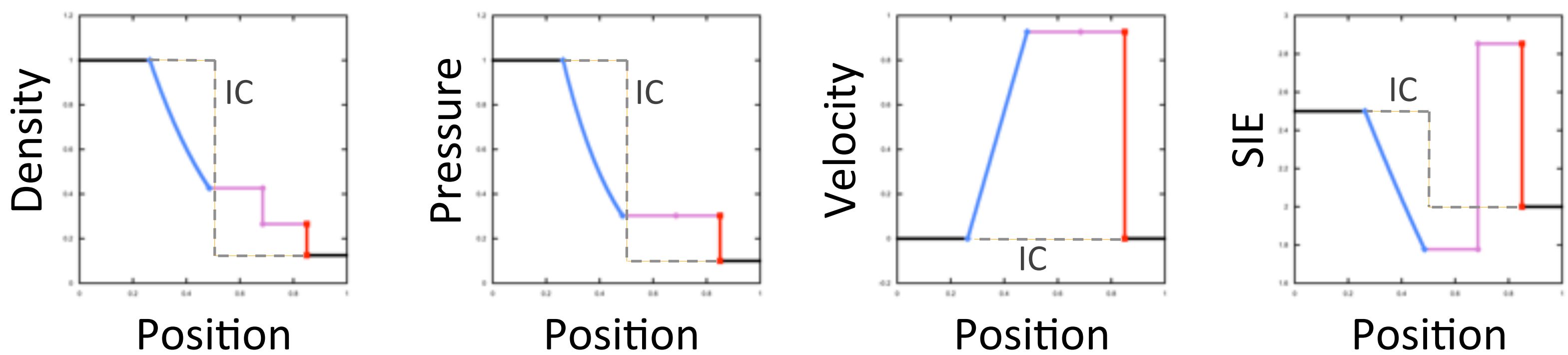
For 1-D Cartesian geometry, you must consider the Riemann problem.

Riemann problems are the canonical IVP, with two constant initial states.

- These lead to the standard “shock tube” solutions of gas dynamics.
- These solutions possess different combinations of the canonical wave structures:

G.F. Bernhard Riemann
(1826-1866)
“the greatest mathematician” *Peter Lax*

Rarefaction Contact Shock



The good news is that these exact solutions for polytropic gases can be readily evaluated.

- Only a single root-solve is required to obtain the entire solution.*

* J.J. Gottlieb, C.P.T. Groth, “Assessment of Riemann Solvers for Unsteady One-Dimensional Inviscid Flows of Perfect Gases,” *J. Comput. Phys*. **78**:437–458 (1988).

The Riemann problem can have different solutions, depending on the initial conditions.

There are five basic solutions for the 1D gas dynamics equations with an ideal gas EOS*.

- These depend on the relative pressures and velocities in the ICs.

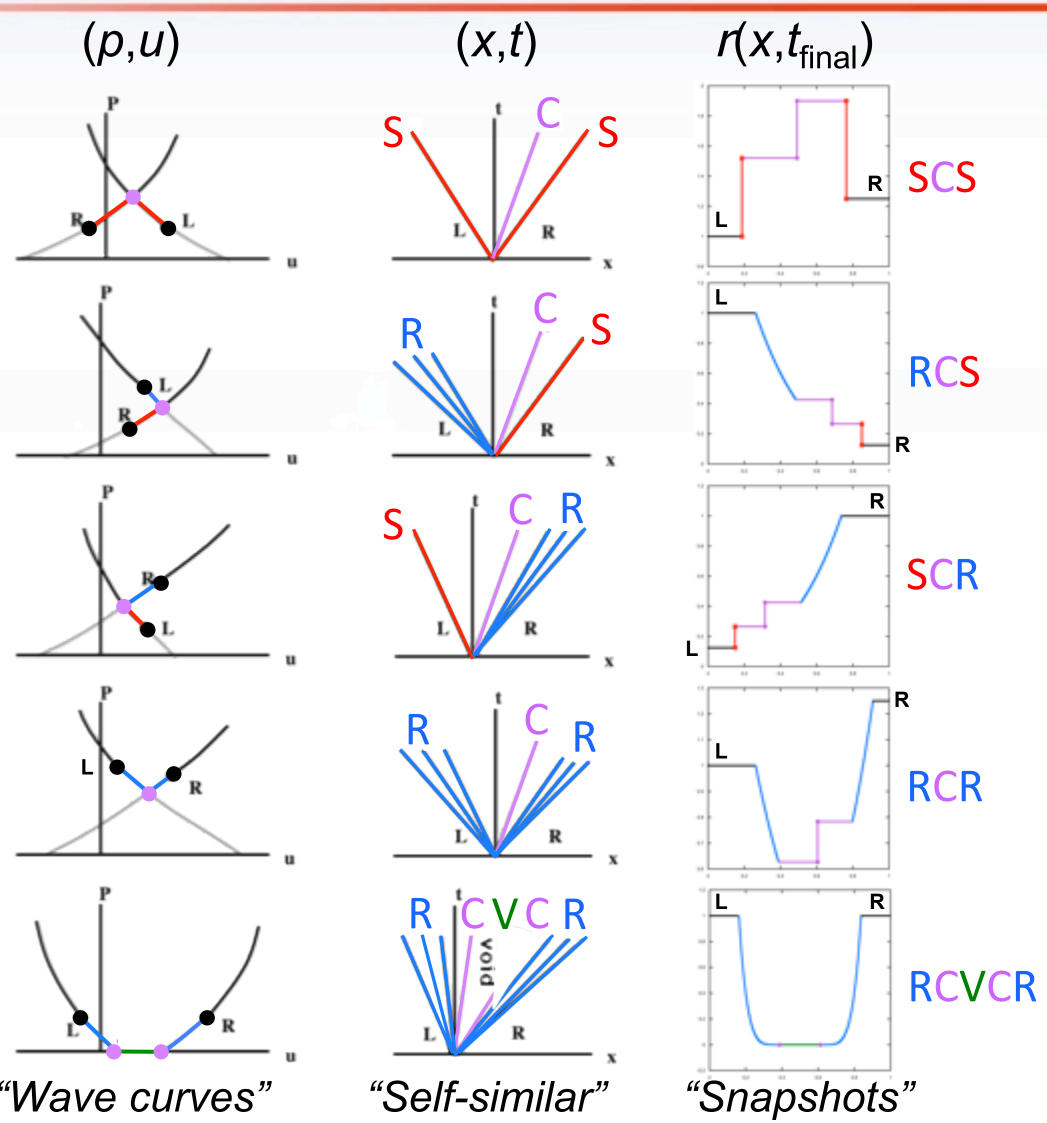
S = Shock

C = Contact

R = Rarefaction

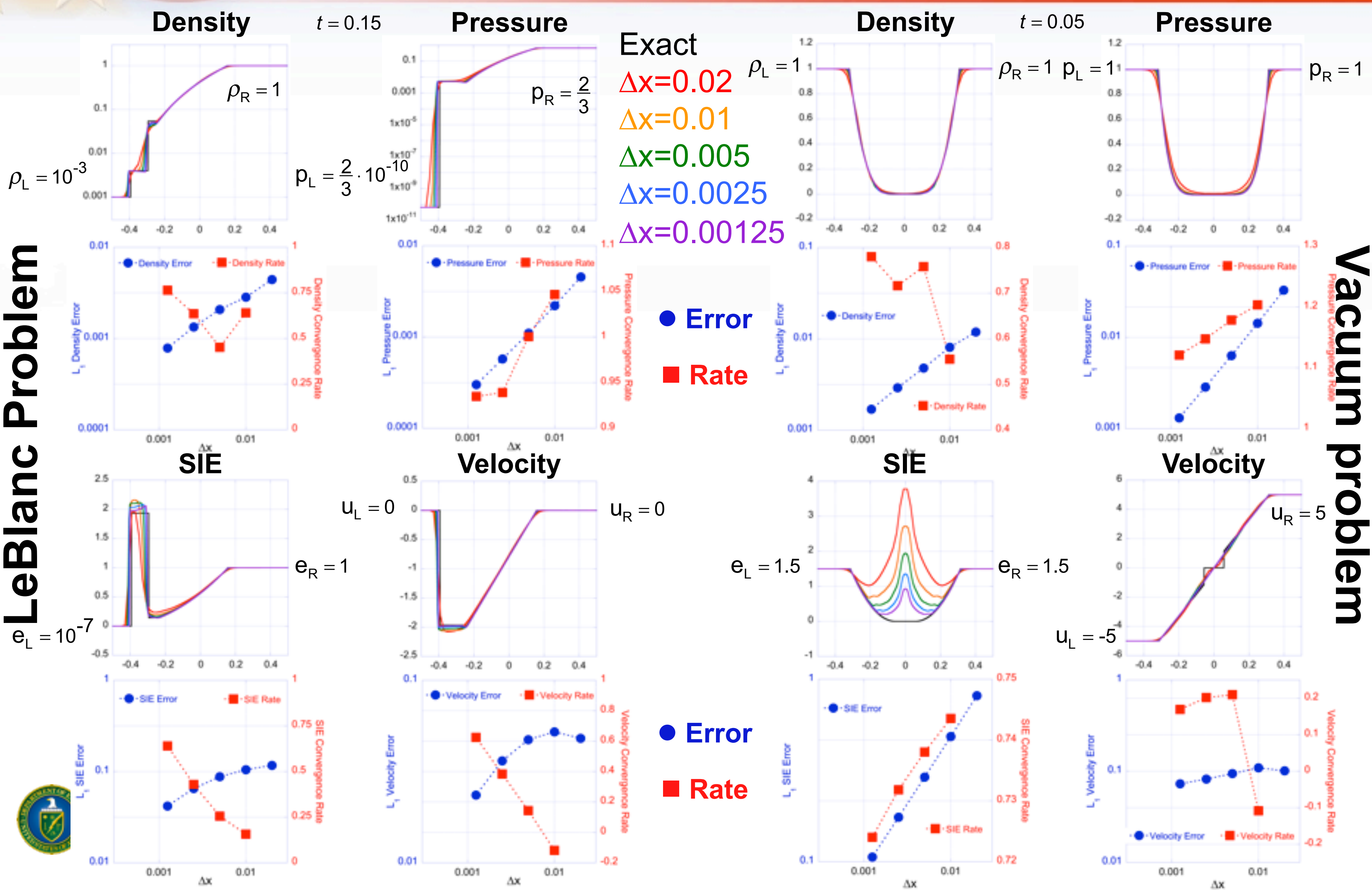
V = Vacuum/Void

Test all five different Riemann solutions!



* R. Menikoff, *Application of Non-Reactive Compressible Fluids*, LANL Report LA-UR-01-273 (2001), E.F. Toro, *Riemann solvers and numerical methods for fluid dynamics*, Springer-Verlag (2009).

Analysis of two challenging RPs demonstrates convergence of a WENO scheme.



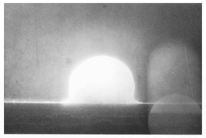
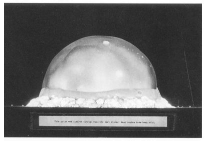
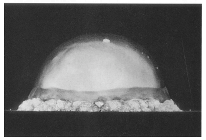
Some details on the WENO scheme used in computing the Riemann problem results…

- **Fifth-order WENO in space, third-order TVD Runge-Kutta time stepping**
  - Shu, C.W., "Essentially non-oscillatory and weighted essentially non-oscillatory schemes for hyperbolic conservation laws", in *Advanced Numerical Approximation of Nonlinear Hyperbolic Equations*, Lecture Notes in Mathematics, Vol. 1697, Springer-Verlag, 1998.
- **Mapped weights modification**
  - Henrick, A.K., Aslam, T.D., Powers, J.M., "Mapped weighted essentially non-oscillatory schemes: Achieving optimal order near critical points", *Journal of Computational Physics*, **207**, 542–567 (2005).
- **First-order monotonicity constraint**
  - Suresh, A., Huynh, H.T., "Accurate monotonicity-preserving schemes with Runge-Kutta time stepping", *Journal of Computational Physics*, **136**, 83–99 (1997).
- **Godunov-type flux difference splitting with HLL Riemann solver**
  - Toro, E.F., *Riemann solvers and numerical methods for fluid dynamics*, Springer-Verlag, 2009.
  - LeVeque, R.J., *Finite volume methods for hyperbolic problems*, Cambridge University Press, 2002.

For spherically symmetric* solutions, there are three cardinal compressible flow problems.

Noh — test the conversion of kinetic energy to internal energy

- The issue of "wall heating" is clearly manifested in this problem.
- A workhorse test problem: easy to set up, easy to evaluate, illuminates particular algorithm features (at the boundary, near the shock).

Sedov — test the conversion of internal energy to kinetic energy

- First used as a model for the relation between source energy and shock distance — and yield estimation, à la Taylor (1945).
- An equally common test problem: set up continues to engender debate, more complicated to evaluate, illuminates particular algorithm features (particularly near the shock).

Guderley — test the transition from converging flow to diverging flow

- Historically underused for verification.
- A seldom seen test problem: tricky to evaluate, complicated to set up, with no established knowledge base to understand its testing of algorithm features.

Reinicke & Meyer-ter-Vehn (RMtV) — Sedov with heat conduction

- A rare — and difficult — coupled-physics code verification test problem.

* Solutions to these problems also exist under the assumption of planar or cylindrically symmetry.

The Noh problem assumes uniform inflow toward the origin as an initial condition.

Noh* obtained a simple, closed-form solution for uniform inflow toward the origin in planar, cylindrical, or spherical symmetry.

- The kinetic energy in the $t = 0$ conditions is converted to internal energy in the $t > 0$ solution.
- Problem is easy to set up and its exact solution is easy to evaluate.
- Behavior at the origin governs the salient structures.

Noh's publications suggest that he pieced together the different elements of his solution.

- Axford† gives a derivation of the solution motivated by Lie group methods…
  - …and extended the solution to other EOSs.
- Gehmyer et al.‡ give the full solution…
  - …and evaluate the solution between the origin and a rigid piston approaching the origin.

* W. Noh, "Errors for calculations of strong shocks using an artificial viscosity and an artificial heat flux," *J. Comput. Phys.* **72**:78–120 (1987).

† R. Axford, "Solutions of the Noh problem for various equations of state using Lie groups," *Lasers Part. Beams* **18**:93–100 (2000).

‡ M. Gehmyer, B. Cheng, D. Mihalas, "Noh's constant-velocity shock problem revisited," *Shock Waves* **7**:255–274 (1997).

The exact Noh solution is easy to evaluate.

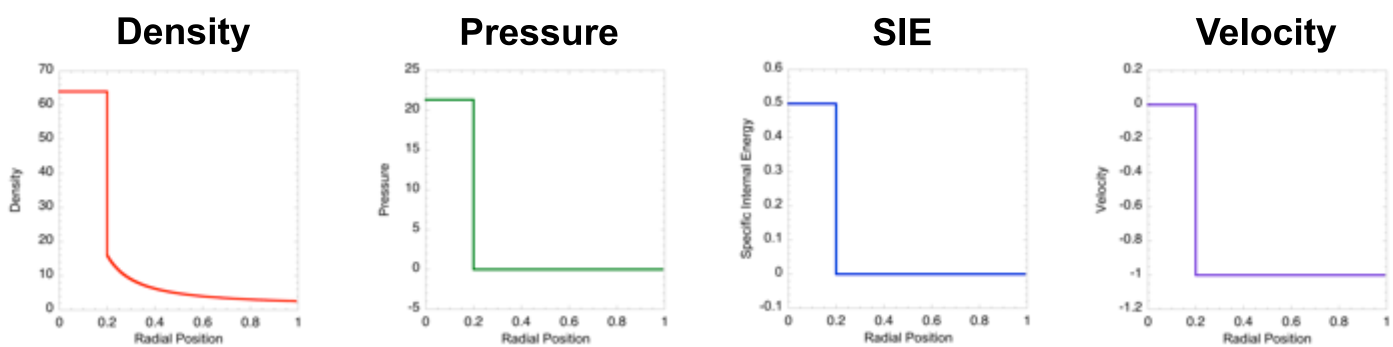
The full solution to the standard Noh problem is easy to evaluate.

- This facilitates comparison between exact and computed solutions.

		Post-shock	Pre-shock
		$r < r_S$	$r > r_S$
Density	$r(r,t) / r_0 =$	$[(g+1)/(g-1)]^d$	$[1-(u_0 t/r)]^{d-1}$
Pressure	$p(r,t) / (r_0 u_0^2/2) =$	$(g+1)^d/(g-1)^{d-1}$	0
SIE	$e(r,t) / (u_0^2/2) =$	1	0
Velocity	$u(r,t) / \lvert u_0 \rvert =$	0	-1

Here, the shock position is: $r_S = U_S t$ with shock speed $U_S = (1/2)(g-1)\,|u|_0$

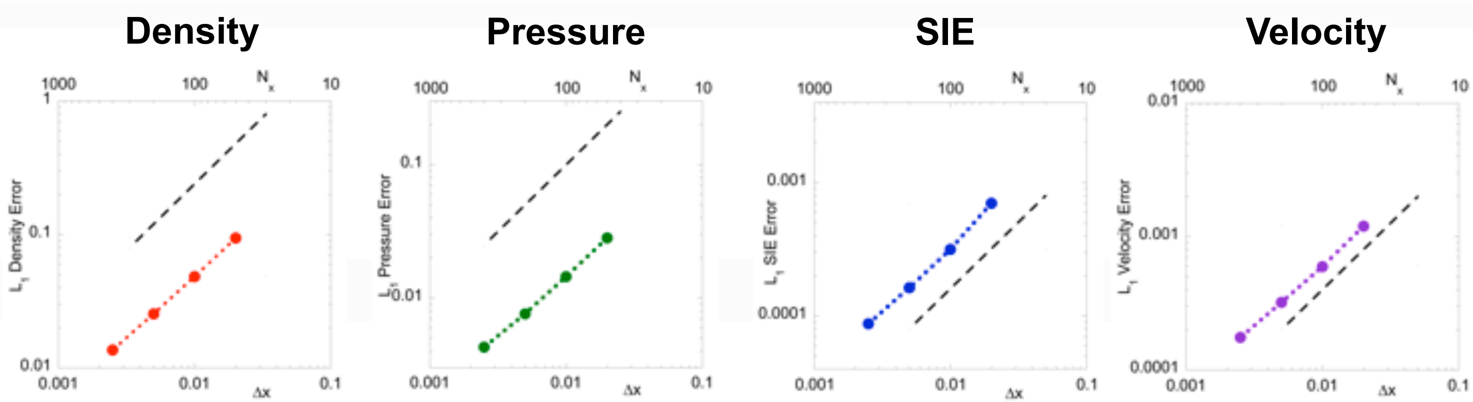
- The canonical hydrocode test case is spherical geometry, $g = 5/3$, $t_{\text{final}} = 0.6$:



‡ M. Gehmyer, B. Cheng, D. Mihalas, "Noh's constant-velocity shock problem revisited," *Shock Waves* **7**:255–274 (1997).

Noh result look good for convergence.

Analysis of 1D hydrocode results look good…



…but the problem remains a workhorse for algorithm developers

- Numerical results give near-axis values that with:
  - Density that is too <u>low</u>
  - SIE that is too <u>high</u>

This is the celebrated "wall heating" problem.*

- The Noh problem remains a "must-do" test for compressible flow codes.

Say "Yes!" to Noh!

* W.J. Rider, "Revisiting Wall Heating," *J. Comput. Phys.* **162**:395–410 (2000).

The Sedov problem assumes an instantaneous energy source at the origin.

Sedov* considered the gas dynamics equations with an intense initial energy source.

- 1D, with planar, cylindrical, or spherical symmetry.
- The initial density is non-zero; other variables initially zero.
- Singular IC is key for the quasi-analytical solution.
- Detail phase-plane analysis elucidates the solution structure.

Leonid I. Sedov
(1907–1999)

Sedov obtained self-similar solution by dimensional analysis:

Non-dim. Position $l = r \,/\, r_s$

Non-dim. Velocity $V(l) = u(r,t)/\,(r/t)$

Non-dim. Density $R(l) = r(r,t) \,/\, (Ar^{-w})$

Non-dim. Pressure $P(l) = p(r,t)/\,(Ar^{2-w}/t^2)$

- A “self-similar solution” means that these scaling functions exist for the governing equations, reducing the governing PDEs to ODEs.

* L.I. Sedov, *Similarity and Dimensional Methods in Mechanics*, Academic Press, New York, p.147 ff. (1959); see also report by Bethe et al., papers by Taylor, Book, books by Korobienikov, Whitham.

“At the London meeting [*International Astronautical Federation, 1959*] Sedov even seemed to enjoy his own doubletalk. When the Russians withdrew an astronomical paper, Sedov admitted to a Russian-speaking colleague that the reason was that British figures proved it erroneous. But when a British reporter asked for corroboration, Sedov offered three other explanations in quick succession: 1) there were too many papers already; 2) it would have been given if the author had been on hand; and 3) there were not enough Russian scientists present to discuss it. He chuckled merrily at each new alibi.” *Time Magazine,* Sept. 21, 1959.

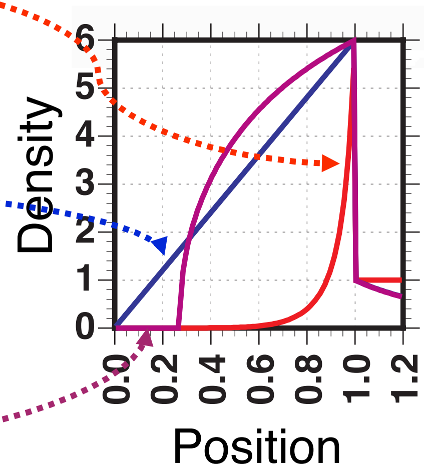
The Sedov problem has three different solutions, depending on the initial conditions.

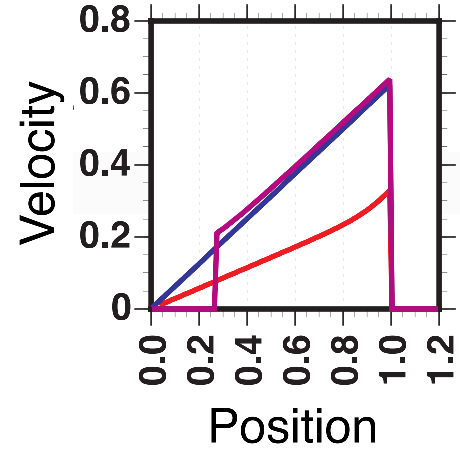
Depending on the value of initial total energy E_0, polytropic index g, and initial density distribution (through parameter w in the initial density $r = r_0 \exp(-wr)$), there are three distinct solution families:

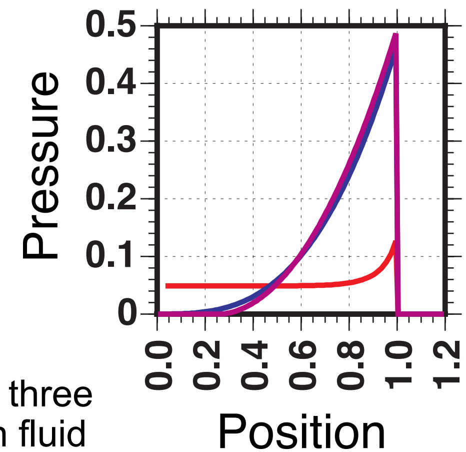
① Standard
constant initial density

② Singular
non-uniform initial density

③ Vacuum
non-uniform initial density







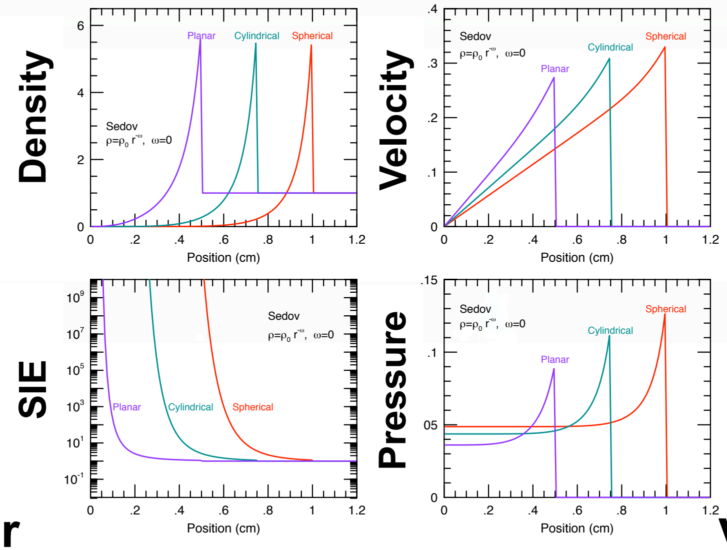
Test all three Sedov solutions!

"Sedov's book, which has gone through ten Russian editions and three English translations, is the bible of the subject of self-similarity in fluid mechanics. But like the Bible, it has been more reverenced (and referenced) than read." D.L. Book, *Shock Waves* **4**:1-10 (1994)

These different Sedov cases exist in the other geometries, as well.

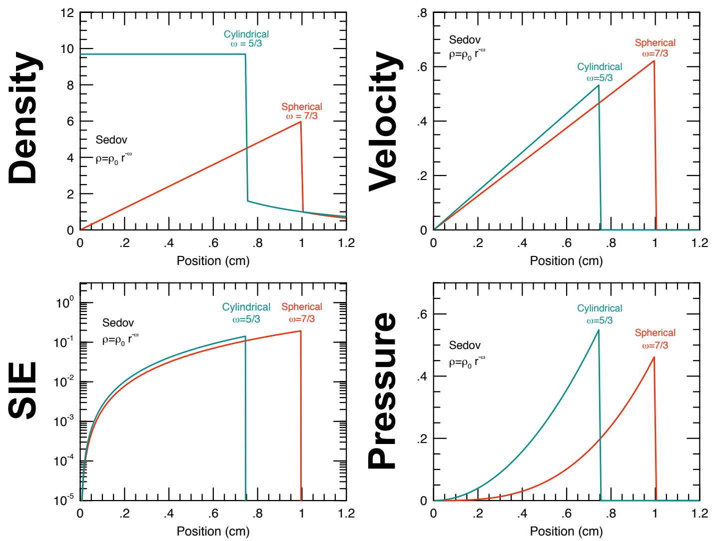
The "standard" solution exist in all geometries, but the "singular" and "vacuum" solutions only exist in cylindrical and spherical geometries.

Standard

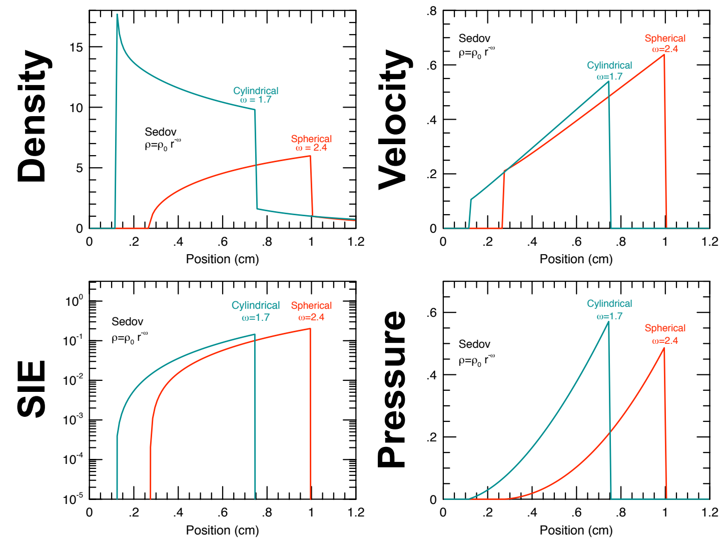


Planar
Cylindrical
Spherical

Singular



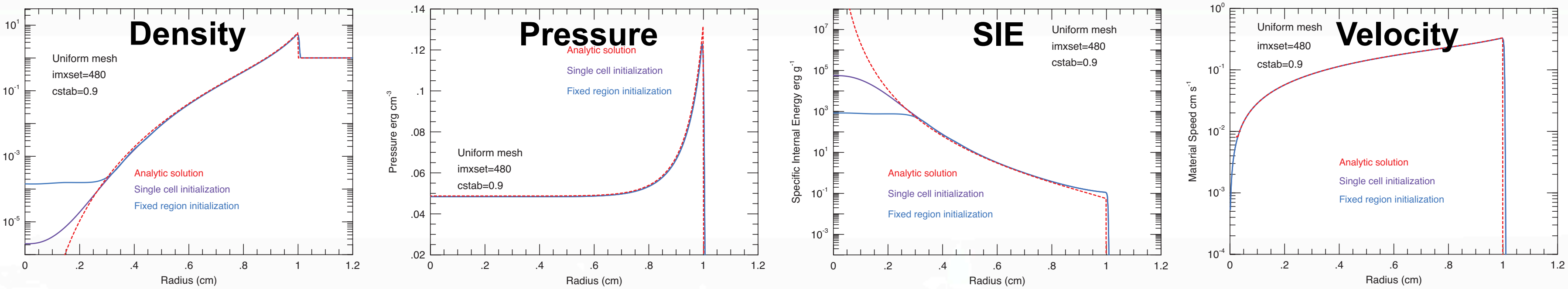
Vacuum



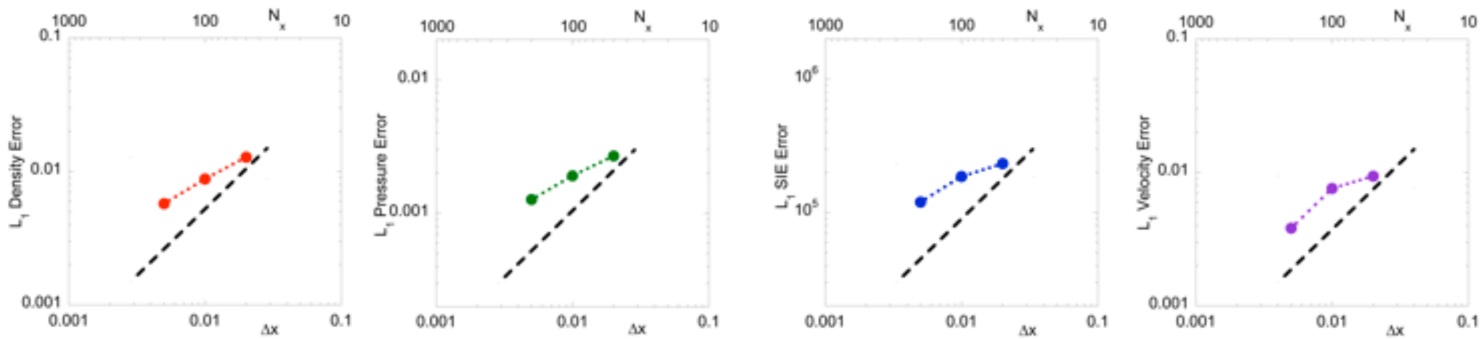
Although the initial conditions can be tricky, the convergence results are readily obtained.

There are "religious wars" about how to set up the problem…

Standard Sedov



…but convergence results are reasonably robust for "standard" Sedov.



Software to evaluate these solutions is readily available*.

- See: http://www.cococubed.asu.edu/
- Our more sophisticated version remains in "research code" form.

* J. Kamm, F. Timmes, *On Efficient Generation of Numerically Robust Sedov Solutions*, LANL Report LA-UR-07-2849 (2007).

The Guderley problem assumes an infinitely weak shock, infinitely far away, infinitely long ago...

Guderley* published an insightful phase plane analysis of the ODEs obtained from self-similar solutions of the Euler equations.

- Reduced equations are obtained from dimensional analysis à la Sedov.
- Equations are ultimately reduced to a single nonlinear ODE, which forms the basis of a nonlinear eigenvalue problem.
- Connection of singular points in the phase plane leads to the “infinitely unusual” initial conditions.
- Meyer-ter-Vehn & Schalk† further elucidated the phase plane analysis.
- Proper integration through the singularities in the phase plane is delicate and numerical evaluation is explained (almost completely) in the spectacular work of Lazarus‡.

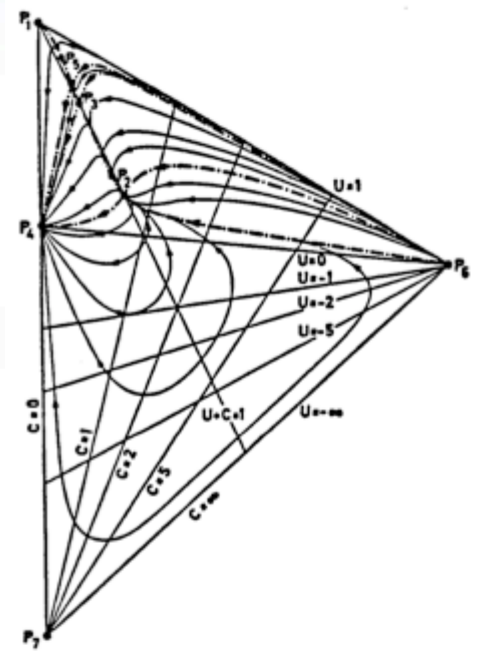


Fig. 2. Guderley's chart of solutions in the U, C plane for $n=3$, $\gamma=7/5$, $\alpha=0.75$ and $\varkappa=0$. Singular points are labelled by P_1 to P_7. Solid curves describe solutions of (19), dash-dotted curves are separatrices. The arrows give the direction of increasing ξ. A projection of the U, C plane has been chosen such that the behaviour of solutions at infinity is seen. The plot has been taken from [1].

From Meyer-ter-Vehn &. Schalk†

* G. Guderley, “Starke kugelige und zylindrische Verdichtungsstöße in der Nähe des Kugelmittelpunktes bzw. der Zylinderasche,” *Luftfahrtforschung* **19**:302–312 (1942).

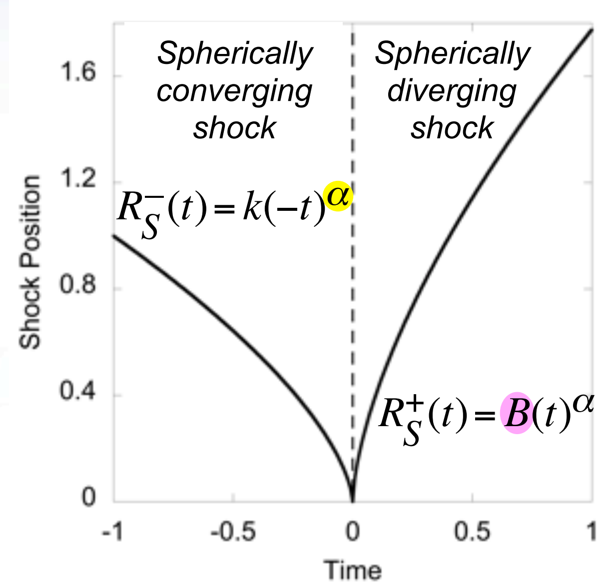
† J. Meyer-ter-Vehn, C. Schalk, “Selfsimilar Spherical Compression Waves in Gas Dynamics,” *Z. Naturforsch. A* **37**:955–969 (1982).

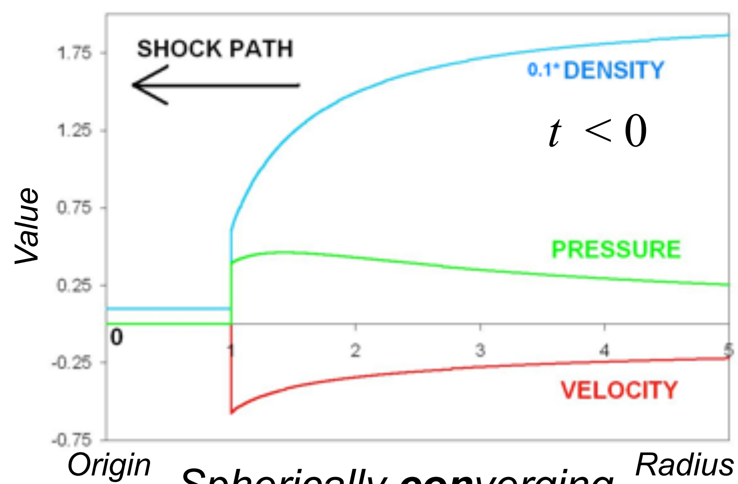
‡ R. Lazarus, “Self-Similar Solutions for Converging Shocks and Collapsing Cavities,” *SIAM J. Numer. Anal.* **18**:316–371 (1981).

The Guderley solution is determined by two nonlinear eigenvalues.

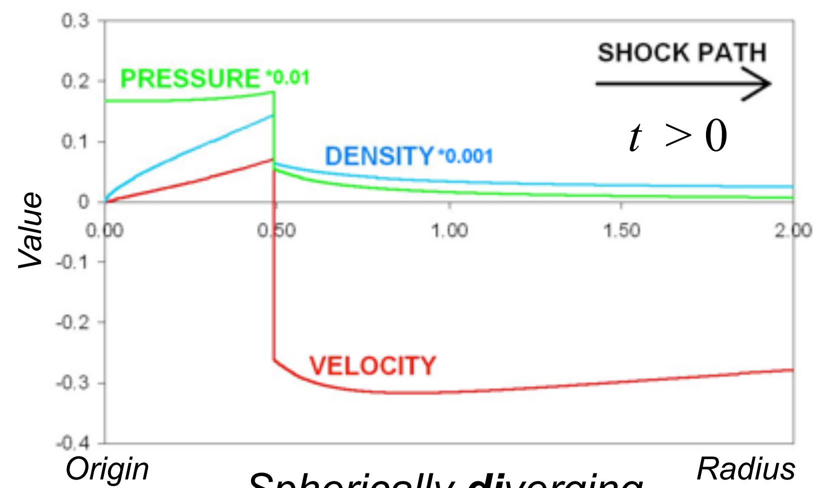
The ODE "Master Equation" and BCs include two unknown parameters:

- The similarity exponent α :
  - Calculated iteratively;
  - Once found, it determines converging solution.
- The reflected shock pre-factor B :
  - Calculated by interconnection between BCs;
  - Once found, it determines diverging solution.
- Solution software remains a research code.





Spherically ***con**verging*



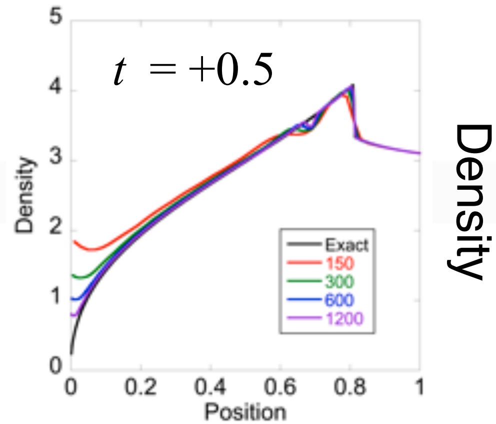
Spherically ***di**verging*

See also: H.G. Hornung et al., *Acta Mechanica* **201**:31–35 (2008), Ponchaut et al., *J. Fluid Mech.* **560**:103–122 (2006).

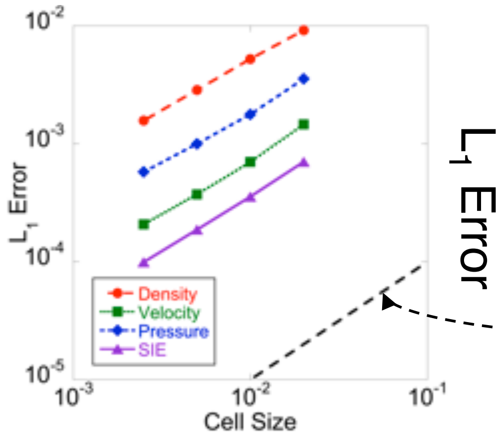
Despite startup errors, the code converged acceptably well — even through reflection*.

Convergent-phase ICs results converge at about 1st order through bounce to divergence.

- Starting at $t = -1$ leads to obvious numerical issues at $t = +0.5$.

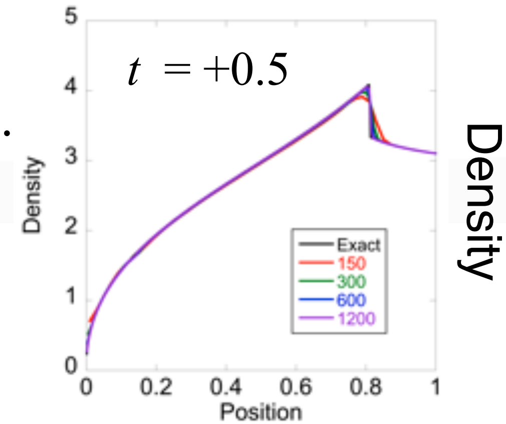


- Almost first order in each variable.

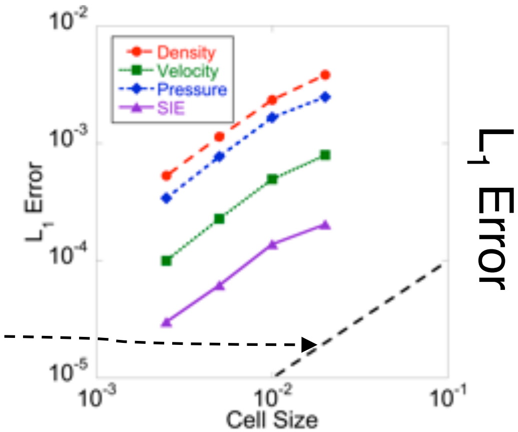


Divergent-phase ICs results converge at about 1st order (without bounce).

- Starting at $t = +0.0186\ldots$ leads to "better-looking" results.



- But with different *absolute* errors.



First order

Give Guderley a go!

* S. Ramsey, J. Kamm, J. Bolstad, "The Guderley Problem Revisited," submitted to *Int. J. Comp. Fluid Dyn.* (2011).

Reinicke & Meyer-ter-Vehn* coupled heat conduction to the Sedov configuration.

RMtV ≈ Sedov + heat conduction

- Coupled physics implies that:
  - The phenomenology is more complex;
  - The solution is <u>*much*</u> more complicated.

Jürgen Meyer-ter-Vehn

- RMtV obtained self-similar solution for delta-function energy ICs using Lie group analysis.
  - Based on the foundational analysis of Coggeshall, RMtV used Lie group analysis to reduce the PDEs to ODEs (+ ICs).
  - To obtain a solution, RMtV wrestled with jump conditions at the shock *and* nontrivial functional behaviors at both the heat front and the origin.
  - The solution method involves Lie group analysis and careful asymptotics based on the mathematical expression of fundamental physical relations.

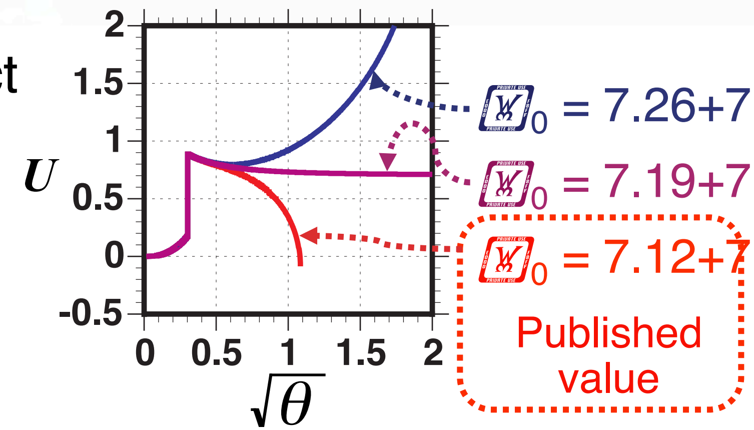
Test coupled physics solutions!

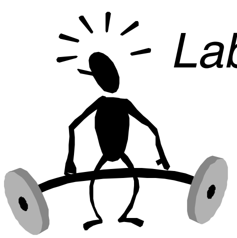
* P. Reinicke & J. Meyer-ter-Vehn, "The point explosion with heat conduction", *Phys. Fluids A* **3**:1807–1818 (1991).

RMtV Problem: The full solution is determined by obtaining the proper value at the origin.

The ODEs form a nonlinear eigenvalue problem in the variables and a parameter b_0.

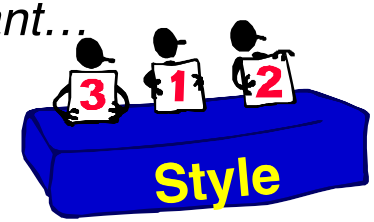
- The appropriate value of b_0 is determined by integrating the solution back from the heat front to the origin (i.e., $r \to 0$).
- Simple "manual bisection" was used to converge to the (ostensibly) correct value of b_0 .
- Comparative evaluation of this result was performed by two separate individuals with two different codes developed completely independently.





Laborious…

Inelegant…



…but it works!

Plots of exact and computed RMtV problem results reveal some discrepancies.

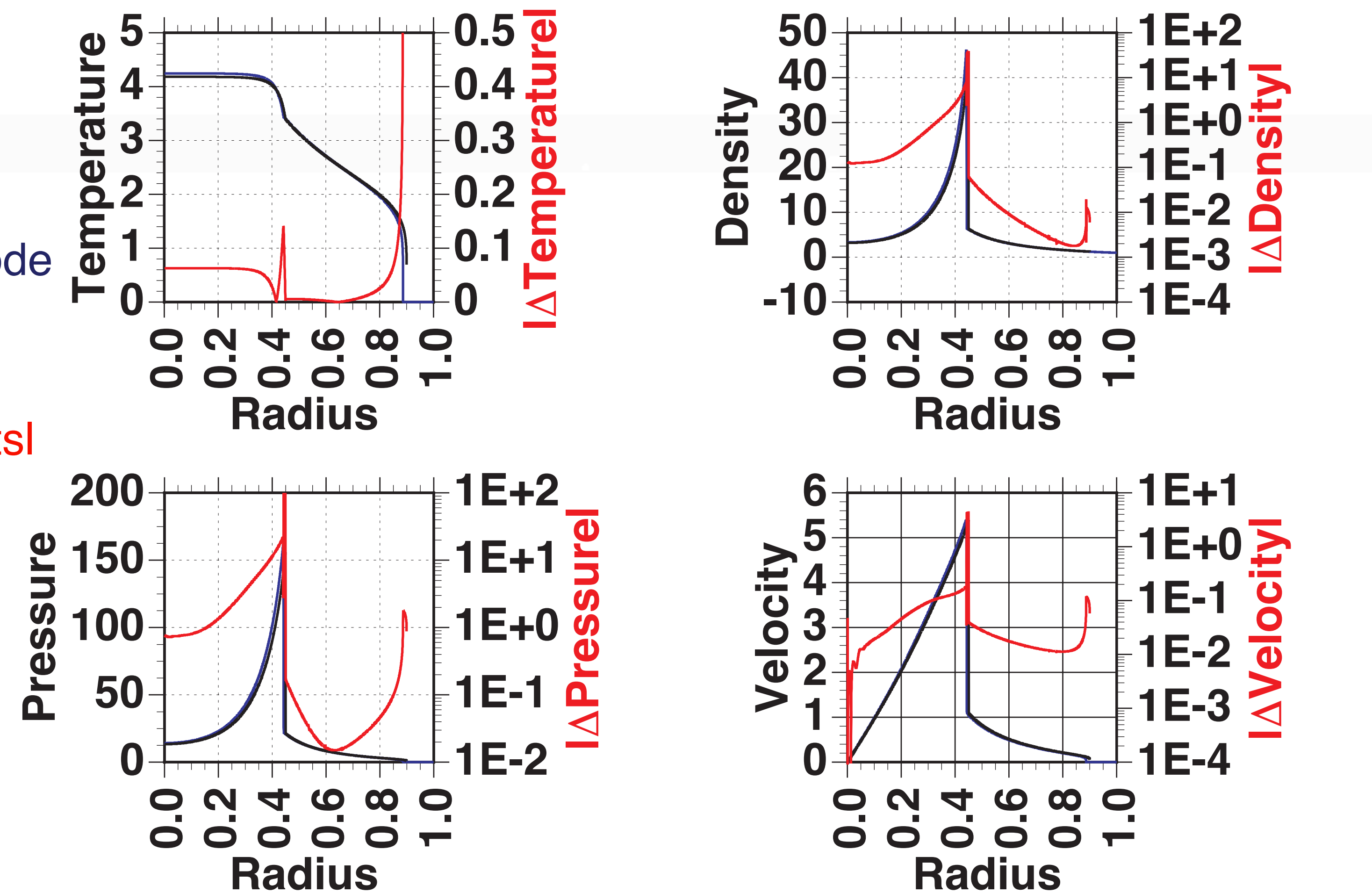
We first solve the ODEs with assigned values, then infer the initial energy, and then use that value in the hydrocode ICs.

- Hydrocode results were computed with with 3200 points on [0,1]:

Hydrocode

“Exact”

IΔResultsI

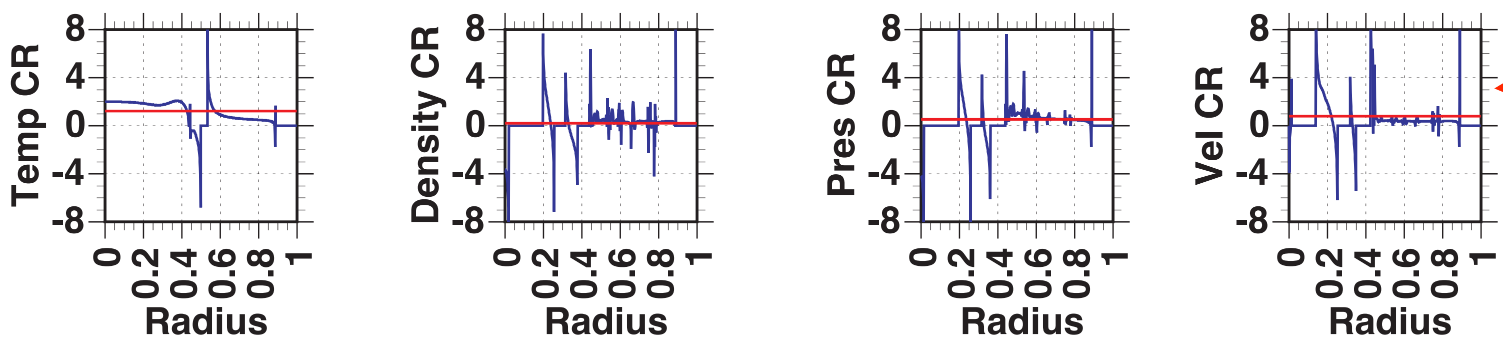


RMtV convergence rates are encouraging but not overwhelming…

Using 1D calculations with 800, 1600, 3200 points on [0,1], convergence rates at the final simulation time were obtained:

Conv. Rate	Dens.	Pres.	Temp.	Vel.
n_{mean}	0.23	0.55	1.22	0.80
n_{L1}	0.39	0.39	0.75	1.25
n_{L2}	0.55	0.55	0.40	0.33
$n_{\mathrm{L\infty}}$	0.09	0.08	-0.03	-0.01

Point-wise convergence rates vs. radius:



"Oldies but goodies" can play key role in the gas dynamics code verification repertoire.

Verification analysis requires a lot of careful bookkeeping.

- Scripting + good coding skills are extremely helpful.

Thanks to countless years of labor by lucky, clever, brilliant, and hard-working technical forebears, there are *many* nontrivial exact solutions for code verification of inviscid, compressible flow.

- Take advantage of this work!
- Test all five Riemann solutions!
- Say "Yes!" to Noh!
- Test all three Sedov solutions!
- *Extra credit*: Give Guderley a go!
- *Extra-extra credit:* Coupled physics!

Fundamental applied math skills remain *vital* in this field.

- Numerics, ODE theory, PDE theory, Lie group theory, asymptotics,…

Take advantage of the solution codes that are out there.

- Check out Frank Timmes' website: www.cococubed.asu.edu

"Whatever you do will be insignificant, but it is very important that you do it."
Mahatma Gandhi

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