LA-UR- 11-04244

Approved for public release; distribution is unlimited.

Title: What the heck are test problems, and what have they done for me lately?

Author(s): Scott D. Ramsey, XCP-8

Intended for: Presentation at the Computational Physics Student Summer Workshop

What the heck are test problems, and what have they done for me lately?

Scott D. Ramsey, XCP-8

Abstract

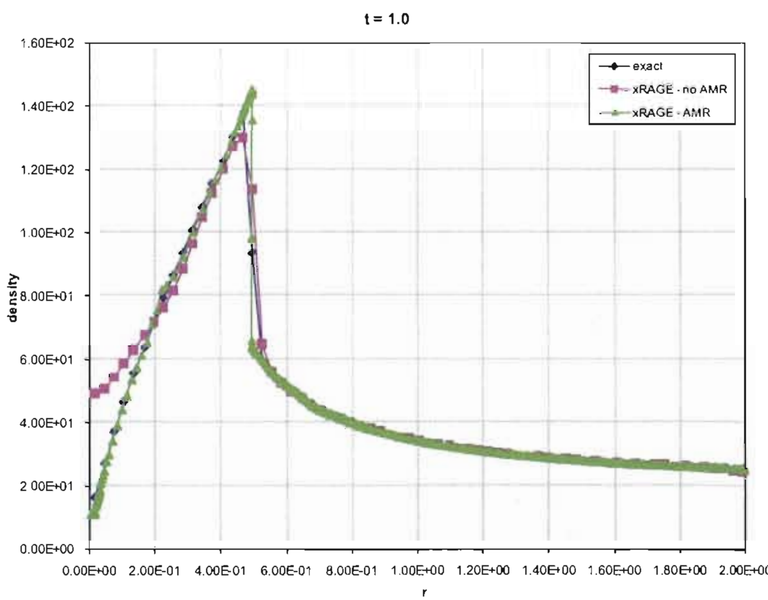
We review various common code verification test problems and associated concepts in this presentation designed for students of the Computational Physics Student Summer Workshop. After a brief overview of code verification and validation concepts, we introduce the three most common test problems used in the compressible flow community: the Noh, Sedov, and Guderley problems. Following a brief discussion of results pertaining to these problems, we investigate their place in a broader class of radiation hydrodynamics test problems that can be systematically derived using Lie group analysis. In the course of this investigation we discuss several example radiation hydrodynamics test problems, including the Kidder, Coggeshall #8, and Reinicke & Meyer-ter-Vehn problems, and variants. Following these developments, we investigate two neutron transport theory test problem sets (the Sood and Ganapol problems) and close the presentation with advice for identifying additional test problems for various physical and computational applications.

What the heck are test problems, and what have they done for me lately?

Scott D. Ramsey, XCP-8

Computational Physics Student Summer Workshop

July 27, 2011

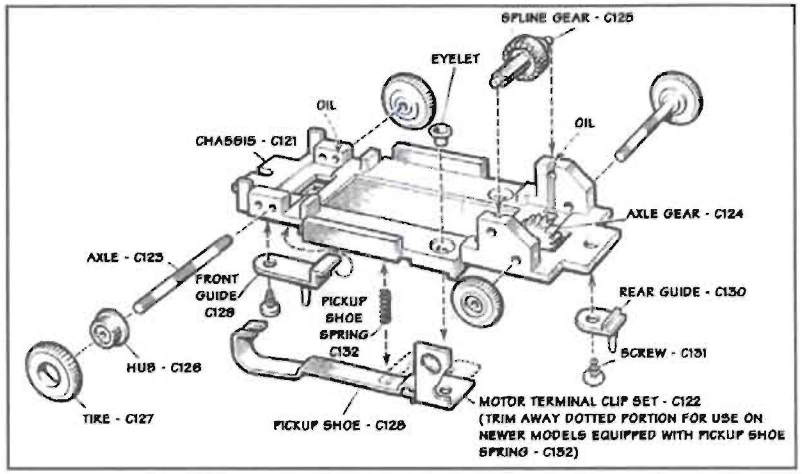


This presentation gives an overview of the test problems we all talk about – and related concepts.

- **Did you get your car checked out before driving to Los Alamos?**
  - Oil change?
  - Rotate tires/check pressure?
  - Anything more serious?
- **Maybe you didn't, and maybe you got here without any problems, but what if … ?**
  - You had a nail in your tire?
  - A cracked engine belt?
  - Identifying problems and getting them fixed before a long trip will surely save you time, money, and effort along the way.

A production code is sort of like a car.

- **A "machine" composed of numerous working parts that are all *supposed* to work together.**
  - For that machine to work as intended, we have to regularly check up on individual or combinations of working parts.
- **For a production code, working parts can be**
  - Physics modules or models,
  - Solution method packages, etc.
- **How do we examine these working parts?**
  - Diagnostics broadly referred to as **test problems**!




```java
public class SetScorer {
    private int[] gamesWon = {0, 0};

    public void gameWon(int player) {
        gamesWon[player-1]++;
    }

    public String getSetScore() {
        int leader = gamesWon[0] > gamesWon[1] ? 1 : 2;
        int leadersGames = gamesWon[leader - 1];
        int opponentsGames = gamesWon[leader == 1 ? 1 : 0];
        String setScoreMessage = null;
        if ((gamesWon[0] < 6 && gamesWon[1] < 6)
                || (leadersGames == 6 && opponentsGames == 5)) {
                    setScoreMessage = "Player" + leader + " leads " +
                      leadersGames + " - " + opponentsGames;
        } else if (gamesWon[0] == gamesWon[1]) {
                    setScoreMessage = "Set is tied at " +
                          leadersGames;
        } else if ((leadersGames - opponentsGames >= 2)
                || (leadersGames == 7)) {
                setScoreMessage = "Player" + leader +
                      " wins the set " + leadersGames + " - " +
                      opponentsGames;
        }
        return setScoreMessage;
    }
}
```

Out of hundreds of choices, we're going to focus on some common test problems.

"How do we get rid of that wall heating error in the Noh problem?"

"These Sedov results with AMR are all screwed up!"

"The Guderley problem will probably barf around bounce time in [insert code name here]..."

- **The idea here is to help you understand what we mean by Noh, Sedov, Guderley, and some others.**
  - … but diagnosing a code can be even simpler.
  - When coding, have you ever put a print statement after a subroutine call to *verify* that things are being read in/written out correctly?
  - Have you ever tested a pre-packaged ODE solver or integration routine on something simple?
  - Even simple tests are valuable for complicated codes.

Outline

- Putting the Vs in "V&V", and just say no to viewgraph norm!
- The hydro triumvirate: the Noh, Sedov, and Guderley problems
- Unification of hydro test problems using Lie groups
- More exotic (multi-physics) animals: Cog8 and Reinicke-Meyer-ter-Vehn
- Unification of rad-hydro test problems using Lie groups
- Blah, weird equations of state, and neutrons, oh my!
- … and that's a wrap!

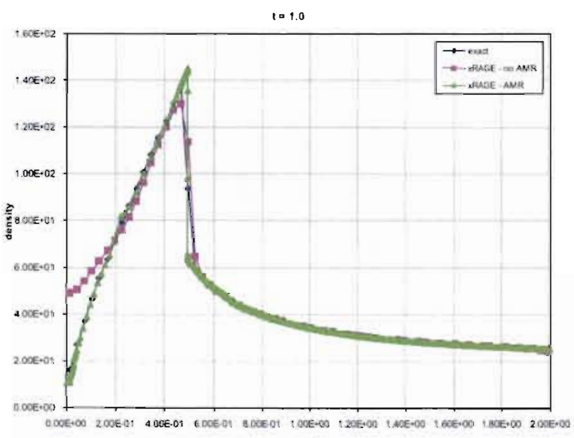
Before we dispense with the preliminaries, here's some obligatory terminology.

- **Code verification: comparison of code output to a known solution of the underlying equations.**
  - *Are we solving the equations correctly?*
  - The first V in "V&V"
- **Code validation: comparison of code output to experimental data.**
  - *Are we solving the correct equations?*
  - The second V in "V&V"
- **Many test problems fall under the scope of these concepts (including all of those we'll be discussing).**
- **Other concepts of interest: calculation verification, uncertainty quantification, calibration, sensitivity analysis, etc...**
  - More on these in an upcoming lecture!

The word "comparison" must be thought about carefully in V&V studies.

Qualitative Metrics

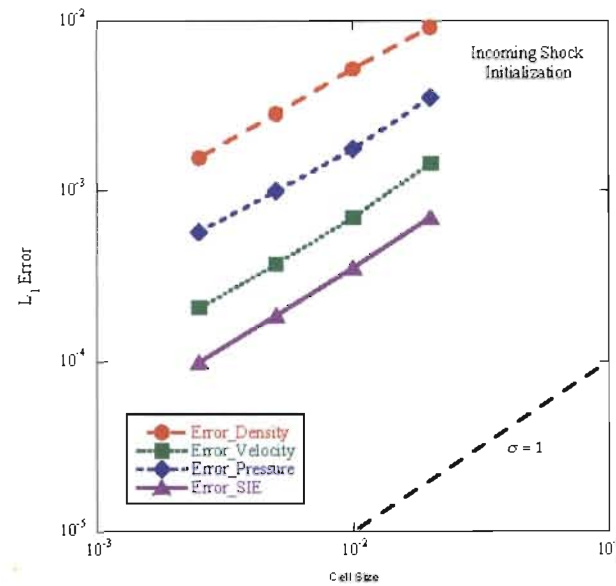
- **"Viewgraph norm"**
  - Plot the known solution and code output on same graph and make a judgment.
  - Manager-friendly…
  - … but not rigorous at all!



"Looks good enough to me!"

Quantitative Metrics

- **Convergence rate**
  - A frequency used error fitting procedure
  - Connected to the code's formal order-of-accuracy



Some of our most well-known hydro test problems didn't start out as test problems!

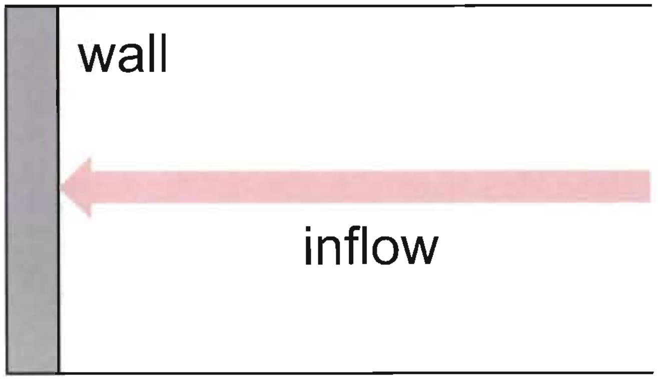
- **You've no doubt recognized that we do a lot of hydro in XCP division!**
  - Three hydro test problems are very well known and extensively used around here – and elsewhere!
  - These problems are special solutions of the compressible flow equations that describe shock wave propagation in simple gases.
  - In some cases, old results derived by the old masters have been reincarnated as test problems.
  - As you work with code, try to remember some simple (and supposedly useless in the real world) derivations from your classes…

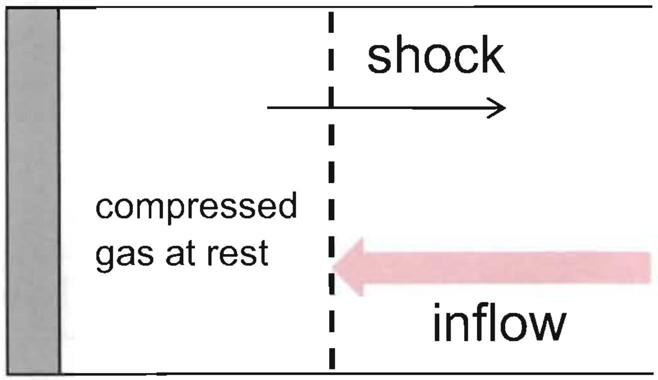

G.I. Taylor


J. von Neumann

The Noh problem is probably the simplest of our three favorite hydro test problems.

- **A big slug of polytropic gas crashing into an immovable wall.**
  - In cylindrical or spherical geometry, the wall is actually an axis/point of symmetry at $r = 0$.
  - The problem starts at the exact moment of impact.
- **Since the “wall” can’t move, the gas that comes into contact with it must come to rest.**
  - A shock wave forms and moves out into the piling-up gas, compressing and bringing it to rest.
  - What is the state of the gas behind the shock? How does the shock move?





For the Noh problem, the state of the shocked gas can be derived in closed-form.

$$u_1 = 0$$

$$\rho_1 = \rho_0 \left(\frac{\gamma + 1}{\gamma - 1} \right)^n$$

$$P_1 = \frac{\rho_0 u_0^2 (\gamma + 1)^{n+1}}{2(\gamma - 1)^n}$$

$$D = -\frac{1}{2}(\gamma - 1) u_0$$

Where:

- Subscript 0 denotes an inflow property
- Subscript 1 denotes a "shocked" property
- n = 1, 2, or 3 for 1D planar, cylindrical, or spherical symmetries
- γ = specific heat ratio
- D = shock speed

- **The post-shock state is a function of symmetry (*n*) and the specific heat ratio (γ) alone. This phenomenon will come up again and again.**

The Noh solution looks simple, but is often difficult for a code to reproduce.

For 1D planar symmetry with γ = 5/3.

The "fly in the ointment" here is the infamous wall-heating error. People much smarter than me have been dealing with this problem for years:

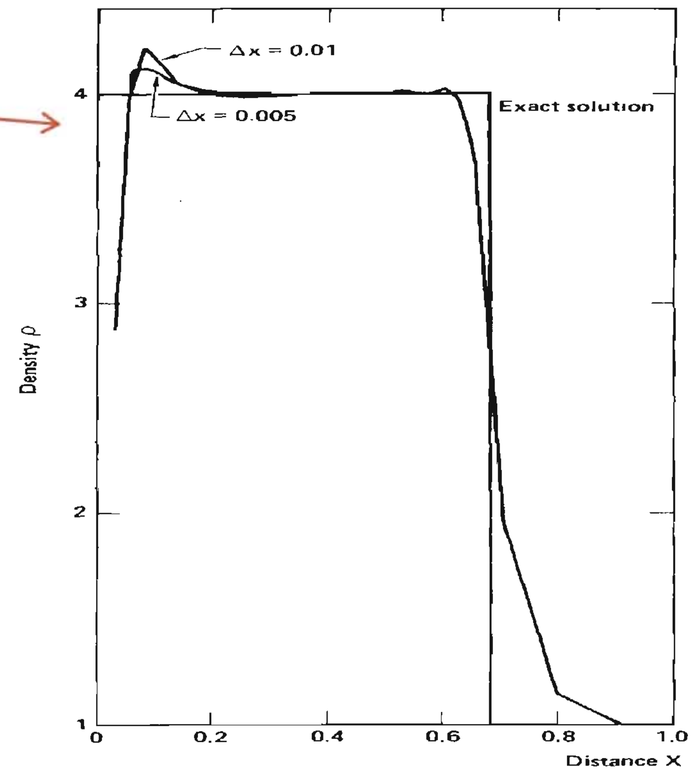
W.F. Noh, "Errors for Calculations of Strong Shocks Using an Artificial Viscosity and an Artificial Heat Flux," *J. Comp. Phys.* **72**, 78-120 (1978).

R.J. Leveque, *Finite Volume Methods for Hyperbolic Problems*, Cambridge University Press, Cambridge, UK (2003).

Where "wall heating" comes from:

$$T \propto 1/\rho$$

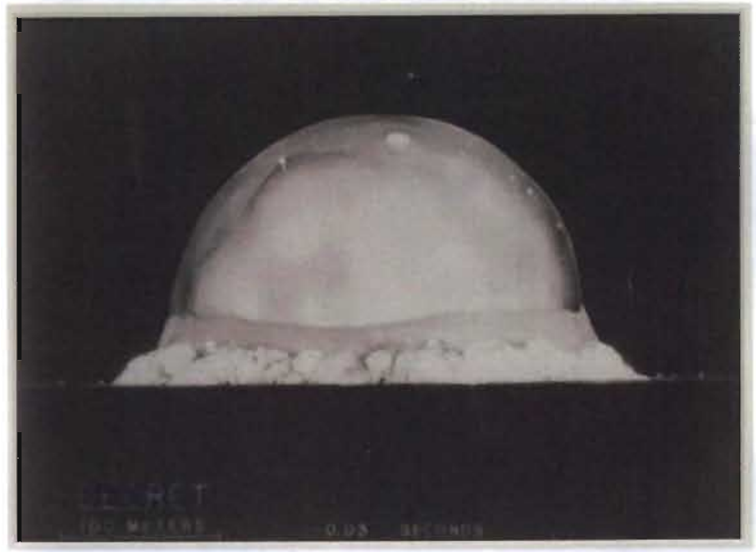
for the polytropic EOS.



(figure borrowed from Noh's awesome paper as referenced on the left)

The Sedov problem is almost as simple as the Noh problem, but for a different reason.

- **Longer name: the Sedov-Taylor-von Neumann problem**
  - Taylor's famous blast wave solution: I first saw this in junior-level hydro
- **A lot of energy instantaneously released at an infinitesimally small point.**
  - By the way, how do you model a point in a finite-sized mesh?
- **A strong shock wave moves out into the surrounding gas.**
  - Typically homogeneous, polytropic.
  - What about the flow behind the shock? How does the shock move?



A whole book about the Sedov problem and variations! Wow!

The Sedov problem has a closed-form solution in terms of the energy released in the explosion.

$$u_1 = 0$$

$$\rho_1 = \rho_0 \left(\frac{\gamma + 1}{\gamma - 1} \right)^n$$

$$P_1 = \frac{\rho_0 u_0^2 (\gamma + 1)^{n+1}}{2(\gamma - 1)^n}$$

$$D = -\frac{1}{2}(\gamma - 1) u_0$$

Where:

- Subscript 0 denotes an inflow property
- Subscript 1 denotes a “shocked” property
- n = 1, 2, or 3 for 1D planar, cylindrical, or spherical symmetries
- γ = specific heat ratio
- D = shock speed

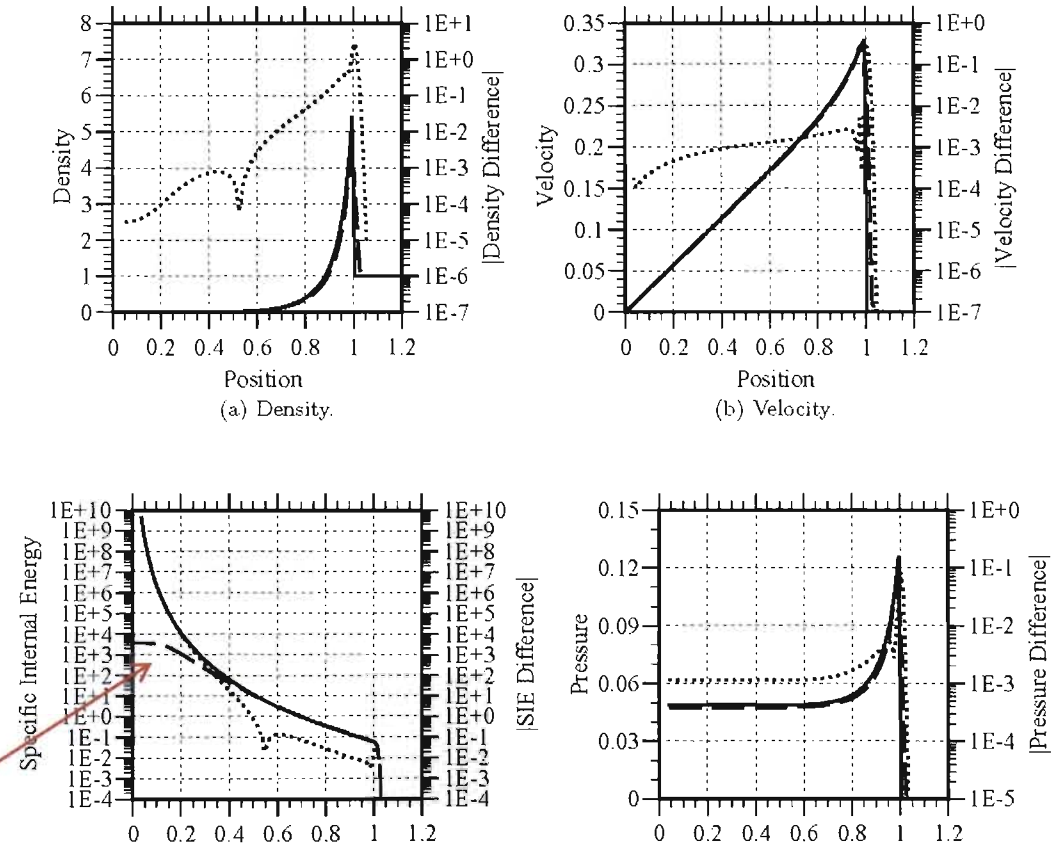
- **The post-shock state is a function of symmetry (*n*) and the specific heat ratio (γ) alone. This phenomenon will come up again and again.**

When simulated in a production code, the Sedov and Noh problems are subject to similar errors.

- For 1D spherical symmetry with $\gamma = 7/5$.
- <u>Solid</u>: exact result
  <u>Dashed</u>: code result
  <u>Dotted</u>: |difference|
- The SIE results show evidence of aof wall error, like the Noh problem.

(Figure borrowed from Jim Kamm's most excellent LANL report, LA-UR-00-6055.)

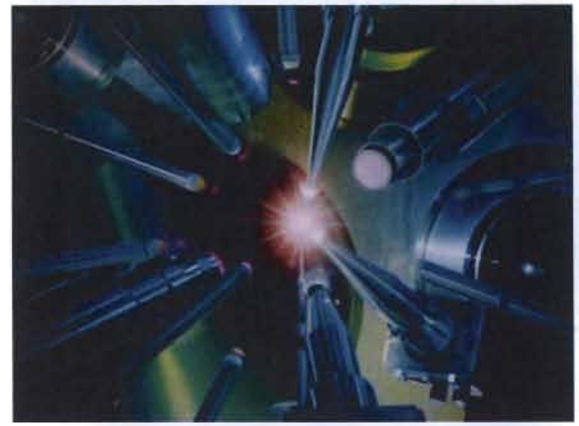
"wall cooling?"

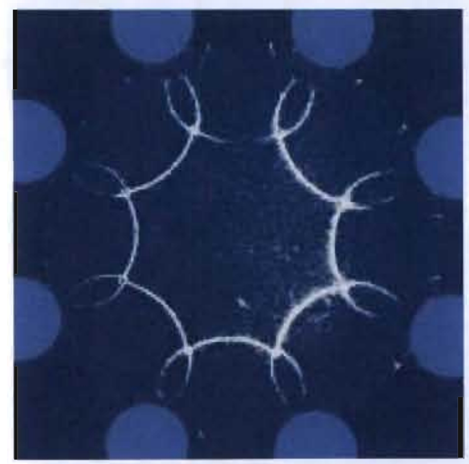


(a) Density. (b) Velocity. (c) Specific Internal Energy. (d) Pressure.

The Guderley problem is the most complicated of our three favorite hydro test problems.

- **A strong shock wave converging into a uniform, non-moving gas.**
  - Where does this shock come from?
  - The pressure increases without limit during shock convergence.
  - What about the flow behind the shock? How does the shock move?
- **The shock "bounces" and propagates back out into the gas.**
  - Bounces off what?
  - How does the flow behave on both sides of the shock? How does the shock move?





Unlike Noh and Sedov, the Guderley problem does not have a closed-form solution.

- **There is no Sedov-like initial energy.**
- **Guderley is a "semi-analytical" test problem - a double nonlinear eigenvalue problem.**
  - It can be reduced from 3 PDEs to a single nonlinear ODE that is more amenable to solution.
- **Some solution approaches:**
  - Phase space and singular analysis →
  - Limiting solution of a cylindrical, spherical shock tube or piston motion
  - Direct solution with high fidelity numerical ODE solvers and root extractors

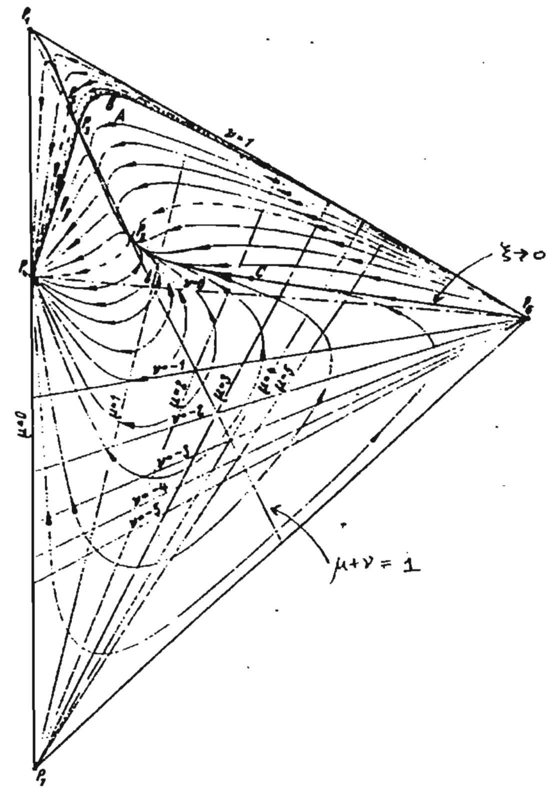


Bild 1. Grundsätzliche Gestalt der Lösungsmannigfaltigkeit in der μν-Ebene.

An example of the phase space analysis approach, borrowed from Guderley's original 1942 paper (in German!)

The Guderley solution seems simple, but the devil is in the details of calculating various important parameters.

$$R(t) = \begin{cases} (-t)^{\alpha}, & t<0 \\ B\,t^{\alpha}, & t>0 \end{cases}$$

$$u = \frac{r}{t}V, \quad \rho = \rho_0 D, \quad c^2 = \frac{r^2}{t^2}C$$

$$\frac{dC}{dV} = \frac{f_1(V)C + f_2(V)C^2}{g_1(V) + g_2(V)C}$$

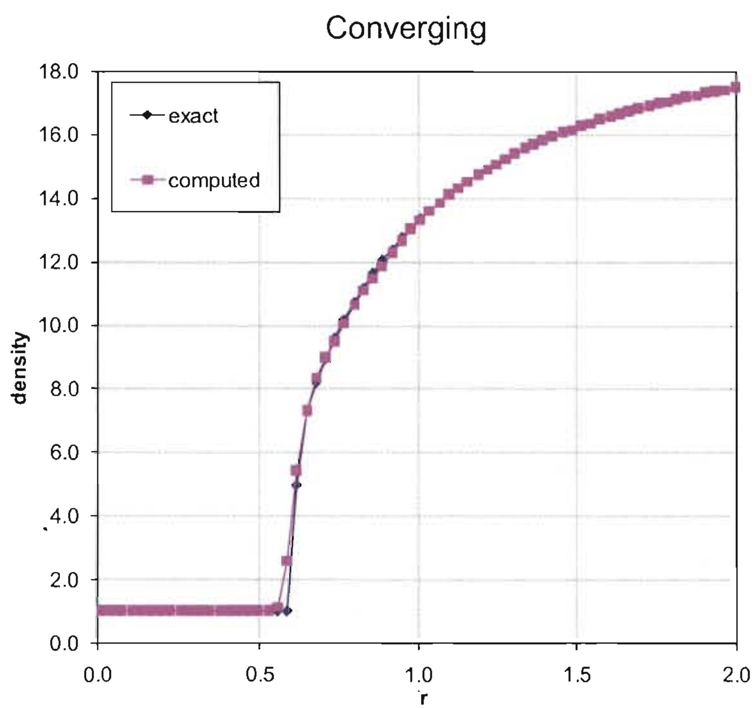
$$\frac{1}{D}\frac{dD}{dV} = \frac{f_3(V) + f_4(V)C + f_5(V)C^2}{g_1(V) + g_2(V)C}$$

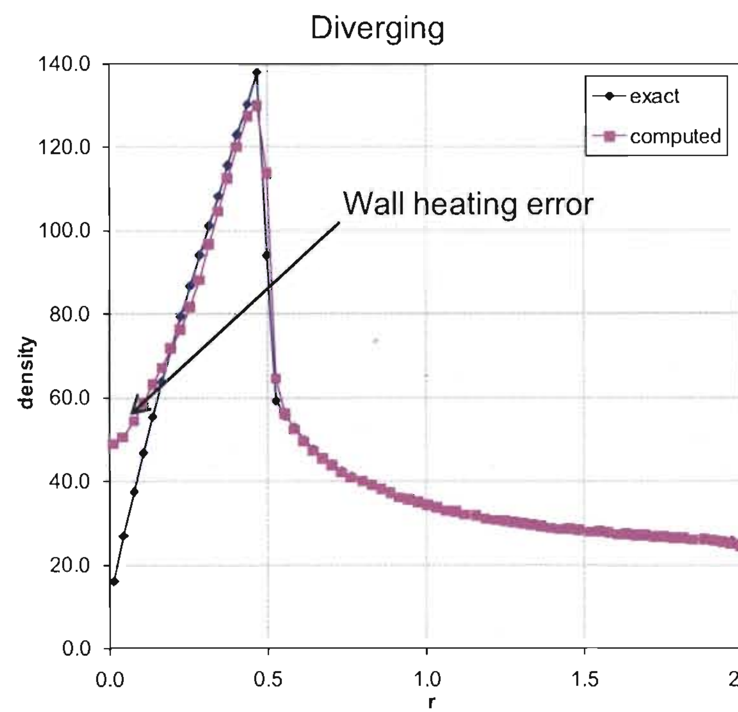
$$\frac{1}{\lambda}\frac{d\lambda}{dV} = \frac{f_6(V) + f_7(V)C + f_8(V)C^2}{g_1(V) + g_2(V)C}$$

- **α = similarity exponent**
  - Root of an analyticity condition
- **B = reflected shock trajectory scale**
  - Determined iteratively with the general-strength shock jump conditions
- **$R(t)$ = shock wave trajectory**
- **V, C, and D = solutions of nonlinear ODEs like that to the left; they are functions of $\lambda(r,t) = r/R(t)$**
- **n = 1, 2, or 3 for 1D planar, cylindrical, or spherical symmetries**
- **γ = specific heat ratio**
- **ρ_0 = density of unshocked medium**

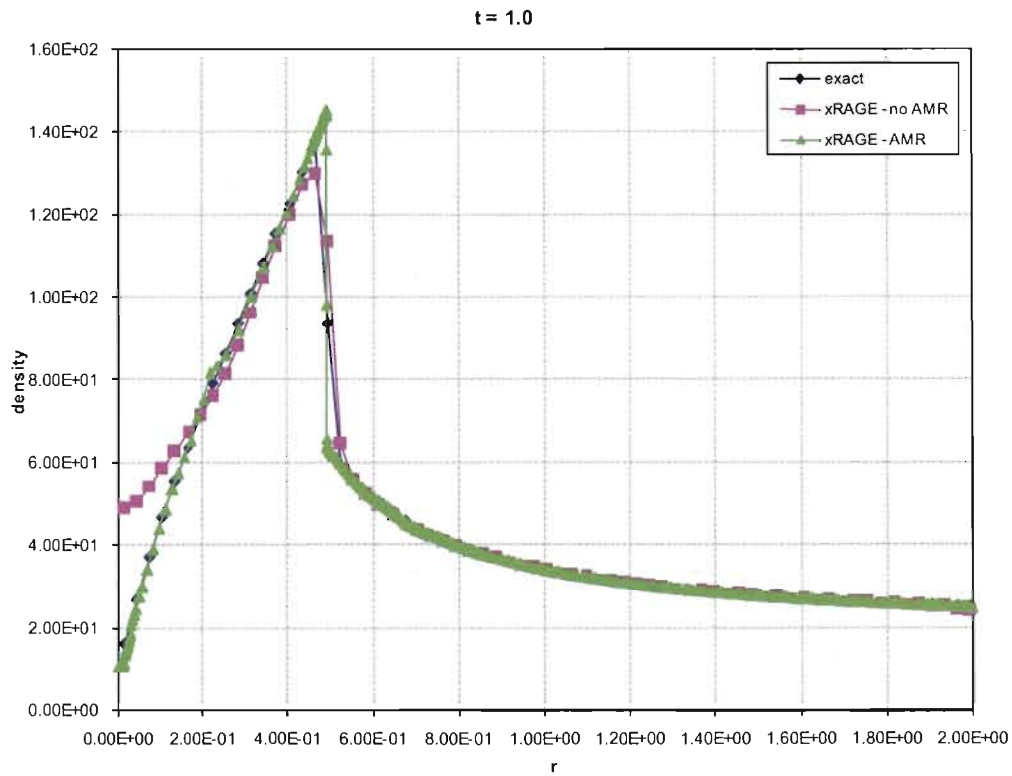
For the Guderley solution, codes suffer from the same pathologies as encountered with Noh and Sedov.

For 1D spherical symmetry with γ = 7/5.





The solutions of the Noh, Sedov, and Guderley problems look suspiciously similar to one another.



The solutions of our favorite hydro problems all look alike because they come from a common family.

- *Common* governing equations

$$\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial r} + \rho\frac{\partial u}{\partial r} + \frac{\rho u(n-1)}{r} = 0$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial r} + \frac{1}{\rho}\frac{\partial P}{\partial r} = 0$$

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

- *Common* scale invariant variable transformations

$$u(r,t) = \frac{r}{t}V(r/R)$$

$$\rho(r,t) = \rho_0 D(r/R)$$

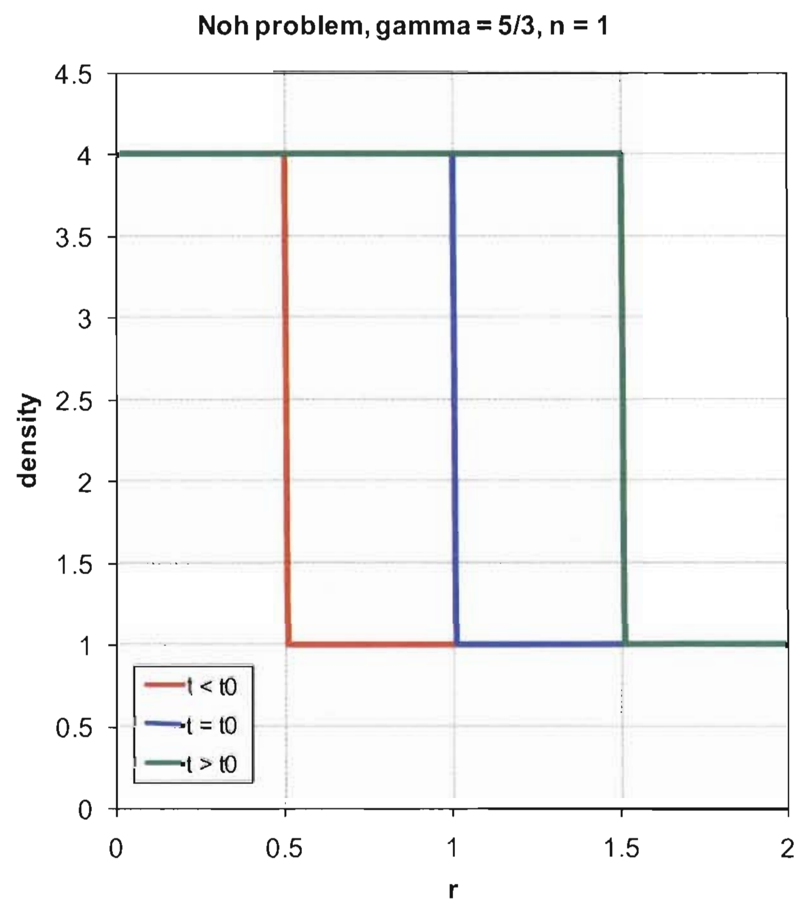
$$c^2(r,t) = \frac{r^2}{t^2}C(r/R)$$

$$R(t) = \begin{cases} (-t)^{\alpha}, & t < 0 \\ Bt^{\alpha}, & t > 0 \end{cases}$$

- The governing equations transform to a *common* system of ODEs.
- Differences arise through initial and boundary conditions.

Scale invariant solutions of the compressible flow equations are said to be "self-similar."

- **The Noh solution has the same shape in space for all times.**
  - Changing the value of time either changes the amplitude of this shape and/or its position along the *x* axis.
  - The units assigned to the *x* and *y* scales depend on initialization (e.g. our choice of units for u_0 and ρ_0).
- **The same is true for the Sedov and Guderley problems.**



Our old friend Sedov again: those Russians know their self-similar problems!

The family of scale-invariant solutions are a part of an even larger family of compressible flow solutions.

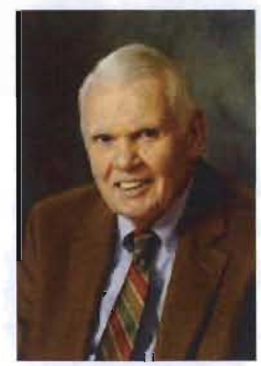
- **The scale invariant variables can be derived using the group invariance properties of the governing equations.**
  - Under what generalized variable transformations do the hydro equations take the same form?
  - This is called Lie group analysis, and involves horrendously involved algebra.
  - Fortunately, most of the work for pure hydro has already been done by Coggeshall (formerly of LANL) and Axford (LANL consultant).

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

$$u = \frac{r}{t} V, \quad \rho = \rho_0 D, \quad c^2 = \frac{r^2}{t^2} C$$

Sophus Lie

Steve Coggeshall



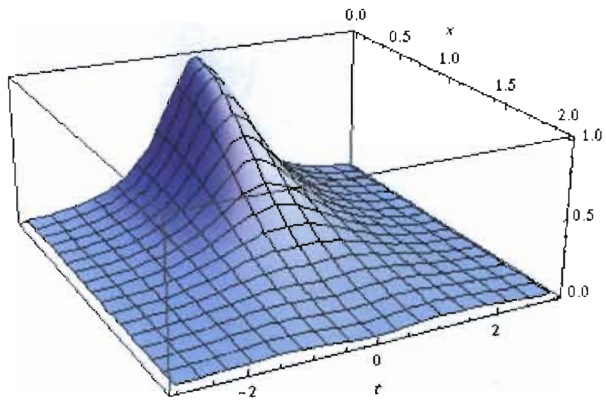
Roy Axford

Many less-familiar hydro solutions can also be found using Lie group analysis.

- **Kidder solution**
  - Shock-free compression and re-expansion of a gas ball

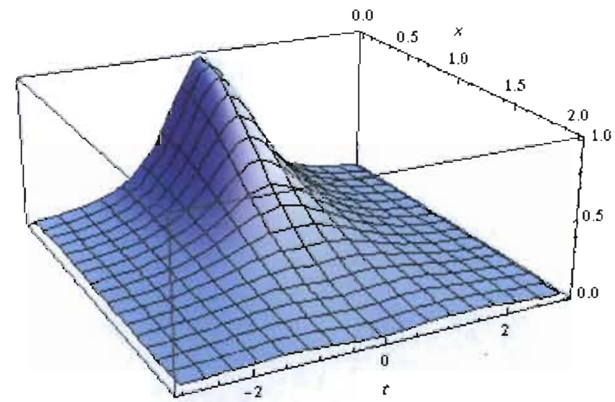
$$\rho(r,t) = \left(1+t^2\right)^{-3/2} \exp\left(-\frac{r^2}{1+t^2}\right)$$

$$u(r,t) = \frac{r\,t}{1+t^2}$$



- **Linear velocity profile family**
  - Shock-free compression and re-expansion of a 1D, arbitrary-shape gas cloud

$$u(r,t) = \frac{\dot{R}(t)}{R(t)} r$$



Coggeshall incorporated additional physics into the Lie group analysis framework.

- **Compressible flow equations with general nonlinear heat conduction**
  - Polytropic gas
  - One temperature for materials and radiation, if included
  - Radiation diffusion approximation to the heat flux *F*, with power law fit to conductivity
  - Can be reduced to classical (linear) heat conduction through appropriate choice of free parameters
- **Lie group analysis yields at least 22 closed-form solutions of these equations, all of which are potential test problems!**

$$\rho_t + u\rho_r + \rho u_r + \frac{(n-1)\rho u}{r} = 0$$

$$u_t + uu_r + \frac{RT\rho_r}{\rho} + RT_r = 0$$

$$\frac{R}{\gamma-1}(T_t + uT_r) + RTu_r + \frac{(n-1)RTu}{r} + \frac{1}{\rho}\left(F_r + \frac{(n-1)F}{r}\right) = 0$$

$$F = -\left(\frac{c\lambda_0}{3}\rho^{c_1}T^{c_2}\right)\nabla aT^4$$

The 8th solution in this series (Coggeshall #8 or Cog8 problem) is a simple multi-physics test problem.

- **This solution represents the shock-free expansion of a *heat conducting* gas cloud.**
  - Similar to the Kidder and linear velocity solutions we've already seen, but with heat conduction added.
- ***n* = 1, 2, or 3 for 1D planar, cylindrical, or spherical symmetries**
- **γ = specific heat ratio**
- **c_1, c_2, ρ_0 and T_0 are arbitrary constants.**

$$\rho(r,t) = \rho_0 r^{(n-2)/(c_2-c_1+4)} \times t^{-n-(n-2)/(c_2-c_1+4)}$$

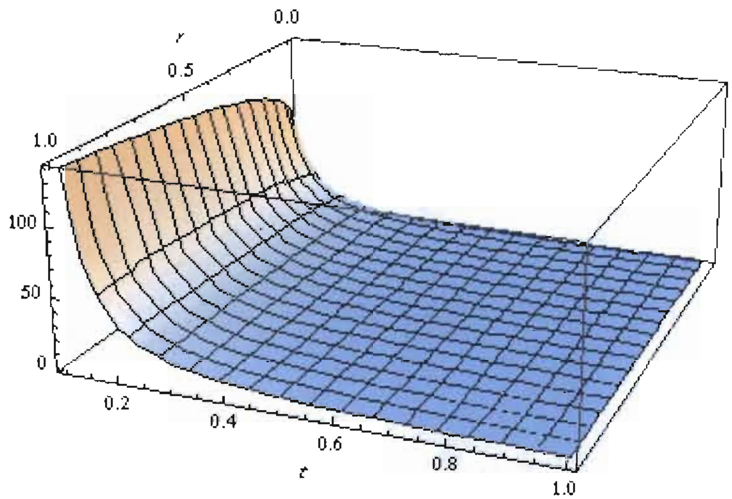
$$u(r,t) = \frac{r}{t}$$

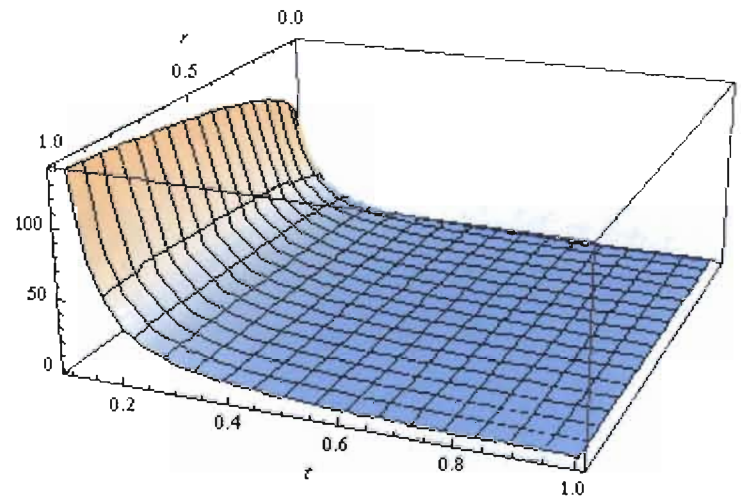
$$T(r,t) = T_0 r^{(2-n)/(c_2-c_1+4)} \times t^{(1-\gamma)n+(n-2)/(c_2-c_1+4)}$$

The standard version of the Cog8 problem includes coupled hydro and radiation diffusion.

- **Radiation diffusion in a spherical ideal gas: $n = 3$, $\gamma = 5/3$, $c_1 = -1$, $c_2 = 2$.**

$$\frac{\rho(r,t)}{\rho_0} = \frac{r^{1/7}}{t^{15/7}} \qquad \frac{T(r,t)}{T_0} = \frac{1}{r^{1/7} t^{13/7}}$$



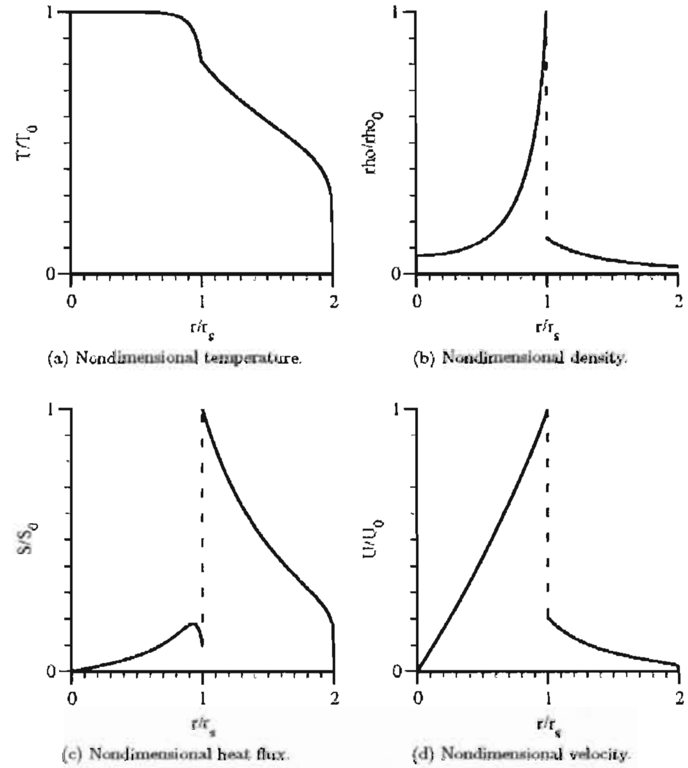


- **Initializing this problem in a code poses some interesting challenges.**

There are many more test problems like Cog8 that have been explored in varying levels of detail.

- **The Reinicke & Meyer-ter-Vehn problem**
  - The Sedov problem with heat conduction.
  - The problem now includes both a shock front and a thermal front.
  - The development and interaction of these two features depends on the material conductivity.
  - Solutions with strong heat conduction tend to be more "smoothed out."

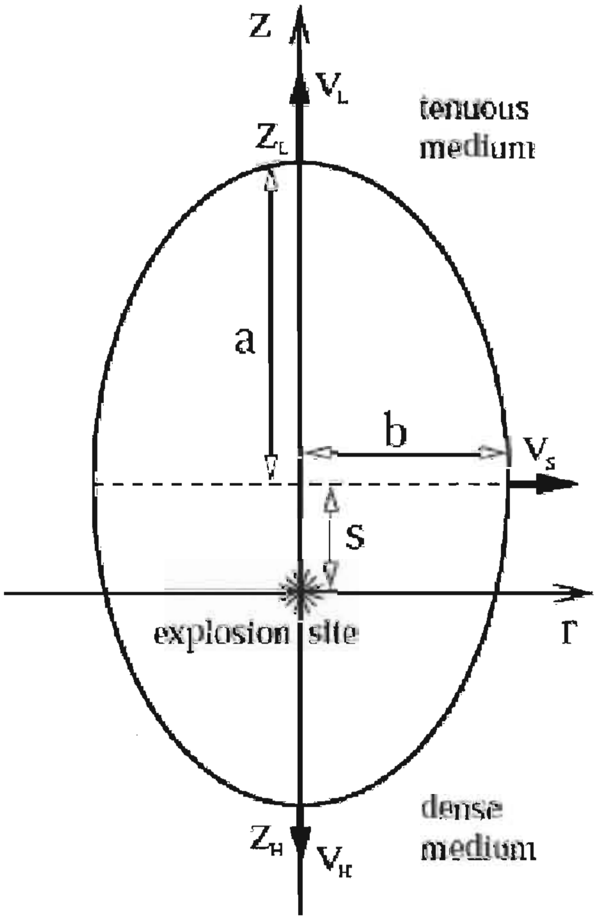
J. Meyer-ter-Vehn: another guy who knows his self-similar problems … and plasma physics … and fusion concepts … and a lot more…



RMtV problem results with strong heat conduction. Figure borrowed from Jim Kamm's most excellent LANL report, LA-UR-00-4304.

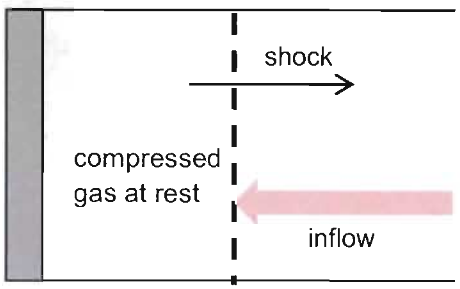
Other "minor changes" to what we've seen can also yield new and non-trivial test problems.

- **Example: what if the ambient gas in the Sedov or Guderley problems is *not* uniform in space?**
  - The Sedov problem becomes an explosion in an inhomogeneous atmosphere when $\rho_0 = \rho_0(r)$
  - The Guderley problem becomes a collapsing bubble when $\rho_0 = 0$
- **Many of these solutions can be found in the literature, and are only waiting to be found and reincarnated as test problems.**



We are also not limited to the polytropic gas equation of state.

- **Lie group analysis can help us identify which equations of state allow for closed-form hydro solutions.**
- **The stiff gas and Mie-Gruneisen equations of state are relatively simple, and allow Noh, Sedov, and Guderley-like hydro solutions.**
- **Example: Noh problem with Mie-Gruneisen EOS**



$$u_1 = 0$$

$$\rho_1 = \rho_0 \left(\frac{\Gamma_1 + 1}{\Gamma_1} \right)^{n+1}$$

$$P_1 = \frac{\rho_0 u_0^2 (\Gamma_1 + 2)^{n+1}}{2\Gamma_1^n}$$

$$D = -\frac{1}{2} \Gamma_1 u_0$$

where $\Gamma_1 = 2/3 + (\Gamma_0 - 2/3) \left[\frac{f_m^2 + 1}{f_m^2 + (\rho_1/\rho_0)^2} \right] \frac{\rho_1}{\rho_0}$

← Transcendental equation for ρ_1

- u_0, ρ_0 = velocity, density of inflowing material
- Γ_0 and f_m = material constants
- Subscript 1 corresponds to shocked material
- D = shock velocity
- N = 1/2/3 for 1D planar/cylindrical/spherical symmetry

We have only scratched the surface when it comes to rad-hydro test problem development.

- **Things we know we can change, and derive test problems**
  - Power-law conductivity fitting parameters
  - Simple EOS model
  - State of the unshocked gas
- **Things we might be able to change and still derive test problems**
  - Different conductivity models?
  - Additional equations of state?
  - Alternatives to radiation diffusion?
  - Include physics beyond rad-hydro?

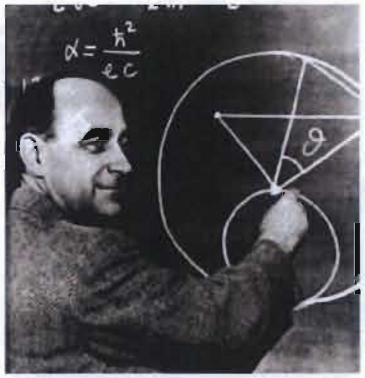
Single-physics test problems are rare and valuable, but multi-physics test problems are even more so!

Hey! What about other types of physics?

- **Neutron transport comes to mind.**
  - The neutron transport equation is arguably even more difficult to solve than the compressible flow equations.
  - Many codes attempt to solve this equation, including MCNP and PARTISN at LANL.

$$
\begin{aligned}
&\nabla \cdot \vec{\Omega}\psi(r,E,\vec{\Omega}) + \sigma(r,E)\psi(r,E,\vec{\Omega}) \\
&\quad = \iint dE' d\Omega' \sigma_S(r,E' \to E, \vec{\Omega}\cdot\vec{\Omega}')\psi(r,E',\vec{\Omega}') \\
&\quad + \frac{1}{k_{\text{eff}}} \iint dE' d\Omega' \chi(r,E' \to E)\nu\sigma_f(r,E')\psi(r,E',\vec{\Omega}') \\
&\quad + Q(r,E,\vec{\Omega})
\end{aligned}
$$

Do neutron transport test problems exist?



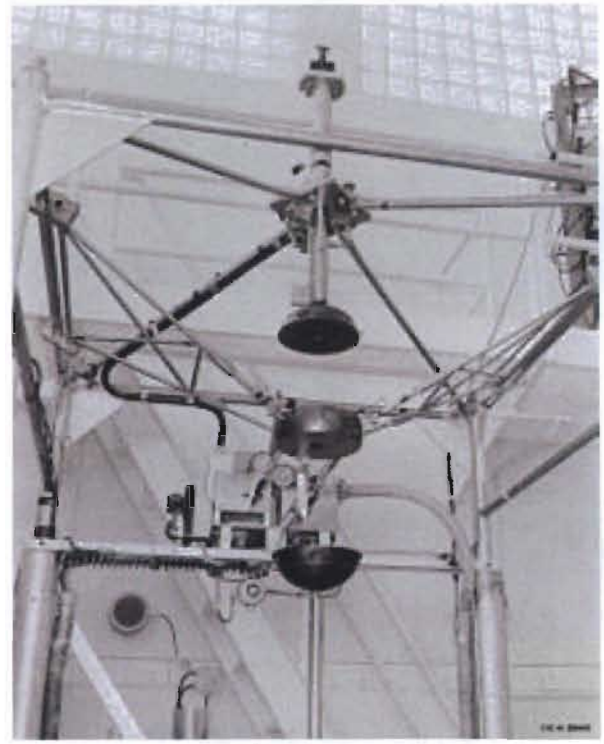
This is the time-independent, inhomogeneous neutron transport equation.

The neutron flux ψ is a function of space, angle, and energy.

Exact solutions of this equation are very difficult to come by!

The Sood problems have more to do with validation than verification, but they're still very useful.

- **Criticality verification benchmark test set**
  - Consists of 75 model U-235 and Pu-239 critical assemblies.
  - Employs the multi-group diffusion approximation to neutron transport.
  - Device dimensions are presented in various configurations (bare, moderated, reflected) so that $k_{eff} = 1.0$ in each case.
- **Verification vs. validation**
  - The Sood problems more likely fall under the purview of validation because they use empirical cross section data.
  - Good for testing cross section data!



Godiva critical assembly

The Ganapol neutron transport test problem set is more diverse.

- **Case studies in neutron transport theory**
  - Neutron slowing down
  - Monoenergetic transport
  - Multigroup transport
- **These problems calculate k_{eff} (when applicable) and more**
  - Lethargies
  - Fluxes
- **To my knowledge, many of these problems have not been implemented for LANL codes**

We are always looking for more test problems in any branch of physics.

- **Test problems in any field are difficult to come by.**
  - Developing them can be tedious, always involving a serious understanding of the underlying equations, and often involving a good deal of analytical work.
  - Attempting to reincarnate results from the literature can be equally tedious.
- **As you work with code, try to remember those simple (and supposedly useless in the real world) derivations from your classes!**

There's an app for that!

- **A smart code developer or user will make use of test problems to assess the physics models included in the code.**
  - Most LANL codes have extensive test suites that are run with regularity, so the impact of changes can be assessed.
- **Test problems aren't just for physics models, and can be developed for…**
  - … solution methods,
  - interface with empirical data,
  - code structure and I/O,
  - … if you can think of a code component, there's a test problem for that!

- **The keys to physics test problem development and use are:**
  - Understand what equations your code is supposed to be solving.
  - Understand what equations your test problem solves.

Who knows – maybe in a few years we'll all be talking about the [your name here] problem…

Summary

- **When you leave the room, remember these five points!**
  - Verification: are we solving the equations correctly? Validation: are we solving the correct equations?
  - Don't be tempted by viewgraph norm!
  - The Noh, Sedov, and Guderley hydro test problems are very "self-similar" to one another (bad test problem pun)!
  - Lie group analysis is a systematic way of constructing more exotic rad-hydro test problems.
  - Test problems aren't limited to rad-hydro or any one branch of physics; they're useful for any code developer or user.
- **Thanks for listening – any questions?**