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An Example of Verification Analysis for an Eulerian Hydrocode (U)

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An important activity in the process of code development is code verification, by which we mean detailed examination of and numerical demonstration that the equations are being solved correctly. This process can entail the comparison of code calculations for problems that possess analytic or quasi-analytic solutions. In this presentation we provide results of a verification analysis of the RAGE hydrocode for two particularly challenging problems: (1) the pure hydrodynamic problem of an adiabatically compressing region, and (2) the coupled hydrodynamics/conduction problem of Reinicke & Meyer-ter-Vehn. We present comparison of code results with the analytic solutions and convergence rates for these cases.

Keywords: verification, validation, Eulerian hydrocode

Introduction

The results of hydrocode calculations may "look good", but can be physically questionable and sometimes inaccurate. A critical step on the path to *science*-based simulation of complex phenomena is the *verification* of the physics in the computer codes that are used. That is, one must demonstrate quantitatively that one is indeed solving the equations that one purports to be solving. We approach this daunting task for the Eulerian hydrocode RAGE by examining two problems: the pure hydrodynamic case of an adiabatically compressing region, and the coupled hydrodynamics/conduction problem of Reinicke & Meyer-ter-Vehn. The former is a completely smooth problem consisting of a converging flow, while the latter involves a point source of energy that expands into a compressible, heat-conducting medium. We first discuss the terminology and philosophy of verification and validation (V+V), then turn our attention to applying those notions to the two problems mentioned. We find that RAGE converges for each of these problems, although the convergence rates obtained exhibit some curious features.

Code Verification

The issue of computational quality is a central theme in the credibility of science-based stockpile stewardship. One of the fundamental pillars upon which this scientific enterprise must be based is code verification, or, more precisely, code physics verification. We follow the evolving standard in our definition of *code verification being the quantitative demonstration that a simulation code accurately represents the chosen description of the model.* More succinctly, code verification is the demonstration that the code is solving the equations correctly.

Code verification is related to but distinct from other fundamental aspects of the code evaluation process (AIAA 1998). More specifically, code verification is **not**

- *code validation*, which is the process of determining the degree to which a code provides an accurate representation of the intended physical phenomena (i.e., that the code is solving the right equations for the physics of interest) and, as such, requires quantitative comparison of code results with experimental data;
- *software V+V*, which involves methods from Software Quality Assurance (SQA) and Software Engineering (SE) and, being intrinsic to the software development process, depends on an individual code's development practices;

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- *benchmarking*, which is another term for *code-to-code comparison*, which, while a critically important activity in the transition from legacy codes to ASCI codes, is technically not part of either verification or validation (perhaps "quasi-validation" is appropriate).

Each of these four processes, viz., code verification, code validation, software V+V, and benchmarking, has unique characteristics and should not be confused with any of the others. Consistent use of nomenclature in this evolving discipline will act to minimize confusion and misunderstanding among researchers. Additionally, each of these procedures has a role to play in the process of establishing the credibility of a simulation process, e.g., a computer code.

As we have observed on numerous previous occasions, one highly dubious practice sometimes witnessed within the simulation community is the use of the "viewgraph norm," which takes its name from the practice of deftly positioning one viewgraph of computational results upon another and claiming "convergence." This practice is predicated upon the inability of the human eye to distinguish between the two results at the scale to which they are plotted. Such a procedure is both virtually meaningless scientifically and inexplicably widespread; we respectfully petition our colleagues to abandon this practice. While we acknowledge the use of "eyeball comparisons" as providing an imminently useful sanity check, the code verification procedure we apply herein obviates the need for attaching any misplaced hope of scientific credibility to the "viewgraph norm."

This appeals begs the question, "How is code verification done?". The simplest answer to this question is "Quantify the error in the computed solution"; more specifically, we offer the following three fundamental approaches, which we describe subsequently in some detail:

1. quantify the solution error with exact or quasi-exact solutions;
2. perform convergence analysis;
3. employ the method of manufactured solutions.

By quantification of the solution error for problems with exact or quasi-exact solutions, we mean compute the difference between the computed and exact solutions. By "quasi-exact solutions" we refer to those obtained under restrictive conditions such that, e.g., the equations reduce to a quadrature, or a set of PDEs can be reduced to a set of ODEs, etc. In such cases, the exact solution provides the "gold standard" with which the error in the computed solution can be calculated in a number of meaningful metrics, e.g., the L_1, L_2, or maximum (L_∞) norms.

Convergence analysis can be accomplished for problems with or *without* exact solutions. The cornerstones of this method are the *Ansätze* that (1) the problem is pointwise deterministic (so that a unique, converged solution can be obtained), and (2) the difference between the exact and computed solutions for a variable ξ can be expanded as a polynomial function of the grid spacing:

$$\xi^* - \xi_i = A(\Delta x_i)^n + o((\Delta x_i)^n)\,, \tag{1}$$

where ξ^* is the exact value, ξ_i is the value computed on the grid of spacing Δx_i, A is a constant (the "convergence factor"), and n is the asymptotic convergence rate. In this expression the notation "$o((\Delta x_i)^n)$" represents terms that approach zero faster than $(\Delta x_i)^n$ as Δx_i becomes vanishingly small. The frequently cited "second-order accuracy" corresponds to the case in which $n = 2$. By computing the solution on three different (uniform) grid spacings, subscripted c for coarse, m for medium, and f for fine, the following expression for the asymptotic convergence rate can be derived:

$$n \approx \log[(\xi_m-\xi_c)/(\xi_f-\xi_m)] \,/\, \log(\Delta x_c/\Delta x_m)\,. \tag{2}$$

Roache (1998) gives a useful overview of this approach, while Kamm and Rider (1998) provide a detailed discussion of this technique as applied to the RAGE hydrocode.

The "method of manufactured solutions" is a procedure that begins with an assumed analytic expression being substituted into the governing equations. Since this expression is, in all likelihood, *not* a solution to the equations, additional terms are created due to the operation of the left-hand side of the equations (i.e., containing the differential operators). These additional terms are used to modify the right-hand side (RHS) of the original equations so that the chosen analytic expression exactly satisfies the modified equation. One must modify the computer code to include the additional RHS terms. Additionally, care must be taken with respect to initial and boundary conditions with this method. Salari & Knupp (2000) provide a detailed discussion of this approach. One restriction of this technique appears to be the inability to capture discontinuous behavior (e.g., shocks) in the manufactured solutions, particularly in more than one dimension; however, this technique is still evolving and may yet overcome this limitation.

The RAGE Hydrocode

The calculations in this paper were performed with the RAGE hydrocode (Baltrusaitis et al. 1996). This code is a 1-, 2-, or 3-D, Eulerian adaptive mesh refinement (AMR) code that uses a high-resolution Godunov method as the hydrodynamics integrator. Additionally, RAGE has packages for the calculation of conduction, gray-diffusion, as well as *many* other useful features. For additional information, the interested reader is referred to the work of Batrusaitis et al. (1996) or encouraged to contact Michael Clover (mrc@lanl.gov).

In the present study, only 1-D, spherically symmetric calculations were performed. The problems considered can be extended to higher dimensions. The problems considered exercised the pure hydrodynamics (adiabatic compression) and the hydrodynamics + conduction (Reinicke & Meyer-ter-Vehn) capabilities of the code.

The Adiabatic Compression Problem

The adiabatic compression problem is one of the many problems catalogued by Coggeshall (1991) that provide an exact solution to the Euler equations of hydrodynamics. This problem provides an ideal verification problem because it has an exact solution and is a 1D, 2D, or 3D problem that tests the entropy and energy conservation of a code–neither the entropy nor energy should change.

The initial condition for this problem are those of uniform initial density and uniform initial specific internal energy (SIE), with an initial inward radial velocity proportional to the radial distance from the origin:

$$\rho_0(r)=1,\ e_0(r)=1,\ u_0(r)=-r\,. \tag{3}$$

The exact solution of the Euler equations for these initial conditions is given by

$$\rho(r,t)=1/(1-t)^3,\quad e(r,t)=1/(1-t)^{3(\gamma-1)},\ u(r,t)=r/(t-1)\,. \tag{4}$$

It is clear from these expressions that the solution becomes singular as time approaches unity, but remains smooth up to that time.

The RAGE results at t=0.9 are shown in Fig. 1, which contains plots of the computed radial velocity (left) and SIE (right). In these plots, the solid lines, plotted against the left axis, denote the computed solution for 100 (red), 200 (green), 400 (blue), and 800 (violet) points on the unit interval; the dashed lines, plotted against the right axis, denote the absolute difference between the computed and exact solutions. For both the velocity and SIE the computed solutions appear to overlay; however, *quantitative comparison* with the exact solutions reveals mesh-dependent variation in the computed solution. Indeed, one might qualitatively infer from these results that the code is performing as expected for this smooth problem, i.e., with ("eyeballed") second order accurate convergence.

Using the pointwise differences in the computed solution one can determine if this is indeed the case by computing both the pointwise and mean asymptotic convergence rates according to Eq. 2. Those results are plotted in Fig. 2 for the velocity (left) and SIE (right). These plots contain the pointwise convergence rates using the 100-200-400 results (red) and the rates using the 200-400-800 (green). The dashed lines in these figures represent the mean convergence rate of the L_2 norm calculated over the unit domain using the 100-200-400 results (blue) and the 200-400-800 results (violet), the results of which are identical to four significant figures for the velocity. For the velocity, the pointwise rate can be computed over only a limited regime, since the terms in the convergence rate expression (Eq. 2) yield nonsensical (i.e., infinite, indeterminate, or imaginary) results otherwise; in the plot, those values are set to a hard zero. Near the origin, the pointwise rate is as expected, i.e., approximately two. The mean L_2 rate is approximately 1.6. Both of these results are within anticipated values for the code. The question remains, however, as to why the convergence rate becomes nonsensical away from the origin. For the SIE, the results unambiguously reveal a convergence rate of approximately one, suggesting that there may be some discrepancy in the values of the SIE either computed or output by the code. One would anticipate that these convergence rate values would be comparable to those of the velocity, i.e., approximately two.

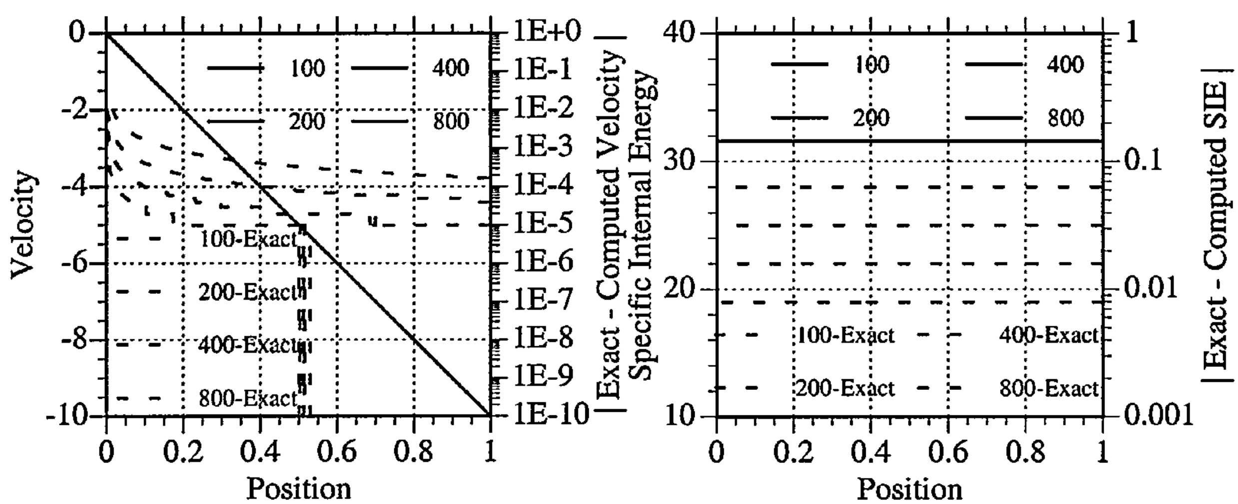

Figure 1. Computed velocity (left) and SIE (right) at t=0.9 for the adiabatic compression problem. The solid lines (left axis) are the calculated values for 100 (red), 200 (green), 400 (blue), and 800 (violet) points on the unit interval. The dashed lines (right axis) are the differences between the calculated and exact values.

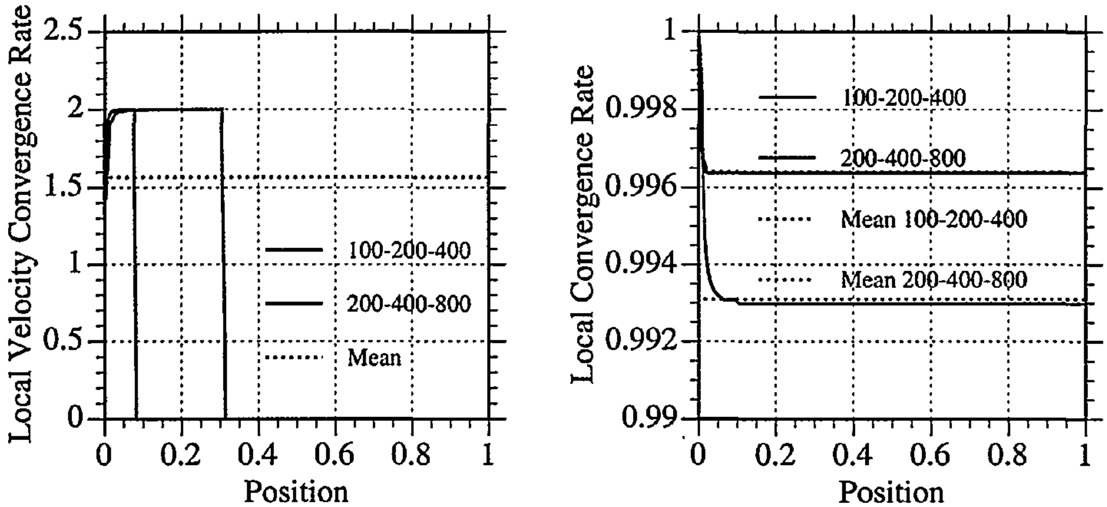

Figure 2. Asymptotic convergence rates for calculated velocity (left) and SIE (right) at t=0.9 for the adiabatic compression problem. The solid lines are the pointwise convergence rates using the 100-200-400 calculations (red)· and 200-400-800 calculations (green). The dashed lines are the mean L2 convergence rates for the 100-200-400 calculations (blue) and 200-400-800 calculations (violet), which match to four significant figures for the velocity.

The Reinicke & Meyer-ter-Vehn Problem

The Reinicke & Meyer-ter-Vehn problem (RMtV) is the 1D, 2D, or 3D spherically symmetric, point-source-of-energy problem, *à la* Sedov (1959), including compressible hydrodynamics and heat conduction. The self-similar case considered by Reinicke & Meyer-ter-Vehn (1991) reduces to a set of ODEs, thereby qualifying this problem as one of the few *multiphysics* verification problems as it has a quasi-exact solution.

A complete explanation of the RMtV problem is given in the publication of Reinicke & Meyer-ter-Vehn (1991), to which the reader is referred for more information; this problem has also been considered in some detail by Shestakov (1999). One key assumption in allowing a self-similar solution is that the heat conductivity χ has the form

$$\chi=\chi_0 \rho^a T^b, \text{ with } a\leq 0 \text{ and } b\geq 1 . \tag{5}$$

The set of ODEs to which the governing equations reduce is given below in Eq. (6).

$$\begin{aligned} U' + (U-1)(\ln H)' &= \sigma - (n+\kappa+\sigma)U \\ (U-1)U' + \Theta(\ln H)' &= U\left(\alpha^{-1} - U\right) + \Theta(2\Omega - \kappa - \sigma) \\ U' + W(\ln H)' + W' &= \Omega[\mu(U-1) + 2W] + \mu\left(\alpha^{-1} - 1\right) \\ &\quad - nU - (n+\kappa+\sigma)W \\ (\ln\Theta)' &= -2(1+\Omega) \end{aligned} \tag{6}$$

In these equations, the variables U, H, W, and Θ are related to the velocity, density, heat flux, and temperature, respectively. The quantities α, n, κ, σ, μ are all parameters related to physical constants, while Ω is a complicated combination of parameters and variables.

The problem we consider is that of an initial energy of approximately 234.2 deposited at zero-time into a polytropic gas with $\gamma = 5/4$. The second key assumption that is critical to the existence of a self-similar solution is that the initial density field varies as an inverse power of the position; for the present case, the initial state is determined by

$$\rho_0(r)=r^{-19/9},\ e_0(r)=0,\ u_0(r)=0\,. \tag{7}$$

A complete explanation of the present RMtV problem is given in Section 4.4 of the report by Kamm (200).

The results for the temperature and density at $t\approx 0.05125$ for this problem are shown in Fig. 3 in the plots on the left and right, respectively. These plots contain the values of these quantities as calculated by RAGE (blue) as well as the results obtained from the ODEs given in Eq. 6 (green). Comparison of the calculated and quasi-exact results indicates slight mismatches in the positions of the shock and the heat front. This discrepancy is related to the slight difference between calculated and quasi-exact values (red). We speculate that this slight inconsistency between the two solutions may be related to the initial conditions imposed on the computation RAGE grid: whereas the quasi-exact solution uses the precise delta-function initial condition (i.e., finite initial energy deposited at r=0 at t=0), the RAGE calculation has the initial energy deposited in the single near-origin zone at the initial time. This difference, while small, has a nontrivial effect on the subsequent flow evolution.

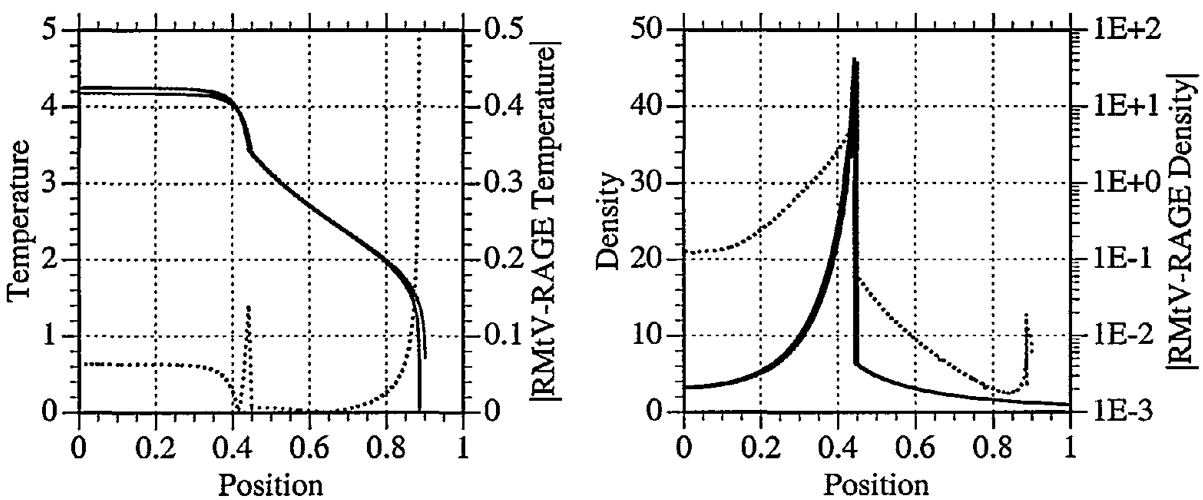

Figure 3. Temperature (left) and density (right) for the strong conduction RMtV problem at t=0.0512512. The solid lines (left axis) are the calculated values (blue) for 3200 points on the unit interval and the quasi-exact values (green) at the identical positions. The dashed line (red), plotted against the right axis, is the difference between the calculated and quasi-exact values.

As in the adiabatic expansion problem, one can compute the pointwise and mean asymptotic convergence rates according to Eq. 2 using the calculated solution on three different grids. Those results are plotted in Fig. 4 for the temperature (left) and density (right). These plots contain the pointwise convergence rates (blue) using results calculated with 800, 1600, and 3200 points on the unit interval. The dashed lines in these figures represent the mean convergence rate of the L_2 norm (red) calculated over the unit domain using the 800-1600-3200 results. For the temperature (left plot in Fig. 4), the pointwise asymptotic convergence rate is seen to hover around the value of two near the origin, to vary significantly in the vicinity of the shock, and to be about one-half near the heat front. For this variable, the mean L_2 asymptotic convergence rate is approximately 0.40. For the density (right plot in Fig. 4), the pointwise convergence rate varies widely throughout the domain. For this quantity, the zero-values correspond to positions at which the terms in the convergence rate expression (Eq. 2) yield nonsensical results (i.e., infinite, indeterminate or imaginary). Between the shock and the heat front, the mean behavior bears some similarity to that of the temperature, although it is much noisier). The mean L_2 rate is approximately 0.55. One might expect a convergence rate on the order of one-half for this type of shock-conduction problem, so the results are nor surprising. It remains to be seen, however, why the difference between the temperature and density convergence rates is so pronounced, and why the density convergence rate behaves so erratically, particularly between the origin and the shock.

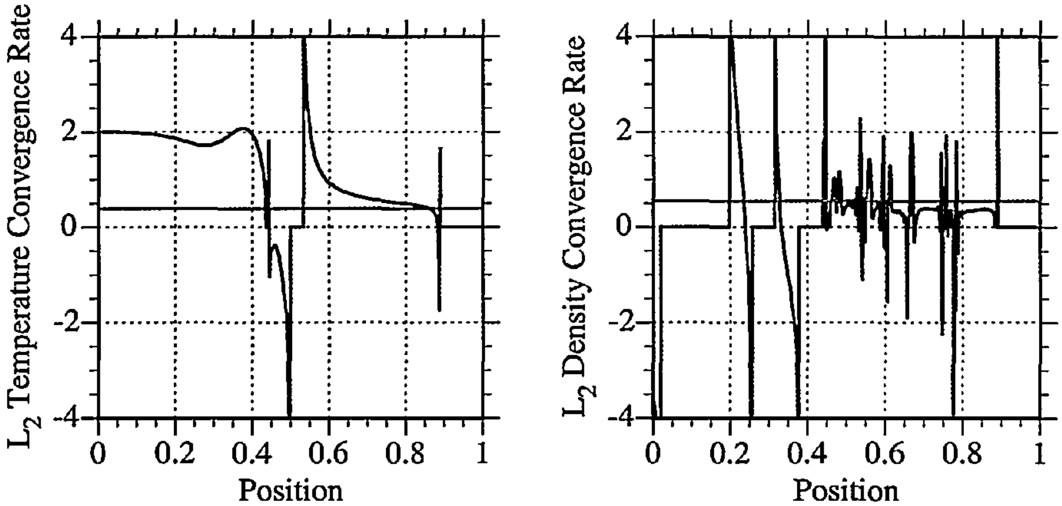

Figure 4. Asymptotic convergence rates for calculated temperature (left) and density (right) for the strong conduction RMtV problem at t=0.0512512. The solid lines are the pointwise convergence rates using the 80016003200 calculations (blue). The dashed lines are the mean L_2 convergence rates for the 800-1600-3200 calculations (red).

Summary

We have defined the notion of code verification, i.e., the demonstration that a code is solving a set of equations correctly. With this approach, we have quantitatively examined the behavior of the RAGE hydrocode in one-dimensional, spherically symmetric geometry on the pure hydrodynamics problem of adiabatic compression, and on the combined hydro-conduction problem of

Reinicke & Meyer-ter-Vehn. In the former case, the code was seen to exhibit anticipated second order convergence in velocity over a limited domain, and inexplicable first-order convergence in specific internal energy. In the latter case, RAGE exhibited mean L_2 convergence of approximately one-half; in this case, the pointwise convergence rate was seen to vary widely between zero and two. Although by no means exhaustive, these two problems cover some of the important regimes of application of the code. Further examination of the convergence properties of RAGE is required, both on different problems and in higher dimensions, to present a compelling case of code verification.

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