Center for Radiative Shock Hydrodynamics

April 2013 TST Meeting

Solution Verification
Bruce Fryxell
The Grid Convergence Index (Roache 1994) can be used to establish a rough estimate for error bars for numerical simulations.

\[ GCI = \frac{F_s}{R^p - 1} \left| \frac{y(\Delta x_F) - y(\Delta x_C)}{y(\Delta x_F)} \right| \]

\( y(\Delta x_C) \) and \( y(\Delta x_F) \) are the solutions on coarse and fine meshes.
\( p \) is the order of the numerical method.
\( R = \frac{\Delta x_C}{\Delta x_F} \) is the refinement ratio.
\( F_s \) is a “safety factor”. Typical values are in the range from 1 to 3.

\[ y_{GCI} \approx y \left( 1 \pm GCI \right) \]
Order of convergence

• If the exact solution to the problem is known, then the order of convergence can be easily calculated from the following equations

\[
\varepsilon_Y(\Delta x_C) = |Y_{\text{Exact}} - Y(\Delta x_C)| = \beta (\Delta x_C)^p + \text{HOT}
\]

\[
\varepsilon_Y(\Delta x_F) = |Y_{\text{Exact}} - Y(\Delta x_F)| = \beta (\Delta x_F)^p + \text{HOT}
\]

\[
p = \frac{\log \left( \frac{\varepsilon_Y(\Delta x_C)}{\varepsilon_Y(\Delta x_F)} \right)}{\log(R)}
\]

• If the exact solution is not known, a “converged” solution computed on a very fine grid can be substituted as a reference solution.
Richardson extrapolation

- Requires solution on three grid sizes
- Assumes that the results are in the asymptotic regime of convergence (i.e. higher order terms are negligible) – If not, the results will not be reliable.
- Also assumes that the convergence is monotonic – If not, the analysis fails.
Richardson extrapolation equations

\[ y(\Delta x_C) = y_{RE} + \beta(\Delta x_C)^p + \text{HOT} \]
\[ y(\Delta x_M) = y_{RE} + \beta(\Delta x_M)^p + \text{HOT} \]
\[ y(\Delta x_F) = y_{RE} + \beta(\Delta x_F)^p + \text{HOT} \]

\( y_{RE} \) is the extrapolated solution

\[
p = \frac{\log \left( \frac{y(\Delta x_M) - y(\Delta x_C)}{y(\Delta x_F) - y(\Delta x_M)} \right)}{\log (R)}
\]

\[ y_{RE} = y(\Delta x_F) + \frac{y(\Delta x_F) - y(\Delta x_M)}{R^p - 1} \]
Shock tube with radiation

Proposed by Lowrie and Morel (1999)

Hydrodynamics plus gray radiation diffusion

\[
\rho_L = 3.123 \quad \rho_R = 1.0
\]
\[
u_L = 6.798 \quad u_R = 0.
\]
\[
\rho_L = 2.874 \quad p_R = 0.6
\]

\[
x = \begin{cases} 0. & 0.25 \end{cases} \quad 1.0
\]

\[
E_r = a_r T^4 \quad F_r = 4/3 \ E_r \ \nu
\]

\[
\gamma = 5/3, \quad a_r = 44.93, \quad c = 100., \quad \sigma_t = 100.
\]
Density profile for six grid resolutions
Convergence of density at a fixed point

Density at x=0.30825

Error bars obtained from GCI (F_S = 3)
Convergence of Maximum Density

Maximum Density

Error bars obtained from GCI ($F_S = 3$)
Oscillatory convergence prevents use of standard Richardson extrapolation method
Analysis of rate of convergence

- Richardson extrapolation fails for this problem, since the convergence is oscillatory rather than monotonic.

- The convergence order of the method can still be computed by assuming that the reference solution is equal to the result from the finest grid.

### Convergence Order of Code

<table>
<thead>
<tr>
<th>Points</th>
<th>$\rho(x=0.30825)$</th>
<th>Maximum $\rho$</th>
<th>Max location</th>
</tr>
</thead>
<tbody>
<tr>
<td>144</td>
<td>0.304</td>
<td>0.554</td>
<td>-1.608</td>
</tr>
<tr>
<td>288</td>
<td>0.741</td>
<td>0.726</td>
<td>0.591</td>
</tr>
<tr>
<td>576</td>
<td>0.807</td>
<td>2.034</td>
<td>0.421</td>
</tr>
<tr>
<td>1152</td>
<td>3.845</td>
<td>3.778</td>
<td>0.277</td>
</tr>
<tr>
<td>2304</td>
<td>2.287</td>
<td>-0.992</td>
<td>-1.338</td>
</tr>
<tr>
<td>4608</td>
<td>1.265</td>
<td>1.672</td>
<td>-0.664</td>
</tr>
<tr>
<td>9216</td>
<td>1.882</td>
<td>5.730</td>
<td>3.464</td>
</tr>
<tr>
<td>18432</td>
<td>0.737</td>
<td>-2.402</td>
<td>0.704</td>
</tr>
</tbody>
</table>
One-dimensional CRASH problem

\[ x_{shk} \]

\[ (x_1, \rho_1) \]

\[ (x_2, \rho_2) \]

\[ (x_3, \rho_3) \]
Density profile for five lowest resolutions

Density peak moves to right and increases in height with increasing resolution for low resolution simulations.
Density profile for four highest resolutions

Density peak moves to left and decreases in height with increasing resolution for high resolution simulations.
Feature locations vs Grid Size (26 ns)

- Error bars obtained from Grid Convergence Index with $F_S = 3$
- Horizontal dashed lines are the extrapolated values obtained from Richardson extrapolation using the three highest resolutions
- $p$ is the order of convergence using the three highest resolutions

$p = 0.23$

$p = 0.04$

$p = 0.29$
Density Values vs Grid Size (26 ns)

- Error bars obtained from Grid Convergence Index with $F_S = 3$
- Horizontal dashed lines are the extrapolated values obtained from Richardson extrapolation using the three highest resolutions
- $p$ is the order of convergence using the three highest resolutions

$p = 0.06$

$p = 0.16$

$p = -0.62$
Multidimensional considerations

When fluid instabilities and/or turbulence are present, convergence is not possible when solving the Euler equations due to lack of physical viscosity.

Higher grid resolutions correspond to larger Reynolds numbers as numerical dissipation effects decrease.

For the problems of interest in our project, the physical Reynolds numbers are much higher than the numerical Reynolds numbers.

Adding a sufficiently large physical viscosity to dominate the numerical viscosity would make it possible to obtain a converged solution, but the increased dissipation would make the result less accurate.
Rayleigh-Taylor instability

Single-mode RT instability simulated with the FLASH code. The growth rate increased and then decreased as resolution increased – changes in the small modes can affect the large modes.
2D CRASH problem

Shock location and morphology changes significantly with grid resolution.

Changes are not monotonic

Uncertainty in shock location is a combination of 1D non-convergence effects plus non-convergence of fluid instabilities due to lack of physical dissipation terms in equations.

Total variation in shock location is approximately 50 μ over this range in grid resolutions.
Conclusions

- CRASH converges for the radiation shock tube problem, but oscillatory convergence prevents using Richardson extrapolation or obtaining a meaningful order of convergence.

- Asymptotic regime of convergence is not achieved for even the 1D CRASH problem due to very narrow peaks in the solution. For 2D and 3D, achieving a converged solution, even with simplified physics, will certainly not be possible.

- Richardson extrapolation indicates that the uncertainty in shock location for the 1D CRASH problem is approximately 60 $\mu$, but this number should not be considered reliable due to lack of convergence.

- In 2D, shock location does not converge due to fluid instabilities but oscillates within a narrow range of about 50 $\mu$.

- The total uncertainty in shock location caused by lack of convergence and multidimensional effects appears to be on the order of 100 $\mu$, which is smaller than the experimental variability.

This research was supported by the DOE NNSA/ASC under the Predictive Science Academic Alliance Program by grant number DEFC52-08NA28616.
Future directions

- Adaptive Mesh Refinement can be used to extend the 1D CRASH simulations to higher resolution to see if the asymptotic regime of convergence can be reached, although it may not be possible to achieve convergence before the buildup of roundoff errors dominates the truncation errors.

- Simulations of the CRASH problem used for this analysis were initiated using HYADES. Simulations initiated with the CRASH laser package should be performed to see if they show similar convergence properties.

- Convergence properties of the multigroup radiation solver should be explored.

- The effect on convergence of the CRASH level set method should be checked.