

VERIFICATION OF A LAGRANGIAN HYDRO-DYNAMICS CODE WITH THE DYNAMIC SPHERE TEST PROBLEM

*François M. Hemez¹, Jerry S. Brock² and James R. Kamm³

Los Alamos National Laboratory, X-Division
X-1, Mail Stop B259, Los Alamos, New Mexico 87545

hemez@lanl.gov, jsbrock@lanl.gov, kammj@lanl.gov

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ABSTRACT

The main goals of code and solution verification (or calculation verification) are to assess the asymptotic convergence of numerical solutions as a function of mesh discretization (Δx) and to quantify solution uncertainty. The challenge is to verify that the approximate solutions of the discretized laws-of-conservation or equations-of-motion converge to the correct solution as $\Delta x \rightarrow 0$. In the case of code verification where the solution of a test problem is known exactly (analytically), common practice is to obtain several discrete solutions from successively refined meshes or grids; calculate L^p or H^p norms of the solution error; verify the rate with which discrete solutions converge to the continuous solution; and, finally, quantify solution error/uncertainty at any grid or mesh size Δx [1, 2]. In the case of solution verification where the exact solution is unknown, the solution error and its norms cannot be computed directly as before. One approach is to reduce the solution fields to scalar quantities, such as peak values or integrands estimated over the computational domain. Working with scalars makes it possible to verify asymptotic convergence from a mesh refinement study and quantify solution error and/or uncertainty, even in the case of joint, space-time (Δx ; Δt) refinement [3, 4].

We propose a new capability to assess asymptotic convergence for entire, discrete solution fields without having to reduce them to scalars. The technique is capable of estimating lower and upper bounds of solution error $\|y^{\text{Exact}} - y(\Delta x)\|_2$ (in the sense of the L^2 norm) when the discrete and exact solutions are entire fields, that is, $y^{\text{Exact}} \in \mathfrak{R}^N$ and $y(\Delta x) \in \mathfrak{R}^N$ for $N \geq 1$, and where the exact solution y^{Exact} need not be known [5].

Furthermore it is not necessary to replace the exact solution by a discrete approximation obtained by running the code with a highly refined mesh, hence, bypassing the commonly-encountered assumption that this discrete solution is “close enough” to the exact-but-unknown solution. It makes the theory relevant to the case of solution verification where an exact solution is unknown. An application is presented to assess the asymptotic convergence of solutions calculated with a general-purpose, hydro-dynamics package developed by the Advanced Scientific Computing Shavano code project at the Los Alamos National Laboratory. The package, written for high-performance computing platforms, provides approximate solutions to the equations of motion in the Lagrangian frame-of-reference for multiple materials and arbitrary geometry.

The application selected for this demonstration is the dynamic sphere test problem that consists of simulating the space-time propagation of a uniform stress wave initiated at the outer surface of a sphere. The calculation must be capable of following the wave pattern

and discontinuities it produces in a perfectly elastic material, as it bounces between the outer and inner surfaces of the sphere [6]. The test problem is relevant because spherical shells are representative of numerous natural and manufactured objects ranging from soap bubbles to marine floats or undersea diving bells. The ability to accurately predict their response to various loading scenarios is essential to many engineering or physics applications. The test problem is also selected because it possesses an exact, analytical solution that can be used to compare the solution error $\|y^{\text{Exact}} - y(\Delta x)\|_2$ estimated by our technique to the actual error. Calculations are performed in “pure Lagrangian” mode without invoking the Arbitrary Lagrangian-Eulerian (ALE) capability of the hydro-code.

How does it work? In a nutshell, several discrete solutions $y(\Delta x_k)$, where sizes Δx_k denote a sequence of mesh refinements, are used to define a functional sub-space of \mathfrak{R}^N . Asymptotic convergence is studied by projecting the discrete solutions $y(\Delta x_k)$ into one of the dimensions of this sub-space. Such operation is equivalent to performing a “modal” decomposition of the discrete solution fields. It is shown that asymptotic convergence of individual projections is a necessary and sufficient condition to reach asymptotic convergence of the entire solution field. It is also demonstrated that the solution error $\|y^{\text{Exact}} - y(\Delta x)\|_2$ can be bounded as a function of mesh size Δx without having to know the exact solution. It is argued that this approach provides acceptable results as long as the sub-space is a “good” approximation of the non-linear manifold within which the discrete solutions are constructed by the numerical method. Results obtained with the dynamic sphere problem support this hypothesis.

Results of a mesh refinement study, where discrete solutions of the dynamic sphere problem are calculated from seven levels of refinement, are presented. Asymptotic convergence is first assessed with scalar response features. It is shown that the theoretical, 2nd-order rate-of-convergence is recovered, more-or-less as expected. The analysis then focuses on the asymptotic convergence of entire solution fields, $y(\Delta x) \in \mathfrak{R}^N$. The technique proposed estimates values of the L^2 norm of solution error $\|y^{\text{Exact}} - y(\Delta x)\|_2$ at different mesh sizes Δx without using the knowledge of the exact solution (even though it is known for this problem). The veracity of the upper and lower bounds of solution error is assessed; it is shown that they compare very favorably to the true values of solution error for this test problem. The results suggest that the analysis technique can be applied with confidence to more complex problems described by continuous equations whose exact solutions are unknown. **(Abstract approved for unlimited, public release on December 18, 2007, LA-UR-07-8360, Unclassified.)**

REFERENCES

- [1] Roache, P.J., **Verification in Computational Science and Engineering**, Hermosa Publishers, Albuquerque, New Mexico, 1998.
- [2] Roache, P.J., “Perspective: A Method for Uniform Reporting of Grid Refinement Studies,” *ASME Journal of Fluids Engineering*, Vol. 116, September 1994, pp. 405-413.
- [3] Kamm, J.R., Rider, W.J., Brock, J.S., “Combined Space and Time Convergence Analyses of a Compressible Flow Algorithm,” *16th AIAA Computational Fluid Dynamics Conference*, Orlando, Florida, July 2003. (Also, LANL Technical Report LA-UR-03-2628.)
- [4] Hemez, F.M., Brock, J.S., Kamm, J.R., “Non-linear Error Ansatz Models in Space and Time for Solution Verification,” *1st Non-deterministic Approaches (NDA) Conference*, Newport, Rhode Island, May 1-4, 2006. (Also, LANL Technical Report LA-UR-06-3705.)
- [5] Hemez, F.M., “Functional Data Analysis of Solution Convergence,” *Technical Report LA-UR-07-5758*, Los Alamos National Laboratory, Los Alamos, New Mexico, August 2007.
- [6] Williams, T.O., Li, S., Brock, J.S., Kamm, J.R., “Spherical Shell Analysis for Material Modeling,” *Technical Report LA-UR-05-8038*, Los Alamos National Laboratory, Los Alamos, New Mexico, September 2005.