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VERIFICATION OF 2-D DETONATION SHOCK DYNAMICS IN CONJUNCTION WITH LOS ALAMOS LAGRANGIAN HYDROCODE

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Abstract

As the latest version of the fast-tube Detonation Shock Dynamics (DSD) solver is linked with the Los Alamos Lagrangian hydrocode, verification problems from a 2006 DSD report (LA-14277 [1]) have been duplicated with some of the verification criteria changed to more quantitative ones. The observed error convergence is as good as or better than reported in [1], quite possibly due to the careful treatment of floating point numbers to ensure that their precision level is maintained throughout the code.

Introduction

This report duplicates the three sample verification problems in LA-14277 [1] using the Los Alamos ASC Lagrangian hydrocode (FLAG), official release of 3.2 Alpha6 with a few modifications. This version of FLAG is linked with the latest fast-tube Detonation Shock Dynamics (DSD) version beta 2 solver released in 2011 as part of the LanlDSD software product [2]. New verification criteria are used for the arcwave problem where two specific locations are chosen for burn arrival time comparison. For this report FLAG's internal driver code prepares the distance function (ψ) and material ID fields from its hydro setup, instead of the stand-alone driver that is being utilized by the other LANL hydrocodes currently interfaced to LanlDSD. As it is implemented in version 3.2 Alpha6, the ψ and material ID fields and other parameters are passed from FLAG to the DSD solver directly, and the burn table is directly passed back to FLAG as part of the calling arguments.

The burn-front arrival time “exact” solutions, mentioned in the sequel for the rate-stick and “arc-wave” problems, are computed using a pair of special-purpose Fortran codes provided by Aslam [3]. In each case an ansatz for the form of the solution is made in which the radius from the detonator center point is used as the independent space coordinate. This leads to a simplified, problem-specific, 1D form of the governing equation. This equation is solved using 2nd-order spatial differencing and the forward Euler method on a very fine temporal and geometric mesh. The boundary conditions are handled exactly at the correct location, with second order accuracy. Care has been taken to ensure that this solution is fully converged. Most other technical details are omitted here as they are comprehensively discussed in [1].

1 Time-Dependent Rate Stick Calculation

The ratestick problems in Section 3 of [1] are reproduced. As per in LA-14277, both the 2D “slab” and “axisymmetric” cases are examined. The specific DSD parameters are $D_{CJ} = 1.0$, $\alpha = 0.1$, $\omega_c = 0.7854$, $\omega_s = 0.5$ with the high explosive occupying $-1.0 \leq x \leq 1.0$, $0.0 \leq y \leq 6.0$, $R = 1.0$, with the detonator located at $(0.0, -24.0)$ with the detonator radius of 25.01999201. The problem geometry is depicted in Fig. 1.

The FLAG hydro mesh for the axisymmetric version is 10×60 where only a half of the geometry is modeled ($0.0 \leq r \leq 1.0$), and 20×60 for the slab version where the whole geometry is modeled ($-1.0 \leq x \leq 1.0$). Since the problem domain (HE) is rectangular Cartesian, this hydro mesh density is deemed fine enough to represent the geometry; increasing the hydro mesh density by an order of magnitude did not change the DSD results.

The burnfront locations are recorded in terms of y at three x or r locations at three burntimes; $x = 0.0, 0.52$ and 0.96 for the slab case and $r = 0.0, 0.4$ and 0.8 for the axisymmetric case. The burntimes of interest for both cases are $t = 1.0, 2.0$ and 5.0 .

Error convergence patterns shown in Figs. 5 and 6 of [1] are reproduced in Figs. 2 (a) and (b). These figures demonstrate the same first-order convergence as in LA-14277, but the errors seen here are roughly $1/3$ of [1] for the slab case and $1/4$ for the axisymmetric case across the board.

Error convergence patterns shown in Figs. 7 and 8 of [1] are reproduced in Figs. 3 (a) and (b). Similarly to the slab case above, these plots for the axisymmetric case demonstrate the same convergence behavior as seen in LA-14277, but the overall errors are much smaller.

Figure 1: Ratestick problem, both slab and axisymmetric cases (Section 3 in [1]).

Figure 2: Resolution study; error in y location with respect to the “exact” solution at $x = 0.0$ and burntime = 5.0.

Figure 3: Resolution study; error in y locations with respect to the “exact” solution at various x or r locations and burntimes.

2 Cylindrically Expanding Detonation Calculation

The cylindrically expanding detonation problem from Section 4 of [1] is insensitive to boundary conditions and is a 1D system. The problem geometry, however, is set up as a concentric quarter-circle in 2D, as shown in Fig. 4 for the DSD code. The detonation is initiated along the inner circle of radius $= r_0$ and the detonation is propagated through two HEs of different $D_n(\kappa)$ relations; $D_n(\kappa) = 0.5 - 0.1\kappa$ for the inner HE (HE1) and $D_n(\kappa) = 1.0 - 0.1\kappa$ for the outer HE (HE2). r_0 is set to 1.0.

Three L1-norms are used as the metrics for numerical convergence on a region-by-region basis, as prescribed in [1]. The formula for the “L1-norm” used here and in [1] is

$$\frac{1}{n} \sum_{i=1}^n \left| bt_i^{exact} - bt_i^{DSD} \right| \quad (1)$$

where n is the total number of DSD grid points that fall within a region of interest. The first region (HE1) covers $1.1 \leq r \leq 1.9$ and $0.157 \leq \theta \leq 1.414$. The second region (HE2) covers $2.1 \leq r \leq 3.9$ and $0.157 \leq \theta \leq 1.414$. The combined or composite region is the union of both ($1.1 \leq r \leq 3.9$ and $0.157 \leq \theta \leq 1.414$). The

Figure 4: Expanding detonation in a concentric 2-HE system from Section 4 in [1]. $r_0 = 1.0$.

“exact” solutions are computed in Mathematica using its built-in integration function [4], and compared against the DSD results with varying grid spacings (dx). The old DSD driver adjusted dx based on the average size (length) of the HE-boundary defining interface segments, thus resulting in dx values that were slightly different from the user-requested ones, as mentioned in Section 5 of [1]. Though not explicitly stated, the irregular dx values for this problem are likely caused by this as well. For the FLAG-based DSD runs, the user-specified dx is used directly to define the grid. Therefore, the dx values from Table 1 of [1] (to an accuracy of 10^{-7}) are used as part of the input for FLAG/DSD.

The results are shown in Table 1 and Fig. 5. The error convergence is second order (or slightly less) for the outer and the composite regions, as observed in [1], but the L1-norm for the inner region maintains the first-order convergence all the way to the finest DSD resolution, unlike [1]. Since the suspected culprit for the accuracy degeneracy, the tube thickness, has not been changed, this is probably due to the new version’s careful declarations/definitions of variables and parameters to ensure that all floating point numbers are double precision.

3 Detonation in an Explosive Arc

The 2D, slab explosive arc of Section 5 of [1] is initiated by a circular detonator on one end. The problem geometry is shown in Fig. 6; the explosive arc spans $-\pi/2.0 \leq \theta \leq \pi/2.0$, centered at $(0.0, 0.0)$, with $r_1 = 2.0$ and $r_2 = 4.0$. The boundary condition on the inside of the arc is free and the outside is fixed.

dx	L1-norm HE1	L1-norm HE2	L1-norm HE1+HE2
0.0588184	0.00226675	0.01677494	0.01412670
0.0294104	0.00124924	0.00596503	0.00511138
0.0147055	0.00068870	0.00188362	0.00167828
0.0073395	0.00036690	0.00053116	0.00051004

Table 1: L1-norms for the 2-HE, expanding cylindrical detonation problem

Figure 5: L1-norm in the 2-HE cylindrically expanding detonation problem; composite, inner and outer regions.

Figure 6: Explosive arc problem geometry from Section 5 in [1]. The detonator is located at $(-4, -3)$ with the radius of $\sqrt{17}$. $r_1 = 2.0$ defines the free inner boundary and $r_2 = 4.0$, the fixed outer boundary.

The hydro mesh that defines the arc in FLAG is a fan mesh, not Cartesian. The mesh density along the arc determines the fidelity of the geometry and affects the accuracy of the distance function (ψ) and consequently the burn times. Since the problem geometry is simple and the analytical ψ for a given DSD grid point that falls within the shaded zones in Fig. 7 is easily calculated, the average pointwise error (the average of $|(\text{calculated } \psi) - (\text{analytical } \psi)|$ for all the DSD grid points in the shaded zones) is used as a metric of how accurately the hydro mesh represents the actual arc. Fig. 8 shows the monotonous, nearly second-order convergence of the average error for the $dx = 0.003125$ case.

This level of convergence, however, does not translate into the accuracy of burn arrival times. Fig. 9 shows the errors in burn arrival times recorded at $(3.5, 0.0)$ and $(1.5, 2.0)$ with respect to the “exact” solutions (discussed below). The errors converge to certain plateau values at about 500 hydro cells along the arc, and these probably are the inherent accuracy limits of DSD, even though the errors appear smaller for the coarser hydro meshes. Those small errors are due to the fact that the coarse hydro meshes create fewer facets. A faceted, or piecewise linear, representation of a curve is unavoidable, and the finer the hydro mesh is, the more line segments there are to approximate the curve. Along the approximate, piecewise linear “curve,” the burn front diffracts at corners between the facets, thus slowing down the burn progression.

Figure 7: Zones for ψ error check. It spans from $-\pi/4$ to $\pi/4$ along the arc and within $4dx$ on each side of the HE boundary.

For coarser hydro meshes, there are fewer corners, and in between the corners the burn travels along a straight line, slowing down *less*. This explains the speedup of burn progression for coarser hydro meshes, thus manifesting as “better” solutions [5].

Therefore, ignoring the coarser hydro meshes, all verification DSD runs below are done with the hydro mesh resolution of 500 cells along the arc.

As alluded above, instead of the burnfront shapes at specified times, as it was done in [1], for this report burn arrival times at two specific points are compared against the “exact” solutions provided by Aslam [3]. The DSD grid spacings are $dx = 0.1, 0.05, 0.025, 0.0125, 0.00625$ and 0.003125 cm. The error convergence patterns which are roughly first-order, are shown in Fig. 10.

References

- [1] Bdzil, J. B., R. J. Henniger and J. W. Walter, “Test Problems for DSD2D,” LA-14277, Los Alamos National Laboratory, Los Alamos, NM, 2006.
- [2] Walter, J. W. and T. Aida, “Software Project Management and Quality Planning for LanlDSD,” *Software Quality Management Document X-LanlDSD-SPMQP*, Los Alamos National Laboratory, Los Alamos, NM, 2011.

Figure 8: Convergence of the average pointwise error in distance function ψ at DSD grid points that fall within the shaded zones in Fig. 7. The DSD grid spacing is 0.003125 cm.

Figure 9: Error in burn arrival times with respect to the “exact” solutions, recorded at (3.5, 0.0) and (1.5, 2.0) with varying hydro mesh resolutions along the arc. The DSD grid spacing is 0.003125 cm for all cases.

Figure 10: Error in burn arrival times with respect to the “exact” solutions, recorded at (3.5, 0.0) and (1.5, 2.0) with varying DSD grid spacings. The hydro resolution is 500 cells along the arc.

- [3] Aslam, T, *Private Communication*, Los Alamos National Laboratory, Los Alamos, NM, 2011.
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