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An iterative Riemann solver for systems of hyperbolic conservation laws, with application to hyperelastic solid mechanics ☆

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Abstract

In this paper, we present a general iterative method for the solution of the Riemann problem for hyperbolic systems of PDEs. The method is based on the multiple shooting method for free boundary value problems. We demonstrate the method by solving one-dimensional Riemann problems for hyperelastic solid mechanics. Even for conditions representative of routine laboratory conditions and military ballistics, dramatic differences are seen between the exact and approximate Riemann solution. The greatest discrepancy arises from misallocation of energy between compressional and thermal modes by the approximate solver, resulting in nonphysical entropy and temperature estimates. Several pathological conditions arise in common practice and modifications to the method to handle these are discussed. These include points where genuine nonlinearity is lost, degeneracies, and eigenvector deficiencies that occur upon melting.

Keywords: Solid mechanics; Shock waves; Godunov method; Elasticity; Hyperelasticity; Riemann solver

1. Introduction

We are interested in solving shock capturing problems in solid mechanics [9], and coupling solid mechanics with fluid dynamics and vacuum boundary conditions [10], in the context of Eulerian Godunov methods. These projects use an approximate Riemann solver which is based on decomposing the jump

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across a discontinuity in a set of right eigenvectors of an effective matrix linearizing the system of partial differential equations. This approximation treats shocks and rarefactions equally and is known to be entropy violating in some circumstances. In order to better diagnose the behavior of this approximate Riemann solver for solid mechanics, and ultimately to develop more accurate approximate schemes, it is desirable to have reference to an "exact" Riemann solver for this system. In addition to its use in validating approximate solvers, exact Riemann solvers may be used in adaptive strategies in which the expensive solver is used judiciously.

Wang et al. [18] report having constructed an exact elastic–plastic Riemann solver for use in front tracking applications but no description of this solver is available. A number of workers have analyzed the properties of Riemann problem solutions in elasticity. Tang and Ting [13] calculate wave curves for an elastically isotropic material under uniaxial deformation. Garaizar [1] outlines an algorithm for solving the elastic Riemann problem under assumptions of elastic isotropy and uniaxial deformation. Trangenstein and Pember [15] present analytical solutions to Riemann problems including elasticity and perfect plasticity.

Godunov [2] proposed an exact iterative Riemann solver for gas dynamics as part of the development of the method that bears his name. Subsequent work in gas dynamics has recognized that an exact Riemann solver is not necessary to achieve high order accuracy in a Godunov method, therefore simpler approximate Riemann solver strategies are generally employed. Toro [14] describes a range of exact and approximate Riemann solvers for gas dynamics.

In Section 2, we present a general algorithm for hyperbolic systems of n conservation laws containing m genuinely nonlinear waves left of the contact and m right of the contact. We assume initially strict genuine nonlinearity and no degeneracy apart from the $n - 2m$ waves forming the contact discontinuity. Assuming also that the underlying equation of state is convex, and that the jump between left and right states is small enough, Lax's implicit function theorem argument [6, Theorem 9.1] holds for the existence and uniqueness of solutions to the Riemann problem. In the context of the method presented in Section 2, these conditions make our iteration scheme a contractive mapping; and this implies both existence and uniqueness of the solution in the neighborhood of the fixed point. When the Riemann problem is well-posed, possessing a single Lax-like solution comprised of simple waves, and when the algorithm described here converges, it converges to the correct entropy solution. More generally, existence and uniqueness of solutions to the Riemann problem is an important open problem except for special systems.

In Section 3, we analyze the equations of motion for elasticity in conservation form and provide details relevant to the implementation of the scheme outlined in Section 2. In Section 4, we present example calculations. In Section 5, we discuss important cases in solid mechanics in which the assumptions employed in Section 2 break down. These are by no means exhaustive discussions, as even in gas dynamics a large number of pathological conditions may occur [8]. Section 5.1 discusses lack of genuine nonlinearity that occurs at special points of high symmetry in configuration space. Section 5.2 deals with degeneracy that occurs on the reference isentropes of elastically isotropic materials. Section 5.3 deals with the degeneracy and eigenvector deficiency that occurs when shear strength is lost as upon melting. Conclusions are summarized in Section 6.

2. An exact iterative Riemann solver

Here, we consider a general hyperbolic system of conservation laws in one dimension,

$$U_t + F(U)_x = 0, \tag{1}$$

with $U, F \in \mathbb{R}^n$. We assume that the matrix A,

$$A = D_U F(U) \tag{2a}$$

with eigenvalue decomposition

$$A = R\Lambda L, \quad L = R^{-1}, \tag{2b}$$

has $2m$ distinct and genuinely nonlinear eigenvalues, with the remaining $n - 2m$ eigenvalues being linearly degenerate and equal. Here, Λ is the diagonal matrix of eigenvalues, assumed ordered:

$$\lambda_1 < \lambda_2 < \cdots < \lambda_m < \lambda_{m+1} = \cdots = \lambda_{n-m} < \lambda_{n+1-m} < \cdots < \lambda_{n-1} < \lambda_n \tag{3}$$

and R is the matrix whose kth column r_k is the kth right eigenvector of A. The conditions of genuine nonlinearity and linear degeneracy are

$$(r_k \cdot D_U)\lambda_k \neq 0, \quad k = 1, \ldots, m, n+1-m, \ldots, n \tag{4a}$$

and

$$(r_k \cdot D_U)\lambda_k = 0, \quad k = m+1, \ldots, n-m, \tag{4b}$$

respectively.

With these assumptions, the solution to the Riemann problem

$$U(x,0) = \begin{cases} U_{\mathrm{L}}, & x \leqslant 0, \\ U_{\mathrm{R}}, & x > 0 \end{cases} \tag{5}$$

will consist of $2m + 2$ constant states bounded by shocks, or rarefaction fans, of the $2m$ nonlinear waves and by a contact discontinuity [7]:

$$U_{\mathrm{L}} = U_0 \underset{1\text{-wave}}{\mid} U_1 \underset{2\text{-wave}}{\mid} U_2 \mid \cdots U_m \underset{\text{contact}}{\mid} U_{m+1} \mid \cdots U_{2m} \underset{2m\text{-wave}}{\mid} U_{2m+1} = U_{\mathrm{R}} \tag{6}$$

with, schematically,

$$U_k = U_{k-1} + \begin{cases} \int r_k(U)\,\mathrm{d}a, & k\text{-rarefaction; or} \\ [F(U_k) - F(U_{k-1})]/s_k, & k\text{-shock}, \end{cases} \tag{7}$$

where s_k is velocity of the k-shock.

The solution $\{U_k\}$, $k = 0, \ldots, 2m+1$, is subject to a consistency requirement; the so-called entropy condition. For k-rarefactions,

$$\lambda_k(U_{k-1}) < \lambda_k(U_k) \tag{8}$$

and for k-shocks,

$$\lambda_k(U_{k-1}) > s_k > \lambda_k(U_k), \tag{9a}$$

$$\lambda_{k-1}(U_{k-1}) < s_k < \lambda_{k+1}(U_k). \tag{9b}$$

Additionally, there is a condition of consistent ordering obtained from consideration of (6), but not contained within (9a), for adjacent shocks:

$$s_k < s_{k+1}. \tag{10}$$

Our approach to obtaining solution (6) is based upon the multiple shooting method for boundary value problems. The Riemann problem is essentially a set of $2m$ boundary value problems: to be determined are the changes in state variables across each wave. The boundaries (the $2m$ interior constant states, or equivalently the end points of each wave or contact) are subject to the condition that the state variables are

continuous functions of wave amplitude from the left and the right. These are free boundary problems since the amplitude of the waves α_k must also be determined.

It is well known [7] that one may choose a parameterization ξ such that for both a k-shock and a k-rarefaction one has

$$U(0) = U_0, \tag{11a}$$

$$\left.\frac{\mathrm{d}}{\mathrm{d}\xi}U(\xi)\right|_{\xi=0} = r_k(U_0), \tag{11b}$$

$$\left.\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}U(\xi)\right|_{\xi=0} = r_k \cdot D_U r_k(U)|_{U=U_0}. \tag{11c}$$

We wish to exploit this second-order continuity in U to choose a wave strength parameterization α. One choice consistent with (11) (and also (22) and (23) below) is

$$\alpha_k(U(\xi)) = l_k(U(0)) \cdot (U(\xi) - U(0)), \tag{12}$$

where $l_k(U(0))$ is the kth left eigenvector of the matrix $A = D_U F(U)$, evaluated at the centering point $U(0)$ of the wave.

To be generally applicable, (12) requires that $\alpha(\xi)$ be monotonic. For general equations of state this cannot be guaranteed for strong shocks, and this is consequently a limitation of the method presented herein. This problem is discussed further in Section 2.1.

Let us denote by $\mathscr{U}_k^{(M)}$ the Mth iterative approximation to U_k, and by $\alpha_k^{(M)}$ the Mth iterative estimate of the strength of the k-wave. For all iteration steps M we have $\mathscr{U}_0^{(M)} = U_{\mathrm{L}}$ and $\mathscr{U}_{2m+1}^{(M)} = U_{\mathrm{R}}$.

Associated with the Mth estimates $\{\mathscr{U}^{(M)}, \alpha^{(M)}\}$ are $2m(n+1)$ scalar measures of error. Across each genuinely nonlinear wave we have a vector error $H_k \in \mathbb{R}^n$:

$$H_k^{\mathrm{L}}(\mathscr{U}_{k-1}, \mathscr{U}_k, \alpha_k) = U_k\left(\mathscr{U}_{k-1}^{(M)}, \alpha_k\right) - \mathscr{U}_k^{(M)}, \tag{13a}$$

$$H_k^{\mathrm{R}}(\mathscr{U}_k, \mathscr{U}_{k+1}, \alpha_k) = U_k\left(\mathscr{U}_{k+1}^{(M)}, \alpha_k\right) - \mathscr{U}_k^{(M)}, \tag{13b}$$

and associated with the contact discontinuities is an error vector $H_c \in \mathbb{R}^{2m}$,

$$H_c(\mathscr{U}_m, \mathscr{U}_{m+1}) = \mathscr{P}(\mathscr{U}_{m+1}) - \mathscr{P}(\mathscr{U}_m), \tag{14}$$

where $\mathscr{P} : \mathbb{R}^n \mapsto \mathbb{R}^{2m}$ is the projection of $\mathscr{U}$ onto the vector space orthogonal to that spanned by the contact discontinuities. Vector $\mathscr{P}$ is a set of independent nonlinear variables which are Riemann invariants of the $(n-2m)$-fold degenerate contact discontinuities. That is, the jump conditions at the contact are satisfied if and only if these variables are continuous at the contact.

Our iterative scheme seeks to zero H_k and H_c using a modified Newton's method to perturb the estimated states $\mathscr{U}_k$ and wave strengths α_k. To the left of the contact, we have

$$0 = H_1^{\mathrm{L}} - I\Delta\mathscr{U}_1 + \frac{\partial H_1^{\mathrm{L}}}{\partial\alpha_1}\Delta\alpha_1, \tag{15a}$$

$$0 = H_2^{\mathrm{L}} - I\Delta\mathscr{U}_2 + \frac{\partial H_2^{\mathrm{L}}}{\partial\alpha_2}\Delta\alpha_2 + \frac{\partial H_2^{\mathrm{L}}}{\partial\mathscr{U}_1}\Delta\mathscr{U}_1, \tag{15b}$$

$$\vdots$$

$$0 = H_m^{\mathrm{L}} - I\Delta\mathscr{U}_m + \frac{\partial H_m^{\mathrm{L}}}{\partial\alpha_m}\Delta\alpha_m + \frac{\partial H_m^{\mathrm{L}}}{\partial\mathscr{U}_{m-1}}\Delta\mathscr{U}_{m-1}, \tag{15c}$$

at the contact we have

$$0 = H_c + D_U\mathscr{P}(\mathscr{U}_{m+1})\Delta\mathscr{U}_{m+1} - D_U\mathscr{P}(\mathscr{U}_m)\Delta\mathscr{U}_m, \tag{15d}$$

and to the right of the contact we have

$$0 = H^{\mathrm{R}}_{m+1} - I\Delta\mathscr{U}_{m+1} + \frac{\partial H^{\mathrm{R}}_{m+1}}{\partial\alpha_{m+1}}\Delta\alpha_{m+1} + \frac{\partial H^{\mathrm{R}}_{m+1}}{\partial\mathscr{U}_{m+2}}\Delta\mathscr{U}_{m+2}, \tag{15e}$$

$$\vdots$$

$$0 = H^{\mathrm{R}}_{2m-1} - I\Delta\mathscr{U}_{2m-1} + \frac{\partial H^{\mathrm{R}}_{2m-1}}{\partial\alpha_{2m-1}}\Delta\alpha_{2m-1} + \frac{\partial H^{\mathrm{R}}_{2m-1}}{\partial\mathscr{U}_{2m}}\Delta\mathscr{U}_{2m}, \tag{15f}$$

$$0 = H^{\mathrm{R}}_{2m} - I\Delta\mathscr{U}_{2m} + \frac{\partial H^{\mathrm{R}}_{2m}}{\partial\alpha_{2m}}\Delta\alpha_{2m} \tag{15g}$$

as defining equations for the perturbations $\Delta\mathscr{U}$ and $\Delta\alpha$ that would zero the error vectors H if they were linear.

In block-factored form, this sparse linear system of $(2mn + 2m)$ equations in $(2mn + 2m)$ variables is

$$\begin{pmatrix}
I & & & & & & & -\frac{\partial H^{\mathrm{L}}_1}{\partial\alpha} \\
-\frac{\partial H^{\mathrm{L}}_2}{\partial\mathscr{U}_1} & I & & & & & & -\frac{\partial H^{\mathrm{L}}_2}{\partial\alpha} \\
 & -\frac{\partial H^{\mathrm{L}}_3}{\partial\mathscr{U}_2} & I & & & & & -\frac{\partial H^{\mathrm{L}}_3}{\partial\alpha} \\
 & & D_U\mathscr{P}(\mathscr{U}_3) & -D_U\mathscr{P}(\mathscr{U}_4) & & & & 0 \\
 & & & I & -\frac{\partial H^{\mathrm{R}}_4}{\partial\mathscr{U}_5} & & & -\frac{\partial H^{\mathrm{R}}_4}{\partial\alpha} \\
 & & & & I & -\frac{\partial H^{\mathrm{R}}_5}{\partial\mathscr{U}_6} & & -\frac{\partial H^{\mathrm{R}}_5}{\partial\alpha} \\
 & & & & & I & & -\frac{\partial H^{\mathrm{R}}_6}{\partial\alpha}
\end{pmatrix}
\begin{pmatrix} \Delta\mathscr{U}_1 \\ \Delta\mathscr{U}_2 \\ \Delta\mathscr{U}_3 \\ \Delta\mathscr{U}_4 \\ \Delta\mathscr{U}_5 \\ \Delta\mathscr{U}_6 \\ \Delta\alpha \end{pmatrix}
=
\begin{pmatrix} H^{\mathrm{L}}_1 \\ H^{\mathrm{L}}_2 \\ H^{\mathrm{L}}_3 \\ H_c \\ H^{\mathrm{R}}_4 \\ H^{\mathrm{R}}_5 \\ H^{\mathrm{R}}_6 \end{pmatrix} \tag{16}$$

(illustrated for the particular case $m = 3$). By a sequence of simple manipulations, this system may be triangularized. First, multiply (15c) by $-D_U\mathscr{P}(\mathscr{U}_m)$ and multiply (15e) by $D_U\mathscr{P}(\mathscr{U}_{m+1})$, then add these equations to (15d) to eliminate $\Delta\mathscr{U}_m$ and $\Delta\mathscr{U}_{m+1}$. Carrying on similarly, a block-triangular form results.

For the case $m = 3$ one obtains

$$\begin{pmatrix}
C & & & & & & \\
-\frac{\partial H^{\mathrm{L}}_1}{\partial\alpha} & I & & & & & \\
-\frac{\partial H^{\mathrm{L}}_2}{\partial\alpha} & -\frac{\partial H^{\mathrm{L}}_2}{\partial\mathscr{U}_1} & I & & & & \\
-\frac{\partial H^{\mathrm{L}}_3}{\partial\alpha} & & -\frac{\partial H^{\mathrm{L}}_3}{\partial\mathscr{U}_2} & I & & & \\
-\frac{\partial H^{\mathrm{L}}_6}{\partial\alpha} & & & & I & & \\
-\frac{\partial H^{\mathrm{L}}_5}{\partial\alpha} & & & & -\frac{\partial H^{\mathrm{R}}_5}{\partial\mathscr{U}_6} & I & \\
-\frac{\partial H^{\mathrm{L}}_4}{\partial\alpha} & & & & & -\frac{\partial H^{\mathrm{R}}_4}{\partial\mathscr{U}_5} & I
\end{pmatrix}
\begin{pmatrix} \Delta\alpha \\ \Delta\mathscr{U}_1 \\ \Delta\mathscr{U}_2 \\ \Delta\mathscr{U}_3 \\ \Delta\mathscr{U}_6 \\ \Delta\mathscr{U}_5 \\ \Delta\mathscr{U}_4 \end{pmatrix}
=
\begin{pmatrix} b \\ H^{\mathrm{L}}_1 \\ H^{\mathrm{L}}_2 \\ H^{\mathrm{L}}_3 \\ H^{\mathrm{R}}_6 \\ H^{\mathrm{R}}_5 \\ H^{\mathrm{R}}_4 \end{pmatrix} \tag{17}$$

in which only one diagonal block element, C, is nontrivial. Thus, instead of solving a single $(2mn + 2m) \times (2mn + 2m)$ system (16), one need only solve a single $(2m) \times (2m)$ system:

$$C\begin{pmatrix} \Delta\alpha_1 \\ \vdots \\ \Delta\alpha_{2m} \end{pmatrix} = b, \tag{18}$$

with

$$C_{ik} = \begin{cases} D_U \mathscr{P}_i(\mathscr{U}_m)\left(\prod_{l=k+1}^{m} \frac{\partial H_l^{\mathrm{L}}}{\partial \mathscr{U}_{l-1}}\right)\frac{\partial H_k^{\mathrm{L}}}{\partial \alpha_k} & \text{if } k \leqslant m; \\ -D_U \mathscr{P}_i(\mathscr{U}_{m+1})\left(\prod_{l=m+1}^{k-1} \frac{\partial H_l^{\mathrm{R}}}{\partial \mathscr{U}_{l+1}}\right)\frac{\partial H_k^{\mathrm{R}}}{\partial \alpha_k} & \text{if } k \geqslant m+1; \end{cases} \tag{19a}$$

$$b_i = -\sum_{k=1}^{m} D_U \mathscr{P}_i(\mathscr{U}_m)\left(\prod_{l=k+1}^{m} \frac{\partial H_l^{\mathrm{L}}}{\partial \mathscr{U}_{l-1}}\right)H_k^{\mathrm{L}} + \sum_{k=m+1}^{2m} D_U \mathscr{P}_i(\mathscr{U}_{m+1})\left(\prod_{l=m+1}^{k-1} \frac{\partial H_l^{\mathrm{R}}}{\partial \mathscr{U}_{l+1}}\right)H_k^{\mathrm{R}} + (H_c)_i. \tag{19b}$$

Then, evaluate sequentially

$$\Delta \mathscr{U}_1 = H_1^{\mathrm{L}} + \frac{\partial H_1^{\mathrm{L}}}{\partial \alpha_1}\Delta\alpha_1, \tag{20a}$$

$$\Delta \mathscr{U}_2 = H_2^{\mathrm{L}} + \frac{\partial H_2^{\mathrm{L}}}{\partial \alpha_2}\Delta\alpha_2 + \frac{\partial H_2^{\mathrm{L}}}{\partial \mathscr{U}_1}\Delta\mathscr{U}_1, \tag{20b}$$

$$\vdots$$

$$\Delta \mathscr{U}_m = H_m^{\mathrm{L}} + \frac{\partial H_m^{\mathrm{L}}}{\partial \alpha_m}\Delta\alpha_m + \frac{\partial H_m^{\mathrm{L}}}{\partial \mathscr{U}_{m-1}}\Delta\mathscr{U}_{m-1}, \tag{20c}$$

and

$$\Delta \mathscr{U}_{2m} = H_{2m}^{\mathrm{R}} + \frac{\partial H_{2m}^{\mathrm{R}}}{\partial \alpha_{2m}}\Delta\alpha_{2m}, \tag{20d}$$

$$\Delta \mathscr{U}_{2m-1} = H_{2m-1}^{\mathrm{R}} + \frac{\partial H_{2m-1}^{\mathrm{R}}}{\partial \alpha_{2m-1}}\Delta\alpha_{2m-1} + \frac{\partial H_{2m-1}^{\mathrm{R}}}{\partial \mathscr{U}_{2m}}\Delta\mathscr{U}_{2m}, \tag{20e}$$

$$\vdots$$

$$\Delta \mathscr{U}_{m+1} = H_{m+1}^{\mathrm{R}} + \frac{\partial H_{m+1}^{\mathrm{R}}}{\partial \alpha_{m+1}}\Delta\alpha_{m+1} + \frac{\partial H_{m+1}^{\mathrm{R}}}{\partial \mathscr{U}_{m+2}}\Delta\mathscr{U}_{m+2} \tag{20f}$$

for the $2m$ n-dimensional state vector perturbations $\Delta\mathscr{U}_k$.

With error vectors H and all derivatives computed at states $\mathscr{U}^{(M)}$ with strengths $\alpha^{(M)}$, we then obtain the $(M+1)$ iterate

$$\mathscr{U}_k^{(M+1)} = \mathscr{U}_k^{(M)} + \zeta\Delta\mathscr{U}_k, \tag{21a}$$

$$\alpha_k^{(M+1)} = \alpha_k^{(M)} + \zeta\Delta\alpha_k \tag{21b}$$

for $k = 1, \ldots, 2m$, with $0 < \zeta \leqslant 1$ a line search parameter in the modified Newton method. We use an approximate line search which seeks the smallest nonnegative integer i such that the sum of squares error for iterative estimate $(M+1)$ with $\zeta = 2^{-i}$ is less that the sum of squares error for estimate (M).

One way to initialize our iterative scheme is with the result of a linear decomposition. We begin by constructing an estimate to (6) by resolving the jump $[\![U]\!] = U_{\mathrm{R}} - U_{\mathrm{L}}$ in right eigenvectors $\tilde{r}$ of a composite matrix of right eigenvectors $\tilde{R}$ after [9]

$$\alpha_k^{(0)} = \pm e_k^{\mathrm{T}}\tilde{R}^{-1}(U_{\mathrm{R}} - U_{\mathrm{L}}), \tag{22a}$$

$$\mathscr{U}_k^{(0)} = \mathscr{U}_{k-1}^{(0)} \pm \alpha_k^{(0)}\tilde{r}_k \tag{22b}$$

for $k = 1, 2, \ldots, m$; and

$$\alpha_k^{(0)} = \pm e_{n+k-2m}^{\mathrm{T}} \tilde{R}^{-1} (U_{\mathrm{R}} - U_{\mathrm{L}}), \tag{23a}$$

$$\mathscr{U}_k^{(0)} = \mathscr{U}_{k+1}^{(0)} \mp \alpha_k^{(0)} \tilde{r}_{n+k-2m} \tag{23b}$$

for $k = m+1, m+2, \ldots, 2m$. The sign ambiguity in (22) and (23) reflects uncertainty in the sign of $r \cdot D_U \lambda$, the change in wave speeds along a simple wave, and the interpretation of $\alpha_k > 0$ as being a shock or a rarefaction. This initial condition is a formally second-order accurate approximation to the converged solution.

A less accurate initial condition comes from taking $\mathscr{U}_k^{(0)} = U_{\mathrm{L}}$ for $k = 1, 2, \ldots, m$; $\mathscr{U}_k^{(0)} = U_{\mathrm{R}}$ for $k = m+1, m+2, \ldots, 2m$; and $\alpha_k^{(0)} = 0$ for all waves. Numerical experiments have shown that this first-order accurate initial condition is sometimes better than the second-order approach, since the second-order approach may select points $\mathscr{U}_k^{(0)}$ in phase space that are not physically valid, and may prevent the algorithm from converging. When the algorithm converges with both sets of initial values, both solutions are numerically equivalent.

2.1. k-Shocks

Our treatment of shocks follows an approach recommended by P. Colella, based on the finite difference Eqs. (24)–(27). Let α_k parameterize the strength of a k-shock centered at state U_0,

$$\alpha_k = l_k \cdot (U - U_0), \tag{24}$$

where l_k is the kth left eigenvector of $A_0 = A(U_0)$, and define the vector ϱ to be

$$\alpha_k \varrho = U - U_0 \tag{25}$$

with normalization

$$l_k \cdot \varrho = 1. \tag{26}$$

Then,

$$\frac{F(U_0 + \alpha_k \varrho) - F(U_0)}{\alpha_k} = s\varrho \tag{27}$$

is a finite difference representation of the shock Hugoniot relations.

To solve (27) we expand ϱ in the right eigenvalues of A_0,

$$\varrho = \sum_i^n \gamma_i r_i, \quad \gamma_k = 1. \tag{28}$$

Then (27) may be viewed as n equations in n unknowns: the shock velocity s, and the $n-1$ nontrivial expansion parameters $\gamma_{i \neq k}$.

For each estimate (γ, s) of the solution there is a vector error measure

$$\psi = \frac{F(U_0 + \alpha_k \varrho) - F(U_0)}{\alpha_k} - s\varrho \tag{29}$$

with derivatives

$$\psi_s = -\varrho \tag{30}$$

and

$$\psi_{\gamma_i} = (A - sI)r_i. \tag{31}$$

A Newton iteration may then be constructed by solving for the change in (γ, s) that would zero ψ if it were linear:

$$\Delta \begin{pmatrix} \vdots \\ \gamma_{i\neq k} \\ \vdots \\ s \end{pmatrix} = -B^{-1}\psi, \tag{32a}$$

$$B = [\cdots \quad (A - sI)r_{i\neq k} \quad \cdots \quad -\varrho\,]. \tag{32b}$$

In the limit of infinitesimal shocks, the matrix approaches

$$\lim_{\alpha_k \to 0} B = [\cdots \quad (A_0 - \lambda_k I)r_i \quad \cdots \quad -r_k\,] = [\cdots \quad (\lambda_i - \lambda_k)r_i \quad \cdots \quad -r_k\,], \tag{33}$$

which is full rank since the vectors $r_{i\neq k}$, r_k form a complete set, and the eigenvalues λ are assumed distinct. This analysis also holds for linearly degenerate contacts of multiplicity one.

For finite strength shocks a proof that B is invertible is lacking. If the state U is near a Hugoniot locus, then $(A - sI)$ will be invertible for the general (nonzero shock strength) case since s is not an eigenvalue of $A(U)$. The matrix appearing in (32) may therefore be written as

$$B = (A - sI)\left[R'_0 \mid -(A - sI)^{-1}\varrho\right], \tag{34}$$

where R'_0 is the $n \times (n-1)$ matrix of right eigenvectors of $A_0 = A(U_0)$, with vector r_k omitted. The overall matrix is therefore invertible if $(A - sI)^{-1}\varrho$ has a component in the nullspace of R'_0, or if

$$l_k^{\mathrm{T}}(A - sI)^{-1}\varrho = \sum_i \gamma_i l_k^{\mathrm{T}}(A - sI)^{-1} r_i \neq 0, \quad \gamma_k = 1. \tag{35}$$

Since $(A - sI)$ is nonsingular and is unrelated to A_0 a failure of (35) would be accidental.

So, given a k-shock strength α_k one may employ a modified Newton iteration based on (32) to compute $U(U_0, \alpha_k)$. This is the shock version of the function employed in (13) for the computation of error vectors $H^{\mathrm{L/R}}$.

The Newton iteration for the multiple shooting method calls for derivatives of $U(U_0, \alpha_k)$ with respect to the centering vector U_0, and with respect to strength α_k. Differentiation of the jump condition $F(U) - F(U_0) = s(U - U_0)$ with respect to the shock wave velocity s, and with respect to the centering vector U_0, gives

$$U(U_0, s)_{U_0} = (A(U) - sI)^{-1}(A_0 - sI), \tag{36a}$$

$$U(U_0, s)_{\mathrm{s}} = (A(U) - sI)^{-1}(U - U_0) \tag{36b}$$

and changing independent variables one obtains

$$U(U_0, \alpha)_{\alpha} = \frac{U(U_0, s)_{\mathrm{s}}}{\alpha(U_0, s)_{\mathrm{s}}}, \tag{37a}$$

$$U(U_0,\alpha)_{U_0} = U(U_0,s)_{U_0} - U(U_0,s)_{\mathrm{s}} \frac{\alpha(U_0,s)_{U_0}}{\alpha(U_0,s)_{\mathrm{s}}}. \tag{37b}$$

Next, differentiation of (24) gives

$$\alpha(U_0,s)_{\mathrm{s}} = l_k^{\mathrm{T}} U(U_0,s)_{\mathrm{s}}, \tag{38a}$$

$$\alpha(U_0,s)_{U_0} = l_k^{\mathrm{T}}(U(U_0,s)_{U_0} - I) + (l_k^{\mathrm{T}})_{U_0}(U - U_0), \tag{38b}$$

and in combination,

$$U(U_0,\alpha)_{\alpha} = \frac{(A(U) - sI)^{-1}(U - U_0)}{l_k^{\mathrm{T}}(A(U) - sI)^{-1}(U - U_0)}, \tag{39a}$$

$$\begin{aligned} U(U_0,\alpha)_{U_0} = {} & (A(U) - sI)^{-1}(A_0 - sI) - U(U_0,\alpha)_{\alpha} \\ & \times \left(l_k^{\mathrm{T}}[(A(U) - sI)^{-1}(A_0 - A(U))] + (l_k^{\mathrm{T}})_{U_0}(U - U_0) \right) \end{aligned} \tag{39b}$$

determine the derivatives necessary to construct $\partial H_k/\partial\alpha$ and $\partial H_k/\partial \mathscr{U}$ for shocks in the multiple shooting method.

If the reparameterization $\alpha(\xi)$ (12) is not monotonic, then two or more values of wave parameter ξ, say ξ' and ξ'', will give the same value of parameter α: $\alpha(\xi') = \alpha(\xi'')$. This implies that the finite difference equation (27) will then have multiple solutions using this value of α. In this case, the solution obtained by the algorithm describe above will be sensitive to the starting value of the iteration sequence.

2.2. k-Rarefactions

For rarefactions, we have the ordinary differential equation based on (11) and (12):

$$\frac{\mathrm{d}U}{\mathrm{d}\alpha} = \frac{\mathrm{d}U}{\mathrm{d}\xi}\frac{\mathrm{d}\xi}{\mathrm{d}\alpha} = \frac{r_k(U)}{l_k^{\mathrm{T}} r_k(U)}, \tag{40a}$$

$$U(0) = U_0. \tag{40b}$$

Since shock and rarefaction branches need be only C^1 for the multiple shooting method to be second-order, it is sufficient to evaluate $\mathrm{d}\xi/\mathrm{d}\alpha$ only at the centering point U_0, where $\mathrm{d}\xi/\mathrm{d}\alpha = 1$. Thus, we have the initial value problem

$$\frac{\mathrm{d}U}{\mathrm{d}\alpha} = r_k(U), \tag{41a}$$

$$U(0) = U_0, \tag{41b}$$

which we solve together with the initial value problem

$$\frac{\mathrm{d}W}{\mathrm{d}\alpha} = (D_U r_k(U(\alpha)))W(\alpha), \tag{42a}$$

$$W(0) = I \tag{42b}$$

derived by differentiation with respect to U_0 of $U'(U_0,\alpha) = f(U_0, U(U_0,\alpha))$. We evaluate these initial value problems with a fourth-order Runge–Kutta method. Then,

$$U(U_0,\alpha)_\alpha = r_k(U(\alpha)), \tag{43a}$$

$$U(U_0,\alpha)_{U_0} = W(\alpha) \tag{43b}$$

determine $\partial H_k/\partial\alpha$ and $\partial H_k/\partial\mathscr{U}$ for rarefactions.

3. Application to hyperelasticity

The one-dimensional (direction η) equations of hyperelasticity may be written as [9]

$$\frac{\partial}{\partial t}\begin{pmatrix} \rho v \\ \rho E \\ g e_1 \\ g e_2 \\ g e_3 \end{pmatrix} + \frac{\partial}{\partial x_\eta}\begin{pmatrix} v_\eta \rho v - e_\eta^{\mathrm{T}}\sigma \\ v_\eta \rho E - e_\eta^{\mathrm{T}}\sigma v \\ g v \delta_{1\eta} \\ g v \delta_{2\eta} \\ g v \delta_{3\eta} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ (v \times (\nabla \times g^{\mathrm{T}}))^{\mathrm{T}} e_1 \\ (v \times (\nabla \times g^{\mathrm{T}}))^{\mathrm{T}} e_2 \\ (v \times (\nabla \times g^{\mathrm{T}}))^{\mathrm{T}} e_3 \end{pmatrix}, \tag{44}$$

where v is the velocity, ρ the mass density, E the total energy, g the inverse deformation tensor, and σ the Cauchy stress.

These equations are based on the kinematics of a solid whose motion is characterized by a time-dependent mapping ϕ from material (Lagrangian) coordinates $\vec{a}$ to spatial (Eulerian) coordinates $\vec{x}$:

$$\vec{x} = \vec{\phi}(\vec{a}, t). \tag{45}$$

The gradient of this mapping is the deformation gradient F,

$$F = \nabla_a \phi; \quad F_{\alpha\beta} = \frac{\mathrm{d}x_\alpha}{\mathrm{d}a_\beta}, \tag{46}$$

and the inverse of F defines g; $g = F^{-1}$. F and g are subject to the equality of mixed partial derivatives; equivalently,

$$\nabla \times g^{\mathrm{T}} = 0. \tag{47}$$

The extra terms $v \times (\nabla \times g^{\mathrm{T}})$ in (44) are therefore zero on the constraint manifold. Their presence guarantees that the system is hyperbolic when $\nabla \times g^{\mathrm{T}}$ differs from 0, as it must in numerical computation [3,4,9].

The weak form of constraint (47) is

$$[\![g e_\tau]\!]_n = 0, \quad \tau \cdot n = 0 \tag{48}$$

that is, the jump in direction n of tangential components ge_τ of tensor g is zero. Analysis of (44) below shows that this condition is satisfied automatically in smooth one-dimensional flow. Therefore, for those Riemann problems where (47) is satisfied by the initial condition, it is satisfied numerically and analytically for all time. Consequently, our analysis of the one-dimensional Riemann problem will ignore the right-hand side nonconservative terms $[v \times (\nabla \times g^{\mathrm{T}})]^{\mathrm{T}}$.

A slightly broader class of problems may be considered in which (47) does not hold strictly in the initial condition. Physically, such a problem may be constructed by tearing the material into two parts, subjecting the parts to independent homogeneous one-dimensional deformations, then rejoining them. At the resulting contact, the underlying Lagrangian coordinate is discontinuous and $\nabla \times g^{\mathrm{T}}$ is not defined. The weak form

of the constraint then gives $[\![ge_\tau]\!]_n = \text{constant}$ at the contact. For such problems the constraint will be obeyed on either side of the contact, and the weak form will hold at the contact for all time. Again, ignoring the nonconservative right hand side terms gives the proper physical result.

The mass density ρ is related to the tensor g,

$$\rho = \rho_0 \det g, \tag{49}$$

where ρ_0 is the density in the undeformed ($F = g = I$) reference frame.

We derive the stress σ as a thermodynamic derivative of the internal energy $\mathscr{E} = E - \frac{1}{2}v^2$,

$$\sigma_{\alpha\beta} = -\rho \frac{\partial \mathscr{E}}{\partial g e_\beta}\bigg|_S g e_\alpha. \tag{50}$$

In our analysis of (44) we will make reference to the η-directed acoustic wave propagation tensor $\mathscr{A}[\eta]$,

$$\mathscr{A}[\eta] = -\frac{\partial \sigma e_\eta}{\partial g e_\eta}\bigg|_S g. \tag{51}$$

Both σ and $\mathscr{A}[\eta]$ are symmetric. The acoustic wave propagation tensor is positive definite for thermodynamically stable substances [9] and may be decomposed to yield the Lagrangian wave speeds $\Lambda_{\mathrm{ac}} = \mathrm{diag}(\lambda_{\mathrm{ac},1}, \lambda_{\mathrm{ac},2}, \lambda_{\mathrm{ac},3})$:

$$\mathscr{A}[\eta] = \rho X_{\mathrm{ac}} \Lambda_{\mathrm{ac}}^2 X_{\mathrm{ac}}^{-1}. \tag{52}$$

We assume without loss of generality that the eigenvalues are ordered, $\lambda_{\mathrm{ac},1} \leqslant \lambda_{\mathrm{ac},2} \leqslant \lambda_{\mathrm{ac},3}$, and that X_{ac} is unitary, $X_{\mathrm{ac}}^{-1} = X_{\mathrm{ac}}^{\mathrm{T}}$.

The linearized matrix $A = D_U F(U)$ derived from (44) is

$$A(U) = \begin{pmatrix} v e_\eta^{\mathrm{T}} + v_\eta I & 0 & \left(-\frac{\partial \sigma e_\eta}{\partial g e_1} - \rho v v_\eta e_1^{\mathrm{T}} F\right) \\ \left(E e_\eta^{\mathrm{T}} - \frac{e_\eta^{\mathrm{T}} \sigma}{\rho}\right) & v_\eta & \left(-\frac{v^{\mathrm{T}} \partial \sigma e_\eta}{\partial g e_1} - \rho E v_\eta e_1^{\mathrm{T}} F + v^{\mathrm{T}} \sigma e_\eta e_1^{\mathrm{T}} F\right) \\ \delta_{1\eta} \frac{g}{\rho} & 0 & (v_\eta I - \delta_{1\eta} g v e_1^{\mathrm{T}} F) \\ \delta_{2\eta} \frac{g}{\rho} & 0 & (-\delta_{2\eta} g v e_1^{\mathrm{T}} F) \\ \delta_{3\eta} \frac{g}{\rho} & 0 & (-\delta_{3\eta} g v e_1^{\mathrm{T}} F) \end{pmatrix}$$

$$\begin{pmatrix} \left(-\frac{\partial \sigma e_\eta}{\partial g e_2} - \rho v v_\eta e_2^{\mathrm{T}} F\right) & \left(-\frac{\partial \sigma e_\eta}{\partial g e_3} - \rho v v_\eta e_3^{\mathrm{T}} F\right) \\ \left(-\frac{v^{\mathrm{T}} \partial \sigma e_\eta}{\partial g e_2} - \rho E v_\eta e_2^{\mathrm{T}} F + v^{\mathrm{T}} \sigma e_\eta e_2^{\mathrm{T}} F\right) & \left(-\frac{v^{\mathrm{T}} \partial \sigma e_\eta}{\partial g e_3} - \rho E v_\eta e_3^{\mathrm{T}} F + v^{\mathrm{T}} \sigma e_\eta e_3^{\mathrm{T}} F\right) \\ (-\delta_{1\eta} g v e_2^{\mathrm{T}} F) & (-\delta_{1\eta} g v e_3^{\mathrm{T}} F) \\ (v_\eta I - \delta_{2\eta} g v e_2^{\mathrm{T}} F) & (-\delta_{2\eta} g v e_3^{\mathrm{T}} F) \\ (-\delta_{3\eta} g v e_2^{\mathrm{T}} F) & (v_\eta I - \delta_{3\eta} g v e_3^{\mathrm{T}} F) \end{pmatrix}, \tag{53}$$

with eigenvalues $\Lambda = \mathrm{diag}(v_\eta I - \pi \Lambda_{\mathrm{ac}}, v_\eta, v_\eta I, v_\eta I, v_\eta I + \Lambda_{\mathrm{ac}})$. Here,

$$\pi = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \tag{54}$$

is a permutation introduced to assist in establishing the canonical ordering (3).

In the special case $\eta = 1$, the right eigenvectors R are:

$$R = \begin{pmatrix} (\rho v e_1^{\mathrm{T}} X_{\mathrm{ac}} - \rho X_{\mathrm{ac}} \Lambda_{\mathrm{ac}})\pi & 0 & \rho v\left[e_2^{\mathrm{T}} - e_1^{\mathrm{T}} \Upsilon_2\right] & \rho v\left[e_3^{\mathrm{T}} - e_1^{\mathrm{T}} \Upsilon_3\right] \\ (\rho E e_1^{\mathrm{T}} X_{\mathrm{ac}} - e_1^{\mathrm{T}} \sigma X_{\mathrm{ac}} - \rho v^{\mathrm{T}} X_{\mathrm{ac}} \Lambda_{\mathrm{ac}})\pi & 1 & \rho E\left[e_2^{\mathrm{T}} - e_1^{\mathrm{T}} \Upsilon_2\right] & \rho E\left[e_3^{\mathrm{T}} - e_1^{\mathrm{T}} \Upsilon_3\right] \\ (g X_{\mathrm{ac}})\pi & 0 & -g\Upsilon_2 & -g\Upsilon_3 \\ 0 & 0 & g & 0 \\ 0 & 0 & 0 & g \end{pmatrix} \begin{pmatrix} (\rho v e_1^{\mathrm{T}} X_{\mathrm{ac}} + \rho X_{\mathrm{ac}} \Lambda_{\mathrm{ac}}) \\ (\rho E e_1^{\mathrm{T}} X_{\mathrm{ac}} - e_1^{\mathrm{T}} \sigma X_{\mathrm{ac}} + \rho v^{\mathrm{T}} X_{\mathrm{ac}} \Lambda_{\mathrm{ac}}) \\ (g X_{\mathrm{ac}}) \\ 0 \\ 0 \end{pmatrix}, \tag{55}$$

and the left eigenvectors $L = R^{-1}$ are:

$$L = \begin{pmatrix} -\frac{1}{2\rho}\pi \Lambda_{\mathrm{ac}}^{-1} X_{\mathrm{ac}}^{-1} & 0 & \frac{1}{2}\pi[X_{\mathrm{ac}}^{-1} + \Lambda_{\mathrm{ac}}^{-1} X_{\mathrm{ac}}^{-1} v e_1^{\mathrm{T}}]F & \frac{1}{2}\pi[X_{\mathrm{ac}}^{-1}\Upsilon_2 + \Lambda_{\mathrm{ac}}^{-1} X_{\mathrm{ac}}^{-1} v e_2^{\mathrm{T}}]F \\ -v^{\mathrm{T}} & 1 & [\rho(v^2 - E)e_1^{\mathrm{T}} + e_1^{\mathrm{T}}\sigma]F & [\rho(v^2 - E)e_2^{\mathrm{T}} + e_1^{\mathrm{T}}\sigma\Upsilon_2]F \\ 0 & 0 & 0 & F \\ 0 & 0 & 0 & 0 \\ +\frac{1}{2\rho}\Lambda_{\mathrm{ac}}^{-1} X_{\mathrm{ac}}^{-1} & 0 & \frac{1}{2}[X_{\mathrm{ac}}^{-1} - \Lambda_{\mathrm{ac}}^{-1} X_{\mathrm{ac}}^{-1} v e_1^{\mathrm{T}}]F & \frac{1}{2}[X_{\mathrm{ac}}^{-1}\Upsilon_2 - \Lambda_{\mathrm{ac}}^{-1} X_{\mathrm{ac}}^{-1} v e_2^{\mathrm{T}}]F \end{pmatrix} \begin{pmatrix} \frac{1}{2}\pi[X_{\mathrm{ac}}^{-1}\Upsilon_3 + \Lambda_{\mathrm{ac}}^{-1} X_{\mathrm{ac}}^{-1} v e_3^{\mathrm{T}}]F \\ [\rho(v^2 - E)e_3^{\mathrm{T}} + e_1^{\mathrm{T}}\sigma\Upsilon_3]F \\ 0 \\ F \\ \frac{1}{2}[X_{\mathrm{ac}}^{-1}\Upsilon_3 - \Lambda_{\mathrm{ac}}^{-1} X_{\mathrm{ac}}^{-1} v e_3^{\mathrm{T}}]F \end{pmatrix}. \tag{56}$$

In (55) and (56) the symbols Υ_2 and Υ_3 denote

$$\Upsilon_2 = \left(\frac{\partial \sigma e_1}{\partial g e_1}\bigg|_S g\right)^{-1}\left(\frac{\partial \sigma e_1}{\partial g e_2}\bigg|_S g\right) = -\frac{1}{\rho} X_{\mathrm{ac}} \Lambda_{\mathrm{ac}}^{-2} X_{\mathrm{ac}}^{-1}\left(\frac{\partial \sigma e_1}{\partial g e_2}\bigg|_S g\right), \tag{57a}$$

$$\Upsilon_3 = \left(\frac{\partial \sigma e_1}{\partial g e_1}\bigg|_S g\right)^{-1}\left(\frac{\partial \sigma e_1}{\partial g e_3}\bigg|_S g\right) = -\frac{1}{\rho} X_{\mathrm{ac}} \Lambda_{\mathrm{ac}}^{-2} X_{\mathrm{ac}}^{-1}\left(\frac{\partial \sigma e_1}{\partial g e_3}\bigg|_S g\right). \tag{57b}$$

In 1-directed flow, it is apparent that the quantities ge_2 and ge_3 may be dropped from consideration in the analysis of the nonlinear waves. Likewise, any passively advected scalar may be dropped, including terms describing the plastic deformation tensor and work hardening parameter [9]. We may therefore restrict ourselves to the reduced system in variables ρv, ρE, and ge_1, for which

$$A = \begin{pmatrix} v e_1^{\mathrm{T}} + v_1 I & 0 & \left(-\frac{\partial \sigma e_1}{\partial g e_1} - \rho v v_1 e_1^{\mathrm{T}} F\right) \\ \left(E e_1^{\mathrm{T}} - \frac{e_1^{\mathrm{T}}\sigma}{\rho}\right) & v_1 & \left(-\frac{v^{\mathrm{T}}\partial \sigma e_1}{\partial g e_1} - \rho E v_1 e_1^{\mathrm{T}} F + v^{\mathrm{T}}\sigma e_1 e_1^{\mathrm{T}} F\right) \\ \frac{g}{\rho} & 0 & (v_1 I - g v e_1^{\mathrm{T}} F) \end{pmatrix}, \tag{58a}$$

$$R = \begin{pmatrix} \rho(ve_1^{\mathrm{T}}X_{\mathrm{ac}} - X_{\mathrm{ac}}\Lambda_{\mathrm{ac}})\pi & 0 & \rho(ve_1^{\mathrm{T}}X_{\mathrm{ac}} + X_{\mathrm{ac}}\Lambda_{\mathrm{ac}}) \\ \rho(e_1^{\mathrm{T}}[EI - \frac{\sigma}{\rho}]X_{\mathrm{ac}} - v^{\mathrm{T}}X_{\mathrm{ac}}\Lambda_{\mathrm{ac}})\pi & 1 & \rho(e_1^{\mathrm{T}}[EI - \frac{\sigma}{\rho}]X_{\mathrm{ac}} + v^{\mathrm{T}}X_{\mathrm{ac}}\Lambda_{\mathrm{ac}}) \\ (gX_{\mathrm{ac}})\pi & 0 & (gX_{\mathrm{ac}}) \end{pmatrix}, \tag{58b}$$

$$L = \begin{pmatrix} -\frac{1}{2\rho}\pi\Lambda_{\mathrm{ac}}^{-1}X_{\mathrm{ac}}^{-1} & 0 & \frac{1}{2}\pi[X_{\mathrm{ac}}^{-1} + \Lambda_{\mathrm{ac}}^{-1}X_{\mathrm{ac}}^{-1}ve_1^{\mathrm{T}}]F \\ -v^{\mathrm{T}} & 1 & [\rho(v^2 - E)e_1^{\mathrm{T}} + e_1^{\mathrm{T}}\sigma]F \\ +\frac{1}{2\rho}\Lambda_{\mathrm{ac}}^{-1}X_{\mathrm{ac}}^{-1} & 0 & \frac{1}{2}[X_{\mathrm{ac}}^{-1} - \Lambda_{\mathrm{ac}}^{-1}X_{\mathrm{ac}}^{-1}ve_1^{\mathrm{T}}]F \end{pmatrix}, \tag{58c}$$

and

$$\Lambda = \mathrm{diag}(v_1 I - \pi\Lambda_{\mathrm{ac}},\ v_1,\ v_1 I + \Lambda_{\mathrm{ac}}). \tag{58d}$$

For this system, then, $m = 3$ and $n = 7$.

Although (55) and (58b) appear to be deterministic analytical formulae, they are not. This is because the acoustic eigenvectors X_{ac}, chosen to be unitary, are determined by (52) only to within a sign. To keep the sense of the eigenvectors consistent across an integral curve, and to maintain consistency with Lax's entropy condition, the sign of columns of X_{ac} must be fixed to some standard. We adopt a standard, which affects interpretation of the wave strengths α_k, by analysis of the condition of genuine nonlinearity. In the present case the test for genuine nonlinearity gives

$$q_4 = r_4 \cdot D_U v_1 = 0, \tag{59a}$$

$$q_{4-\gamma} = (r_{4-\gamma} \cdot D_U)(v_1 - \lambda_{\mathrm{ac},\gamma}) = -\lambda_{\mathrm{ac},\gamma}X_{\mathrm{ac},1\gamma} - \left.\frac{\partial\lambda_{\mathrm{ac},\gamma}}{\partial g_{\alpha 1}}\right|_S g_{\alpha\beta}X_{\mathrm{ac},\beta\gamma}, \tag{59b}$$

$$q_{4+\gamma} = (r_{4+\gamma} \cdot D_U)(v_1 + \lambda_{\mathrm{ac},\gamma}) = +\lambda_{\mathrm{ac},\gamma}X_{\mathrm{ac},1\gamma} + \left.\frac{\partial\lambda_{\mathrm{ac},\gamma}}{\partial g_{\alpha 1}}\right|_S g_{\alpha\beta}X_{\mathrm{ac},\beta\gamma} \tag{59c}$$

for $\gamma = 1, 2, 3$. We choose, arbitrarily, to fix the sign of columns of X_{ac} to make q_γ, $\gamma = 1, 2, 3$, negative. With this choice, H_k^{L} (13a) calls for rarefaction when $\alpha < 0$, and a shock when $\alpha > 0$. The sense of integration is different for H_k^{R} (13b) because for these terms the wave is centered on the right state. Thus, the limits of integration are effectively reversed at the same time that the sign of q is reversed. So, again, $\alpha < 0$ calls for a rarefaction and $\alpha > 0$ a shock.

Consideration of (55) shows that the linearly degenerate eigenvectors r_k obey

$$(r_k \cdot D_U)\sigma e_1 = 0, \tag{60a}$$

$$(r_k \cdot D_U)v = 0, \tag{60b}$$

where the derivative of σe_1 is taken at constant entropy. It follows therefore that the six-dimensional projection $\mathscr{P}$ maps from $(\rho v, E, ge_1)$ onto $(v, \sigma e_1)$ (see (15d)):

$$\mathscr{P}(U;\quad ge_2, ge_3) = \begin{pmatrix} v \\ \sigma e_1 \end{pmatrix}, \tag{61}$$

and therefore (see (19)):

$$D_U\mathscr{P} = \begin{pmatrix} \left(\frac{1}{\rho}I\right) & 0 & \left(-ve_1^{\mathrm{T}}F^{\mathrm{T}}\right) \\ \left(-\left.\frac{\partial\sigma e_1}{\partial\mathscr{E}}\right|_g \frac{v^{\mathrm{T}}}{\rho}\right) & \left(\frac{1}{\rho}\left.\frac{\partial\sigma e_1}{\partial\mathscr{E}}\right|_g\right) & \left(\left.\frac{\partial\sigma e_1}{\partial ge_1}\right|_{\mathscr{E}} + (v^2 - E)\left.\frac{\partial\sigma e_1}{\partial\mathscr{E}}\right|_g e_1^{\mathrm{T}}F\right) \end{pmatrix}. \tag{62}$$

The derivatives $D_U l_k$ and $D_U r_k$ appear in the shock and rarefaction wave curve derivatives (39b) and (42a). These terms require determination of $D_U X_{\rm ac}$ and of $D_U \Lambda_{\rm ac}$: a first-order perturbation problem.

Denote the eigenvalues of $\mathscr{A}[1]$ by the diagonal matrix Q ($Q = \rho \Lambda_{\rm ac}^2$), then,

$$\mathscr{A} X_{\rm ac} = X_{\rm ac} Q, \tag{63a}$$

$$\mathscr{A}_U X_{\rm ac} + \mathscr{A}(X_{\rm ac})_U = (X_{\rm ac})_U Q + X_{\rm ac} Q_U, \tag{63b}$$

$$X_{\rm ac}^{-1} \mathscr{A}_U X_{\rm ac} + Q X_{\rm ac}^{-1} (X_{\rm ac})_U = X_{\rm ac}^{-1} (X_{\rm ac})_U Q + Q_U. \tag{63c}$$

The diagonal entries of (63c) give

$$(Q_{kk})_U = (X_{\rm ac} e_k)^{\rm T} \mathscr{A}_U (X_{\rm ac} e_k) \tag{64a}$$

and with Q_{kk}, $k = 1, 2, 3$ distinct, the off-diagonal entries give

$$(X_{\rm ac} e_k)_U = \sum_{j \neq k} \frac{(X_{\rm ac} e_j)^{\rm T} \mathscr{A}_U (X_{\rm ac} e_k)}{Q_{kk} - Q_{jj}} (X_{\rm ac} e_j). \tag{64b}$$

Partial derivatives with respect to conserved variables $(\rho v, \rho E, g)$ are obtained from partial derivatives with respect to primitive variables $(v, \mathscr{E}, g)$ with:

$$\left.\frac{\partial}{\partial \rho v_\alpha}\right|_{\rho E, g} = \frac{1}{\rho} \left.\frac{\partial}{\partial v_\alpha}\right|_{g, \mathscr{E}} - \frac{v_\alpha}{\rho} \left.\frac{\partial}{\partial \mathscr{E}}\right|_{g, v}, \tag{65a}$$

$$\left.\frac{\partial}{\partial \rho E}\right|_{g, \rho v} = \frac{1}{\rho} \left.\frac{\partial}{\partial \mathscr{E}}\right|_{g, v}, \tag{65b}$$

$$\left.\frac{\partial}{\partial g_{\alpha\beta}}\right|_{\rho E, \rho v} = \left.\frac{\partial}{\partial g_{\alpha\beta}}\right|_{\mathscr{E}, v} + (v_\gamma v_\gamma - E) F_{\beta\alpha} \left.\frac{\partial}{\partial \mathscr{E}}\right|_{g, v} - v_\gamma F_{\beta\alpha} \left.\frac{\partial}{\partial v_\gamma}\right|_{g, \mathscr{E}}. \tag{65c}$$

4. Examples

4.1. Hyperelastic equation of state

To illustrate the method with sample calculations we use a hyperelastic equation of state model after [10]. We assume a separation of the total internal energy as follows:

$$\mathscr{E}(C^{\rm e}, S) = \mathscr{E}_{\rm h}(I_3) + \mathscr{E}_{\rm t}(I_3, S) + \mathscr{E}_{\rm s}(I_1, I_2, I_3), \tag{66}$$

where $\mathscr{E}_{\rm h}$ describes the isentropic, hydrostatic compressional energy; $\mathscr{E}_{\rm t}$ is the thermal energy associated with changing entropy at constant volume; and $\mathscr{E}_{\rm s}$ is the energy associated with isochoric shearing. In (66) I_1, I_2, and I_3 are the isotropic invariants of the elastic Green tensor $C^{\rm e}$:

$$C^{\rm e} = F^{\rm T} F, \tag{67a}$$

$$I_1(C^{\rm e}) = {\rm tr}(C^{\rm e}), \tag{67b}$$

$$I_2(C^{\mathrm{e}}) = \frac{1}{2}\left[(\mathrm{tr}C^{\mathrm{e}})^2 - \mathrm{tr}(C^{\mathrm{e}})^2\right], \tag{67c}$$

$$I_3(C^{\mathrm{e}}) = \det(C^{\mathrm{e}}) = \left(\frac{\rho_0}{\rho}\right)^2. \tag{67d}$$

The hydrostatic energy is given by the universal equation of state [12,16,17], determined by the zero pressure isentropic bulk modulus K_{0S} and by the isentropic pressure derivative of the isentropic bulk modulus at zero pressure, K'_{0S}:

$$\mathscr{E}_{\mathrm{h}}(I_3) = -\frac{4K_{0S}}{\rho_0(K'_{0S}-1)^2}(1+r_K)\,\mathrm{e}^{-r_K}, \tag{68}$$

with

$$r_K = \frac{3(K'_{0S}-1)}{2}\left[\left(\frac{\rho_0}{\rho}\right)^{1/3} - 1\right]. \tag{69}$$

Density ρ is understood to depend on I_3 through (67d).

$\mathscr{E}_{\mathrm{t}}(I_3, S)$ is the thermal part, modeled on a Mie–Grüneisen form

$$\mathscr{E}_{\mathrm{t}}(I_3, S) = C_{\mathrm{V}}T_0\left(\exp\left[\frac{S-S_0}{C_{\mathrm{V}}}\right] - 1\right)\exp\left[\frac{\gamma_0 - \gamma(I_3)}{q}\right], \tag{70}$$

where C_{V} is a constant heat capacity, S_0 and T_0 are the entropy and temperature in the reference configuration (at zero pressure and density ρ_0), and where $\gamma(I_3)$ is the thermodynamic Grüneisen parameter given by the model equation

$$\gamma = \gamma_0\left(\frac{\rho_0}{\rho}\right)^q, \tag{71}$$

with γ_0 and $q \neq 0$ constants.

The energy change due to shearing motion at constant volume is given by

$$\mathscr{E}_{\mathrm{s}}(I_1, I_2, I_3) = \frac{G(\rho)}{2\rho}\left[\beta I_1 I_3^{-1/3} + (1-\beta)I_2 I_3^{-2/3} - 3\right]. \tag{72}$$

The parameter β, $0 \leqslant \beta \leqslant 1$, is an adjustable parameter chosen to control the symmetry of the shear potential away from the hydrostat (see [11]). The function $G(\rho)$ is the shear modulus, also constructed to follow the universal equation of state formalism, and determined by the zero pressure shear modulus G_0 and the pressure derivative of the shear modulus G'_0, also evaluated at zero pressure:

$$G(\rho) = G_0\left[(1-r_G)\left(\frac{\rho}{\rho_0}\right)^{1/3} - \frac{4}{3}r_G\left(\frac{K_{0S}}{G_0}G'_0 - 1\right)^{-1}\left(\frac{\rho}{\rho_0}\right)^{2/3}\right]\mathrm{e}^{-r_G}, \tag{73}$$

where

$$r_G = \frac{3}{2}\left[\frac{K_{0S}}{G_0}G'_0 - 1\right]\left[\left(\frac{\rho_0}{\rho}\right)^{1/3} - 1\right]. \tag{74}$$

Note that on the hydrostat of an elastically isotropic solid $I_1 = 3I_3^{1/3}$ and $I_2 = 3I_3^{2/3}$, and so $\mathscr{E}_{\mathrm{s}} = 0$.

To determine temperature T as a function of g and $\mathscr{E}$ we first rearrange (66) to solve for $\mathscr{E}_t$,

$$\mathscr{E}_t = \mathscr{E} - \mathscr{E}_h(I_3) - \mathscr{E}_s(I_1, I_2, I_3) \tag{75}$$

and then differentiate to obtain

$$T = \left.\frac{\partial \mathscr{E}}{\partial S}\right|_{C^e} = \frac{\mathscr{E}_t}{C_V} + T_0 \exp\left[\frac{\gamma_0 - \gamma}{q}\right]. \tag{76}$$

Parameters for this model, chosen to approximate the elastically isotropic response of copper, are given in Table 1.

4.2. Solution of the Riemann problem

Here, we illustrate the use of our method in the computation of a simple Riemann problem solution. Left and right states U_L and U_R are constructed from the parameters in Table 2. The components of g were chosen arbitrarily, but so as to avoid some of the pathological conditions described in Section 5. These initial conditions represent a moderate strength longitudinal compression, with a small component of shear.

Table 1
EOS parameters for elastically isotropic approximation to copper

Parameter	Value	Units
ρ_0	8.93	g/cm^2
K_{0S}	138	GPa
K'_{0S}	4.96	–
$G_0 2$	46.9	GPa
G'_0	0.57	–
β	0	–
T_0	300	K
C_V	3.9×10^{-4}	kJ/g·K
γ_0	1.96	–
q	1	–

Table 2
Initial conditions for calculation shown in Fig. 1

Parameter	Value	Units
Left state		
$\mathscr{E}_L$	−3.1	kJ/g
g_L	$\begin{pmatrix} 1 & 0 & 0 \\ 0.01 & 1.1 & 0 \\ 0.02 & 0 & 1.2 \end{pmatrix}$	–
v_L	$\begin{pmatrix} 2 \\ 0 \\ 0.1 \end{pmatrix}$	km/s
Right state		
$\mathscr{E}_R$	−3.1	kJ/g
g_R	$\begin{pmatrix} 1 & 0 & 0 \\ -0.02 & 1.1 & 0 \\ 0.01 & 0 & 1.2 \end{pmatrix}$	–
v_R	$\begin{pmatrix} 0 \\ -0.03 \\ -0.01 \end{pmatrix}$	km/s

The strength is in the range attainable by single-stage propellant-driven guns, but represents less than 10% of the velocity range of planetary impacts.

Even with these relatively mundane conditions, significant discrepancies between the exact solution and the approximate solution are observed for some variables. The approximate solution, shown in Fig. 1 by dashed lines and open symbols, was obtained by the procedure described in [9] using a primitive variable representation of A (i.e., ρ, v, $\mathscr{E}$, and ge_1, in place of the conservation form variables ρv, ρE, and ge_1). The exact results are displayed with solid lines and filled symbols. Circles represent the end points of the six nonlinear wave systems, and squares represent the contact discontinuity.

The exact solution consists of a 1-shock, a 2-rarefaction, a 3-shock, a 4-shock, a 5-rarefaction, and a 6-shock. Each wave system obeys the Lax entropy conditions. The existence of rarefactions is not

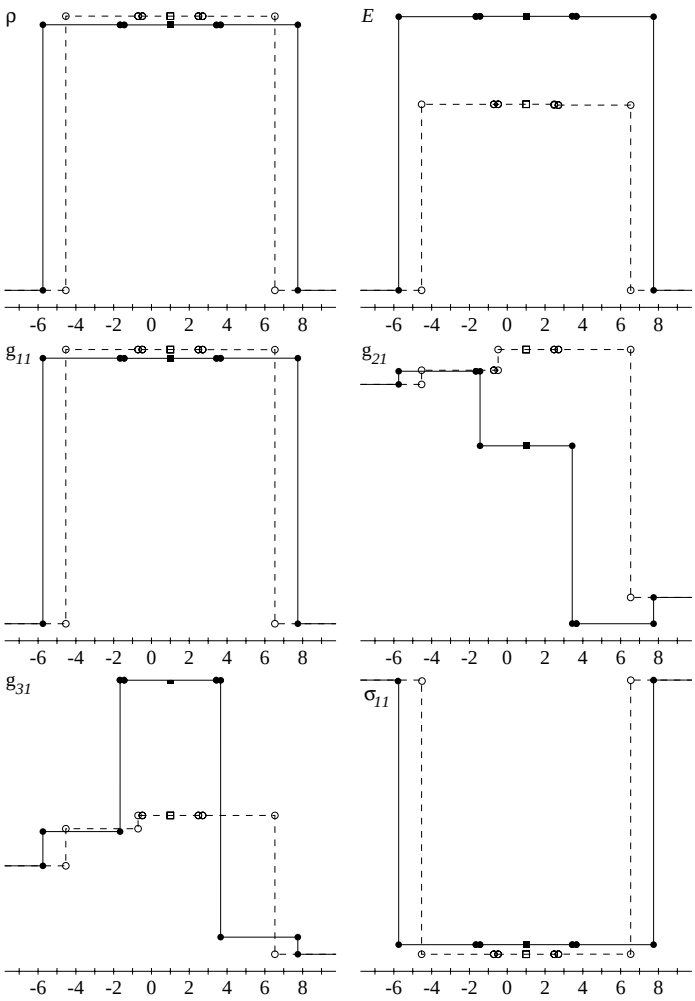

Fig. 1. Test problem showing approximate Riemann solution (IC in Table 2) after [9] (dash line, open symbols), and 'exact' result (solid line, filled symbols). The abscissa is wave velocity in km/s. Density ρ (range 11.7876–13.5924 g/cm^2), internal energy $\mathscr{E}$ (−3.1 to −1.925 kJ/g), inverse deformation tensor g_{11} (1–1.153), g_{21} (−0.024–0.015), and g_{31} (0.01–0.041), normal stress σ_{11} (−155.9 to −62.00 GPa), shear stresses σ_{21} (−1.094–1.735 GPa) and σ_{31} (−3.273 to −0.720 GPa), entropy S (0–1.808 $\times 10^{-5}$ kJ/g·K), temperature T (−478–612 K), velocities v_x (0–2 km/s), v_y (−0.035–0.021 km/s), and v_z (−0.01–0.1 km/s).

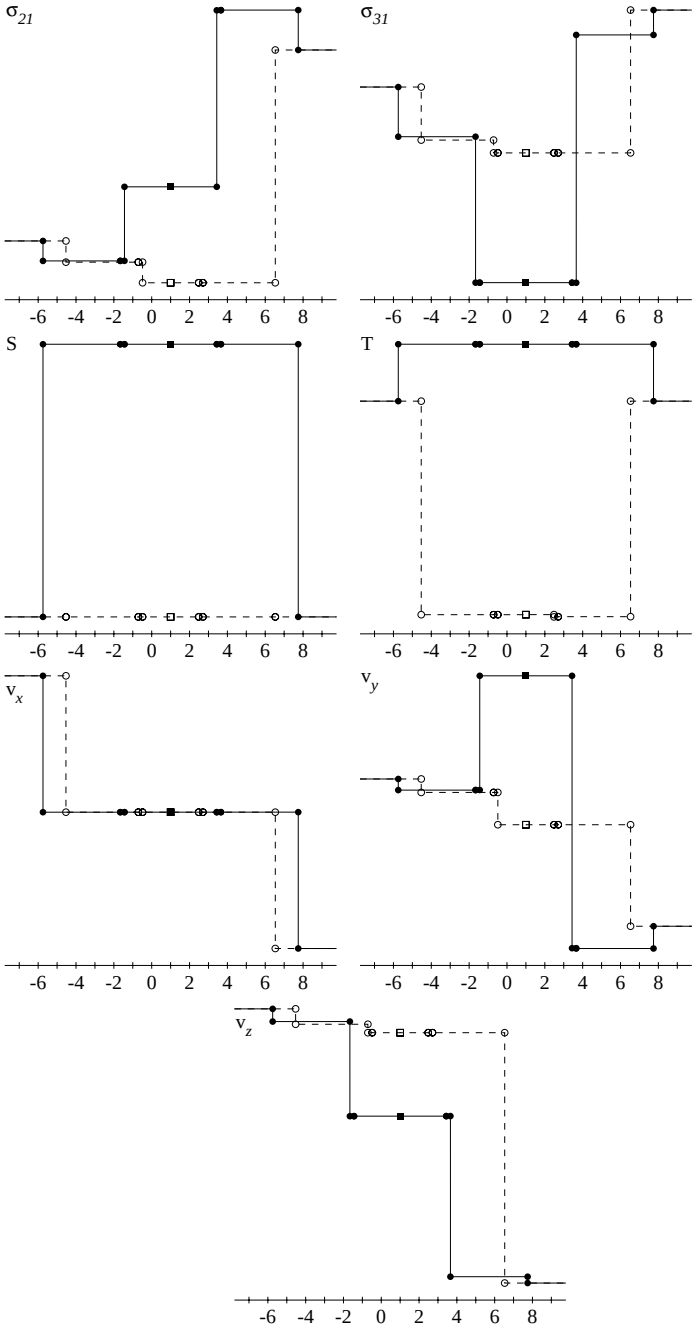

Fig. 1. (*continued*)

immediately obvious in the figures because the width of the wave fans is small. The 2-rarefaction is spread from only −1.6606 to −1.6600 km/s, and the 5-rarefaction from only 3.6600 to 3.6608 km/s.

A dramatic failure of the approximate solver is seen in the temperature and entropy fields. The approximate solver predicts negative temperatures, and pure imaginary entropy (the zero real part is plotted in the figure). The internal energy calculation is not unreasonable, but the partitioning of internal energy between compression ($\mathscr{E}_h$ and $\mathscr{E}_s$) and thermal ($\mathscr{E}_t$) terms is incorrect. The result is a nonphysical approximate solution.

Fig. 2 shows the result of a calculation using the initial conditions of Table 3. This test problem is similar to the first, but has initial states consistent with uniaxial deformation. In this case, the 2- and 5-waves are

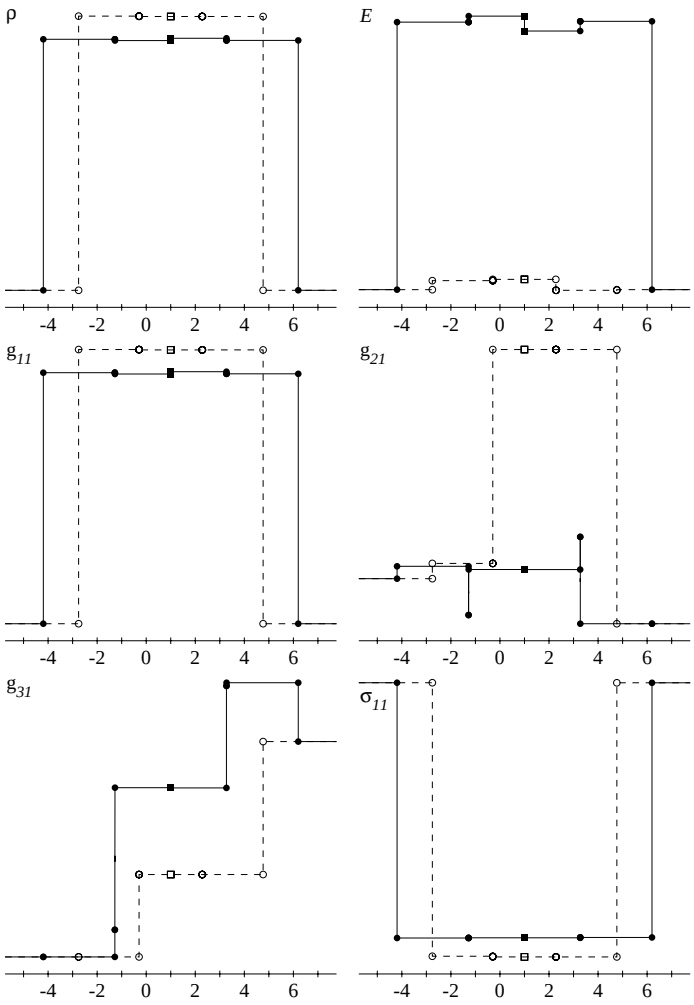

Fig. 2. Uniaxial isotropic case with degeneracy (IC in Table 3). Approximate solution after [9] (dash line, open symbols), and 'exact' result (solid line, filled symbols). The abscissa is wave velocity in km/s. Density ρ (range 8.930–10.810 g/cm^2), internal energy $\mathscr{E}$ (−3.901 to −3.374 kJ/g), inverse deformation tensor g_{11} (1–1.211), g_{21} (0–0.0608), and g_{31} (0–0.127), normal stress σ_{11} (−60.20 to −0.73 GPa), shear stresses σ_{21} (−3.40–0 GPa) and σ_{31} (−7.03–0 GPa), entropy S (0–2.509 $\times 10^{-4}$ kJ/g·K), temperature T (−759–784 K), velocities v_x (0–2 km/s), v_y (−0.115–0.020 km/s), and v_z (−0.08–0.1 km/s).

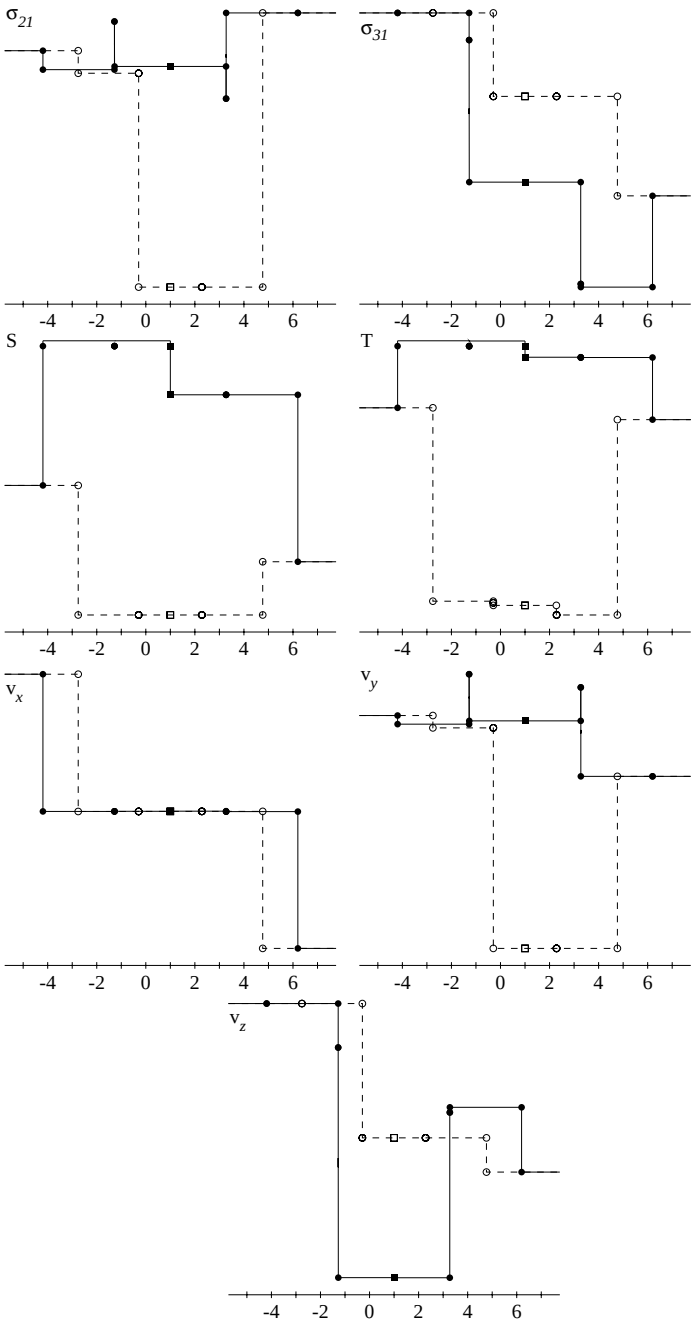

Fig. 2. (*continued*)

linearly degenerate across the wave system. The solution consists of a 1-shock, a linearly degenerate 2-shock (a contact discontinuity), a 3-rarefaction, a 4-shock, a linearly degenerate 5-shock (another contact discontinuity), and a 6-shock.

Table 3
Initial conditions for calculation shown in Fig. 2

Parameter	Value	Units
Left state		
$\mathscr{E}_L$	−3.9	kJ/g
g_L	$\begin{pmatrix} 1 & 0 & 0 \\ 0.01 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	–
v_L	$\begin{pmatrix} 2 \\ 0 \\ 0.1 \end{pmatrix}$	km/s
Right state		
$\mathscr{E}_R$	−3.9	kJ/g
g_R	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0.1 & 0 & 1 \end{pmatrix}$	–
v_R	$\begin{pmatrix} 0 \\ -0.03 \\ -0.01 \end{pmatrix}$	km/s

The state space encountered in this example violates several of the assumptions made in Section 2. In particular, the 2 and 3, and the 4 and 5-waves are degenerate at points across the wave system. Solution of this problem requires modifications to the algorithm of Section 2 described in Section 5.2.

5. Some pathological conditions

In this section, we consider some pathological conditions that occur in solid mechanics. This treatment is not exhaustive, but covers several special cases that occur commonly with the simple elastically isotropic model presented in Section 4.

5.1. Lack of genuine nonlinearity at points of high symmetry

When g is diagonal but not proportional to I, C^e is also diagonal and not proportional to I, with the result that X_{ac} will be proportional to a permutation of I. The three acoustic waves are aligned with the principal directions. The fast ($\lambda_{ac,3}$; $\lambda_1 = v_1 - \lambda_{ac,3}$) wave is a longitudinal mode, $X_{ac}e_3 = e_1$, and the slow waves are orthogonal transverse modes. At these special points, $r_1 \cdot D_U\lambda_1$ is nonzero, and the ordering method (59) may be used without ambiguity. However, the transverse wave speeds are local extrema, hence $r_2 \cdot D_U\lambda_2 = 0$, etc.

Let us suppose this circumstance, with λ_2 a local minimum. Then, whether α_2 is positive or negative, a finite perturbation $\mathrm{d}U = \alpha_2 r_2$ will increase λ_2: a rarefaction is required whatever the sign of α_2. Conversely, if λ_2 is a local maximum, then a shock is required whatever the sign of α_2.

Therefore, to obtain a solution obeying Lax's entropy condition it is insufficient to select the wave type by the sign of α_k when $r_k \cdot D_U\lambda_k = 0$ at the centering point.

Also, a simple wave trajectory passing though such a point of genuine nonlinearity must terminate at this point in order to obey the constraint that wave speeds vary monotonically across the wave. Computationally, this will occur if the acoustic eigenvector sign convention ((59) and subsequent discussion) is enforced. However, doing this makes the sign of $\partial U/\partial\alpha$ calculated on the rarefaction indeterminate, and this in turn may cause the overall multiple shooting method to fail to converge. Therefore, to assure convergence, the sign of vectors X_{ac} must be constant along the rarefaction integral, even though this may

violate wave monotonicity constraints on a given iteration. At the start of a rarefaction wave curve integration, the sign of $X_{\rm ac}$ is determined as described by (59). Subsequent evaluations of $X_{\rm ac}$ choose the sign to maximize the inner product of the appropriate columns of $X_{\rm ac}$ with the column obtained in the previously evaluation on the wave curve.

5.2. Degeneracy I: $0 < \lambda_{ac1} = \lambda_{ac2} < \lambda_{ac3}$

The analysis above assumes genuine nonlinearity and distinct eigenvectors. Both of these assumptions break down in a very common circumstance in elastically isotropic materials. In common practice, one constructs the hyperelastic energy function for an elastically isotopic material as a shear perturbation to a hydrostatic reference configuration. When evaluated at a point on the hydrostat, the shear modes are degenerate by virtue of symmetry. Further, since the shear energy is a minimum on the hydrostat the shear modes are linearly degenerate on the hydrostat, although they are genuinely nonlinear elsewhere.

Two problems arise in this case. First, given $\lambda_d = \lambda_{\rm ac1} = \lambda_{\rm ac2}$, the eigenvectors $X_{\rm ac}e_1$ and $X_{\rm ac}e_2$ of the acoustic tensor are not uniquely determined: any linear combination of these eigenvectors is itself an eigenvector with eigenvalue λ_d. Neither the shock nor the rarefaction algorithms are uniquely defined in this case. Second, the perturbation analysis (64b) is not appropriate. Both problems may be addressed if the degeneracy local: i.e., if upon perturbation of the centering state along either a shock Hugoniot locus or a rarefaction wave curve the degeneracy is lifted.

We first examine the problem of degeneracy alone (neglecting the lack of genuine nonlinearity) from a formal point of view to analyze the solution properties. Across a wave k that is degenerate, the degeneracy may be broken. In the particular case of an elastically isotropic hyperelastic solid constructed from an isentropic reference curve, this will always happen. Consideration of (63), (64) shows that if n_d degenerate waves are hybridized

$$\begin{pmatrix} X'_{\rm ac}e_{d_1} \\ \vdots \\ X'_{\rm ac}e_{d_{n_d}} \end{pmatrix} = \begin{pmatrix} X_{\rm ac}e_{d_1} \\ \vdots \\ X_{\rm ac}e_{d_{n_d}} \end{pmatrix} \Theta \tag{77}$$

in such a way that

$$\begin{pmatrix} (X'_{\rm ac}e_{d_1})^{\rm T}\mathscr{A}_U(X'_{\rm ac}e_{d_1}) & \cdots & (X'_{\rm ac}e_{d_1})^{\rm T}\mathscr{A}_U(X'_{\rm ac}e_{d_{n_d}}) \\ \vdots & \ddots & \vdots \\ (X'_{\rm ac}e_{d_{n_d}})^{\rm T}\mathscr{A}_U(X'_{\rm ac}e_{d_1}) & \cdots & (X'_{\rm ac}e_{d_{n_d}})^{\rm T}\mathscr{A}_U(X'_{\rm ac}e_{d_{n_d}}) \end{pmatrix} \tag{78}$$

is diagonal, then terms $(X'_{\rm ac}e_{d_i})^{\rm T}\mathscr{A}_U(X'_{\rm ac}e_{d_j})$, $i \neq j$ will be identically zero, and the singularities that would otherwise occur in (64b) will disappear.

In the present circumstance, let us perturb $\mathscr{A}$ not by differentiation, but by the action of the r_k degenerate wave, $\Delta\mathscr{A} = r_k \cdot D_U\mathscr{A}$. Combining (77) with (78) we obtain an eigenvalue problem, with eigenvectors Θ being the hybridization matrix, and eigenvalues ΔQ corresponding to the change in eigenvalue upon perturbation Δ (cf, (64a)):

$$\begin{pmatrix} (X_{\rm ac}e_{d_1})^{\rm T}\Delta\mathscr{A}X_{\rm ac}e_{d_1} & \cdots & (X_{\rm ac}e_{d_1})^{\rm T}\Delta\mathscr{A}X_{\rm ac}e_{d_{n_d}} \\ \vdots & \ddots & \vdots \\ (X_{\rm ac}e_{d_{n_d}})^{\rm T}\Delta\mathscr{A}X_{\rm ac}e_{d_1} & \cdots & (X_{\rm ac}e_{d_{n_d}})^{\rm T}\Delta\mathscr{A}X_{\rm ac}e_{d_{n_d}} \end{pmatrix} \theta = \theta\,{\rm diag}(\Delta Q_{d_1d_1}, \ldots, \Delta Q_{d_{n_d}d_{n_d}}). \tag{79}$$

The matrix $\left(X_{\mathrm{ac}}^{\mathrm{T}}\Delta\mathscr{A}X_{\mathrm{ac}}\right)$ is symmetric, with real eigenvalues, and Θ is unitary, $\Theta^{-1}=\Theta^{\mathrm{T}}$. In the $n_d=2$ case Θ may be represented as a rotation

$$\Theta=\begin{pmatrix}\cos\theta & \sin\theta\\ \sin\theta & -\cos\theta\end{pmatrix}. \tag{80}$$

To be specific, let us suppose that we are interested in computing state $\mathscr{U}_2$ from state $\mathscr{U}_1$ in the degenerate case. The relevant eigenvector r_2 depends on $X_{\mathrm{ac},2}$, which is not yet uniquely defined. According to (58b), across wave 2 we have perturbations

$$\Delta g e_1 = g e_1 X'_{\mathrm{ac},2}, \tag{81a}$$

$$\Delta\mathscr{E} = -e_1^{\mathrm{T}}\sigma X'_{\mathrm{ac},2}, \tag{81b}$$

$$\Delta\mathscr{A}_{\gamma\mu} = \frac{\partial\mathscr{A}_{\gamma\mu}}{\partial g e_1} g e_1 X'_{\mathrm{ac},2} - \frac{\partial\mathscr{A}_{\gamma\mu}}{\partial\mathscr{E}} e_1^{\mathrm{T}}\sigma X'_{\mathrm{ac},2}, \tag{81c}$$

$$\Delta\lambda_{\mathrm{ac}} = \frac{\Delta Q - Q e_1^{\mathrm{T}} X'_{\mathrm{ac},2}}{2\rho\lambda_{\mathrm{ac}}}. \tag{81d}$$

The Δr_2 perturbation will break the symmetry and lift the degeneracy because the symmetric reference configuration is defined for zero shear.

By virtue of (80), we may consider (79) with (81c) as a set of simultaneous equations in θ. Two solutions may be obtained in general, one of which satisfies the wave ordering denoted in Fig. 3. One solution comes from considering the solid line $\lambda(\alpha)$ in Fig. 3 as $\lambda_{\mathrm{ac},2}$; the other from considering the dashed line.

This settles the question of uniqueness: a self-consistent prescription is given above for lifting the degeneracy and identifying the relevant vector $X_{\mathrm{ac}}e_2$ for the computation of the 2-wave. Unresolved are the derivatives $D_U l_k$ and $D_U r_k$ appearing in (39b) and (42a) respectively. The $D_U r_k$ derivatives are evaluated along the rarefaction integral curve, where degeneracy will already be lifted by the perturbation $r_2\cdot D_U\cdot$, and so these derivatives pose no special problem. The derivatives $D_U l_k$ appearing in the shock problem are centered at the degenerate point U_0, however, and there the formal analysis breaks down.

For any perturbation $f\cdot D_U\mathscr{A}$, a different hybridization $\Theta(f/|f|)$ is required to cancel singularities in (64b). Since the hybridization depends on the direction of the perturbation, and not its strength, X_{ac} is not continuous at U_0 and therefore the derivative $D_U X_{\mathrm{ac}}$ does not exist.

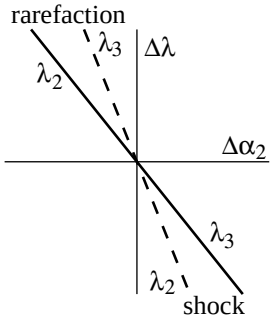

Fig. 3. Wave labeling conventions upon lifting λ_2,λ_3 degeneracy in state $\mathscr{U}_1$ with perturbation $\mathrm{d}r_2$, chosen to enforce canonical ordering.

However, if the degeneracy is local, in the present case when evaluated at $\mathscr{U}_1$, then unless $\alpha_2 = 0$ we expect the degeneracy to be lifted in $\mathscr{U}_2$. Then, instead of

$$H_2^{\mathrm{L}} = U_2(\mathscr{U}_1, \alpha_2) - \mathscr{U}_2, \tag{82a}$$

$$0 = H_2^{\mathrm{L}} - I\Delta\mathscr{U}_2 + \frac{\partial H_2^{\mathrm{L}}}{\partial \alpha_2}\Delta\alpha_2 + \frac{\partial H_2^{\mathrm{L}}}{\partial \mathscr{U}_1}\Delta\mathscr{U}_1 \tag{82b}$$

we may integrate across the wave starting from the nondegenerate point $\mathscr{U}_2$ with

$$H_2^{\prime\mathrm{L}} = \mathscr{U}_1(\mathscr{U}_2, -\alpha_2) - \mathscr{U}_1, \tag{83a}$$

$$0 = -\left(\frac{\partial H_2^{\prime\mathrm{L}}}{\partial \mathscr{U}_2}\right)^{-1} H_2^{\prime\mathrm{L}} - \Delta\mathscr{U}_2 - \left(\frac{\partial H_2^{\prime\mathrm{L}}}{\partial \mathscr{U}_2}\right)^{-1}\frac{\partial H_2^{\prime\mathrm{L}}}{\partial \alpha_2}\Delta\alpha_2 + \left(\frac{\partial H_2^{\prime\mathrm{L}}}{\partial \mathscr{U}_2}\right)^{-1}\Delta\mathscr{U}_1. \tag{83b}$$

That is, we may use the formal machinery developed in Section 2, with a redefinition of the terms related to H_2^{L} corresponding to a reversed centering.

If $\alpha_2 = 0$ then the derivatives $\partial H/\partial U$ and $\partial H/\partial\alpha$ are trivial, and again there is no problem. If $|\alpha_2|$ is small, such that the multiple shooting iterations may oscillate between shock and rarefaction solutions, then the reversed centering (82) should be used consistently from iteration to iteration to preserve the interpretation of α_k (which is different for forward- and reverse-centerings on the shock branch).

The analysis of a combined point of degeneracy and lack of genuine nonlinearity follows the procedure described above. However, in this case the degeneracy is not lifted by a first order perturbation $(r \cdot D_U)$, but must be lifted by the second order perturbation $(r \cdot D_U)^2$. The wave ordering in this case is not given as indicated in Fig. 3, but may be as indicated in Fig. 4. As in the simpler genuinely nonlinear case, backward centering of the solution (82) may be used to compute the desired solution.

If degeneracy occurs along a rarefaction wave curve, but not necessarily at the end points, then reverse centering will not resolve the eigenvector ambiguity. This circumstance occurred in the calculation shown in Fig. 2. At each point along the rarefaction wave curve, if degeneracy is detected then an appropriate hybridization must be calculated.

5.3. Degeneracy II: $0 = \lambda_{ac1} = \lambda_{ac2} < \lambda_{ac3}$

This circumstance corresponds to a so-called "soft acoustic mode": a thermodynamic loss of shear strength encountered upon melting. When $\lambda_{\mathrm{ac1}} = \lambda_{\mathrm{ac2}} = 0$, r_3 and r_5 become linearly degenerate and equal, and so do r_2 and r_6: there is a double eigenvector deficiency.

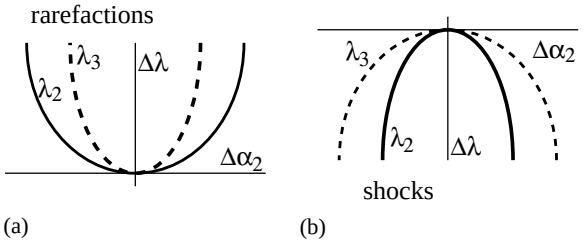

Fig. 4. Wave labeling conventions upon lifting λ_2, λ_3 degeneracy in state $\mathscr{U}_1$ with second-order perturbation $\mathrm{d}r_2$, chosen to enforce canonical ordering.

First we analyze the condition that this degeneracy exists in initial states U_{L} and U_{R}, and persists in all intermediate states. Then we have

$$\sigma = \begin{pmatrix} \sigma_{11} & 0 & 0 \\ 0 & \sigma_{11} & 0 \\ 0 & 0 & \sigma_{11} \end{pmatrix}, \tag{84a}$$

$$\mathscr{A} = \begin{pmatrix} \rho c^2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{84b}$$

and $X_{\mathrm{ac}} = \pi$ (54), $\Lambda_{\mathrm{ac}} = \mathrm{diag}(0,\ 0,\ c)$.

Without loss of generality we may at any point perform a "virtual remap" of the underlying Lagrangian reference coordinate $\vec{a}$. That is, set

$$\tilde{g} := g \tag{85}$$

and then

$$g := \begin{pmatrix} g_{11} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad F := \begin{pmatrix} 1/g_{11} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{86}$$

with initially $g_{11} = 1$. Then in place of $\mathscr{E}(g, S)$ we construct the internal energy function from $\mathscr{E}(g\tilde{g}, S)$. This mixed symbolic and numeric representation (86), together with (84a), (84b), expose the decoupling of variables ρv_2, ρv_3, g_{12}, and g_{13} in the matrix A (58a). Thus, in the case of melting we have $U = (\rho v_1,\ \rho E,\ g_{11})$, $U \in \mathbb{R}^3$, and

$$A = \begin{pmatrix} 2v_1 & 0 & \frac{\rho}{g_{11}}(c^2 - v_1^2) \\ E - \frac{\sigma_{11}}{\rho} & v_1 & (\rho v_1(c^2 - E) + v_1\sigma_{11})\frac{1}{g_{11}} \\ \frac{g_{11}}{\rho} & 0 & 0 \end{pmatrix}, \tag{87a}$$

$$R = \begin{pmatrix} \rho(v_1 - c) & 0 & \rho(v_1 + c) \\ (\rho E - \sigma_{11} - \rho c v_1) & 1 & (\rho E - \sigma_{11} + \rho c v_1) \\ g_{11} & 0 & g_{11} \end{pmatrix}, \tag{87b}$$

$$L = \begin{pmatrix} -\frac{1}{2\rho c} & 0 & \frac{1}{2g_{11}}\left(1 + \frac{v_1}{c}\right) \\ -v_1 & 1 & [\rho(v_1^2 - E) + \sigma_{11}]/g_{11} \\ +\frac{1}{2\rho c} & 0 & \frac{1}{2g_{11}}\left(1 - \frac{v_1}{c}\right) \end{pmatrix}, \tag{87c}$$

$$\Lambda = \mathrm{diag}(v_1 - c,\ v_1,\ v_1 + c), \tag{87d}$$

and

$$\mathscr{P} = \begin{pmatrix} v_1 \\ \sigma_{11} \end{pmatrix}. \tag{87e}$$

These equations describe the Euler equations in conservation form, with $P = -\sigma_{11}$ and ρc^2 the bulk modulus $K_S = \partial P/\partial \ln\rho|_S$, with c the bulk sound speed. This system of dimension $n = 3$, $m = 1$, contains two genuinely nonlinear waves and a single linearly degenerate contact discontinuity.

The more interesting problem arises when U_L and U_R are not initially degenerate, but that melting occurs for example across the 1 wave, so that states U_1, U_2, and U_3 are molten. In this case, the treatment of the 1 wave and of waves 4, 5, 6 follows the prescription of Section 2. The 2- and 3-waves are linearly degenerate, and let us suppose initially that they could be treated in the manner of a simple wave. The degenerate vectors 2 and 3 are

$$r_d = \begin{pmatrix} \rho v e_1^{\mathrm{T}} X_{\mathrm{ac}} \pi e_d \\ \rho\left(E - \frac{\sigma_{11}}{\rho}\right) e_1^{\mathrm{T}} X_{\mathrm{ac}} \pi e_d \\ g X_{\mathrm{ac}} \pi e_d \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ g_{1d} \\ g_{2d} \\ g_{3d} \end{pmatrix}, \quad d = 2, 3 \tag{88}$$

since $X_{\mathrm{ac}}\pi = I$ in this case. These vectors are constant, since in 1-directed flow ($\eta = 1$) the variables ge_2 and ge_3 are treated as parameters, constant on each side of the contact. Thus,

$$U_d(U_0, \alpha_d) = U_0 + \alpha_d r_d, \tag{89a}$$

$$D_{U_0} U_d(U_0, \alpha_d) = I, \tag{89b}$$

$$\frac{\partial}{\partial \alpha_d} U_d(U_0, \alpha_d) = r_d \tag{89c}$$

must apply across these degenerate waves if they were to be treated as genuine waves. However a consequence of (89) and (62) is that columns 2 and 3 of the matrix C (19a) become

$$\begin{pmatrix} 0 \\ 0 \\ 0 \\ \frac{\partial \sigma_{11}}{\partial g e_1}\Big|_{\mathscr{E}} g e_2 = 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ \frac{\partial \sigma_{11}}{\partial g e_1}\Big|_{\mathscr{E}} g e_3 = 0 \\ 0 \\ 0 \end{pmatrix} \tag{90}$$

and so C must be singular. The hypothesis that we may solve this problem as a 6-wave system is false. Instead, we must recognize that a phase change has occurred across the 1 wave, and so now the projection $\mathscr{P}$ acting across the contacts (including waves 2 and 3) is

$$\mathscr{P} : \mathbb{R}^7 \mapsto \mathbb{R}^4, \quad \mathscr{P}(U) = \begin{pmatrix} v_1 \\ \sigma_{11} \\ \sigma_{21} \\ \sigma_{31} \end{pmatrix} \tag{91}$$

describing fluid–solid coupling [10].

6. Conclusions

A general iterative solution to the Riemann problem for systems of conservation laws is presented. Under conditions where Lax's [6] existence and uniqueness argument holds, our iterative method converges

to this unique solution. The structure of the method is quite simple although the thermodynamic derivatives required may be complicated.

An analysis of the equations of hyperelastic solid mechanics reveals that the key assumptions of genuine nonlinearity and distinct eigenvalues are not always valid. In fact, these pathological conditions occur under very common conditions for equations of state with high symmetry. For these conditions, relatively straightforward modifications are recommended to obtain the correct entropy solution.

Using an elastically isotropic hyperelastic model approximating copper, a comparison of exact and approximate Riemann solutions reveals some significant discrepancies. In the examples of a predominately normal impact, with a small component of shear, the approximate solver obtains reasonable results for the hydrodynamic variables density ρ, normal velocity v_x, and normal stress σ_{11}. For the internal energy $\mathscr{E}$ the approximate solver is in error by approximately 30%. Entropy S and the derived temperature are non-physical in the approximate solution.

These results suggest that the approximate solver employed in [9,10] may be inadequate for certain computations. In particular, problems with temperature-dependent rates of chemical reaction, or temperature- and rate-dependent plasticity, may interact poorly with the approximate solver. Despite the surprisingly discrepant results between the exact and approximate Riemann solutions, numerical methods based on the approximate solver perform well and do converge to the correct state values and wave speeds [9,10]. This occurs because the approximate method is $\mathscr{O}(\Delta U \Delta A) \approx \mathscr{O}(\Delta U^2)$ and so consistent, and stable and consistent conservation-form methods converge to weak solutions of the conservation laws [5].

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