A Well-Balanced Path-Integral f-wave Method for Hyperbolic Problems with Source Terms

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Abstract. Systems of hyperbolic partial differential equations with source terms (balance laws) arise in many applications where it is important to compute accurate time-dependent solutions modeling small perturbations of equilibrium solutions in which the source terms balance the hyperbolic part. The f-wave version of the wave-propagation algorithm is one approach, but requires the use of a particular averaged value of the source terms at each cell interface in order to be "well balanced" and exactly maintain steady states. A general approach to choosing this average is developed using the theory of path conservative methods. A scalar advection equation with a decay or growth term is introduced as a model problem for numerical experiments.

Keywords: Hyperbolic partial differential equations, source terms, well-balanced methods.

1 Introduction

The goal of this paper is to present a new approach to incorporating source terms into high-resolution finite volume methods for problems of the form

$$q_t + f(q)_x = \psi(q)\sigma_x(x) \tag{1}$$

or

$$q_t + A(q)q_x = \psi(q)\sigma_x(x) \tag{2}$$

where $q(x,t) \in \mathbb{R}^m$, $\psi : \mathbb{R}^m \to \mathbb{R}^m$, $\sigma : \mathbb{R} \to \mathbb{R}$ and we either have a flux function $f : \mathbb{R}^m \to \mathbb{R}^m$ in (1) or a matrix-valued function $A : \mathbb{R}^m \to \mathbb{R}^{m\times m}$ in (2). The equation (1) can be written in the quasi-linear form (2) by defining the Jacobian $A(q) = f'(q)$, but (2) is more general. In any case we assume the homogeneous equation with $\psi \equiv 0$ is hyperbolic, i.e. that $f'(q)$ or $A(q)$ is diagonalizable with real eigenvalues.

The method is designed to work for problems where the solution is near a steady state equilibrium solution for which $q_t = 0$ and the source terms exactly balance the hyperbolic terms. In practical problems it is often necessary to solve "quasi-steady" problems close to such steady states. It is well known that fractional step methods, in which one alternates between solving the homogeneous equation and the pure source term problem, often fails for quasi-steady problems (see, e.g., [22]).

A method is called "well-balanced" if equilibrium initial data is exactly preserved by the method. The hope is that the method then also accurately resolves solutions that are small perturbations to equilibrium data. Many different well-balanced methods have been developed for specific problems, particularly shallow water equations, see for example [2, 5, 6, 7, 8, 10, 16, 17, 18, 21, 26, 27, 28]. However, there are still problems for which it is not clear how to define such a method and the need for more general strategies.

In [3] an approach was proposed using the f-wave version of the wave-propagation algorithm, which is reviewed in Section 2. These methods are based on solving Riemann problems at the interface between each pair of grid cells, so that the jump from Q_{i-1} and Q_i is resolved into waves propagating into neighboring cells. The main idea of the f-wave approach is to split the flux difference $f(Q_i) - f(Q_{i-1})$ into waves. Source terms are incorporated by modifying the flux difference by a quantity based on some average of the source terms between the two states before doing the splitting. For some problems, such as the "ocean-at-rest" steady state in the shallow water equations, a simple

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averaging formula yields a well-balanced method (as reviewed in Section 3). However, for other problems it is not clear how to define a suitable average.

In this paper an approach is explored that is based on the idea of "path conservative" methods for solving nonconservative problems of the form (2). The idea of an f-wave method is extended to this problem by replacing the flux difference by an integral of $A(\widehat{q}(s))\widehat{q}\,'(s)$ over a path in state space connecting Q_{i-1} to Q_i. The source term is incorporated in this path in a manner that effectively defines the proper average to use for quasi-steady problem, although in the formulation below the source term itself drops out of the resulting equations. This approach is based on incorporating $\sigma(x)$ as an additional component in an augmented vector $w = (q, \sigma)$ and considering the Riemann problem for the resulting hyperbolic system. This idea appears in several previous papers on source terms of this form, including the work of Gosse [16, 17], who introduced a similar approach to using the path conservative framework based on Riemann solutions to this expanded system. The simplified paths chosen here to define an approximate Riemann solution and its use in high resolution f-wave methods appears to be different from previous suggestions and may be a promising general approach to developing high-resolution well-balanced methods for a wide class of systems of this form. The details are explained in Section 5 after reviewing the existing methods that form the basis for the new approach.

Some examples are used to illustrate the method, including both the ocean-at-rest and more general flowing equilibria for shallow water equations in Section 3, and a new model problem of scalar advection with a source term in Section 7. Numerical results are presented for the latter problem. The tests are done using Clawpack [24] and all codes and additional plots may be found at `www.clawpack.org/links/wbfwave10`.

2 The f-wave approach

One approach to developing well-balanced finite volume methods is the so-called f-wave approach first formulated in [3, 25]. General discussions can also be found in [23] and [7]. This approach has been used in a number of applications with success, e.g. [1, 4, 20, 29, 30]. The f-wave formulation is a variant of the "wave-propagation algorithms" described in detail in [23] and implemented in Clawpack [24].

We assume familiarity with these methods and review them briefly to recall the main ideas and specify notation. In one dimension Q_i^n represents the cell average over grid cell i, which is the interval $[x_{i-1/2}, x_{i+1/2}]$. The Riemann problem between states Q_{i-1} and Q_i consists of the homogeneous hyperbolic equation with piecewise constant data, and the solution consists of M_w waves propagating away from $x_{i-1/2}$. Typically $M_w = m$ for a system of m equations, though approximate solvers may use a different number (e.g., HLLE uses $M_w = 2$). In the classic formulation of the wave-propagation algorithm the jump in q between neighboring cell averages is split into waves,

$$Q_i - Q_{i-1} = \sum_{p=1}^{M_w} \mathcal{W}_{i-1/2}^p \tag{3}$$

and these waves $\mathcal{W}_{i-1/2}^p \in \mathbb{R}^m$ are simply vectors represnting jump discontinuities propagating at some speeds $s_{i-1/2}^p$. For nonlinear problems with rarefaction wave solutions, these are typically obtained by some linearization of the problem, taking the $\mathcal{W}_{i-1/2}^p$ to be eigenvectors of a Roe-averaged Jacobian matrix, for example, and the speeds to be the corresponding eigenvalues. If $\ell_{i-1/2}^p$ and $r_{i-1/2}^p$ are the left and right eigenvectors of the approximate Jacobian $\widehat{A}_{i-1/2}$, then $\mathcal{W}_{i-1/2}^p = (\ell_{i-1/2}^p)^T(Q_i - Q_{i-1})r_{i-1/2}^p$.

The first-order upwind method can then be written as

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x}[\mathcal{A}^+\Delta Q_{i-1/2} + \mathcal{A}^-\Delta Q_{i+1/2}] \tag{4}$$

where the symbols $\mathcal{A}^{\pm}\Delta Q_{i-1/2}$ represent the "fluctuations", the vectors

$$\mathcal{A}^{\pm}\Delta Q_{i-1/2} = \sum_p (s^p_{i-1/2})^{\pm} \mathcal{W}^p_{i-1/2} \tag{5}$$

where $s^+ = \max(s, 0)$ and $s^- = \min(s, 0)$. Second order correction terms can be added that depend on the waves and speeds, and by applying limiters to the waves it is possible to develop a very general formulation of a high-resolution method that avoids oscillations near discontinuities while giving second-order accuracy in smooth regions of the flow. The Clawpack software [24] is based on this approach, and written in a general framework that easily applies to many hyperbolic systems.

The idea of the f-wave splitting for $q_t + f(q)_x = 0$ is to decompose the flux difference $f(Q_i) - f(Q_{i-1})$ into waves rather than the q-difference used in (3), i.e. we split

$$f(Q_i) - f(Q_{i-1}) = \sum_{p=1}^{M_w} \mathcal{Z}^p_{i-1/2} \tag{6}$$

for some vectors $\mathcal{Z}^p_{i-1/2} \in \mathbb{R}^m$, e.g. again as eigenvectors of the approximate Jacobian: $\mathcal{Z}^p_{i-1/2} = (\ell^p_{i-1/2})^T (f(Q_i) - f(Q_{i-1}))r^p_{i-1/2}$.

The upwind method still has the form (4) but now with

$$\mathcal{A}^{\pm}\Delta Q_{i-1/2} = \sum_p \text{sgn}(s^p_{i-1/2}) \mathcal{Z}^p_{i-1/2} \tag{7}$$

where sgn is the sign-function with $\text{sgn}(0) = 1/2$. If eigenvector-splittings for an approximate Jacobian are used as suggested above, then (7) agrees exactly with (5) provided that $\widehat{A}_{i-1/2}(Q_i - Q_{i-1}) = f(Q_i) - f(Q_{i-1})$, exactly the Roe condition for a Roe-averaged Jacobian. Second order correction terms have a similar minor modification and for Roe solvers are equivalent in the two formulations except that in the f-wave formulation, limiters are applied to the f-waves $\mathcal{Z}^p$ of (6) rather than to the waves $\mathcal{W}^p$.

One advantage of the formulation (6), (7) over (3), (5) is that the method will be conservative even if the Roe condition is not satsified on the averaged Jacobian $\widehat{A}_{i-1/2}$. Another advantage discussed extensively in [3] is that it naturally extends to spatially varying flux functions $f(q, x)$.

A third advantage is of particular interest here: one can often incorporate source terms directly into the f-wave splitting in a well balanced manner. A simple extension of the approach of [3] to (2) suggests that the waves $\mathcal{Z}^p_{i-1/2}$ should be obtained by splitting

$$f(Q_i) - f(Q_{i-1}) - \Psi_{i-1/2}(\sigma_i - \sigma_{i-1}) \tag{8}$$

into eigenvectors. Here $\Psi_{i-1/2}$ is some suitable average of $\psi(q, x)$ between the neighboring states and $\sigma_i - \sigma_{i-1} = \sigma(x_i) - \sigma(x_{i-1})$ reduces to Δx for the case $\sigma(x) = x$ considered in [3].

We expect the possibility of a well-balanced method because an equilibrium solution $q^e(x)$ satisfies

$$\int_{x_{i-1}}^{x_i} f(q^e(x))_x - \psi(q^e(x))\sigma'(x)\, dx = 0 \tag{9}$$

The term (8) is an approximation to this integral, and so if $\Psi_{i-1/2}$ is chosen properly we can hope that the vector (8) will reduce to the zero vector. Decomposing this into waves gives zero-strength waves and fluctuations, and hence a solution that does not change in time. Moreover, for quasi-steady solutions that are near steady state, the limiters and second-order correction terms are applied to the deviations from steady state modeled by (8), typically yielding very good accuracy even for extremely small perturbations of a steady state.

The trick is choosing an appropriate averaging of the source term. In the next section we see that this can be easily done in one standard problem, but it is not always obvious how to do so in general. The remainder of the paper provides a possible approach.

3 Applications

We briefly review two problems where well-balanced methods are useful: shallow water flow over topography and gas dynamics in a stratified atmosphere. In Section 7 a simpler scalar equation is also used as a model problem.

Underwater topography is generally called *bathymetry* and we use $B(x)$ to denote the bathymetry. The shallow water equations then take the form

$$\begin{aligned} h_t + (hu)_x &= 0 \\ (hu)_t + \left(hu^2 + \frac{1}{2}gh^2\right)_x &= -ghB_x(x). \end{aligned} \tag{10}$$

This has the form (1) with

$$q = \begin{bmatrix} h \\ hu \end{bmatrix}, \quad f(q) = \begin{bmatrix} hu \\ hu^2 + \frac{1}{2}gh^2 \end{bmatrix}, \quad \psi(q) = \begin{bmatrix} 0 \\ -gh \end{bmatrix}, \quad \sigma(x) = B(x). \tag{11}$$

Example I (ocean-at-rest): An important special case for many applications is the *ocean-at-rest* equilibrium where $u^e(x) \equiv 0$ and $h^e(x) + B(x) \equiv \bar{\eta}$, so the top surface of the water is flat at sea level $\bar{\eta}$. The f-wave method for this problem is well-balanced if we choose the arithmetic average of h_{i-1} and h_i in the source term, yielding

$$\Psi_{i-1/2}(\sigma_i - \sigma_{i-1}) = \begin{bmatrix} 0 \\ -\frac{g}{2}(h_{i-1} + h_i)(B_i - B_{i-1}) \end{bmatrix}, \tag{12}$$

where we use $\sigma = B$.

Since the steady state solution has $u_{i-1} = u_i = 0$, the second component of the flux difference reduces to $\frac{g}{2}(h_i^2 - h_{i-1}^2)$. Moreover, in this steady state $h_{i-1} + b_{i-1} = h_i + B_i = \bar{\eta}$, from which it can be checked that this flux difference exactly cancels out with (12) and so (8) reduces to the zero vector. The f-wave formulation of the shallow water equations has been used extensively in tsunami modeling, an application where it is crucial that small perturbations on the ocean-at-rest be accurately captured since the magnitude of a tsunami wave is generally one meter or less while the bathymetry varies on the order of several kilometers. For more discussion of this application see for example [13, 14, 15].

Note that this exact cancellation occurs when the arithmetic average is used in the source term only because the hydrostatic pressure $\frac{1}{2}gh^2$ is quadratic in the depth and $h_i^2 - h_{i-1}^2 = (h_i + h_{i-1})(h_i - h_{i-1})$.

Example II (flowing shallow water): There are equilibrium solutions to the one-dimensional shallow water equations in which the velocity is not zero, corresponding to steady flow through a channel. In this case the momentum hu (also called the "discharge" in this context) must be constant in space from the first equation of (10). Call this constant value of the momentum $\bar{m}$. For smooth steady states without shock waves, it can be shown by manipulating (10) that the energy

$$\frac{1}{2}u^2 + g(h + B) \tag{13}$$

must also be constant. Replacing u in this equation by $\bar{m}/h$ and multiplying by h^2 gives a cubic equation for h in terms of B that can be solved to obtain the equilibrium solution for a given bathymetry $B(x)$. (In this paper we only consider the nonresonant case for which this is possible.)

Given an equilibrium solution of this form, using the f-wave method with the source term approximated by (12) does not give a method that is exactly well balanced. It typically performs quite well, however, and from the literature it is not clear how important having an exactly well-balanced method is for this case. Nonetheless, some methods have been developed that achieve this, such as the method of Gosse [16] or the WENO method proposed in [28]. The method of this paper gives another approach.

Example III (atmosphere-at-rest): A problem closely related to Example I is the atmosphere-at-rest problem, in which a vertical pressure gradient exactly balances the force of gravity. Accurately

computing small amplitude disturbances propagating through such an atmosphere again requires well-balanced methods. In one space dimension, with x now the vertical coordinate and u the vertical velocity, the simplest compressible equations are the equations of polytropic gas dynamics,

$$\begin{aligned} \rho_t + (\rho u)_x &= 0, \\ (\rho u)_t + (\rho u^2 + p(\rho))_x &= -g\rho, \end{aligned} \tag{14}$$

where $p(\rho)$ gives the pressure as a function of density, e.g. by the polytropic equation of state

$$p(\rho) = K\rho^\gamma \tag{15}$$

for some constants K and γ. This is of the form (1) if we set

$$\psi(q,\sigma) = \begin{bmatrix} 0 \\ -g\rho \end{bmatrix}, \qquad \sigma(x) = x. \tag{16}$$

Note the special case $K = 1/2,\ \gamma = 2$, in which case (14) is just the shallow water equations on a linear beach with $B(x) = x$. For air, $\gamma \approx 1.4$ and the pressure is not a quadratic function, which means that using the arithmetic average $\frac{1}{2}(\rho_{i-1} + \rho_i)$ in defining $\Psi_{i-1/2}$ in (8) will not yield a well-balanced method. An averaging formula that does give a well-balanced method is derived in Section 6. The full Euler equations in which (14) is augmented by an energy equation is also briefly discussed in Section 6.

4 Path conservative methods

Path conservative methods were introduced to extend the idea of conservative finite volume methods to equations containing nonconservative products such as (2) (see, e.g., [9, 10, 11, 12]). First consider the homogeneous system $q_t + A(q)q_x = 0$ and the Riemann problem between states Q_{i-1} and Q_i. Suppose we know the physically correct solution to the Riemann problem, a similarity solution depending only on $(x - x_{i-1/2})/t$. This similarity solution corresponds to some path $\widehat{q}(s)$ in state space connecting Q_{i-1} and Q_i, as the parameter s goes from 0 to 1. Then we can define an f-wave method in which we split

$$\mathcal{A}\Delta Q_{i-1/2} \equiv \int_0^1 A(\widehat{q}(s))\widehat{q}\,'(s)\,ds \tag{17}$$

into left- and right-going fluctuations $\mathcal{A}^\pm \Delta Q_{i-1/2}$, and further into waves $\mathcal{Z}^p_{i-1/2}$ for second-order corrections. If $A(q)$ is the Jacobian of a flux function, $A(q) = f'(q)$, then (17) reduces to $f(Q_i) - f(Q_{i-1})$ regardless of what path is chosen and we recover the standard f-wave method. However, more generally the value of $\mathcal{A}\Delta Q_{i-1/2}$ defined by (17) depends on the path.

Note that if the Riemann solution involves discontinuities then q_x contains delta functions supported at the same points where $A(q)$ is discontinuous, and so the "nonconservative product" $A(q)q_x$ is not well defined, even in the distribution sense. The path chosen in state space resolves this ambiguity by determining how q varies *within* the discontinuity, since the path $\widehat{q}(s)$ is continuous in state space even for the portion of the path that corresponds to the jump discontinuity. This is the power of the path conservative approach: it makes sense of the nonconservative product. But we can only do so properly by assuming we know the correct path for each Riemann problem that arises, which generally requires more knowledge about the physics of the problem. For example, we may need to know what higher-order terms are ignored in deriving the hyperbolic problem, since, for example, adding a diffusive term and letting the coefficient vanish may give different limiting paths depending on the form of diffusion chosen.

Unfortunately, in practical problems it is frequently difficult to determine the correct path and often a straight-line path is used to compute the integral (17) in numerical methods, i.e.,

$$\widehat{q}(s) = (1-s)Q_{i-1} + sQ_i \qquad \text{for } 0 \le s \le 1. \tag{18}$$

This at least resolves the ambiguity in some manner, and experiments have shown that this may be adaquate for some practical problems. See [9] for more discussion and some examples. The choice of correct path for specific applications is an active area of research. In this paper we choose paths to simplify the integrals that arise when source terms are included.

To incorporate source terms, note that (2) can be rewritten as a homogeneous system if we view $\sigma(x)$ as another component in the hyperbolic system satisfying $\sigma_t = 0$. We set

$$w = \begin{bmatrix} q \\ \sigma \end{bmatrix}, \qquad B(w) = \begin{bmatrix} A(q) & -\psi(q) \\ 0 & 0 \end{bmatrix} \tag{19}$$

and then (2) becomes

$$w_t + B(w)w_x = 0. \tag{20}$$

For this problem a path in state space takes the form $\widehat{w}(s) = (\widehat{q}(s),\, \widehat{\sigma}(s))$. Using a path-conservative method for this problem, we find that (17) is replaced by

$$\mathcal{A}\Delta Q_{i-1/2} \equiv \int_0^1 A(\widehat{q}(s))\widehat{q}\,'(s) - \psi(\widehat{q}(s))\widehat{\sigma}'(s)\, ds. \tag{21}$$

If $A(q)$ is a Jacobian, i.e., if we had started with (1), then the first term of the integral would be path-independent and this reduces to

$$\begin{aligned} \mathcal{A}\Delta Q_{i-1/2} &= \int_0^1 f'(\widehat{q}(s))\widehat{q}\,'(s) - \psi(\widehat{q}(s))\widehat{\sigma}'(s)\, ds \\ &= f(Q_i) - f(Q_{i-1}) - \int_0^1 \psi(\widehat{q}(s))\widehat{\sigma}'(s)\, ds. \end{aligned} \tag{22}$$

We will only consider this case for the remainder of the paper, since the examples considered all have the form (1), but the ideas should carry over more generally to equations of the form (2).

Note that choosing an approximation to the remaining integral in (22) can be viewed as equivalent to choosing an average $\Psi_{i-1/2}$ as discussed in Section 2, since if we approximate $\psi(\widehat{q}(s)) \approx \Psi_{i-1/2}$ for $0 \le s \le 1$ and pull this out of the integral then (22) reduces to (8). However, in order to use the path integral idea to choose such an average we will keep $\mathcal{A}\Delta Q_{i-1/2}$ in the form of the first line of equation (22).

The eigenvalues of $B(w)$ consist of the eigenvalues of $A(q)$ together with $\lambda = 0$, corresponding to a new linearly degenerate field introduced by adding $\sigma(x)$ as an element of w. If the original system is hyperbolic ($A(q)$ diagonalizable with real eigenvalues) then so is the extended system provided that 0 is not an eigenvalue of $A(q)$. The "resonant case" where A is singular and B has $\lambda = 0$ as a repeated eigenvalue can be more difficult. Note that for the shallow water equations the eigenvalues of A are $u \pm \sqrt{gh}$ and the ocean-at-rest case is non-resonant for $h > 0$. The moving-water equilibrium is non-resonant in the subcritical case with $|u| < \sqrt{gh}$. The transcritical case is more subtle and an equilibrium typically contains stationary shock waves where the solution jumps from one solution of the cubic equation described in Section 3 to another. Here we concentrate on the non-resonant case.

Consider a state $w_* = (q_*,\ \sigma_*)$ for which $A(q_*)$ is nonsingular. The matrix $B(w_*)$ has m eigenvectors given by the vectors $(r^p, 0)^T$, where r^p is the pth eigenvector of $A(q_*)$. In the non-resonant case, the eigenvector for the new linearly degenerate field can be written as

$$\begin{bmatrix} r_* \\ 1 \end{bmatrix}, \tag{23}$$

with $r_* = A(q_*)^{-1}\psi(q_*) \in \mathbb{R}^m$. Through the point w_* there is a unique 1-parameter integral curve $\widehat{w}(s) = (\widehat{q}(s),\ \widehat{\sigma}(s))$ of the linearly degenerate field satisfying

$$A(\widehat{q}(s))\widehat{q}\,'(s) - \psi(\widehat{q}(s))\widehat{\sigma}'(s) = 0 \tag{24}$$

at each point. Note that this is exactly the expression appearing as the integrand in (21), which will be important below. These means that varying w along the integral curve through w_* yields nearby states that are in equilibrium with w_*.

Since the final component of the eigenvector (23) is nonzero, we can view q as a function of σ along this path, at least sufficiently close to w_*, and we will denote this path by

$$w^{[*]}(\sigma) = (q^{[*]}(\sigma),\ \sigma) \tag{25}$$

for σ near σ_*.

Now recall that σ is a function of x. Let w_* be the solution at one point x, then $w^{[*]}(\sigma(x))$ gives a solution that varies in x. The fact that (24) is satisfied along this solution means that the given state w_* can be viewed as one pointwise state of an equilibrium solution as σ varies near σ_*. Some examples follow.

For Example I from Section 3 (the ocean-at-rest), given any state $w_* = (h_*,\ 0,\ B_*)$ with zero velocity, some non-negative depth h_*, and bathymetry B_*, this is clearly one state in an ocean at rest. Given any other bathymetry value B, the corresponding depth is $h^{[*]}(B) = \min(h_* + B_* - B,\ 0)$ (taking the minimum to allow dry states). In this case $\sigma = B$ and $w^{[*]}(s) = (h^{[*]}(B(s)),\ 0,\ B(s))$. Example III (atmosphere-at-rest) is similar and is considered further in Section 6.

For Example II (a flowing equilibrium), consider a state $w_* = (h_*, m_*, B_*)$ where the momentum $m_* = (hu)_*$ need not be zero (but is subcritical). Then for a nearby bathymetry value B we can follow the integral curve to find $w^{[*]}(B) = (h(B, m_*),\ m_*,\ B)$, where $h(B, m_*)$ is obtained by solving a cubic equation as described in Section 3.

5 A well-balanced path conservative method

Finally we come to the main idea of the new approach. Given states Q_{i-1} and Q_i for which we wish to define $\mathcal{A}\Delta Q_{i-1/2}$ via (22), construct the local equilibrium solution $Q^{[i-1]}(\sigma)$ passing through (Q_{i-1}, σ_{i-1}) and let $\widehat{Q}_i = Q^{[i-1]}(\sigma_i)$ be the value of this local equilibrium solution at σ_i. We do this by following the integral curve of the linearly degenerate field as discussed in the previous section.

Now consider the following path in state space:

$$(Q_{i-1}, \sigma_{i-1}) \quad \longrightarrow \quad (\widehat{Q}_i, \sigma_i) \quad \longrightarrow \quad (Q_i, \sigma_i) \tag{26}$$

with an arbitrary parameterization $s \in [0, 1]$, chosen with the intermediate point $(\widehat{Q}_i, \sigma_i)$ reached at $s = 1/2$. Along the first half of this path, σ varies from σ_{i-1} to σ_i while moving along the local equilibrium solution. Along the second half, Q varies from $\widehat{Q}_i$ to Q_i while keeping σ constant. Splitting the path integral (22) into two pieces yields

$$\int_0^{1/2} f'(\widehat{q}(s))\widehat{q}\,'(s) - \psi(\widehat{q}(s))\widehat{\sigma}'(s)\,ds + \int_{1/2}^1 f'(\widehat{q}(s))\widehat{q}\,'(s) - \psi(\widehat{q}(s))\widehat{\sigma}'(s)\,ds. \tag{27}$$

By our choice of path, the first integral is zero (since we move along an equilibrium solution) while in the second integral the source term vanishes (since $\widehat{\sigma}$ is constant for $s \in [1/2, 1]$ and so $\widehat{\sigma}'(s) = 0$). Hence the only remaining term is the integral of f over the second portion of the path and the entire integral reduces to

$$f(Q_i) - f(\widehat{Q}_i) \tag{28}$$

regardless of the parameterization.

There is a second equally plausible choice of paths:

$$(Q_{i-1}, \sigma_{i-1}) \quad \longrightarrow \quad (\widehat{Q}_{i-1}, \sigma_{i-1}) \quad \longrightarrow \quad (Q_i, \sigma_i) \tag{29}$$

where $\widehat{Q}_{i-1} = Q^{[i]}(\sigma_{i-1})$. On this path we first hold $\widehat{\sigma}$ constant at σ_{i-1} for the first half and then move along the local equilibrium solution $Q^{[i]}(\sigma)$ through (Q_i, σ_i). A similar computation of the integral from (22) along this path shows that it reduces to

$$f(\widehat{Q}_{i-1}) - f(Q_{i-1}) \tag{30}$$

regardless of the parameterization. In general neither path corresponds to the exact solution of the Riemann problem for (20) (See Notes 5 and 6 below), but a simple general approach to obtaining a well-balanced method is to average expressions (28) and (30) and take

$$\mathcal{A}\Delta Q_{i-1/2} = \frac{1}{2}[f(Q_i) - f(\widehat{Q}_i) + f(\widehat{Q}_{i-1}) - f(Q_{i-1})]. \tag{31}$$

This is the vector that is split into f-waves $\mathcal{Z}^p_{i-1/2}$ and into left- and right-going fluctuations $\mathcal{A}^{\pm}\Delta Q_{i-1/2}$.

Note the following:

1. This method is well-balanced. If the data (Q_{i-1}, σ_{i-1}) and (Q_i, σ_i) are sampled from an equilibrium solution then our constructions above give $\widehat{Q}_{i-1} = Q_{i-1}$ and $\widehat{Q}_i = Q_i$ and so (31) gives $\mathcal{A}\Delta Q_{i-1/2} = 0$ as desired.

2. We can rewrite $\mathcal{A}\Delta Q_{i-1/2}$ from (31) as

$$\mathcal{A}\Delta Q_{i-1/2} = f(Q_i) - f(Q_{i-1}) + \frac{1}{2}[-f(Q_i) - f(\widehat{Q}_i) + f(\widehat{Q}_{i-1}) + f(Q_{i-1})] \tag{32}$$

   and interpret the final term as the approximation to the source term to be used in place of $\Psi_{i-1/2}(\sigma_i - \sigma_{i-1})$ in (8). This seems odd since the source term does not explicitly appear in this term, but of course it implicitly comes into the calculation of $\widehat{Q}_i$ and $\widehat{Q}_{i-1}$.

3. For Example I (ocean-at-rest), it is easy to verify that the expression (32) reduces to (8) with (12).

4. For Example II (flowing shallow water), it is not easy to write down a closed expression for $\mathcal{A}^+\Delta Q_{i-1/2}$ from (31) for this example since two cubic equations must be solved to evaluate it. Numerically it has been verified that use of this formula for a standard test problem of subcritical flow over a bump maintains a steady state to machine precision. One advantage of this formulation is that the local equilibrium solution is determined for each state separately and there is no *a priori* assumption of a particular equilibrium that the method should be well balanced with respect to. The equilibrium state can evolve from one to another via time-dependent boundary conditions, for example, and the method will be well-balanced on both. This case is the subject of on-going investigation and will be reported on elsewhere.

5. Instead of using the paths defined above, one could in principle correctly solve the Riemann problem for the extended system $w_t + B(w)w_x = 0$ and use the resulting waves in the wave propagation algorithm. This would correspond to using the path

$$(Q_{i-1}, \sigma_{i-1}) \quad \longrightarrow \quad (\widetilde{Q}_{i-1}, \sigma_{i-1}) \quad \longrightarrow \quad (\widetilde{Q}_i, \sigma_i) \quad \longrightarrow \quad (Q_i, \sigma_i) \tag{33}$$

   where Q_{i-1} is connected to $\widetilde{Q}_{i-1}$ by left-going waves corresponding to negative eigenvalues of A, the transition from $\widetilde{Q}_{i-1}$ to $\widetilde{Q}_i$ corresponds to moving along the equilibrium solution as σ varies and gives the linearly degenerate wave moving at speed 0 in the Riemann solution, and then $\widetilde{Q}_i$ is connected to Q_i by right-going waves corresponding to positive eigenvalues of A. Similar analysis as above would then suggest that we take

$$\mathcal{A}^-\Delta Q = f(\widetilde{Q}_{i-1}) - f(Q_{i-1}), \qquad \mathcal{A}^+\Delta Q = f(Q_i) - f(\widetilde{Q}_i). \tag{34}$$

   The problem with this approach is that it may be quite difficult to determine $\widetilde{Q}_{i-1}$ and $\widetilde{Q}_i$ analytically and it is not clear how to use this approach in the context of an approximate Riemann solver. Gosse [17] discusses the use of an approximate Riemann solver of the type developed by Toumi [31] for non-conservative systems and develops a method of this form that is well balanced to high order but not exactly.

6. Note that the path (26) in fact agrees with (33) in the special case where all eigenvalues of A are positive and the path (29) agrees with (33) if all eigenvalues of A are negative. In one of these cases it would make most sense to use only the appropriate path rather than averaging results from the two, although averaging still gives a well-balanced method. This is discussed further in Section 7 where numerical results are compared for a scalar advection example where A has only a single eigenvalue. In the scalar case the equilibrium paths $q^{[*]}$ discussed above correspond to the paths in Theorem 3.1 of Gosse [17].

6 Atmosphere at rest

As another example, we apply this idea to Example III from Section 3, an atmosphere at rest. In this case we will not attempt to make the method well-balanced for a moving atmosphere and so we will assume that $u_{i-1} = u_i = 0$ (though the resulting method works well also for small amplitude perturbations where the velocity is nonzero). The result can be interpreted as defining a source term averaging $\Psi_{i-1/2}$ that can the be used also in a moving atmosphere near this equilibrium, just as the simple averaging of (12) can be used for problems near the ocean-at-rest equilibrium even when the velocities are not identically zero.

For the equations (14), the equilibrium solution passing through a specified value ρ_* at $x = x_*$ is given by

$$\rho^{[*]}(x) = \left(\rho_*^{\gamma-1} - \frac{g(\gamma-1)(x-x_*)}{\gamma K}\right)^{1/(\gamma-1)} \tag{35}$$

So given states (ρ_{i-1}, x_{i-1}) and (ρ_i, x_i) (and assuming $u_{i-1} = u_i = 0$) we find that

$$\begin{aligned} \widehat{\rho}_i = \rho^{[i-1]}(x_i) &= \left(\rho_{i-1}^{\gamma-1} - \frac{g(\gamma-1)\Delta x}{\gamma K}\right)^{1/(\gamma-1)} \\ \widehat{\rho}_{i-1} = \rho^{[i]}(x_{i-1}) &= \left(\rho_i^{\gamma-1} + \frac{g(\gamma-1)\Delta x}{\gamma K}\right)^{1/(\gamma-1)} \end{aligned} \tag{36}$$

Using these expressions in (32) we find that the second component of $\mathcal{A}\Delta Q_{i-1/2}$ takes the form (still assuming $u_{i-1} = u_i = 0$)

$$K(\rho_i^\gamma - \rho_{i-1}^\gamma) + \frac{K}{2}[-\rho_i^\gamma - \widehat{\rho}_i^\gamma + \widehat{\rho}_{i-1}^\gamma + \rho_{i-1}^\gamma] \tag{37}$$

The first term is just the momentum flux difference and the second term can be interpreted as the desired average of the source term for use in (8):

$$\begin{aligned} \Psi_{i-1/2}\Delta x = -\frac{K}{2}\Bigg[&-\rho_i^\gamma - \left(\rho_{i-1}^{\gamma-1} - \frac{g(\gamma-1)\Delta x}{\gamma K}\right)^{\gamma/(\gamma-1)} \\ &+ \left(\rho_i^{\gamma-1} + \frac{g(\gamma-1)\Delta x}{\gamma K}\right)^{\gamma/(\gamma-1)} + \rho_{i-1}^\gamma\Bigg]. \end{aligned} \tag{38}$$

Taylor series expansion for small Δx shows that this is in fact a consistent average of the source term from the two sides:

$$\Psi_{i-1/2}\Delta x = -\frac{g}{2}(\rho_{i-1} + \rho_i)\Delta x + \mathcal{O}(\Delta x^2) \tag{39}$$

and tests confirm that (38) maintains an atmosphere at rest to machine precision, which is not true if the $\mathcal{O}(\Delta x^2)$ terms are dropped in (39) (except of course if $\gamma = 2$, the shallow water equations, in which case the $\mathcal{O}(\Delta x^2)$ terms are identically zero).

The full Euler equations in which (14) is augmented by an energy equation and the equation of state relates p to ρ and E has steady states with a similar form. However, there are multiple steady states with the same pressure variations (but different entropy stratifications) and this complicates

the problem, as discussed in [6]. In this case the Jacobian matrix has an eigenvalue equal to zero for the entropy waves (jumps in density but not pressure), again a resonant case. In this case there is a two-dimensional manifold of equilibrium paths through a given state q_*. It is possible to choose an equilibrium path by reconstructing the entropy variation from nearby points and this may be sufficient for studying small amplitude perturbations [6]. Experiments are underway to further explore this idea, which is being used in joint work with Carsten Gundlach on the study of shock waves near vacuum at the outer limit of a neutron star [19].

7 A scalar model problem

To further illustrate how the new path integral method uses local steady states to incorporate source terms, we consider the simple model problem given by

$$q_t(x,t) + uq_x(x,t) = -q(x,t)\sigma_x(x). \tag{40}$$

This is an advection equation (with a constant advection velocity $u > 0$) with a source term that leads to exponential decay (when $\sigma_x > 0$) or growth (when $\sigma_x < 0$) along characteristics.

First consider the case $\sigma(x) = x$, for which the solution decays as it propagates and for any initial data $q(x,0) = q^0(x)$ the solution to the Cauchy problem is simply

$$q(x,t) = e^{-t/u} q^0(x - ut). \tag{41}$$

The boundary value problem on $0 \le x \le L$ with inflow boundary conditions $q(0,t) = \mu$ has the equilibrium solution

$$q^e(x) = \mu e^{-x/u}. \tag{42}$$

Note that if we apply a fractional step method then in each step the decaying exponential shifts to the right in the advection step and then decays downward in the source term step (see Figure 17.4 of [23]). Ideally these two steps would cancel exactly, but they will not numerically since very different numerical methods are used for the two steps.

The f-wave approach of [3] would use

$$\mathcal{A}\Delta Q_{i-1/2} = uQ_i - uQ_{i-1} + \Delta x \bar{Q}_{i-1/2}, \tag{43}$$

where $\bar{Q}_{i-1/2}$ is some average value based on Q_{i-1} and Q_i. We would then set

$$\mathcal{A}^+\Delta Q_{i-1/2} = \mathcal{A}\Delta Q_{i-1/2}, \quad \mathcal{A}^-\Delta Q_{i-1/2} = 0, \quad \mathcal{Z}^1_{i-1/2} = \mathcal{A}\Delta Q_{i-1/2} \tag{44}$$

since we have assumed $u > 0$ so there is a single right-going wave.

It is not obvious how to choose the average $\bar{Q}_{i-1/2}$. For example, using the arithmetic average does not give a well-balanced method and results shown for a related problem below illustrate that this may not be sufficient (see the last column of Figure 2).

The method proposed in this paper yields better expressions for this average. For this example, given a state $w_* = (Q_*, x_*)$ (recall that $\sigma(x) = x$ here), there is a unique equilibrium solution passing through this point:

$$Q^{[*]}(x) = Q_* e^{-(x-x_*)/u} \tag{45}$$

and so from the Riemann problem states Q_{i-1} and Q_i we find that

$$\widehat{Q}_{i-1} = Q^{[i]}(x_{i-1}) = Q_i e^{-(x_{i-1}-x_i)/u} = Q_i e^{\Delta x/u} \tag{46}$$

and

$$\widehat{Q}_i = Q^{[i-1]}(x_i) = Q_{i-1} e^{-(x_i - x_{i-1})/u} = Q_{i-1} e^{-\Delta x/u} \tag{47}$$

The formula (31) then gives (using $f(q) = uq$):

$$\begin{aligned}
\mathcal{A}\Delta Q_{i-1/2} &= \frac{u}{2}[Q_i - \widehat{Q}_i + \widehat{Q}_{i-1} - Q_{i-1}] \\
&= \frac{u}{2}\left[Q_i(1 + e^{\Delta x/u}) - Q_{i-1}(1 + e^{-\Delta x/u})\right] \\
&= u(Q_i - Q_{i-1}) + \frac{u}{2}\left[Q_i(-1 + e^{\Delta x/u}) - Q_{i-1}(-1 + e^{-\Delta x/u})\right] \\
&= u(Q_i - Q_{i-1}) + \frac{\Delta x}{2}(Q_i + Q_{i-1}) + \frac{\Delta x^2}{4u}(Q_i - Q_{i-1}) + \mathcal{O}(\Delta x^3).
\end{aligned} \tag{48}$$

In practice the second or third line is used in the Riemann solver. The last line shows that this choice differs only in the $\mathcal{O}(\Delta x^2)$ terms from the simple arithmetic average, though for smooth solutions we expect $Q_i - Q_{i-1} = \mathcal{O}(\Delta x)$ and so this term is in fact $\mathcal{O}(\Delta x^3)$. Since $u > 0$ there is a single f-wave $\mathcal{Z}^1_{i-1/2} = \mathcal{A}^+\Delta Q_{i-1/2} = \mathcal{A}\Delta Q_{i-1/2}$ while $\mathcal{A}^-\Delta Q_{i-1/2} = 0$.

For this scalar problem with $u > 0$, Note 6 at the end of Section 5 suggests that we might do better to use only the path (26) rather than averaging results with path (29). This would give

$$\begin{aligned}
\mathcal{A}\Delta Q_{i-1/2} &= u[Q_i - \widehat{Q}_i] \\
&= u\left[Q_i - Q_{i-1}e^{-\Delta x/u}\right] \\
&= u(Q_i - Q_{i-1}) + u\left[Q_{i-1}(1 - e^{-\Delta x/u})\right] \\
&= u(Q_i - Q_{i-1}) + \Delta x Q_{i-1} - \Delta x^2 Q_{i-1}/u + \mathcal{O}(\Delta x^3).
\end{aligned} \tag{49}$$

Again there is a single f-wave $\mathcal{Z}^1_{i-1/2} = \mathcal{A}^+\Delta Q_{i-1/2} = \mathcal{A}\Delta Q_{i-1/2}$ while $\mathcal{A}^-\Delta Q_{i-1/2} = 0$.

Numerical experiments show that both (48) and (49) give well balanced methods but the latter is slightly more accurate.

The methods just described are easily generalized to problems of the form (40) where $\sigma(x) \neq x$. One need only replace Δx by $\sigma(x_i) - \sigma(x_{i-1})$ in the formulas above. An example of this is considered in the numerical experiments below.

7.1 Numerical experiments

As an example we consider a more difficult problem where $u = 1$ and

$$\sigma(x) = Ae^{-(x-5)^2} + B(\tanh(x - 5) + 1), \tag{50}$$

where $A = 8$ and $B = -\frac{1}{2}\log(1.4)$. We solve the equation (40) on the interval $0 \le x \le 10$ with inflow boundary data at $x = 0$ and the steady state solution as initial data:

$$q(x, 0) = q^e(x) = e^{-\sigma(x)/u}. \tag{51}$$

We specify the boundary data at $x = 0$ as $q(0, t) = q^{\text{true}}(0, t)$, where

$$q^{\text{true}}(x, t) = q^0(x - ut)\exp((\sigma(x - ut) - \sigma(x))/u) \tag{52}$$

with

$$q^0(x) = \begin{cases} q^e(x) + 0.2 & \text{if } -11 < x < -10.5 \\ q^e(x) & \text{otherwise} \end{cases} \tag{53}$$

The true solution is then given by (52). Initially it is just the equilibrium solution on the domain $0 < x < 10$ but there is a square pulse that enters the domain about time $t = 10.5$ and propagates against the background steady state solution, leaving the right boundary by time $t = 21$.

The function $\sigma(x)$ is chosen to be near zero at the boundaries of our domain. As q propagates through the domain, σ_x is first positive, leading to decay of the solution (including the propagating pulse) to nearly zero, and then negative causing the equilibrium solution to grow again to a different value 1.4 near the right boundary.

This gives a fairly severe test of a method since any errors made in the solution in the region where it has decayed to nearly zero are magnified exponentially as the solution grows again.

Figure 1 shows the results on the method proposed in this paper on a grid with 100 cells. The left column shows results when the two paths are averaged as in (48). The right column shows the better results obtained with the correct path, as in (49). In each figure the solid red curve is the exact solution and the blue curve with cell values as circles shows the computed results.

Results are shown at four times. At time $t = 10$ the equilibrium solution is observed. This is before the pulse has entered the domain but after more than 100 time steps, so the fact that the error is at the level of machine precision shows that both methods are well balanced. At time $t = 12$ the pulse is seen at $x = 1$, shortly after entering at the left boundary. At time $t = 15$ the pulse is located around $x = 4$ and has decayed to the point where it is invisible in the plot. At time $t = 20$ it has grown to be visible again at $x = 9$. This is the best time to observe the relative difference in accuracy of the two methods. For time $t > 21$ the pulse has left the domain and the solution should return to the equilibrium. These frames are not shown, but for both methods look identical to the $t = 12$ frames in the top row of Figure 1, with the error again at the level of machine precision.

For contrast, Figure 2 shows the same computation with two other methods. The left column shows results obtained with a fractional step method, where solving the homogenous hyperbolic equation is alternated with the exact solution of $q_t = -q\sigma_x(x)$ in each grid cell. Clearly this method produces very poor results. The initial data $q(x, 0) = q^e(x)$ is not preserved well, particularly in the rightmost portion of the domain after the exponential growth of errors. The right column shows results obtained with the f-wave method using arithmetic averaging for the source term. This gives much better results, but examining the error at $t = 10$ shows it is not well balanced. The pulse is also not as well resolved at $t = 20$.

These results were obtained using Clawpack Version 4.4. The second-order wave-propagation method with the superbee limiter and Courant number 0.9 were used. The computer code used to generate these figures can be examined or downloaded at `www.clawpack.org/links/wbfwave10`. Additional frames and animations of the computations and errors are also available there.

8 Summary and further comments

An approach has been presented for choosing an appropriate discretization of the source term to use as $\Psi_{i-1/2}$, the average of ψ between cells $i - 1$ and i, for use in the f-wave formulation of the wave-propagation algorithms implemented in Clawpack. This approach is based on studying the Riemann problem for an augmented hyperbolic system where the source terms are eliminated and instead a nonconservative product appears. A path conservative approach is then used where the paths in state space are chosen to simplify evaluation of the source term approximation.

For some simple problems, such as the model advection equation studied in Section 7, the path in state space corresponding to the exact Riemann solution of the augmented system is easily constructed, leading to a slightly more accurate method. In this case the path can also dictate the choice of the resulting fluctuation splitting and f-waves.

More generally, the choice of path for computing $\Psi_{i-1/2}$ is decoupled from the decompositon of the resulting $\mathcal{A}\Delta Q$ into fluctuations and f-waves. The method will be well-balanced regardless of the latter choice, which can be based on the eigenstructure of the original hyperbolic problem or standard approximate Riemann solvers for the original problem.

In this paper we assumed the non-resonant case, where the original hyperbolic system has no zero eigenvalues (or eigenvalues that change sign between grid cells), as would happen for transcritical flow in the shallow water equations.

We have also only considered the one-dimensional problem. Maintaining exact equilibrium solutions in two space dimensions is in general more challenging, since there is typically a balance between the x- and y-derivatives in the divergence of the flux as well as between these and the source terms. The two-dimensional shallow water equations for the ocean at rest over varying bathymetry is again a special case, since the source term in the each momentum equation exactly balances the hydrostatic pressure jump in the same equation, and arithmetic averages of the bathymetry in each

one-dimensional f-wave splitting yields a well balanced method (e.g., [4, 13, 15]. For an atmosphere at rest on a Cartesian grid the approach of this paper should apply directly since the source term appears only in the vertical momentum equation and again should balance the pressure gradient in this equation. On a non-Cartesian grid maintaining balance can be more difficult, see for example [6].

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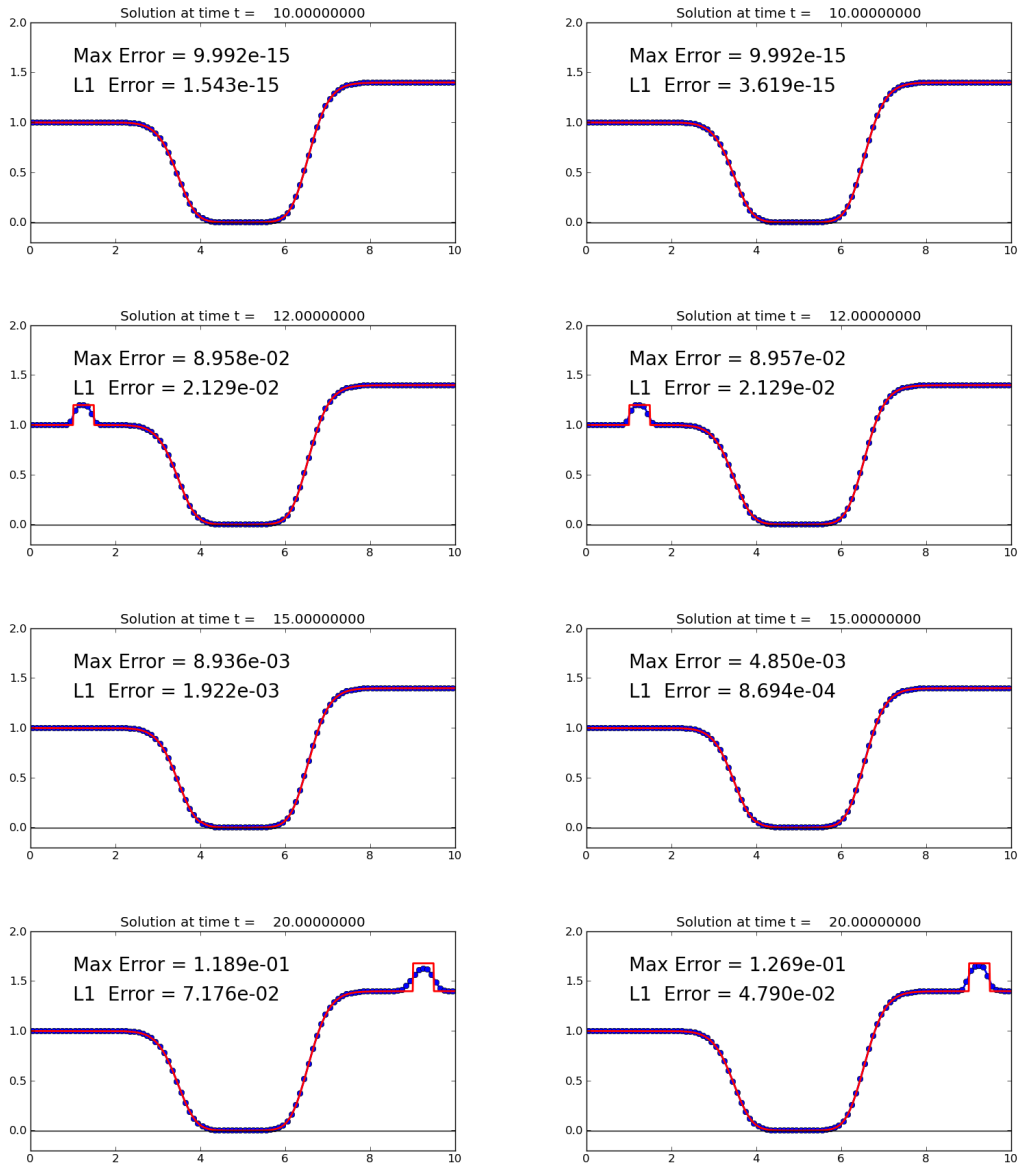

Figure 1: Computed results for the scalar test problem as described in the text. The left column shows results obtained using (48) and the right column using (49).

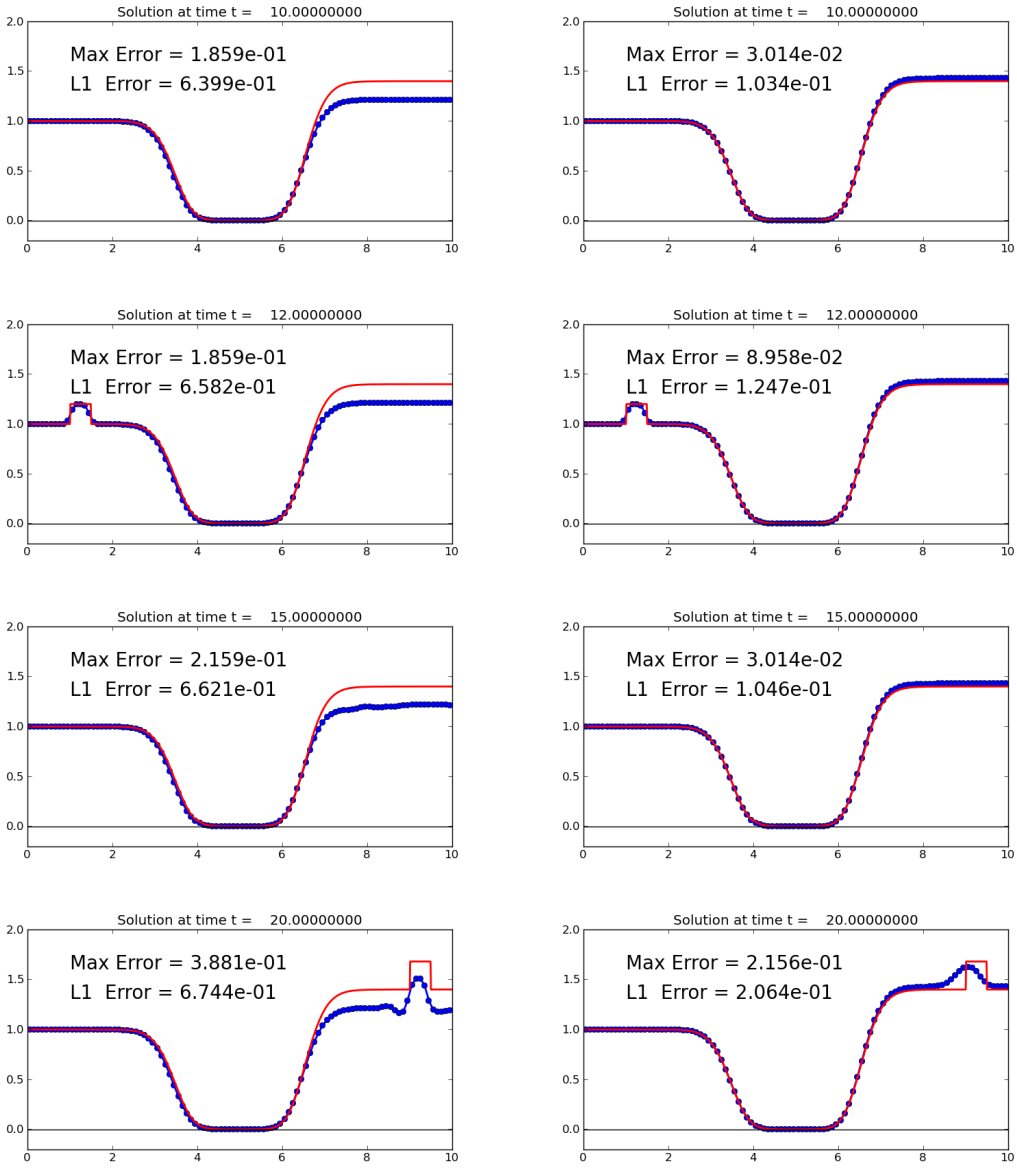

Figure 2: The same experiments as in Figure 1, but using methods that are not well balanced. The left column shows results obtained with a fractional step method and the right column using the f-wave method with arithmetic average of Q in the source term.