THE RANDOM PROJECTION METHOD

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Dedicated to Professor Hong-ci Huang on the occasion of his retirement

Abstract. In this note we review the random projection methods, recently introduced by the authors, for numerical simulations of the hyperbolic conservation laws with stiff reaction terms:

$$U_t + F(U)_x = \frac{1}{\varepsilon}\Psi(U).$$

In this problem, the reaction time ε is small, making the problem numerically stiff. A classic spurious numerical phenomenon – the incorrect shock speed – occurs when the reaction time scale is not properly resolved numerically. The random projection method, a fractional step method that solves the homogeneous convection by any shock capturing method, followed by a random projection for the reaction term, was introduced in [1] to handle this numerical difficulty. For a scalar model problem, one can prove that the random projection methods capture the correct shock speed with a first order accuracy, if a monotonicity-preserving method is used in the convection step. This method can also be extended to compute stiff detonation waves by randomizing the ignition temperature. Numerical results on an unstable detonation wave will be presented.

Key words. the random projection method, hyperbolic conservation law, stiff reaction term

AMS subject classifications. 65N06,76N15,62N99

1. Introduction.

In this note we review the random projection methods proposed recently by the authors [1, 2] for numerical simulations of the hyperbolic conservation laws with stiff reaction terms:

$$U_t + F(U)_x = \frac{1}{\varepsilon}\Psi(U), \tag{1.1}$$

where U is the vector of dependent variables with components mass, momentum, total energy, and densities or concentration for each species in the reacting mixture, respectively. The flux function $F(U)$ describes the fluid dynamical convection while the source term $\Psi(U)$ arises from the chemistry of the reacting species. ε is the reaction time. In a reacting flow, the reacting time ε is much smaller than the characteristic time scale of the fluid, making the source term in (1.1) stiff.

Numerical methods for the stiff reaction term has attracted lots of attention in the last decade. It was first observed by Colella, Majda and Roytburd [8] that underresolved numerical methods, where ε is not resolved by suitable small time steps and grid sizes, lead to spurious shock that travels one grid per time step. Since then, lots of attention have been paid to study this peculiar numerical phenomenon (see [3], [16], [17], [4] and references therein) and or find a robust way to fix it (see [9, 10]). It is known that the numerical shock profile, an essential mechanism in all shock capturing methods, leads to too early chemical reaction once the smeared value in the numerical shock layer is above the ignition temperature.

Recently we proposed the random projection method for the hyperbolic systems with stiff reaction terms (1.1) [1, 2]. Unlike the classical random choice method for reacting flow [6], originated from Glimm's scheme [12, 5], which requires solving a

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generalized Riemann problem for hyperbolic systems with source terms, our method is a fraction step method, which combines a standard –no Riemann solver is needed –shock capturing method for the homogeneous convection with a strikingly simple random projection step for the reaction term. In the random projection step, the ignition temperature is chosen to be uniformly distributed random variable between the initial left and right states. Although at each time step, this random projection will move the shock with an incorrect speed, the statistical average yields the correct speed, even though the small time scale ε is not numerically resolved. In particular, when the random number is chosen to be the equidistributed van der Corput sampling sequence [13, 7], we can prove, for a scalar model problem, a first order accuracy if a monotonicity-preserving method is used in the convection step. This method can be extended straightforwardly to the calculation of detonation waves, where in the projection step for the reaction terms, the ignition temperature is made random. A large amount of numerical experiments for one and two dimensional detonation waves demonstrate the robustness of this novel approach [1].

The note is organized as follows: In section 2 we review the global and the local random projection methods introduced in [1, 2] and their error estimates for a scalar model problem. In section 3 we present the local random projection method for one-dimensional detonation waves. In section 4 we report numerical results for an unstable detonation wave.

2. A scalar model problem. In this section we review the random projection methods introduced in [1, 2] for the following hyperbolic conservation law with stiff reaction term,

$$u_t + f(u)_x = -\frac{1}{\varepsilon}(u-\alpha)(u^2-1), \qquad -1<\alpha<1, \tag{2.1}$$

with piecewise constant initial data

$$u(x,0) = u_0(x) = \begin{cases} 1, & x \le x_0, \\ -1, & x > x_0. \end{cases} \tag{2.2}$$

Here ε is the reaction time, f is a convex function of u, i.e. $f''(u) > 0$, and x_0 is a given point.

The source term in (2.1) admits three local equilibria, i.e., the unstable one α, and the stable ones ± 1. When the solution is at equilibria, the reaction term has no effect. Thus the exact solution is a shock discontinuity connecting $u = 1$ with $u = -1$ and propagating to the right with the speed determined by the Rankine-Hugoniot jump condition [16] [11]:

$$s = \frac{1}{2}[f(1) - f(-1)]\,. \tag{2.3}$$

Namely,

$$u(x,t) = \begin{cases} 1, & \text{if } x \le x_0 + st, \\ -1, & \text{if } x > x_0 + st. \end{cases} \tag{2.4}$$

Let h be the spatial increment and k be the time step, such that x_0 is a grid point, i.e. $x_0 = l(0)h$ with $l(0)$ an integer. The numerical solution is evaluated at the points (ih, nk), $i = 0, \pm 1, \pm 2, \cdots$, $n = 0, 1, 2, \cdots$. Let u_i^n approximate $u(ih, nk)$ and u^n be the solution vector of $u(\cdot, nk)$ at time $t = t_n = nk$. When the reaction term is resolved, i.e. $k = O(h) << \varepsilon$, any method which works well for the homogeneous hyperbolic conservation law still works well here. Here we are interested in the underresolved case, where $k = O(h) \geq \varepsilon$.

2.1. The global random projection method. The random projection method is a fractional step method that solves the homogeneous equation

$$u_t + f(u)_x = 0 \tag{2.5}$$

by a standard shock capturing method S_c for one time step, followed by a projection step. In the projection step, we replace the unstable equilibrium, or the critical value, α, by a uniformly distributed random sequence $\theta_n \in (-1, 1)$. Let $u^+ = S_c(k)u^n$. We define the **global random projection** operator $S_\theta(k)$ by

$$S_\theta(k): \quad u_j^{n+1} = \begin{cases} 1, & \text{if } u_j^+ > \theta_n; \\ -1, & \text{if } u_j^+ \leq \theta_n\,. \end{cases} \tag{2.6}$$

In this method, one random value of θ_n will be selected per time step. The combination of the two steps gives the numerical scheme

$$S_{gp}(k): \qquad u^{n+1} = S_\theta(k)S_c(k)u^n. \tag{2.7}$$

The stability condition for this method, as well as the local random projection method (2.10), are the usual CFL condition determined by the convection term.

While effective most of the time, the global random projection method fails when there are waves that are at most m points away from the detonation fronts, where m is the number of smeared points after the convection $S_c(k)$ [1]. The reason for this is that, during each step, the random projection operator could move the detonation front, forward or backward, by m grid points, forcing it to interact, unphysically, with the neighboring wave. This motivates the introduction of the **local random projection method**, which allows the front to move at most one grid point per time step. Another advantage of the local random projection method is that it can be easily applied to more general reaction terms [2].

2.2. The local random projection method. First, notice that, although u may have some intermediate values between -1 and 1 after the convection step, the projection step always makes u either -1 or 1. Therefore, at any time step $t_n = nk$, there is an $l(n) = j_0$, j_0 an integer, such that

$$u_j^n = \begin{cases} 1, & \text{if } j \leq l(n), \\ -1, & \text{if } j > l(n). \end{cases} \tag{2.8}$$

Let $u^+ = S_c(k)u^n$. The local random projection operator $\tilde{S}_\theta(k)$ is defined as

$$\begin{aligned} &\tilde{S}_\theta(k) : \text{Set } l(n+1) := l(n) - 1, \\ &\qquad \text{For } \ j = l(n) - 1, \cdots, l(n) + 1 \quad \text{do}: \ \ l(n+1) = j, \quad \text{if } \ u_j^+ > \theta_n; \end{aligned}$$

$$u_j^{n+1} = \begin{cases} 1, & \text{if } \ j \leq l(n+1), \\ -1, & \text{if } \ j > l(n+1). \end{cases} \tag{2.9}$$

Again in this method, one random value of θ_n will be selected per time step. The combination of the two steps gives the numerical method:

$$S_{lp}(k): \qquad u^{n+1} = \tilde{S}_\theta(k)S_c(k)u^n. \tag{2.10}$$

The difference between the local random projection method and its global counterpart is that the local one allows, after each time step, the front to move–forward or backward–at most one grid point. When the number of smeared values of u by S_c is at most 2 after the convection step, for example, when one uses the first order upwind scheme or Lax-Friedrichs scheme for the convection part, the local random projection operator (2.9) is identical to the global random projection operator (2.6). However, when there are more than 2 smeared values of u between -1 and 1 after the convection, these two methods are different. For problems where waves are well-separated, these two methods generate essentially the same numerical results. However, the local method is more adequate for problems involving complex wave interactions.

2.3. The choice of the random sequence θ_n. Here and in our practical computations, we always use van der Corput's sampling scheme. The merit of this scheme is that it produces an equidistributed sequence on the interval $[0, 1]$ and among all known uniformly distributed sequences the deviation of van der Corput's sequence is minimal [13, 7]. The detailed scheme is the following. Let $1 \le n = \sum_{k=0}^{m} i_k 2^k$, $i_k = 0, 1$, be the binary expansion of the integer n. Then one gets a random number generator on $[0, 1]$:

$$\vartheta_n = \sum_{k=0}^{m} i_k 2^{-(k+1)}, \qquad n = 1, 2, \cdots. \tag{2.11}$$

We rescale it in order to get a random number generator θ_n on $[-1, 1]$:

$$\theta_n = 2\vartheta_n - 1, \qquad n = 1, 2, \cdots. \tag{2.12}$$

In fact, the binary van der Corput's sampling sequence $\{\vartheta_n,\ n = 1, 2, \cdots\}$ is equidistributed on the interval $[0, 1]$, see [13, 7] for detail. Thus the sequence $\{\theta_n,\ n = 1, 2, \cdots\}$ is equidistributed on the interval $[-1, 1]$.

2.4. Error estimates on the numerical shock speed. We have proved that the global random projection method, when a monotonicity-preserving method is used for the convection term, see [2] for detail, can capture the correct location of discontinuities for the scalar model problem (2.1) with a first order accuracy. The proof is similar to that of Glimm's scheme [7], and the error estimate made in [1] for first order schemes in the convection.

THEOREM 2.1. *The difference between the shock location of the exact solution, $x_0 + st_n$, and the numerical one, $l(n)h$, as determined by the global random projection method (2.7), in which any conservative, monotonicity-preserving scheme is used for the convection part, has the following estimate:*

$$|x_0 + st_n - l(n)h| \le h\left[C_1 + C_2 \ln(2st_n/\lambda h)\right], \tag{2.13}$$

where $t_n = nk$ is a fixed time, $\lambda = sk/h$ and C_1 and C_2 are two constants independent of t_n, n, h and k.

From this theorem, we know that the global random projection method yields the correct shock speed with an error of $O(h \ln h)$ when a monotonicity-preserving method is used. Since the solution is a step function, this error estimate holds for the l^1-norm between the numerical solution of (2.1) and the exact solution.

It is easy to see that the local random projection (2.10) is identical to its global counterpart, when one uses the first order upwind scheme or Lax-Friedrichs scheme for the convection part. Thus, clearly, the above theorem imply that, if the first order upwind or Lax-Friedichs scheme is used for the convection, the local random projection method yields a first order convergence in the shock location, or the solution in l^1. Since a second order TVD method reduces to a first order scheme, and in particular, if the solution at t_n is a step function with the discontinuity at $x_{l(n)}$, it is easy to check that after the convection, the second order TVD scheme gives exactly the same numerical results as its first order counterpart. Thus for the local random projection method, when one uses any TVD scheme for the convection part, we have (see [2] for detail)

THEOREM 2.2. *If we choose $S_c(k)$ as any TVD method without intermediate time step between t_n and t_{n+1}, then (2.13) holds.*

3. The detonation waves. In this section, we review the random projection method for the computation of one dimensional detonation waves. The key idea is to **make the ignition temperature random**.

Consider the Euler equations that model the time-dependent flow of an inviscid, compressible, reactive gas in one space dimension. Without heat conduction and viscosity, the equations take the form

$$U_t + F(U)_x = \frac{1}{\varepsilon}\Psi(U), \tag{3.1}$$

$$U = \begin{pmatrix} \rho \\ m \\ e \\ \rho z \end{pmatrix}, \quad F(U) = \begin{pmatrix} m \\ m^2/\rho + p \\ m(e+p)/\rho \\ mz \end{pmatrix}, \quad \Psi(U) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -\rho z e^{-T_0/T} \end{pmatrix} \equiv \begin{pmatrix} 0 \\ 0 \\ 0 \\ \psi(U) \end{pmatrix}.$$

The dependent variables $\rho(x,t)$, $m(x,t)$, $e(x,t)$ and $z(x,t)$ are the density, momentum, total energy and the fraction of unreacted fluid, respectively. The pressure is given by

$$p = (\gamma - 1)\left(e - \frac{m^2}{2\rho} - q_0 \rho z\right)$$

and the temperature is defined as $T = p/\rho$. Let $u = m/\rho$ be the velocity. The parameters q_0, T_0, γ and ε correspond to chemical heat release, ignition temperature, c_p to c_v ratio, and reaction time.

We will focus on the discontinuous solutions of detonation waves. For these waves the viscosity is not as important as for the slower deflagration wave solutions.

We refer to (3.1) as the reactive Euler equations with Arrhenius kinetics. We will also consider (3.1) with

$$-\frac{1}{\varepsilon}\rho z e^{-T_0/T}$$

replaced by the Heaviside kinetics

$$-\frac{1}{\varepsilon}\rho z H(T - T_0),$$

where $H(x) = 1$ for $x > 0$ and $H(x) = 0$ for $x < 0$. Actually the stiffness issue with the Heaviside kinetics is the more severe one [10].

Now we will describe the random projection method to the problem (3.1) with piecewise constant initial data

$$(\rho(x,0),u(x,0),p(x,0),z(x,0)) = \begin{cases} (\rho_l,u_l,p_l,0), & \text{if } x \le x_0, \\ (\rho_r,u_r,p_r,1), & \text{if } x > x_0; \end{cases} \tag{3.2}$$

where x_0 is a given point. Let $U_j^n = (\rho_j^n, m_j^n, e_j^n, (\rho z)_j^n)$ be the approximate solution of $U = (\rho, m, e, \rho z)$ at $(x_j, t_n) = (jh, nk)$. Similar to the scalar model problem, a fractional step method is used. In the first step, the inviscid compressible Euler equations

$$U_t + F(U)_x = 0, \tag{3.3}$$

are solved using a standard shock capturing method $S_F(k)$. Since any shock capturing method will have a few grid points in the shock profile, and corresponding temperature values, once above the critical temperature T_0, may trigger a too early chemical reaction, causing non-physical waves [8] [3].

In the second step of the fractional step method, we solve the chemical reaction term

$$\rho_t = 0, \qquad m_t = 0, \qquad e_t = 0, \qquad (\rho z)_t = \frac{1}{\varepsilon}\psi(U)\,, \tag{3.4}$$

using a local random projection method. Here the ignition temperature T_0 is made random. This can be successful since the speed of the front does not depend on the specific value of T_0, as far as it is in the range between the left and right states. Notice that, although z may have some intermediate values between 0 and 1 after the convection step, the projection step always makes z either 0 or 1. Therefore, at any time step t_n, there is an $l(n) = j_0$, j_0 an integer, such that

$$z_j^n = \begin{cases} 0, & \text{if } j \le l(n), \\ 1, & \text{if } j > l(n). \end{cases}$$

Here $l(n)$ is the location of the jump for z in the approximate solution at time t_n. The algorithm for the local random projection is:

$$\begin{aligned} \tilde{S}_\theta(k) :& \rho_j^{n+1} = \rho_j^*, \qquad m_j^{n+1} = m_j^*, \qquad e_j^{n+1} = e_j^*, \\ & \text{Set } l(n+1) := l(n) - 1, \\ & \text{For } \ j = l(n)-1, \cdots, l(n)+1 \quad \text{do}: \ \ l(n+1) = j, \ \ \text{if } T_j^* > \theta_n; \\ & z_j^{n+1} = \begin{cases} 0, & \text{if } \ j \le l(n+1), \\ 1, & \text{if } \ j > l(n+1); \end{cases} \end{aligned} \tag{3.5}$$

where

$$\theta_n = (T_l - T_r)\vartheta_n + T_r, \tag{3.6}$$

with

$$T_l = \frac{p_l}{\rho_l}, \qquad T_r = \frac{p_r}{\rho_r}. \tag{3.7}$$

Then the corresponding algorithm is

$$S_1(k): \qquad U^{n+1} = \tilde{S}_\theta(k)\, S_F(k) U^n. \tag{3.8}$$

The stability condition for this algorithm is the usual CFL condition determined by the convection term.

4. A numerical example. We consider an example defining an overdrive detonation wave with overdrive factor $f = 1.6$. The data is taken from [14]. Let $\gamma = 1.2$, $q_0 = 50$, $T_0 = 3.0$ and $\frac{1}{\varepsilon} = K = 230.75$. The initial state was given by

$$(\rho, u, p, z) = \begin{cases} (\rho_0, u_0, p_0, 1), & \text{if } x > 10, \\ (\rho_1, u_1, p_1, 0), & \text{if } x \le 10; \end{cases}$$

where $p_0 = 1.0$, $\rho_0 = 1.0$, $u_0 = 0$, and $p_1 = 54.8244$, $\rho_1 = 3.64282$, $u_1 = 6.2489$. By selecting these data, the "half reaction length" $L_{\frac{1}{2}}$ is the spatial unit 1.

This problem is solved on the interval $[0, 100]$. The 'exact' solutions are obtained by using an explicit scheme with fine mesh $h = 0.005$ (i.e. 20001 grid points on the interval $[0, 100]$) and $k = 0.00025$. These mesh size and time step resolve both the dynamical scale and the chemical scale. Now we compare the underresolved results obtained by the local random projection method (3.8) and the results by the deterministic method where T_0 is fixed by the given value. In these results $S_F(U)$ is the second order relaxed scheme proposed in [15].

Figure 1 shows the numerical solutions by using the random projection method (3.8) with $h = 1.0$ (i.e. 101 grid points for the interval $[0, 100]$) and $k = 0.05$ at time $t = 8.0$. Figure 2 shows the numerical solutions by using the deterministic method with $h = 1.0$ and $k = 0.05$ at time $t = 4.0$.

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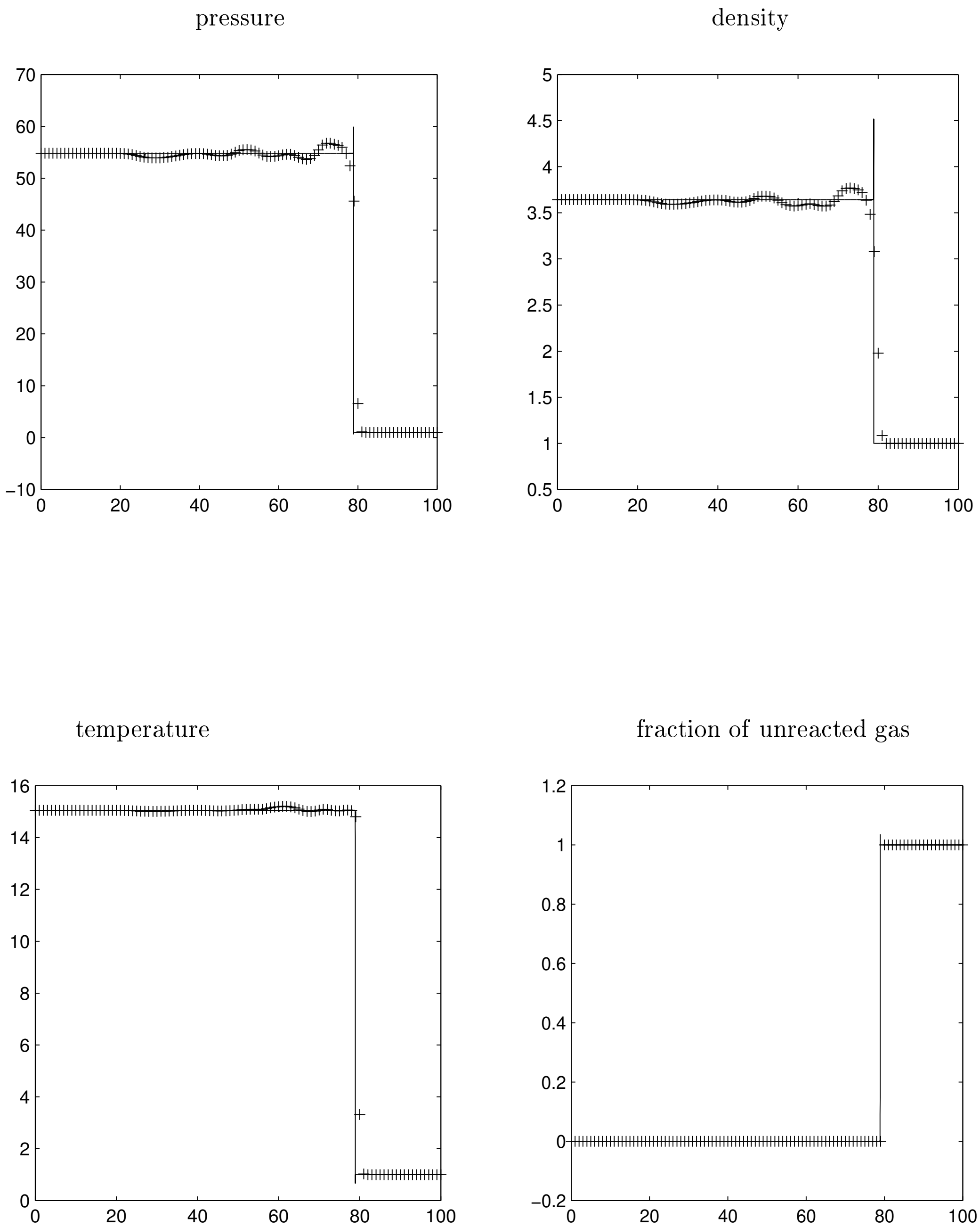

Figure 1 Numerical results for an unstable detonation using the local random projection method (3.8) at time $t = 8$. $h = 1$, $k = 0.05$. $-$: 'exact' solutions; $++$: computed solutions.

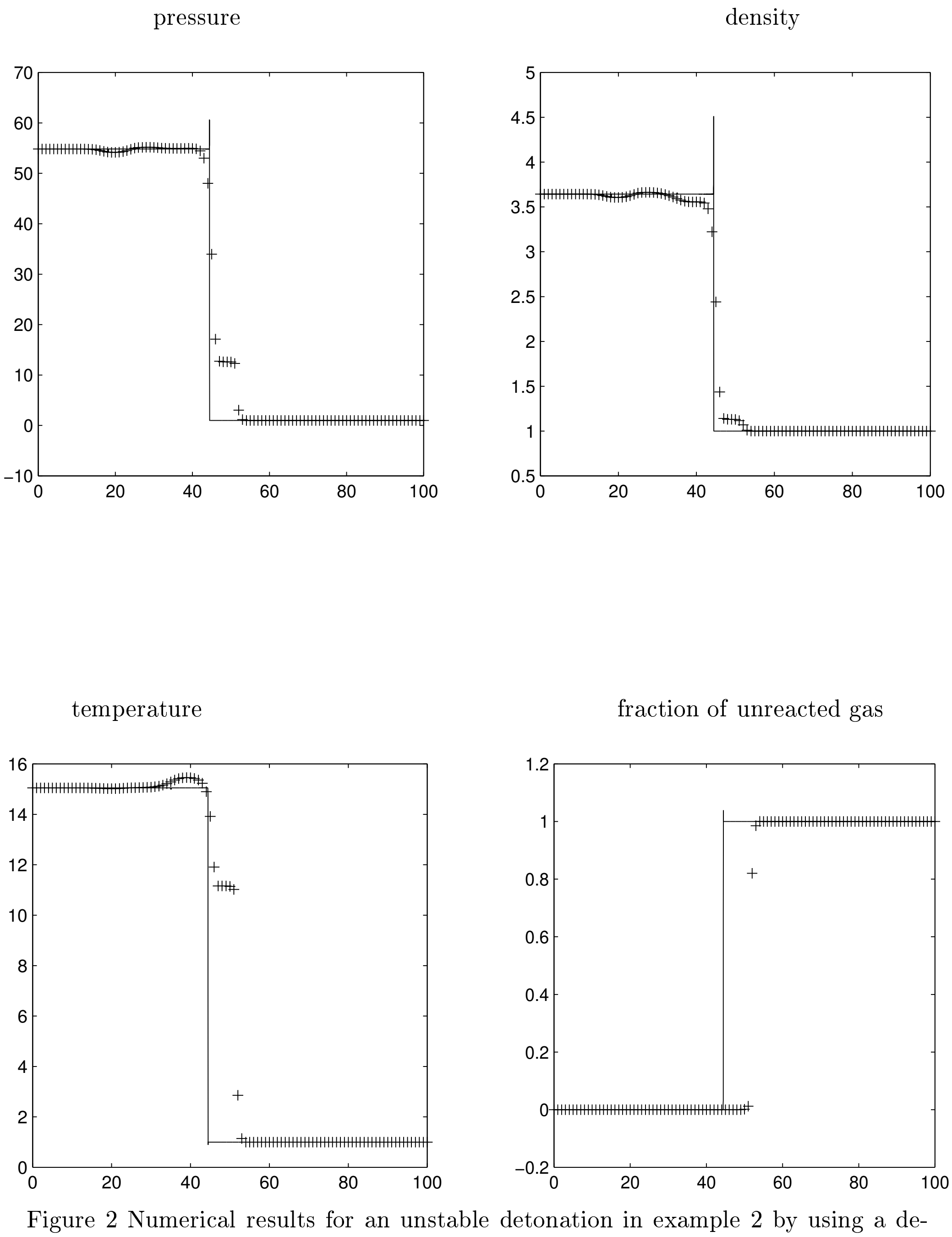

Figure 2 Numerical results for an unstable detonation in example 2 by using a deterministic method (where the ignition temperature is a given value) at time $t = 4$. $h = 1$, $k = 0.05$. $-$: 'exact' solutions; $++$: computed solutions.