The random projection method for stiff detonation waves

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Abstract

In this paper we present a simple and robust random projection method for underresolved numerical simulation of stiff detonation waves in chemically reacting flows. This method is based on the random projection method proposed by the authors for general hyperbolic systems with stiff reaction terms [1], where the ignition temperature is randomized in a suitable domain. It is simplified using the equations of instantaneous reaction, and then extended to handle the interactions of detonations. Extensive numerical experiments, including interaction of detonation waves, and in two dimensions, demonstrate the reliability and robustness of this novel method.

1 Introduction

We consider the reactive Euler equations that model the time-dependent flow of an inviscid, compressible, reacting flow. Without heat conduction and viscosity, the equations take the form

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

$$U = \begin{pmatrix} \rho \\ m \\ n \\ e \\ \rho z \end{pmatrix}, \quad F(U) = \begin{pmatrix} m \\ m^2/\rho + p \\ mn/\rho \\ m(e+p)/\rho \\ mz \end{pmatrix}, \quad G(U) = \begin{pmatrix} m \\ mn/\rho \\ n^2/\rho + p \\ n(e+p)/\rho \\ nz \end{pmatrix}, \tag{1.2}$$

$$\Psi(U) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ -\rho z e^{-T_c/T} \end{pmatrix} \equiv \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \psi(U) \end{pmatrix}. \tag{1.3}$$

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The dependent variables $\rho(x,y,t)$, $m(x,y,t)$, $n(x,y,t)$, $e(x,y,t)$ and $z(x,y,t)$ are the density, x- and y-momentum, total energy and the fraction of unburnt fluid, respectively. The pressure for ideal gas is given by

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

and the temperature is defined as $T = p/\rho$. Let $(u,v) = (m/\rho, n/\rho)$ be the velocity. The parameters q_0, T_c, γ and ε correspond to chemical heat release, ignition temperature, c_p to c_v ratio, and reaction time, respectively. The equations have been nondimensionalized, leaving the choice of these four parameters to completely determine the problem.

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

We refer to (1.1)-(1.3) as the reactive Euler equations with Arrhenius kinetics. We will also consider (1.1)-(1.3) with

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

replaced by the Heaviside kinetics

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

where $H(x) = 1$ for $x > 0$ and $H(x) = 0$ for $x < 0$.

One of the main numerical challenges for reacting flows is that the kinetics equations (1.1) often include reactions with widely varying time scales. The chemical time scales, as characterized by ε, may be orders of magnitude faster than the fluid dynamical time scale. This leads to problems of severe numerical stiffness. Actually the stiffness issue with the Heaviside kinetics is the more severe one [10]. Even a stable numerical scheme may lead to spurious unphysical solutions unless the small chemical time scale is fully resolved numerically.

Numerical methods for this kind of problems have attracted a great deal of attentions in the last decade. In particular, many works have contributed to the analysis and development of underresolved numerical methods which are capable of capturing the physically relevant solutions. Of course, when one does not resolve the chemical scale numerically (using grid size larger than the reaction zone of width $O(\varepsilon)$), it is impossible to capture the pressure spike in the reaction zone. Thus the best one can hope is to capture the speed of detonation as well as other features of fluid dynamics. It was first observed by Colella, Majda and Roytburd [8] that an underresolved numerical method, where ε is not resolved by suitably small time steps and grid sizes, leads to spurious weak detonation wave that travels one grid per time step. Since then, lots of attention have been paid to study this peculiar numerical phenomenon (see [4], [17], [18], [12], [5]). It is known that numerical shock profile, an essential mechanism in all shock capturing methods, leads to too early chemical reaction once the smeared value of the temperature in the numerical shock layer is above the ignition temperature. Various approaches have been suggested to fix this numerical problem. For examples, in [10], a temperature extrapolation technique was proposed. In [3] the ignition temperature is artificially raised. In [19] the reaction time ε was replaced by a larger one thus the reaction zone is made much wider than the physical one. Recently, a modified fractional step method was introduced [14], where the structure of the Riemann solution of the homogeneous part is used to determine where burning should occur in each time step

Recently we proposed the random projection method as a general and systematic method to solve hyperbolic systems with stiff reaction term, applicable to reacting flow problems [1]. Unlike the random choice method of Chorin for reacting flow [6], which was originated from Glimm's scheme [11], and requires solving a generalized Riemann problem for hyperbolic systems with source terms [4], our method is a fractional 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 an uniformly distributed random variable between two stable equilibria. 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], we can prove, for a model scalar problem, a first order accuracy on the shock speed if a monotonicity-preserving method, which includes all TVD schemes, is used in the convection step [1], [2]. A large amount of numerical experiments for one and two dimensional detonation waves demonstrate the robustness of this novel approach.

In this paper, we conduct extensive numerical experiments to examine the applicability of the random projection method for reacting flows. We focus on stiff detonation waves and their interactions with other waves, including the interaction of detonation waves. To this aim, we first simplify the convection step using the reacting flow model of zero reaction zone, meaning that the chemical heat is released instantaneously. Since we are to develop underresolved method, where the reaction zone is much smaller than a grid size, the equation reduces effectively to the zero reaction model, which is given by [9]:

$$U_t + F(U)_x + G(U)_y = 0, \tag{1.4}$$

$$U = \begin{pmatrix} \rho \\ m \\ n \\ e \end{pmatrix}, \quad F(U) = \begin{pmatrix} m \\ m^2/\rho + p \\ mn/\rho \\ m(e+p)/\rho \end{pmatrix}, \quad G(U) = \begin{pmatrix} m \\ mn/\rho \\ n^2/\rho + p \\ n(e+p)/\rho \end{pmatrix}, \tag{1.5}$$

$$\tag{1.6}$$

with equation of state

$$p = (\gamma - 1)\left(e - \frac{1}{2}\left(m^2 + n^2\right)/\rho - q_0\rho z\right) \tag{1.7}$$

and the fraction of unburnt gas

$$z = \begin{cases} 0, & \text{if } T > T_c, \\ 1, & \text{if } T < T_c. \end{cases} \tag{1.8}$$

The random projection method consists of two steps, with the first being any standard shock capturing method for (1.4), followed by a random projection for the fraction variable z in (1.8), with T_c replaced by a uniformly distributed random sequence. Here the convection step is slightly simpler than the original one proposed in [1] where the full convection equation, including the homogeneous part of the species equation in (1.1)-(1.3), is solved. Algorithms for the collision of detonation waves are also introduced. Many numerical examples, including the C-J detonation, strong detonation, unstable detonation, collisions of detonation with shocks, rarefaction wave, or another detonation, as well as two dimensional examples, will be used to justify the robustness of this novel approach.

The paper is organized as follows. In section 2 we provide a random project method for the problem (1.4)-(1.8) in one space dimension with general initial data. Algorithms for multi-detonations are also introduced. In section 3 this method is extended to two space dimension. In section 4 many numerical examples will be presented. In section 5 some conclusions are drawn.

2 One-dimensional detonations

In this section, we shall describe the random projection method for (1.4)-(1.8) in one space dimension. Moreover, we will describe its implementation for the case of interaction of detonation waves. The problem to be solved is given by

$$U_t + F(U)_x = 0, \tag{2.1}$$

$$U = \begin{pmatrix} \rho \\ m \\ e \end{pmatrix}, \qquad F(U) = \begin{pmatrix} m \\ m^2/\rho + p \\ m(e+p)/\rho \end{pmatrix}, \tag{2.2}$$

with equation of state

$$p = (\gamma - 1)\left(e - \frac{1}{2}m^2/\rho - q_0\rho z\right) \tag{2.3}$$

and the fraction of unburnt gas

$$z = \begin{cases} 0, & \text{if } T > T_c, \\ 1, & \text{if } T < T_c. \end{cases} \tag{2.4}$$

Let the grid points be x_i, $i = \cdots, -1, 0, 1, \cdots$, with equal mesh spacing $h = x_{i+1} - x_i$. The time level $t_0 = 0$, t_1, t_2, $\cdots$ are also uniformly spaced with time step $k = t_{n+1} - t_n$. We use $U_i^n = (\rho_i^n, m_i^n, e_i^n, (\rho z)_i^n)$ to denote the approximate solution of $U = (\rho, m, e, \rho z)$ at the point $(x_i, t_n) = (ih, nk)$. Our main interest is an underresolved numerical method which allows $k = O(h) >> \varepsilon$ and still obtains physically relevant numerical solutions.

The random projection method is a fractional step method that consists of a standard shock capturing method for (2.1), denoted by $S_F(k)$ for one time step, followed by a random projection step for the fraction variable z defined by (2.4) where T_c, the ignition temperature, is randomized in a suitable domain. Let $U^{n+1} = S_F(k)U^n$. To obtain z^{n+1}, we replace (2.4) by

$$z_j^{n+1} = \begin{cases} 0, & \text{if } T_j^{n+1} > \theta_n, \\ 1, & \text{if } T_j^{n+1} < \theta_n, \end{cases} \tag{2.5}$$

where $T_j^{n+1} = p_j^{n+1}/\rho_j^{n+1}$ and θ_n is a random number, chosen one per time step, between two equilibrium temperatures on both sides of the detonation. To be more precise, consider the initial data

$$(\rho(x,0), u(x,0), p(x,0), z(x,0)) = \begin{cases} (\rho_l(x), u_l(x), p_l(x), 0)\,, & \text{if } x \le x_0, \\ (\rho_r(x), u_r(x), p_r(x), 1)\,, & \text{if } x > x_0; \end{cases} \tag{2.6}$$

where x_0 is a given point. Without loss of generality these data are chosen such that the detonation, initially at $x = x_0$, moves to the right. The case when the detonation moved to the left can be treated similarly. Since our projection always makes z either 1 or 0, therefore, at any time step t_n, there is an $l(n) = j_0$, j_0 an integer, such that

$$z_j^n = \begin{cases} 0, & \text{if } i \le l(n), \\ 1, & \text{if } l > l(n). \end{cases} \tag{2.7}$$

Here $l(n)$ is the location of the jump for z in the approximate solution at time t_n and we assume $x_0 = l(0)h$ be a grid point. Let

$$\theta_n = (T_l - T_r)\vartheta_n + T_r, \qquad T_l = \min_{x<x_0} \frac{p_l(x,0)}{\rho_l(x,0)}, \qquad T_r = \max_{x>x_0} \frac{p_r(x,0)}{\rho_r(x,0)}, \tag{2.8}$$

with ϑ_n being the van der Corput's sampling sequence on the interval $[0,1]$. The van der Corput sequence is an equidistributed sequence with the minimal deviation among all random sequences [13]. It is obtained as follows: let $1 \le n = \sum_{k=0}^m i_k 2^k$, $i_k = 0, 1$, be the binary expansion of the integer n. One gets ϑ_n on $[0,1]$ as:

$$\vartheta_n = \sum_{k=0}^{m} i_k 2^{-(k+1)}, \qquad n = 1, 2, \cdots. \tag{2.9}$$

Since there are other waves in the domain, one cannot project z according to (2.5) in the whole domain. Instead, we do it around the denotation, a procedure called *local random projection* in [1]. Specifically, We move the jump of z according to the following algorithm:

$$\begin{aligned} S_{sp}(k): \quad & \text{set } l(n+1) := l(n) - 1; \\ & \text{For } j = l(n)-1, l(n), \cdots, l(n)+d, \text{ do} \\ & \quad l(n+1) := j, \quad \text{if } T_j^{n+1} > \theta_n; \\ & z_j^{n+1} = \begin{cases} 0, & \text{if } j \le l(n+1), \\ 1, & \text{if } j > l(n+1); \end{cases} \end{aligned} \tag{2.10}$$

where d is the number of smeared points in the shock layer. From our numerical experience, for C-J detonations and strong detonations, $d = 1$ works very well. In the above algorithm, only $d+2$ points will be scanned.

The stability condition for this algorithm, as well as the algorithms for multi-detonations (2.15) and (2.20), is the usual CFL condition determined by the operator $S_F(k)$ for the convection terms.

For numerical comparison, we also mention the *deterministic* projection method using the given deterministic ignition temperature T_c in (2.4).

We now extend the random projection method to handle the problems involving more than one detonation waves. For clarity of presentation we only present the case of two detonations. It is straightforward to extend to the case where there are more than two detonations.

Consider (2.1)-(2.4) with initial data

$$(\rho(x,0),u(x,0),p(x,0),z(x,0)) = \begin{cases} (\rho_l(x),u_l(x),p_l(x),0)\,, & \text{if } x \le x_1, \\ (\rho_m(x),u_m(x),p_m(x),1)\,, & \text{if } x_1 < x < x_2, \\ (\rho_r(x),u_r(x),p_r(x),0)\,, & \text{if } x_2 \le x. \end{cases} \tag{2.11}$$

These data are chosen such that the two detonations move toward each other, i.e. the detonation initially at $x = x_1$ moves to the right and the one initially at $x = x_2$ moves to the left. Thus after some time, the two detonations will collide.

Let

$$T_l = \min_{x<x_1} \frac{p_l(x)}{\rho_l(x)}, \qquad T_m = \max_{x_1<x<x_2} \frac{p_m(x)}{\rho_m(x)}, \qquad T_r = \min_{x>x_2} \frac{p_r(x)}{\rho_r(x)} \tag{2.12}$$

and

$$\theta_n^{(1)} = (T_l - T_m)\vartheta_n + T_m, \qquad \theta_n^{(2)} = (T_r - T_m)\vartheta_n + T_m. \tag{2.13}$$

Since the projection always makes z either 1 or 0, the profile of z at any time step is a piecewise constant function. Therefore, at any time step t_n, there are $l_1(n) = j_1$ and $l_2(n) = j_2$ with $j_1 \le j_2$ integers, such that

$$z_j^n = \begin{cases} 0, & \text{if } j \le l_1(n), \\ 1, & \text{if } l_1(n) < j < l_2(n), \\ 0, & \text{if } l_2(n) \le j. \end{cases} \tag{2.14}$$

Here we assume that $x_1 = l_1(0)h$, and $x_2 = l_2(0)h$ are grid points. Since $x_1 \le x_2$, then $l_1(0) \le l_2(0)$. One can use the following algorithm to obtain z^{n+1}, if the positions of the two detonations at time t_n, i.e. $l_1(n)$ and $l_2(n)$, are known. The detailed algorithm to find z^{n+1} is

$$\begin{aligned} S_{cp}(k): \quad & l_{\text{mid}} = (l_1(n) + l_2(n))/2; \\ & \text{set } l_1(n+1) := l_1(n) - 1; \\ & \text{For } j = l_1(n)-1, l_1(n), \cdots, \min\{l_1(n)+d,\ l_{\text{mid}}+1\} \text{ do} \\ & \qquad l_1(n+1) := j, \quad \text{if } T_j^{n+1} > \theta_n^{(1)}; \\ & \text{set } l_2(n+1) := l_2(n) + 1; \\ & \text{For } j = l_2(n)+1, l_2(n), \cdots, \max\{l_2(n)-d,\ l_{\text{mid}}-1\} \text{ do} \\ & \qquad l_2(n+1) := j, \quad \text{if } T_j^{n+1} > \theta_n^{(2)}; \\ & z_j^{n+1} = \begin{cases} 0, & \text{if } j \le l_1(n+1), \\ 1, & \text{if } l_1(n+1) < j < l_2(n+1), \\ 0, & \text{if } l_2(n+1) \le j. \end{cases} \end{aligned} \tag{2.15}$$

Another case is when two detonations move away from each other. Consider the initial data

$$(\rho(x,0),u(x,0),p(x,0),z(x,0)) = \begin{cases} (\rho_l(x),u_l(x),p_l(x),1)\,, & \text{if } x < x_1, \\ (\rho_m(x),u_m(x),p_m(x),0)\,, & \text{if } x_1 \le x \le x_2, \\ (\rho_r(x),u_r(x),p_r(x),1)\,, & \text{if } x_2 < x. \end{cases} \tag{2.16}$$

These data are chosen such that the two detonations move away from each other, i.e. the detonation initially at $x = x_1$ moves to the left and the one initially at $x = x_2$ moves to the right. In this case, there is no collision of detonations at all.

Let

$$T_l = \max_{x<x_1} \frac{p_l(x)}{\rho_l(x)}, \qquad T_m = \min_{x_1<x<x_2} \frac{p_m(x)}{\rho_m(x)}, \qquad T_r = \max_{x>x_2} \frac{p_r(x)}{\rho_r(x)} \tag{2.17}$$

and

$$\theta_n^{(1)} = (T_m - T_l)\vartheta_n + T_l, \qquad \theta_n^{(2)} = (T_m - T_r)\vartheta_n + T_r. \tag{2.18}$$

At any time step t_n, there are $l_1(n) = j_1$ and $l_2(n) = j_2$ with $j_1 \le j_2$ integers, such that

$$z_j^n = \begin{cases} 1, & \text{if } j < l_1(n), \\ 0, & \text{if } l_1(n) \le j \le l_2(n), \\ 1, & \text{if } l_2(n) < j. \end{cases} \tag{2.19}$$

The detailed algorithm to find z^{n+1} is:

$$\begin{aligned} S_{bp}(k): \quad & \text{set } l_1(n+1) := l_1(n) + 1; \\ & \text{For } j = l_1(n)+1, l_1(n), \cdots, l_1(n) - d, \text{ do} \\ & \qquad l_1(n+1) := j, \quad \text{if } T_j^{n+1} > \theta_n^{(1)}; \\ & \text{set } l_2(n+1) := l_2(n) - 1; \\ & \text{For } j = l_2(n)-1, l_2(n), \cdots, l_2(n) + d, \text{ do} \\ & \qquad l_2(n+1) := j, \quad \text{if } T_j^{n+1} > \theta_n^{(2)}; \\ & z_j^{n+1} = \begin{cases} 1, & \text{if } j < l_1(n+1), \\ 0, & \text{if } l_1(n+1) \le j \le l_2(n+1), \\ 1, & \text{if } l_2(n+1) < j. \end{cases} \end{aligned} \tag{2.20}$$

3 The two-dimensional method

In this section, the random projection method is extended to two space dimensional problem (1.4)-(1.8). For simplicity, we consider the detonation waves in a two dimensional channel. Let the initial data be

$$(\rho(x,y,0),u(x,y,0),v(x,y,0),p(x,y,0),z(x,y,0)) = \begin{cases} (\rho_l,u_l,0,p_l,0), & \text{if } x \le \xi(y), \\ (\rho_r,u_r,0,p_r,1), & \text{if } x > \xi(y); \end{cases} \tag{3.1}$$

where $\xi(y)$ is a given function of y and these data are chosen such that the detonation moves to the right. Let

$$\theta_n = (T_l - T_r)\vartheta_n + T_r, \qquad T_l = \frac{p_l}{\rho_l}, \qquad T_r = \frac{p_r}{\rho_r}, \tag{3.2}$$

and ϑ_n (see (2.9) for detail) being the van der Corput's sampling sequence on the interval $[0, 1]$.

Let the grid points $(x_i, y_j) = (ih, jh), i, j = \cdots, -1, 0, 1, \cdots$, with equal mesh spacing h. The time level $t_n = nk$, $k = 0, 1, 2, \cdots$ are also uniformly spaced with time step k. Let $U^n_{i,j} = \left(\rho^n_{i,j}, m^n_{i,j}, n^n_{i,j}, e^n_{i,j}, (\rho z)^n_{i,j}\right)$ be the approximate solution of $U = (\rho, m, n, e, (\rho z))$ at $(x_i, y_j, t_n) = (ih, jh, nk)$. Let $S_{FG}(k)$ be a standard shock capturing method for (1.4). Notice that, at any time step, for each j, there is an $l_j(n) = j_n$, j_n an integer, such that

$$z^n_{i,j} = \begin{cases} 0, & \text{if } j \le l_j(n), \\ 1, & \text{if } i > l_j(n). \end{cases} \tag{3.3}$$

Here $l_j(n)$ is the location of the jump for z at the grid line $y = y_j$ in the approximate solution at time $t_n = nk$. Then the random project algorithm to find z^{n+1} follows:

$$\begin{aligned} S_{2p}(k): \quad & \text{For } j \text{ do} \\ & \quad \text{Set } l_j(n+1) := l_j(n) - 1, \\ & \quad \text{For } m = l_j(n) - 1, l_j(n), \cdots, l_j(n) + d, \text{ do} \\ & \quad\quad l_j(n+1) := m, \quad \text{if } T^{n+1}_{m,j} > \theta_n, \\ & \quad z^{n+1}_{i,j} = \begin{cases} 0, & \text{if } i \le l_j(n+1), \\ 1, & \text{if } i > l_j(n+1). \end{cases} \end{aligned} \tag{3.4}$$

The stability condition for this algorithm is still the usual CFL condition determined from the convection step $S_{FG}(k)$.

4 Numerical examples

In order to verify the performance of the random projection method proposed in this paper, we conduct extensive numerical experiments, including the Chapman-Jouguet (C-J) detonation, strong detonation, unstable detonation, collision of a detonation with a shock, a rarefaction wave, and another detonation. We also give two dimensional examples. In our computation, the operator $S_F(k)$ and $S_{FG}(k)$ are chosen as the second order relaxed scheme [16], which is a TVD scheme without the usage of Riemann solvers or local characteristic decompositions. We choose $d = 5$ in (2.10), (2.15), (2.20) and (3.4) in our computations in this section.

Example 4.1: A Chapman-Jouguet (C-J) detonation. This is the example 4.1 in [1] revisited. We choose here the case of ozone decomposition C-J detonation discussed and computed in [8] and [4]. We use CGS units and the following parameter values:

$$\gamma = 1.4, \qquad q_0 = 0.5196 \times 10^{10}, \qquad \frac{1}{\varepsilon} = K = 0.5825 \times 10^{10}, \qquad T_c = 0.1155 \times 10^{10}.$$

The initial data are taken as the piecewise constant data defining a C-J detonation as a single wave (recall that in the Chapman-Jouguet model a C-J detonation corresponds to a sonic detonation, or, in other words, a sharp reaction wave that moves at minimal speed relative to the unburnt gas). The initial state was given by

$$(\rho, u, p, z)(x, 0) = \begin{cases} (\rho_l, u_l, p_l, 0), & \text{if } x \le 0.005, \\ (\rho_r, u_r, p_r, 1), & \text{if } x > 0.005; \end{cases}$$

where $p_l = p_{CJ} = 6.270 \times 10^6$, $\rho_l = \rho_{CJ} = 1.945 \times 10^{-3}$, $u_l = u_{CJ} = 4.162 \times 10^4$; and $p_r = 8.321 \times 10^5$, $\rho_r = 1.201 \times 10^{-3}$, $u_r = 0$. The speed of the sharp front in this example is $D = D_{CJ} = 1.088 \times 10^5$. In this example the width of the reaction zone is approximately 5×10^{-5} ([4] and [8]).

This problem is solved on the interval $[0, 0.05]$. The 'exact' solution is obtained by using a resolved calculation with $h = 5 \times 10^{-6}$ (i.e. 10001 grid points on the interval $[0, 0.05]$) and $k = 5 \times 10^{-12}$. The mesh size and time step resolve the chemical scale. Now we compare the results obtained by the random projection method and the deterministic method when the reaction time is underresolved. We use $h = 5 \times 10^{-4}$ (i.e. 101 grid points for the interval $[0, 0.05]$) and $k = 5 \times 10^{-10}$ and output the numerical solution at $t = 2 \times 10^{-7}$.

Figure 4.1(a) shows the numerical solution by using the random projection method (2.10), while Figure 4.1(b) shows the numerical solution obtained by the deterministic method. It can be seen that the random projection method can capture the correct speed of the discontinuity of the C-J detonation wave even when the chemical reaction scale is not numerical resolved. As mentioned earlier, with an underresolved method it is impossible to capture the pressure spike which has a width in the order of reaction scale ε. there are small post shock statistical fluctuations due to the random nature of the method, but they are at an acceptable level. The deterministic method produces spurious waves, as was observed in earlier literatures.

In all of the following examples, the deterministic method always produces spurious waves when the chemical scale is not resolved. We will not report those results, and will only present the solutions obtained by the random projection method.

Example 4.2: A strong detonation. This is Example 4.3 in [1] revisited. The set up of this example is similar to those in Example 4.1 (i.e. γ, q_0, $K = \frac{1}{\varepsilon}$ and T_c are the same) except that the initial data are changed to

$$(\rho, u, p, z)(x, 0) = \begin{cases} (\rho_l, u_l, p_l, 0), & \text{if } x \le 0.005; \\ (\rho_r, u_r, p_r, 1), & \text{if } x > 0.005, \end{cases}$$

where $u_l = 9.162 \times 10^4 > u_{CJ}$, $\rho_l = \rho_{CJ}$, $p_l = 8.27 \times 10^6 > p_{CJ}$ and p_r, u_r, ρ_r, p_{CJ}, u_{CJ} and ρ_{CJ} are the same as those in Example 4.1. In this case there is a strong detonation, a contact discontinuity and a shock, all moving to the right.

The 'exact' solution is obtained similarly as that in Example 4.1. Figure 4.2 shows the numerical solutions by the random projection method (2.10) with $h = 5 \times 10^{-4}$ (i.e. 101 grid points for the interval $[0, 0.05]$) and $k = 5 \times 10^{-10}$ at time $t = 2 \times 10^{-7}$.

Example 4.3: An unstable detonation. We consider an example defining an overdrive detonation wave with overdrive factor $f = 1.6$. The data is taken from [15]. Let $\gamma = 1.2$,

$q_0 = 50$, $T_c = 3.0$ and $\frac{1}{\varepsilon} = K = 230.75$. The initial state was given by

$$(\rho, u, p, z)(x, 0) = \begin{cases} (\rho_l, u_l, p_l, 0), & \text{if } x \le 10; \\ (\rho_r, u_r, p_r, 1), & \text{if } x > 10, \end{cases}$$

where $p_r = 1.0$, $\rho_r = 1.0$, $u_r = 0$, and $p_l = 54.8244$, $\rho_l = 3.64282$, $u_l = 6.2489$. By selecting these data, the "half reaction length" $L_{\frac{1}{2}}$ is the spatial unit 1 [15].

This problem is solved on the interval $[0, 100]$. The 'exact' solution are obtained by using a resolved calculation $h = 0.005$ (i.e. 20001 grid points on the interval $[0, 100]$) and $k = 0.00025$. Figure 4.3 shows the numerical solution using the random projection method (2.10) with $h = 1.0$ (i.e. 101 grid points for the interval $[0, 100]$) and $k = 0.05$ at time $t = 8.0$.

Example 4.4: Collision of a detonation with a rarefaction wave. The set up of this example is similar to those in Example 4.3 (i.e. γ, q_0, $K = \frac{1}{\varepsilon}$ and T_c are the same) except the following change in initial data:

$$(\rho, u, p, z)(x, 0) = \begin{cases} (\rho_l, u_l, p_l, 0), & \text{if } x \le 10, \\ (\rho_m, u_m, p_m, 0), & \text{if } 10 < x \le 20, \\ (\rho_r, u_r, p_r, 1), & \text{if } 20 < x; \end{cases}$$

where $p_l = 40.0$, $\rho_l = 2.0$, $u_l = 4.0$; $p_m = 54.8244$, $\rho_m = 3.64282$, $u_m = 6.2489$ and $p_r = 1.0$, $\rho_r = 1.0$, $u_r = 0$.

In this example there is a right moving detonation, a right moving rarefaction wave, a right moving contact discontinuity, and a left moving rarefaction wave before the collision happens. After some time, there is a collision between the detonation and the right moving rarefaction wave.

The 'exact' solution is obtained similarly as those in Example 4.3. Figure 4.4 shows the numerical solution by using the random projection method (2.10) with $h = 0.25$ (i.e. 401 grid points for the interval $[0, 100]$) and $k = 0.01$ at time $t = 2$ (before collision) and $t = 8.0$ (after collision), respectively.

Example 4.5: A detonation interacting with an oscillatory profile. The set up of this problem is similar to those in Example 4.3 (i.e. γ, q_0, and T_c are the same) except that we change $K = 1000.0$ and the initial data to:

$$(\rho, u, p, z)(x, 0) = \begin{cases} (\rho_l, u_l, p_l, 0), & \text{if } x \le \frac{\pi}{2}, \\ (\rho_r(x), u_r, p_r, 1), & \text{if } \frac{\pi}{2} < x; \end{cases}$$

where $p_l = 21.53134$, $\rho_l = 1.79463$, $u_l = 3.0151$; and $p_r = 1.0$, $\rho_r(x) = 1.0 + 0.5 \sin 2x$, $u_r = 0$.

This problem is solved on the interval $[0, 2\pi]$. The 'exact' solutions are obtained by using $h = \frac{\pi}{10000}$ (i.e. 20001 grid points on the interval $[0, 2\pi]$) and $k = \frac{h}{20}$. This is a resolved calculation.

Figure 4.5 shows the numerical solutions by using the random projection method (2.10) with $h = \frac{\pi}{400}$ (i.e. 801 grid points for the interval $[0, 2\pi]$) and $k = \frac{h}{20}$ at time $t = \frac{\pi}{20}$ and $t = \frac{\pi}{5}$, respectively.

Example 4.6: Collision of a detonation with a shock and a rarefaction. The set up of this problem is similar to those in Example 4.3 (i.e. γ, q_0, $K = \frac{1}{\varepsilon}$ and T_c are the same) except that we change the initial data to:

$$(\rho, u, p, z)(x, 0) = \begin{cases} (\rho_l, u_l, p_l, 0), & \text{if } x \leq 10, \\ (\rho_m, u_m, p_m, 1), & \text{if } 10 < x \leq 40, \\ (\rho_r, u_r, p_r, 1), & \text{if } 40 < x; \end{cases}$$

where $p_l = 54.8244$, $\rho_l = 3.64282$, $u_l = 6.2489$; $p_m = 1.0$, $\rho_m = 1.0$, $u_m = 0.0$ and $p_r = 10.0$, $\rho_r = 4.0$, $u_r = 0$.

In this example there is a right moving detonation, a right moving rarefaction, a stationary contact discontinuity, and a left moving shock before the collision happens. After some time, there are collisions of detonation with the shock and the rarefaction.

The 'exact' solution is obtained similarly as that in Example 4.3. Figure 4.6 (a)-(c) show the numerical solution by using the random projection method (2.10) with $h = 0.125$ (i.e. 801 grid points for the interval $[0, 100]$) and $k = 0.005$ at time $t = 2$ (before collision), $t = 4$ (during collision), and $t = 8.0$ (after collision), respectively.

This example shows that the random projection method works very well before, during and after collisions. It captures precisely the collision time.

Example 4.7: Collision of two detonations. The set up in this example is similar to those in Example 4.3 (i.e. γ, q_0, $K = \frac{1}{\varepsilon}$ and T_c are the same) except that we change the initial data to

$$(\rho, u, p, z)(x, 0) = \begin{cases} (\rho_l, u_l, p_l, 0), & \text{if } x \leq 10, \\ (\rho_m, u_m, p_m, 1), & \text{if } 10 < x < 90, \\ (\rho_r, u_r, p_r, 0), & \text{if } 90 \leq x; \end{cases}$$

where $p_l = 30.0$, $\rho_l = 1.79463$, $u_l = 3.0151$; $p_m = 1.0$, $\rho_m = 1.0$, $u_m = 0.0$ and $p_r = 21.53134$, $\rho_r = 1.79463$, $u_r = -8.0$.

In this example there is a right moving detonation, a left moving strong detonation and other waves. After some time, there is a collision between the two detonations.

The 'exact' solution is obtained similarly as that in Example 4.3. Figure 4.7 shows the numerical solution by using the random projection method (2.15) with $h = 0.25$ (i.e. 401 grid points for the interval $[0, 100]$) and $k = 0.01$ at time $t = 4$ (before collision), and $t = 6.0$ (after collision), respectively.

From the above examples, we can see that our random project method works very well for one dimensional detonation wave problems even if the reaction scale is not numerically resolved. It not only captures the correct speeds of detonations but also is able to handle the interactions between detonations, and between a detonation with another wave.

Example 4.8: A two-dimensional detonation wave. We consider the problem (1.4)-(1.8) in a two dimensional channel, the upper and lower boundaries are solid walls. We choose γ, q_0, $K = \frac{1}{\varepsilon}$ and T_c the same as those in Example 4.3. The initial data (3.1) are chosen as $p_l = 54.8244$, $\rho_l = 3.64282$, $u_l = 6.2489$, $v_l = 0.0$; and $p_r = 1.0$, $\rho_r = 1.0$, $u_r = 0.0$, $v_r = 0.0$. This problem is solved on $[0, 300] \times [0, 50]$ with a 301×51 mesh, and

$$\xi(y) = \begin{cases} 10 & |y - 25| \geq 15, \\ 25 - |y - 25| & |y - 25| < 15. \end{cases}$$

Thus the mesh size $h = 1$. The time step is chosen as $k = 0.01$.

Figure 4.8 shows density contours at several different times. One can see that the triple points, which is the important feature of the solution, travel in the transverse direction and bounce back and forth against the upper and lower walls. On the contrary, the triple points cease to move after some time by using the usual deterministic method [10].

Example 4.9: Another two-dimensional detonation wave. This example is similar to Example 4.8 (i.e. the setup, boundary condition, the parameters γ, q_0, $K = \frac{1}{\varepsilon}$ and T_c are the same) except that we choose $p_l = 21.53134$, $\rho_l = 1.79463$, $u_l = 6.015114$, $v_l = 0.0$; $p_r = 1.0$, $\rho_r = 1.0$, $u_r = 0.0$, $v_r = 0.0$ and

$$\xi(y) = \begin{cases} 10 & 0 \leq y \leq 5 \text{ or } 35 \leq y \leq 50, \\ 25 - |y - 20| & 5 < y < 35. \end{cases}$$

This problem is solved on $[0, 300] \times [0, 50]$ with a 301×51 mesh. Thus the mesh size $h = 1$. The time step is chosen as $k = 0.01$.

Figure 4.9 shows profiles of pressure, p, temperature, T, and 10 times the fraction of unreacted fluid, $10z$ (here we show $10z$ not z in order to make it visible in one picture for the three profiles) on the line $y = 25$ at four different times, i.e. $t = 8$, $t = 16$, $t = 24$, $t = 32$ by using the random projection method (3.4). On the other hand, if one uses the deterministic method, spurious wave is generated if the same grid size and time step are used.

5 Conclusions

In this paper we presented a simple and robust random projection method for underresolved numerical simulation of stiff detonation waves in chemically reacting flows. This method is based on the random projection method proposed by the authors for general hyperbolic systems with stiff reaction terms [1], where the ignition temperature is randomized in a suitable domain. The method is simplified using the equations of instantaneous reaction, and then extended to handle the interactions of detonations. Extensive numerical experiments, including interaction of detonation waves, and in two dimensions, demonstrate that this method, although very simple and efficient, are very reliable and robust in calculating a wide range of problems in reacting flows.

In the future we hope to generalize this method to multispecies reactions.

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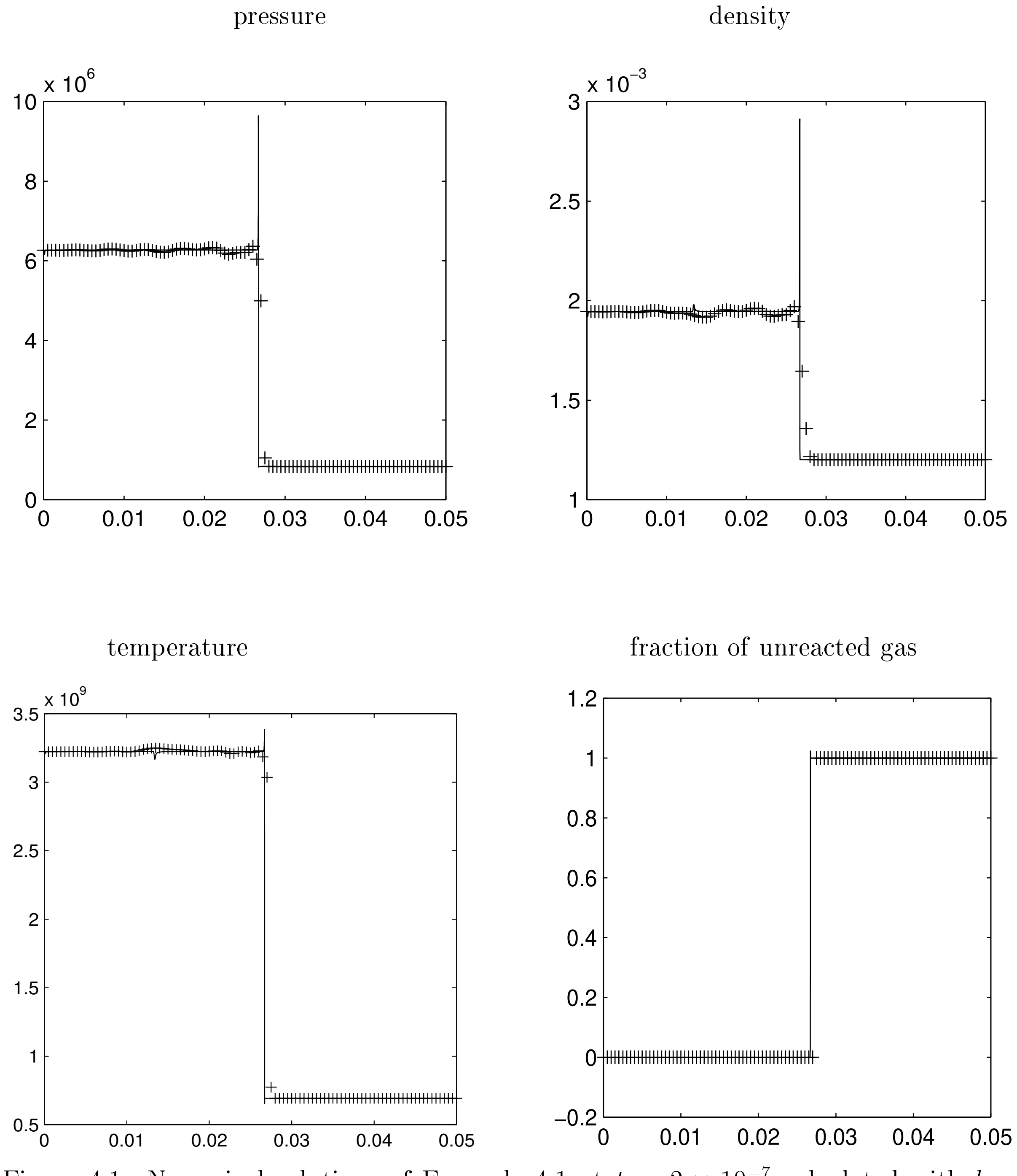

Figure 4.1: Numerical solutions of Example 4.1 at $t = 2 \times 10^{-7}$ calculated with $h = 5 \times 10^{-4}$, $k = 5 \times 10^{-10}$. $-$: 'exact' solutions; $++$: computed solutions. (a): the random projection method.

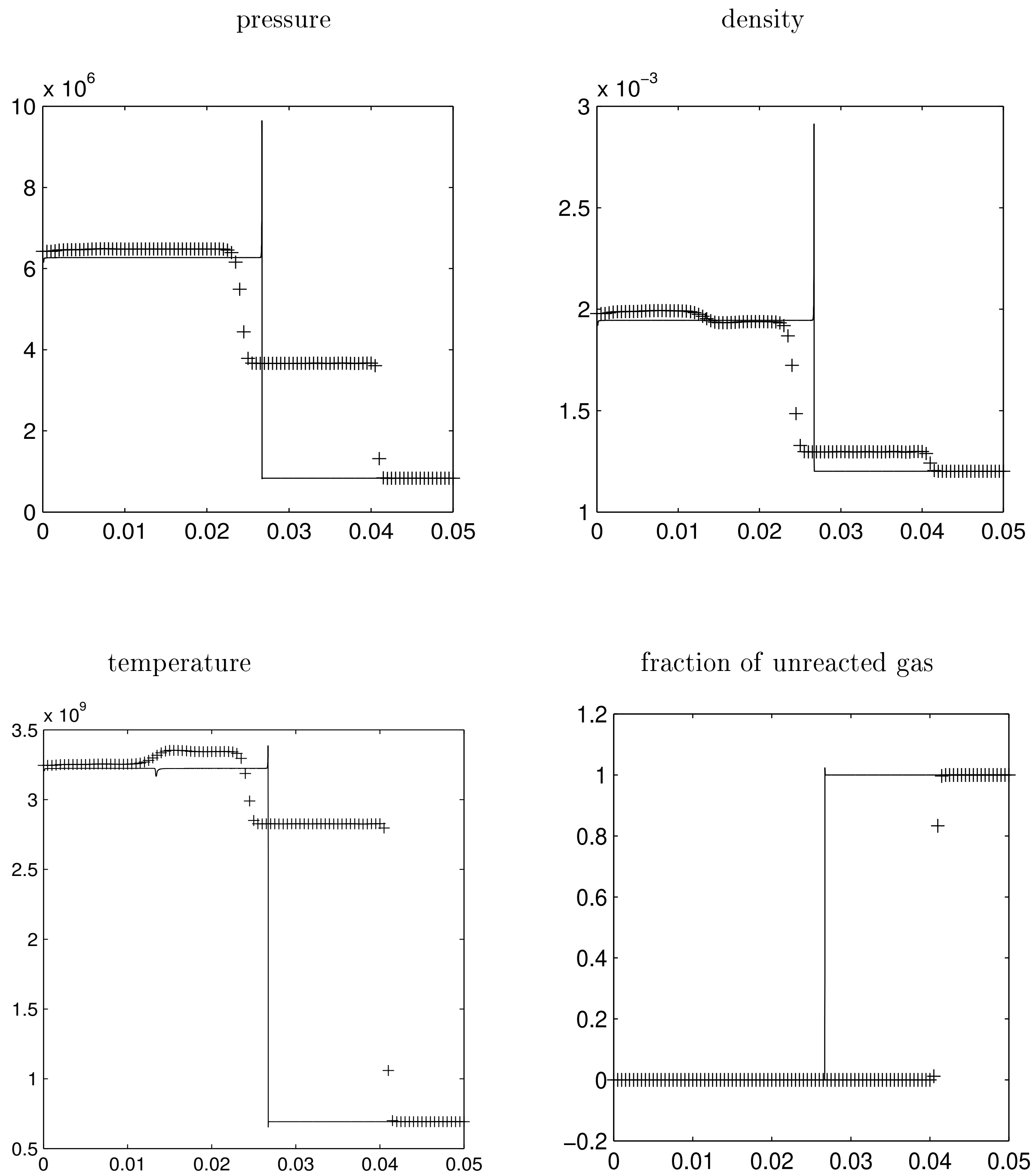

Figure 4.1 (cont'd). (b): the deterministic method.

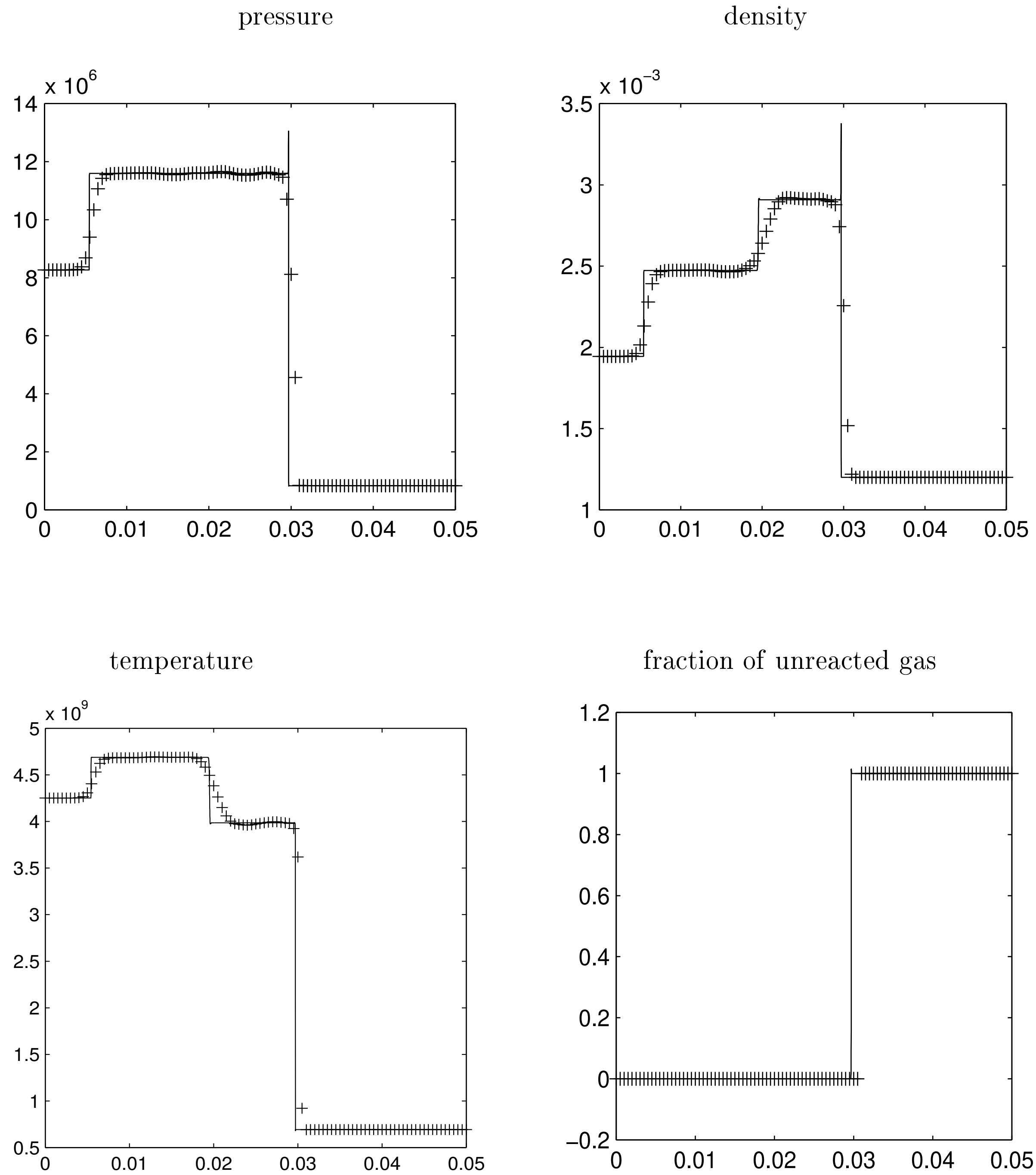

Figure 4.2: Numerical results at $t = 2 \times 10^{-7}$ for a strong detonation in Example 4.2 calculated by the random projection method (2.10). $h = 5 \times 10^{-4}$, $k = 5 \times 10^{-10}$. $-$: 'exact' solutions; $++$: computed solutions.

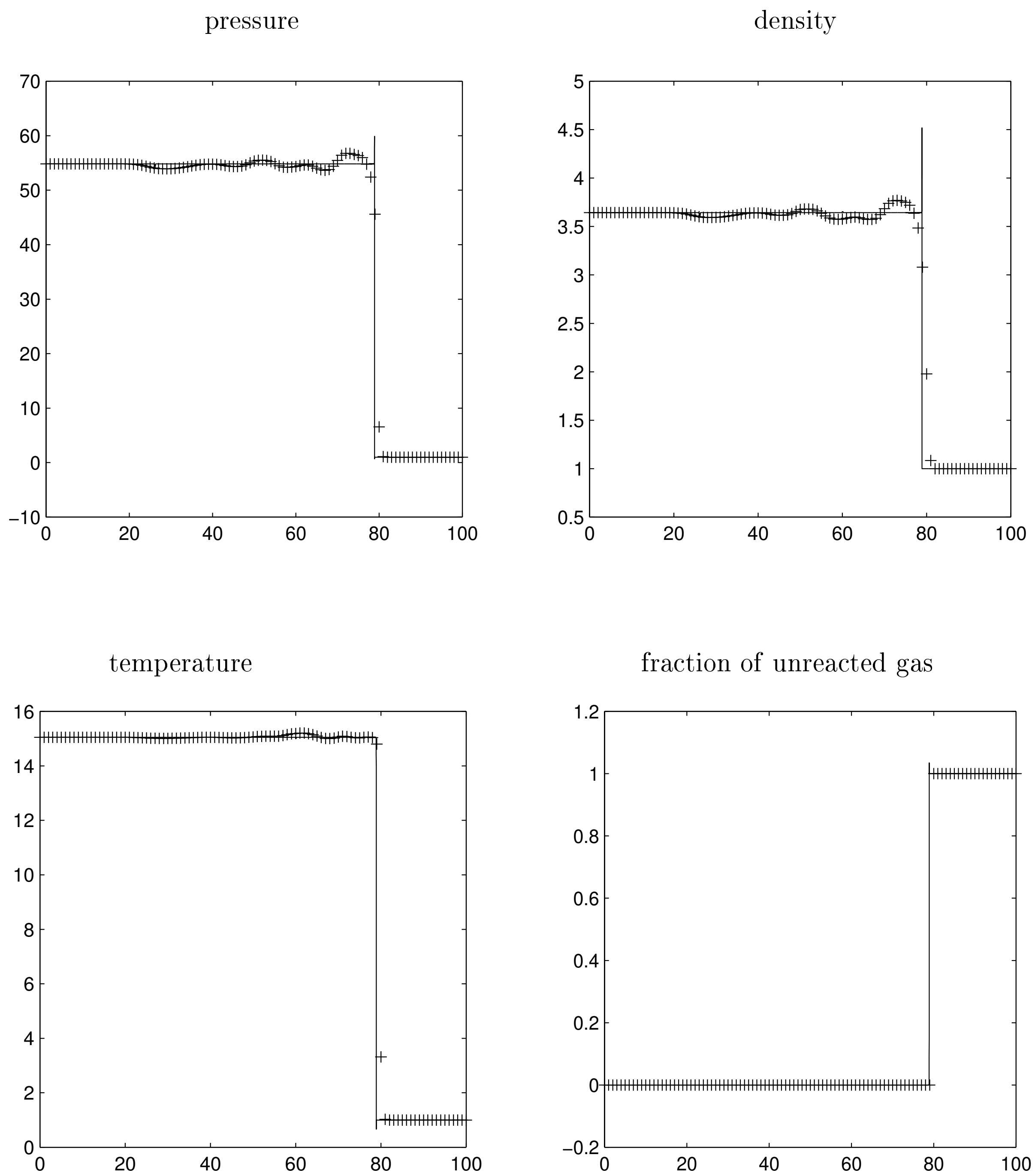

Figure 4.3: Numerical results of an unstable detonation in Example 4.3 using the random projection method (2.10). $h = 1$, $k = 0.05$, $t = 8$. $-$: 'exact' solutions; $++$: computed solutions.

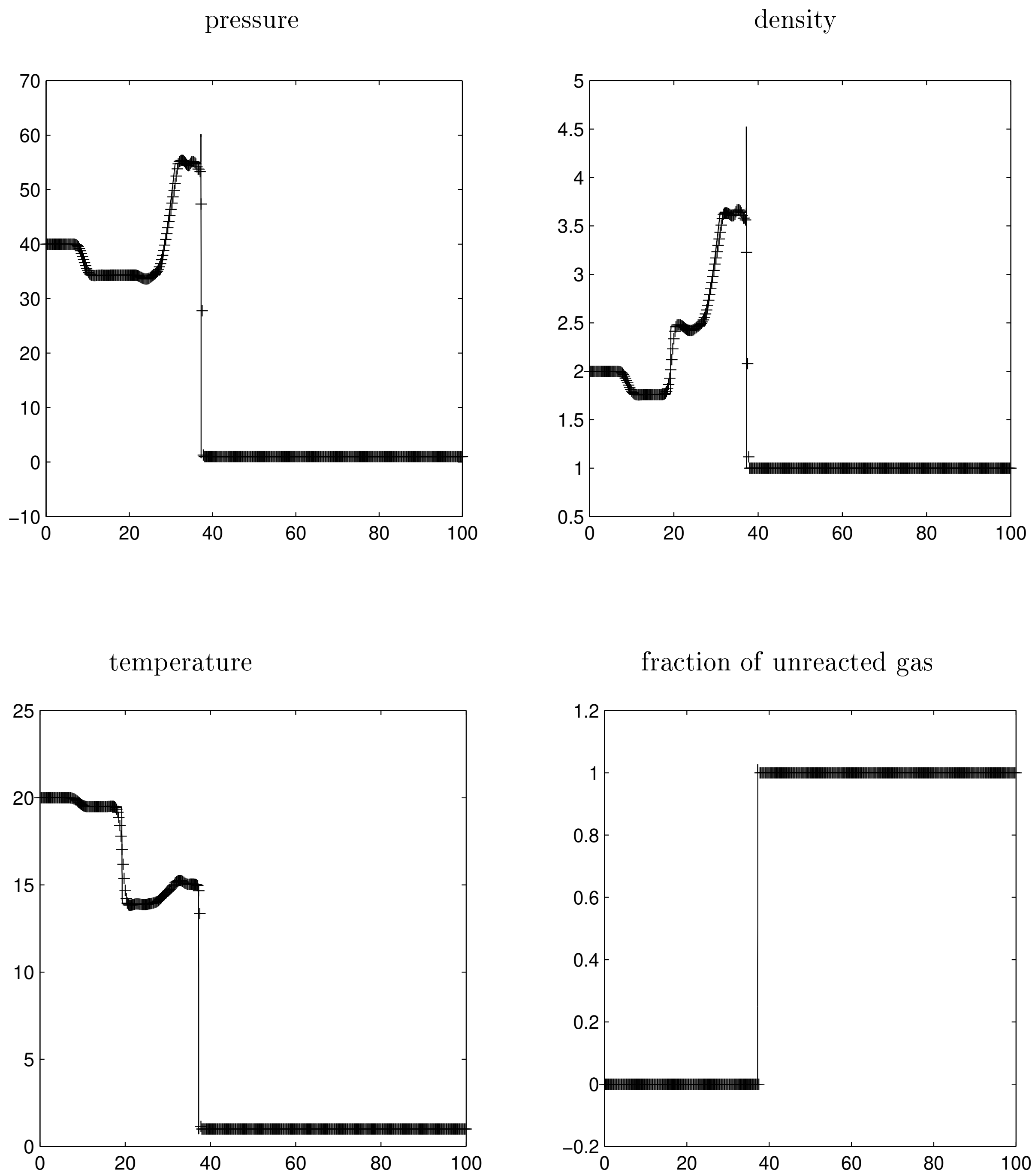

Figure 4.4: Numerical results of Example 4.4 involving the collision of a detonation with a rarefaction wave using the random projection method (2.10). $h = 0.25$, $k = 0.01$. $-$: 'exact' solutions; $++$: computed solutions. (a): $t = 2$ (before collision).

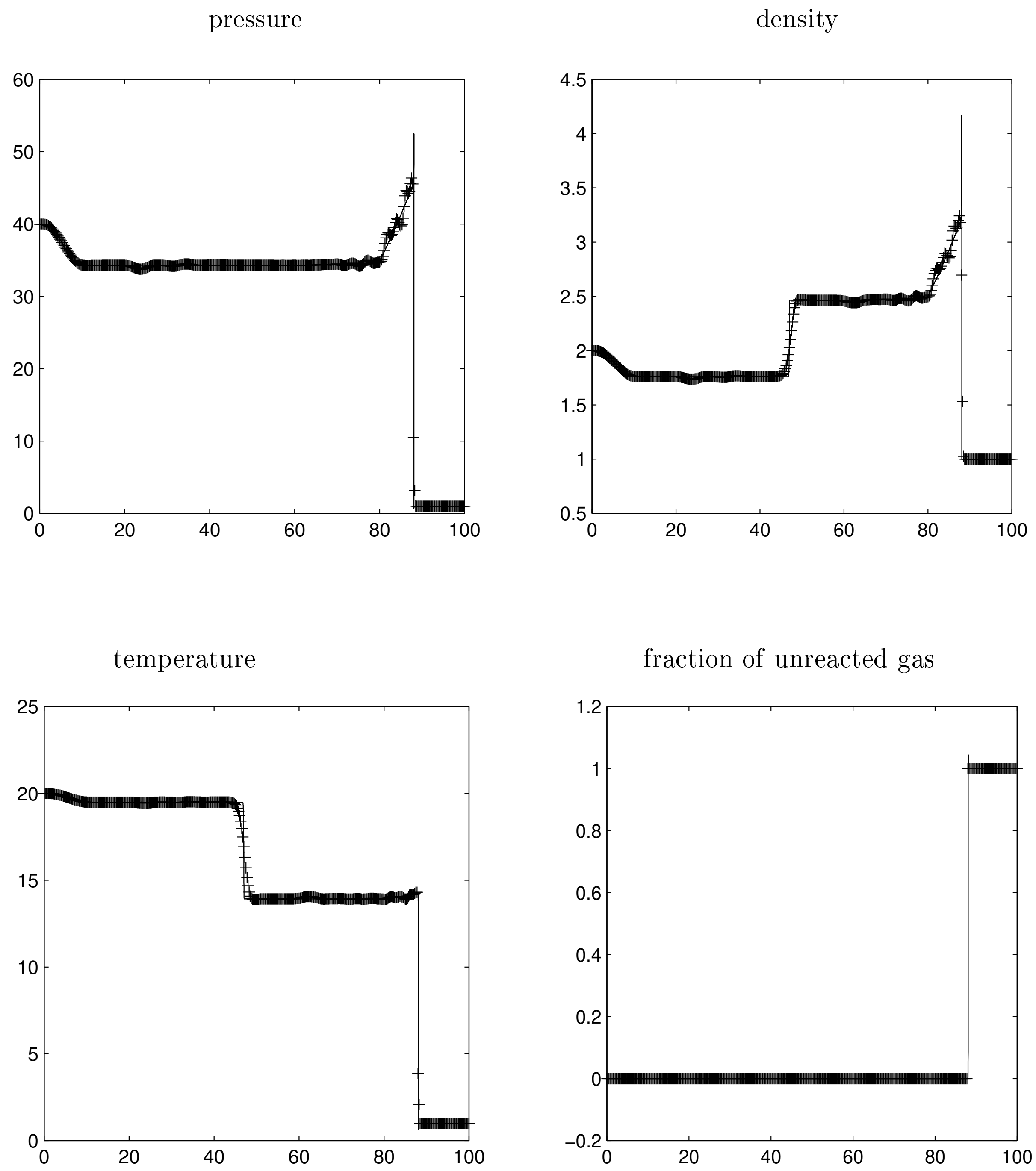

Figure 4.4 (cont'd). (b) $t = 8$ (after collision).

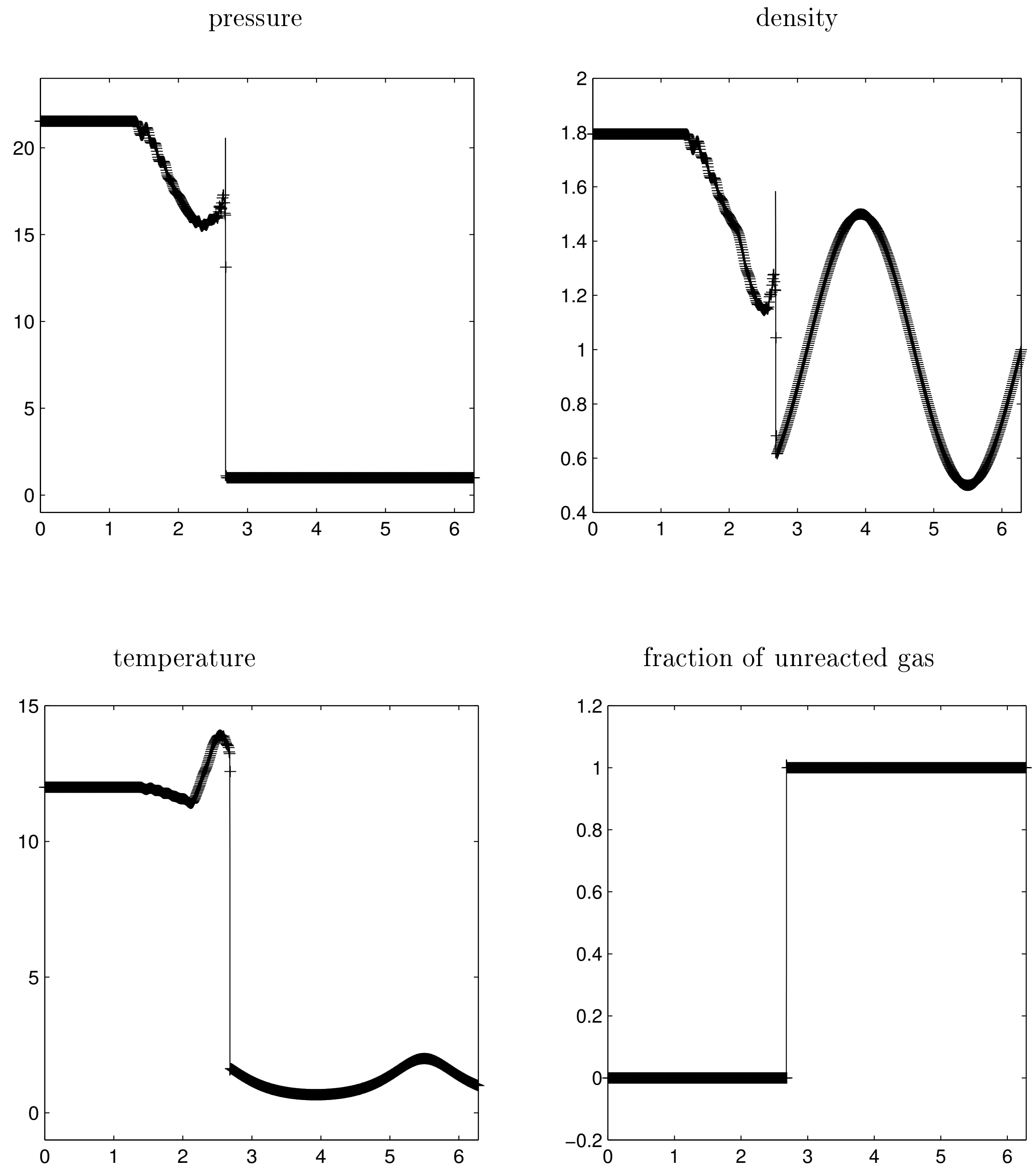

Figure 4.5: Numerical results of Example 4.5 by the random projection method (2.10). $h = \frac{\pi}{400}$, $k = \frac{h}{20}$. $-$: 'exact' solutions; $++$: computed solutions. (a). $t = \frac{\pi}{20}$.

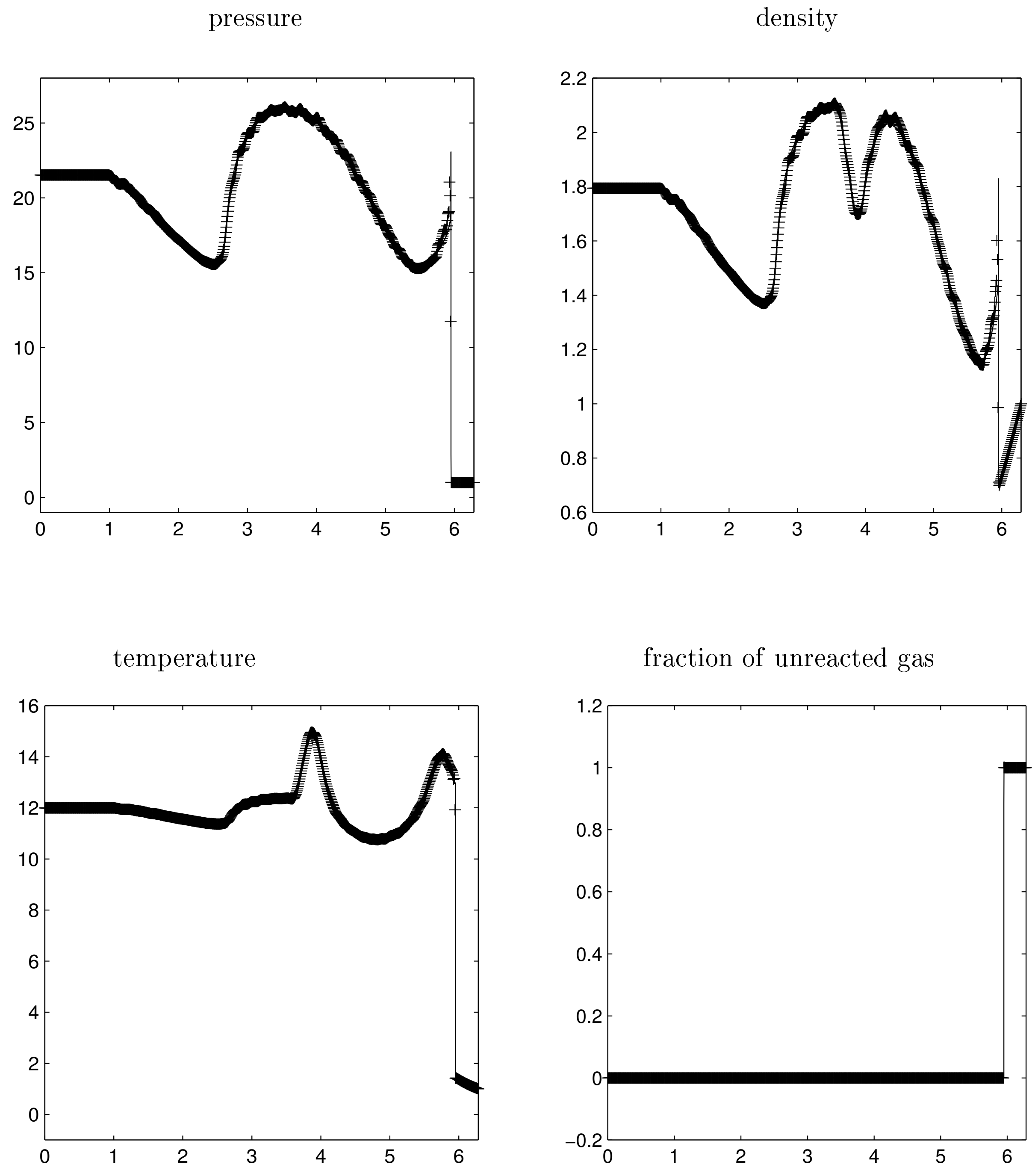

Figure 4.5 (cont'd). (b) $t = \frac{\pi}{5}$.

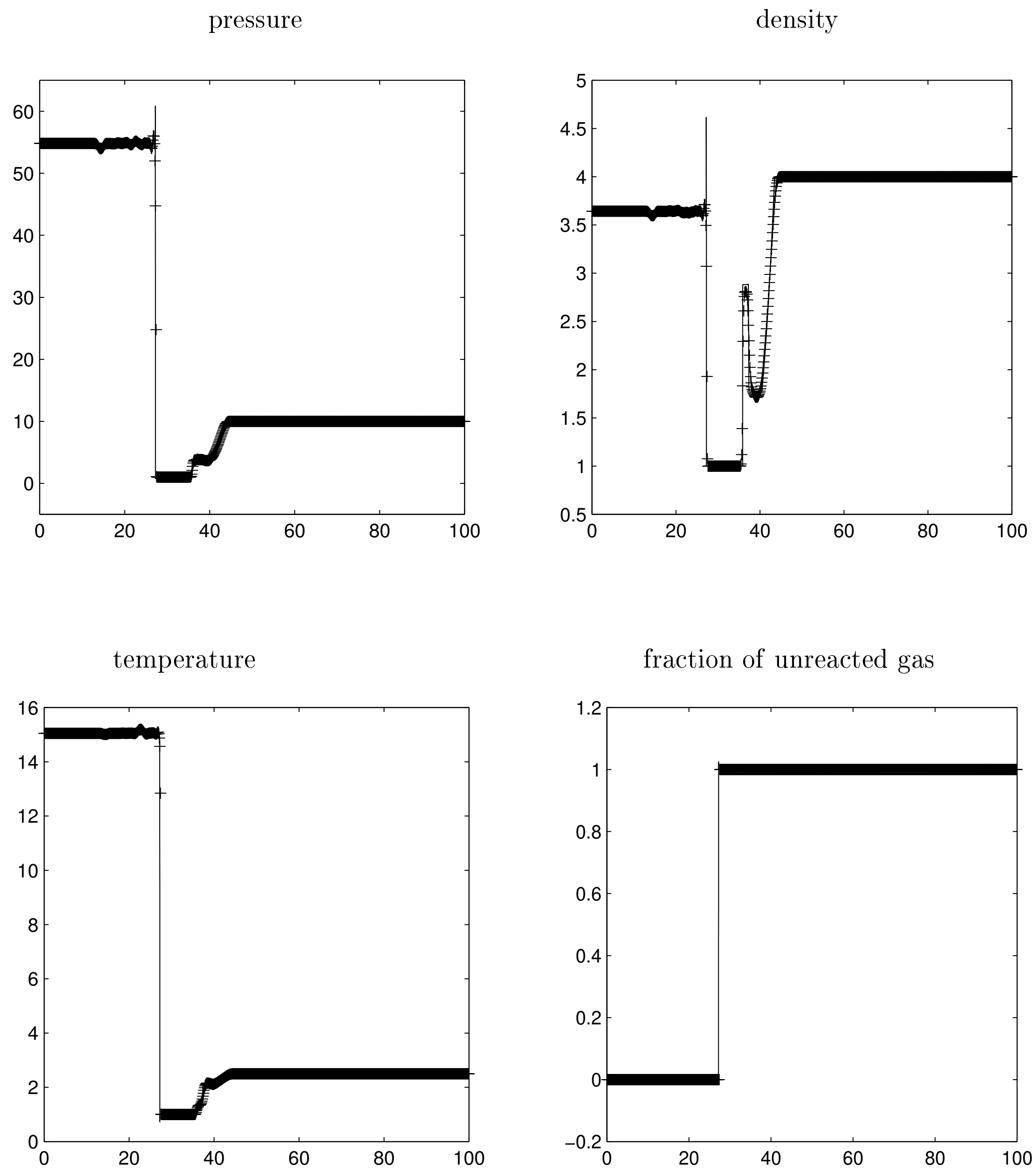

Figure 4.6: Numerical results of Example 4.6 involving the collisons of a detonation with a shock and then a rarefaction wave by the random projection method (2.10). $h = 0.125$, $k = 0.005$. $-$: 'exact' solutions; $++$: computed solutions. (a): $t = 2$ (before collision).

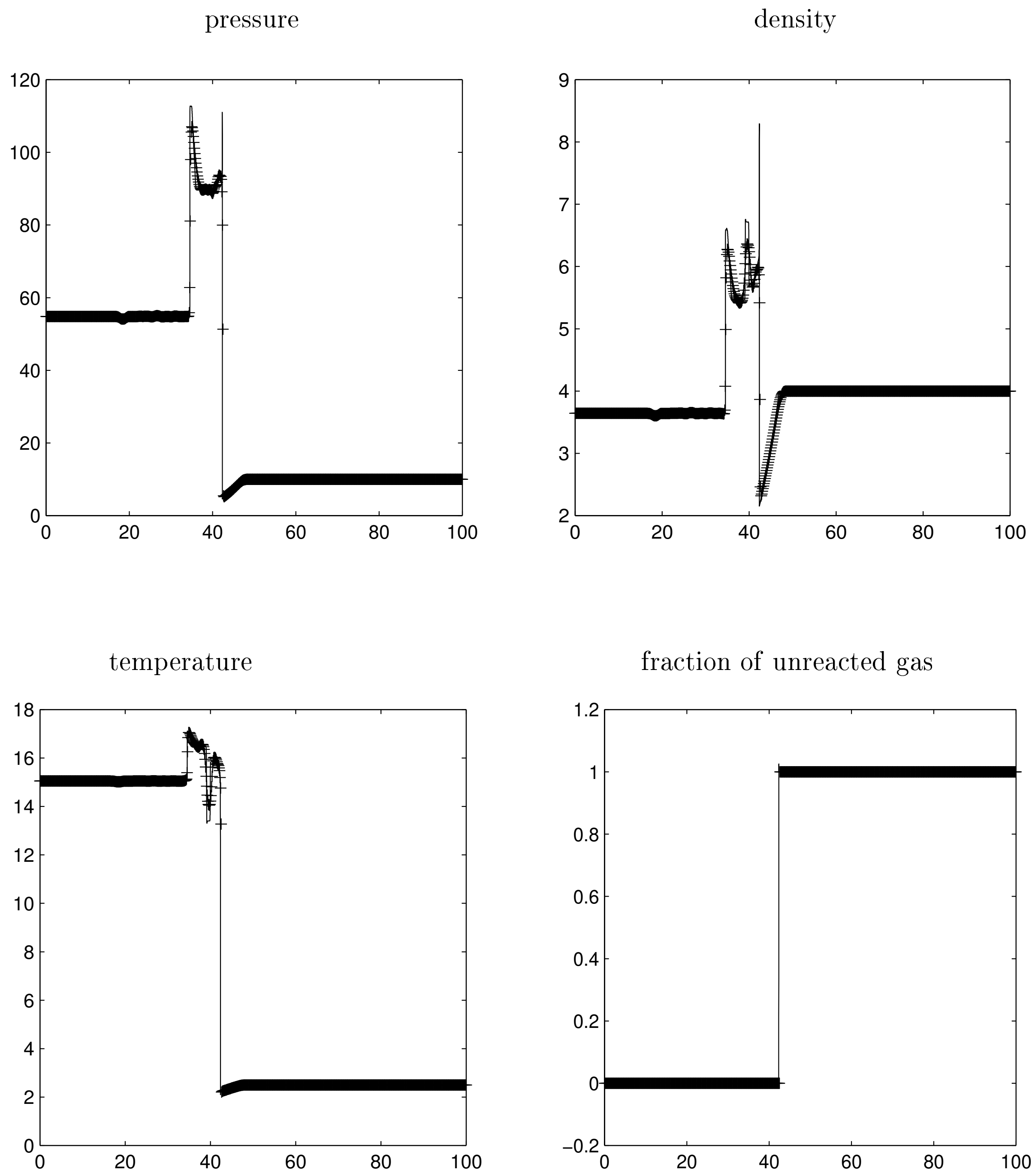

Figure 4.6 (cont'd) (b): $t = 4$ (during collision).

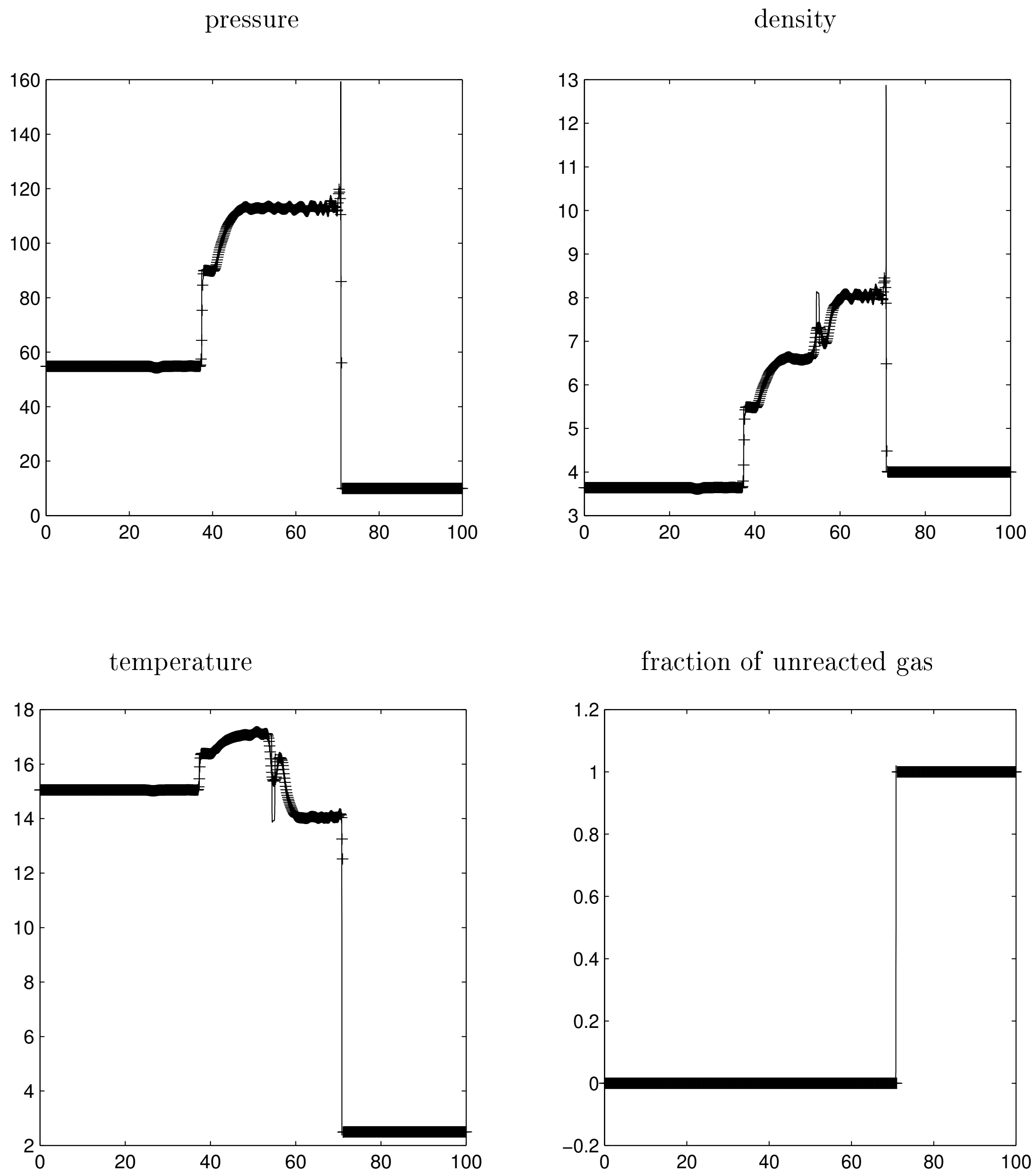

Figure 4.6 (cont'd) (c): $t = 8$ (after collision).

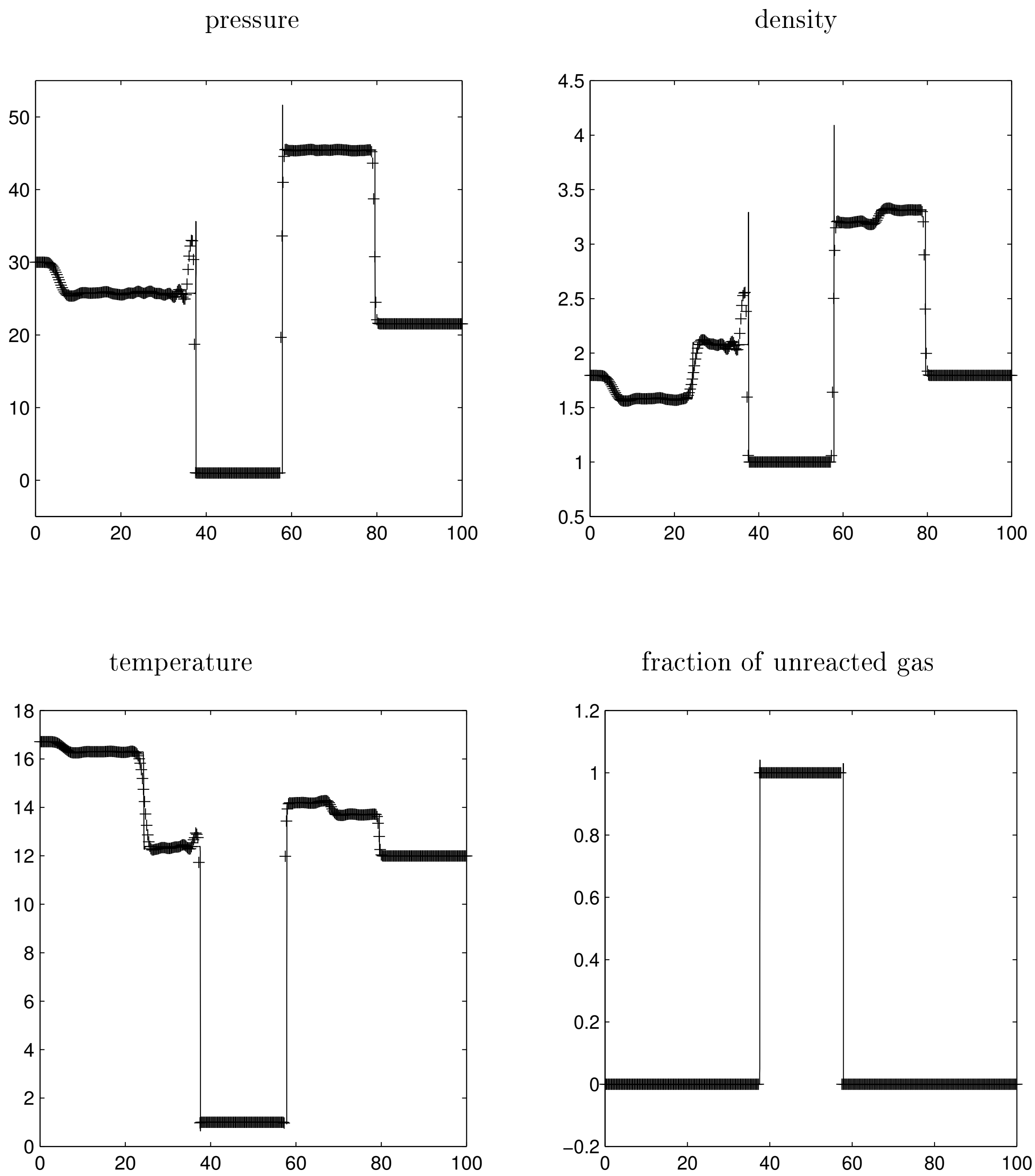

Figure 4.7: Numerical results of Example 4.7 involving the collision of two detonations by the random projection method (2.15). $h = 0.25$, $k = 0.01$. $-$: 'exact' solutions; $++$: computed solutions. (a): at $t = 4$ (before collision).

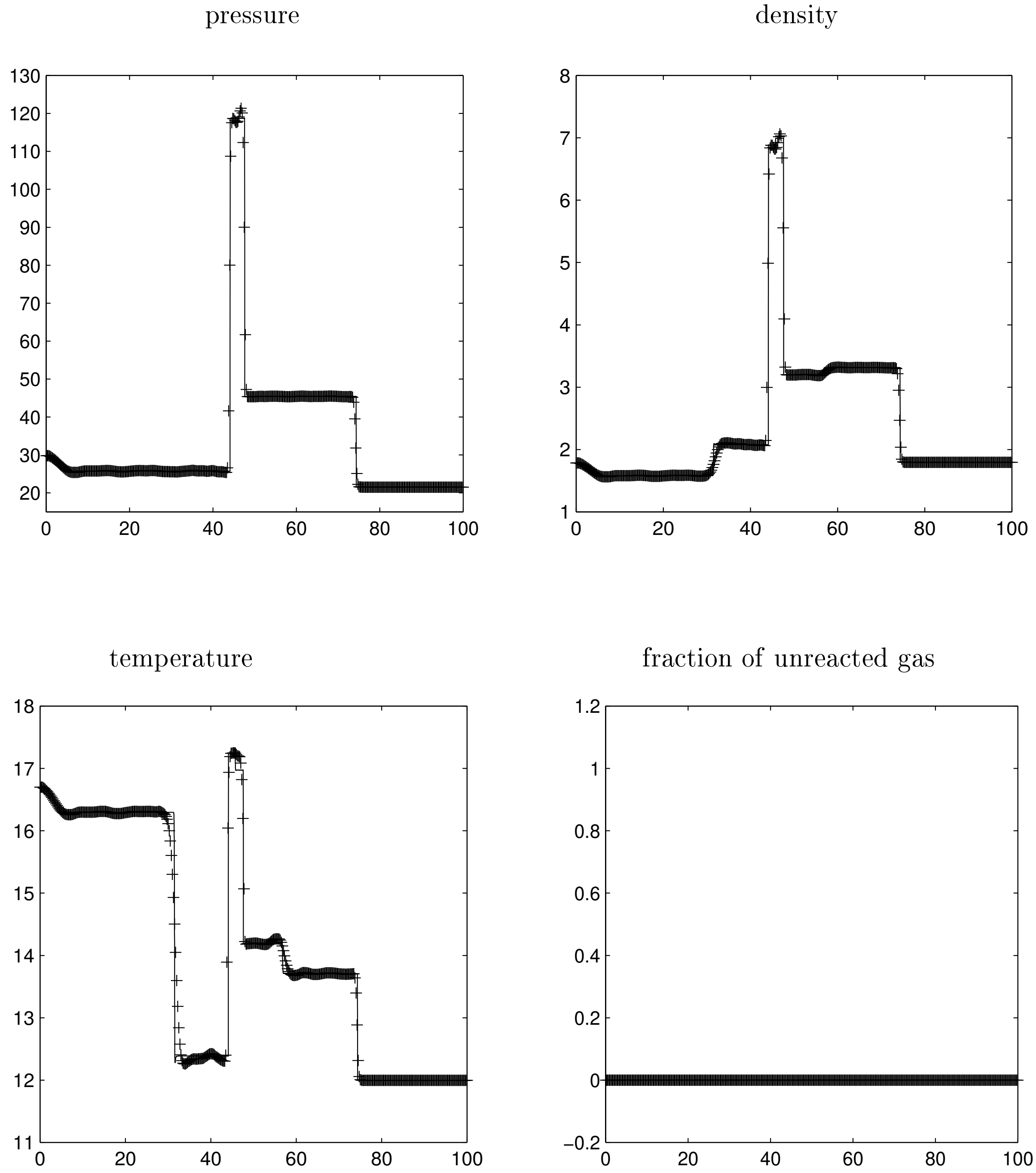

Figure 4.7 (cont'd). (b): at $t = 6$ (after collision).

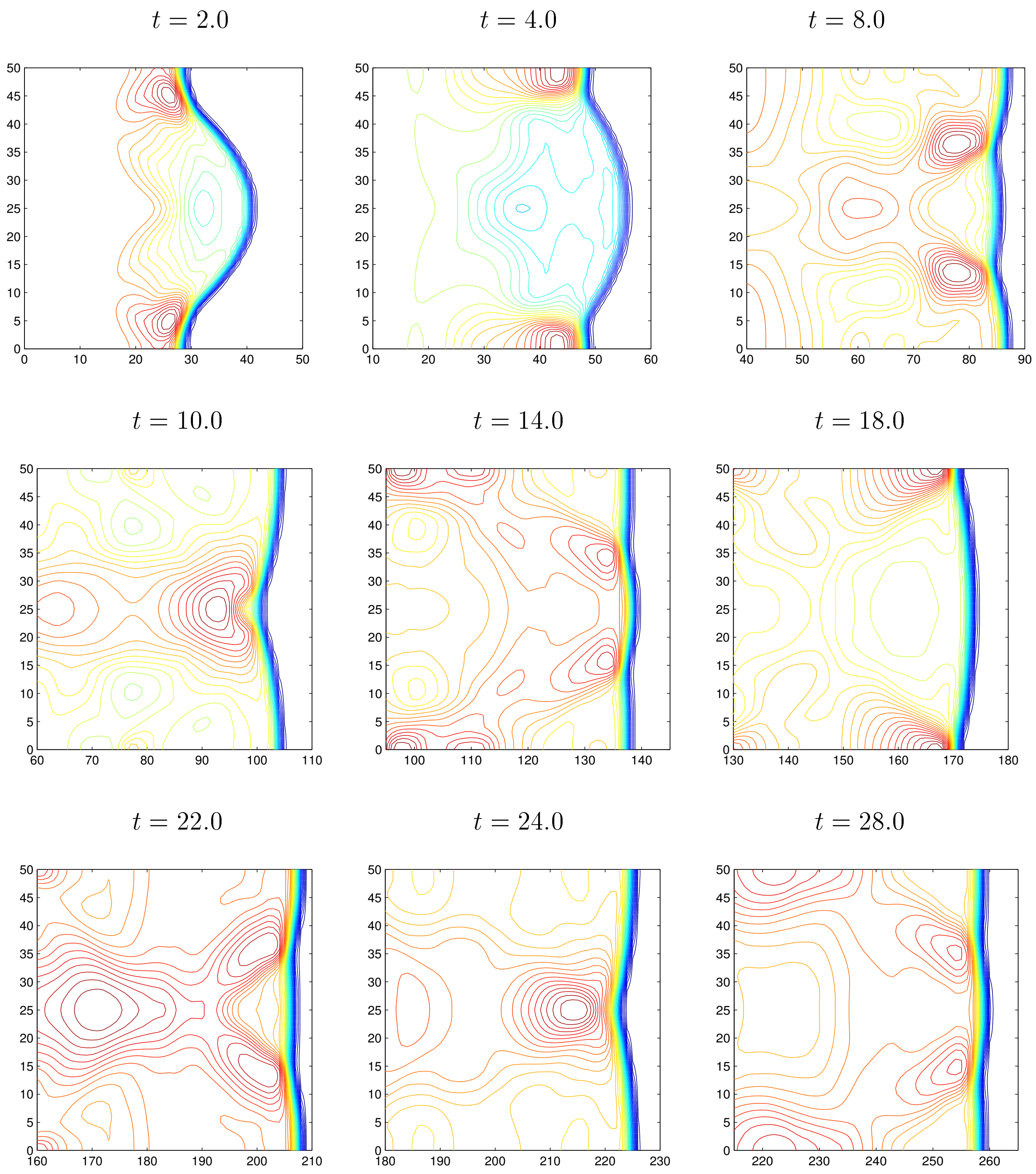

Figure 4.8. Numerical density contours for Example 4.8 by the 2d random projection method (3.4). $h = 1.0$, $k = 0.01$.

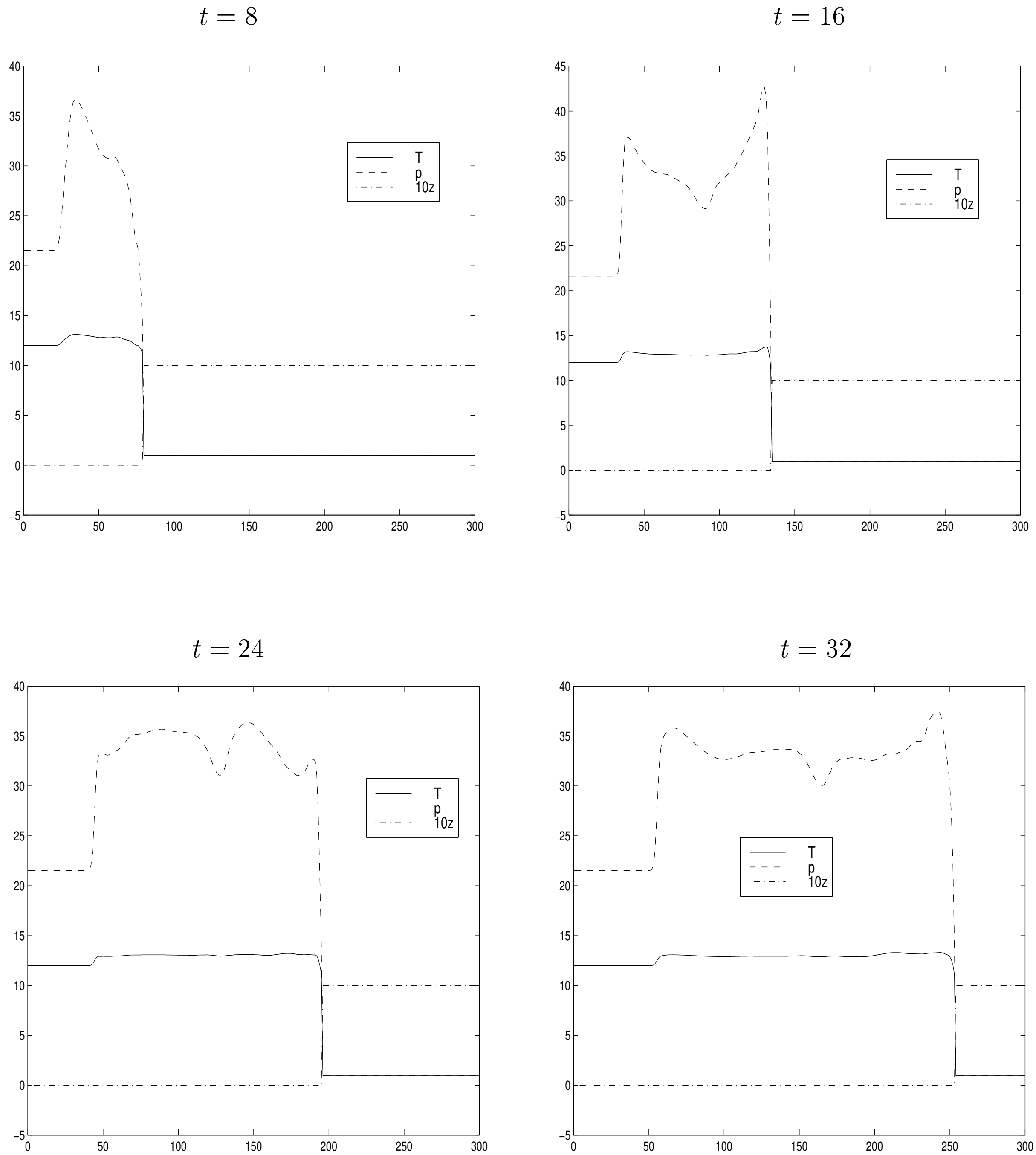

Figure 4.9: Profiles of pressure, p, temperature, T, and the fraction of unreacted fluid multiplied by 10, $10z$, on the line $y = 25$ for different times in Example 4.9 by using the 2d random projection method (3.4). $h = 1.0$, $k = 0.01$.