

# Numerical Calculation of Unstable Detonations by the Method of Space-Time Conservation Element and Solution Element

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## ABSTRACT

In the present paper, we report the two-dimensional calculations of propagating detonation waves by the method of Space-Time Conservation Element and Solution Element, or the CE/SE method for short. The two-dimensional Euler equations in conjunction with a species equation are solved in a time-accurate manner. The chemical reaction is modeled by a one-step Arrhenius kinetic model. The stiff source term is treated by a volumetric integration over a space-time region. As a contrast to the modern upwind methods, the present method does not use the Riemann solver, reconstruction methods, and/or directional splitting as the building blocks. Thus the logic and rational is significantly simpler. Two examples are reported: detonation initiation and two-dimensional propagating detonations. Special flow features of detonations are crisply resolved, including cellular structure, triple points, unburned pocket, and transverse waves. It is clearly that the present space-time method is a viable approach for solving unsteady detonation waves.

## 1. INTRODUCTION

Research of detonation waves [1] was pioneered by Zeldovich, von Neumann, and Doering, i.e., the ZND model, in which a steadily propagating detonation wave consisting of an ordinary compressible flow shock followed by a finite-rate reaction zone is postulated. This remarkable insight of the flow physics provided the preliminary knowledge of detonations. Further experimental evidences showed

that detonation waves are often unstable with transverse wave structure, and the pressure level of the pressure spike is significantly higher than that predicted by the ZND model.

Capability of accurate calculation of stable and unstable detonation waves is imperative for the further development of new numerical methods for detonations. To this end, the ZND model is an ideal proofing ground. Many important works about the development and application of numerical methods for detonations have been reported. A brief account of previous works, which are beneficial to the present research, is provided in the following.

Numerical calculation of the ZND detonation model was pioneered by Fickett and Wood [2,3]. They solved the one-dimensional equations using the method of characteristics in conjunction with a shock fitting method. Longitudinal instability waves were accurately simulated.

Taki and Fujiwara [4,5] applied Van Leer's upwind method to calculate two-dimensional traveling detonation waves. They solved the Euler equations coupled with two species equations. The chemical reaction was simulated by a two-step finite-rate model. The shock front was perturbed to trigger transverse instabilities and triple points.

Oran, Kailasanath and coworkers [6,7,8] extended the Flux-Corrected Transport (FCT) algorithm for detonations. The FCT approach is the most popular method in calculating detonation. The software has been widely used for one, two, and three-dimensional calculations.

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Bourlioux *et al.* [9,10] developed an advanced numerical method, composed of a high-order upwind scheme, a front tracking method, and an adaptive refinement algorithm, for direct calculations of detonations. They presented detailed comparisons between the theoretical solution and their numerical solution. The results in [9,10] are used as the guideline of our development of the CE/SE method for detonations.

Quirk [11] addressed the particular deficiency of the Godunov type upwind schemes when solving complex flows such as detonations. As a result, he developed a strategy to overcome the weakness. By using his modified upwind method, he successfully simulated the galloping one and two-dimensional detonations

Yungster and Radhakrishnan [12] developed a fully implicit, time-accurate upwind method for supersonic combustion. An efficient Successive Gauss Seidel (SGS) iteration method was used to invert the matrix. They have reported numerical results related to projectile moving in a hydrogen-air mixture.

Papalexandris [13] developed an unsplit upwind method for hyperbolic conservation laws with stiff source term. The method is based on integrating the flow equations along the characteristic manifolds in space-time. We will repeat Case C reported in [13] in the present paper.

The objective of the present work is to extend the Space-Time CE/SE method, originally developed by Chang and coworkers [14,15,16,17,18], to calculate the two-dimensional unstable detonations. We want to access the efficiency and the accuracy of the method in calculating the complex flow features of detonations. The rest of this paper is organized as follows. In Section 2, a brief account of the CE/SE method will be provided. The numerical treatment for the stiff source terms associated with the finite-rate chemistry will be discussed. In Section 3, the numerical solutions by the CE/SE method for two-dimensional unsteady ZND waves will be reported. We then offer the concluding remarks.

## 2 THE SPACE-TIME CE/SE METHOD

The details of the Space-Time CE/SE method have been extensively illustrated in [14,15]. Here, a brief discussion of the essentially steps of the method is provided. The basic idea of the CE/SE method is an equal footing treatment of space and time in calculating the space-time flux balance. Consider an

initial-value problem involving the partial differential equation,

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} + b \frac{\partial u}{\partial y} = \tau(u) \quad (2.1)$$

where  $a$  and  $b$  are constants and the source term  $\tau(u)$  is a function of  $u$ . Let  $x_1 = x$ ,  $x_2 = y$  and  $x_3 = t$  be the coordinates of a three-dimensional Euclidean space  $E_3$ . Equation. (2.1) can be reformulated as a divergence free condition,

$$\nabla \cdot \mathbf{h} = \tau(u) \quad (2.2)$$

where the current density vector  $\mathbf{h} = (au, bu, u)$ . By using Gauss' divergence theorem in  $E_3$ , it can be shown that Eq. (2.1) is the differential form of the integral conservation law:

$$\oint_{S(R)} \mathbf{h} \cdot d\mathbf{s} = \int_R \tau(u) dR \quad (2.3)$$

Here  $S(R)$  is the boundary of an arbitrary space-time region  $R$  in  $E_3$ ,  $d\mathbf{s} = d\sigma \mathbf{\bar{n}}$  with  $d\sigma$  and  $\mathbf{\bar{n}}$ , the area of a surface element normal on  $S(R)$ , and its outward unit, respectively. In Eq. (2.3),  $R$  is the volume of a space-time volume inside  $S(R)$ , and  $\mathbf{h} \cdot d\mathbf{s}$  is the space-time flux  $\mathbf{h}$  leaving the region  $R$  through the surface element  $d\mathbf{s}$ . All mathematical operations can be carried out as if  $E_3$  were an ordinary three-dimensional Euclidean space. We remark that space and time are treated in an equal-footing manner. Therefore, there is no restriction on the space-time geometry of the conservation elements over which the space-time flux is imposed.

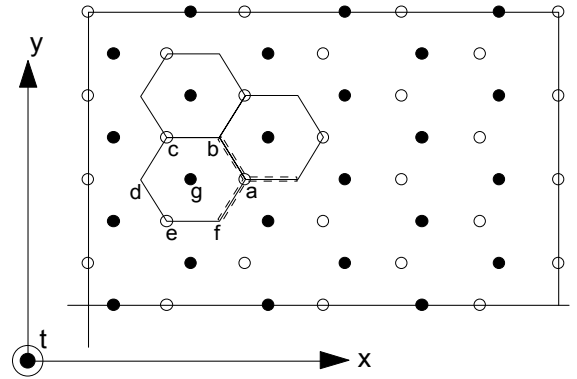


Fig. 2.1 A space-time mesh of the two-dimensional CE/SE method; solid circles for the time step  $n$ , and the filled circles are for the time step  $n+1/2$ .

Two sets of space-time nodes are used in the present method, i.e., the solid circles and the open circles in Fig. 2.1. Each node is denoted by  $(j, k, n)$ , with  $n$  being a time index, and  $(j, k)$  the spatial indices. Associated with each node  $(j, k, n)$ , the

solution element  $SE(j, k, n)$  is the space-time region in the immediate neighborhood of three vertical planes and one hexagonal plane. Note the vertical direction is referred to the time marching direction. In Fig. 2.1, the projection of the three vertical planes on the x-y plane associated with point  $a$  is illustrated. For detailed description, refer to [14,15].

To proceed, for any  $(x, y, t) \in SE(j, k, n)$ , let  $u(x, y, t)$  be approximated by  $u^*(x, y, t; j, k, n)$ , which is defined as

$$u^*(x, y, t; j, k, n) = u_{j,k}^n + (u_x)_{j,k}^n(x - x_j) + (u_y)_{j,k}^n(y - y_k) + (u_t)_{j,k}^n(t - t^n), \quad (2-4)$$

where (i)  $u_{j,k}^n$ ,  $(u_x)_{j,k}^n$ ,  $(u_y)_{j,k}^n$  and  $(u_t)_{j,k}^n$  are constants in  $SE(j, k, n)$ , and (ii)  $(x_j, y_k, t^n)$  are the coordinates of the mesh point  $(j, k, n)$ . Here, we shall assume that

$$(u_t)_{j,k}^n = -a_x(u_x)_{j,k}^n - a_y(u_y)_{j,k}^n \quad (2.5)$$

Combining Eqs. (2.4) and (2.5), one has

$$u^*(x, y, t; j, k, n) = u_{j,k}^n + (u_x)_{j,k}^n[(x - x_j) - a_x(t - t^n)] + (u_y)_{j,k}^n[(y - y_k) - a_y(t - t^n)], \quad (2.6)$$

where  $(x, y, t) \in SE(j, k, n)$ . As a result, there are three independent marching variables  $u_{j,k}^n$ ,  $(u_x)_{j,k}^n$  and  $(u_y)_{j,k}^n$  associated with each  $(j, k, n) \in \Omega$ . Furthermore, because  $\mathbf{h} = (a_x, a_y, u)$ , we define

$$\mathbf{h}^*(x, y, t; j, k, n) = (a_x u^*(x, y, t; j, k, n), a_y u^*(x, y, t; j, k, n), u^*(x, y, t; j, k, n)) \quad (2.7)$$

Let  $E_3$  be divided into non-overlapping hexagonal-based-column regions with its projection to the x-y plane as the area  $\Delta A$  in Fig.2.1, referred to as conservation elements (CEs). As depicted in Fig. 2.1, the CE with the midpoint of its top face being a mesh point  $(j, k, n)$  is denoted by  $CE(j, k, n)$  and the discrete approximation of Eq. (2.3) is expressed as

$$\oint_{S(CE(j,k,n))} \mathbf{h} \cdot d\mathbf{S} = \tau(u_{j,k}^n) \frac{\Delta A \Delta t}{2}. \quad (2.8)$$

Here  $\tau(u_{j,k}^n)$  is assumed to be the average value of  $\tau(u)$  in  $CE(j, k, n)$ . Because  $(\Delta A \Delta t)/2$  is the volume of  $CE(j, k, n)$ , Eq. (2.8) simply states that the total space-time flux of  $\mathbf{h}^*$  leaving the boundary of any CE is equal to the source integral over the CE. Because the surface integration over any interface separating two neighboring CEs is evaluated using the information from a single SE, the local conservation relation Eq. (2.8) leads to a global flux conservation relation. Thus, the total flux of  $\mathbf{h}^*$  leaving the boundary of any space-time region that is the union of any combination of CEs is equal to the source integral over the same space-time region.

To justify Eq. (2.8), we shall assume that the value of  $u$  on a macro scale, i.e., the value of  $u$  obtained from an averaging process involving a few neighboring CEs, will not vary significantly as a result of redistribution of  $\tau$  over each CE is held constant. We take the liberty to redistribute the source term such that there is no source present within each SE. Thus, with the aid of Eq. (2.4), Eq. (2.5) is the result of substituting  $u = u^*(x, y, t; j, k, n)$  into Eq. (2.3). Because the boundary of  $CE(j, k, n)$  is a subset of the union of  $SE(a)$ ,  $SE(c)$ ,  $SE(e)$  (refer to Fig. 2.1), Eq. (2.8) imply that

$$u_{j,k}^n - \frac{\Delta t}{2} \tau(u_{j,k}^n) = f_1(u_{j,k}^{n-1/2}(a), u_x^{n-1/2}(a), u_y^{n-1/2}(a)) + f_2(u_{j,k}^{n-1/2}(c), u_x^{n-1/2}(c), u_y^{n-1/2}(c)) + f_3(u_{j,k}^{n-1/2}(e), u_x^{n-1/2}(e), u_y^{n-1/2}(e)). \quad (2.9)$$

Given the values of the marching variables at the  $(n-1/2)$ th time level,  $u_{j,k}^n$  is determined by solving Eq. (2.9) with the aid of Newton's iteration method. Note the initial condition for Newton's iterations is calculated by assuming that the source term is zero. After  $u_{j,k}^n$  is known,  $(u_x)_{j,k}^n$  and  $(u_y)_{j,k}^n$  are calculated by the standard a- $\epsilon$  scheme. The resultant  $(u_x)_{j,k}^n$  and  $(u_y)_{j,k}^n$  are further modified by a reweighted-procedure to catch shock. These treatments are fully illustrated in [14,15]. The detailed the stiff source term treatment in the context of the CE/SE scheme for one-dimensional problems can be found in [16].

### 3. THEORETICAL MODEL

The classical ZND model of the two-dimensional detonation waves can be formulated by the Euler equations coupled with a species equation. The five equations can be cast to a vector form:

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial t} + \frac{\partial F}{\partial t} = S \quad (3.1)$$

where  $Q$  is the unknown vector,  $E$  and  $F$  are the flux vector, and  $S$  is the source term:

$$Q = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \\ \rho Y \end{pmatrix}, E = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (\rho E + p)u \\ \rho u Y \end{pmatrix},$$

$$F = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (\rho E + p)v \\ \rho v Y \end{pmatrix}, S = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \dot{\omega} \end{pmatrix}. \quad (3.2)$$

The five equations here are the continuity, moment, energy, and species equations, respectively. In the equation set,  $\rho$  is density,  $u$  and  $v$  are velocity,  $p$  is pressure,  $Y$  is the mass fraction of the reactant, and  $E = e + Yq + (u^2 + v^2)/2$  is the total energy with  $e$  as the internal energy and  $q$  as the heat release. In the species equation, a source term exists due to a one-step, irreversible chemical reaction, modeled by finite-rate kinetics. The source term can be expressed as

$$\dot{\omega} = -K \exp(-E^+/RT) \rho Y \quad (3.3)$$

where  $K$  is the pre-exponential factor of the Arrhenius kinetics,  $E^+$  is the activation energy, and  $R$  is the universal gas constant.

To proceed, the above equations are non-dimensionalized based on density, pressure, and a reference velocity (defined similar to the speed of sound) of the unburned gas, i.e.,  $\rho_0$ ,  $p_0$ , and  $\sqrt{RT_0}$ . Note that subscript 0 denotes the unburned state. In order to keep the flow equations consistent, the total energy, internal energy, and the activation energy in the governing equations are nondimensionalized by  $RT_0$ . The reaction rate constant  $K$  is a parameter, which sets the spatial and temporal scales. Typically,  $K$  is chosen such that the half-reaction length,  $L_{1/2}$ , of the ZND wave is unity. Note that  $L_{1/2}$  is defined as the distance between the detonation front and the point where half of the reactant is consumed. In addition, we also assume that the fluid is polytropic, i.e., the molecular weights and the specific heats are constants for the unburned and the burned gases.

#### 4. RESULTS AND DISCUSSIONS

In one of our previous papers [12], we have reported the one-dimensional stable and unstable ZND waves, calculated by the CE/SE method. We also conducted the mesh refinement study to assess the accuracy of the CE/SE method for resolving the longitudinal instabilities. Essentially, five mesh nodes per half reaction length are required for satisfactory results. The findings of the one-dimensional calculations will be used as the yardstick for the two-dimensional calculations in this paper.

In Ref. [18], two types of the ZND problems were simulated; i.e., the piston problem and the instability problem. In the piston problem, the detonation is initialized by a driving piston running into the fresh reactant gas. As a result, a shock is created, which in turn ignites the reactant and creates a detonation. In this case, the detonation would run away from the piston and a long computational domain is required.

To avoid the complexity of the start-up process in the piston problem, we also calculate the instability problem, in which the analytical solution of a stationary ZND detonation is used as the initial condition. The spatial coordinate is chosen such that the origin of the coordinate system is placed at the shock front, and the coordinate system is moving at the same velocity as the detonation. As such, we were able to fully control the flow condition and conduct the detailed comparison between the CFD results and the analytical solution. For completeness, a typical one-dimensional instability solution is provided in Fig. 4.1.

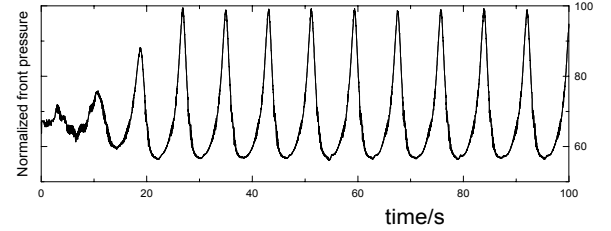


Fig.4.1 Shock pressure history for a calculation with 20 mesh cells per half-reaction length.

The parameters of the flow field are  $q = 50$ ,  $E^+ = 50$ ,  $\gamma = 1.2$ , and the overdrive factor  $f$  is 1.6. The calculation was started with the analytical ZND solution as initial condition. According to the classical theory for detonation instability, the above flow parameters would trigger longitudinal instability. Figure 4.1 shows the temporal evolution of the pressure level of the shock front. Twenty grid nodes per half reaction zone were used. Note that this mesh resolution is not necessary for one-dimensional calculations. This calculation is done as the benchmark for the two-dimensional calculation. The pressure trace in Fig. 4.1 compares well with Bourlioux's result [6]. Moreover, the average peak pressure is in close agreement with the value given by Fickett and Wood [2].

Based on the exactly the same flow condition, a two-dimensional simulation of a travelling detonation is calculated. Figure 4.2 shows the peak pressure history for two-dimensional detonation waves and it compares with that of the one-dimensional detonation and the analytical ZND solution at the



same flow condition. The numerical result shows that the value of peak pressure for two-dimensional structure is much higher than that of the one-dimensional case and the frequency is much higher. This plot shows the fundamental difference between the one and two-dimensional calculations of detonations.

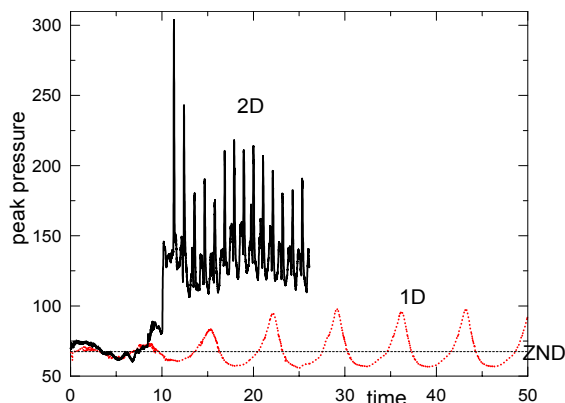


Fig. 4.2 Shock peak pressure history in one and two-dimensional detonation waves as compared to the analytical ZND solution.

In Figures 4.3-6, we present snapshots of the mass fraction, pressure, vorticity, and temperature, respectively. The width of the computational domain is 7.6 half-reaction lengths, and the height is 9.5. The mesh size is the 190x152. The grid points are distributed evenly. A periodic boundary condition is imposed along the two lateral boundaries. The detonation is traveling from bottom to top. The numerical result is plotted twice to enhance the visual interpretation. In each plot, ten snapshots are provided to show the initiation of the transverse instability and its development to the triple point shocks. The first snapshot is taken when  $t=8$ . Note that the time unit is nondimensionalized by a characteristic time period, which defined as the ratio of the reference velocity  $\sqrt{RT_0}$  to  $L_{1/2}$ . The time increment between the snapshots is 0.5. The computation is initialized by the analytical solution of the stationary ZND wave, and twenty mesh nodes are used in the half-reaction zone. No perturbation is imposed to trigger the instability. The computation was done using a regular Pentium II PC. It took about three hours to reach a stationary solution. Note that at this point, no effort was made to optimize the computational efficiency.

Similar to that in the one-dimensional detonations, the flow field is composed of: (i) the quiescent state

of the reactant before the shock, (ii) a von Neumann spike with finite rate reaction, and (iii) the equilibrium state after the reaction zone. However, due to the two-dimensional cellular structure of the detonation, the flow field is much more complex. The shock front is characterized by mushroom-shaped incident shocks interacting with a Mach stem. The width of the Mach stem changes in a periodic fashion and tremendous vortices are created during the process.

From this sequence, we can confirm the classical picture of “explosion within explosions,” sustained by the propagation of the transverse cells in the detonation front. The vorticity contours show high concentration of vortex at the triple points. At each collision of triple points, a new pair of vortices with opposite signs will be created and propagated downstream. Due to these vortices, some unburned reactant is engulfed into the flame zone and the unburned pockets behind the flame zone are created. The continuous burning of the unburned pockets behind the flame zone greatly extended the effective flame zone. In general, the flow features shown in Figs. 4.3-6 are consistent with previous reported numerical and experimental results.

## CONCLUDING REMARKS

The space-time CE/SE method was conceived from a global CFD perspective and designed to avoid the limitation of traditional methods. It was built from a foundation, which is solid in physics and yet mathematically simple enough that one can build from it a coherent, robust, and accurate CFD framework for complex flow fields.

In the present paper, the space-time CE/SE method has been extended to solve the two-dimensional detonations. All special features of this complex flow are crisply resolved, including transverse wave structure, triple points, Mach stem, counter rotating vortices, and unburned pockets. The result obtained is consistent with the previous experimental and numerical results.

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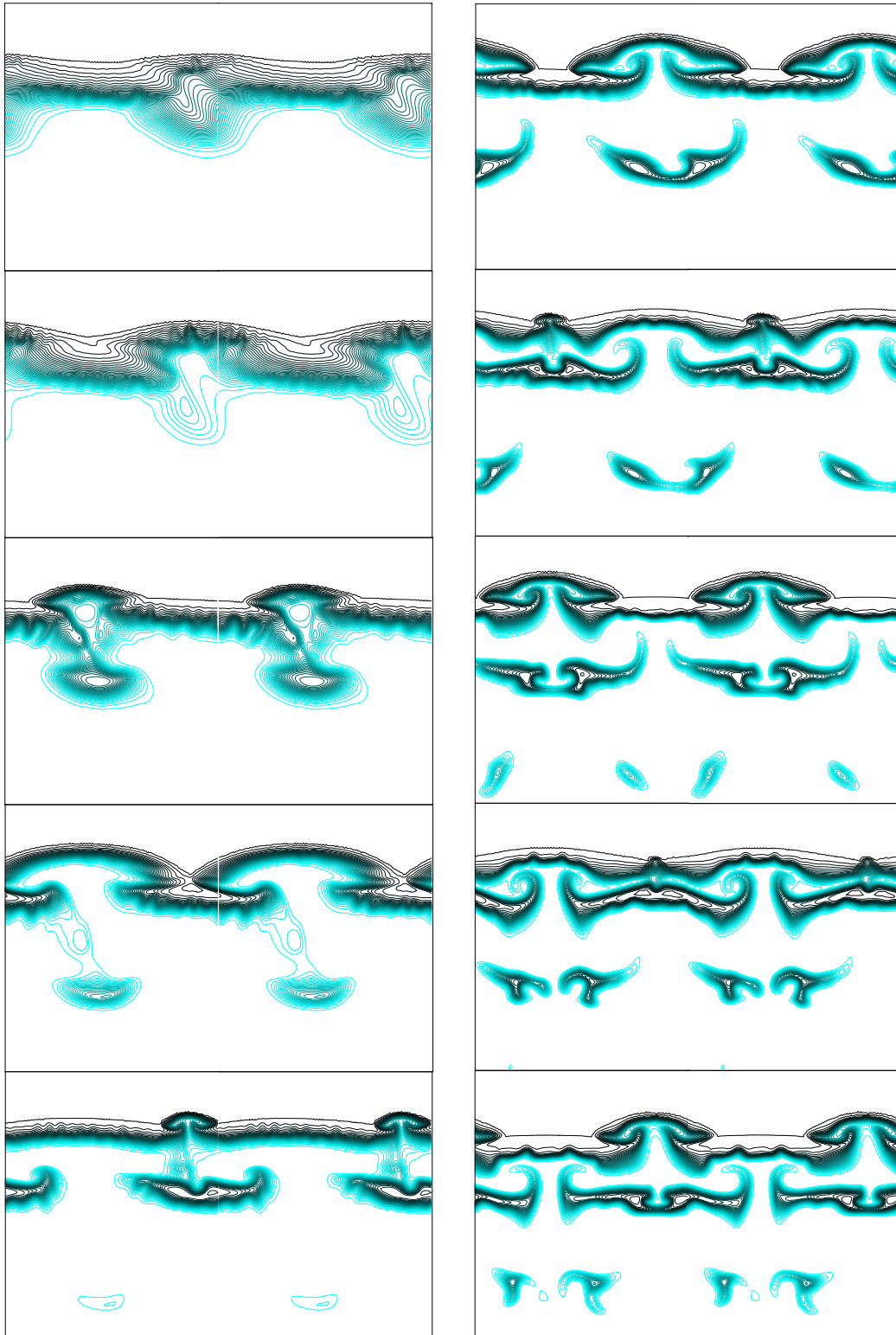


Fig. 4.4 Sequence of ten snapshots of pressure. Time increases from top left to bottom right, and shock moves upwards. The flow condition is  $E^+ = 50$ ,  $q_0 = 50$  and  $f = 1.6$ .

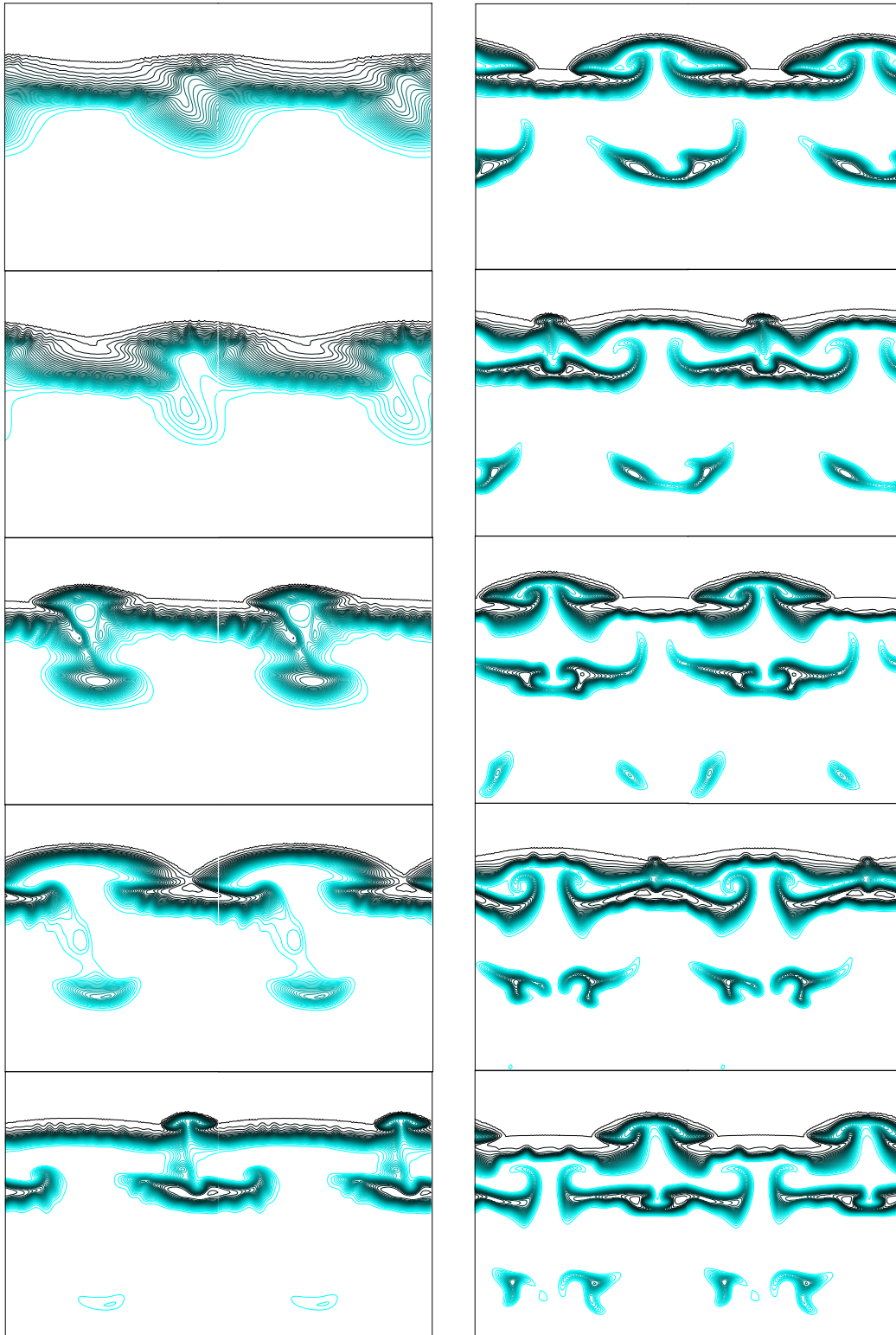


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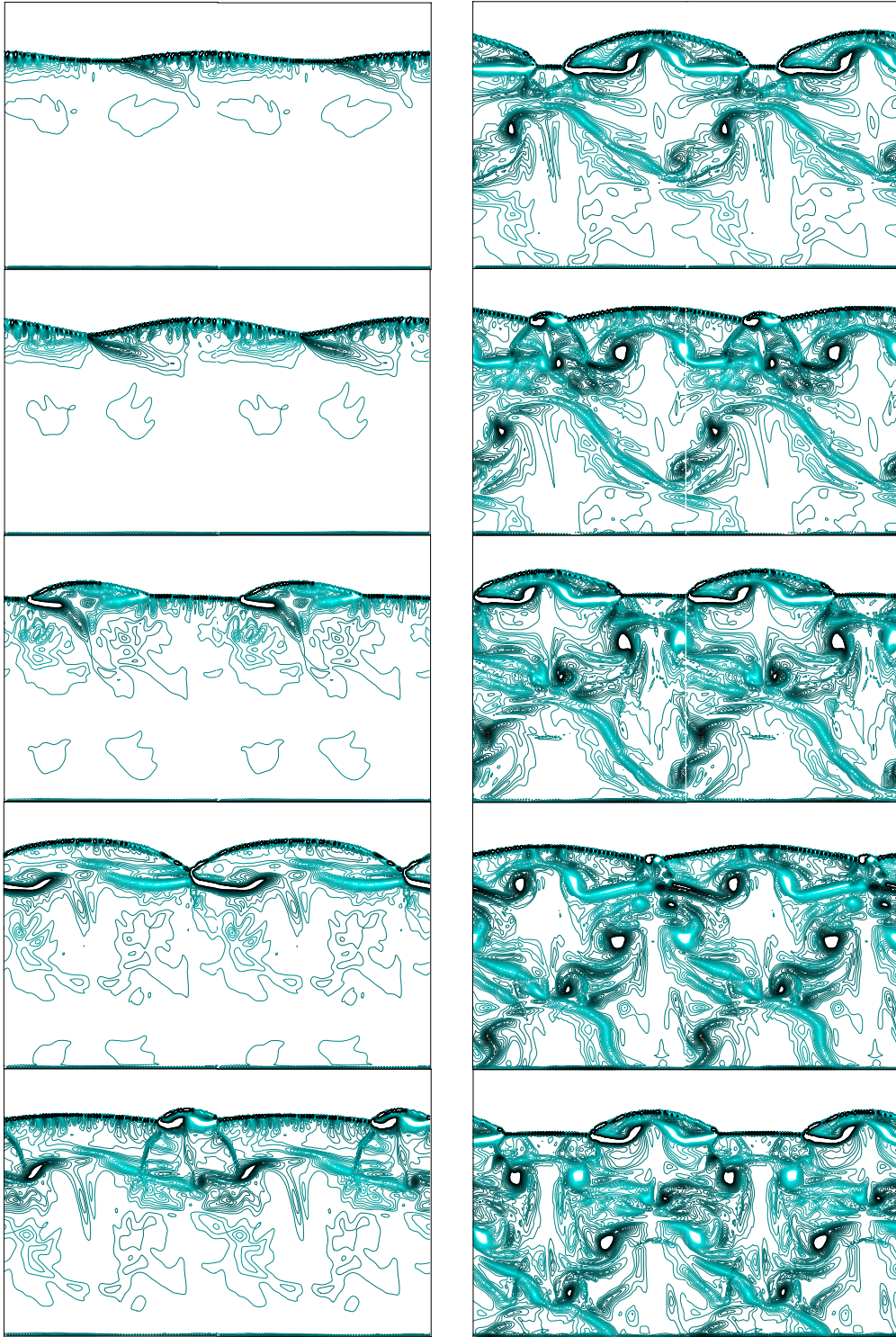


Fig. 4.5 Sequence of ten snapshots of vorticity. Time increases from top left to bottom right, and shock moves upwards. The flow condition is  $E^+ = 50$ ,  $q_0 = 50$  and  $f=1.6$ .

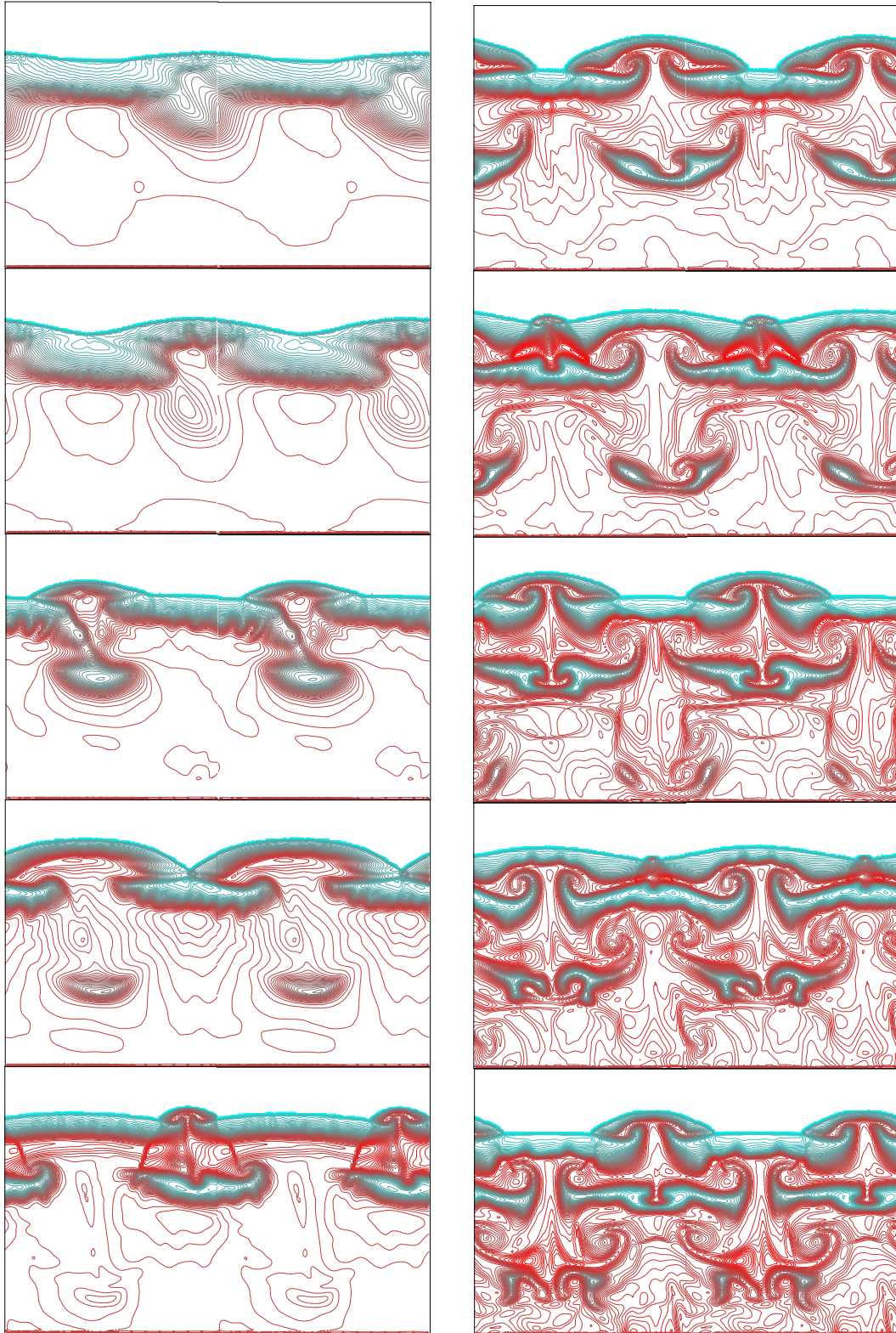


Fig. 4.6 Sequence of ten snapshots of temperature. Time increases from top left to bottom right, and shock moves upwards. The flow condition is  $E^+ = 50$ ,  $q_0 = 50$  and  $f=1.6$ .