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AN ENTROPY STABLE FINITE VOLUME METHOD FOR A COMPRESSIBLE TWO PHASE MODEL

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Abstract. We study a binary mixture of compressible viscous fluids modelled by the Navier-Stokes-Allen-Cahn system with isentropic or ideal gas law. We propose a finite volume method for the approximation of the system based on upwinding and artificial diffusion approaches. We prove the entropy stability of the numerical method and present several numerical experiments to support the theory.

Keywords: compressible Navier-Stokes-Allen-Cahn; finite volume method; entropy stability

MSC 2020: 65M12, 76N06, 76Txx

1. Introduction

Binary mixture of compressible fluids finds its wide applications in physics. Despite the existence of a rich mathematical theory of such problems [1], [2], [7], [9], the corresponding numerical analysis is far from well understood. In this paper, we are interested in a finite volume approximation of the following model in the time space cylinder $(0,T)\times\Omega$, $\Omega\subset\mathbb{R}^d$ an open and bounded domain, $d=2,3$:

$$\partial_t \varrho + \operatorname{div}_x(\varrho\mathbf{u}) = 0, \tag{1.1a}$$

$$\partial_t(\varrho\mathbf{u}) + \operatorname{div}_x(\varrho\mathbf{u}\otimes\mathbf{u}) + \nabla_x p = -\operatorname{div}_x\left(\nabla_x\chi\otimes\nabla_x\chi - \tfrac{1}{2}|\nabla_x\chi|^2\mathbb{I}\right) + \operatorname{div}_x\mathbb{S} + \nabla_x\mathcal{F}(\chi) \tag{1.1b}$$

$$\partial_t\chi + \mathbf{u}\cdot\nabla_x\chi = \Delta_x\chi - \frac{\partial\mathcal{F}(\chi)}{\partial\chi}, \tag{1.1c}$$

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where ϱ, $\mathbf{u}$ and χ represent the fluid density, velocity, and the order parameter, respectively. Moreover, $\mathcal{F} = \mathcal{F}(\chi)$ is Ginzburg-Landau potential, $\mathbb{S} = \mathbb{S}(\nabla_x \mathbf{u})$ is the viscous stress

$$\mathbb{S} = 2\mu\Big[\mathbb{D}_x\mathbf{u} - \frac{1}{d}\operatorname{div}_x \mathbf{u}\mathbb{I}\Big] + \eta \operatorname{div}_x \mathbf{u}\mathbb{I}, \quad \mathbb{D}_x\mathbf{u} = \frac{1}{2}(\nabla_x\mathbf{u} + \nabla_x^t\mathbf{u}).$$

The fluid pressure p is determined by the state equation. In this paper, we consider two variants of state equations:

Isentropic case. The pressure is a function of density:

$$p = p(\varrho) = \varrho^\gamma. \tag{1.2a}$$

Non-isothermal case. The pressure is a function of density and absolute temperature ϑ:

$$\begin{aligned} p = p(\varrho, \vartheta) = \varrho\vartheta \quad \text{with} \quad & c_v(\partial_t(\varrho\vartheta) + \operatorname{div}_x(\varrho\vartheta\mathbf{u})) - \kappa\Delta_x\vartheta \\ & = -p\operatorname{div}_x\mathbf{u} + \mathbb{S} : \mathbb{D}_x\mathbf{u} + (\Delta_x\chi - \mathcal{F}'(\chi))^2. \end{aligned} \tag{1.2b}$$

For the sake of simplicity, we suppose the no-slip boundary conditions for the velocity, together with the Neumann boundary conditions for the order parameter, i.e.,

$$\begin{aligned} \mathbf{u}|_{\partial\Omega} = 0, \quad & \nabla_x\chi \cdot \mathbf{n}|_{\partial\Omega} = 0 \text{ for the isentropic case,} \\ & \text{and in addition, } \nabla_x\vartheta \cdot \mathbf{n}|_{\partial\Omega} = 0 \text{ for the non-isothermal case.} \end{aligned} \tag{1.3}$$

To close the system we impose the initial conditions

$$\begin{aligned} (\varrho, \chi, \mathbf{u})(0) = (\varrho_0, \chi_0, \mathbf{u}_0) & \text{ with } \varrho_0 > 0 \text{ for the isentropic case} \\ & \text{and in addition, } \vartheta(0) = \vartheta_0 > 0 \text{ for the non-isothermal case.} \end{aligned} \tag{1.4}$$

1.1. Stability of the system. It is easy to check system (1.1)–(1.4) satisfies the energy balance equation

$$\frac{\mathrm{d}}{\mathrm{dt}}\int_\Omega E\,\mathrm{d}x + \int_\Omega (\mathbb{S} : \mathbb{D}_x\mathbf{u} + (\Delta_x\chi - \mathcal{F}'(\chi))^2)\,\mathrm{d}x = 0 \tag{1.5a}$$

for the isentropic case, and

$$\frac{\mathrm{d}}{\mathrm{dt}}\int_\Omega E\,\mathrm{d}x = 0 \tag{1.5b}$$

for the non-isothermal case, where E is the total energy function of the system

$$E = \begin{cases} \frac{1}{2}\varrho|\mathbf{u}|^2 + \frac{1}{2}|\nabla_x\chi|^2 + \mathcal{H}(\varrho) + \mathcal{F}(\chi) & \text{for the isentropic case,} \\ \frac{1}{2}\varrho|\mathbf{u}|^2 + \frac{1}{2}|\nabla_x\chi|^2 + c_v\varrho\vartheta + \mathcal{F}(\chi) & \text{for the non-isothermal case,} \end{cases}$$

where $\mathcal{H}(\varrho) = c_v\varrho^\gamma$ and $c_v = 1/(\gamma - 1)$.

For the isentropic case, the total energy plays the role of the mathematical entropy. When considering the non-isothermal case, the system satisfies the entropy balance

$$\frac{\mathrm{d}}{\mathrm{dt}}\int_\Omega \varrho s \,\mathrm{d}x \geqslant \int_\Omega \frac{1}{\vartheta}\Big[\mathbb{S} : \mathbb{D}_x\mathbf{u} + (\Delta_x\chi - \mathcal{F}'(\chi))^2 + \frac{\kappa|\nabla_x\vartheta|^2}{\vartheta}\Big]\,\mathrm{d}x, \tag{1.6}$$

where $s = \log(\vartheta^{c_v}/\varrho)$ is the specific entropy.

The goal of this paper is to propose a finite volume method preserving the discrete variant of the above stabilities (1.5a)–(1.6), namely the entropy/energy stability. The rest of the paper is organized as follows. In Section 2 we introduce a finite volume method for the approximation of the problem. In Section 3 we analyze the energy/entropy stability of the numerical solutions. Further, in Section 4 we validate the theoretical results by numerical experiments. Section 5 is the conclusion.

2. Numerical method

In this section we propose a finite volume method for the approximation of system (1.1)–(1.4).

Primary grid. Let Ω_h be either a regular and quasi-uniform unstructured triangulation of Ω in the sense of Ciarlet [3] or a uniform structured mesh of Ω with the following notations:

- ▷ We denote by K a generic element such that $\Omega = \bigcup_{K\in\Omega_h} K$, where in the case of unstructured mesh, K is either a triangle for $d = 2$ or a tetrahedron for $d = 3$, and in the case of structured mesh, K is either a rectangle for $d = 2$ or a cuboid for $d = 3$.
- ▷ For any element K we denote by $|K|$ its volume and by h_K its diameter. Further, we define by $h = \max_{K\in\Omega_h} h_K$ the size of the mesh.
- ▷ We denote by $\mathcal{E}$ the set of all faces, $\mathcal{E}_B$ the set of all faces on the boundary, $\mathcal{E}_I = \mathcal{E}\setminus\mathcal{E}_B$ the set of all interior faces, and $\mathcal{E}(K)$ the set of all faces of the element $K \in \Omega_h$. Further, we denote by $\sigma = K|L$ the common face of two neighbouring elements K and L.

- ▹ For each face $\sigma \in \mathcal{E}$, we denote by $|\sigma|$ its Lebesgue measure, and $\mathbf{n}$ its outer normal vector. If furthermore $\sigma \in \mathcal{E}(K)$, we write it as $\mathbf{n}_K$.
- ▹ Let $\mathbb{P}_x = \{x_K \mid x_K \in K \in \Omega_h\}$ be a set of control points such that for any $\sigma = K|L$ the segment $\overrightarrow{x_K x_L}$ is perpendicular to σ. Then we denote by d_σ the Euclidean distance between x_K and x_L for $\sigma = K|L$.

Hereafter, we call Ω_h the primary grid and introduce a dual grid for convenience of notations.

Dual grid. We denote $\mathcal{D}_h = \bigcup\limits_{\sigma \in \mathcal{E}} D_\sigma$ as the dual grid, where D_σ is the dual cell associated to the face σ. On the one hand, for any exterior face $\sigma \in \mathcal{E}(K) \cap \mathcal{E}_B$ we define its dual cell as $D_\sigma = D_{\sigma,K}$, where $D_{\sigma,K}$ is the domain obtained by connecting the control point x_K with the $(d-1)$ vertices of σ. On the other hand, for any interior face $\sigma = K_1|K_2 \in \mathcal{E}_I$ we define $D_\sigma = D_{\sigma,K_1} \cup D_{\sigma,K_2}$.

Remark 2.1. For a uniform structured mesh, $\mathbb{P}_x$ can be chosen as the barycenters. Concerning unstructured, we refer to VanderZee et al. [10] for the discussion of a well-centered mesh, where the control points are chosen as the circumcenters.

For a piecewise (elementwise) continuous function v we define

$$v^{\mathrm{in}}(x) = \lim_{\delta \to 0+} v(x - \delta \mathbf{n}) \quad \forall\, x \in \sigma \in \mathcal{E} \text{ and } v^{\mathrm{out}}(x) = \lim_{\delta \to 0+} v(x + \delta \mathbf{n}) \quad \forall\, x \in \sigma \in \mathcal{E}_I.$$

Moreover, for $x \in \sigma \in \mathcal{E}_B$ we specify $v^{\mathrm{out}}(x)$ according to the boundary conditions:

$$v^{\mathrm{out}} = \begin{cases} v^{\mathrm{in}} & \text{for no flux condition, s.t. } [\![v]\!] = 0, \\ -v^{\mathrm{in}} & \text{for zero-Dirichlet condition, s.t. } \{\{v\}\} = 0, \end{cases}$$

where

$$\{\{v\}\}(x) = \frac{v^{\mathrm{in}}(x) + v^{\mathrm{out}}(x)}{2}, \quad [\![v]\!](x) = v^{\mathrm{out}}(x) - v^{\mathrm{in}}(x).$$

Function spaces. We define Q_h and W_h, respectively, as the space of piecewise constant functions on the primary grid Ω_h and the dual grid $\mathcal{D}_h$. Moreover, we mean by $\mathbf{v} \in \mathbf{Q}_h$ (or $\mathbf{v} \in \mathbf{W}_h$) that $\mathbf{v} \in Q_h(\Omega; R^d)$ (or $\mathbf{v} \in W_h(\Omega; R^d)$), i.e., $v_i \in Q_h$ (or $v_i \in W_h$) for all $i = 1, \ldots, d$. The interpolation operator associated to Q_h reads

$$\Pi_Q \varphi = \sum_{K \in \Omega_h} \frac{1_K(x)}{|K|} \int_K \varphi \, \mathrm{d}x, \quad 1_K(x) = \begin{cases} 1 & \text{if } x \in K, \\ 0 & \text{otherwise.} \end{cases}$$

Diffusive upwind flux. Given the velocity field $\mathbf{v} \in \mathbf{Q}_h$, the upwind flux for any function $r \in Q_h$ is specified at each face $\sigma \in \mathcal{E}$ by

$$\mathrm{Up}[r,\mathbf{v}]|_\sigma = r^{\mathrm{up}} \mathbf{v}_\sigma \cdot \mathbf{n} = r^{\mathrm{in}} [\mathbf{v}_\sigma \cdot \mathbf{n}]^+ + r^{\mathrm{out}} [\mathbf{v}_\sigma \cdot \mathbf{n}]^- = \{\{r\}\} \mathbf{v}_\sigma \cdot \mathbf{n} - \frac{1}{2} |\mathbf{v}_\sigma \cdot \mathbf{n}| [\![r]\!],$$

where

$$\mathbf{v}_\sigma = \{\{\mathbf{v}\}\}|_\sigma, \quad [f]^\pm = \frac{f \pm |f|}{2} \quad \text{and} \quad r^{\mathrm{up}} = \begin{cases} r^{\mathrm{in}} & \text{if } \mathbf{v}_\sigma \cdot \mathbf{n} \geqslant 0, \\ r^{\mathrm{out}} & \text{if } \mathbf{v}_\sigma \cdot \mathbf{n} < 0. \end{cases}$$

Furthermore, we consider a diffusive numerical flux function of the form

$$F_\varepsilon^{\mathrm{up}}(r,\mathbf{v}) = \mathrm{Up}[r,\mathbf{v}] - h^\varepsilon [\![r]\!], \quad \varepsilon > -1. \tag{2.1}$$

Discrete operators. For piecewise constant functions we define the discrete gradient, divergence and Laplace operators elementwisely on the primary grid as

$$\begin{aligned}
\nabla_h r_h(x) &= \sum_{K \in \Omega_h} (\nabla_h r_h)_K 1_K(x), & (\nabla_h r_h)_K &= \sum_{\sigma \in \mathcal{E}(K)} \frac{|\sigma|}{|K|} \{\{r_h\}\} \mathbf{n}, \\
\mathrm{div}_h \mathbf{v}_h(x) &= \sum_{K \in \Omega_h} (\mathrm{div}_h \mathbf{v}_h)_K 1_K(x), & (\mathrm{div}_h \mathbf{v}_h)_K &= \sum_{\sigma \in \mathcal{E}(K)} \frac{|\sigma|}{|K|} \{\{\mathbf{v}_h\}\} \cdot \mathbf{n}, \\
\Delta_h r_h(x) &= \sum_{K \in \Omega_h} (\Delta_h r_h)_K 1_K(x), & (\Delta_h r_h)_K &= \sum_{\sigma \in \mathcal{E}(K)} \frac{|\sigma|}{|K|} \frac{[\![r_h]\!]}{d_\sigma}
\end{aligned}$$

for any $r_h \in Q_h$ and $\mathbf{v}_h \in \mathbf{Q}_h$. Further, we define discrete difference operator that involves the dual grid. For any $r_h \in Q_h$ and $\mathbf{q} \in \mathbf{W}_h$ we define

$$\nabla_{\mathcal{E}} r_h(x) = \sum_{\sigma \in \mathcal{E}} 1_{D_\sigma} (\nabla_{\mathcal{E}} r_h)_{D_\sigma}, \quad (\nabla_{\mathcal{E}} r_h)_{D_\sigma} := \sqrt{d} \frac{[\![r]\!]}{d_\sigma} \mathbf{n} \quad \forall\, \sigma \in \mathcal{E}_I.$$

It is easy to check for any $r_h, \varphi_h \in Q_h$ that

$$\begin{aligned}
\int_\Omega \Delta_h r_h \varphi_h \,\mathrm{d}x &= -\int_{\mathcal{E}_I} \frac{1}{d_\sigma} [\![r_h]\!] [\![\varphi_h]\!] \,\mathrm{d}S_x \\
&= -\int_\Omega \nabla_{\mathcal{E}} r_h \cdot \nabla_{\mathcal{E}} \varphi_h \,\mathrm{d}x \quad \text{if } [\![r_h]\!]_\sigma = 0 \quad \forall\, \sigma \in \mathcal{E}_B.
\end{aligned} \tag{2.2}$$

Time discretization. For a given time step $\Delta t > 0$, we denote the approximation of a generic discrete function v_h at time $t^k = k\Delta t$ by v_h^k for $k = 1, \ldots, N_T (= T/\Delta t)$, and define

$$D_t v_h^k = \frac{v_h^k - v_h^{k-1}}{\Delta t}.$$

2.1. A finite volume method. Now we introduce a finite volume (FV) method for the approximation of phase field model (1.1)–(1.4). First, we consider the isentropic case (1.2a).

Scheme A: An FV method for the isentropic model.

Let $(\varrho_h^0, \mathbf{u}_h^0, \chi_h^0) = (\Pi_Q \varrho_0, \Pi_Q \chi_0, \Pi_Q \mathbf{u}_0)$. Given $(\varrho_h^{k-1}, \chi_h^{k-1}, \mathbf{u}_h^{k-1}) \in Q_h \times Q_h \times \mathbf{Q}_h$ for any $k = 1, \dots, N_T$, we say that the triple $(\varrho_h^k, \chi_h^k, \mathbf{u}_h^k) \in Q_h \times Q_h \times \mathbf{Q}_h$ is an FV approximation of the Navier-Stokes-Allen-Cahn system (1.1), (1.2a), (1.3)–(1.4) at time t^k if the following system of algebraic equations holds:

$$\int_\Omega D_t \varrho_h^k \varphi_h \,\mathrm{d}x - \int_{\mathcal{E}} F_\varepsilon^{\mathrm{up}}(\varrho_h^k, \mathbf{u}_h^k) [\![\varphi_h]\!] \,\mathrm{d}S_x = 0 \quad \forall \varphi_h \in Q_h; \tag{2.3a}$$

$$\begin{aligned} \int_\Omega D_t(\varrho_h^k \mathbf{u}_h^k) \cdot \boldsymbol{\varphi}_h \,\mathrm{d}x &- \int_{\mathcal{E}} F_\varepsilon^{\mathrm{up}}(\varrho_h^k \mathbf{u}_h^k, \mathbf{u}_h^k) \cdot [\![\boldsymbol{\varphi}_h]\!] \,\mathrm{d}S_x \\ &+ \int_\Omega (2\mu \mathbb{D}_h \mathbf{u}_h^k : \nabla_h \boldsymbol{\varphi}_h + \lambda \mathrm{div}_h \mathbf{u}_h^k \mathrm{div}_h \boldsymbol{\varphi}_h) \,\mathrm{d}x \\ &= \int_\Omega p_h^k \mathrm{div}_h \boldsymbol{\varphi}_h \,\mathrm{d}x \\ &+ \int_\Omega (f_h^k - \Delta_h \chi_h^k) \nabla_h \chi_h^k \cdot \boldsymbol{\varphi}_h \,\mathrm{d}x \quad \forall \boldsymbol{\varphi}_h \in \mathbf{Q}_h, \end{aligned} \tag{2.3b}$$

$$\int_\Omega (D_t \chi_h^k + \mathbf{u}_h^k \cdot \nabla_h \chi_h^k) \psi_h \,\mathrm{d}x = \int_\Omega (\Delta_h \chi_h^k - f_h^k) \psi_h \,\mathrm{d}x \quad \forall \psi_h \in Q_h; \tag{2.3c}$$

where $p_h^k = (\varrho_h^k)^\gamma$, $\mathbb{D}_h \mathbf{u}_h = (\nabla_h \mathbf{u}_h + \nabla_h^t \mathbf{u}_h)/2$, $\lambda = \eta - 2\mu/d$, and the approximation of $\mathcal{F}'$ follows the so-called convex-concave splitting technique

$$f_h^k = \mathcal{F}_a'(\chi_h^k) + \mathcal{F}_b'(\chi_h^{k-1}), \tag{2.4}$$

where $\mathcal{F}_a$ and $\mathcal{F}_b$ are the convex and concave part of $\mathcal{F}$, respectively.

Further, we propose an FV method for the non-isothermal case (1.2b).

Scheme B: An FV method for the non-isothermal model.

Let $(\varrho_h^0, \vartheta_h^0, \mathbf{u}_h^0, \chi_h^0) = (\Pi_Q \varrho_0, \Pi_Q \vartheta_0, \Pi_Q \chi_0, \Pi_Q \mathbf{u}_0)$. Given $(\varrho_h^{k-1}, \vartheta_h^{k-1}, \chi_h^{k-1}, \mathbf{u}_h^{k-1}) \in Q_h \times Q_h \times Q_h \times \mathbf{Q}_h$ for any $k = 1, \dots, N_T$, we say that the quadruple $(\varrho_h^k, \vartheta_h^k, \chi_h^k, \mathbf{u}_h^k) \in Q_h \times Q_h \times Q_h \times \mathbf{Q}_h$ is an FV approximation of the Navier-Stokes-Allen-Cahn system (1.1), (1.2b), (1.3)–(1.4) at time t^k if it satisfies (2.3) and

$$\begin{aligned} c_v \int_{\Omega_h} D_t(\varrho_h^k \vartheta_h^k) \varphi_h \,\mathrm{d}x - c_v \int_{\mathcal{E}_I} F_\varepsilon^{\mathrm{up}}(\varrho_h^k \vartheta_h^k, \mathbf{u}_h^k) [\![\varphi_h]\!] \,\mathrm{d}S_x + \int_{\mathcal{E}_I} \frac{\kappa}{d_\sigma} [\![\vartheta_h^k]\!] [\![\varphi_h]\!] \,\mathrm{d}S_x \\ = \int_{\Omega_h} (\mathbb{S}(\nabla_h \mathbf{u}_h^k) : \nabla_h \mathbf{u}_h^k - p_h^k \mathrm{div}_h \mathbf{u}_h^k + |\Delta_h \chi_h^k - f_h^k|^2) \varphi_h \,\mathrm{d}x \quad \forall \varphi_h \in Q_h. \end{aligned} \tag{2.5}$$

Here, f_h is the same as in scheme A, and the discrete pressure is defined as $p_h = \varrho_h \vartheta_h$ for $\vartheta_h \geqslant 0$ with an extension to the non-physical regime for $\vartheta_h < 0$ that $p_h(\varrho_h, \vartheta_h) = 0$.

3. Stability

In this section we show the stability of the FV schemes. Before that we recall some important properties satisfied by our numerical approximation. First, we recall from [5] that the density scheme (2.3a) satisfies the positivity of density and conservation of mass.

Lemma 3.1 (Positivity of density and conservation of mass). *Let* $(\varrho_h, \mathbf{u}_h)$ *satisfy* (2.3a) *with* $\varrho_0 > 0$. *Then for any* $t \in (0, T)$,

$$\varrho_h(t, x) > 0 \quad \forall\, x \in \Omega \quad \textit{and} \quad \int_\Omega \varrho_h(t) \,\mathrm{d}x = \int_\Omega \varrho_0 \,\mathrm{d}x.$$

Next, we test the density scheme (2.3a) by $\varphi_h = \mathcal{H}'(\varrho_h^k)$, and find the following lemma, see [5], Lemma 11.2.

Lemma 3.2 (Discrete renormalized continuity equation). *Let* $(\varrho_h^k, \mathbf{u}_h^k) \in Q_h \times \mathbf{Q}_h$ *satisfy the discrete continuity equation* (2.3a) *for any* $k \in \{1, \ldots, N_T\}$. *Then there exist* $\varrho_\xi^k \in \mathrm{co}\{\varrho_h^{k-1}, \varrho_h^k\}$ *and* $\varrho_\zeta^k \in \mathrm{co}\{\varrho_K^k, \varrho_L^k\}$ *for any* $\sigma = K|L \in \mathcal{E}_I$ *such that*

(3.1)

$$\begin{aligned}&\int_\Omega D_t \mathcal{H}(\varrho_h^k) \,\mathrm{d}x + \int_\Omega (\varrho_h^k)^\gamma \mathrm{div}_h \mathbf{u}_h^k \,\mathrm{d}x \\ &\quad = -\frac{\Delta t}{2} \int_\Omega \mathcal{H}''(\varrho_\xi^k) |D_t \varrho_h^k|^2 \,\mathrm{d}x - \int_{\mathcal{E}_I} \mathcal{H}''(\varrho_\zeta^k) [\![\varrho_h^k]\!]^2 \Big(h^\varepsilon + \frac{1}{2} |\mathbf{u}_\sigma^k \cdot \mathbf{n}|\Big) \,\mathrm{d}S_x \leqslant 0.\end{aligned}$$

Note that $\mathrm{co}\{a, b\} = [\min\{a, b\}, \max\{a, b\}]$. Further, we report the positivity of the temperature, see [6], Lemma 3.5.

Lemma 3.3 (Positivity of temperature). *Let* $(\varrho_h, \vartheta_h, \chi_h, \mathbf{u}_h)$ *satisfy* (2.5) *with* $\varrho_0 > 0, \vartheta_0 > 0$. *Then for any* $t \in (0, T)$,

$$\vartheta_h(t, x) > 0 \quad \forall\, x \in \Omega.$$

Theorem 3.4 (Existence of numerical solution). *For every* $k = 1, \ldots, N_T$, *there exist a solution* $(\varrho_h^k, \chi_h^k, \mathbf{u}_h^k) \in Q_h \times Q_h \times \mathbf{Q}_h$ *to the FV method scheme A, and a solution* $(\varrho_h^k, \vartheta_h^k, \chi_h^k, \mathbf{u}_h^k) \in Q_h \times Q_h \times Q_h \times \mathbf{Q}_h$ *to the FV method scheme B*

The proof can be done analogously as [5], Lemma 11.3.

3.1. Stability of Scheme A.

Here we derive the energy stability of Scheme A for compressible Navier-Stokes-Allen-Cahn system with isentropic state equation (1.2a).

Theorem 3.5 (Discrete energy balance). *Let $(\varrho_h, \chi_h, \mathbf{u}_h)$ be a solution of the FV method* (2.3). *Then we have the energy estimate*

$$
\begin{aligned}
(3.2)\qquad D_t \int_\Omega \Big(\frac{1}{2}\varrho_h^k |\mathbf{u}_h|^2 + \mathcal{H}(\varrho_h^k) + F(\chi_h^k) + \frac{1}{2}|\nabla_{\mathcal{E}}\chi_h|^2\Big)\,\mathrm{d}x \\
+ 2\mu\|\mathbb{D}_h \mathbf{u}_h^k\|_{L^2}^2 + \lambda\|\mathrm{div}_h \mathbf{u}_h^k\|_{L^2}^2 + \|\Delta_h \chi_h^k - f_h^k\|_{L^2}^2 = -D_A^k,
\end{aligned}
$$

where $D_A^k \geqslant 0$ is the numerical dissipation

$$
\begin{aligned}
D_A^k = {} & \frac{\Delta t}{2}\int_{\Omega_h} (\varrho_h^{k-1}|D_t \mathbf{u}_h^k|^2 + (\mathcal{F}_a'(\chi_\xi^k) - \mathcal{F}_b'(\chi_\zeta^k))|D_t\chi_h^k|^2 + |\nabla_{\mathcal{E}} D_t \chi_h^k|^2)\,\mathrm{d}x \\
& + \frac{\Delta t}{2}\int_\Omega \mathcal{H}''(\varrho_\xi^k)|D_t\varrho_h^k|^2\,\mathrm{d}x + \int_{\mathcal{E}_I}\mathcal{H}''(\varrho_\zeta^k)[\![\varrho_h^k]\!]^2\Big(h^\varepsilon + \frac{1}{2}|\{\{\mathbf{u}_h^k\}\}\cdot\mathbf{n}|\Big)\,\mathrm{d}S_x \\
& + \int_{\mathcal{E}_I}\Big(h^\varepsilon\{\{\varrho_h^k\}\} + \frac{1}{2}\varrho_h^{k,\mathrm{up}}|\{\{\mathbf{u}_h^k\}\}\cdot\mathbf{n}|\Big)|[\![\mathbf{u}_h^k]\!]|^2\,\mathrm{d}S_x,
\end{aligned}
$$

where χ_ξ^k, $\chi_\zeta^k \in \mathrm{co}\{\chi_h^{k-1}, \chi_h^k\}$.

Proof. First, we sum up (2.3a) and (2.3b) with $\varphi_h = -\frac{1}{2}|\mathbf{u}_h^k|^2 \in Q_h$ and $\boldsymbol{\varphi}_h = \mathbf{u}_h^k \in \mathbf{Q}_h$ to get the kinetic energy balance

$$
\begin{aligned}
(3.3)\qquad D_t\int_{\Omega_h}\frac{1}{2}\varrho_h^k|\mathbf{u}_h^k|^2\,\mathrm{d}x + \frac{\Delta t}{2}\int_{\Omega_h}\varrho_h^{k-1}|D_t\mathbf{u}_h^k|^2\,\mathrm{d}x \\
+ \int_{\mathcal{E}_I}\Big(h^\varepsilon\{\{\varrho_h^k\}\} + \frac{1}{2}\varrho_h^{k,\mathrm{up}}|\{\{\mathbf{u}_h^k\}\}\cdot\mathbf{n}|\Big)|[\![\mathbf{u}_h^k]\!]|^2\,\mathrm{d}S_x \\
+ 2\mu\|\mathbb{D}_h\mathbf{u}_h^k\|_{L^2}^2 + \lambda\|\mathrm{div}_h\mathbf{u}_h^k\|_{L^2}^2 \\
= \int_{\Omega_h}(\varrho_h^k)^\gamma \mathrm{div}_h\mathbf{u}_h^k\,\mathrm{d}x + \int_{\Omega_h}(f_h^k - \Delta_h\chi_h^k)\nabla_h\chi_h^k\cdot\mathbf{u}_h^k\,\mathrm{d}x,
\end{aligned}
$$

see, e.g. [4], eq. 3.4 for more details.

Next, by choosing $\psi_h = (\Delta_h\chi_h^k - f_h^k) \in Q_h$ in (2.3c) we derive

$$
\begin{aligned}
(3.4)\qquad \int_{\Omega_h}(\Delta_h\chi_h^k - f_h^k)^2\,\mathrm{d}x &= \int_\Omega\Big(\Delta_h\chi_h^k - f_h^k\Big)(D_t\chi_h^k + \mathbf{u}_h^k\cdot\nabla_h\chi_h^k)\,\mathrm{d}x \\
&= -D_t\int_\Omega\frac{1}{2}|\nabla_{\mathcal{E}}\chi_h^k|^2\,\mathrm{d}x - \frac{\Delta t}{2}\int_\Omega|\nabla_{\mathcal{E}}D_t\chi_h^k|^2\,\mathrm{d}x \\
&\quad - D_t\int_{\Omega_h}\mathcal{F}(\chi_h^k)\,\mathrm{d}x \\
&\quad - \frac{\Delta t}{2}\int_{\Omega_h}(\mathcal{F}_a''(\chi_\xi^k) - \mathcal{F}_b''(\chi_\zeta^k))|D_t\chi_h^k|^2\,\mathrm{d}x \\
&\quad + \int_\Omega(\Delta_h\chi_h^k - f_h^k)\mathbf{u}_h^k\cdot\nabla_h\chi_h^k\,\mathrm{d}x,
\end{aligned}
$$

where χ_ξ^k, $\chi_\zeta^k \in \mathrm{co}\{\chi_h^{k-1}, \chi_h^k\}$. Finally, summing up (3.3) and (3.4) together with (3.1) completes the proof. $\square$

3.2. Stability of Scheme B. Considering the compressible Navier-Stokes-Allen-Cahn system with non-isothermal state equation (1.2b), its stability includes not only the energy stability but also the entropy stability. First, we derive the energy stability of Scheme B.

Theorem 3.6 (Energy stability)**.** *Let $(\varrho_h, \vartheta_h, \chi_h, \mathbf{u}_h)$ be a solution of scheme B. Then*

$$D_t \int_{\Omega_h} \Big(\frac{1}{2}\varrho_h^k |\mathbf{u}_h|^2 + c_v \varrho_h^k \vartheta_h^k + F(\chi_h^k) + \frac{1}{2}|\nabla \varepsilon \chi_h^k|^2\Big)\,\mathrm{d}x = -D_B^k, \tag{3.5}$$

where $D_B^k \geqslant 0$ is the numerical dissipation

$$\begin{aligned} D_B^k = \frac{\Delta t}{2}\int_{\Omega_h} &(\varrho_h^{k-1}|D_t \mathbf{u}_h^k|^2 + (\mathcal{F}_a''(\chi_\xi^k) - \mathcal{F}_b''(\chi_\zeta^k))|D_t\chi_h^k|^2 + |\nabla\varepsilon D_t \chi_h^k|^2)\,\mathrm{d}x \\ &+ \int_{\mathcal{E}_I} \Big(h^\varepsilon \{\{\varrho_h^k\}\} + \frac{1}{2}\varrho_h^{k,\mathrm{up}} |\{\{\mathbf{u}_h^k\}\}\cdot \mathbf{n}|\Big) |[[\mathbf{u}_h^k]]|^2\,\mathrm{d}S_x, \end{aligned}$$

where $\chi_\xi^k, \chi_\zeta^k \in \mathrm{co}\{\chi_h^{k-1}, \chi_h^k\}$.

P r o o f. First, following the proof of Theorem 3.5, we set $\varphi_h = -\frac{1}{2}|\mathbf{u}_h^k|^2 Q_h$ in (2.3a), $\boldsymbol{\varphi}_h = \mathbf{u}_h^k \in \mathbf{Q}_h$ in (2.3b) and $\psi_h = (\Delta_h \chi_h^k - f_h^k) \in Q_h$ in (2.3c) to get

$$\begin{aligned} D_t \int_{\Omega_h} \frac{1}{2}\varrho_h^k |\mathbf{u}_h^k|^2\,\mathrm{d}x + \frac{\Delta t}{2}\int_{\Omega_h} \varrho_h^{k-1}|D_t\mathbf{u}_h^k|^2\,\mathrm{d}x + 2\mu\|\mathbb{D}_h \mathbf{u}_h^k\|_{L^2}^2 \\ + \lambda\|\mathrm{div}_h \mathbf{u}_h^k\|_{L^2}^2 + \|\Delta_h\chi_h^k - f_h^k\|_{L^2}^2 \\ = \int_{\Omega_h} p_h^k \mathrm{div}_h \mathbf{u}_h^k\,\mathrm{d}x - D_t\int_{\Omega} \frac{1}{2}|\nabla\varepsilon\chi_h^k|^2\,\mathrm{d}x \\ - \frac{\Delta t}{2}\int_{\Omega} |\nabla \varepsilon D_t \chi_h^k|^2\,\mathrm{d}x - D_t \int_{\Omega_h} \mathcal{F}(\chi_h^k)\,\mathrm{d}x \\ - \frac{\Delta t}{2}\int_{\Omega_h} \Big(\mathcal{F}_a''(\chi_\xi^k) - \mathcal{F}_b''(\chi_\zeta^k)\Big)|D_t\chi_h^k|^2\,\mathrm{d}x \\ - \int_{\mathcal{E}_I} \Big(h^\varepsilon\{\{\varrho_h^k\}\} + \frac{1}{2}\varrho_h^{k,\mathrm{up}}|\{\{\mathbf{u}_h^k\}\}\cdot\mathbf{n}|\Big)|[[\mathbf{u}_h^k]]|^2\,\mathrm{d}S_x. \end{aligned} \tag{3.6}$$

Next, by setting $\varphi_h = 1 \in Q_h$ in (2.5) we obtain

$$D_t \int_{\Omega_h} c_v \varrho_h^k \vartheta_h^k\,\mathrm{d}x = \int_{\Omega_h} (\mathbb{S}(\nabla_h \mathbf{u}_h^k) : \nabla_h \mathbf{u}_h^k - p_h(\varrho_h^k, \vartheta_h^k)\mathrm{div}_h \mathbf{u}_h^k)\,\mathrm{d}x + \|\Delta_h\chi_h^k - f_h^k\|_{L^2}^2. \tag{3.7}$$

Further, summing up (3.6) and (3.7) yields the desired result. $\square$

Next, following [6], Theorem 3.7 we report the entropy inequality for Scheme B.

Lemma 3.7 (Entropy inequality). *Let $(\varrho_h, \vartheta_h, \chi_h, \mathbf{u}_h)$ be a solution of Scheme B. Then*

$$
\begin{aligned}
(3.8) \qquad D_t \int_\Omega \varrho_h^k s_h^k \,\mathrm{d}x = &- \int_\Omega \kappa \nabla_{\mathcal{E}} \vartheta_h^k \cdot \nabla_{\mathcal{E}} \Big(\frac{1}{\vartheta_h^k}\Big) \,\mathrm{d}x \\
&+ \int_\Omega \frac{1}{\vartheta_h^k} (2\mu |\mathbb{D}_h(\mathbf{u}_h^k)|^2 + \lambda |\mathrm{div}_h \mathbf{u}_h^k|^2) \,\mathrm{d}x \\
&+ \int_{\Omega_h} \frac{1}{\vartheta_h^k} (\Delta_h \chi_h^k - f_h^k)^2 \,\mathrm{d}x + D_S^k \\
\geqslant &\ 0,
\end{aligned}
$$

where

$$
\begin{aligned}
D_S^k = &\frac{\Delta t}{2\xi_{\varrho,h}^k} |D_t \varrho_h^k|^2 + \frac{h}{2\eta_{\varrho,h}^k} |\nabla_{\mathcal{E}} \varrho_h^k|^2 |\overline{\mathbf{u}_h^k} \cdot \mathbf{n}| + \frac{c_v \Delta t}{2|\xi_{\vartheta,h}^k|^2} \varrho_h^{k-1} |D_t \vartheta_h^k|^2 \\
&- \frac{c_v h}{2|\eta_{\vartheta,h}^k|^2} |\nabla_{\mathcal{E}} \vartheta_h^k|^2 (\varrho_h^k)^{\mathrm{out}} [\overline{\mathbf{u}_h^k} \cdot \mathbf{n}]^- + h^{\varepsilon+1} \nabla_{\mathcal{E}} \varrho_h^k \cdot \nabla_{\mathcal{E}} (\nabla_\varrho (-\varrho_h^k s_h^k)) \\
&+ h^{\varepsilon+1} \nabla_{\mathcal{E}} p_h^k \cdot \nabla_{\mathcal{E}} (\nabla_p (-\varrho_h^k s_h^k)) \\
\geqslant &\ 0
\end{aligned}
$$

where $\xi_{\varrho_h}^k \in \mathrm{co}\{\varrho_h^{k-1}, \varrho_h^k\}$, $\xi_{\vartheta_h}^k \in \mathrm{co}\{\vartheta_h^{k-1}, \vartheta_h^k\}$, and $\eta_{\varrho_h}^k \in \mathrm{co}\{\varrho_h^{k,\mathrm{in}}, \varrho_h^{k,\mathrm{out}}\}$, $\eta_{\vartheta_h}^k \in \mathrm{co}\{\vartheta_h^{k,\mathrm{in}}, \vartheta_h^{k,\mathrm{out}}\}$ for any $\sigma \in \mathcal{E}$.

Remark 3.8. The inequality in Lemma 3.7 implies that the total (physical) entropy is non-decreasing. Hereafter we refer to the above inequality as entropy stability.

4. Numerical experiments

In our experiments, we consider the computational domain to be $\Omega = [-1, 1]^2$, divided into 80^2 uniform squares. To solve the nonlinear schemes, we use the fix-point iteration method and solve an explicit and linear system at each sub-iteration, which requires the so-called CFL condition. To fulfill this condition, we take a small time step $\Delta t = 10^{-4}$. The potential function $\mathcal{F}(\chi)$ and its discrete derivative f_h denoted in (2.4) are respectively taken as

$$
\mathcal{F}(\chi) = \frac{1}{4}(\chi^2 - 1)^2 \quad \text{and} \quad f_h^k = (\chi_h^k)^3 - \chi_h^{k-1}.
$$

4.1. Experiment 1—barotropic case. In this experiment, we consider the barotropic case. Initially, one of the fluids occupies two circular areas located at $x_l = (-0.12, 0)$ and $x_r = (0.1, 0)$ of the radii 0.08 and 0.1, respectively, while the other fluid stays in the rest of the domain. The initial data read

$$\mathbf{u} = 0, (\varrho_0, \chi_0) = \begin{cases} (\varrho_1, 1) & \text{if } |x - x_l| < 0.08 \text{ or } |x - x_r| < 0.12, \\ (\varrho_2, 0) & \text{otherwise,} \end{cases}$$

$$(\varrho_1, \varrho_2) = \begin{cases} (1, 1) & \text{Case A,} \\ (1, 2) & \text{Case B,} \\ (2, 1) & \text{Case C.} \end{cases}$$

In Figure 1 we present the time evolution of the total mass and energy, which clearly supports the conservation of mass and stability of energy. Further, we show the time evolution of ϱ and χ in Figure 2 and Figure 3, respectively.

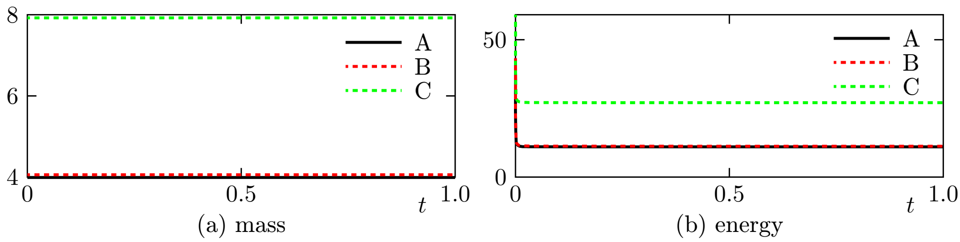


Figure 1. Time evolution of the total mass and energy.

Experiment 2—Non-isothermal case. In this experiment, we consider the non-isothermal case. Analogously to experiment 1, one of the fluids occupies two circular areas located at $x_l = (-0.12, 0)$ and $x_r = (0.1, 0)$ of the radii 0.08 and 0.1, respectively, while the other fluid stays in the rest of the domain. We take the initial data for density, velocity and order parameter, and moreover $\vartheta_0 = 1$.

In Figure 4 we present the time evolution of the total mass, energy and entropy, which clearly supports the conservation of mass and stability of energy, and entropy. Further, we show the time evolution of ϱ_h and χ_h and ϑ_h in Figures 5–7, respectively.

5. Conclusion

In this paper, we have studied the compressible Navier-Stokes-Allen-Cahn system with both isentropic gas law and ideal gas law. By using central difference, upwinding, and artificial diffusion techniques, we have proposed a finite volume method. We have shown that the finite volume method is entropy stable for both isentropic and ideal gas laws. We have also validated the theoretical results by numerical experiments.

R e m a r k 5.1. Here we open a few technical discussions.

▷ We point out that the artificial diffusion term $h^{\varepsilon}[\![r_h]\!]$ is not necessary for the proof of stability, but plays an important role if one wants to show the consistency of the methods, see [5]. Indeed, when setting $\varepsilon = \infty$, we have $h^{\varepsilon} = 0$ and the diffusive flux $F_{\varepsilon}^{\rm up}$ defined in (2.1) becomes the standard upwind flux.

▷ The current paper can be viewed as the preceding chapter of the convergence analysis of the method, see our recent work on the barotropic Navier-Stokes-Allen-Cahn [8] and Navier-Stokes-Fourier [6].

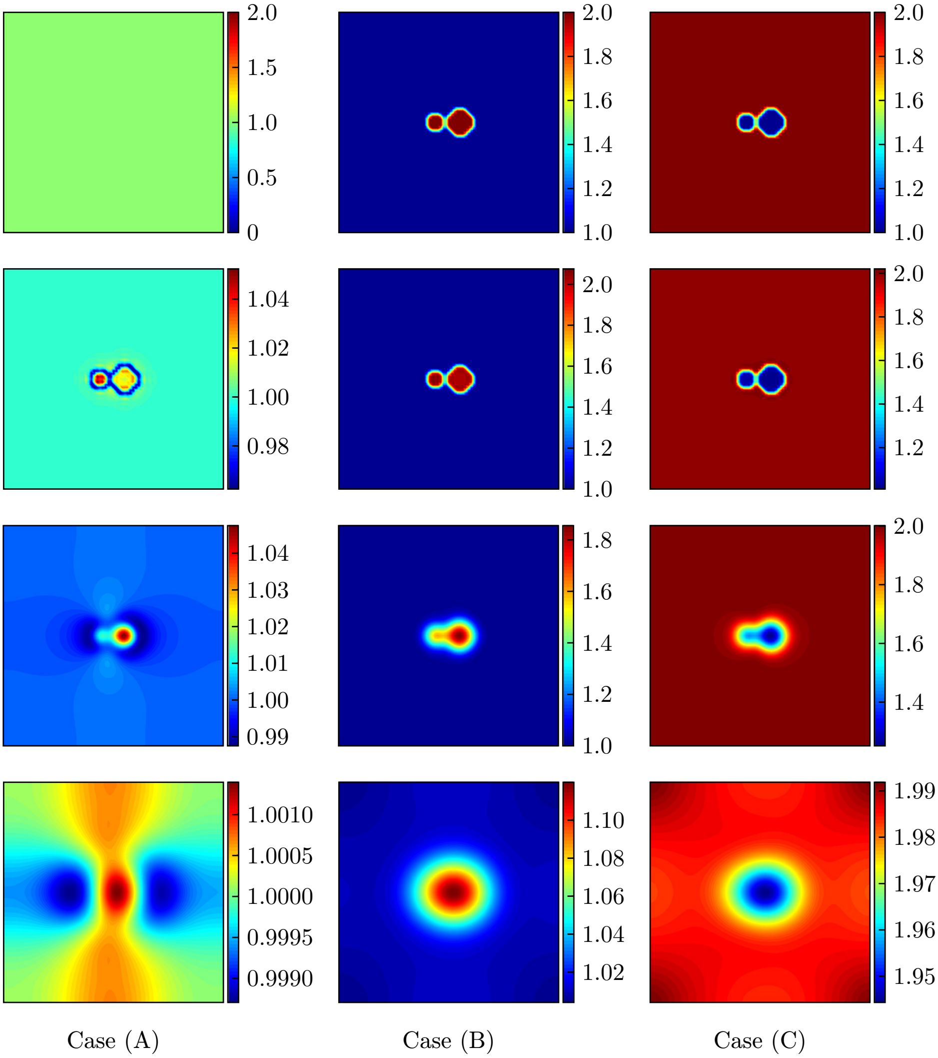


Figure 2. Experiment 1: time evolution of ϱ, from top to bottom are $t = 0, 0.001, 0.1, 1$.

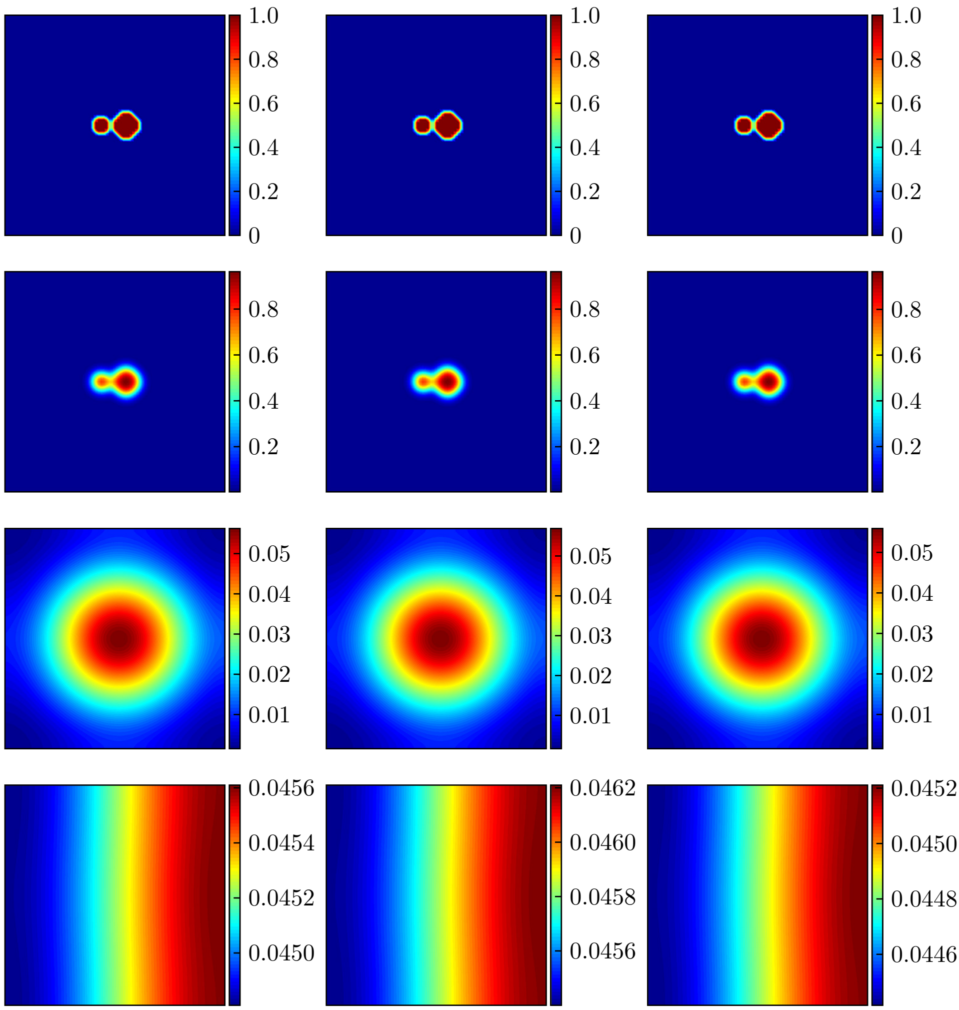
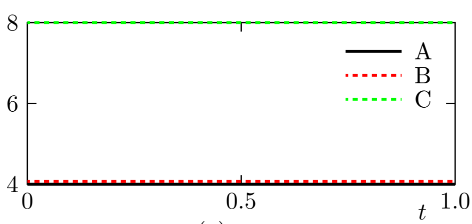
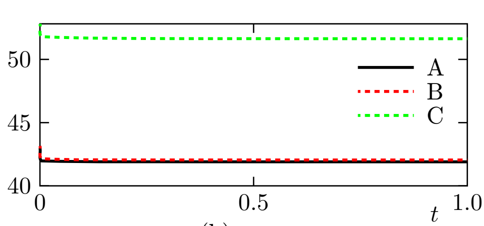


Figure 3. Experiment 1: time evolution of χ, from top to bottom are $t = 0, 0.001, 0.1, 1$.

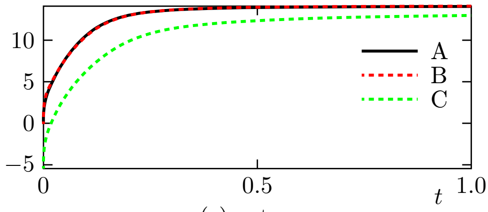


(a) mass



(b) energy

Figure 4. Time evolution of the total mass, energy and entropy (continued).



(c) entropy

Figure 4. Time evolution of the total mass, energy and entropy.

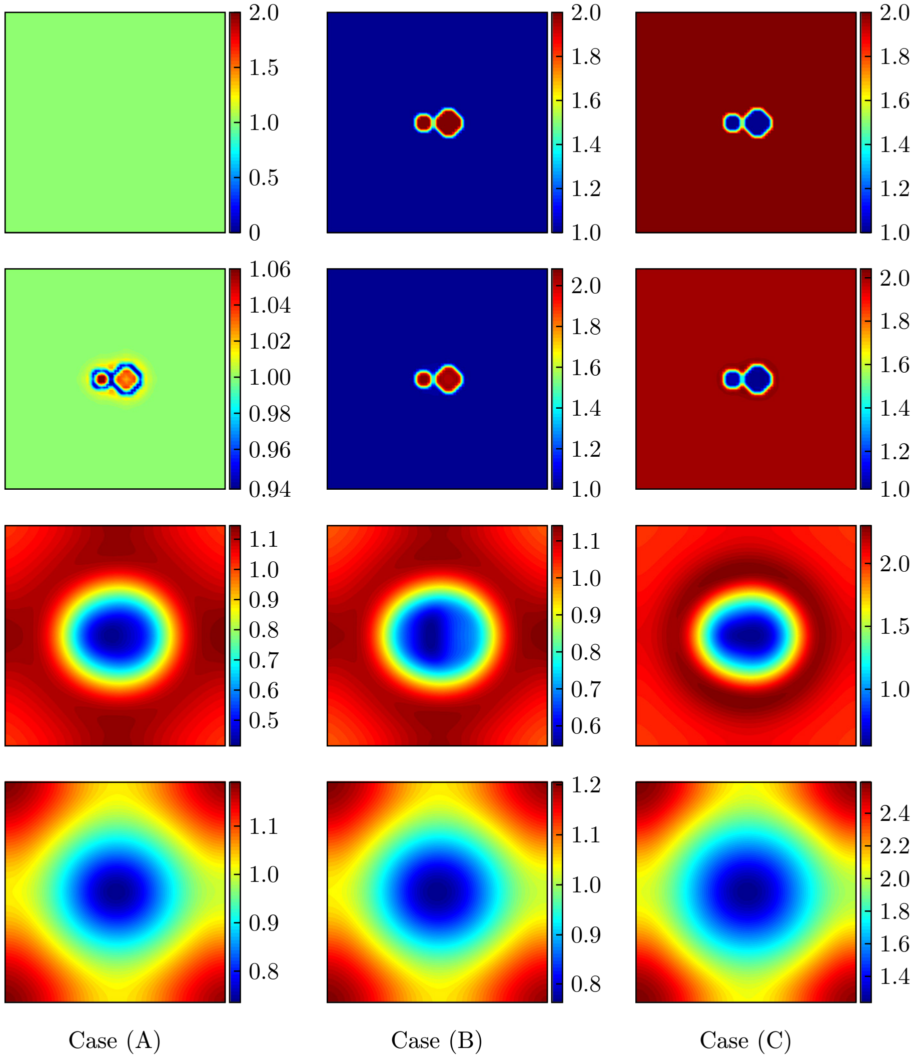
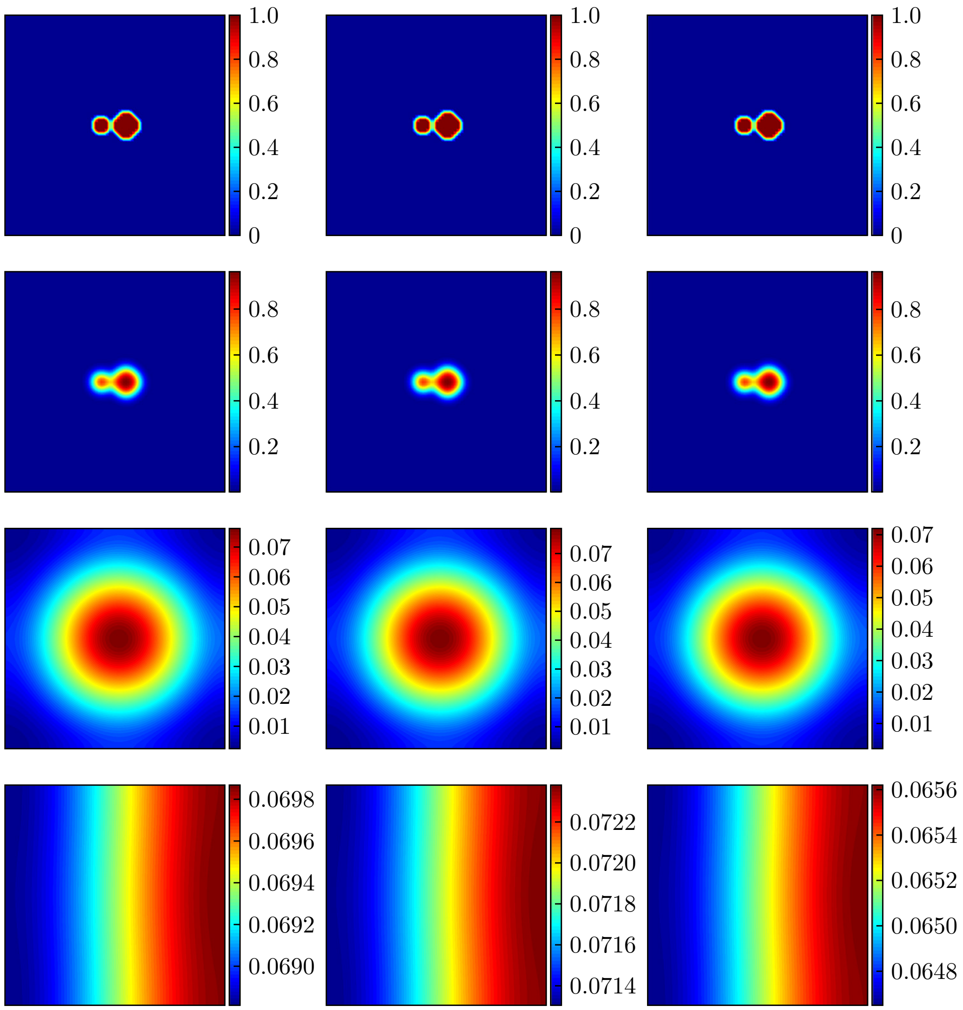


Figure 5. Experiment 2: time evolution of ϱ, from top to bottom are $t = 0, 0.001, 0.1, 1$.



Case (A) Case (B) Case (C)

Figure 6. Experiment 2: time evolution of χ, from top to bottom are $t = 0, 0.001, 0.1, 1$.

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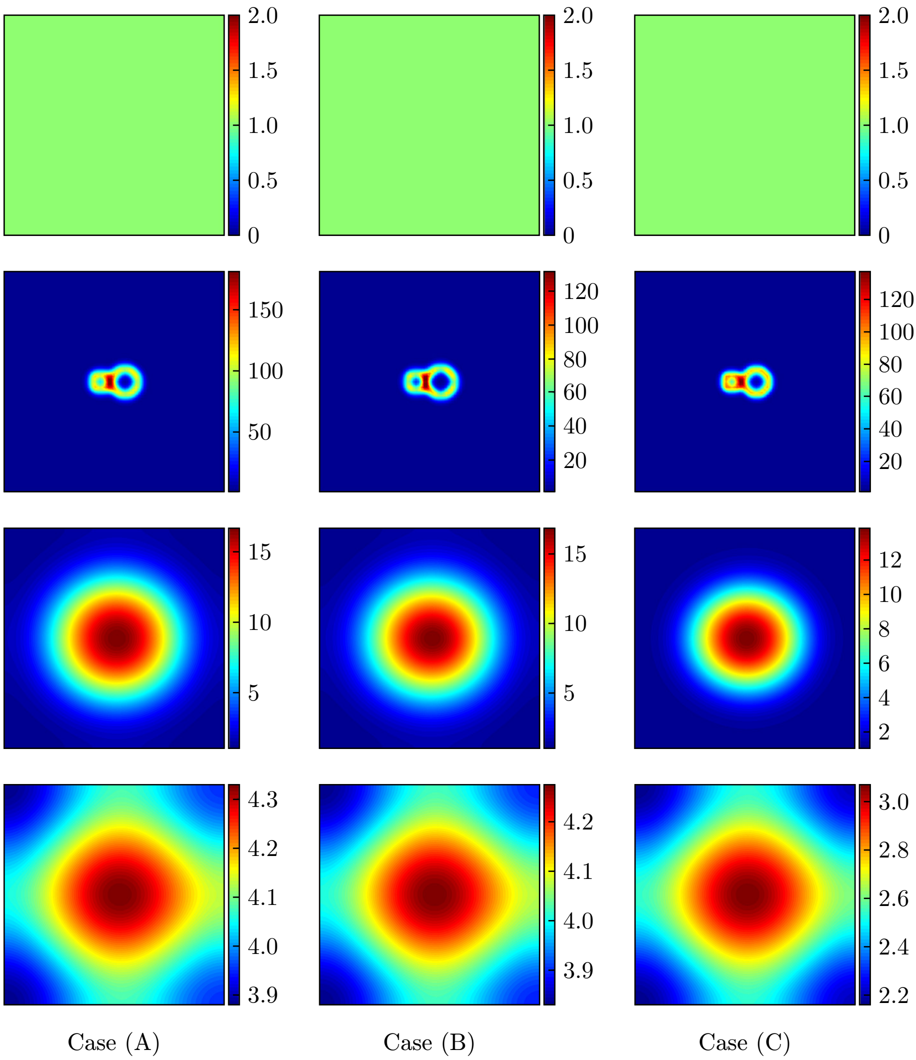

Figure 7. Experiment 2: time evolution of ϑ_h, from top to bottom are $t = 0, 0.001, 0.1, 1$.

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