An Anti-Diffusive Method for Simulating Interface Flows with a Five-Equation Model

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Numerical Methods for Multi-material Fluid Flows
Sept 10–14 2007

Outline

1. Introduction
2. Five-Equation Model
3. Lagrange-Remap Method
4. The Numerical Scheme
5. iso-(P, U) Profiles
6. Numerical Results

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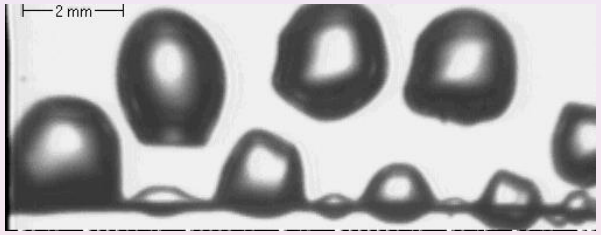
A Target (Open) Problem for Nuclear Safety Simulation

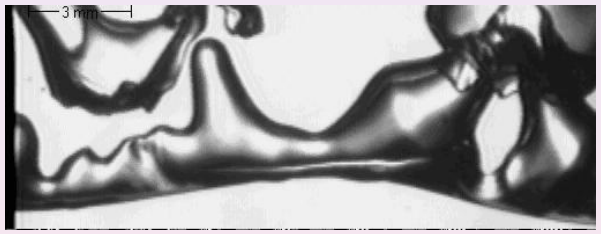
Phenomenon

- Liquid phase heated by a wall (pool boiling) at a given temperature T_{wall}.
- As T_{wall} increases there is a transition from the Nucleate Boiling Regime to the Film Boiling Regime. This transition is still misunderstood.

Nucleate Boiling



Critical Flux



Film Boiling

source : `http://www.spaceflight.esa.int/users/fluids/TT_boiling.htm`

A difficult problem

- Determining the most significant physical scale is still an open issue
- Performing experiments is difficult.

Simulation Framework

Physical Framework

- Simulation of two-phase flows with interfaces
- Each fluid $k = 0, 1$ is compressible, EOS: $(\rho_k, \varepsilon_k) \mapsto P_k$
- The interface is passively advected
- Model choice: Five-Equation Model (Allaire,Clerc,Kokh and also Murrone, Guillard, Massoni, Saurel, Périgaud,...)

Numerical Method

- Interface Capture Method: the interface is located by the mean of a color function z
- The variable z is updated thanks to an advection PDE that is directly discretized

Issues & Questions

Drawback

The discretization for z tends to smear the interface

Possible Cures

- Level-Set Type Method: conservativity issue (Osher, Sethian, Fedkiw, Smereka, Sussman, Gibou...)
- Anti-diffusive schemes (Després-Lagoutière, and also Reservoir Schemes : Alouges, Lorin, Le Coq, ...)

Is it possible to design an anti-diffusive solver for the Five-Equation system? Can we "extend" the Després-Lagoutière strategy to models different from its original framework?

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The Five-Equation Model with Isobaric Closure

$$\begin{cases} \partial_t \rho y + \mathrm{div}(\rho y \mathbf{u}) = 0 \\ \partial_t \rho + \mathrm{div}(\rho \mathbf{u}) = 0 \\ \partial_t \rho \mathbf{u} + \mathrm{div}[\rho \mathbf{u} \otimes \mathbf{u} + P(z, y, \rho, \varepsilon)\mathrm{Id}] = 0 \\ \partial_t \rho e + \mathrm{div}\left[(\rho e + P)\,\mathbf{u}\right] = 0 \\ \partial_t z + \mathbf{u} \cdot \nabla z = 0 \\ P_1(\rho_1, \varepsilon_1) = P_0(\rho_0, \varepsilon_0) = P \end{cases}$$

$$\rho = z\rho_1 + (1-z)\rho_0, \quad \rho\varepsilon = z\rho_1\varepsilon_1 + (1-z)\rho_0\varepsilon_0$$

$$e = \varepsilon + \frac{|u|^2}{2}, \qquad y = \frac{z\rho_1}{\rho}$$

Model Main Properties

- The system can be expressed in a fully conservative form
- Hyperbolicity is ensured when

$$\xi_k = \left(\frac{\partial \rho_k \varepsilon_k}{\partial P_k}\right)_{\rho_k} > 0 \quad \text{(reads } \gamma_k > 1 \text{ for perfect gases)}$$

- Eigenstructure of the system: $\{u - c, u, u, u, u + c\}$
- Sound velocity c given by

$$\xi c^2 = y\xi_1 c_1^2 + (1 - y)\xi_0 c_0^2,$$

$$\xi = z\xi_1 + (1 - z)\xi_0, \quad c_k = \text{pure fluid } k \text{ sound velocity}$$

- No entropy so far for the general case...

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The system reads (for regular solutions)

$$\begin{cases} \mathrm{D}_t z = 0, \quad \mathrm{D}_t y = 0 \\ \rho \mathrm{D}_t \begin{bmatrix} 1/\rho \\ u \\ e \end{bmatrix} + \begin{bmatrix} -u \\ P \\ Pu \end{bmatrix}_x = 0 \end{cases}$$

$$\mathrm{D}_t \cdot = \partial_t \cdot + u \partial_x \cdot$$

Euler Coord. $a(x,t)$ $\longleftrightarrow$ Lagrange Coord. $\widetilde{a}(\mathrm{X},t)$

$$(\mathrm{L}) \begin{cases} \widetilde{z}_t = 0, \quad \widetilde{y}_t = 0 \\ \widetilde{\rho} \begin{bmatrix} 1/\widetilde{\rho} \\ \widetilde{u} \\ \widetilde{e} \end{bmatrix}_t + \begin{bmatrix} -\widetilde{u} \\ \widetilde{P} \\ \widetilde{P}\widetilde{u} \end{bmatrix}_{\mathrm{X}} = 0 \end{cases}$$

Lagrange-Remap process

Map the Euler variable onto the Lagrange variable.	Update the Lagrange variable by solving (L)	Remap the Lagrange variable onto the Euler variable
$a^n \longrightarrow \widetilde{a}^n$	$\widetilde{a}^n \longrightarrow \widetilde{a}^{n+1}$	$\widetilde{a}^{n+1} \longrightarrow a^{n+1}$

Notations

We only consider a single timestep: $t^n \longrightarrow t^{n+1}$.

Initial Lagrange & Euler Variable

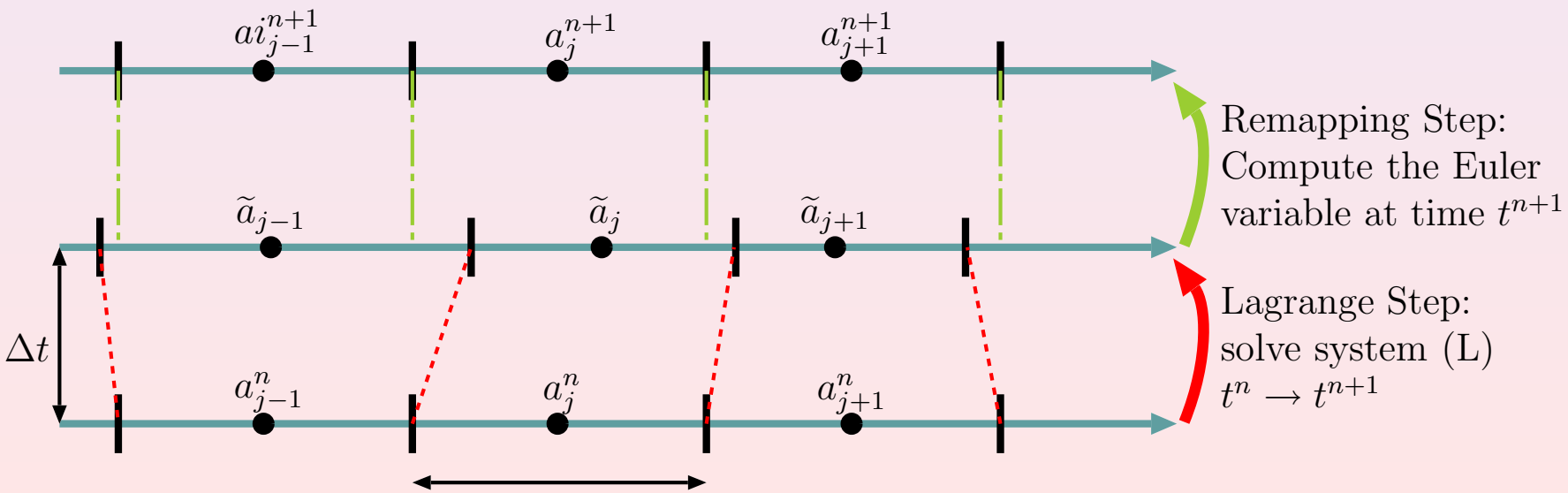
$$a_j^n = \widetilde{a}_j^n$$

Updated Lagrange Variable

$$\widetilde{a}_j^{n+1} \sim \widetilde{a}_j$$

Final Euler Variable

$$a_j^{n+1}$$



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Scheme for the Lagrange Step

Acoustic Scheme (Després)

$$\begin{cases} \begin{pmatrix} 1/\widetilde{\rho}_j - 1/\rho_j^n \\ \widetilde{u}_j - u_j^n \\ \widetilde{e}_j - e_j^n \end{pmatrix} + \frac{\lambda}{\rho_j^n} \begin{pmatrix} -u_{j+1/2} + u_{j-1/2} \\ P_{j+1/2} - P_{j-1/2} \\ P_{j+1/2}u_{j+1/2} - P_{j-1/2}u_{j-1/2} \end{pmatrix} = 0 \\ \widetilde{z}_j = z_j^n, \quad \widetilde{y}_j = y_j^n, \quad \lambda = \Delta t/\Delta x \end{cases}$$

Flux Formulas

$$(\rho c)^*_{j+1/2} = \sqrt{\max[\rho_j^n (c_j^n)^2, \rho_{j+1}^n (c_{j+1}^n)^2] \min(\rho_j^n, \rho_{j+1}^n)}$$

$$P_{j+1/2} = \frac{1}{2}(P_j^n + P_{j+1}^n) - \frac{1}{2}(\rho c)^*_{j+1/2}(u_{j+1}^n - u_j^n)$$

$$u_{j+1/2} = \frac{1}{2}(u_j^n + u_{j+1}^n) - \frac{1}{2}\frac{1}{(\rho c)^*_{j+1/2}}(P_{j+1}^n - P_j^n)$$

This step preserves (P, u)-constant profiles.

Scheme for the Remapping Step

General Form

$$\rho \mathbf{W} = (\rho y, \rho, \rho u, \rho e)^T$$

$$\rho_j^{n+1} \mathbf{W}_j^{n+1} - \rho_j \widetilde{\mathbf{W}}_j + \lambda \Big(u_{j+1/2} \widetilde{\rho}_{j+1/2} \widetilde{\mathbf{W}}_{j+1/2} - u_{j-1/2} \widetilde{\rho}_{j-1/2} \widetilde{\mathbf{W}}_{j-1/2} \Big) = 0$$

$$(z_j^{n+1} - z_j^n) + \lambda (u_{j+1/2} \widetilde{z}_{j+1/2} - u_{j-1/2} \widetilde{z}_{j-1/2}) - \lambda z_j^n (u_{j+1/2} - u_{j-1/2}) = 0$$

Building the scheme boils down to specify the following terms

$$\widetilde{y}_{j+1/2}, \quad \widetilde{\rho}_{j+1/2}, \quad \widetilde{u}_{j+1/2}, \quad \widetilde{\varepsilon}_{j+1/2}, \quad \widetilde{z}_{j+1/2}$$

Defining the Fluxes

$$\widetilde{z}_{j+1/2} = ?$$

$$\widetilde{u}_{j+1/2} = ?$$

$$\widetilde{y}_{j+1/2} = ?$$

$$\widetilde{\rho}_{j+1/2} = ?$$

$$\widetilde{(\rho\varepsilon)}_{j+1/2} = ?$$

Enforce consistency for $\widetilde{y}_{j+1/2}$, $\widetilde{\rho}_{j+1/2}$, $\widetilde{\varepsilon}_{j+1/2}$.

Upwind choice ($j + 1/2 = \mathrm{upw}$) according to the sign of $u_{j+1/2}$ for phasic quantities ρ_0, ρ_1 and $\rho_0\varepsilon_0$, $\rho_1\varepsilon_1$.

Upwind choice too for u

Defining the Fluxes

$$\widetilde{z}_{j+1/2} = ?$$

$$\widetilde{u}_{j+1/2} = ?$$

$$\widetilde{y}_{j+1/2} = \widetilde{z}_{j+1/2}\widetilde{(\rho_1)}_{j+1/2}/\widetilde{\rho}_{j+1/2}$$

$$\widetilde{\rho}_{j+1/2} = \widetilde{z}_{j+1/2}\widetilde{(\rho_1)}_{j+1/2} + (1-\widetilde{z}_{j+1/2})\widetilde{(\rho_0)}_{j+1/2}$$

$$\widetilde{(\rho\varepsilon)}_{j+1/2} = \widetilde{z}_{j+1/2}\widetilde{(\rho_1\varepsilon_1)}_{j+1/2} + (1-\widetilde{z}_{j+1/2})\widetilde{(\rho_0\varepsilon_0)}_{j+1/2}$$

Enforce consistency for $\widetilde{y}_{j+1/2}$, $\widetilde{\rho}_{j+1/2}$, $\widetilde{\varepsilon}_{j+1/2}$.

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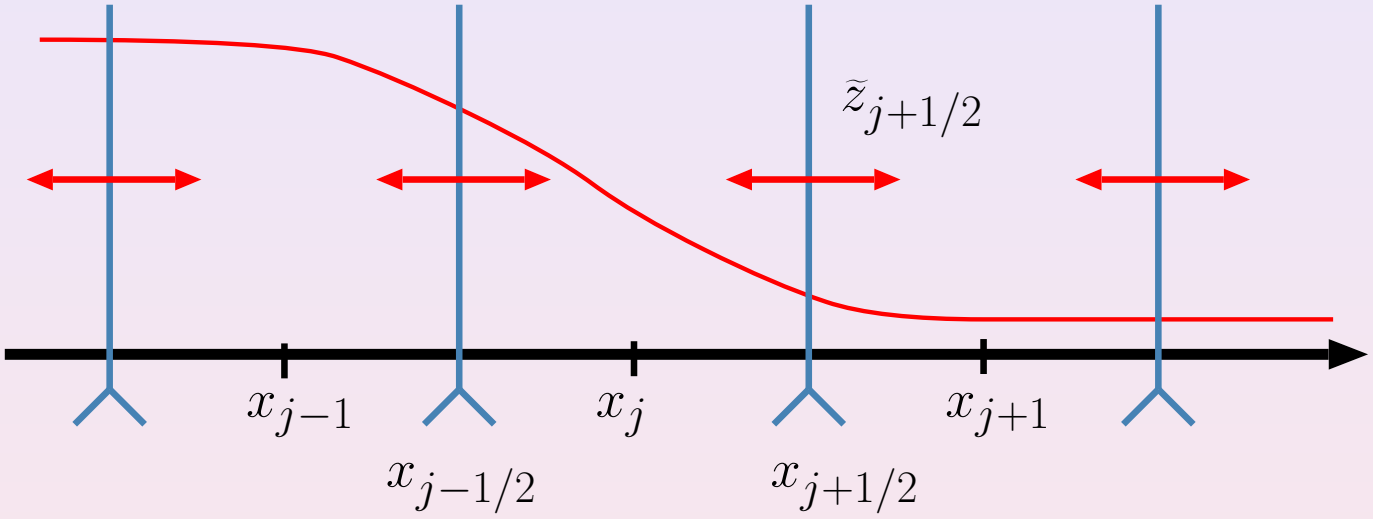
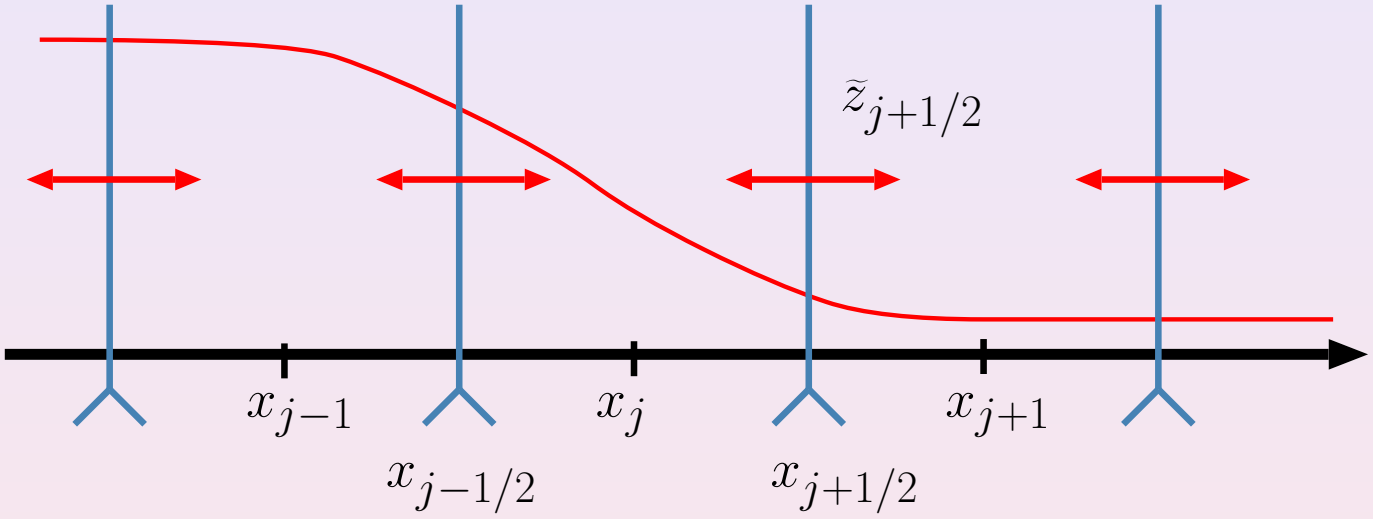
Upwind choice too for u

Consistency for the Flux $\widetilde{z}_{j+1/2}$



$$\min(z_j^n, z_{j+1}^n) \leq \widetilde{z}_{j+1/2} \leq \max(z_j^n, z_{j+1}^n) \quad \Longrightarrow \quad \text{consistency}$$

Consistency for the Flux $\widetilde{z}_{j+1/2}$



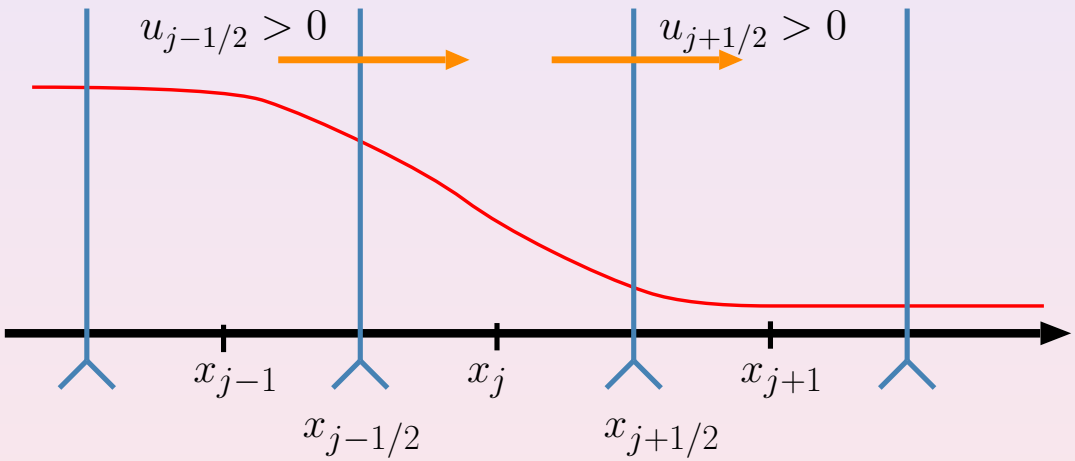
$$\left.\begin{array}{r}\text{Consistency "Trust Interval"}\\ \widetilde{z}_{j+1/2} \in [m_{j+1/2}, M_{j+1/2}]\end{array}\right\} \quad \Longrightarrow \quad \text{consistency}$$

$$m_{j+1/2} = \min(z_j^n, z_{j+1}^n), \quad M_{j+1/2} = \max(z_j^n, z_{j+1}^n)$$

Stability for the Color Function z

Ad hoc properties provide a simple stability criterion.

Suppose $u_{j+1/2} > 0$
Examine the jth cell if $u_{j-1/2} > 0$



Stability Criterion

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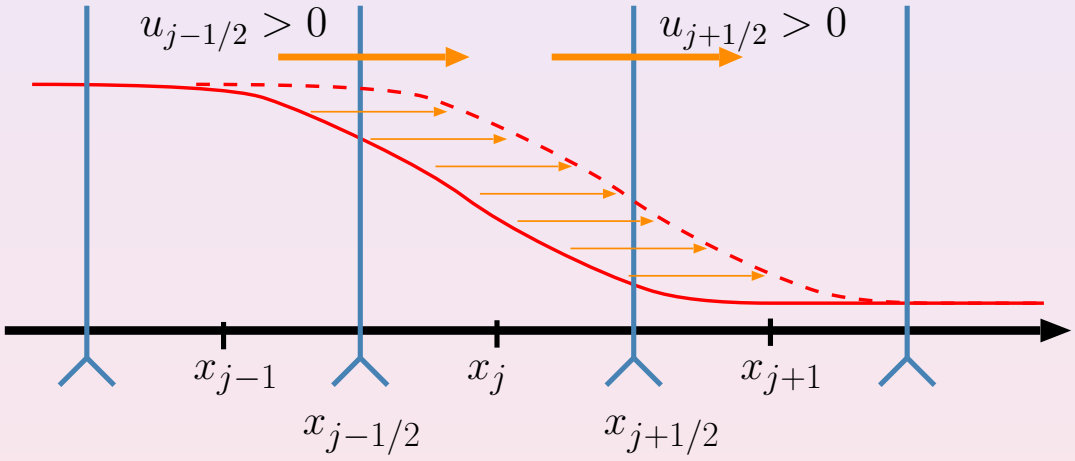

Stability Criterion

$$z_j^{n+1} \in [m_{j-1/2}, M_{j-1/2}] \Longrightarrow \text{Stability}$$

Stability for the Color Function z

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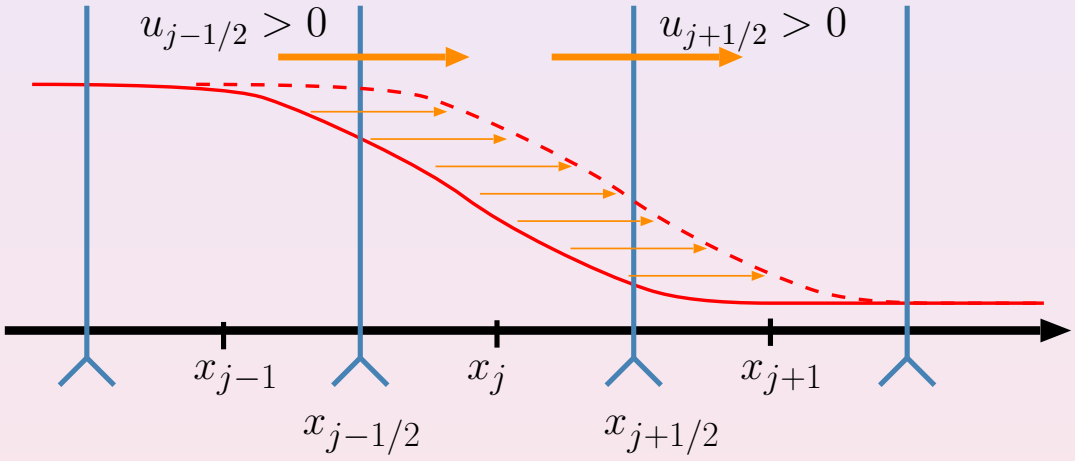

Stability Criterion

$$\widetilde{z}_{j+1/2} \ ? \Longrightarrow \quad z_j^{n+1} \in [m_{j-1/2}, M_{j-1/2}] \Longrightarrow \text{Stability}$$

Sufficient Stability Condition (case $u_{j-1/2} > 0$ and $u_{j+1/2} > 0$)

$$\widetilde{z}_{j+1/2} \ ?$$

$$\Downarrow$$

$$z_j^{n+1} \in [m_{j-1/2}, M_{j-1/2}] \Longrightarrow \text{Stability for } z$$

$$\begin{cases} a_j = z_j^n + \left(\dfrac{u_{j-1/2}}{u_{j+1/2}} - \dfrac{1}{\lambda u_{j+1/2}}\right)(m_{j-1/2} - z_j^n) \\ A_j = z_j^n + \left(\dfrac{u_{j-1/2}}{u_{j+1/2}} - \dfrac{1}{\lambda u_{j+1/2}}\right)(M_{j-1/2} - z_j^n) \end{cases}, \quad \begin{cases} m_{j+1/2} = \min(z_j^n, z_{j+1}^n) \\ M_{j+1/2} = \max(z_j^n, z_{j+1}^n) \end{cases}$$

Sufficient Stability Condition (case $u_{j-1/2} > 0$ and $u_{j+1/2} > 0$)

$$\widetilde{z}_{j+1/2} \in [a_j, A_j]$$

$$\Downarrow$$

$$z_j^{n+1} \in [m_{j-1/2}, M_{j-1/2}] \Longrightarrow \text{Stability for } z$$

Stability and Consistency Trust Interval for z

$$\widetilde{z}_{j+1/2} \in \left[a_j, A_j\right] \bigcap \left[m_{j+1/2}, M_{j+1/2}\right]$$

Stability for the Mass Fraction y

Suppose $u_{j-1/2} > 0$ and $u_{j+1/2} > 0$.

Similar Lines

$$\text{Stability for } y$$

$$\Uparrow$$

$$y_j^{n+1} \in [m^y_{j-1/2}, M^y_{j-1/2}]$$

$$\Uparrow$$

$$\widetilde{y}_{j+1/2} = \frac{(\widetilde{\rho}_0)_j \widetilde{z}_{j+1/2}}{\widetilde{\rho}_{j+1/2}} \in \left[d_j, D_j\right]$$

$$\Uparrow$$

$$\widetilde{z}_{j+1/2} \in [b_j, B_j]$$

$$\begin{cases} m^y_{j-1/2} = \min(y^n_{j-1}, y^n_j) \\ M^y_{j-1/2} = \max(y^n_{j-1}, y^n_j) \end{cases}$$

$$\begin{cases} d_j = M^y_{j-1/2} + \dfrac{\rho^n_j}{\lambda u_{j+1/2} \widetilde{\rho}_{j+1/2}} (y^n_j - M^y_{j-1/2}) \\ D_j = m^y_{j-1/2} + \dfrac{\rho^n_j}{\lambda u_{j+1/2} \widetilde{\rho}_{j+1/2}} (y^n_j - m^y_{j-1/2}) \end{cases}$$

$$\begin{cases} b_j = z^n_j + \dfrac{\rho^n_j (y^n_j - M^y_{j-1/2}) \left(\frac{1}{\lambda u_{j+1/2}} - \frac{u_{j-1/2}}{u_{j+1/2}} \right)}{(\rho_1)_j (1 - M^y_{j+1/2}) + (\rho_2)_j M^y_{j+1/2}} \\ B_j = z^n_j + \dfrac{\rho^n_j (y^n_j - m^y_{j-1/2}) \left(\frac{1}{\lambda u_{j+1/2}} - \frac{u_{j-1/2}}{u_{j+1/2}} \right)}{(\rho_1)^n_j (1 - m^y_{j+1/2}) + (\rho_2)^n_j m^y_{j+1/2}} \end{cases}$$

Stability for the Mass Fraction y

Suppose $u_{j-1/2} > 0$ and $u_{j+1/2} > 0$.

Similar Lines

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$$y_j^{n+1} \in [m^y_{j-1/2}, M^y_{j-1/2}]$$

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$$\widetilde{y}_{j+1/2} = \frac{(\widetilde{\rho}_0)_j \widetilde{z}_{j+1/2}}{\widetilde{\rho}_{j+1/2}} \in \left[d_j, D_j\right]$$

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$$\begin{cases} m^y_{j-1/2} = \min(y^n_{j-1}, y^n_j) \\ M^y_{j-1/2} = \max(y^n_{j-1}, y^n_j) \end{cases}$$

explicit expression for d_j, D_j, b_j, B_j.

Constraints for the flux $\widetilde{z}_{j+1/2}$

Suppose $u_{j-1/2} > 0$ and $u_{j+1/2} > 0$.

We have a "trust interval" for $\widetilde{z}_{j+1/2}$ that ensures stability for both y and z, and consistency for the flux $\widetilde{z}_{j+1/2}$.

$$\widetilde{z}_{j+1/2} \in \left[m_{j-1/2}, M_{j-1/2}\right] \bigcap \left[a_j, A_j\right] \bigcap \left[b_j, B_j\right]$$

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How should we choose $\widetilde{z}_{j+1/2}$?

Choosing the z-flux $\widetilde{z}_{j+1/2}$ (1)

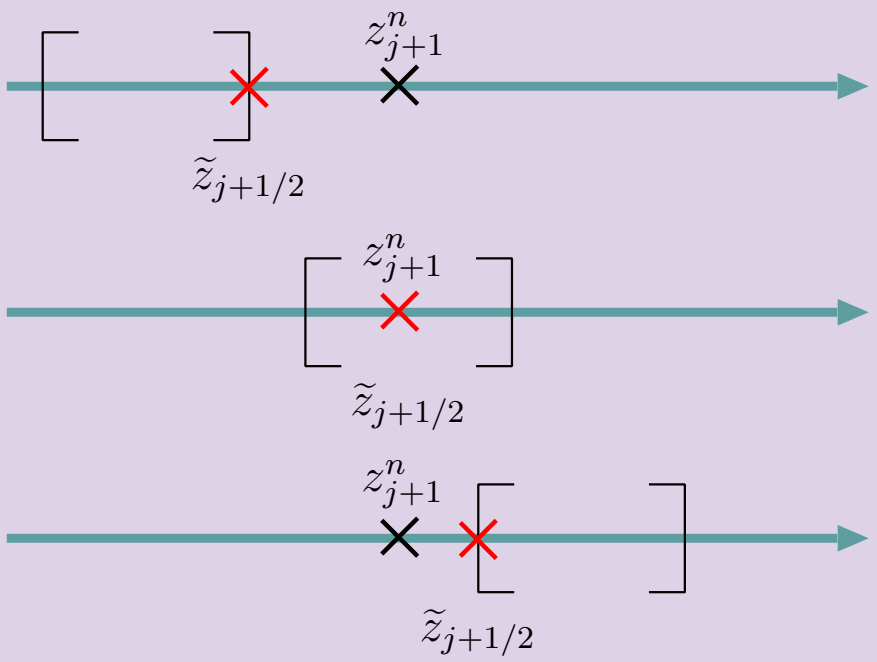
Suppose $u_{j-1/2} > 0$ and $u_{j+1/2} > 0$.

Després-Lagoutière strategy

We choose the most downwind possible value for $\widetilde{z}_{j+1/2}$ such that

$$\widetilde{z}_{j+1/2} \in \left[m_{j-1/2}, M_{j-1/2}\right] \bigcap \left[a_j, A_j\right] \bigcap \left[b_j, B_j\right]$$

$\widetilde{z}_{j+1/2}$ values axis



Choosing the $\widetilde{z}_{j+1/2}$ value is also an explicit step: no CPU cost is needed, nor any recursive procedure.

Choosing the flux $\widetilde{z}_{j+1/2}$ (2)

What if $u_{j-1/2} < 0$ and $u_{j+1/2} > 0$?

For sake of "security" we opt for the upwind choice, i.e.

$$\widetilde{z}_{j+1/2} = z_j^n$$

Other cases

The cases $u_{j-1/2} > 0$, $u_{j+1/2} < 0$ and $u_{j-1/2} < 0$, $u_{j+1/2} < 0$ can be examined following the same lines and provide similar formulas for the flux $\widetilde{z}_{j+1/2}$.

Quasi-Conservative Form

The overall scheme reads

$$\begin{cases} \rho_j^{n+1}\mathbf{W}_j^{n+1} - \rho_j^n\mathbf{W}_j^n + \lambda\left(\mathbf{F}_{j+1/2} - \mathbf{F}_{j-1/2}\right) = 0 \\ (z_j^{n+1} - z_j^n) + \lambda(u_{j+1/2}\widetilde{z}_{j+1/2} - u_{j-1/2}\widetilde{z}_{j-1/2}) \\ \qquad - \lambda z_j^n(u_{j+1/2} - u_{j-1/2}) = 0 \end{cases}$$

$$\begin{cases} \rho\mathbf{W} = (\rho y, \rho, \rho u, \rho e)^T \\ \mathbf{F}_{j+1/2} = \widetilde{\rho}_{j+1/2}\widetilde{\mathbf{W}}_{j+1/2}u_{j+1/2} + \left(0, 0, P_{j+1/2}, P_{j+1/2}u_{j+1/2}\right)^T \end{cases}$$

Outline

1. Introduction
2. Five-Equation Model
3. Lagrange-Remap Method
4. The Numerical Scheme
5. iso-(P, U) Profiles
6. Numerical Results

iso-(P, U) Profiles

The scheme inherits the properties of the original Five-Equation and solver.

If $(\rho\mathbf{W}, z)^n$ is such that

1. $\forall j,\ P_j^n = P$ and $u_j^n = u$
2. If z varies across the cell interface $j + 1/2$ then $(\rho_k)_j^n = (\rho_k)_{j+1}^n,\ k = 0, 1$

Then $\forall j,\ P_j^{n+1} = P$ and $u_j^{n+1} = u$

Remark

Assumption (2) is not necessary for some EOS (Perfect Gases, Stiffened Gas)

Outline

1. Introduction
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Interface Advection (1)

Test Description

Advection of a 1D "bubble" (pulse) involving two perfect gases

Inner bubble state

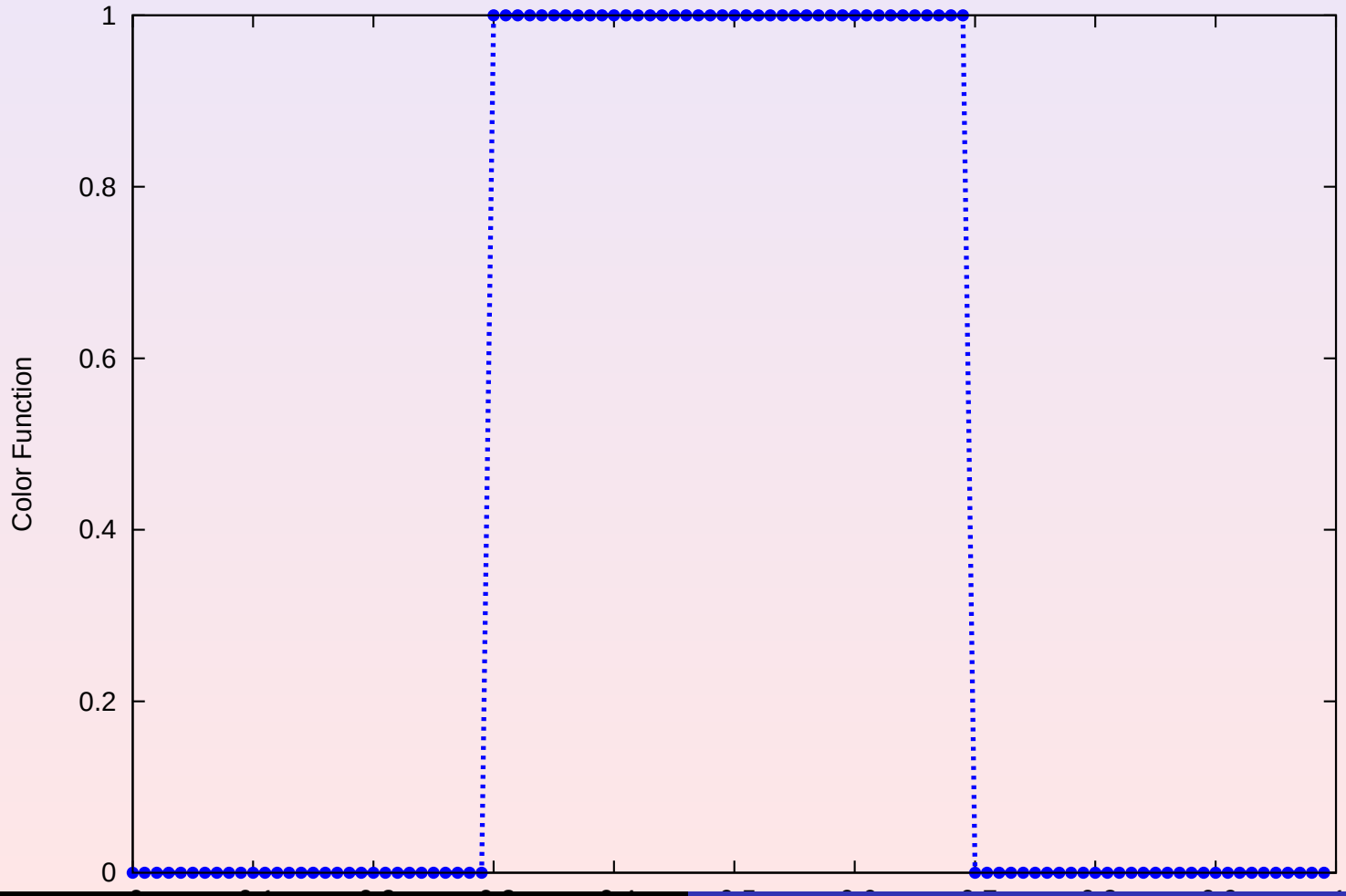
$$\gamma = 1.4, \quad \rho = 50.0$$
$$P = 10^5, \quad u = 1.0$$

Outter bubble State

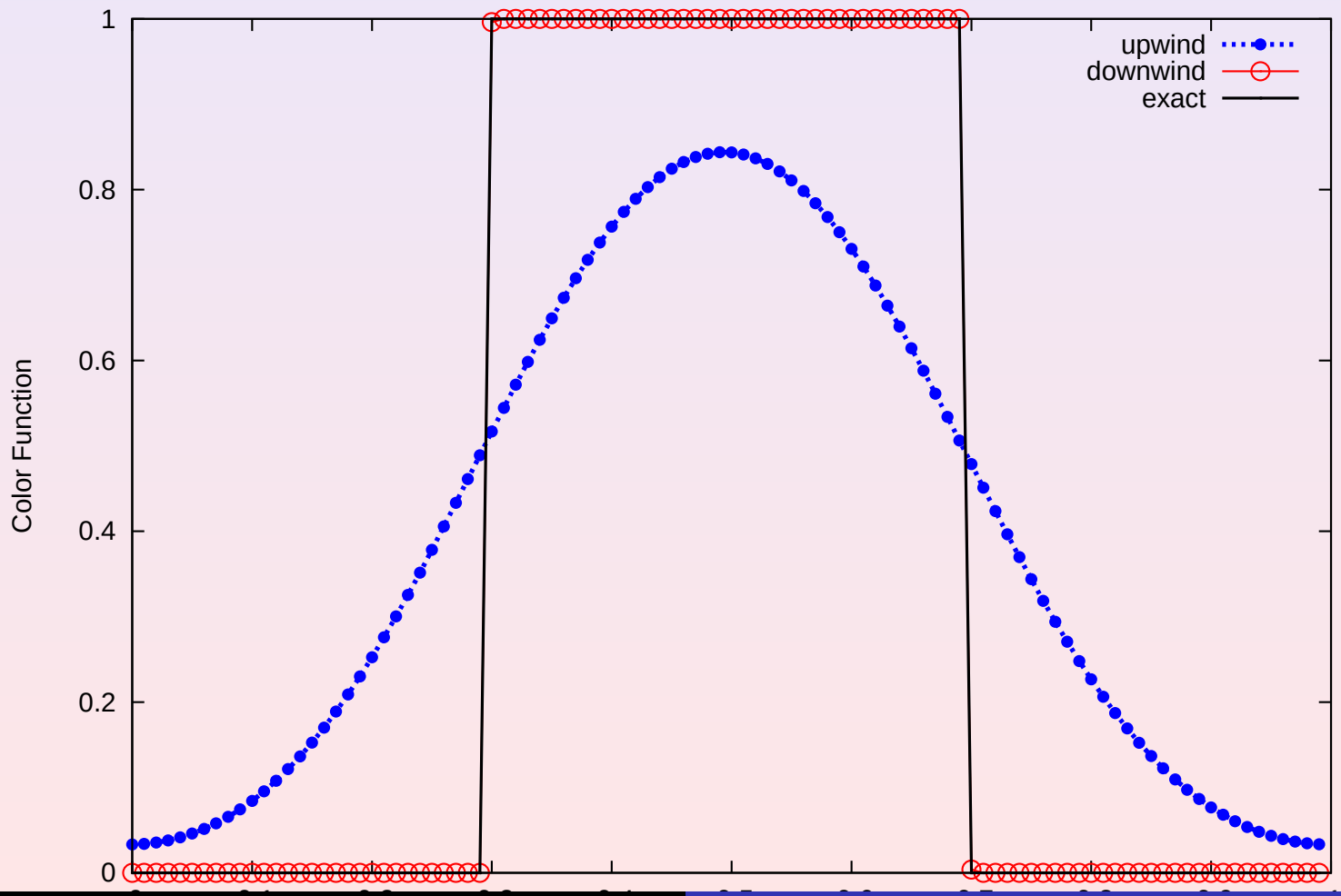
$$\gamma = 4.4, \quad \rho = 100$$
$$P = 10^5, \quad u = 1.0$$

- The domain is discretized over a 100 cells mesh
- Periodic boundary conditions
- $t = 1000\ \mathrm{s}$ (1000 turns)

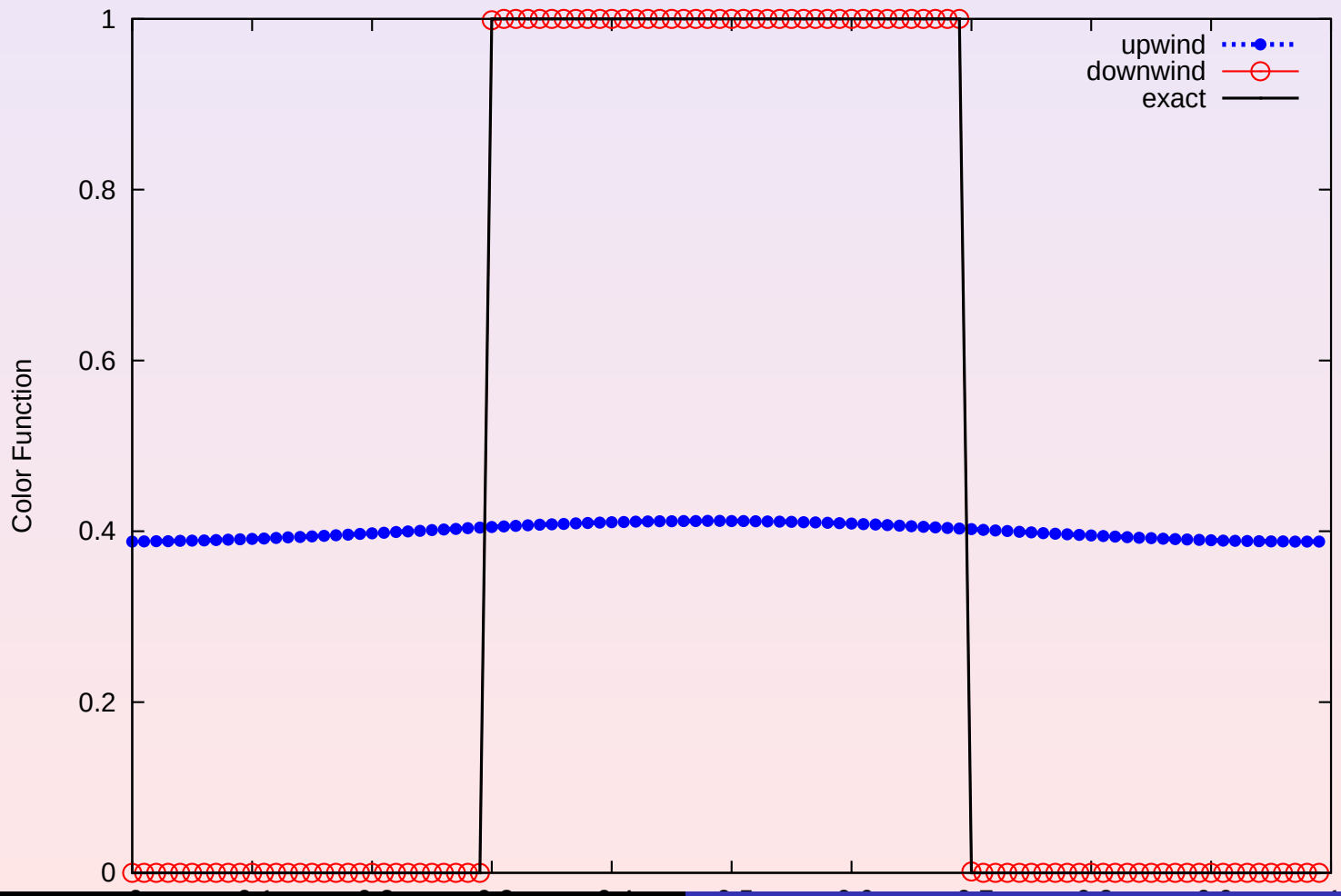
Interface Advection (2): Initial State



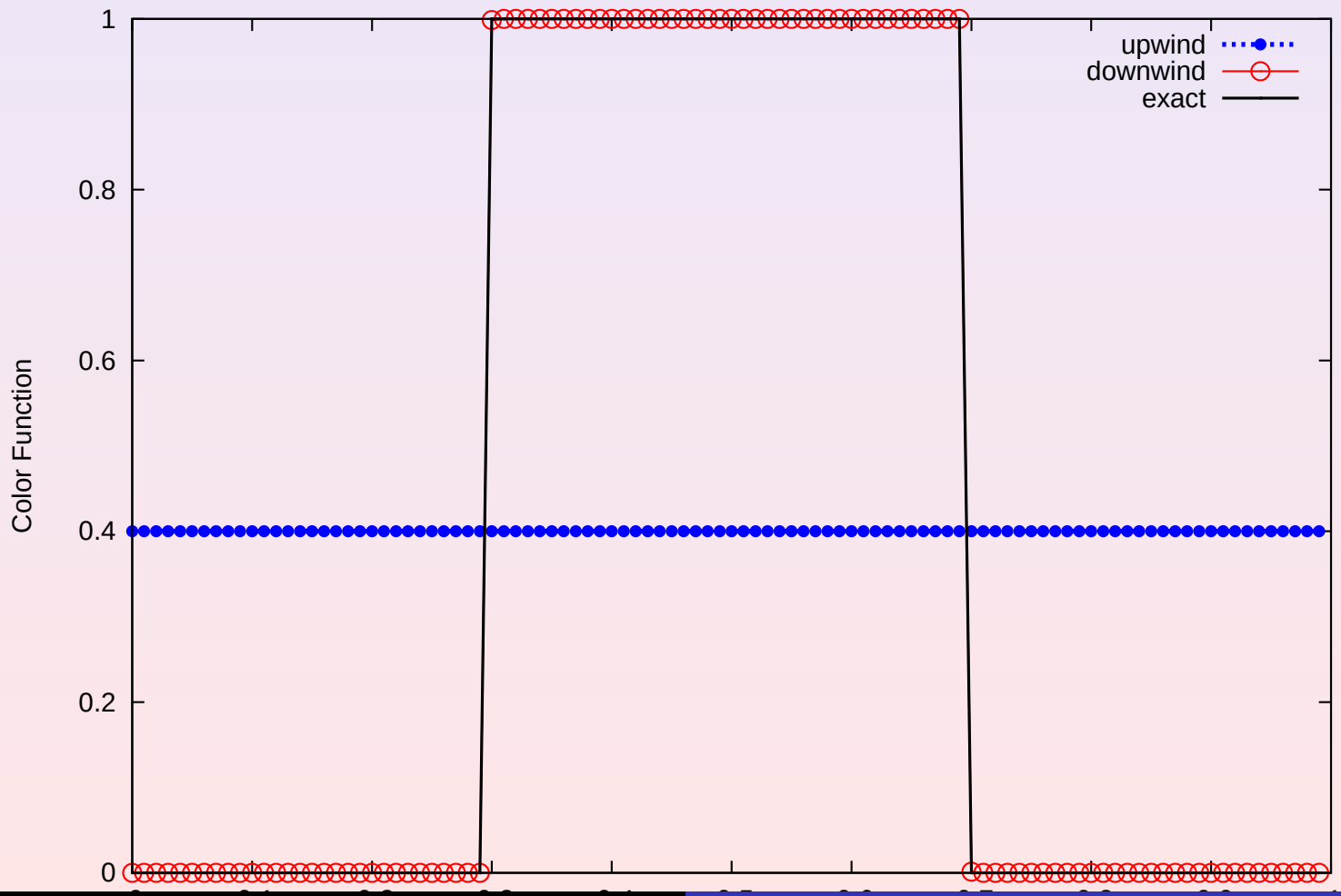
Interface Advection (3): Color Function at $t = 2$ s



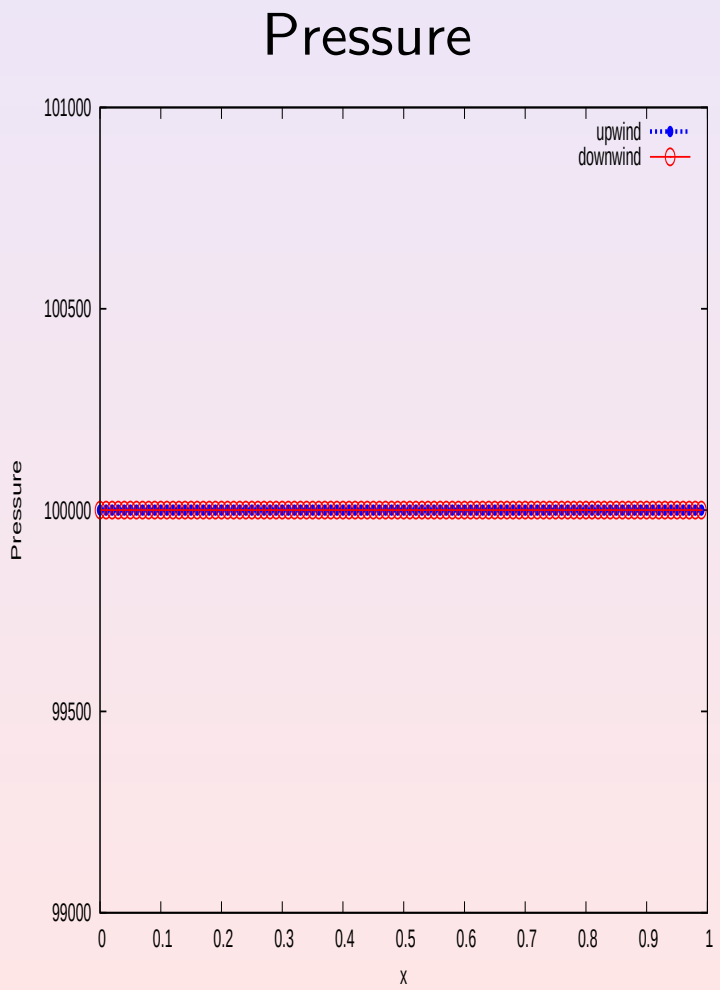
Interface Advection (4): Color Function at $t = 20$ s

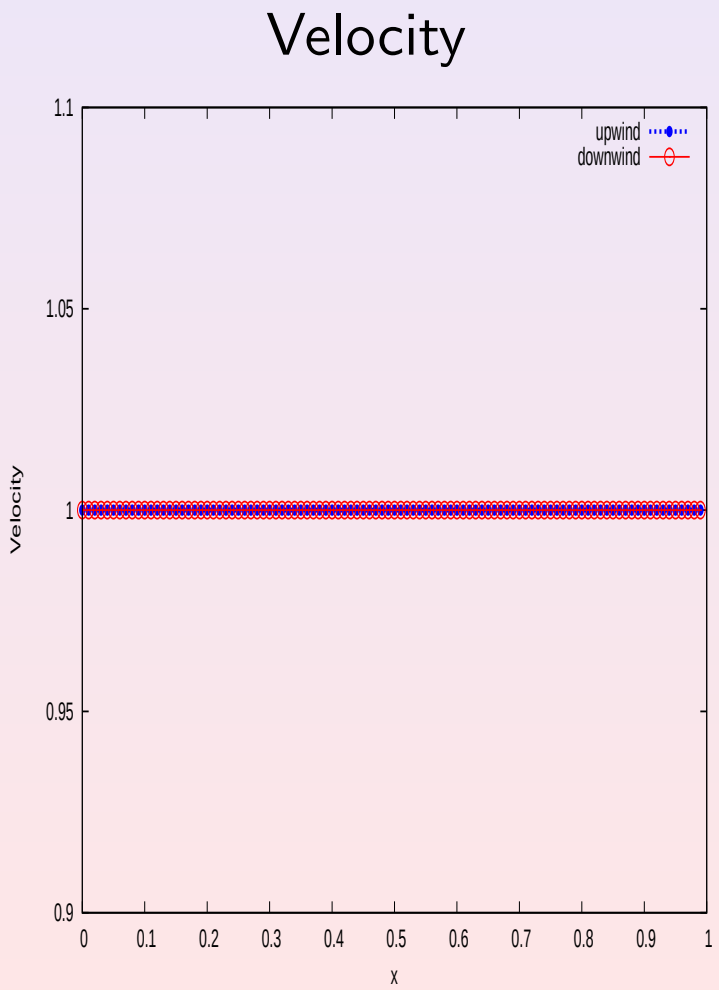


Interface Advection (5): Color Function at $t = 1000$ s

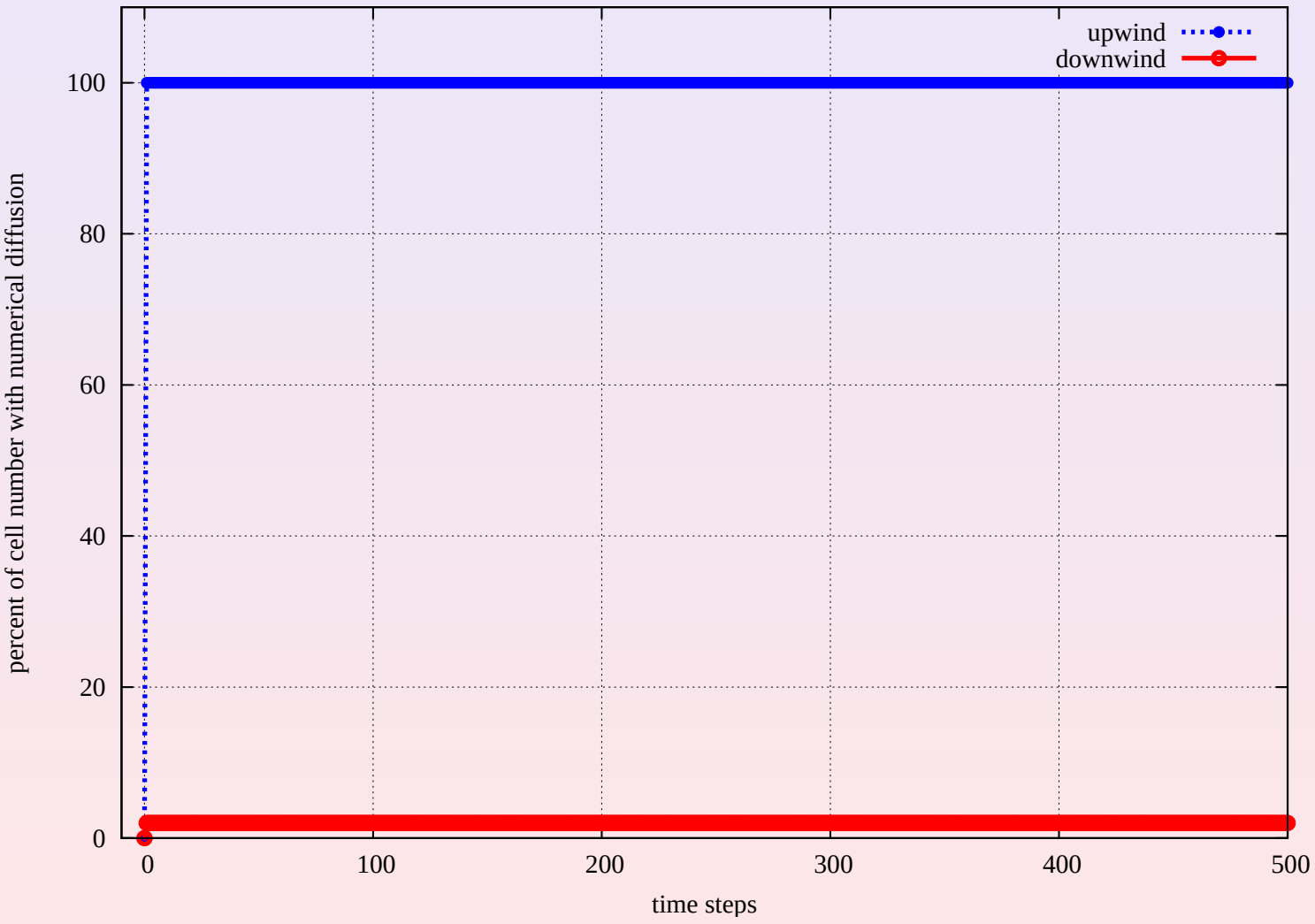


Interface Advection (6): Pressure & Velocity at $t = 1000$ s





Interface Advection (7): Numerical Diffusion of the Color Function



Shock Tube 1 (1)

Test Description

Riemann Problem with two perfect gases

Left State

$\gamma = 1.4$

$\rho = 1.0$

$P = 1.0$

$u = 0.0$

Right State

$\gamma = 2.4$

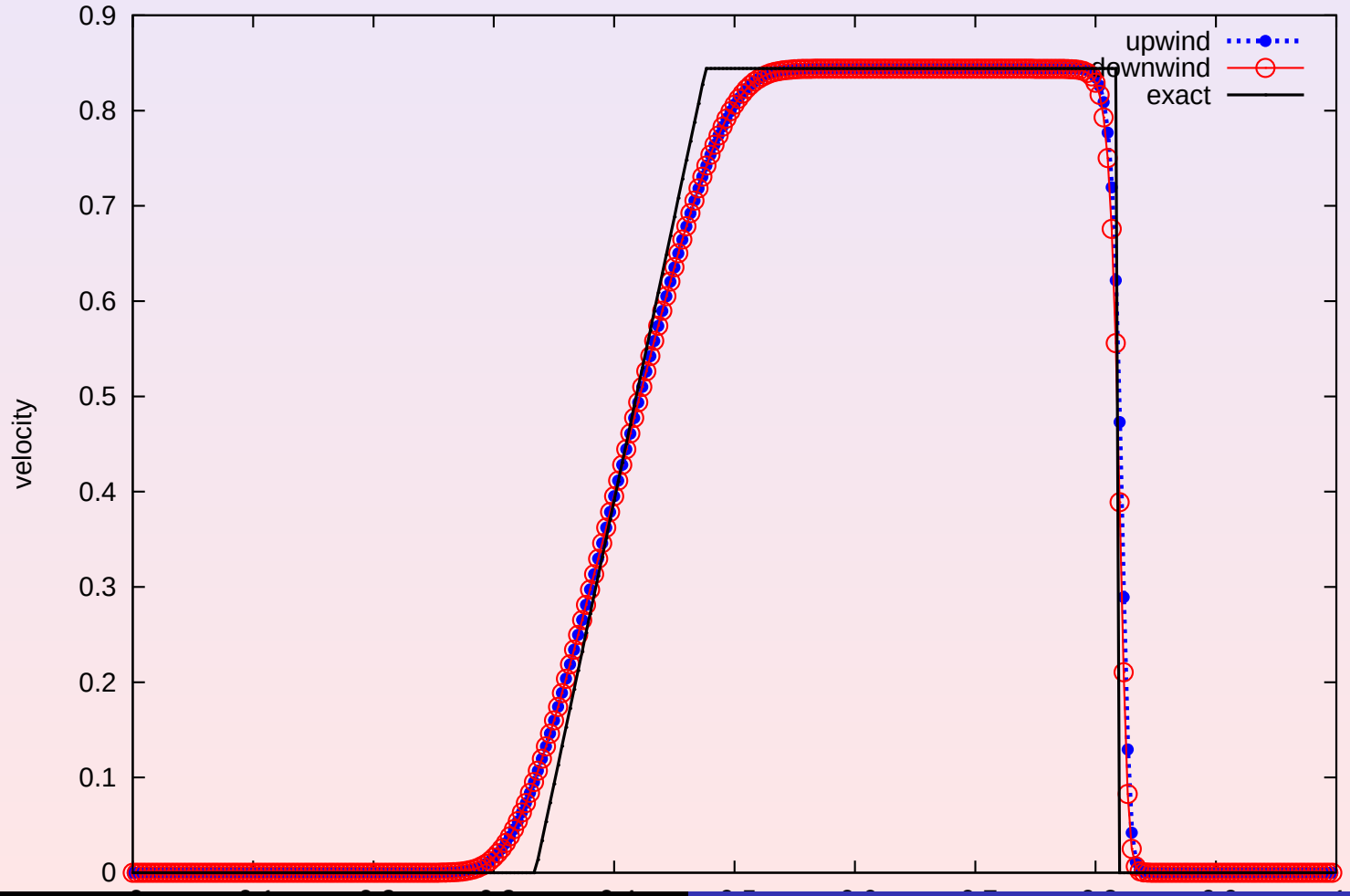
$\rho = 0.125$

$P = 0.1$

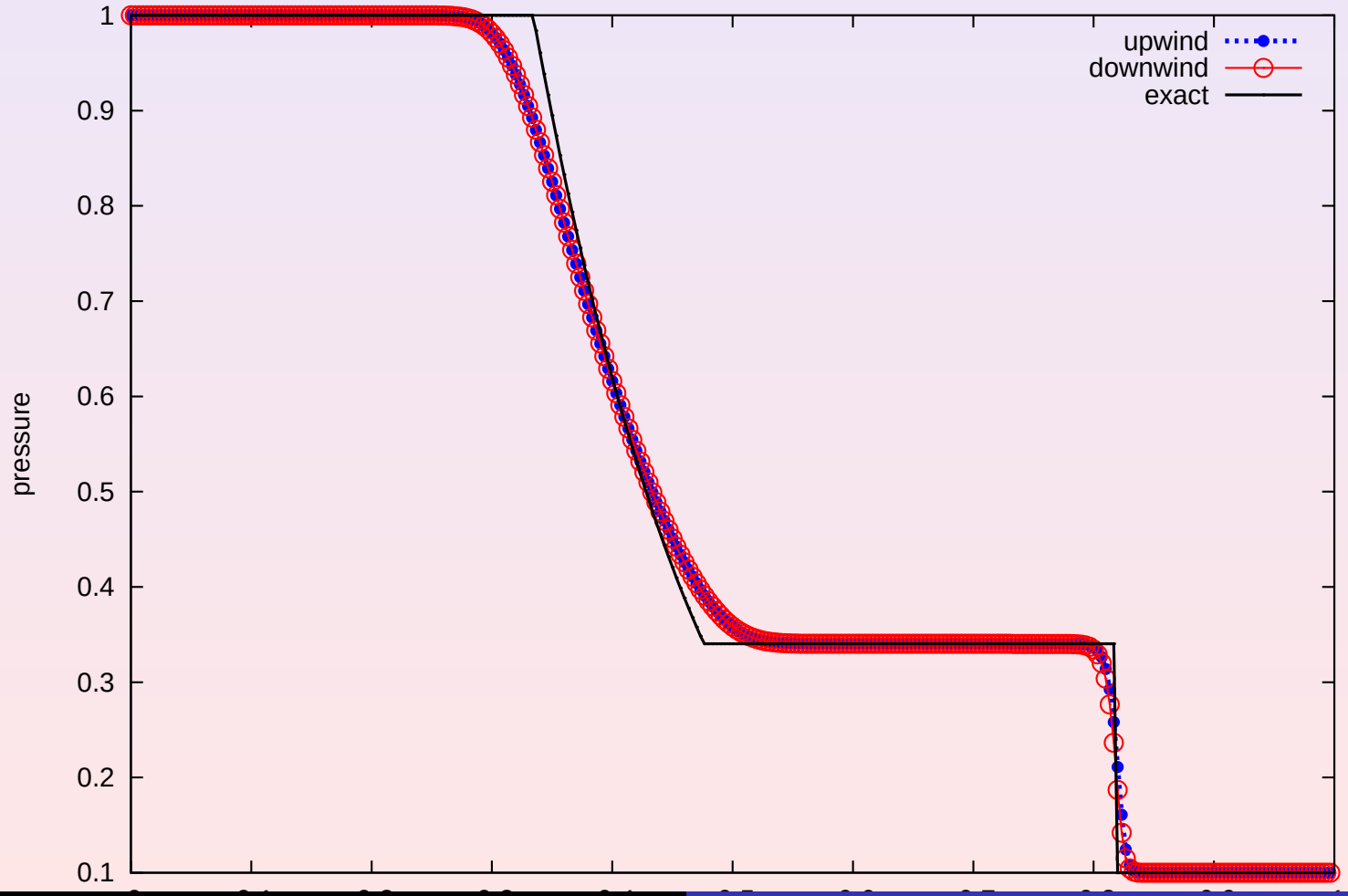
$u = 0.0$

- The domain is discretized over a 300 cells mesh.
- $t = 0.14s$

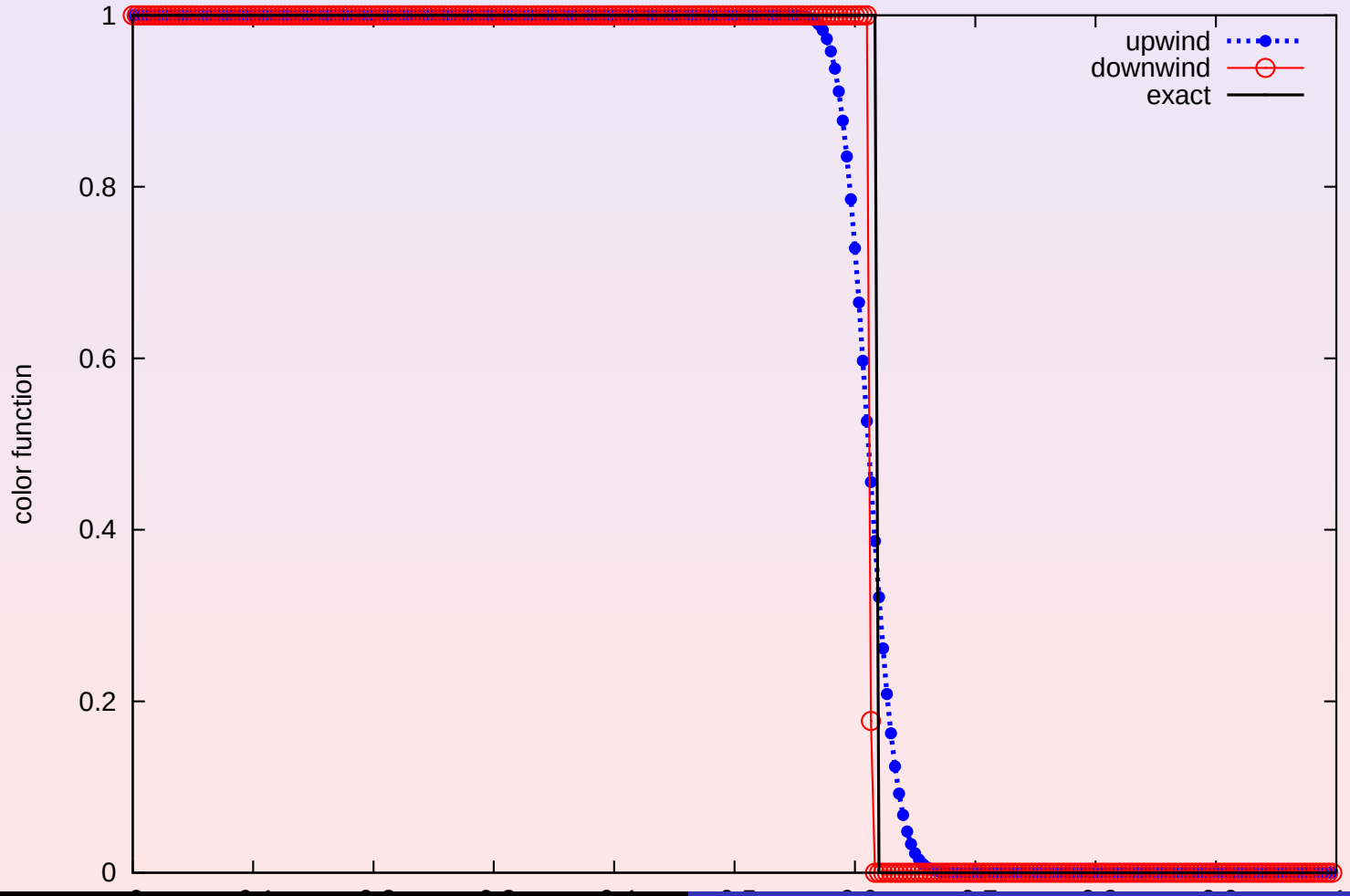
Shock Tube 1 (2): Velocity



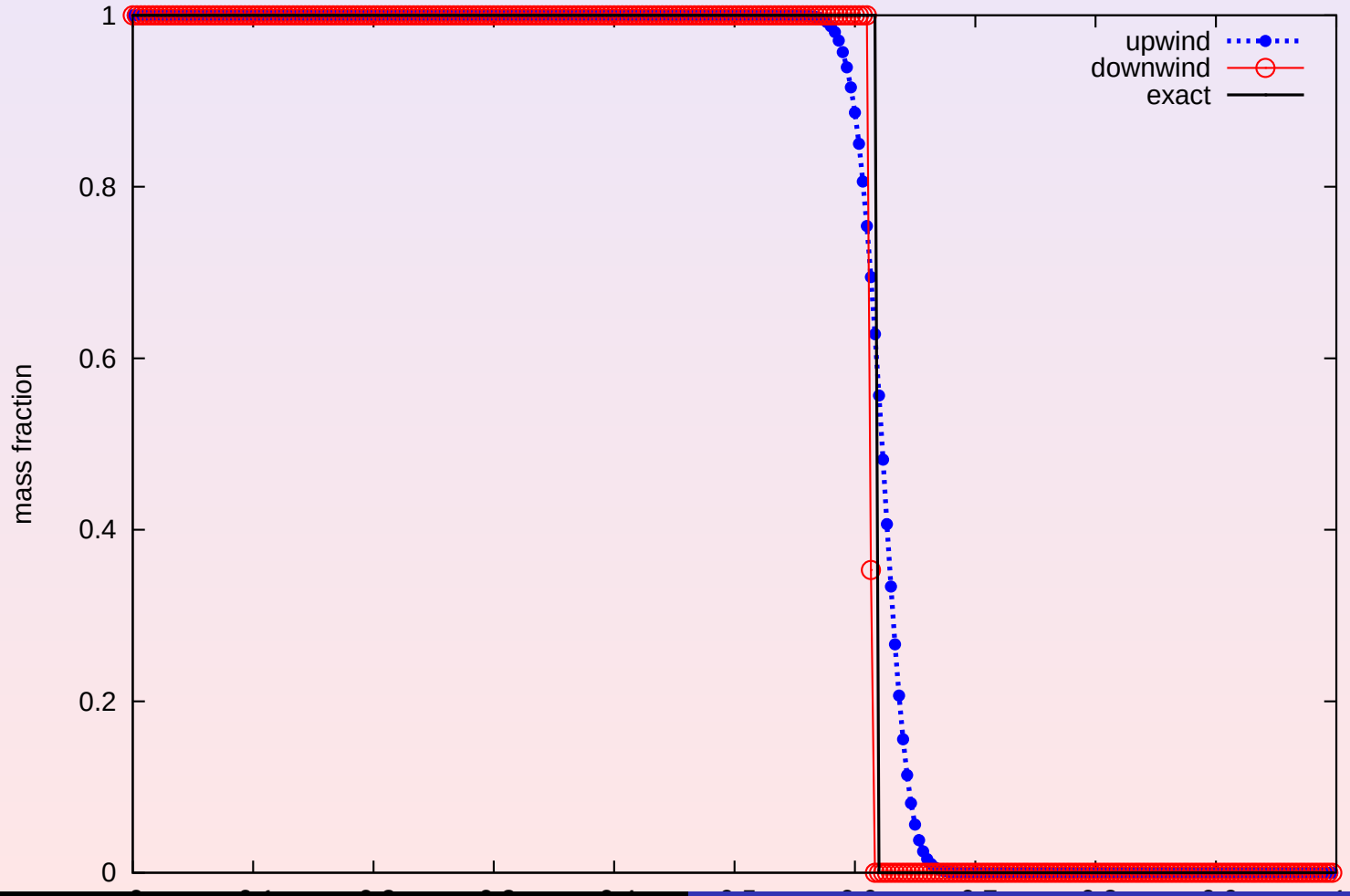
Shock Tube 1 (3): Pressure



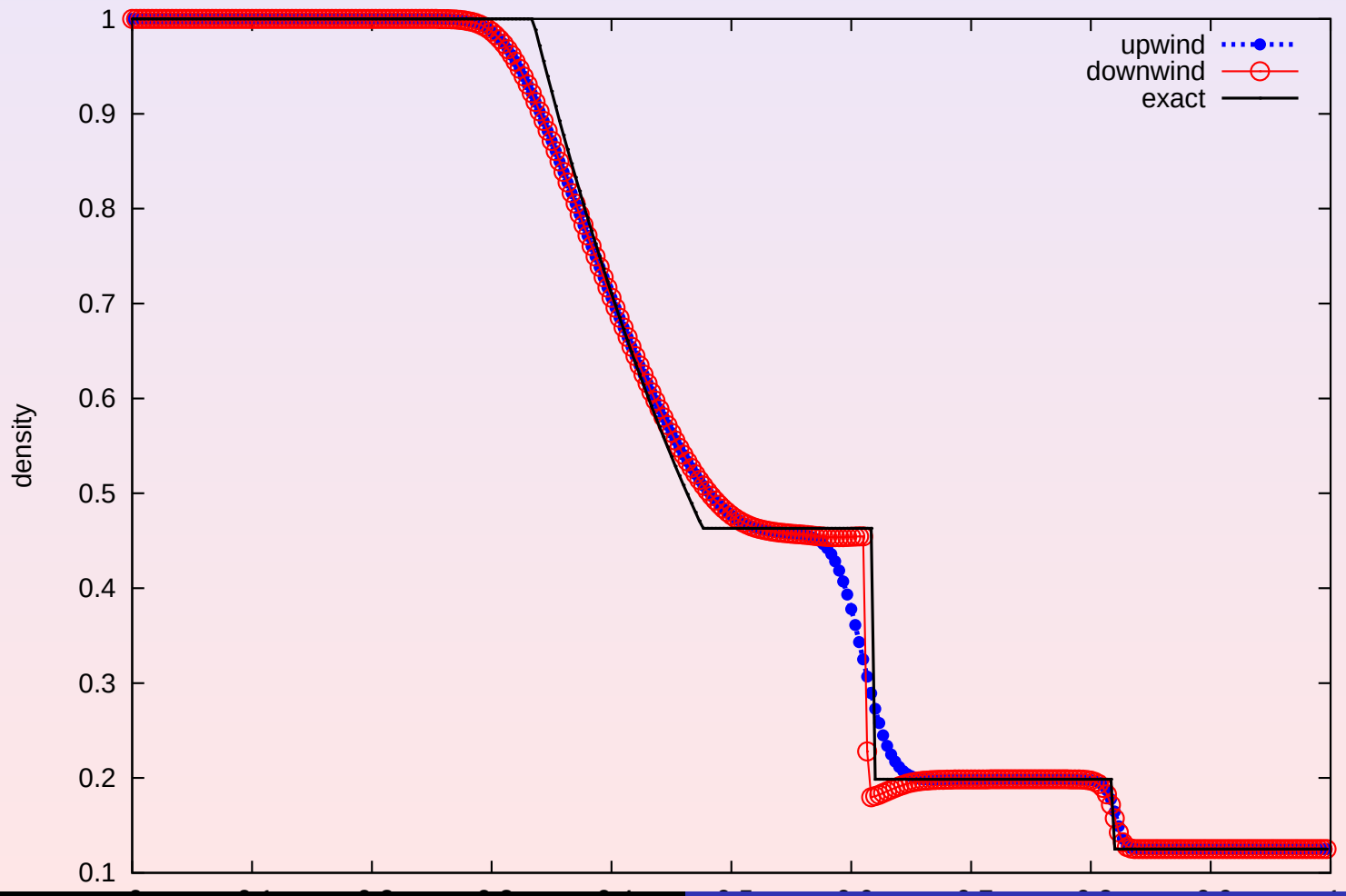
Shock Tube 1 (4): Color Function



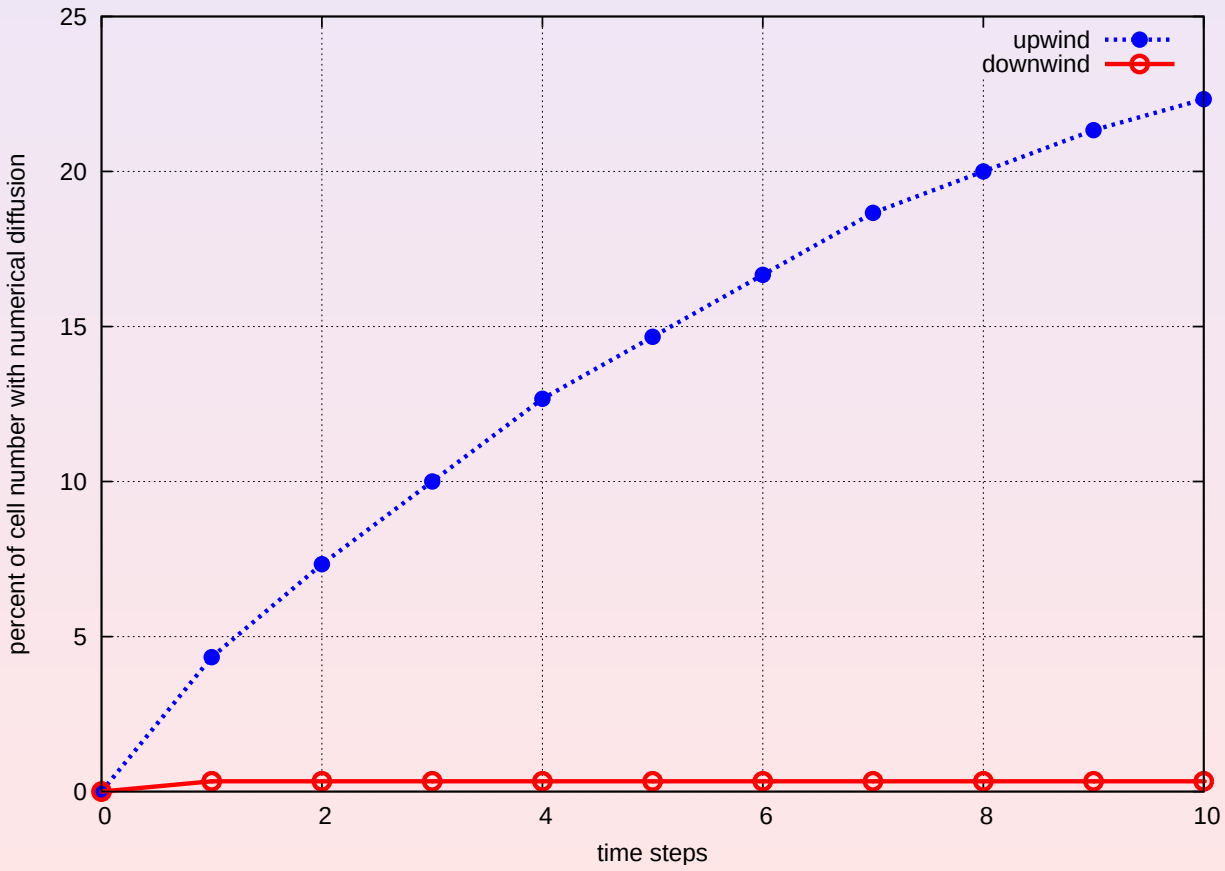
Shock Tube 1 (5): Mass Fraction



Shock Tube 1 (6): Density



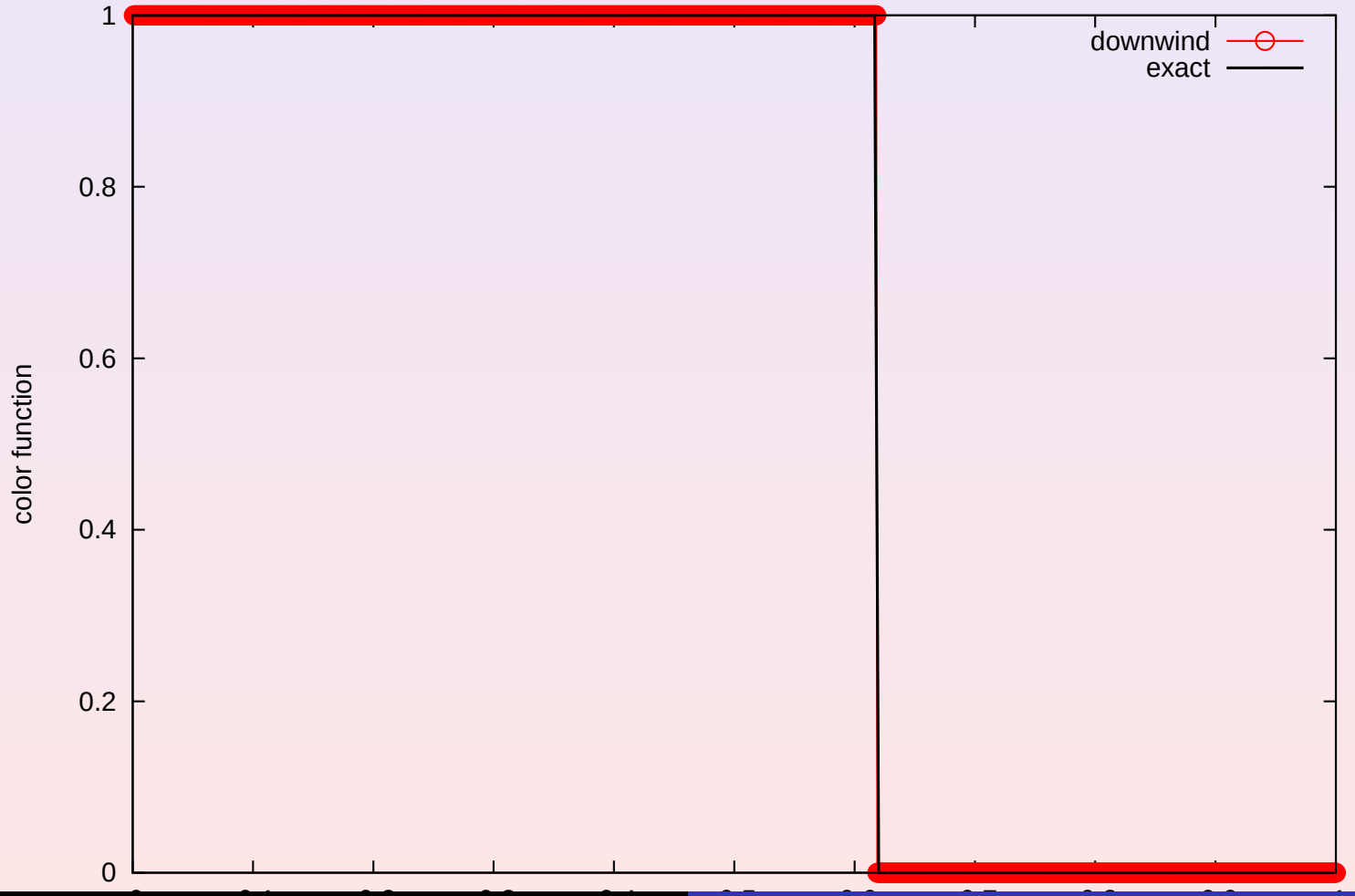
Shock Tube 1 (7): Numerical Diffusion of The Color Function



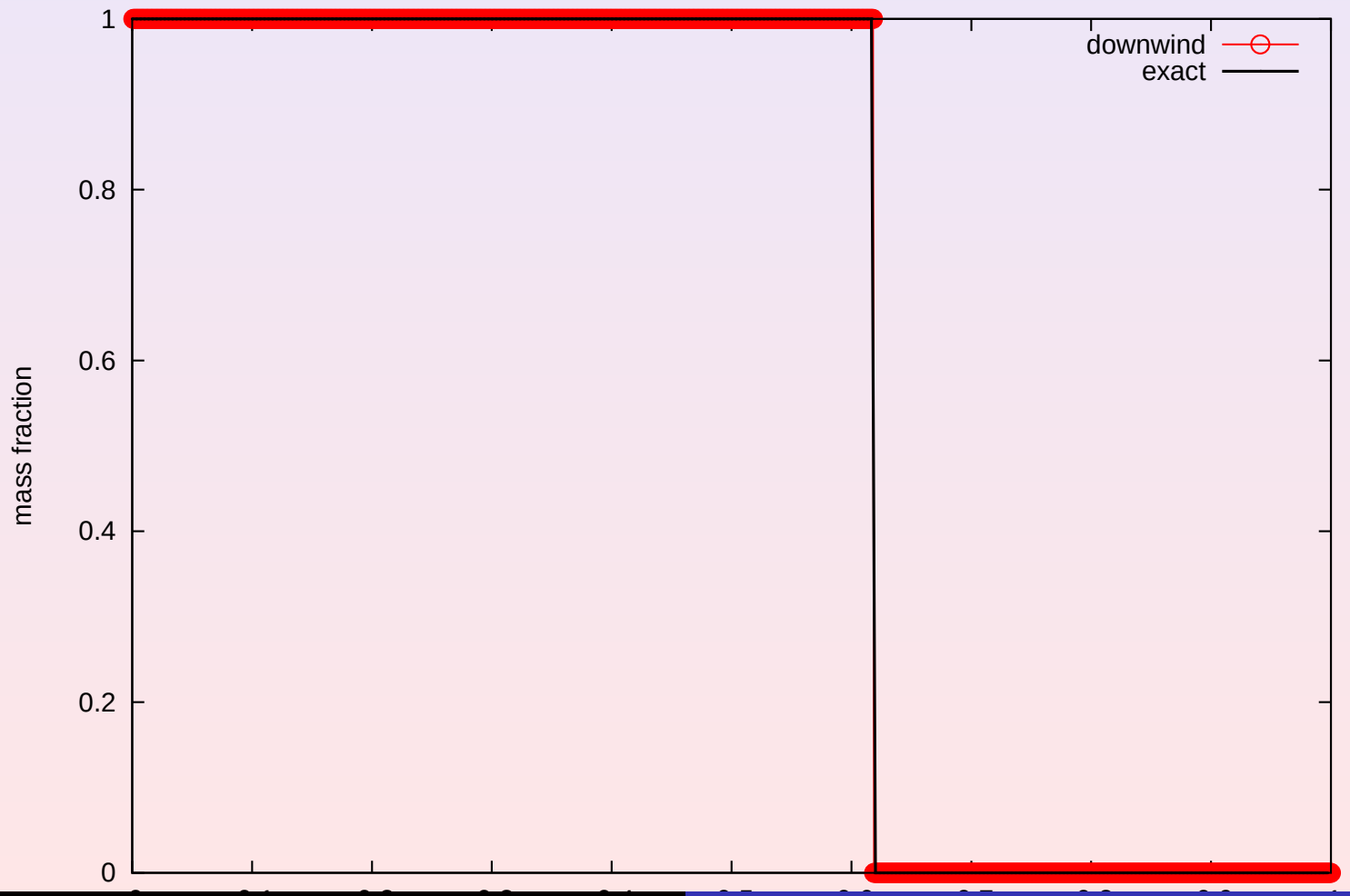
Shock Tube 1 (8): Velocity (50000 cells)

Shock Tube 1 (9): Pressure (50000 cells)

Shock Tube 1 (10): Color Function (50000 cells)



Shock Tube 1 (11): Mass Fraction (50000 cells)



Shock Tube 1 (12): Density (50000 cells)

Shock Tube 2 (1)

Test Description

Riemann Problem with two perfect gases

Left State

$\gamma = 1.67$

$\rho = 14.549030$

$P = 194.0 \times 10^5$

$u = 0.0$

Right State

$\gamma = 1.40$

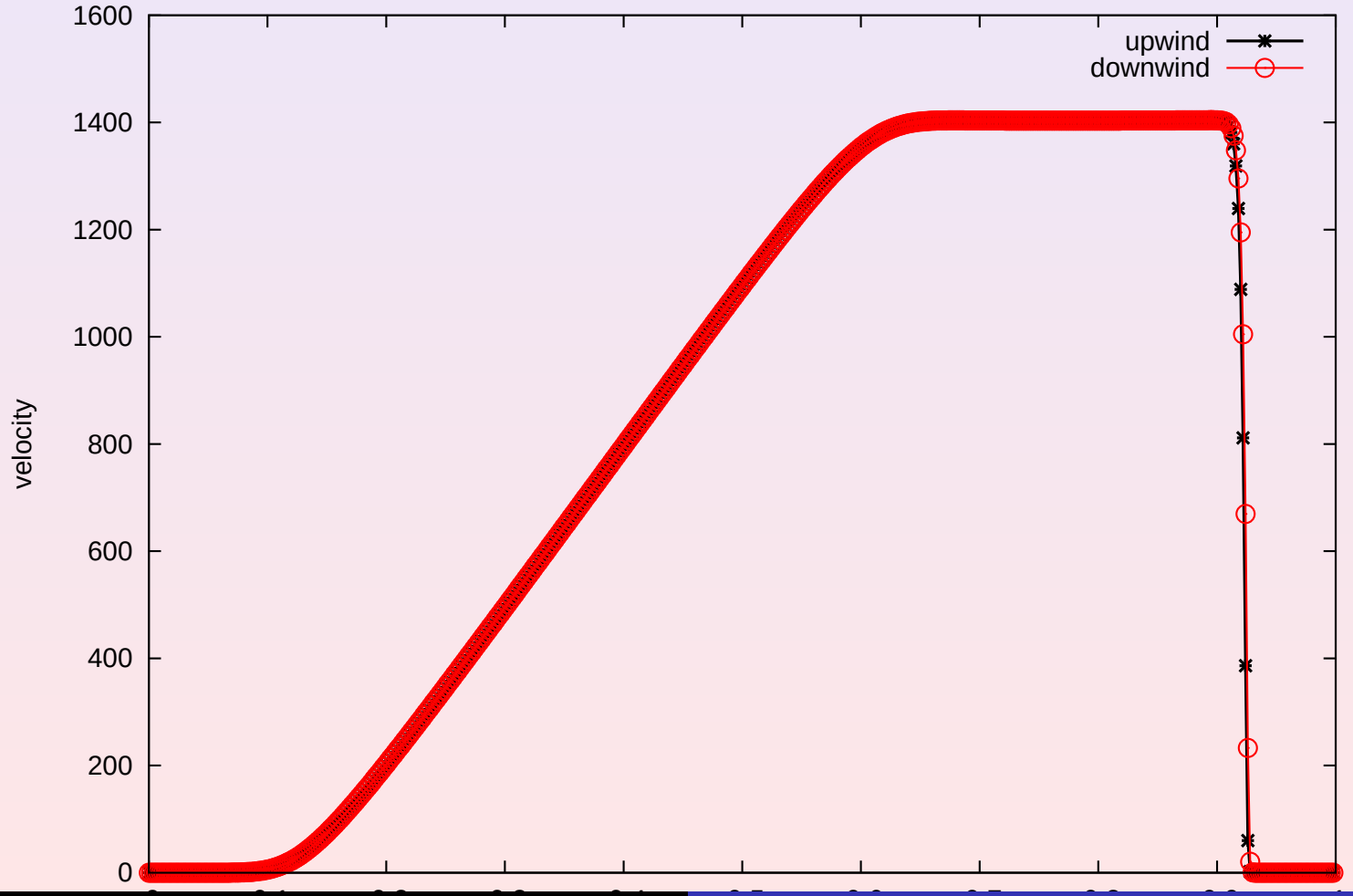
$\rho = 1.163550$

$P = 10^5$

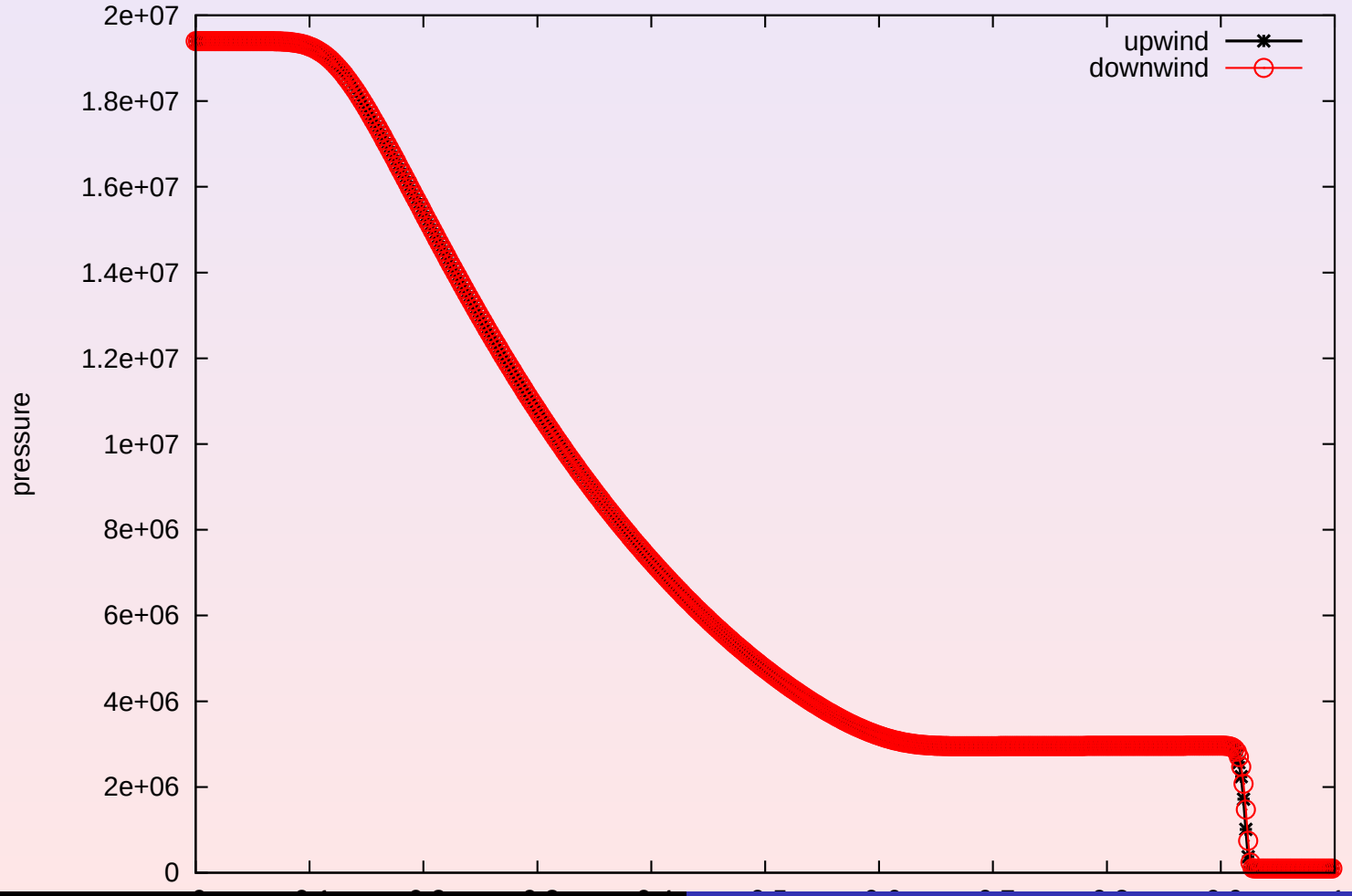
$u = 0.0$

- The domain is discretized over a 500 cells mesh.
- $t = 2.4 \times 10^{-4}$ s

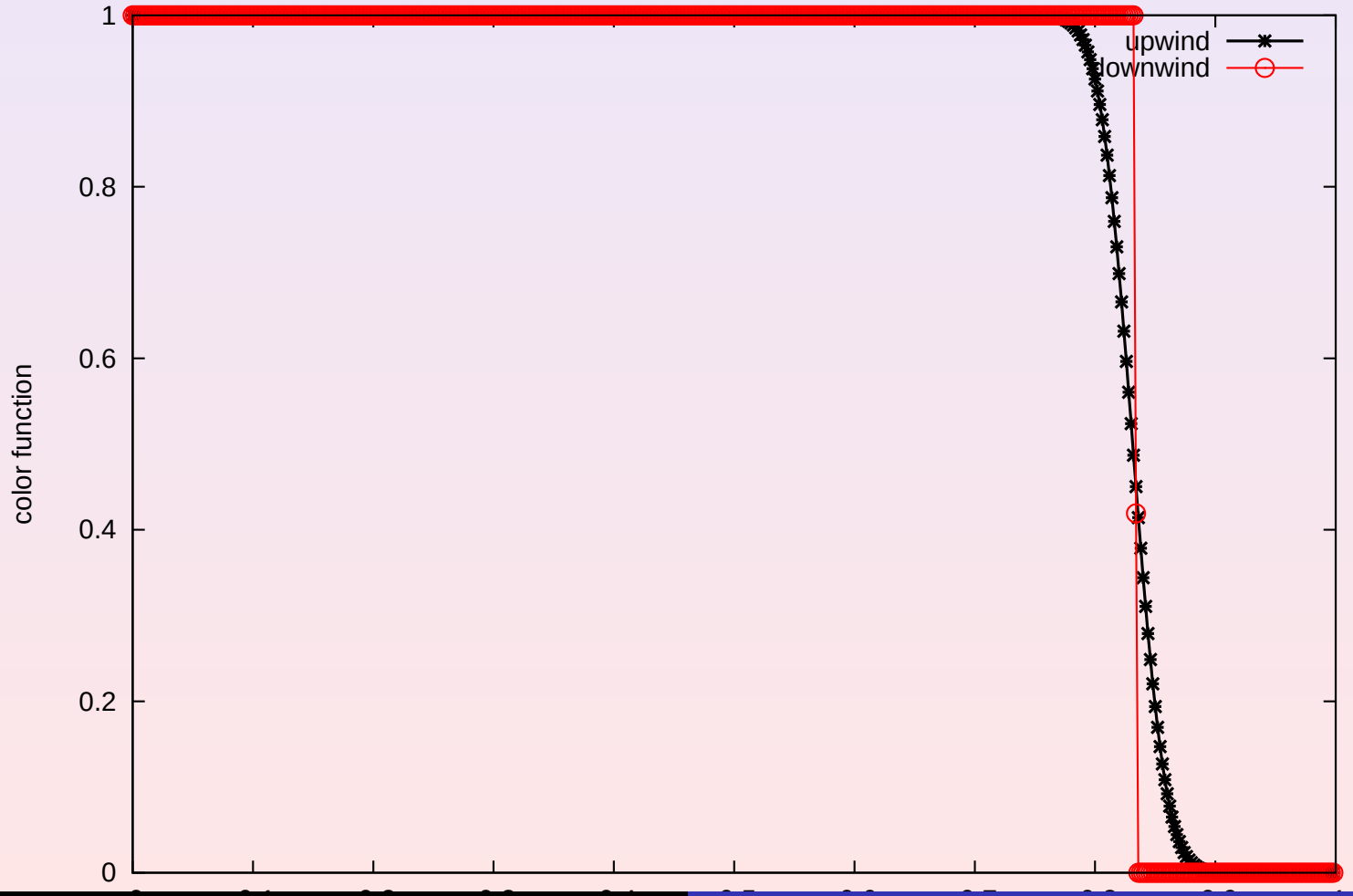
Shock Tube 2 (2): Velocity



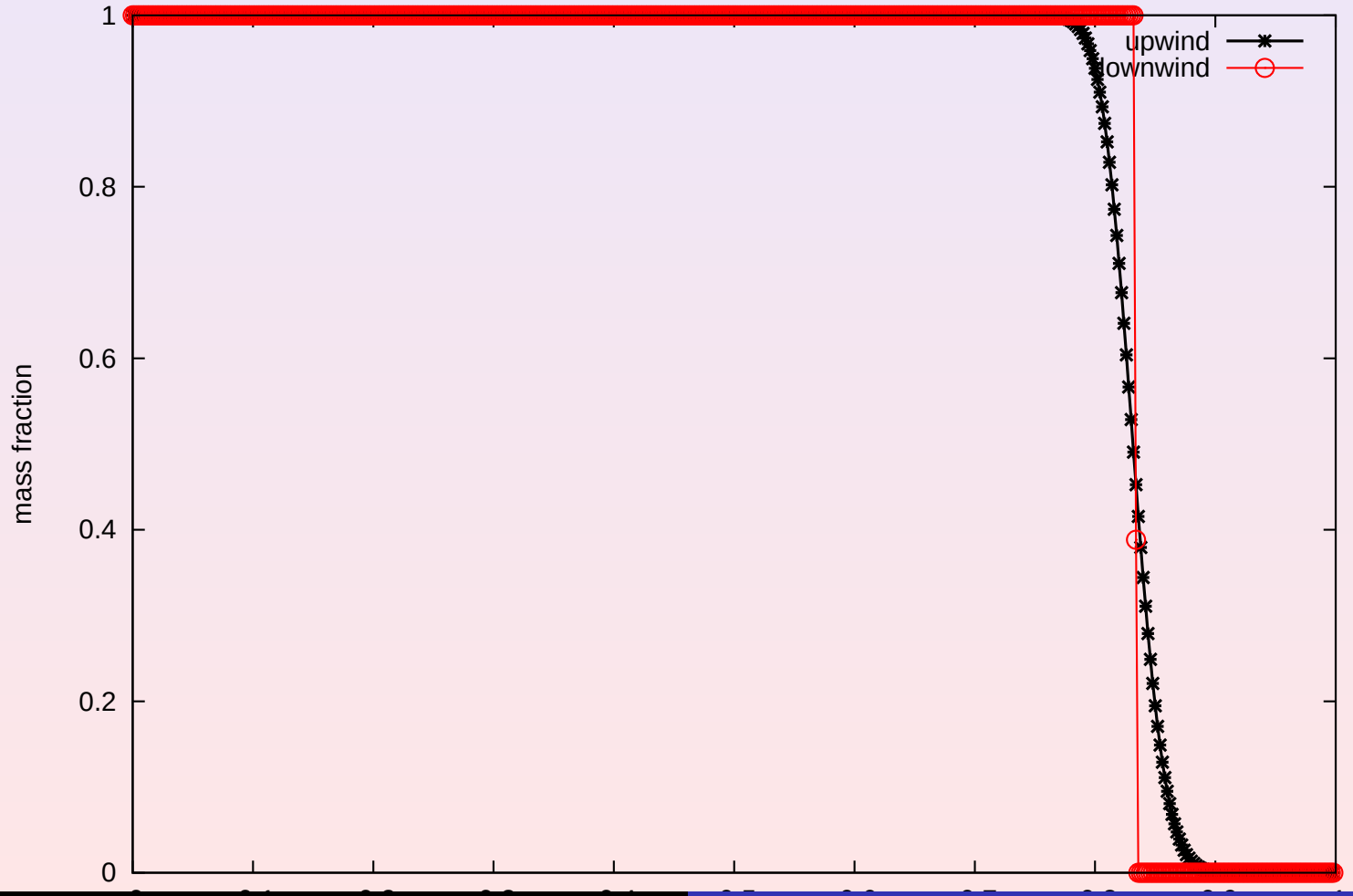
Shock Tube 2 (3): Pressure



Shock Tube 2 (4): Color Function

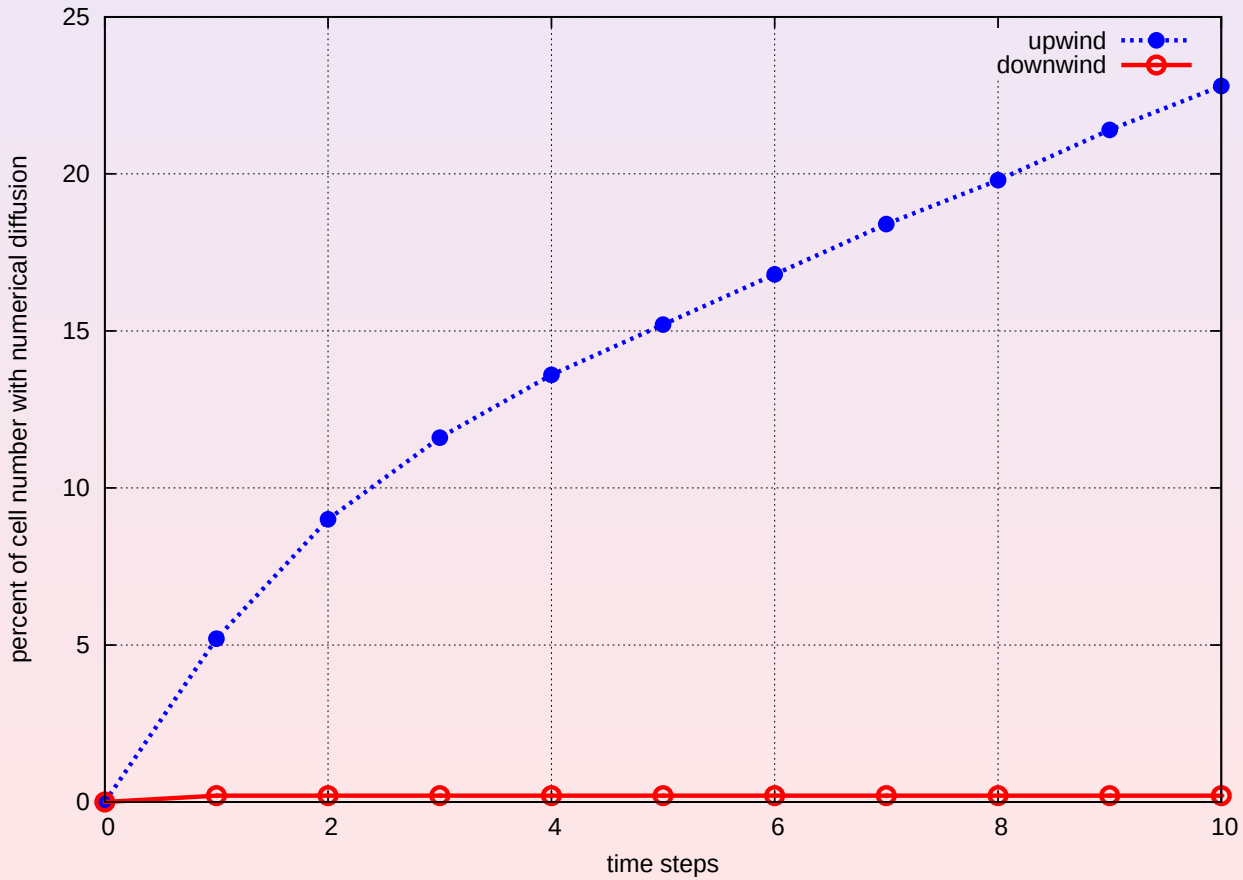


Shock Tube 2 (5): Mass Fraction



Shock Tube 2 (6): Density

Shock Tube 2 (7): Numerical Diffusion of The Color Function



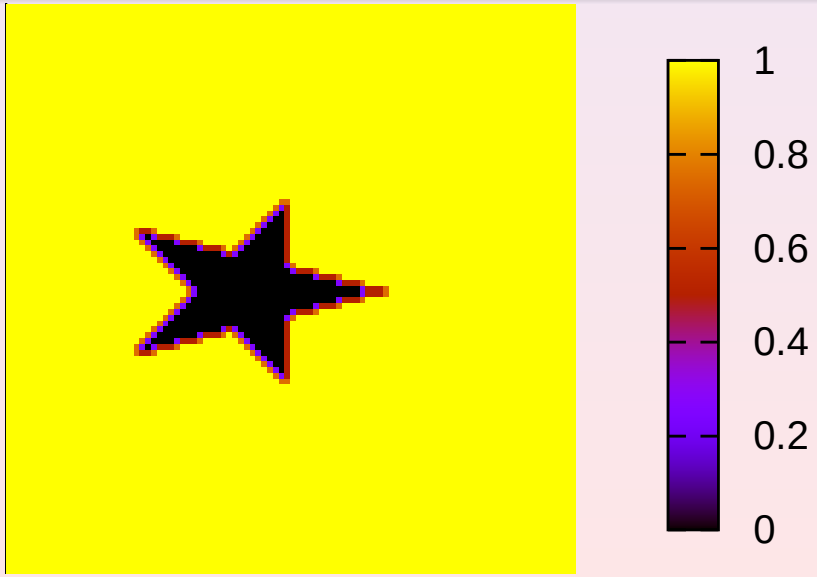
Advection of a 2D Interface (1)

Test Description

advect a 2D inteface

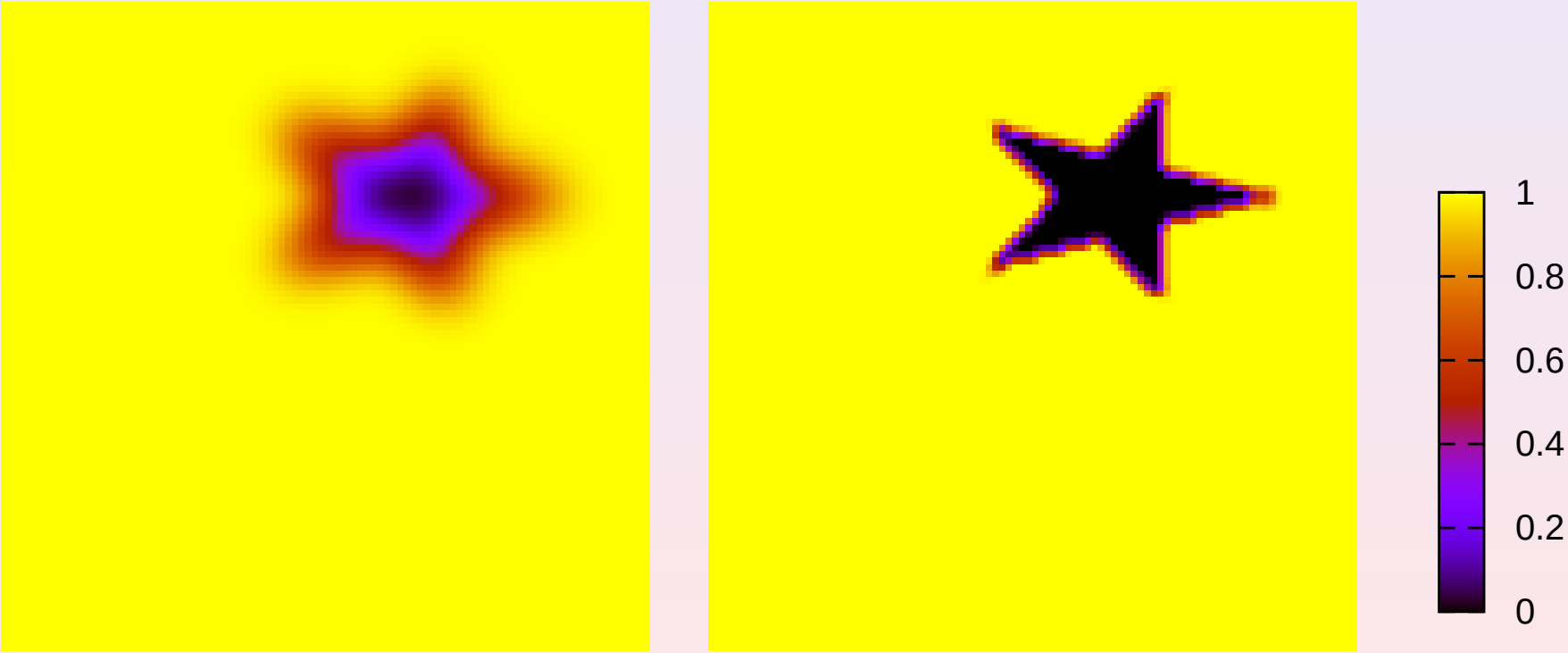
- Domain discretized over a 100×100 mesh
- Velocity $(u_x, u_y) = (1.0, 1.0)$

Color Function
$(t = 0)$



Advection of a 2D Interface (2)

Color Function at $t = 0.2$ s

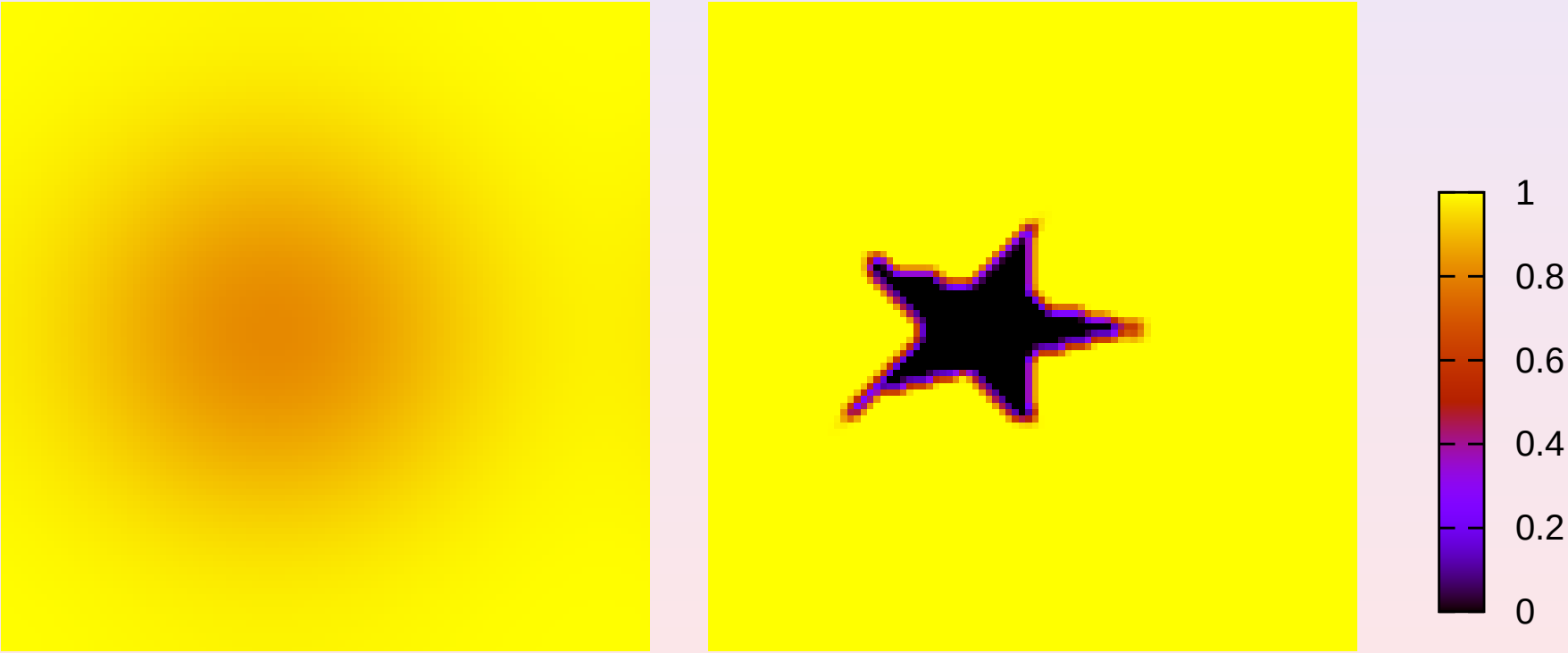


upwind

downwind

Advection of a 2D Interface (3)

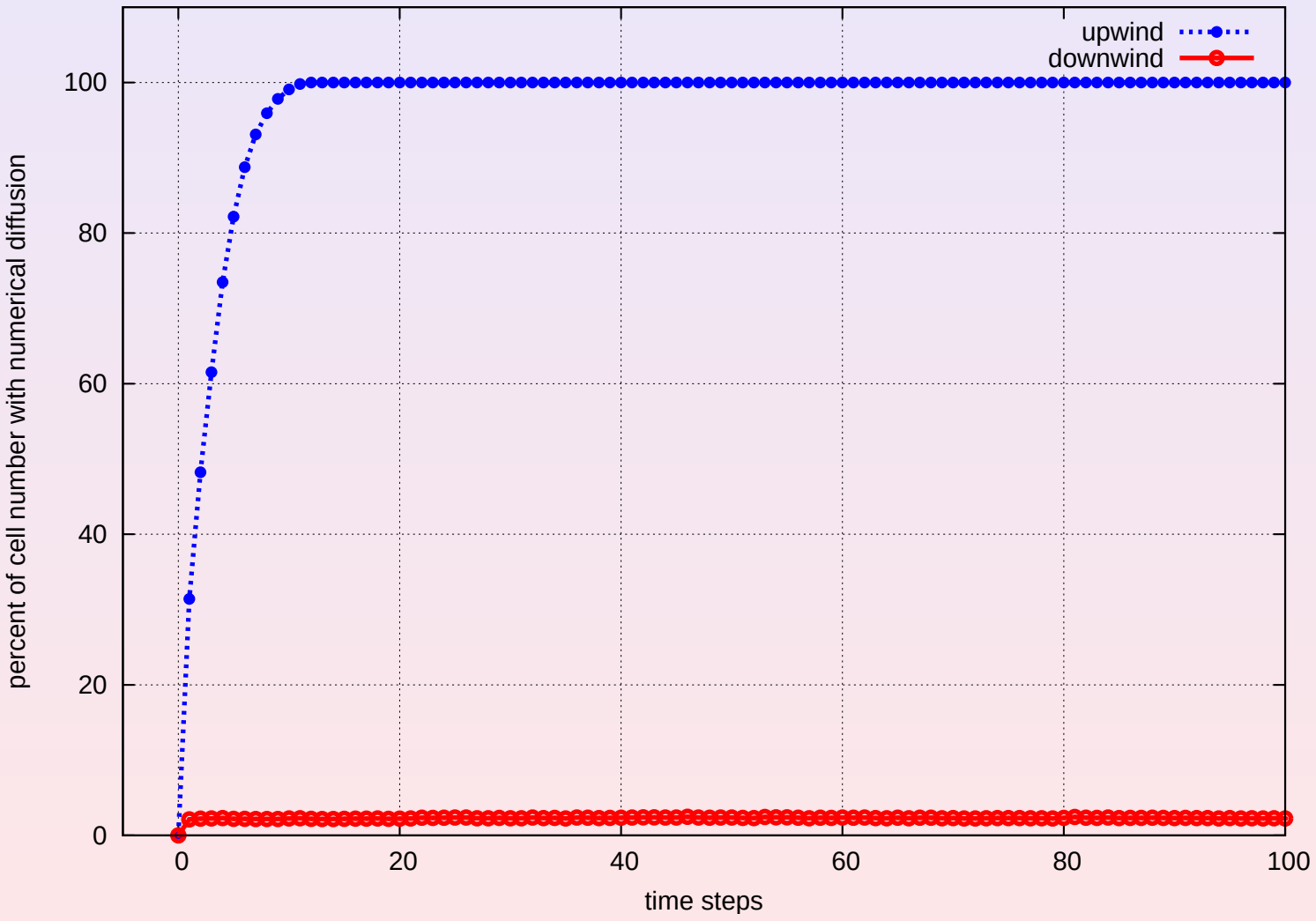
Color Function at $t = 5$ s



upwind

downwind

Advection of a 2D Interface (4): Numerical Diffusion of the Color Function

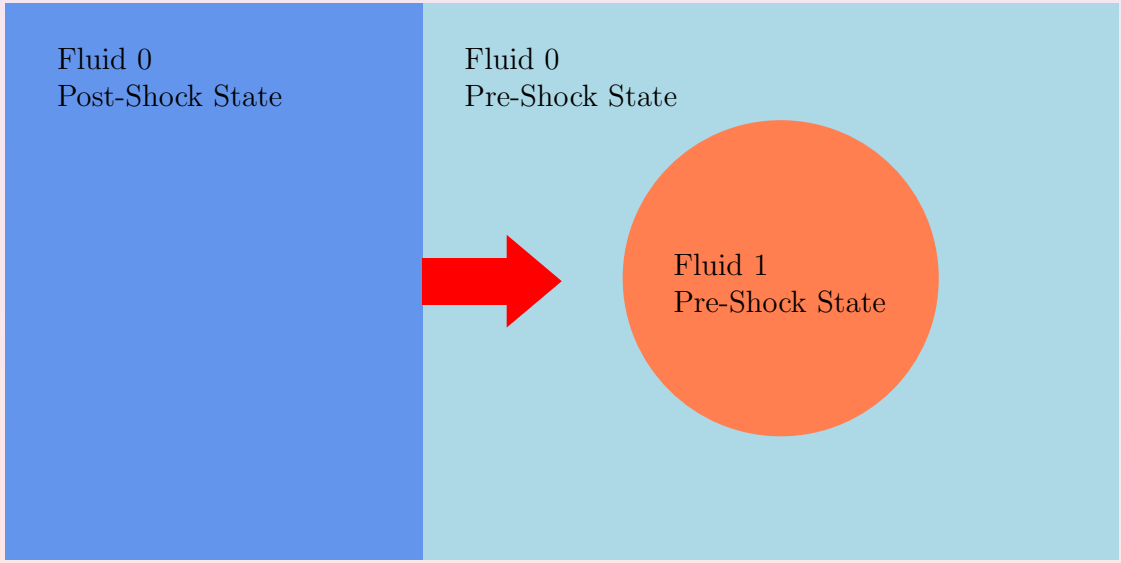


2D Shock/Interface Interaction (1)

Test Description

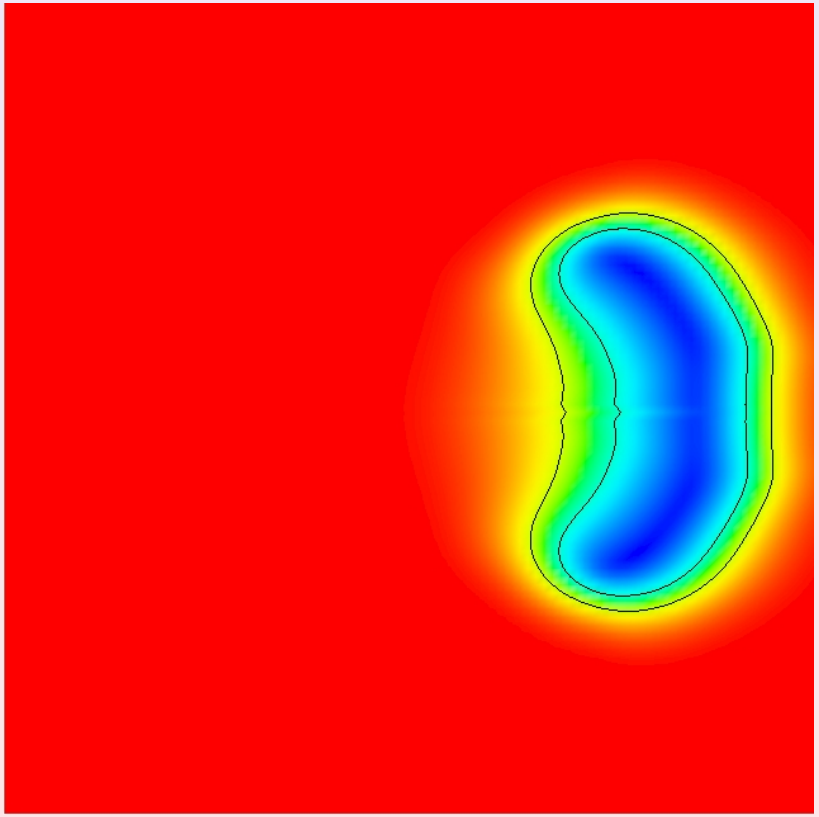
A planar shock hits a bubble initially at rest.

- Domain discretized over a 100×100 mesh
- Two perfect gases

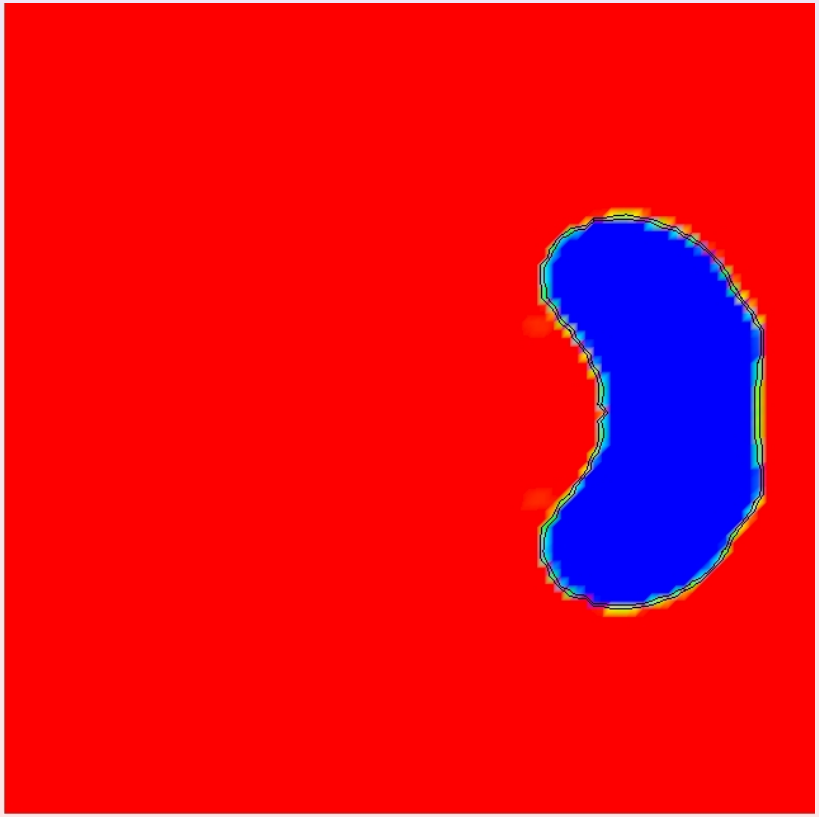


2D Shock/Interface Interaction (2)

Color Function at $t = 0.7$ s



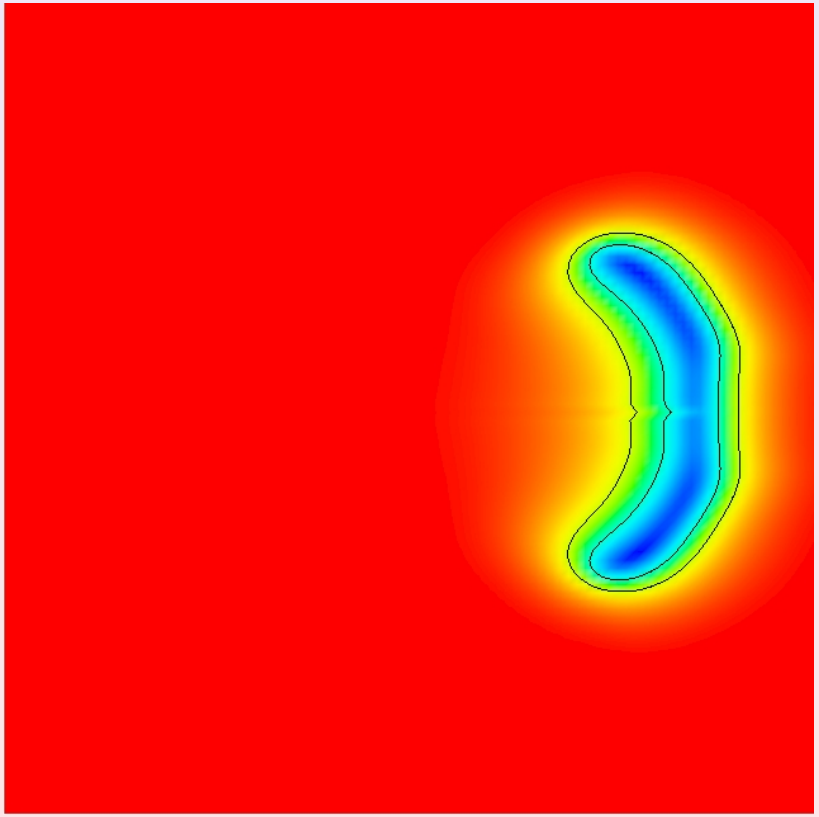
upwind



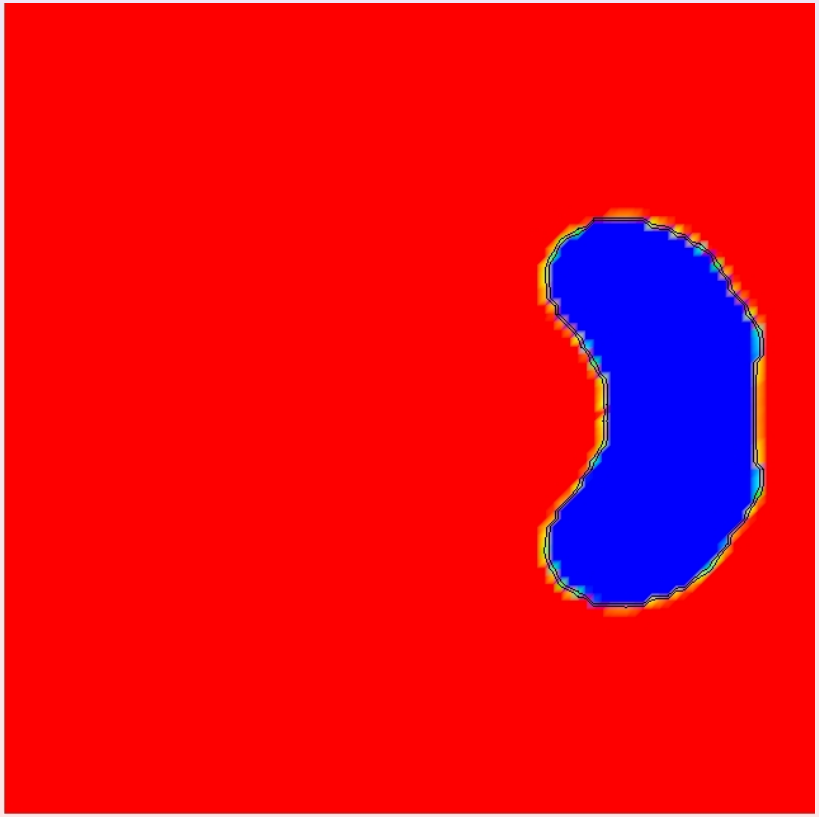
downwind

2D Shock/Interface Interaction (3)

Mass Fraction at $t = 0.7$ s



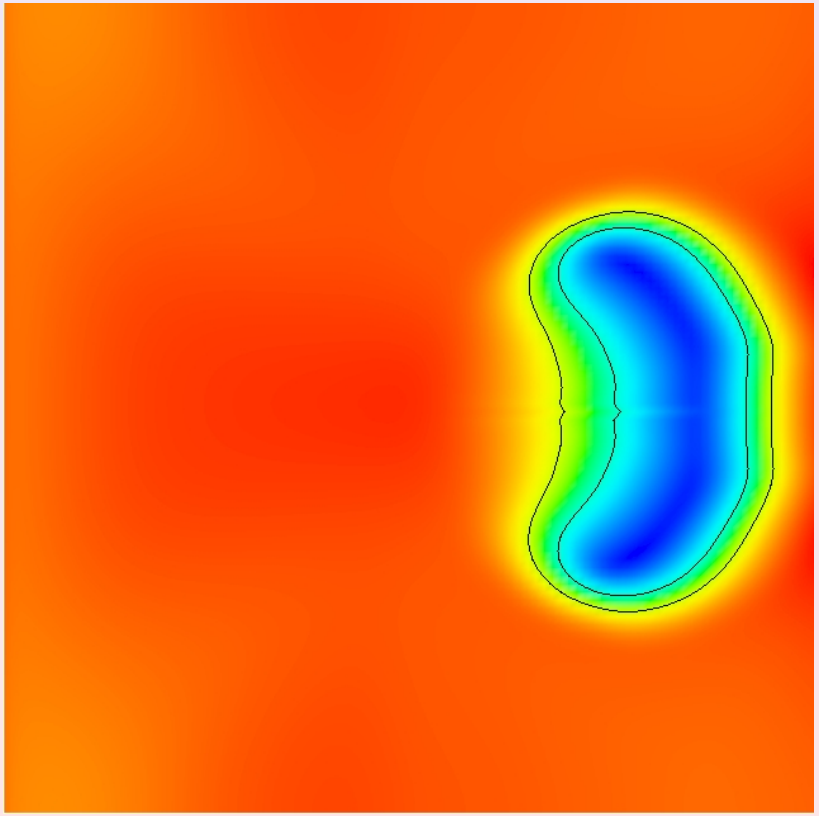
upwind



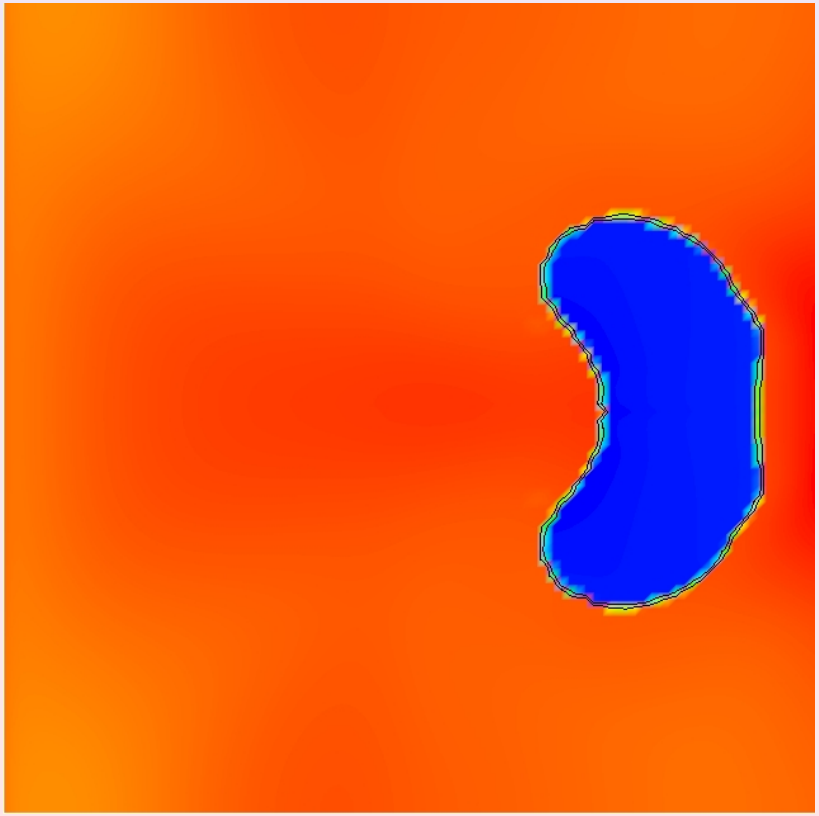
downwind

2D Shock/Interface Interaction (4)

Density at $t = 0.7$ s

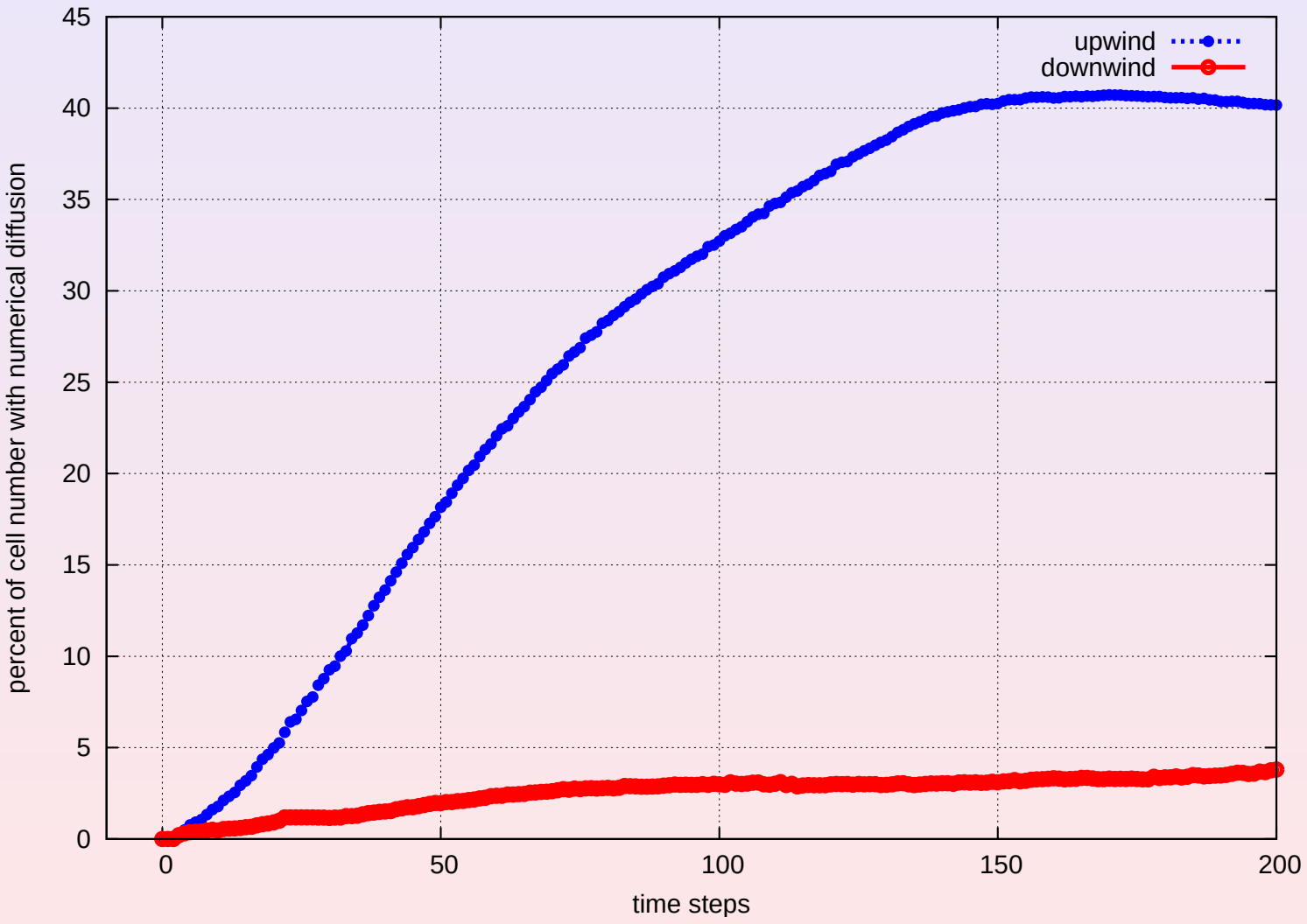


upwind

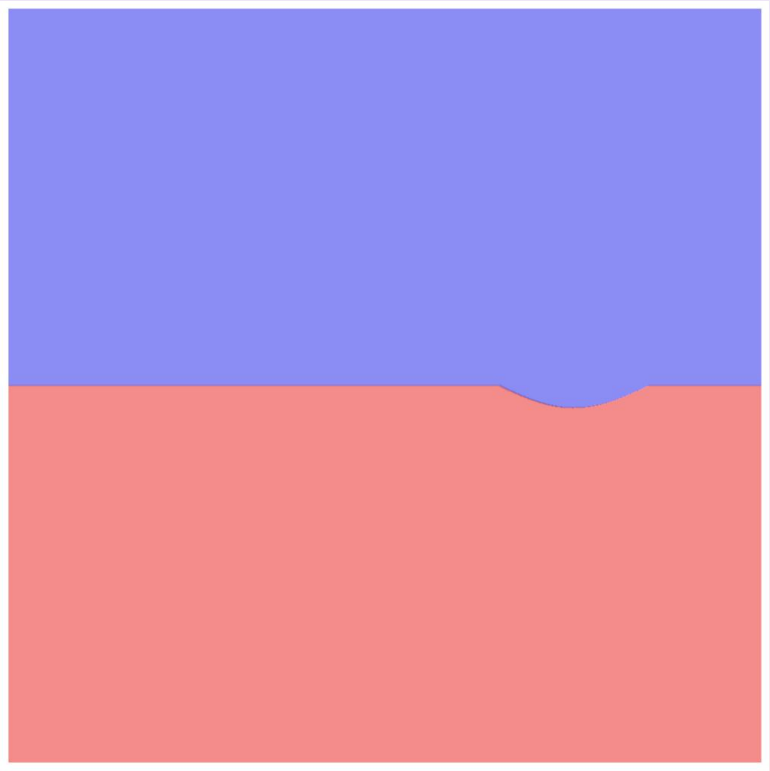


downwind

2D Shock/Interface Interaction (5): Numerical Diffusion of the Color Function



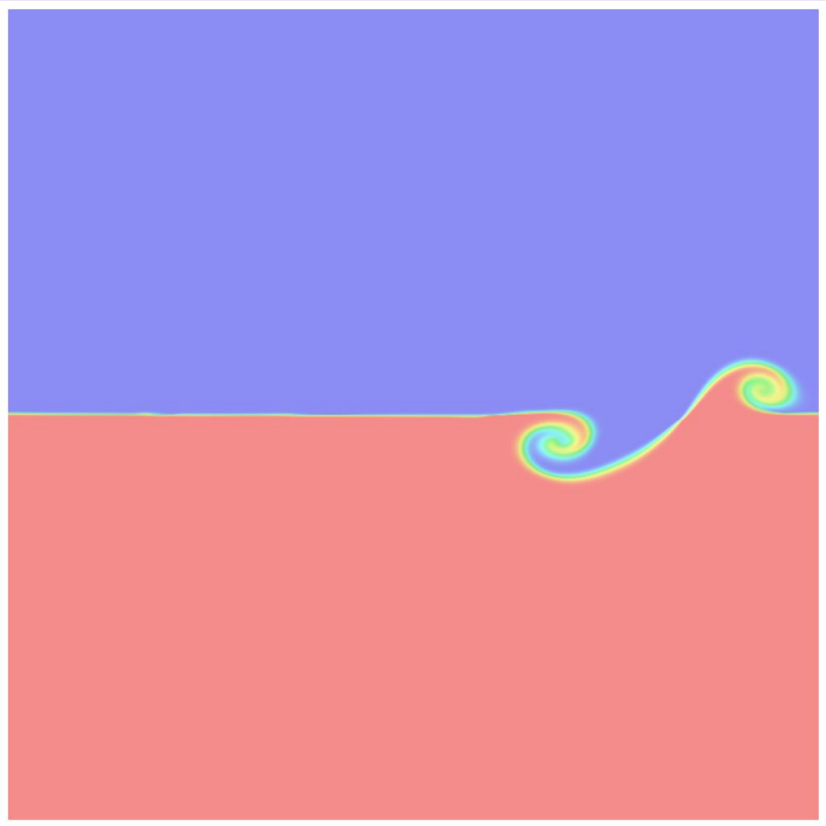
Kelvin-Helmholtz Instability (1)



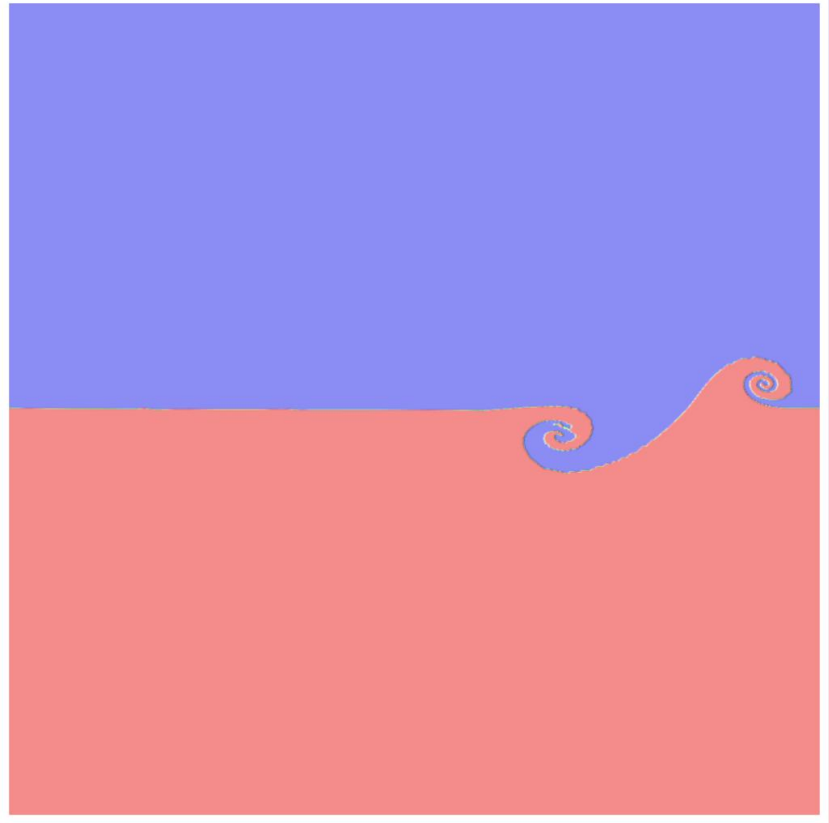
The domain is discretized over a 1000×1000 mesh

Kelvin-Helmholtz Instability (2)

upwind

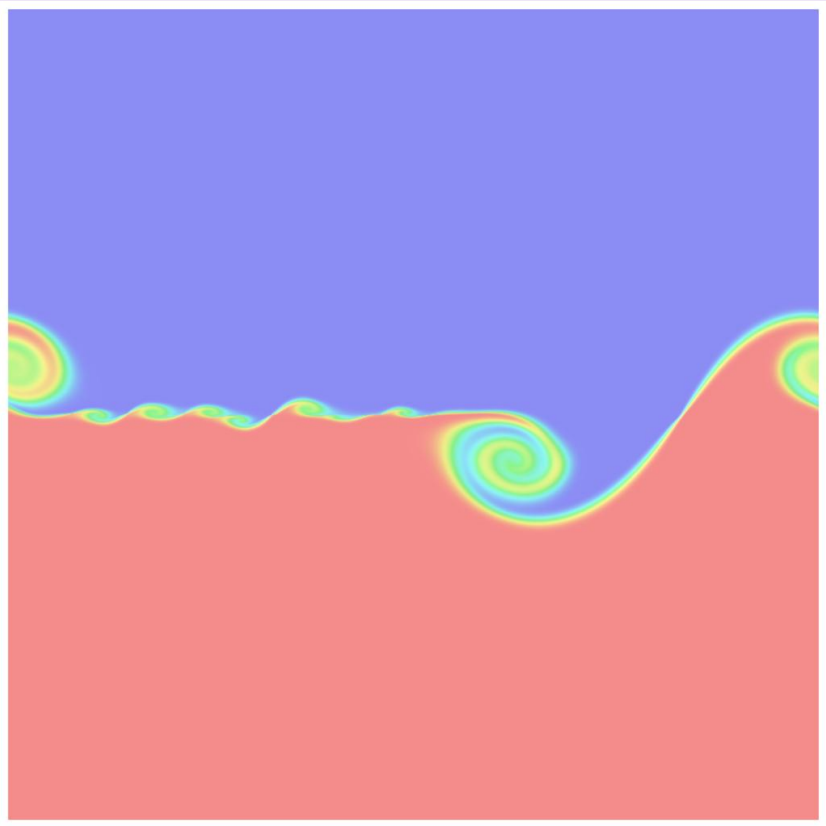


downwind

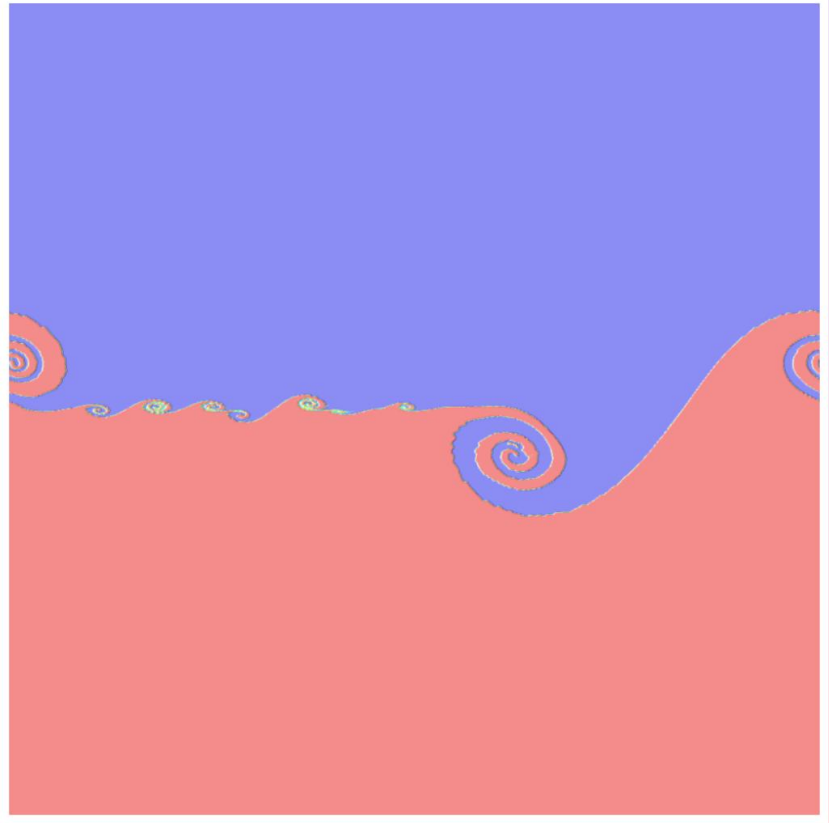


Kelvin-Helmholtz Instability (3)

upwind

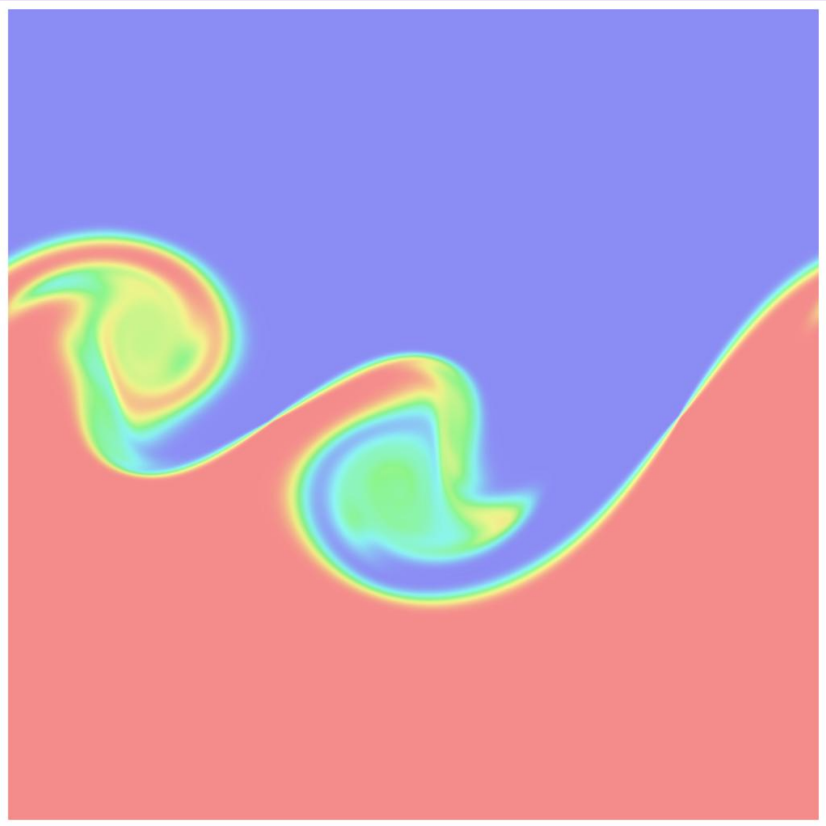


downwind

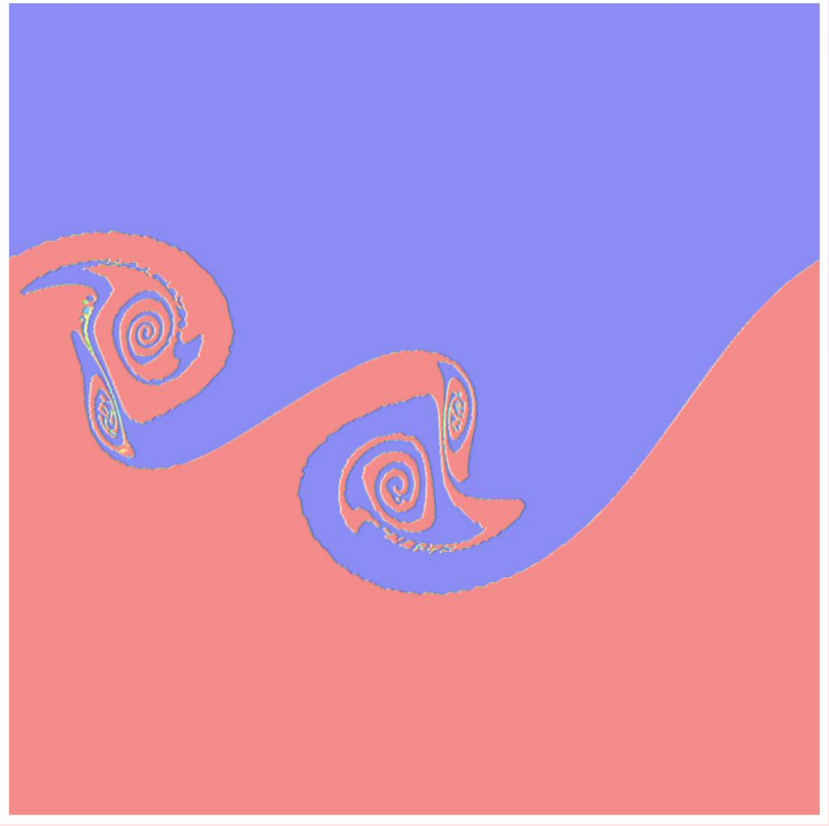


Kelvin-Helmholtz Instability (4)

upwind

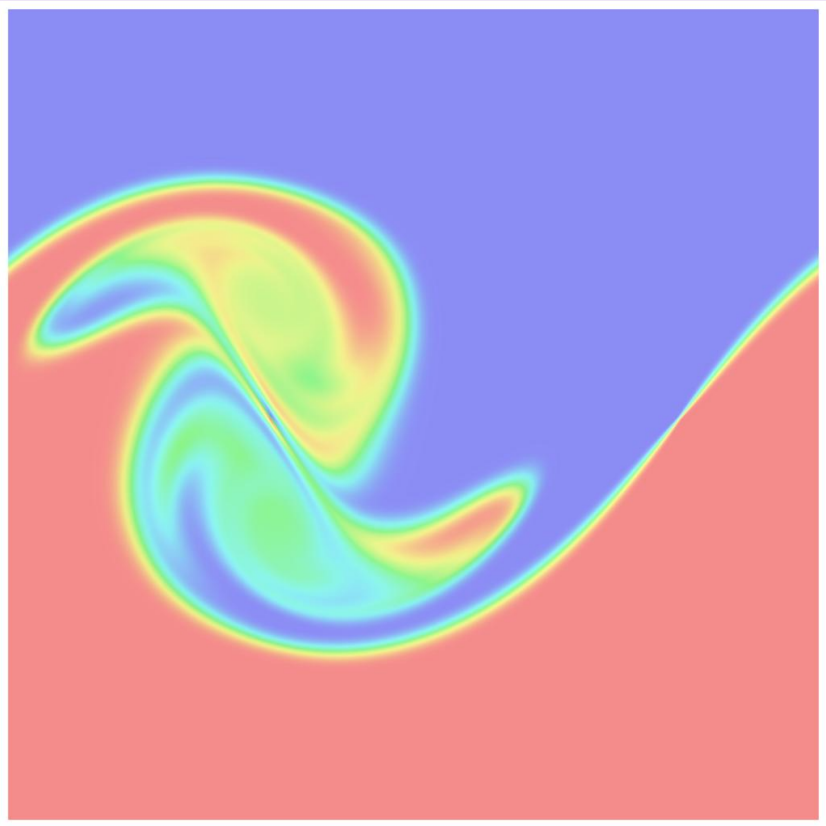


downwind

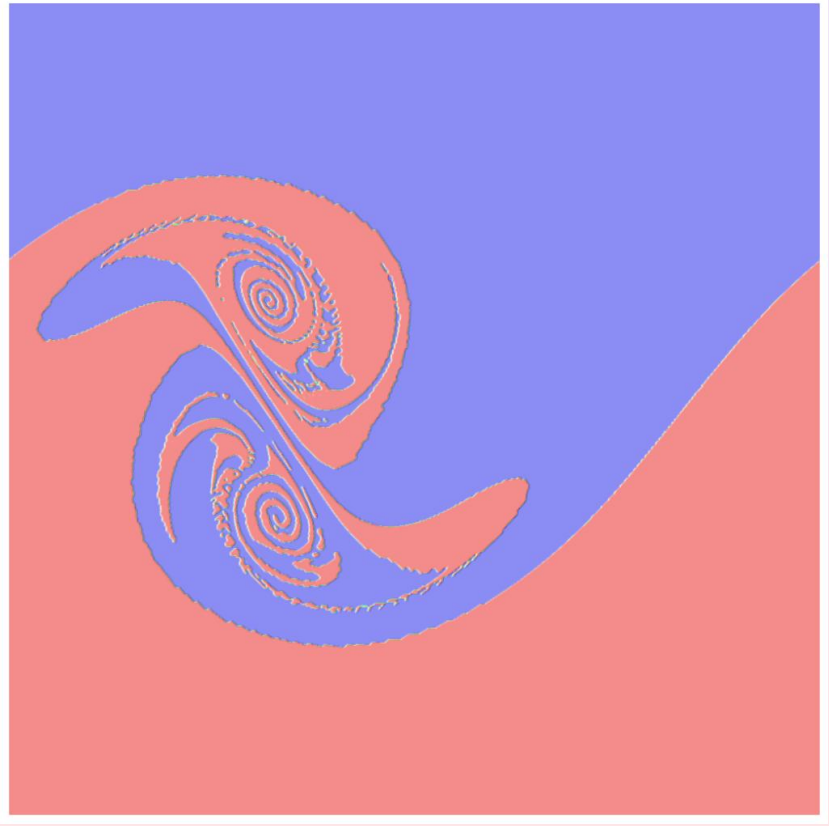


Kelvin-Helmholtz Instability (5)

upwind

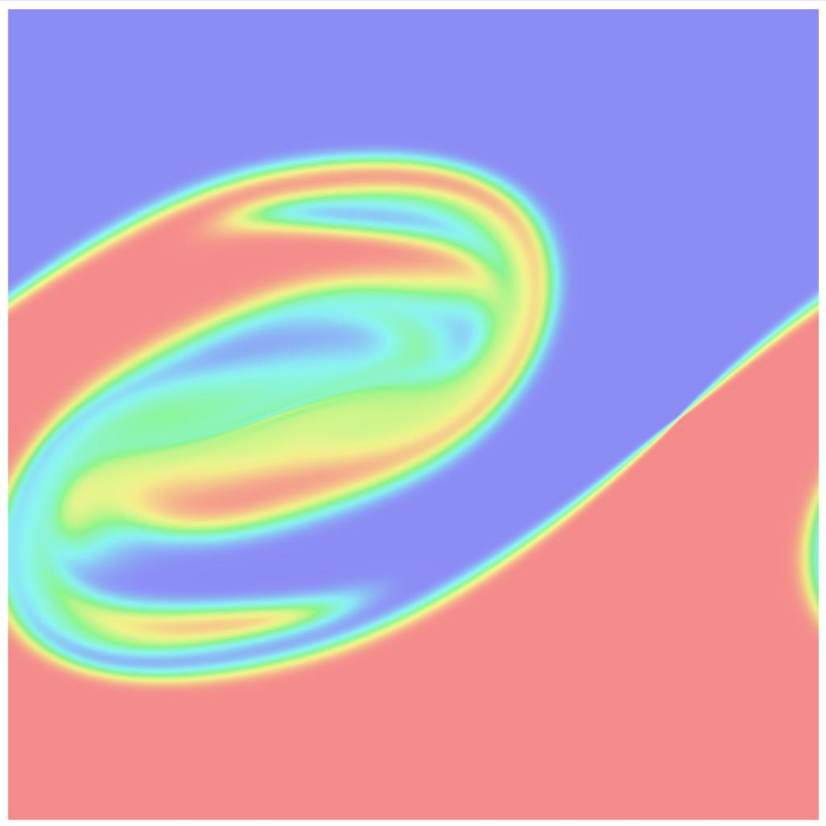


downwind

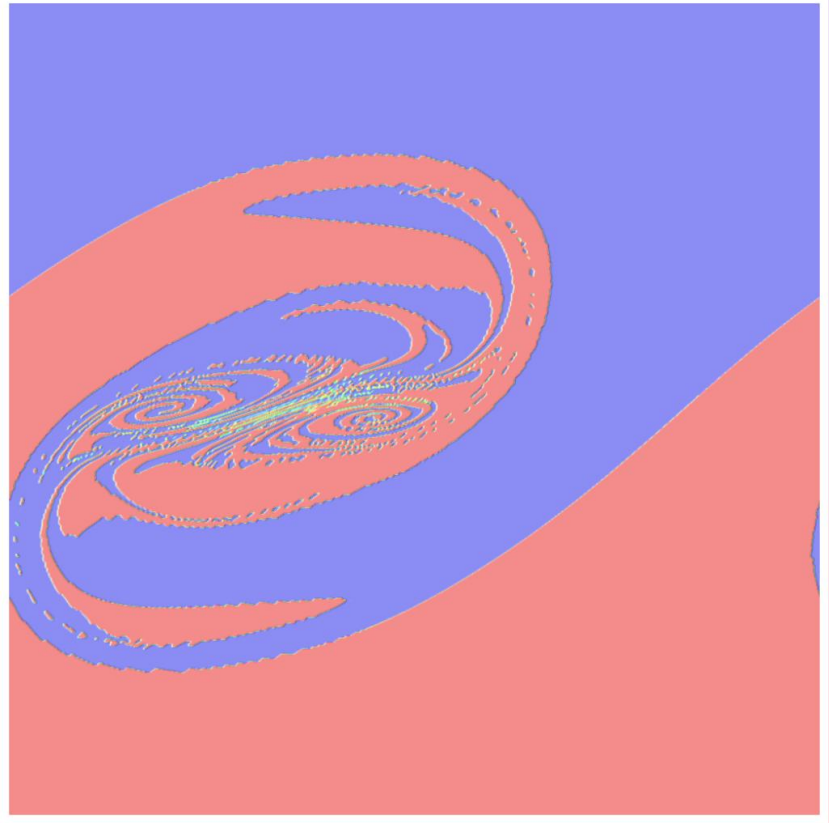


Kelvin-Helmholtz Instability (6)

upwind

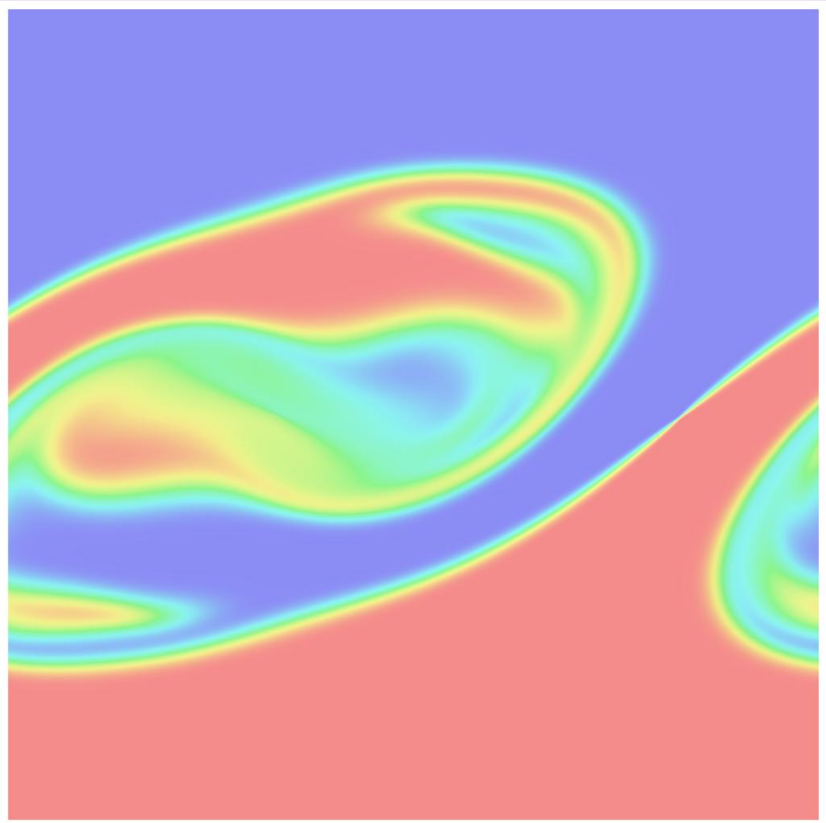


downwind

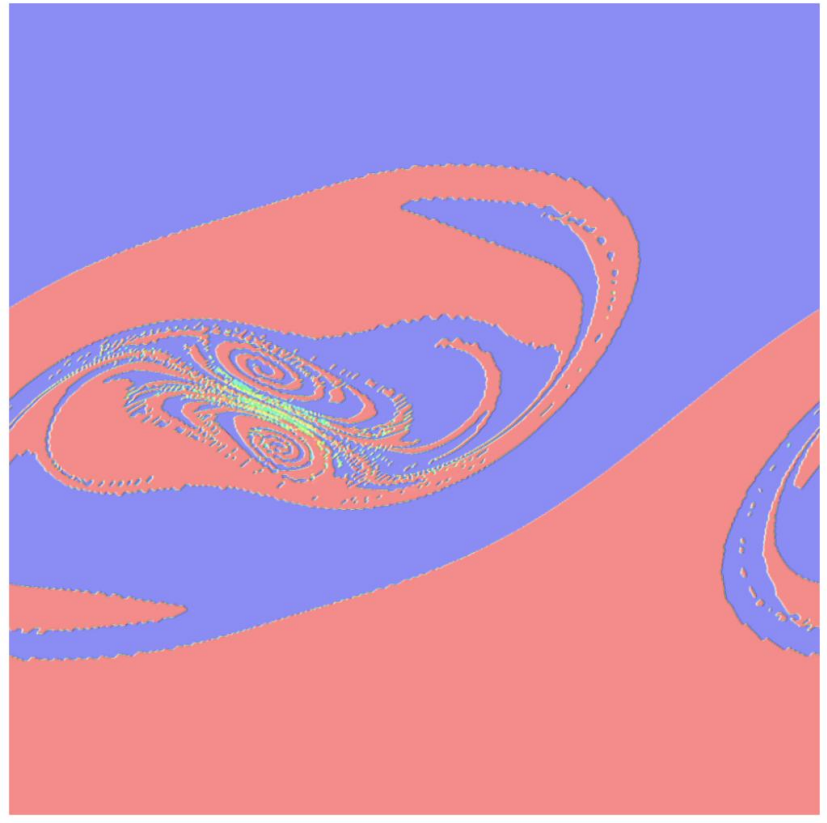


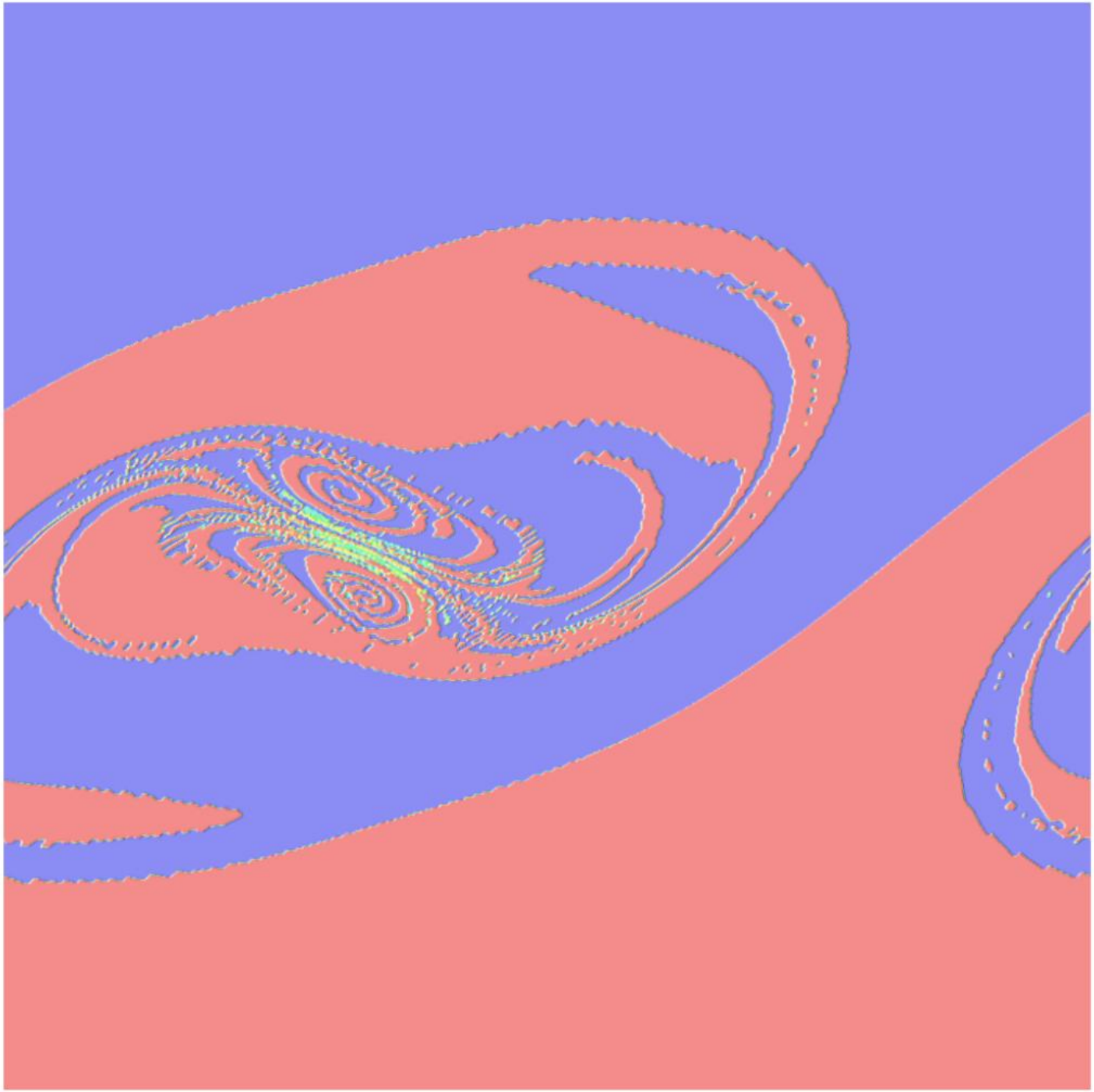
Kelvin-Helmholtz Instability (7)

upwind

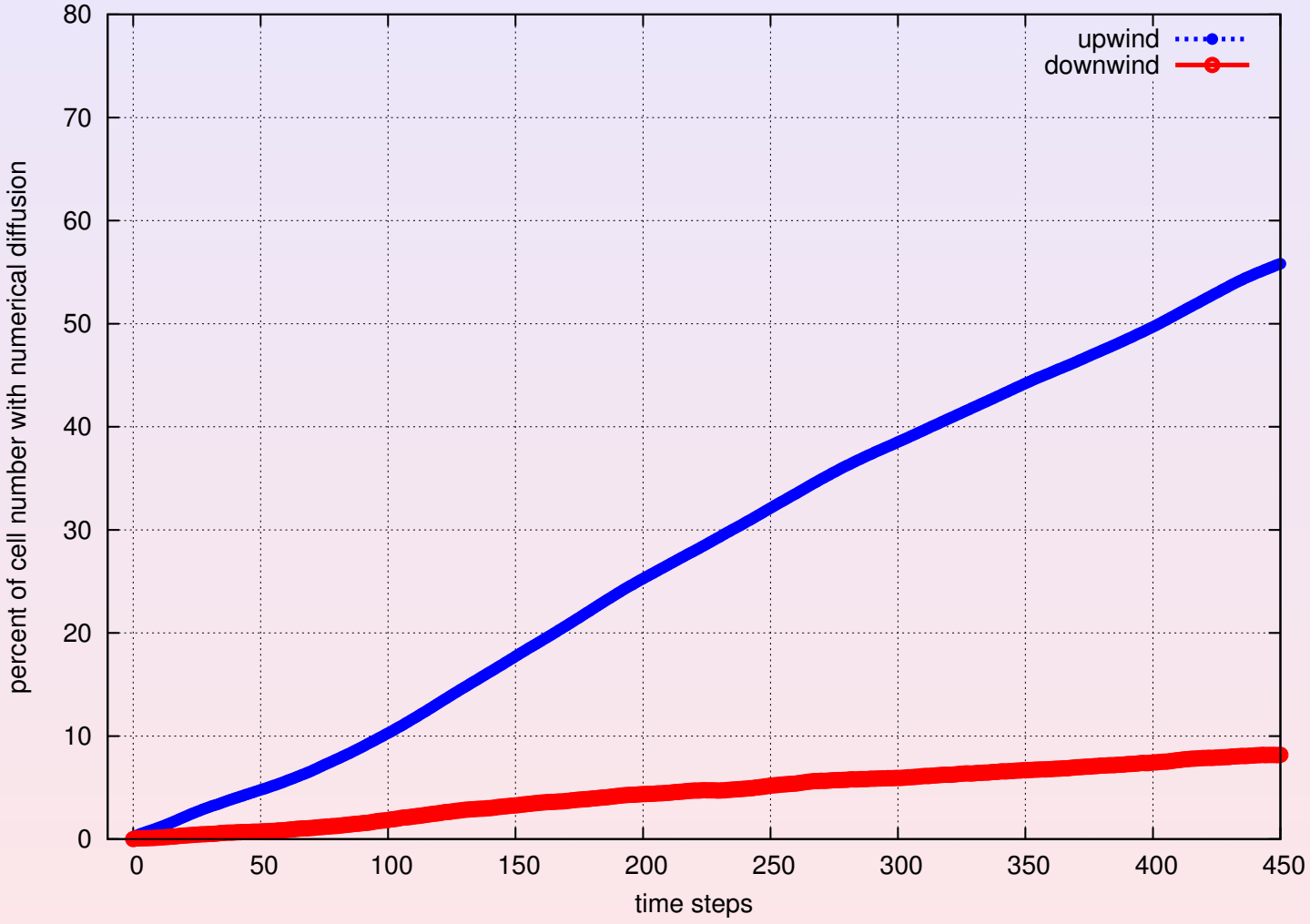


downwind





Kelvin-Helmholtz Instability (9): Numerical Diffusion

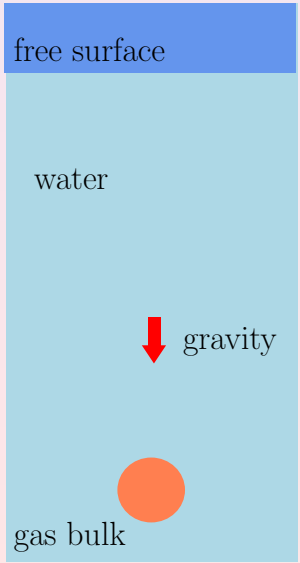


Gas Bulk Rising Towards a Free Surface (1)

Joint work with O. Grégoire (CEA) & P. Salvatore (CEA).

Test Description

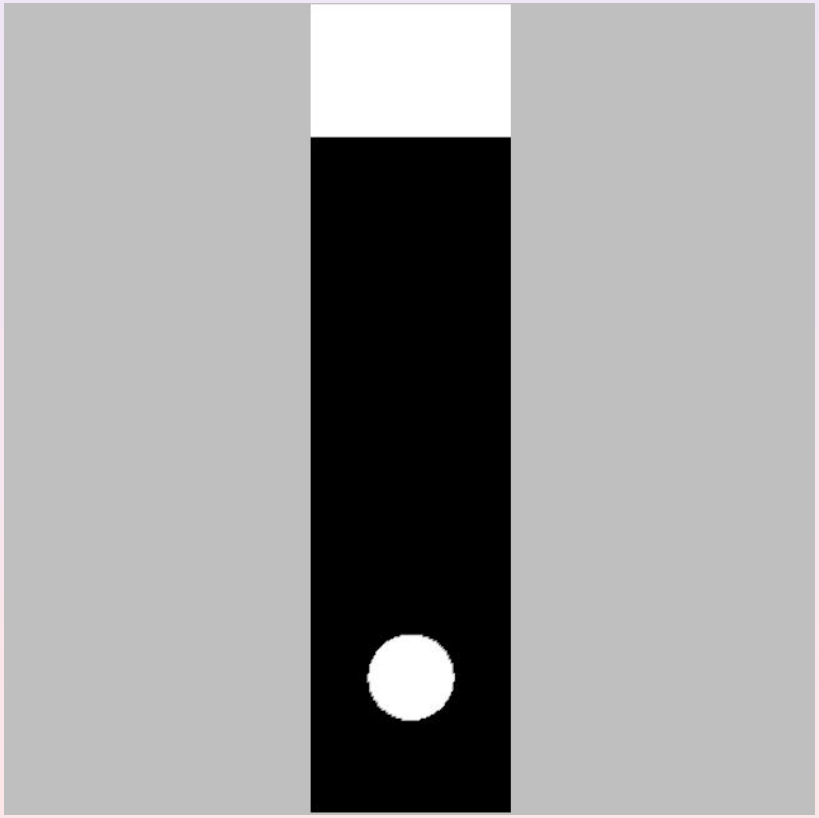
A $1\,\mathrm{m}^3$ volume of gas (Perfect Gas) initially located near the bottom of a $10\,\mathrm{m}$ high water colum (Stiffened Gas) starts rising towards the surface.



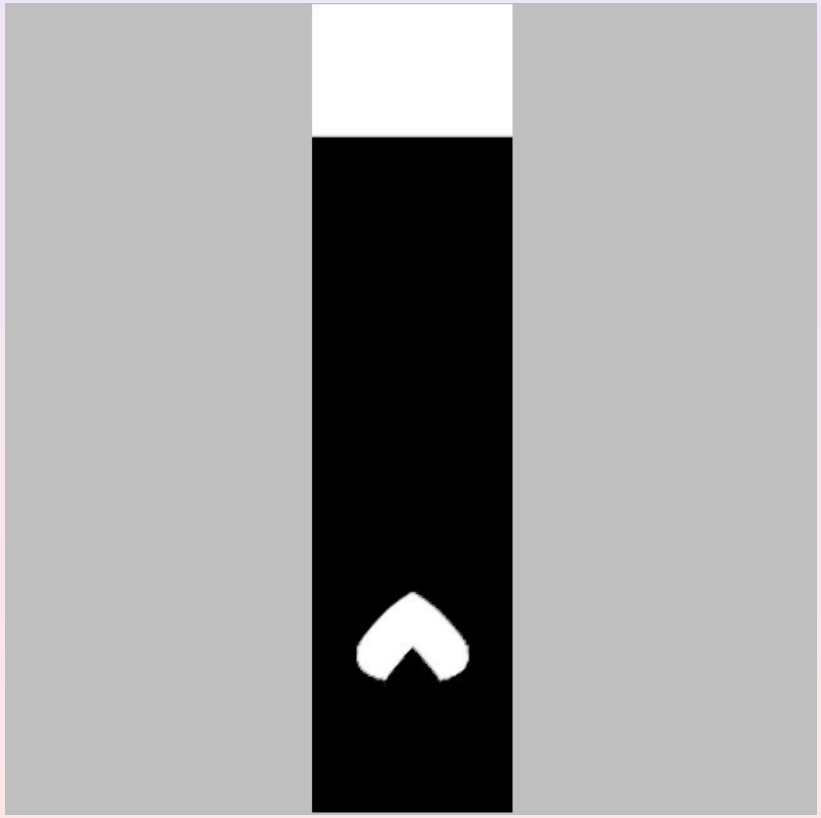
- The domain discretized over a 100×400 mesh
- Density ratio is 500
- Surface Tension via CSF Method (Brackbill)
- MUSCL reconstruction for the interface states

Gas Bulk Rising Towards a Free Surface (2)

Color Function



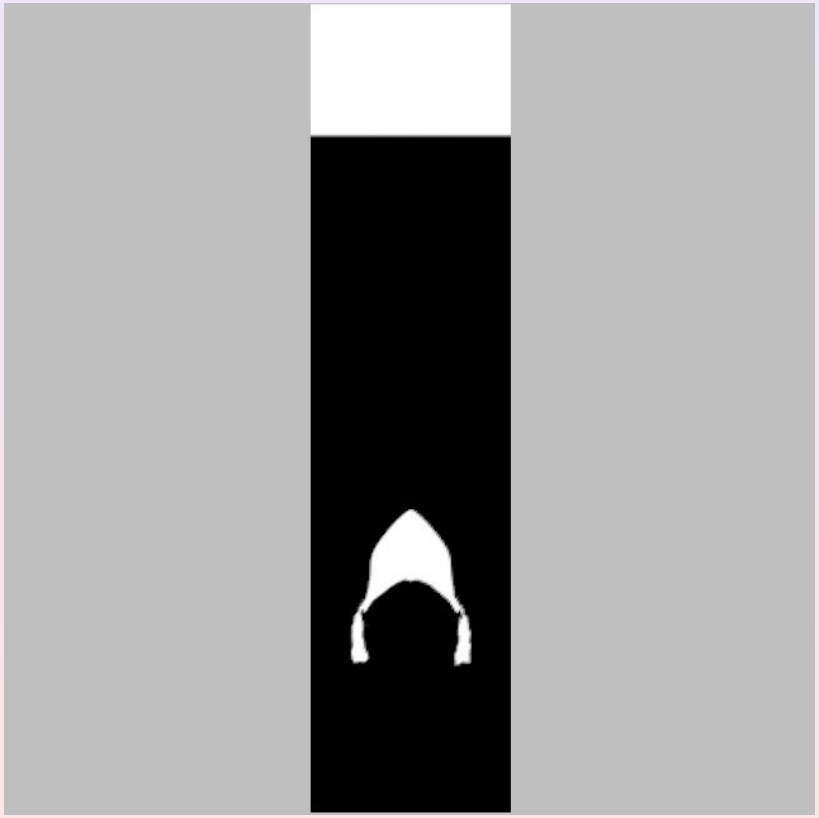
$t = 0$ s



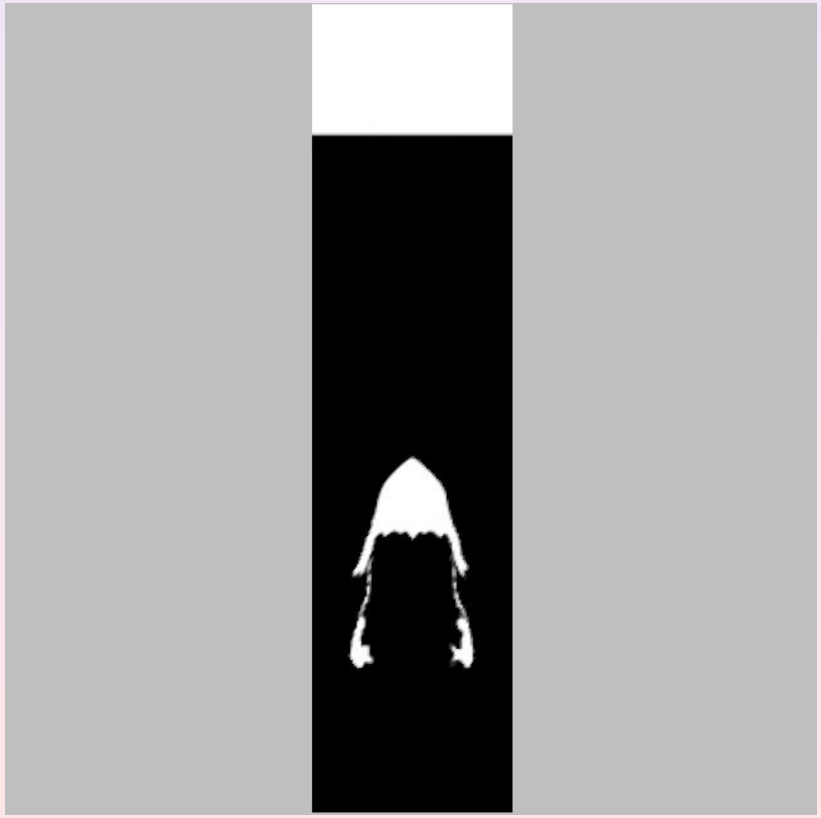
$t = 0.5$ s

Gas Bulk Rising Towards a Free Surface (3)

Color Function



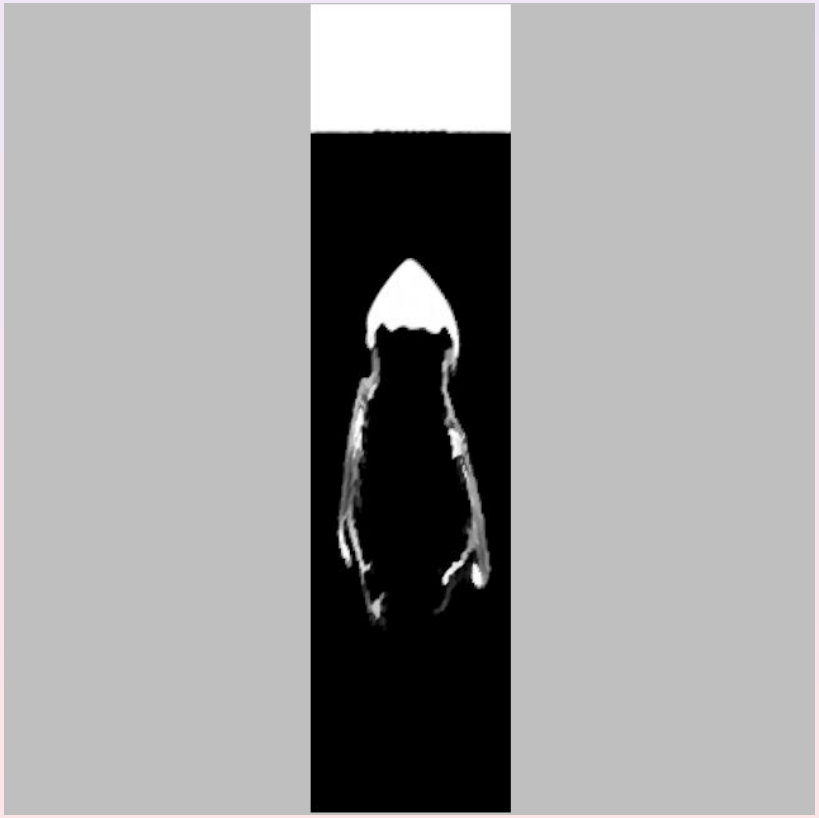
$t = 1.04$ s



$t = 1.37$ s

Gas Bulk Rising Towards a Free Surface (4)

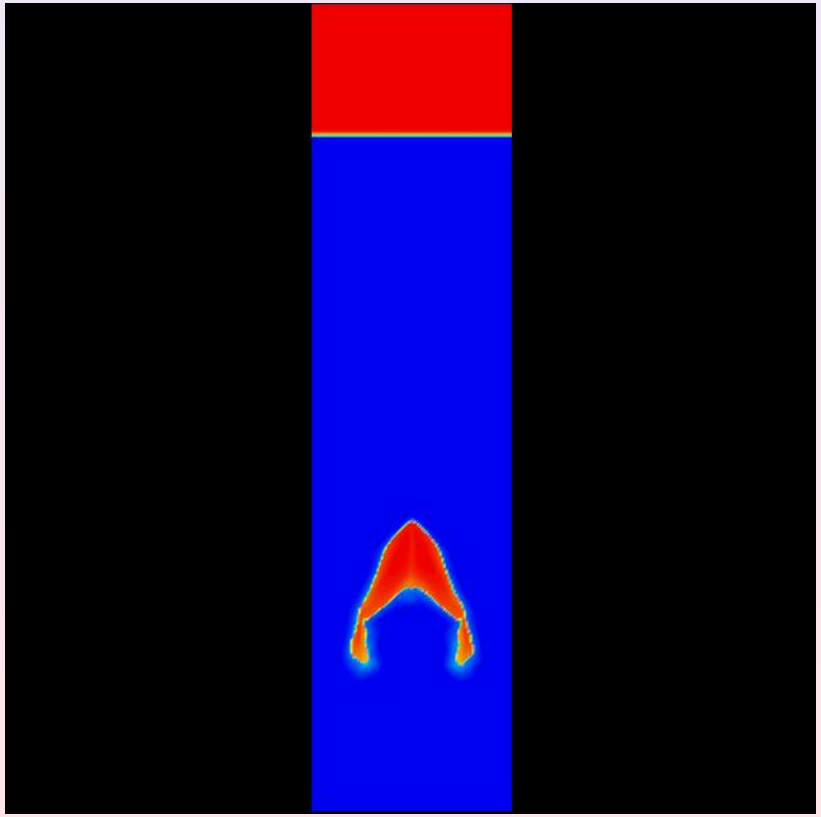
Color Function



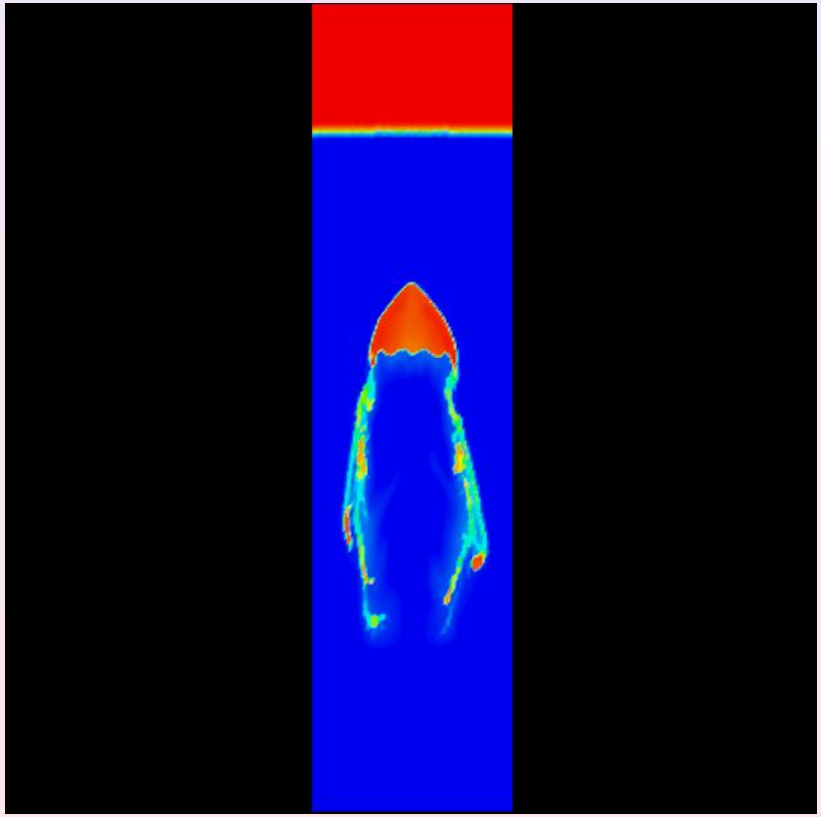
$t = 2.78$ s

Gas Bulk Rising Towards a Free Surface (5)

Density



$t = 0.96$ s



$t = 2.62$ s

Conclusion & Perspectives

- Design of a Lagrange-Remap scheme for the Five-Equation system with isobaric closure
- The scheme is conservative for ρy, ρ, ρu, ρe
- Good treatment of the Riemann Invariants across the material interface
- The scheme works "out of the box": no specific "numerical tuning" is required to optimize the scheme performance
- Anti-diffusive interface advection for both mass fraction y & color function z
- "Positivity" for both y & z variables
- no extra CPU cost
- The Després-Lagoutière approach is not restricted to its originating framework

Application to other models (see Dellacherie, Jaouen)?