SPH improvements for Multi-phase problems in mesoscopic fluids

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Introduction

The objective is show our experience in the implementation:

- **The mesoscopic flows approximation** (S. Litvinov, Ellero, Hu, & Adams, 2010; Vázquez-Quesada, Ellero, & Español, 2009, 2012).
- **Surface-tension formulation** (Adami, Hu, & Adams, 2010; Hu & Adams, 2006).
- **Solid Wall Boundary Condition "dummy particle"** (Adami et al. 2012).

Method

- Consideramos las ecuaciones de *Navier-Stokes em un marco lagrangiano*:

$$\frac{d\rho}{dt} = -\rho\nabla\cdot\mathbf{v}$$

Tension surface force

Pressure

$$\frac{d\mathbf{v}}{dt} = -\frac{1}{\rho}\nabla P + \mathbf{F}^{(\nu)} + \frac{\mathbf{F}^{(ST)}}{\rho}$$

Viscosity force

Method

Equation of state (Pressure)

$$P = B_f \left[\left(\frac{\rho}{\rho_0} \right)^{\gamma} - 1 \right]$$

Viscosity force

$$\mathbf{F}^{(\nu)} = \nu \nabla^2 \mathbf{v}$$

For an immiscible mixture the surface force

$$\mathbf{F}^{(TS)} = \alpha \left(\nabla \cdot \hat{\mathbf{n}} \right) \hat{\mathbf{n}}$$

SPH – Macroscopic flow

- **Density equation**

$$\langle \rho_i \rangle = \sum_{j=1}^{N} m_j W_{ij},$$

- **Pressure[1]**

$$\left\langle \frac{d\mathbf{v}^{(P)}}{dt} \right\rangle = -\frac{1}{\rho}\nabla P = -\frac{1}{m_i}\sum_{j=1}^{N}\left(P_i V_i^2 + P_j V_j^2\right)\frac{\partial W_{ij}}{\partial r_{ij}}\boldsymbol{\eta}_{ij},$$

[1]Adami, Hu, & Adams, 2010; Hu & Adams, 2006.

SPH – Macroscopic flow

- **Viscosity force**[1]

$$\left\langle \frac{d\mathbf{v}^{(\nu)}}{dt} \right\rangle = \mathbf{F}^{(\nu)} = \frac{1}{m_i} \sum_{j=1}^{N} \frac{2\eta_j \eta_i}{\eta_j + \eta_i} \left(V_i^2 + V_j^2 \right) \frac{(\mathbf{v}_i - \mathbf{v}_j)}{r_{ij}} \frac{\partial W_{ij}}{\partial r_{ij}}$$

- **Surface force**[2]

$$\mathbf{F}^{(ST)} = \nabla \times \prod^{(TS)}$$

Continuous Surface Force model (CSF)[1]

$$\prod^{(TS)} = \alpha \frac{1}{|\nabla C|} \left(\frac{1}{d} \mathbf{I} |\nabla C|^2 - \nabla C \nabla C \right)$$

[1]Adami, Hu, & Adams, 2010; [2] Morris, 2000 .

SPH – Macroscopic flow

- **Surface force**

The part of the acceleration particle due to surface tension (CSF)[1]:

$$\left\langle \frac{d\mathbf{v}^P}{dt} \right\rangle = \mathbf{F}^{(TS)} = \frac{1}{m_i} \sum_{j=1}^{N} \left(\Pi_i^{(TS)} V_i^2 + \Pi_j^{(TS)} V_j^2 \right) \cdot \frac{\partial W_{ij}}{\partial r_{ij}} \boldsymbol{\eta}_{ij},$$

$$\nabla C_i^{kl} = \sigma_i \sum_{j=1}^{N} \left[\frac{C_i^l}{\sigma_i^2} + \frac{C_j^l}{\sigma_j^2} \right] \frac{\partial W_{ij}}{\partial r_{ij}} \boldsymbol{\eta}_{ij}, \qquad l \neq k$$

$$\Pi_{kl}^{(TS)} = \alpha^{kl} \frac{1}{|\nabla C^{kl}|} \left(\frac{1}{d} \mathbf{I} \left| \nabla C^{kl} \right|^2 - \nabla C^{kl} \nabla C^{kl} \right), \qquad l \neq k$$

$$\Pi_i^{(TS)} = \sum_{l=1}^{N} \Pi_{ij}^{(TS)}, \quad l \neq k$$

[1] Hu & Adams, 2006.

SPH – Mesoscopic hydrodynamics

- **GENERIC Methodology[1]:** SDPD formulation.

Thermal fluctuations

$$d\tilde{m}_i = 0,$$

$$d\tilde{\mathbf{P}}_i = \sum_{j=1}^{N} B_{ij} d\overline{\overline{W}}_{ij} \boldsymbol{\eta}_{ij},$$

$d\overline{\overline{W}}_{ij} =$ The traceless symmetric part of a tensor of indepent increments of wiener process

Boltzmann constant and Temperature

$$B_{ij} = \left[-\frac{8k_B T \eta_i \eta_j}{\eta_i + \eta_j} \left(V_i^2 + V_j^2 \right) \frac{1}{r_{ij}} \frac{\partial W_{ij}}{\partial r_{ij}} \right]^{\frac{1}{2}}$$

[1]S. Litvinov, Ellero, Hu, & Adams, 2010; Español & Revenga 2003.

SPH – Mesoscopic hydrodynamics

- **GENERIC Methodology[1]:** SDPD formulation.

$$d\mathbf{v}_i = \left\langle \frac{d\mathbf{v}^{(P)}}{dt} \right\rangle dt + \mathbf{F}^{(\nu)} dt + \mathbf{F}^{(TS)} dt + \frac{1}{m_i} d\tilde{\mathbf{P}}_i,$$

Characteristics with SDPD[1]:

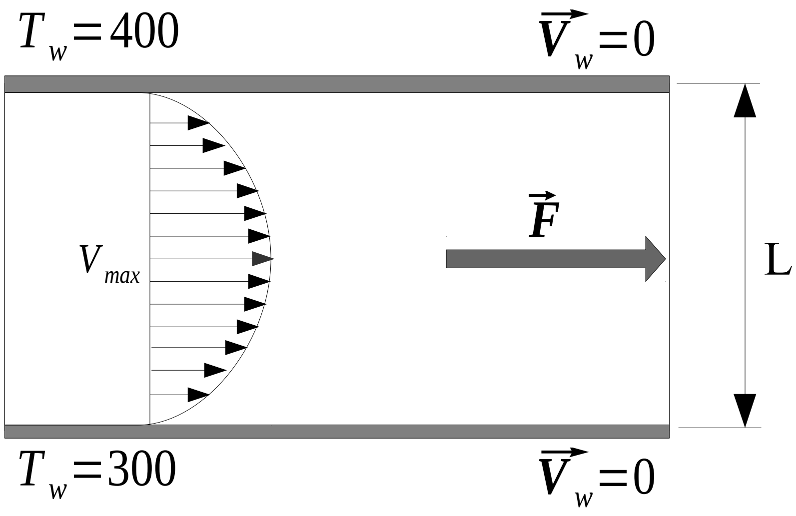
- *SDPD is used to simulate low-Reynolds-number and mesoscopic liquid flow.*
- *Successfully simulates in micro-fluids probems in micro-channels.*
- *The method can be faithfully applied to both macroscopic and mesoscopic multiphase flows.*

[1]Español & Revenga , 2003; Vázquez-Quesada, Ellero, & Español, 2012, .

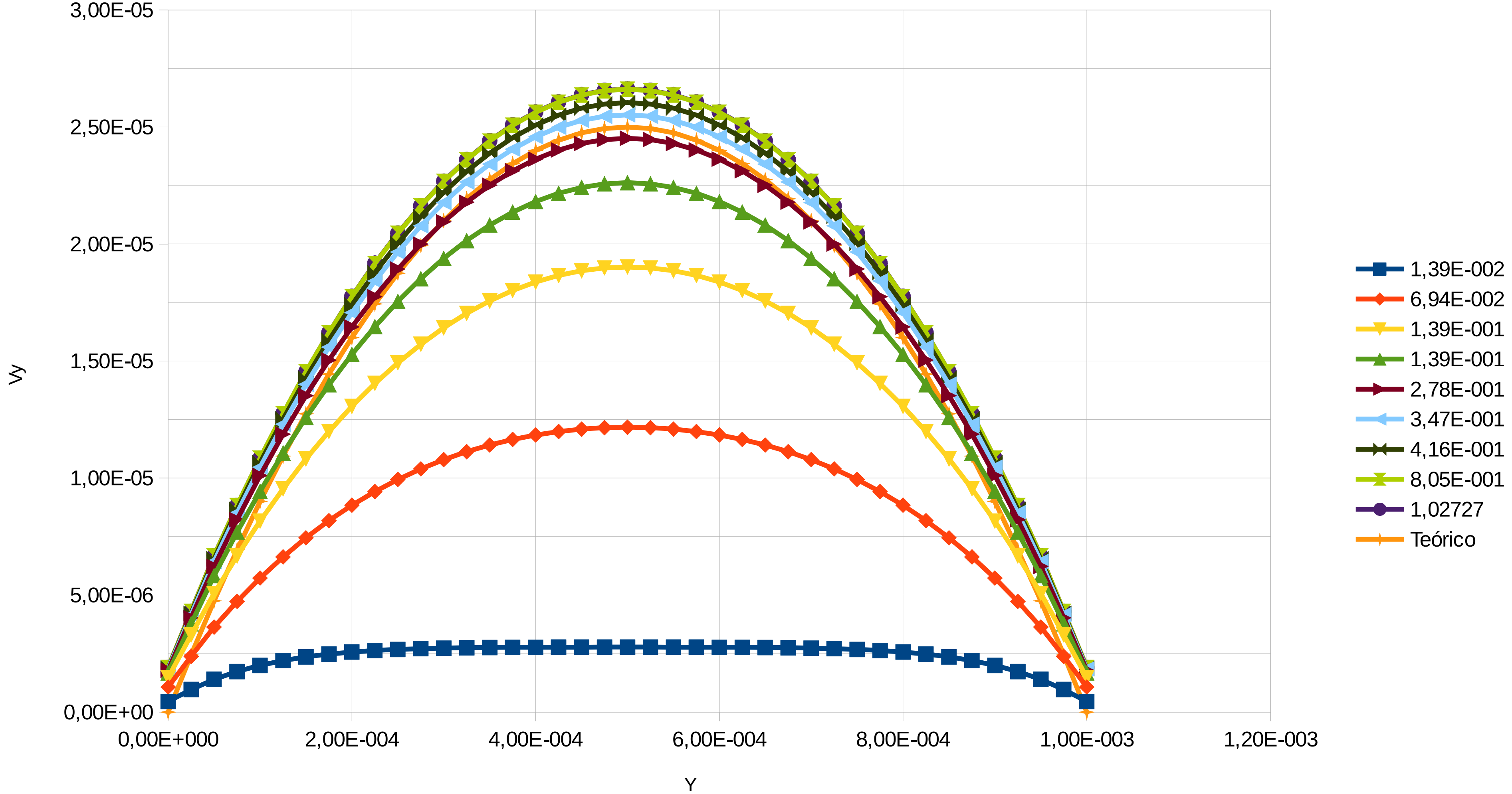
Numerical examples

Poiseuille:

- Viscosity $\eta = 1\text{x } 10^{-3}$ Pa.s
- Density
- $\rho = 1000$ kg/m^3
- F= 1 x 10^{-2}m/s^2.
- $V_0 \approx 3{,}125 \text{ x } 10^{-4}$ m/s.
- Re= 0,15625.

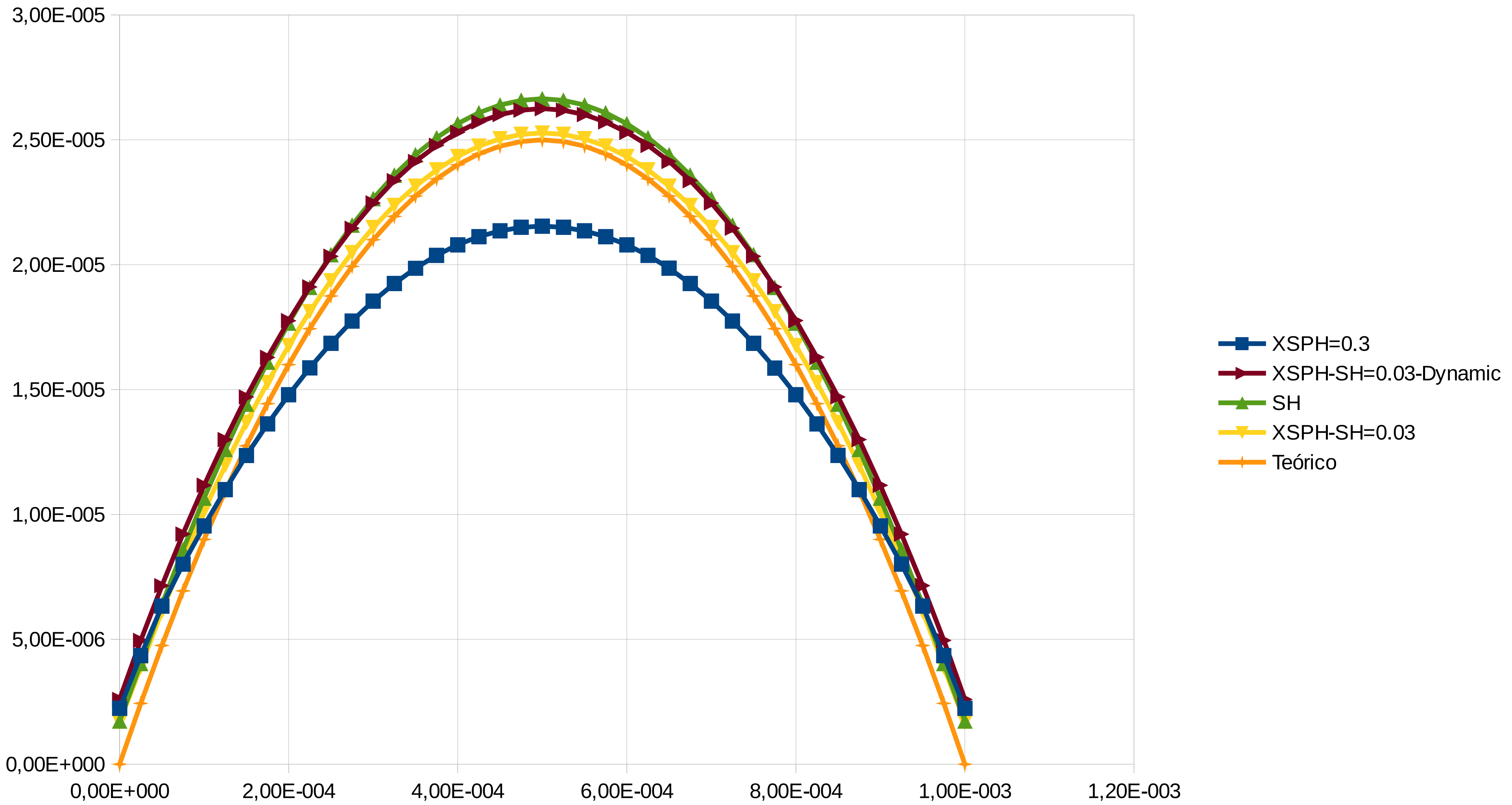


Boundary Condition (dummy particle)

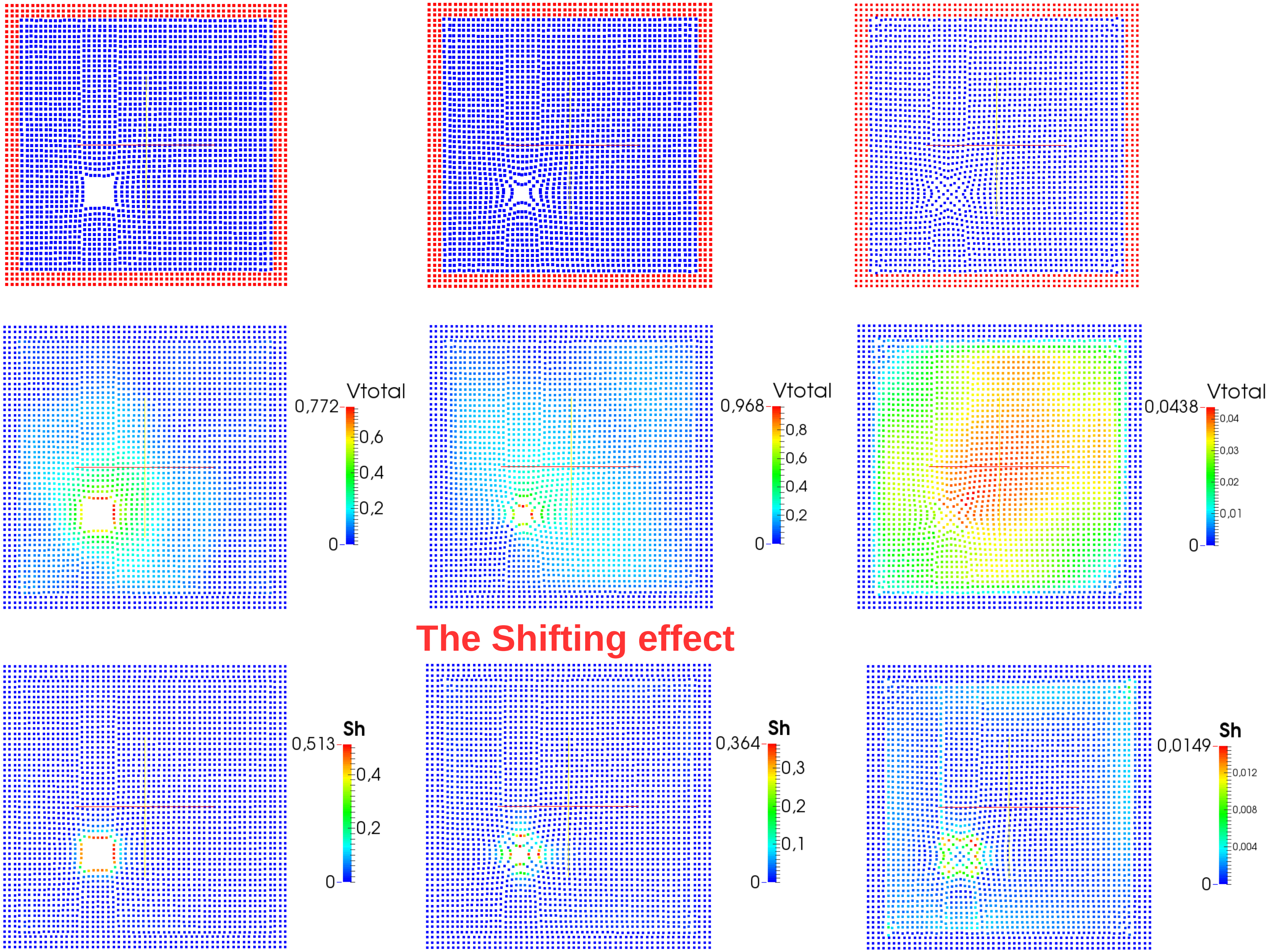


(Adami et al. 2012)

Dummy Vs Dynamics

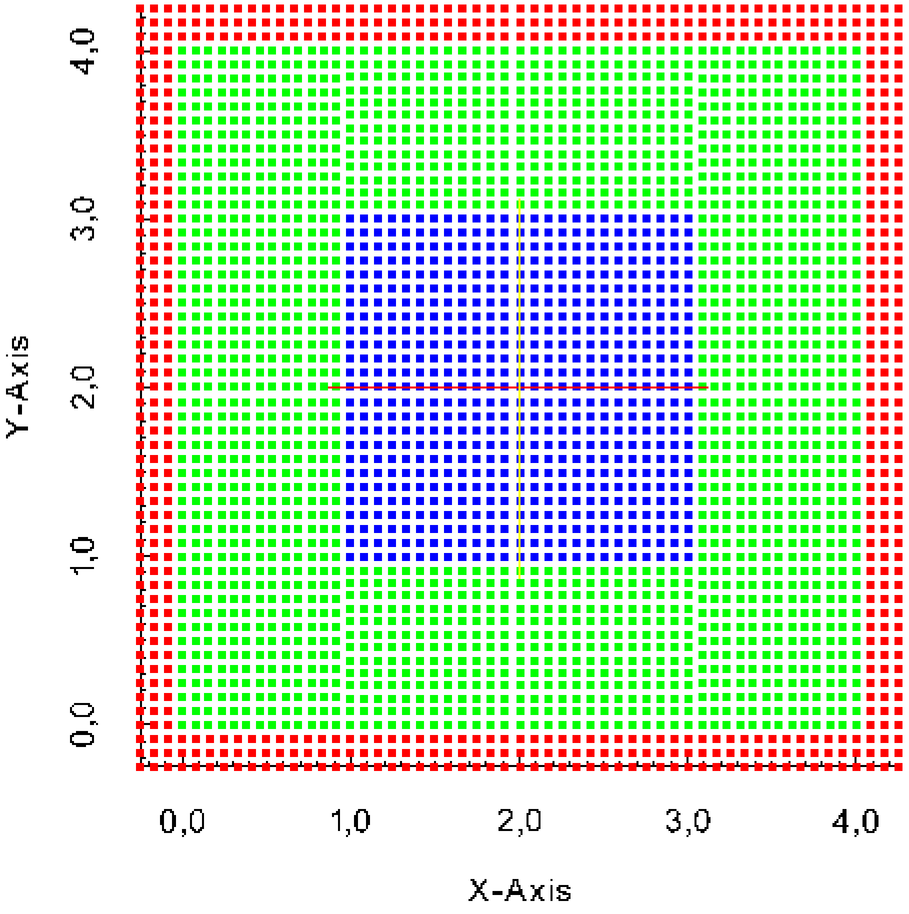


Shifting Implementation



Numerical examples

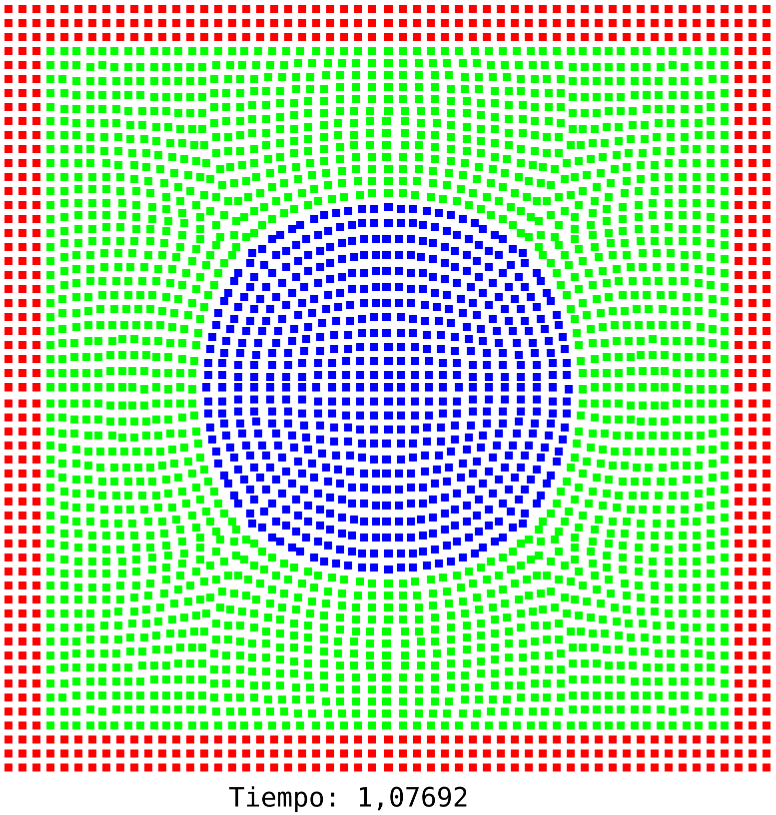
Square-Droplet deformation:

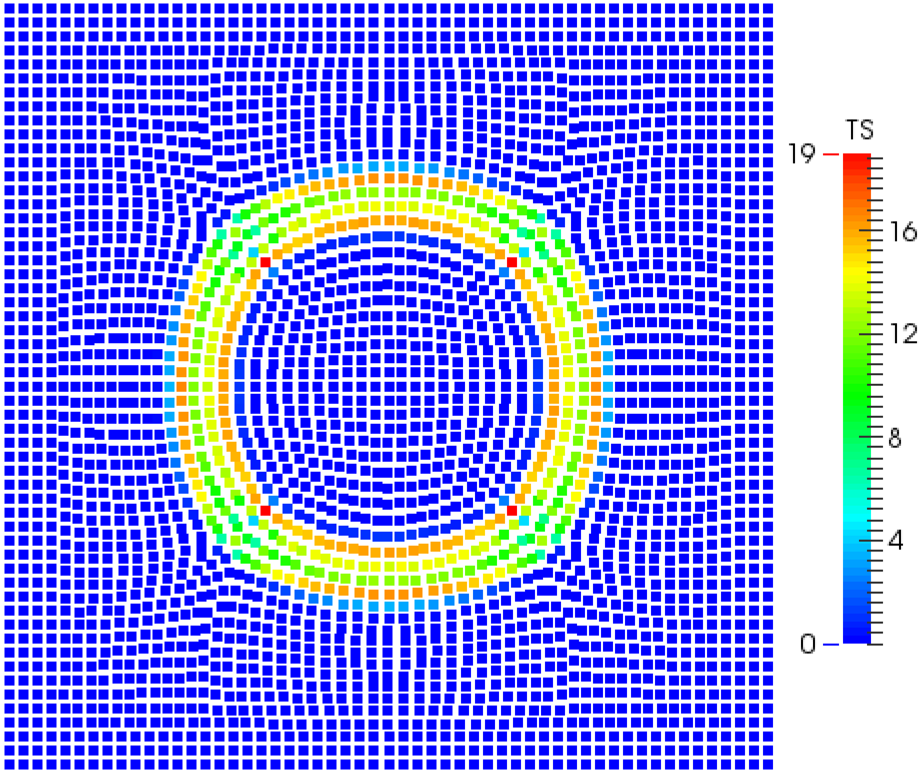


- Viscosity = 2×10^{-2}
- Density ρ= 1
- The surface-tension coefficient α = 1.
- $\rho_l / \rho_L = 1$
- External square = 4 X 4
- Internal squere = 2 X 2

Surface Tension

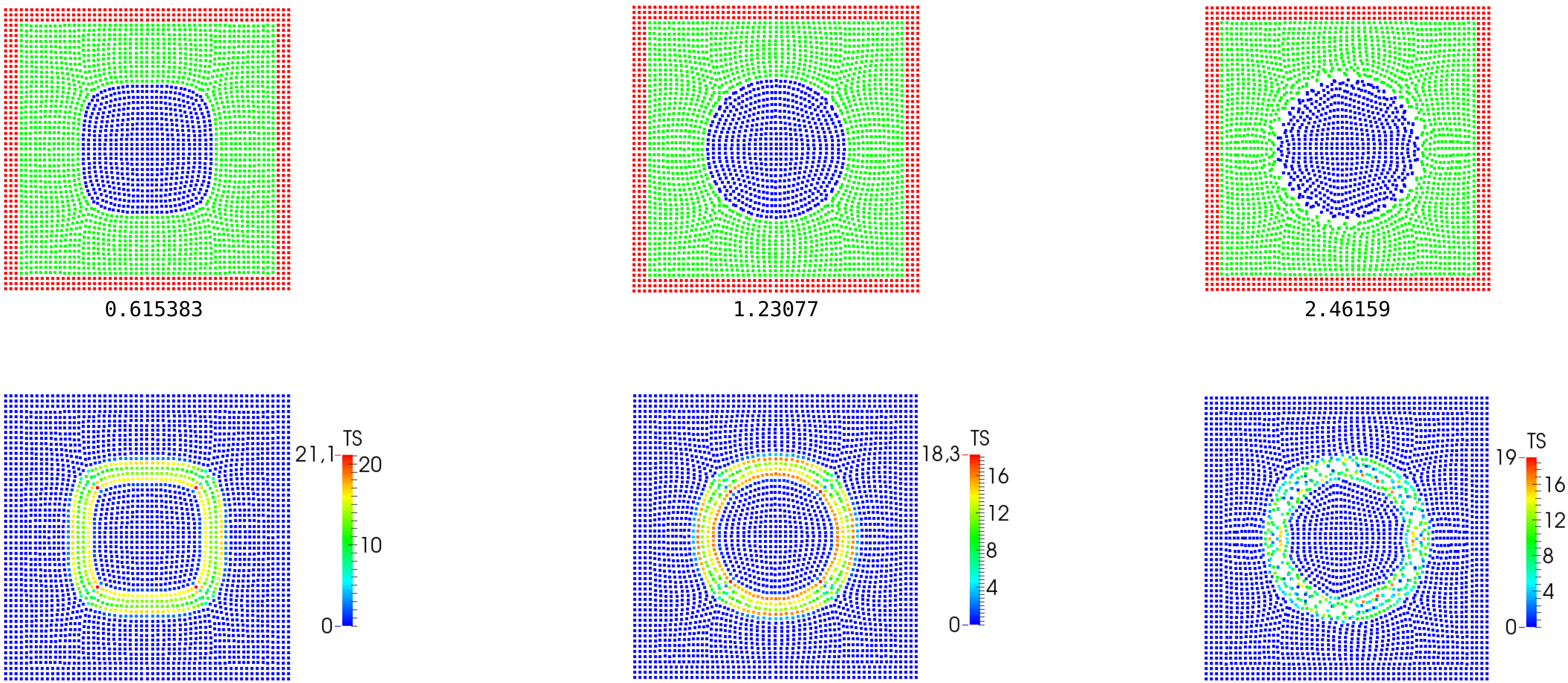
Surface Tension Implementation (Hu & Adams, 2006)





Surface Tension

Surface Tension Implementation (Hu & Adams, 2006)



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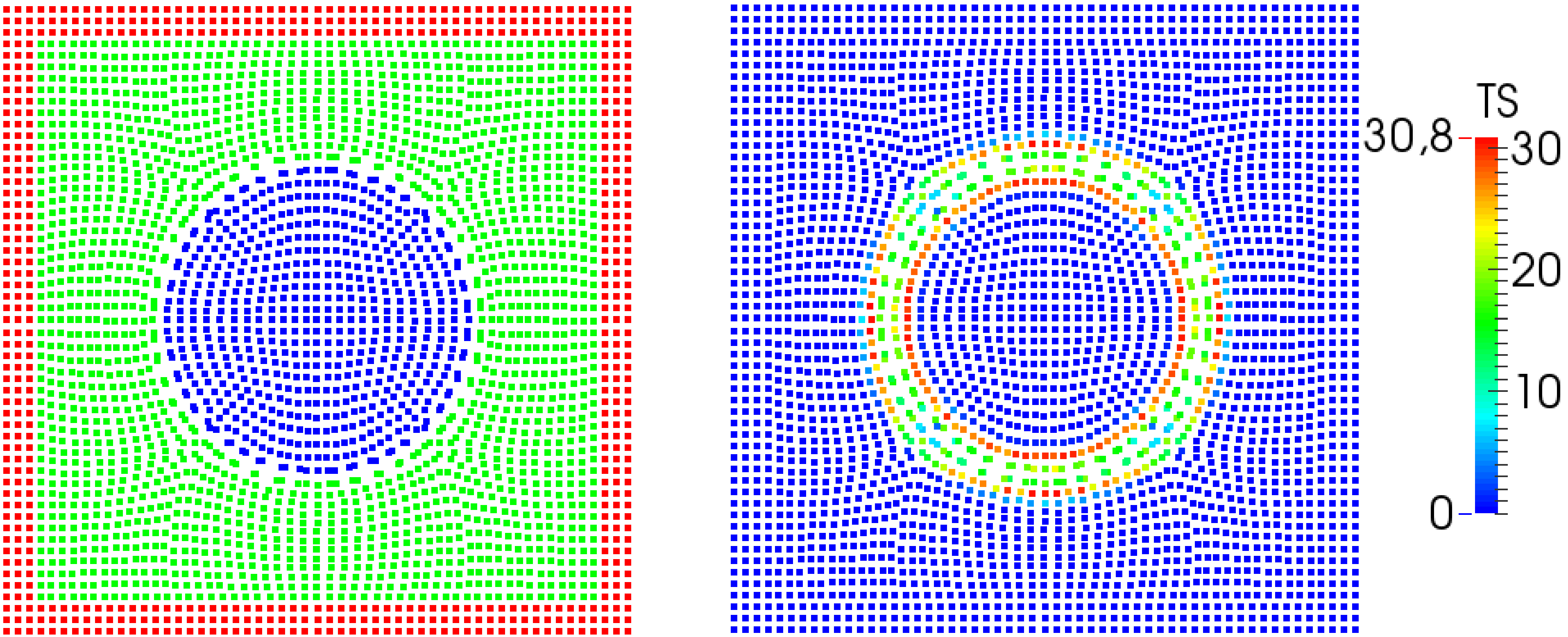
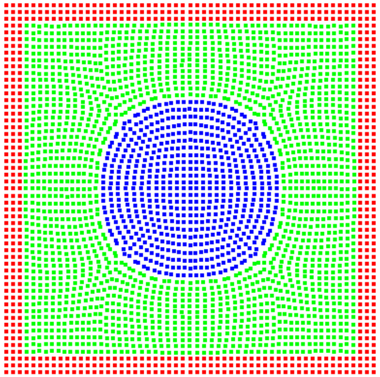
Surface Tension Implementation (Adami et al. 2010)



Tiempo: 0.769228

Surface Tension

Surface Tension Implementation (Adami et al. 2010)



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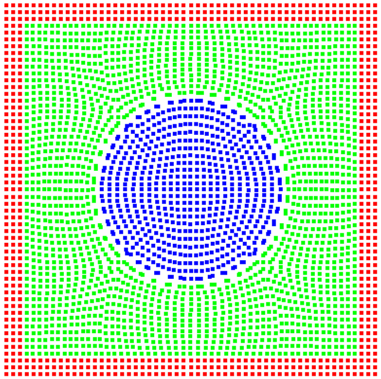

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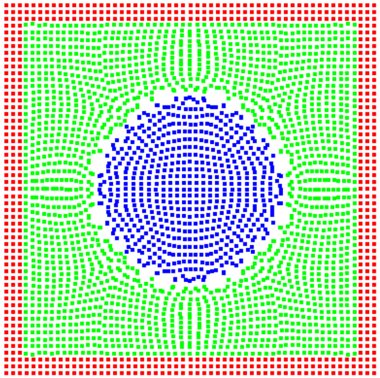

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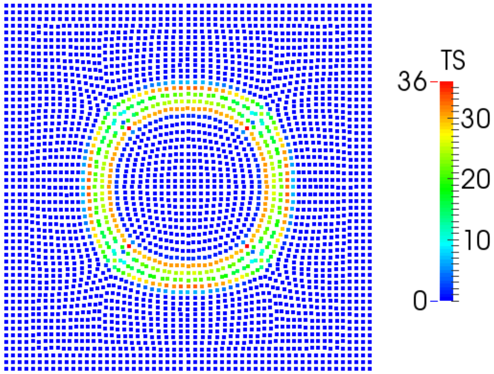
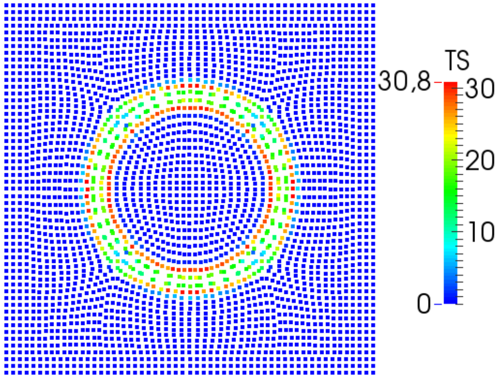
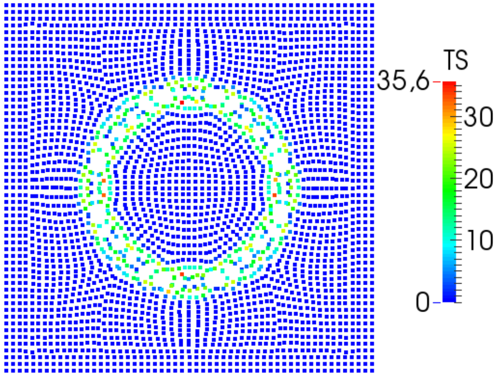
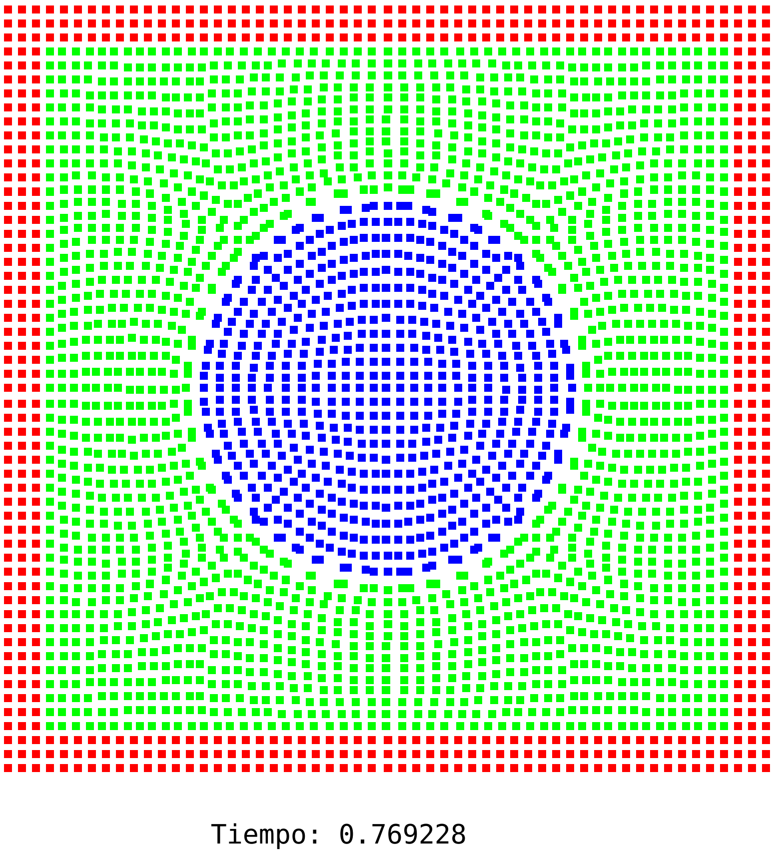


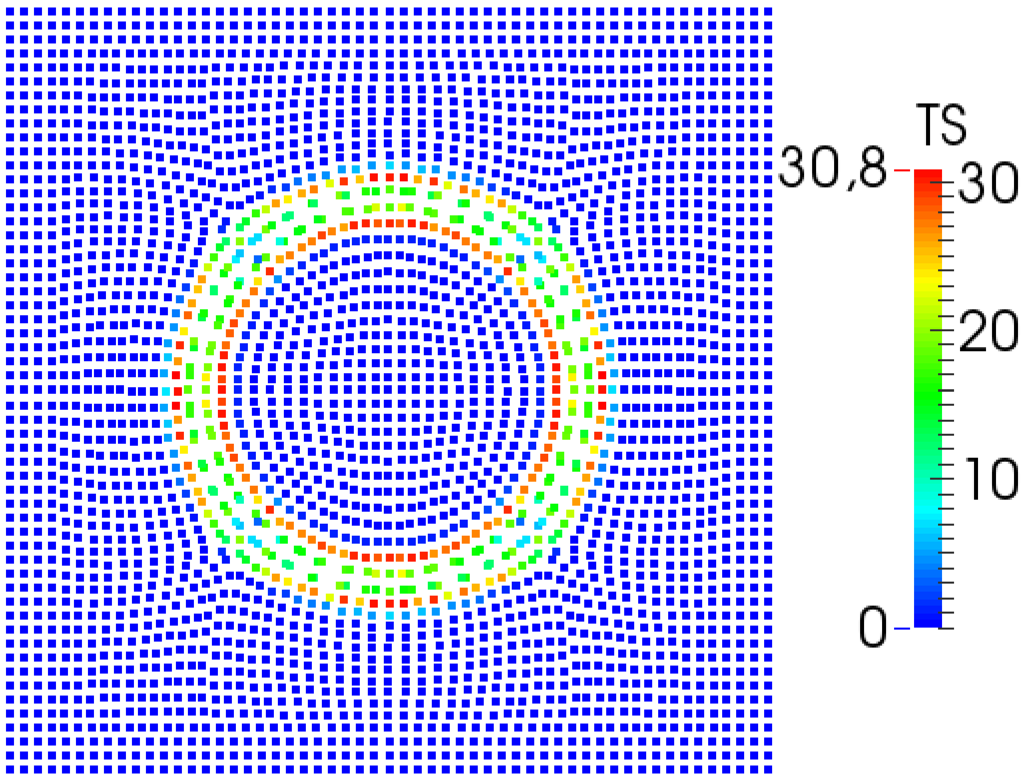




Surface Tension

Surface Tension Implementation (Morris 2000)





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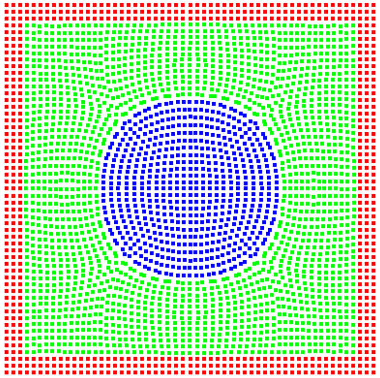

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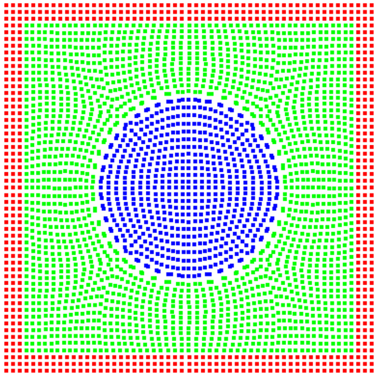

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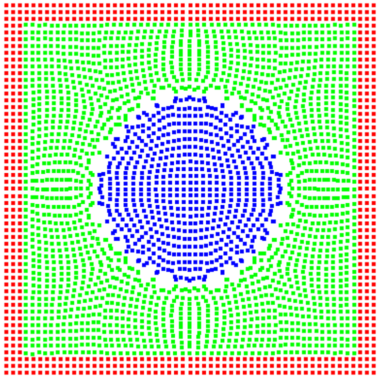

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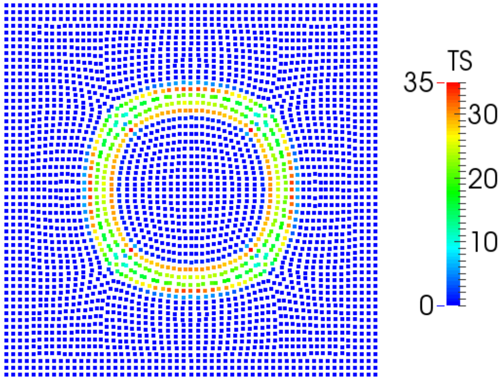
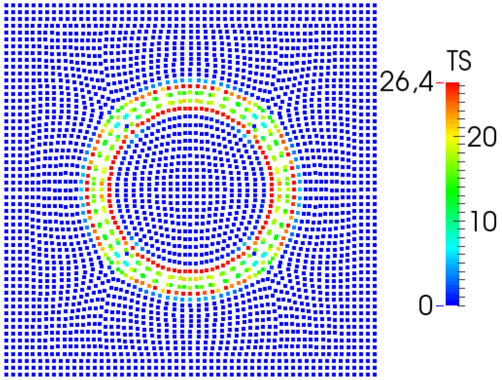
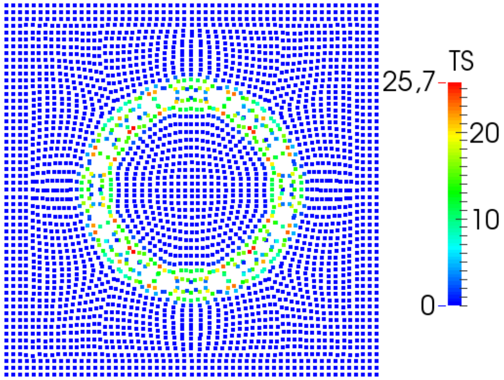
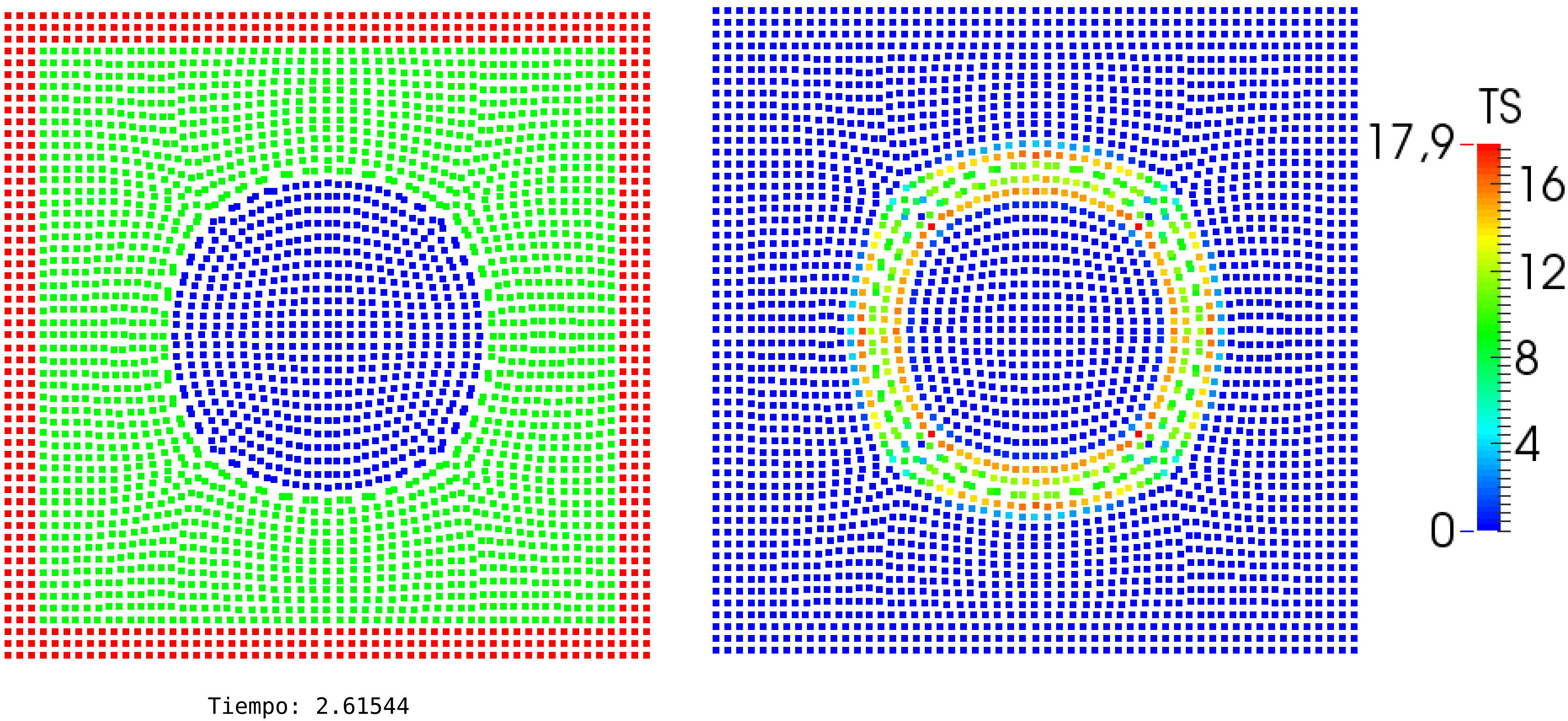






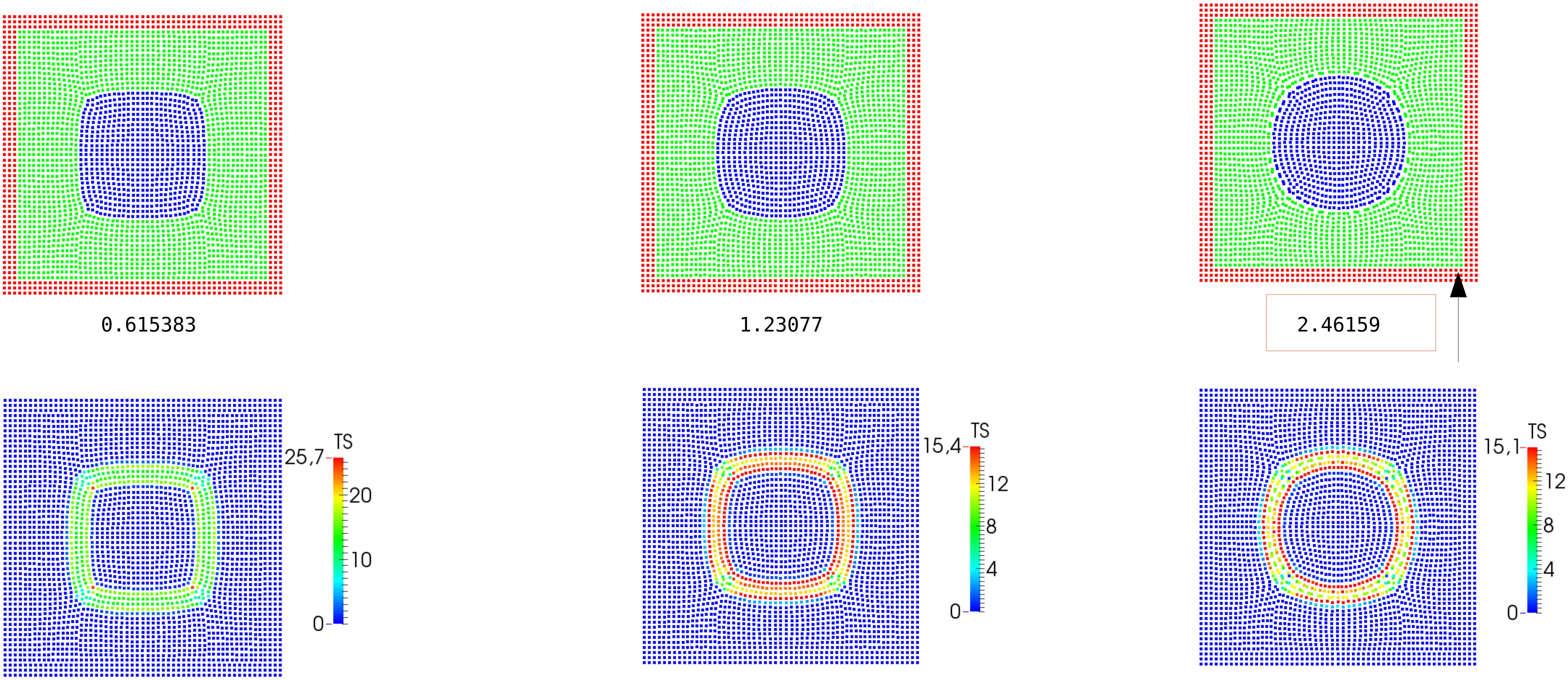
Surface Tension

Surface Tension Implementation (Hu & Adams, 2006) with XSPH (e=0,03)



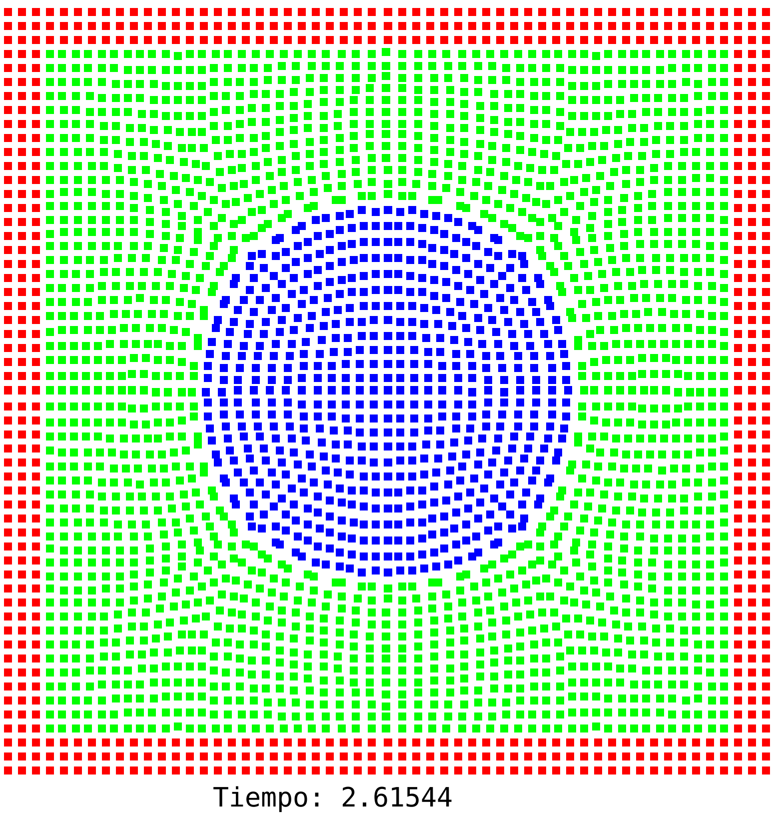
Surface Tension

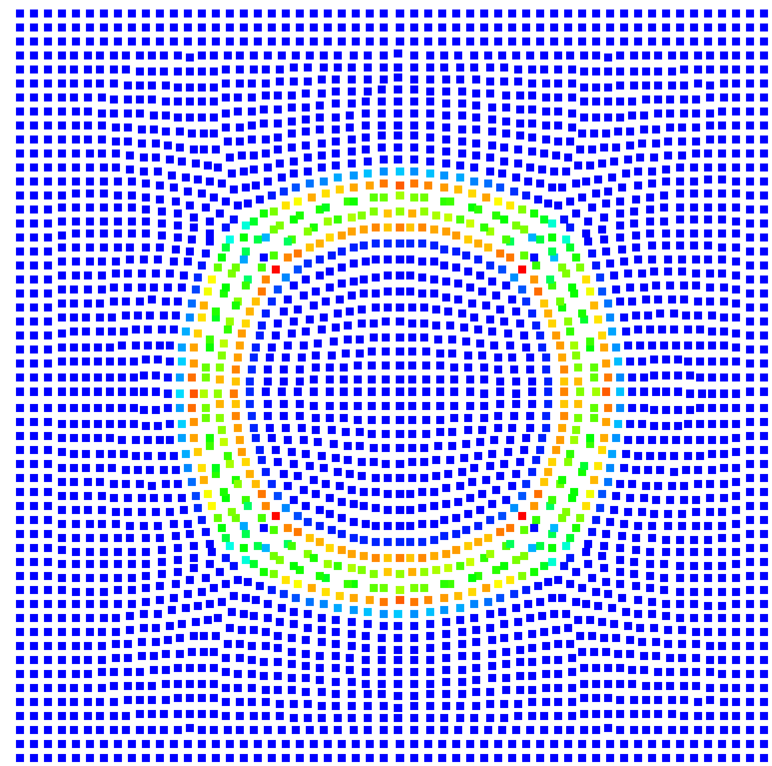
Surface Tension Implementation (Hu & Adams, 2006) with XSPH (e=0,03)



Surface Tension

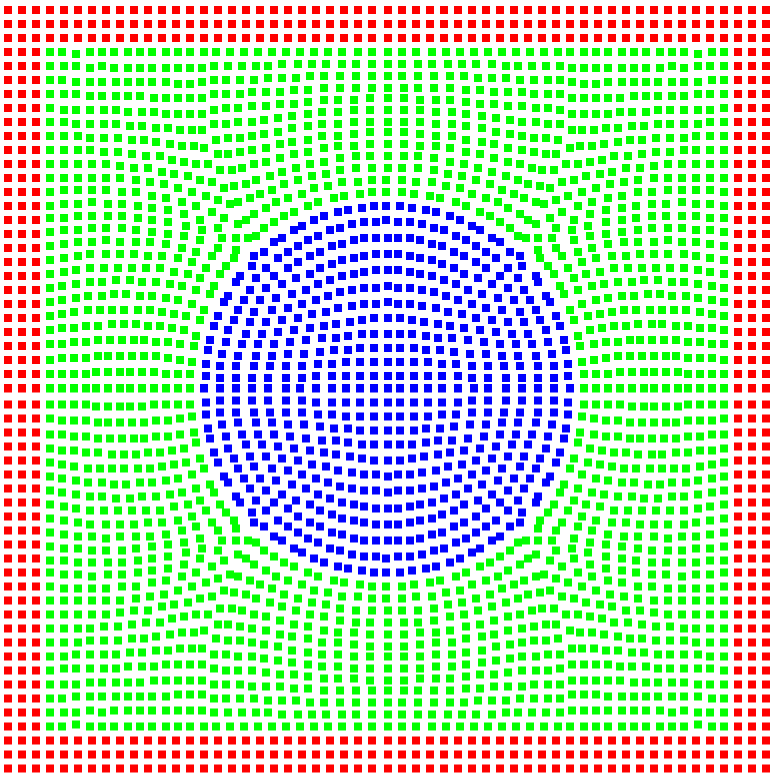
Surface Tension Implementation (Hu & Adams, 2006) with XSPH (e=0,03) and Dynamics Bundary condition

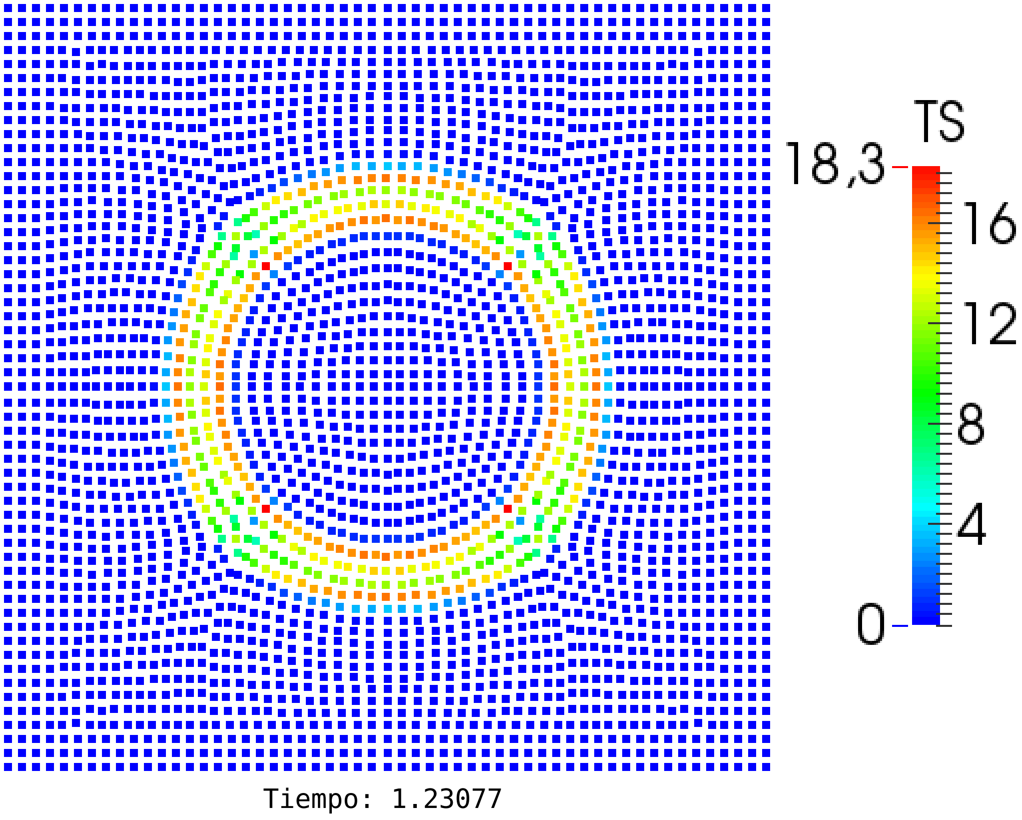




Surface Tension

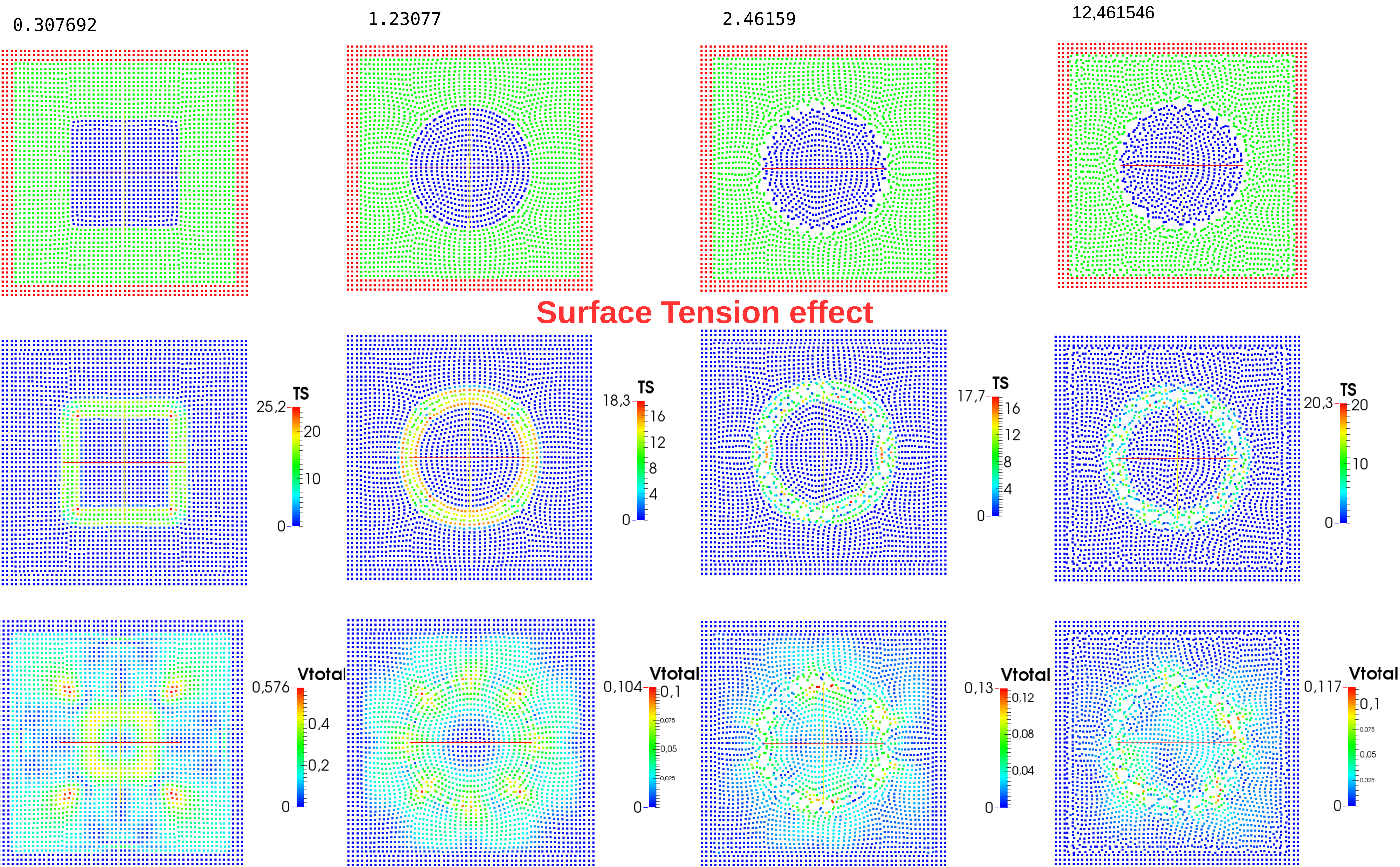
Surface Tension Implementation (Hu & Adams, 2006) with Dynamics Bundary condition





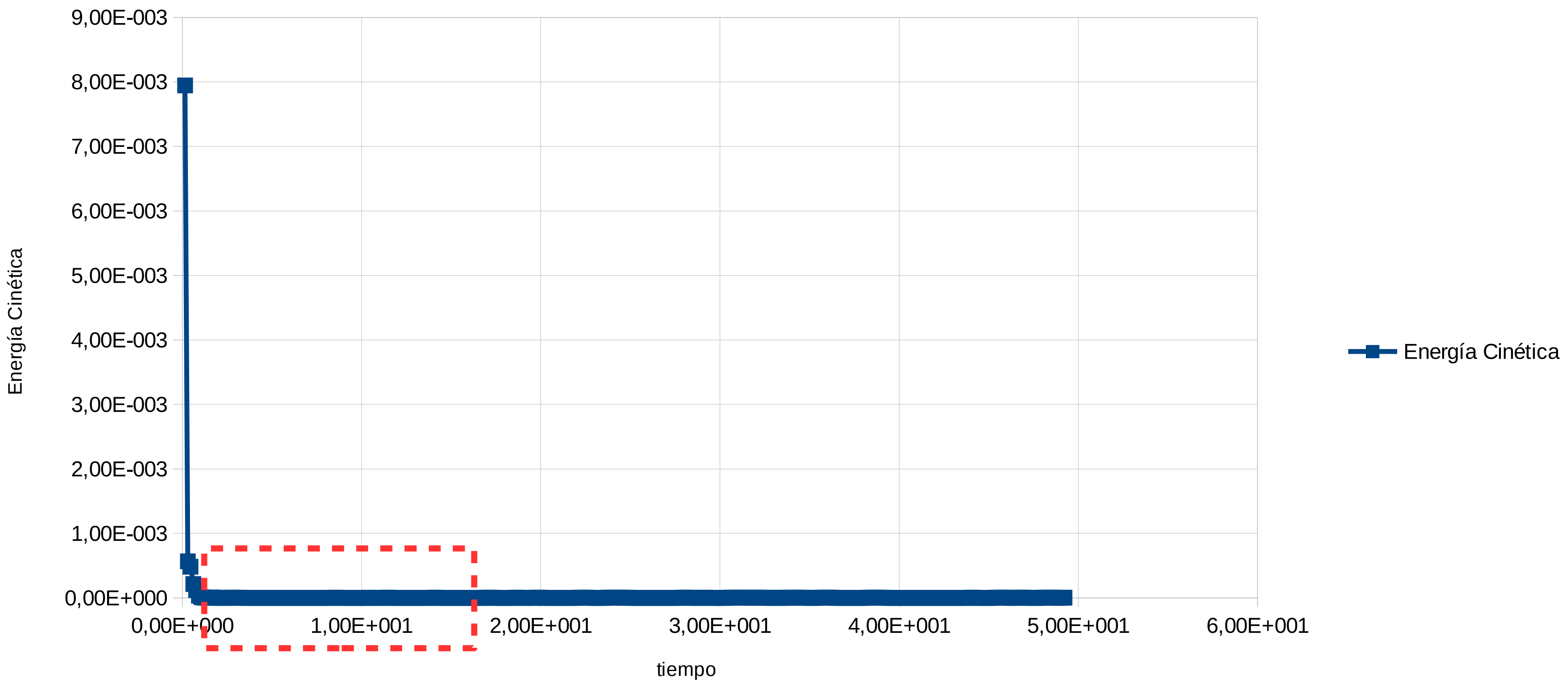
Surface Tension

Adami-Hu 2006



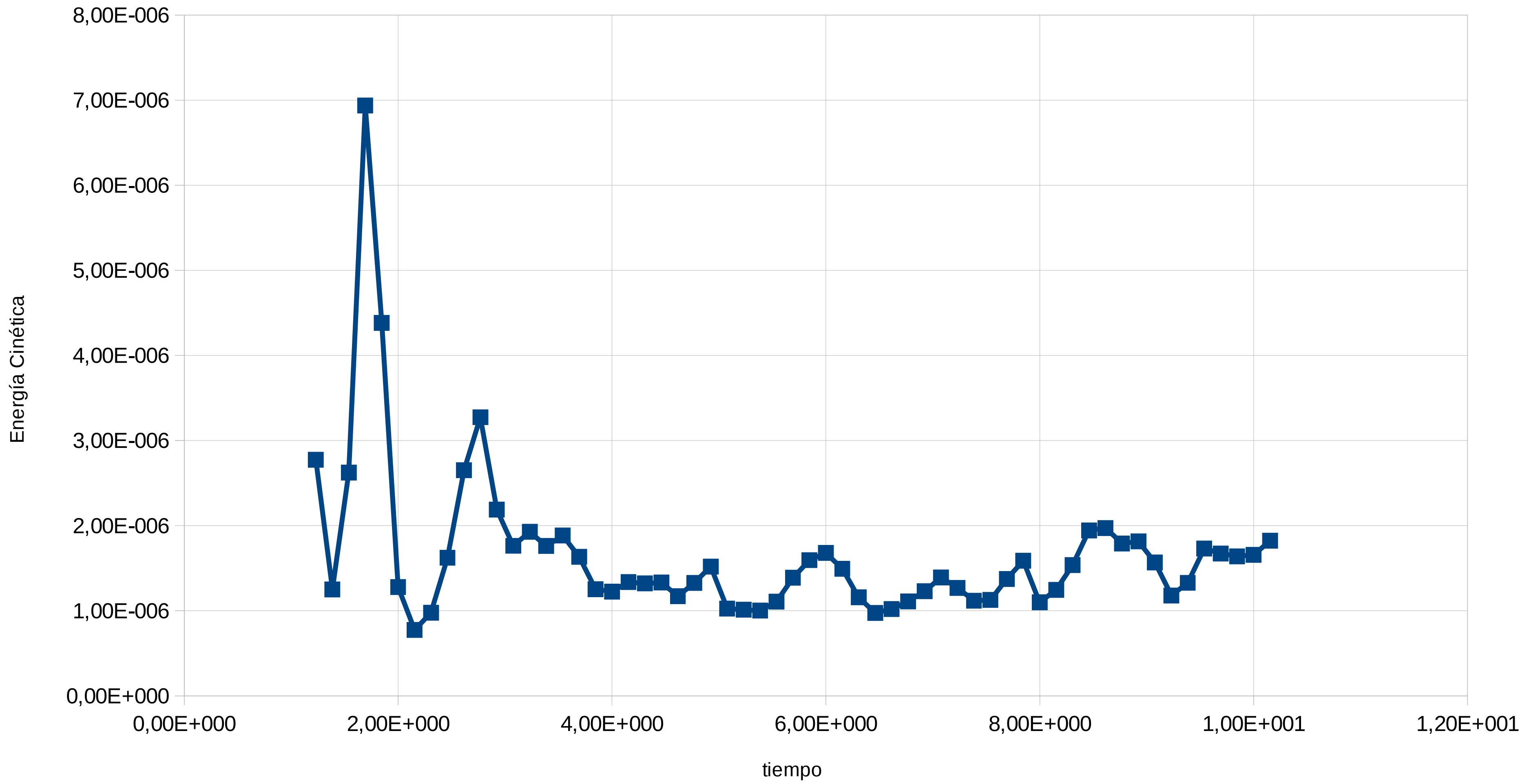
Surface Tension

Adami-Hu 2006

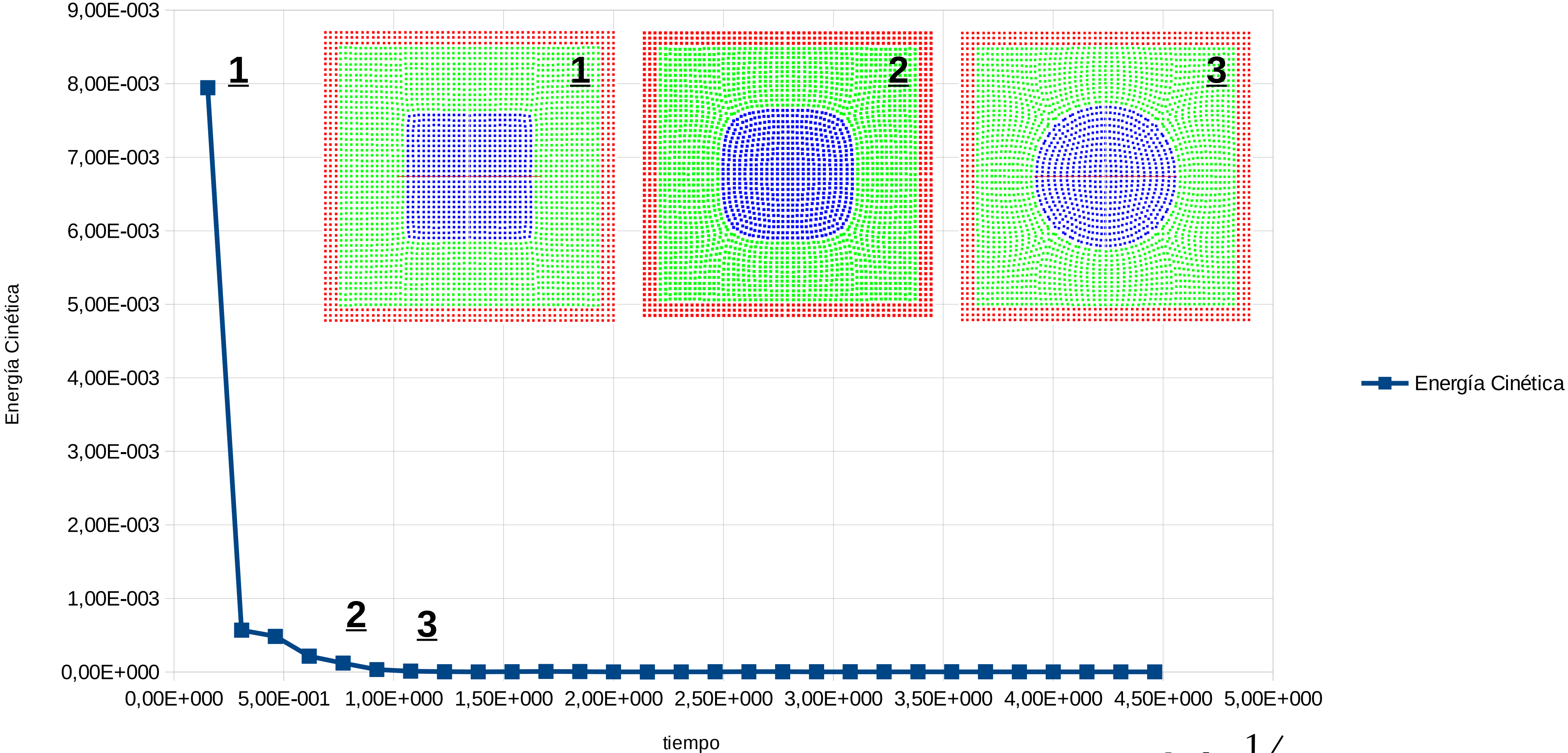


Surface Tension

Adami-Hu 2006



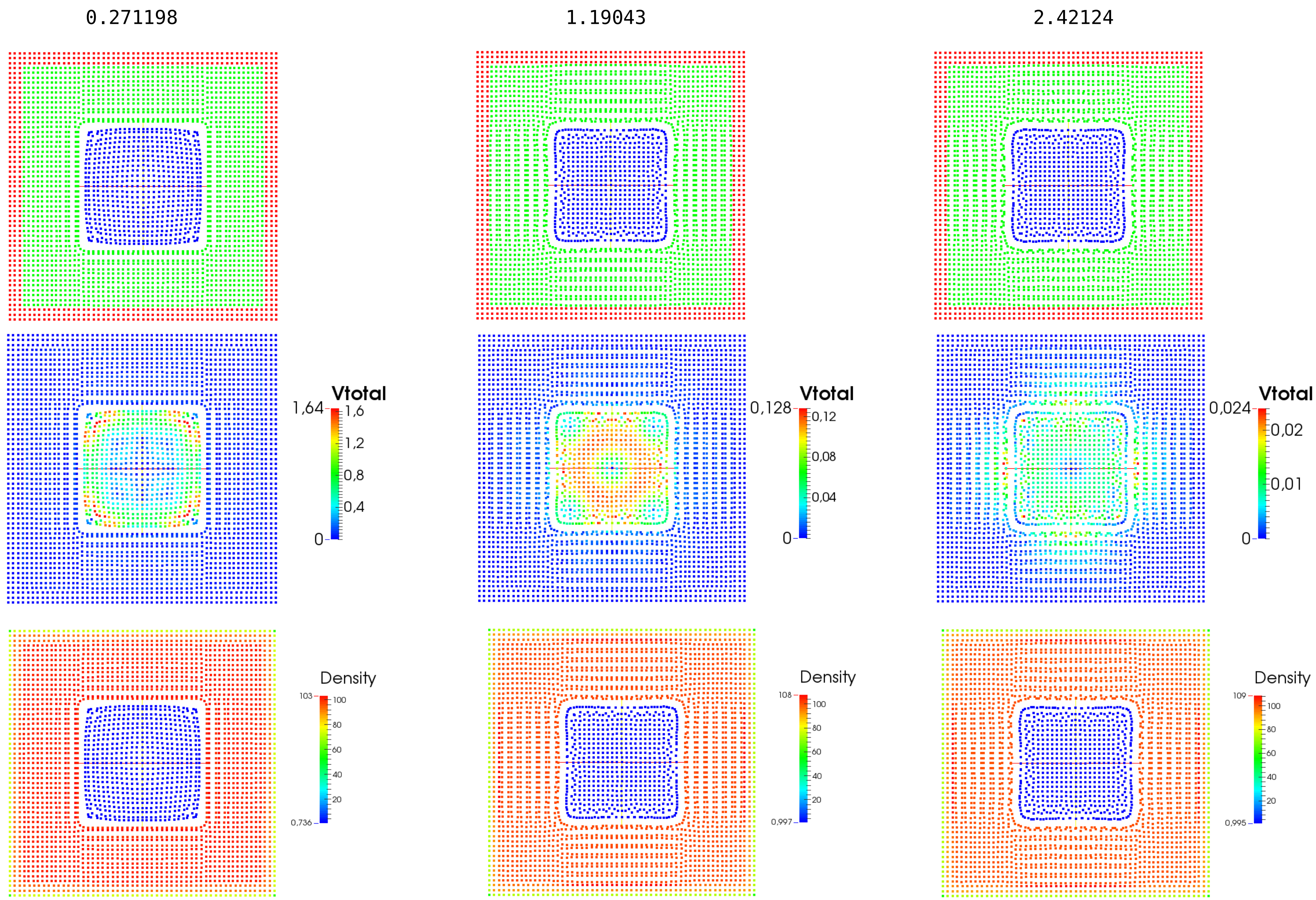
Surface Tension



$$Densidad = {}^{1}\!/_{1}$$

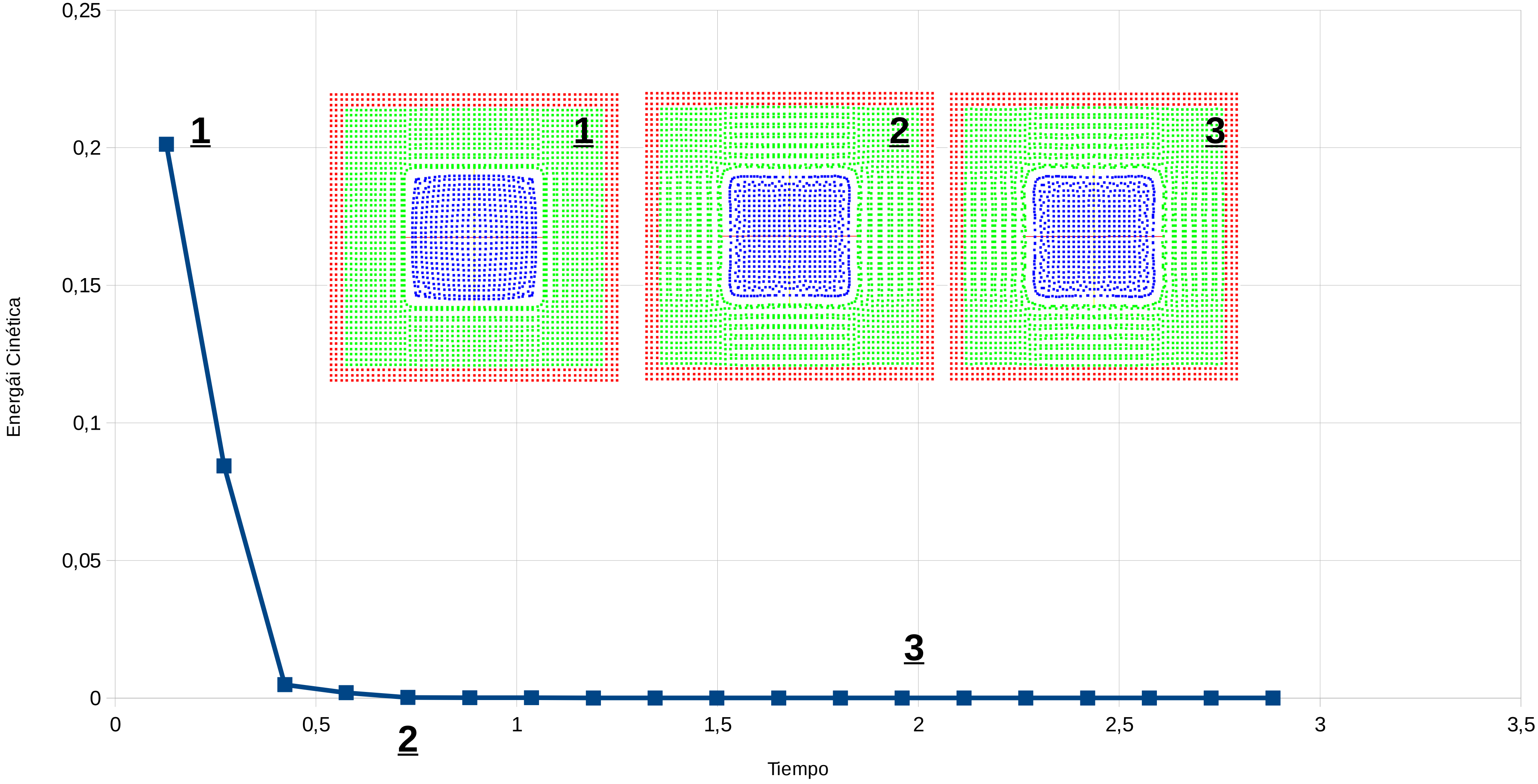
$$Densidad = {}^{1}\!/_{100}$$

Surface Tension



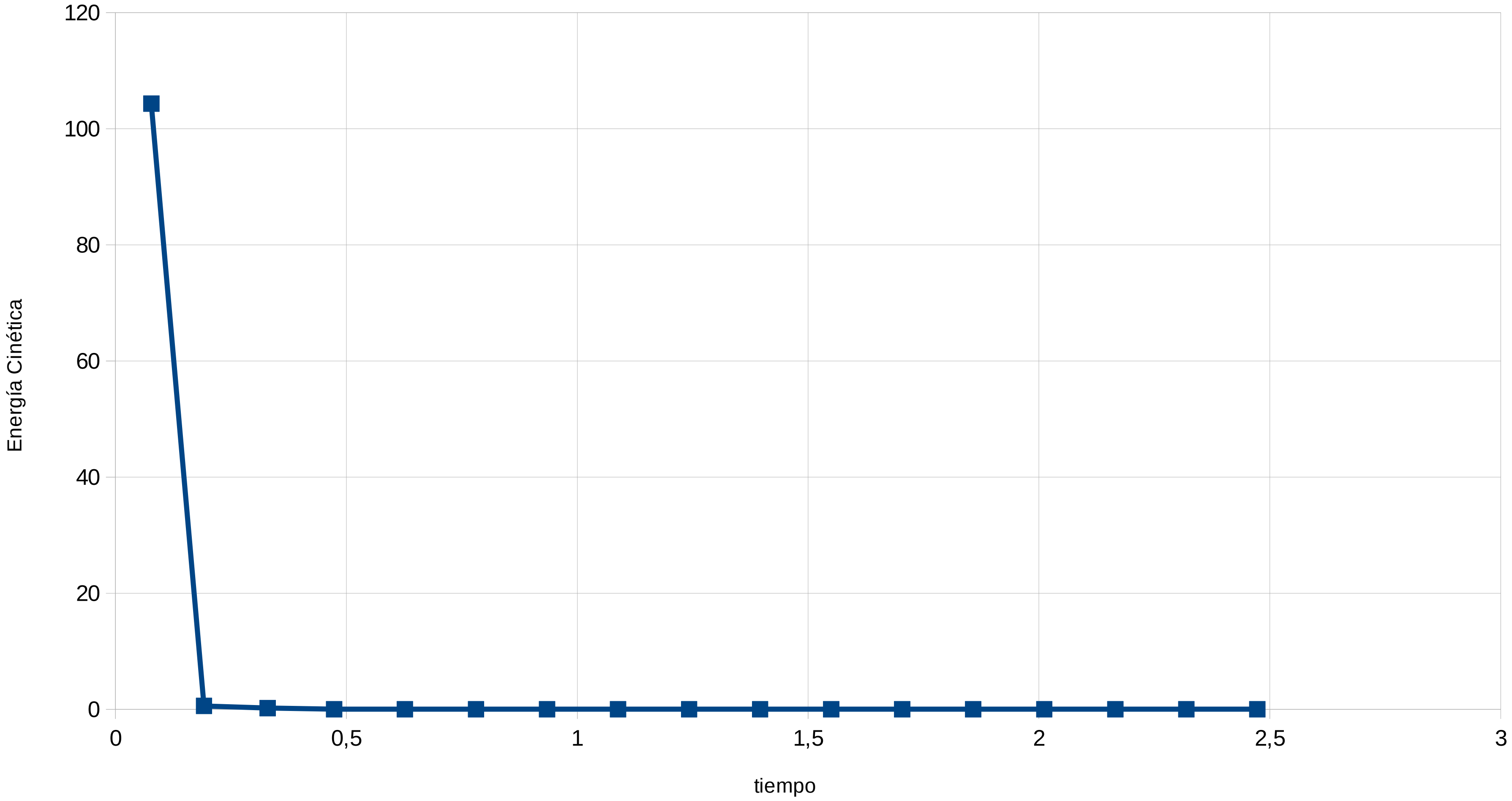
$$Densidad = {}^{1}\!/_{100}$$

Surface Tension



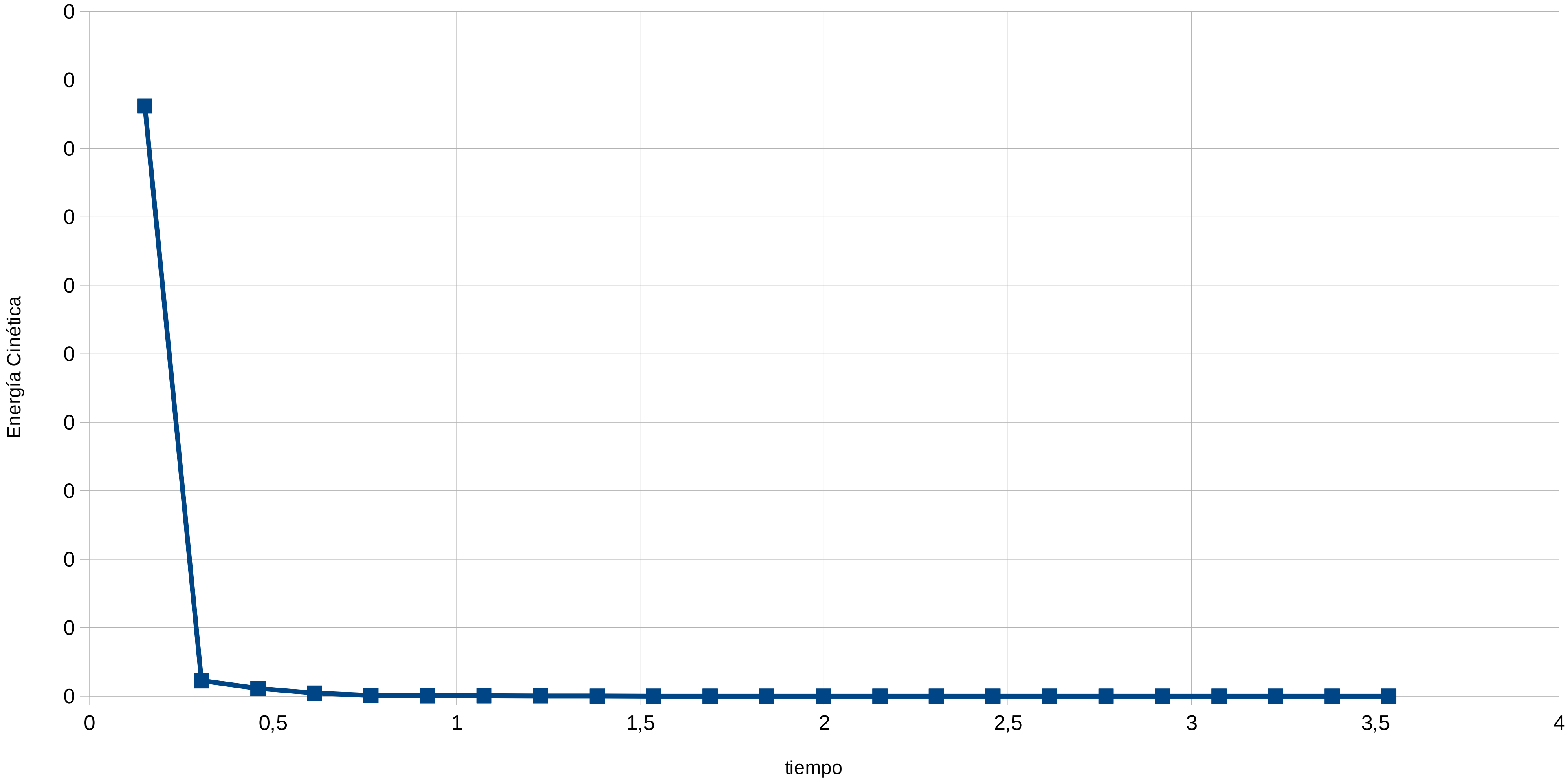
$$Densidad = \frac{1}{1000}$$

Surface Tension



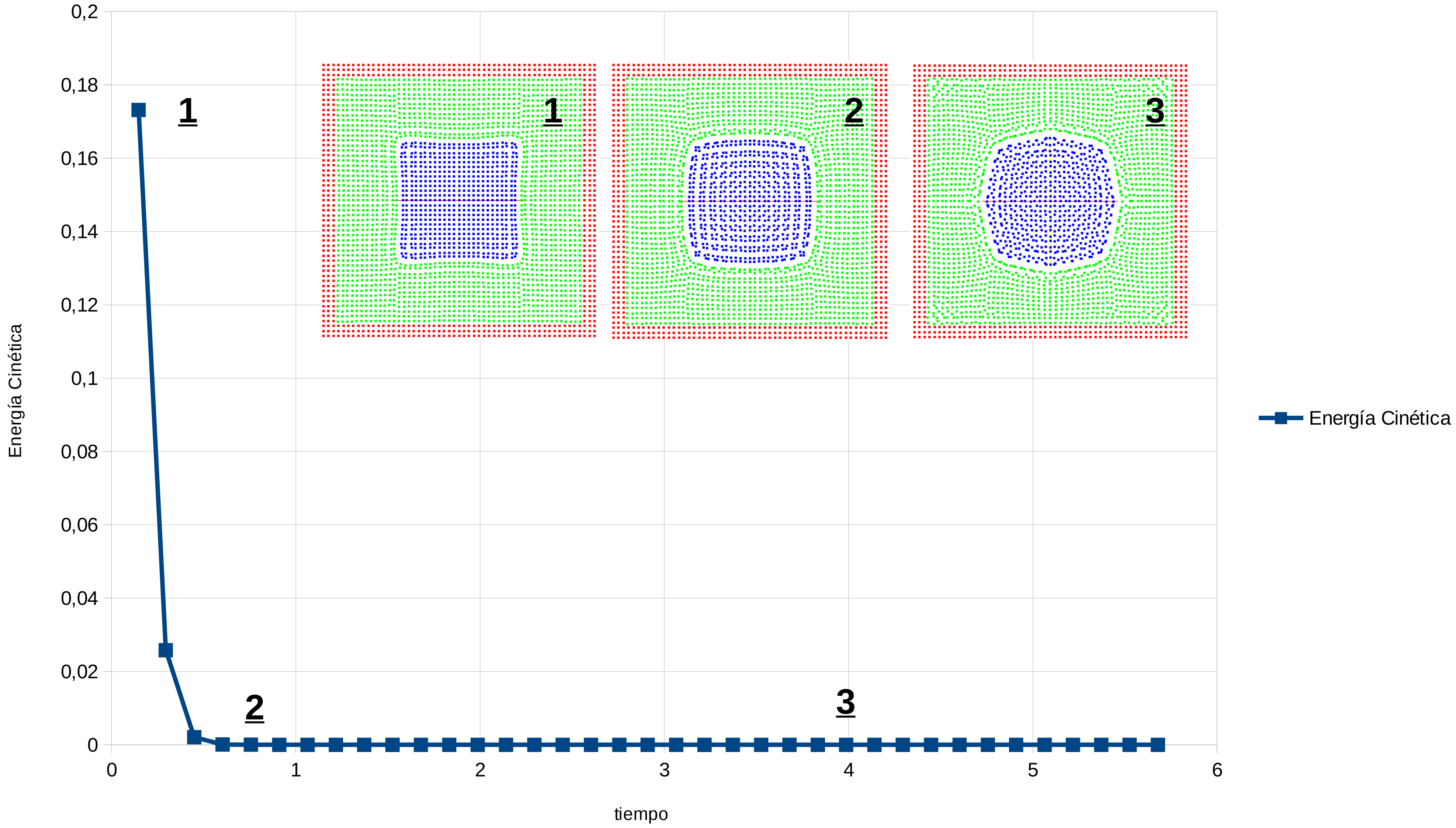
$$Densidad = {}^{1}\!/\!_{10}$$

Surface Tension



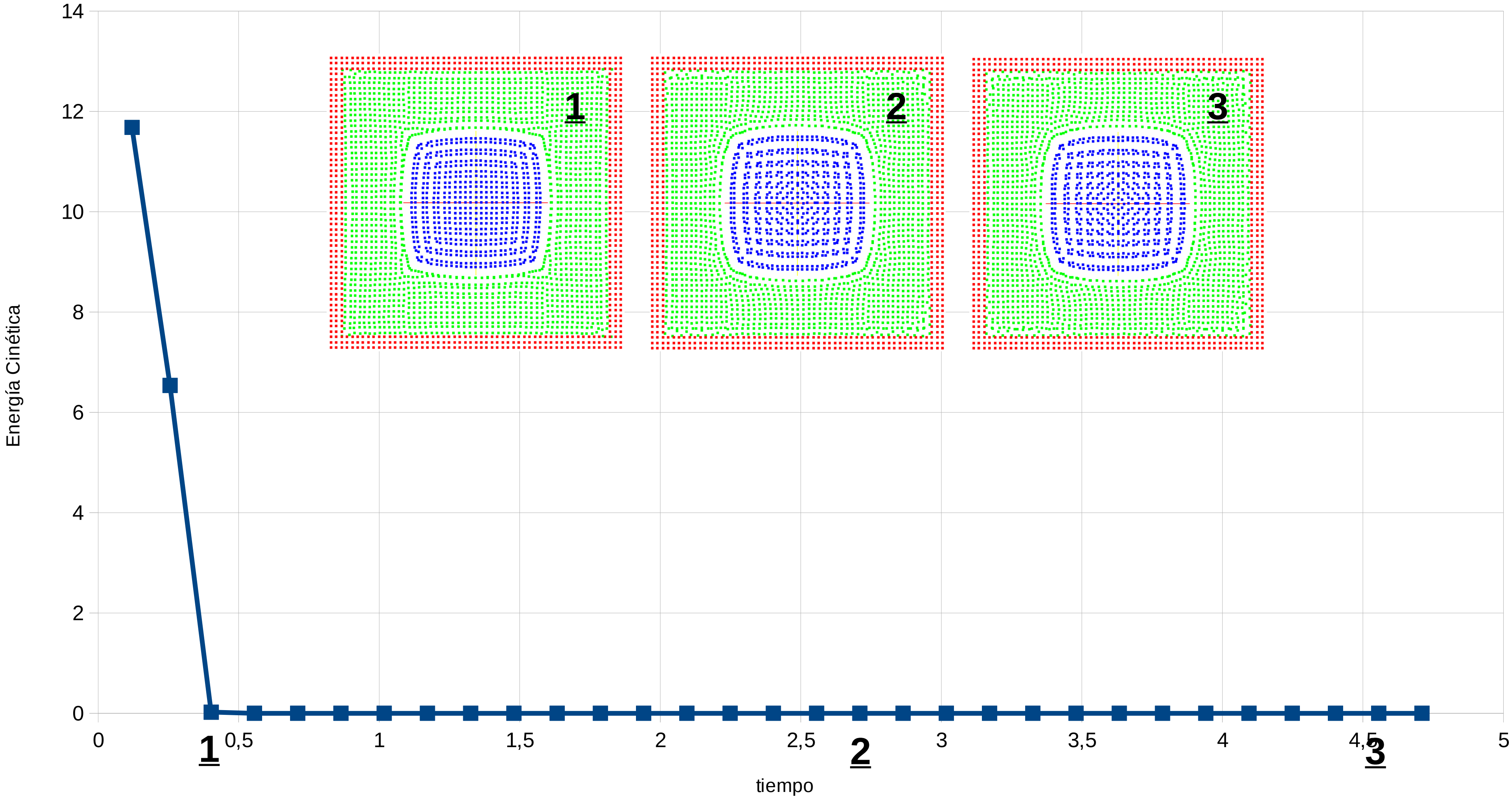
$$Densidad = {}^{10}\!/\!{}_{1}$$

Surface Tension



Surface Tension

$$Densidad = {}^{1000}\!/_{1}$$



Surface Tension with Shifting

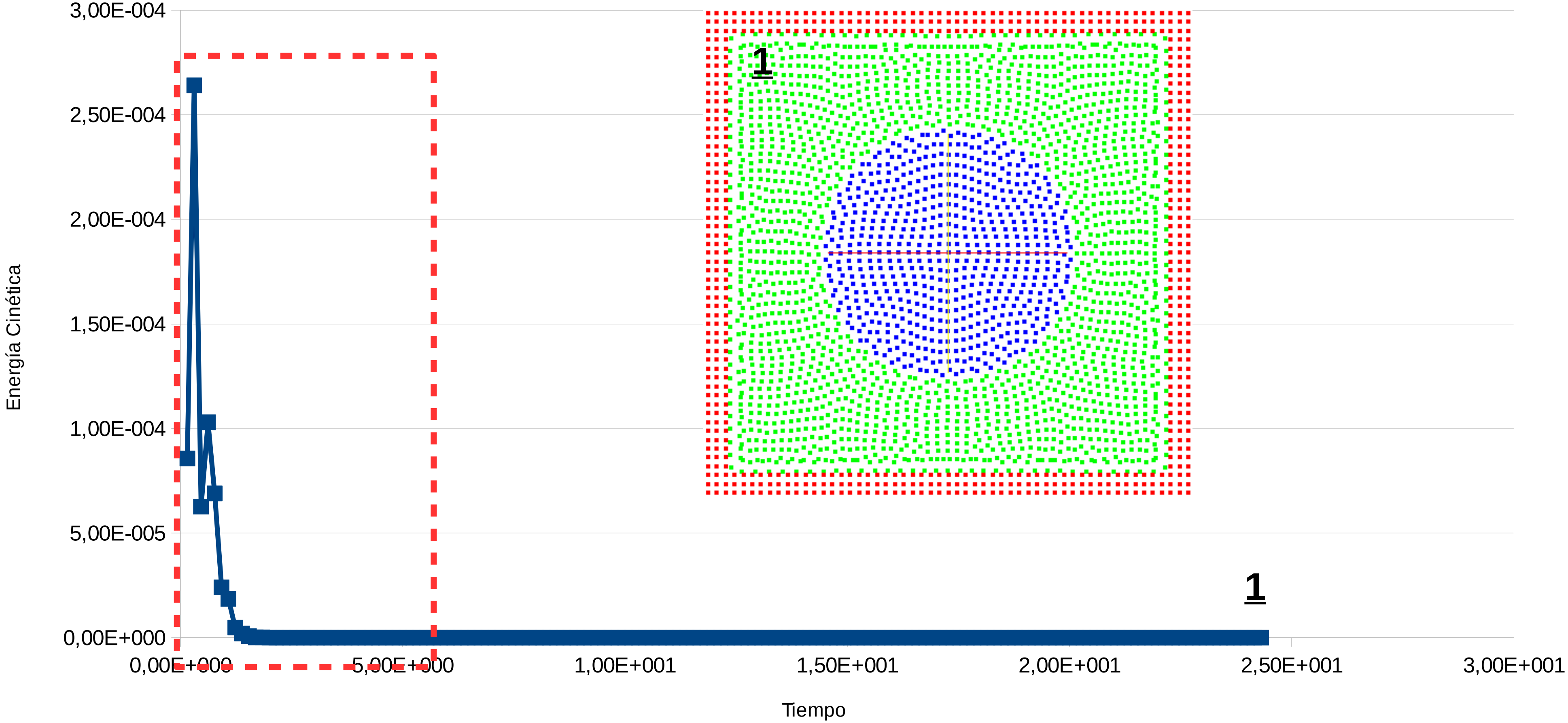
Shifting algorithm (Crespo et al. 2016)

$$\delta \mathbf{r}_s = -D \nabla C_i$$

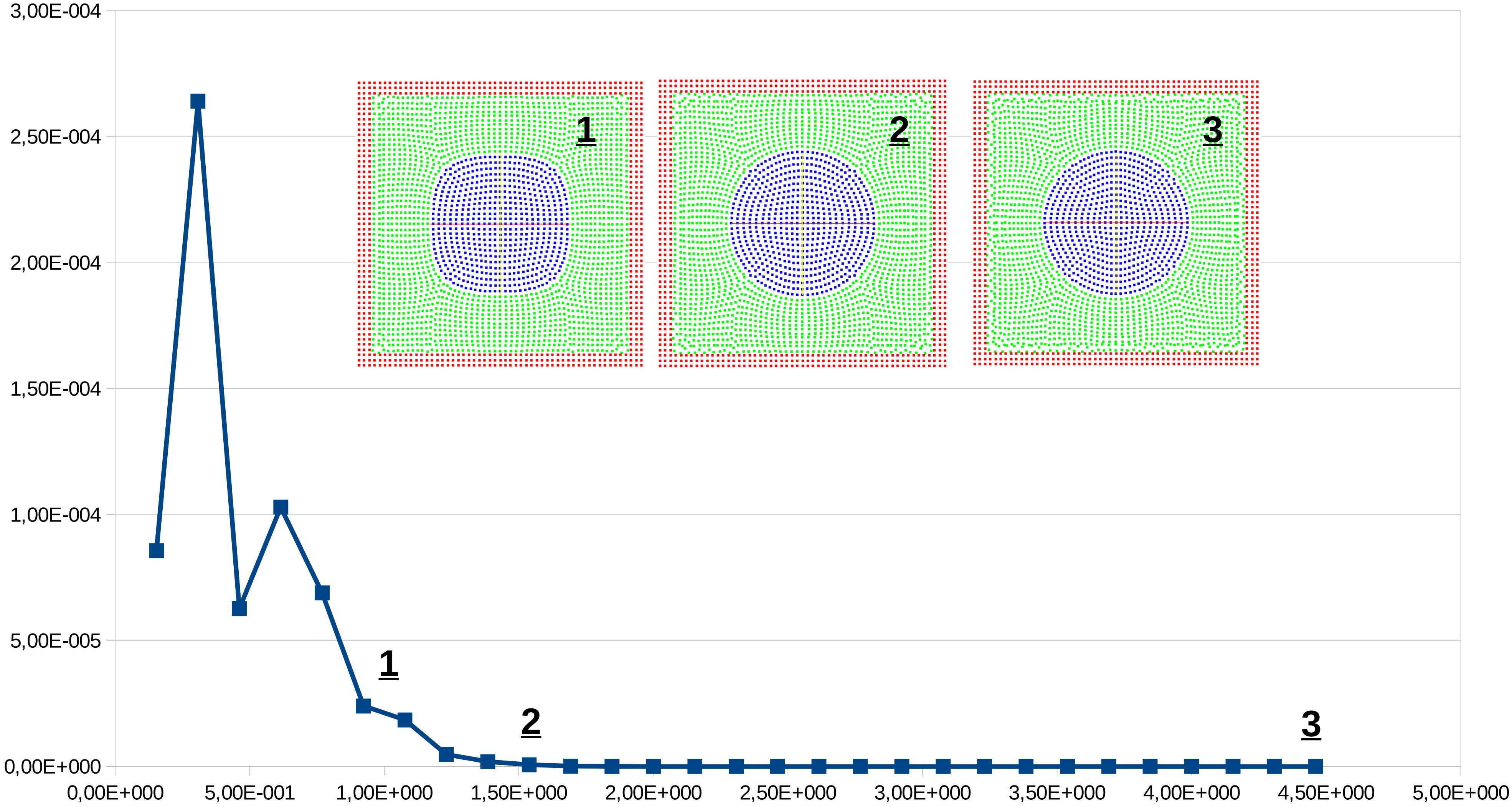
$$\nabla C_i = \sum_j \frac{m_j}{\rho_j} \nabla W_{ij}$$

$$D = Ah \|\boldsymbol{u}\|_i \Delta t$$

Surface Tension with Shifting

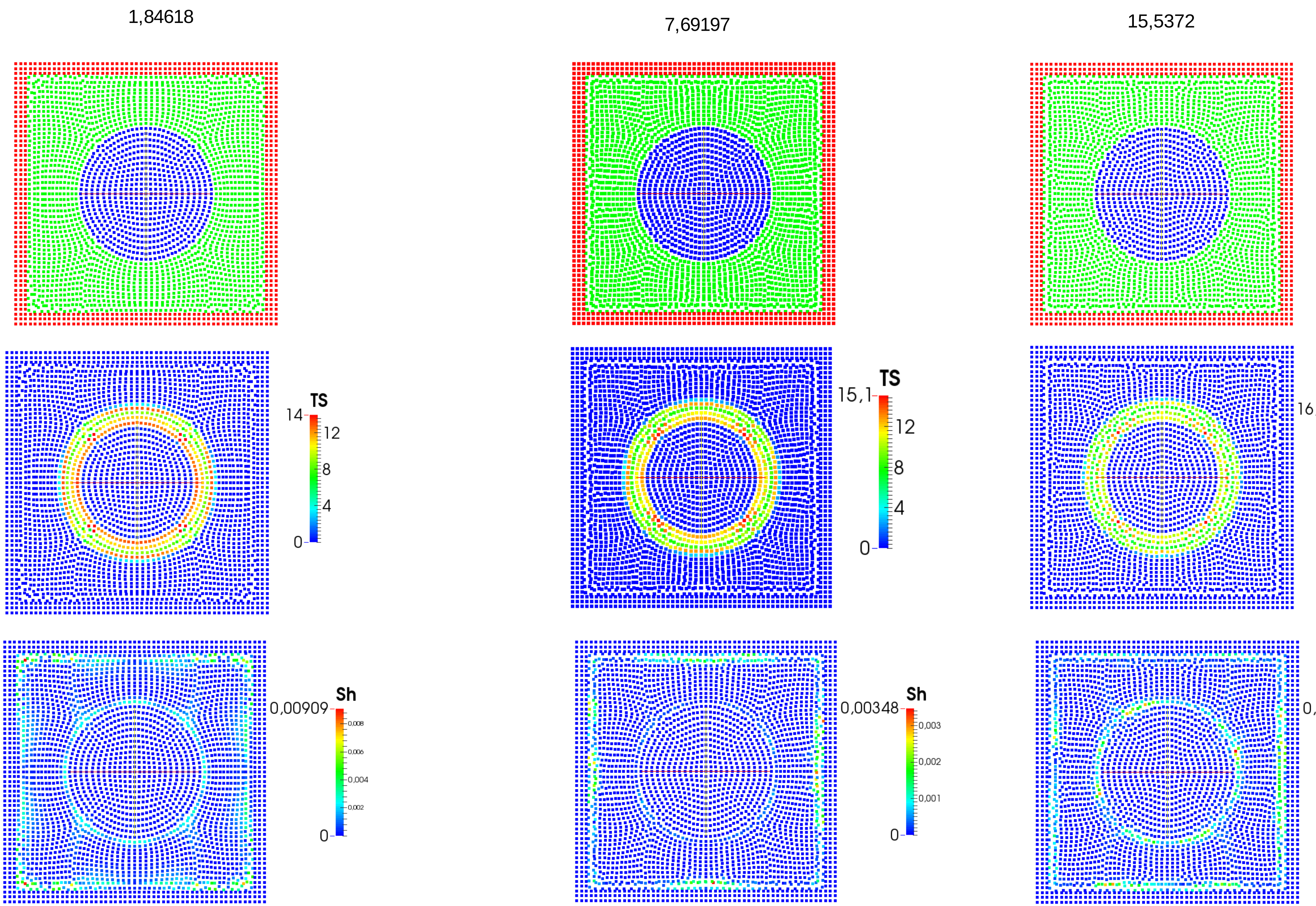


Surface Tension with Shifting

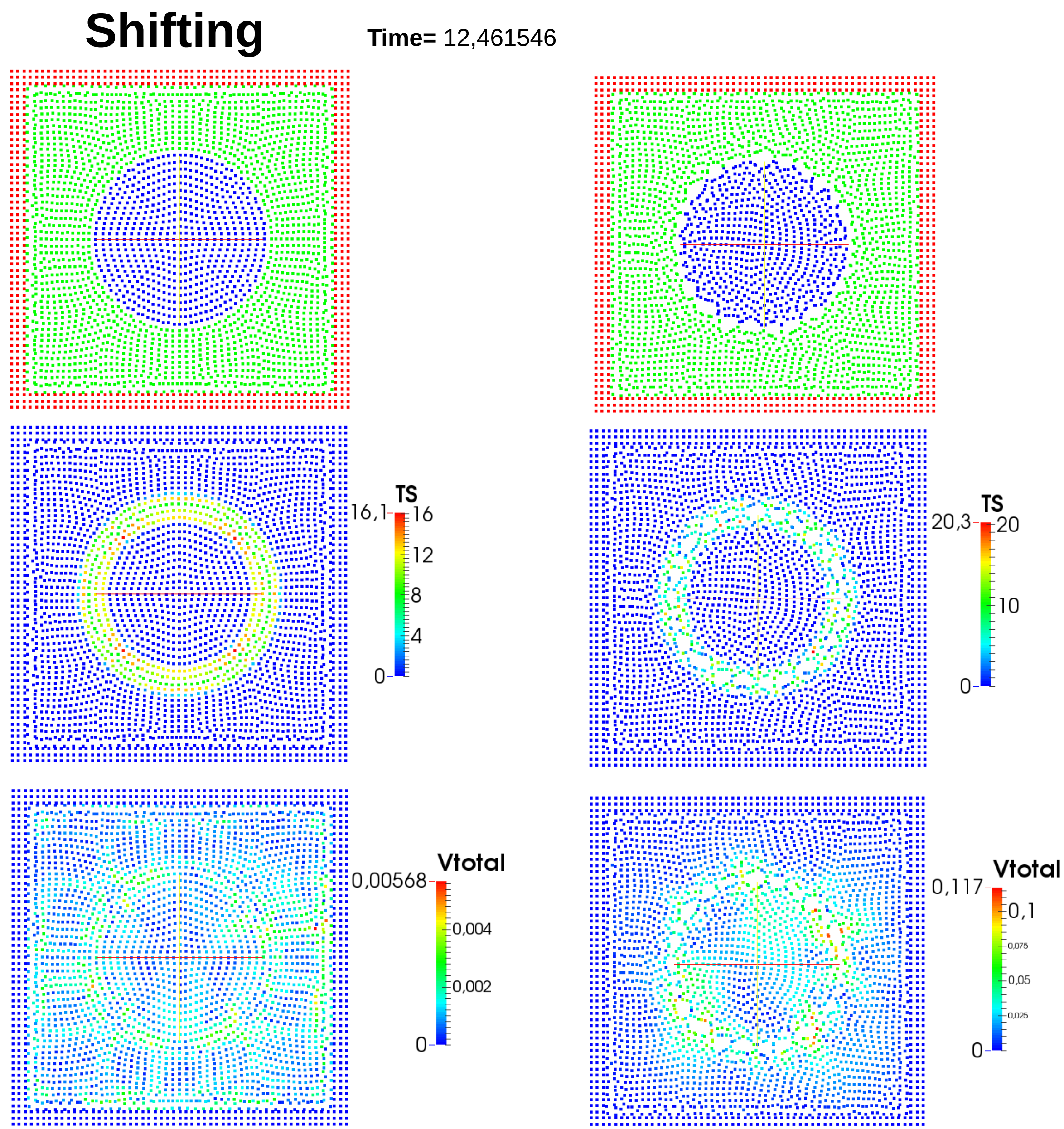


$$Densidad = {}^{1}\!/_{1}$$

Surface Tension with Shifting



Surface Tension with Shifting

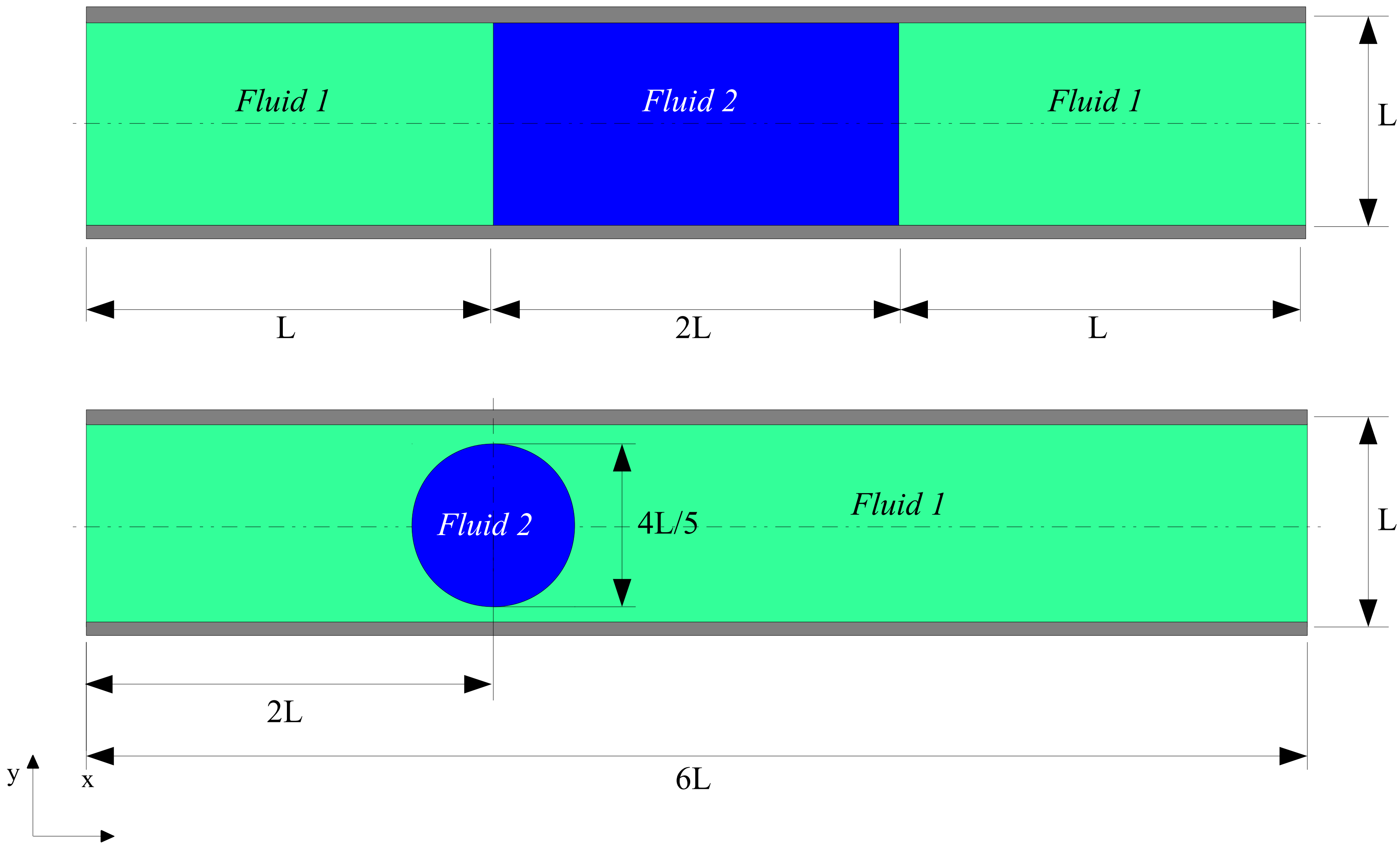


Conclusions

- Eliminated the dependence with:
  - XSPH
  - Shepard
- Boundary condition is improved, using:
  - BC Dummy of Adami, Hu and Adams.
- Shifting is presented as a viable alternative for implementation of multi-phase problems.

Numerical examples

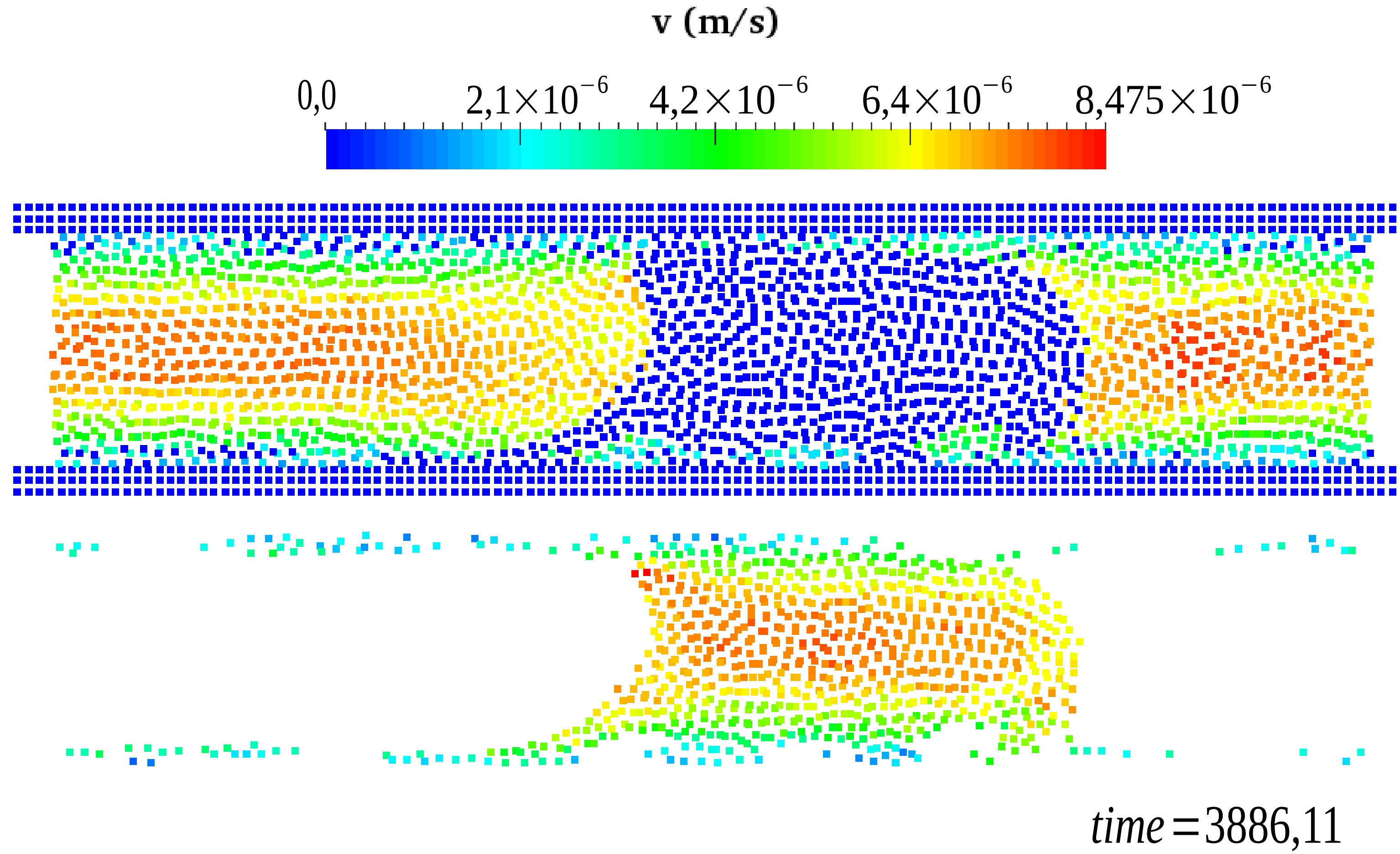
Mesoscopic flow in a channel



Numerical examples

Mesoscopic flow in a channel

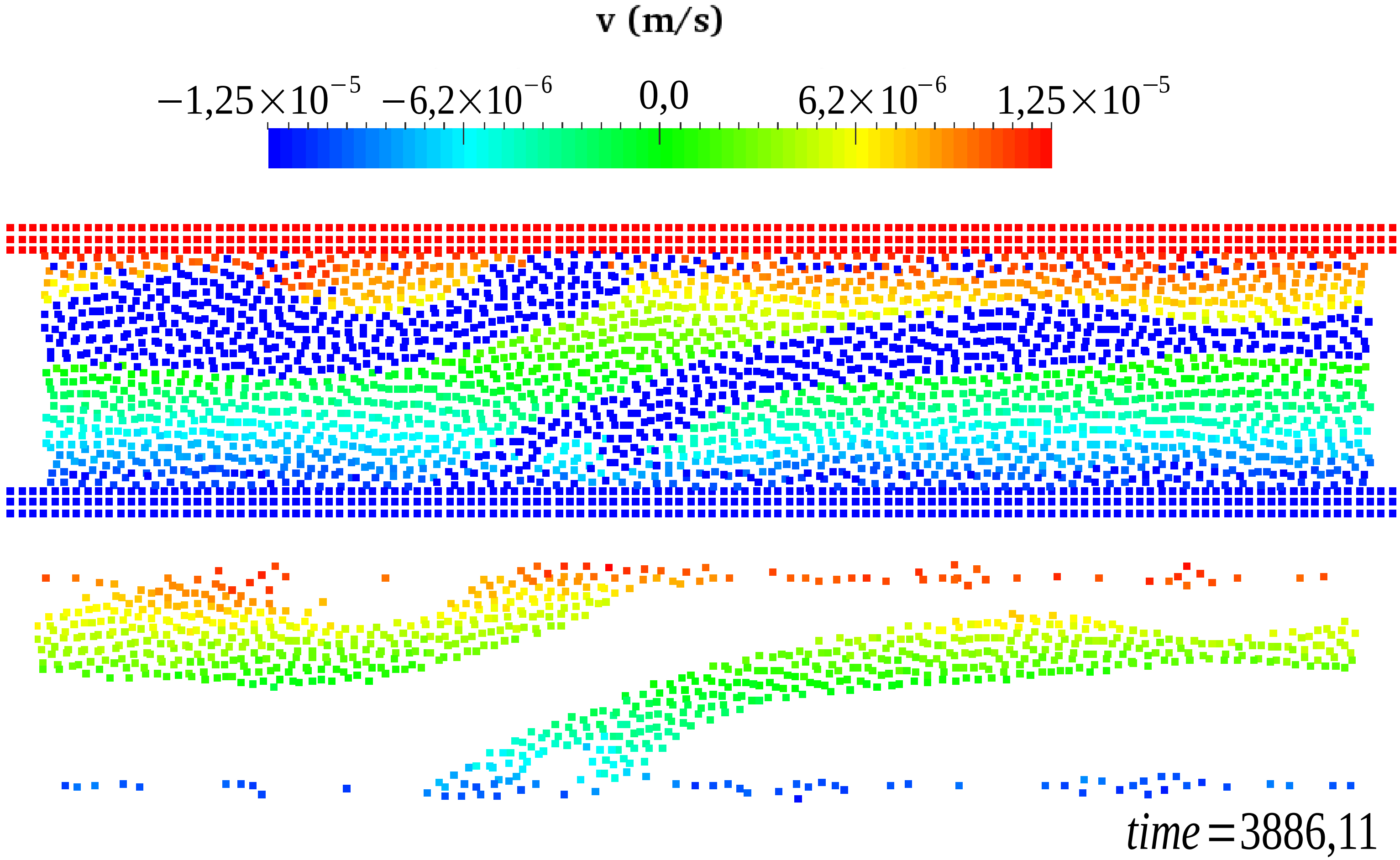
Poiseuille



Numerical examples

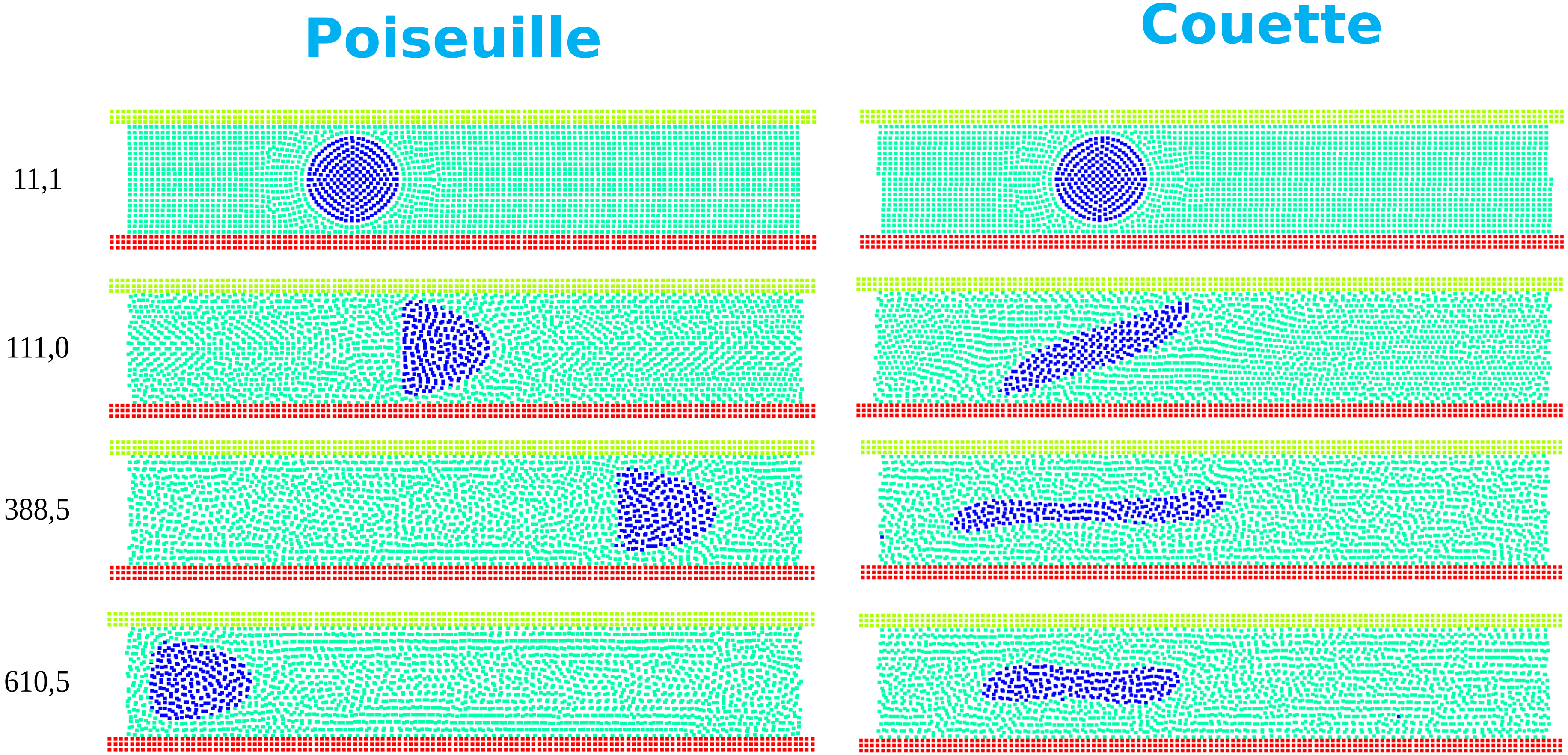
Mesoscopic flow in a channel

Couette



Future implementations

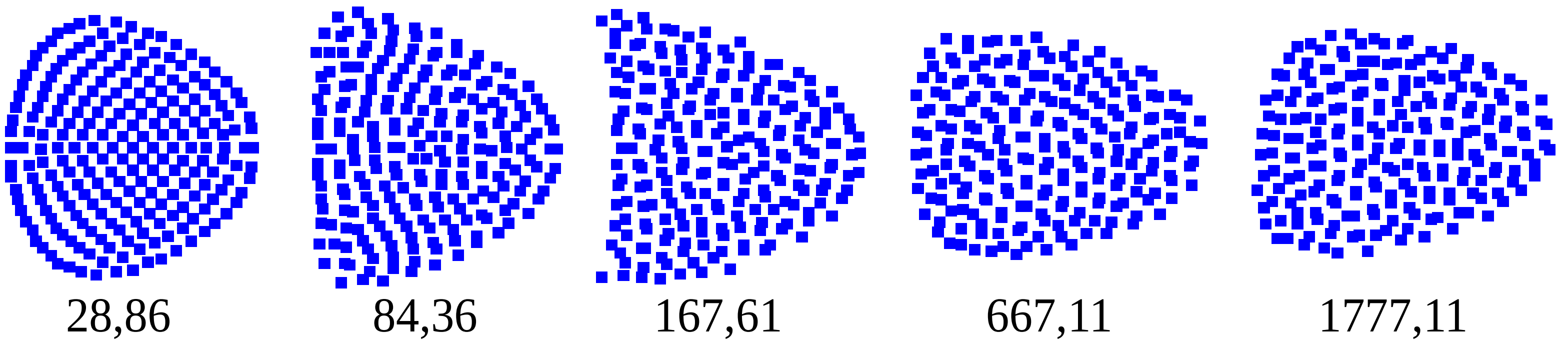
Mesoscopic flow in a channel

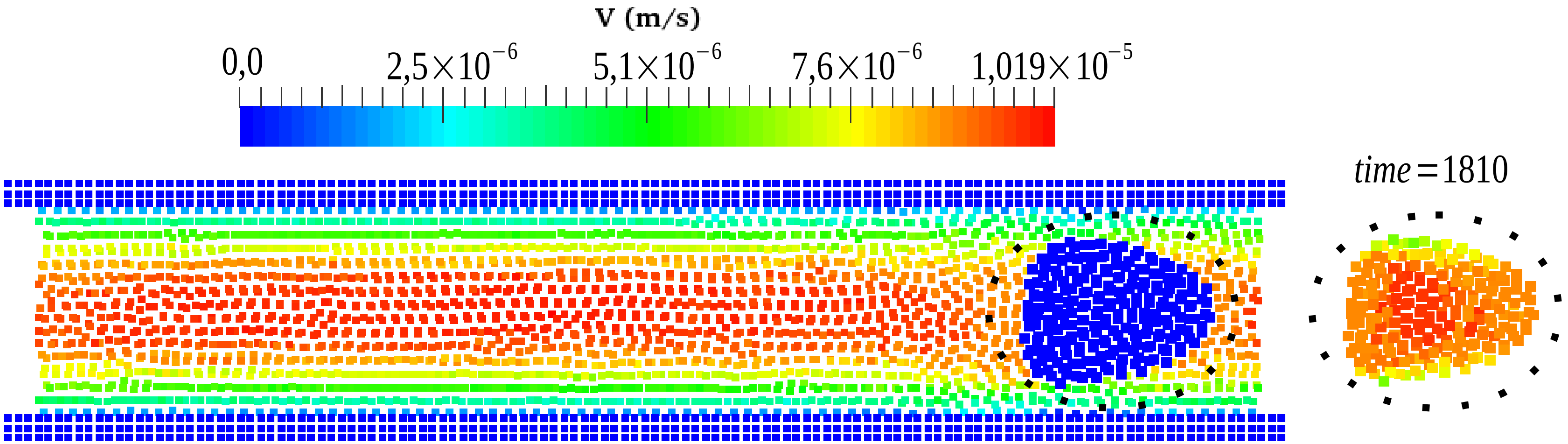


Future implementations

Mesoscopic flow in a channel

Poiseuille





Numerical examples

Mesoscopic flow in a channel

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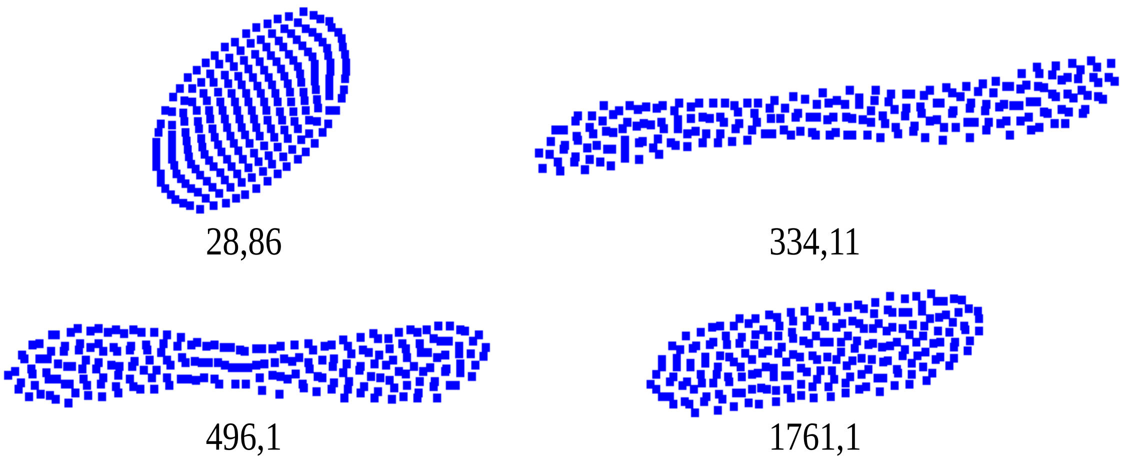
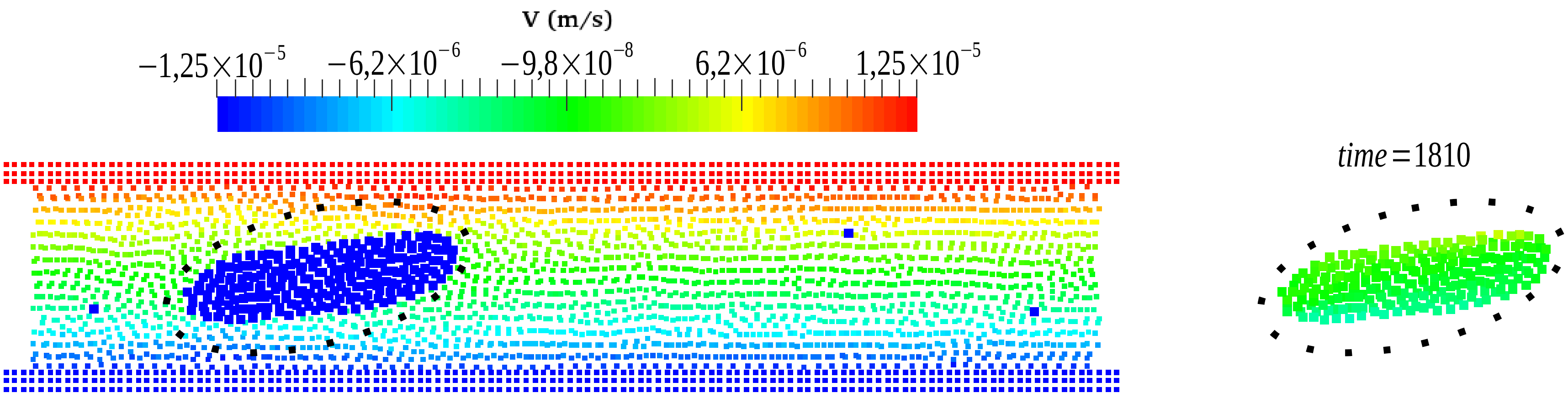
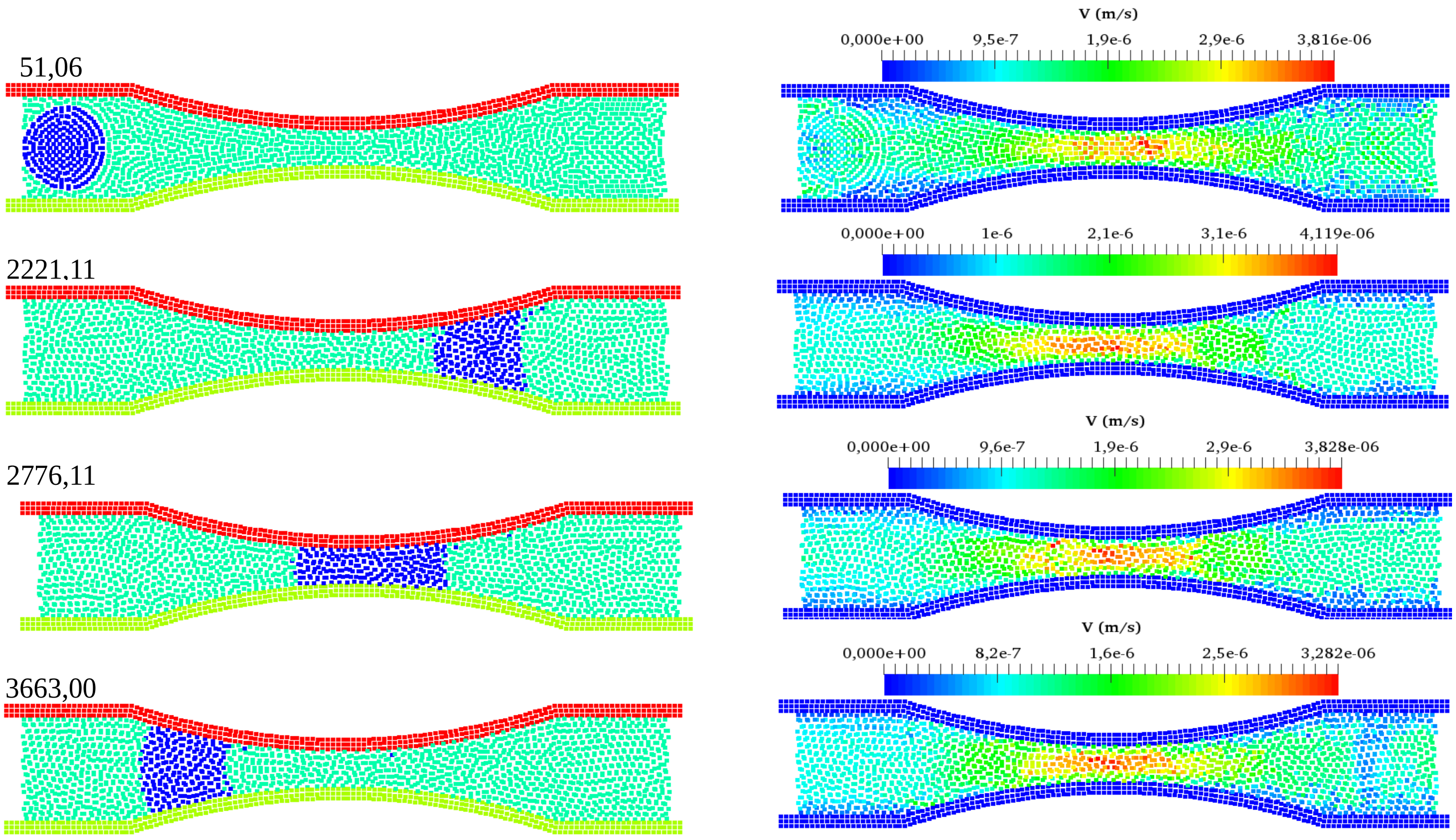




Future implementations

Developing work:

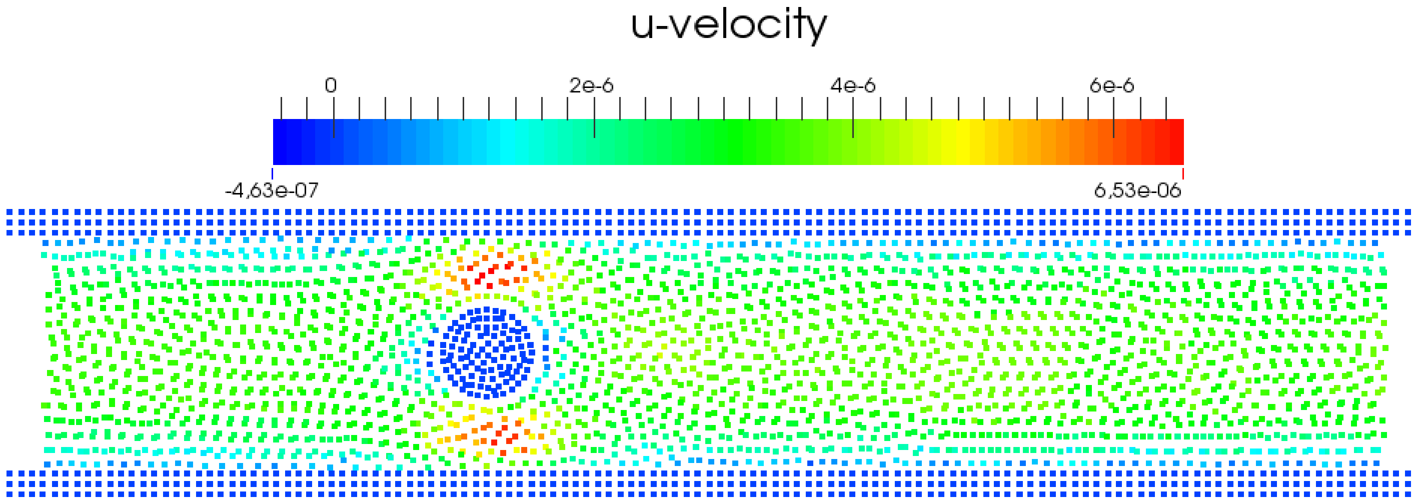
- Porous cavities and micro-channels



Future implementations

Developing work:

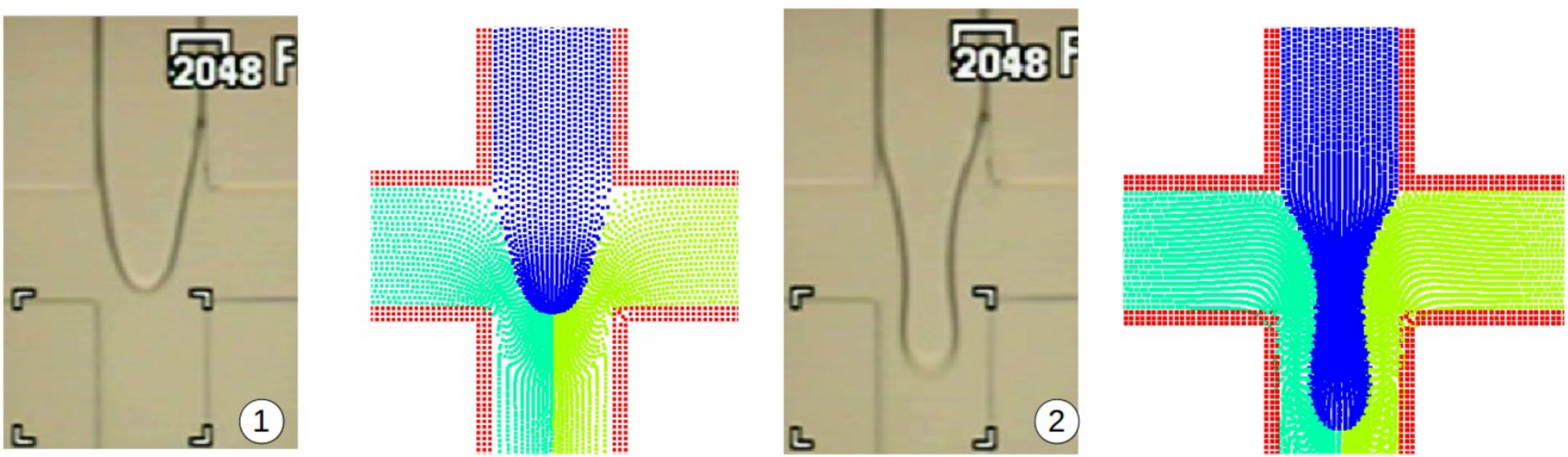
- Porous cavities



Future implementations

Developing work:

- Microfluidic devices



Thank you

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