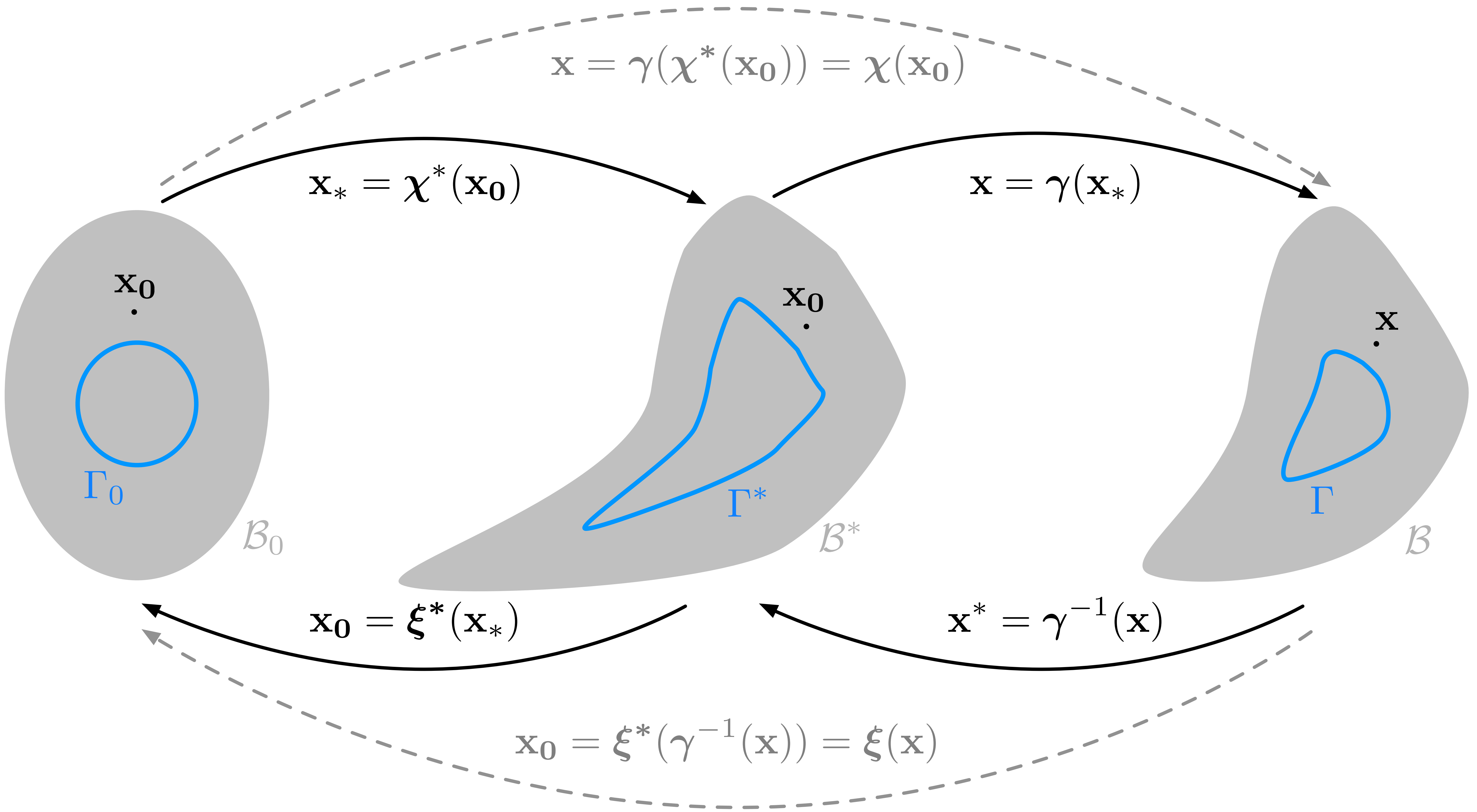
A Volume-Preserving Reference Map Method for the Level Set Representation



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The VIP* Method

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**Volume and Interface Preserving*

UC Merced

UC MERCED BOBCATS

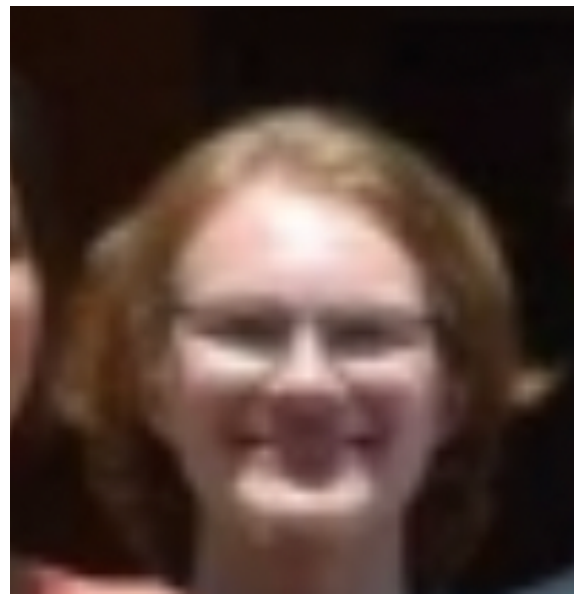
Applied Mathematics @ UC Merced

- **Scientific and Data Enabled Computing**
- Non-linear waves and Optimization
- **Computational biology**
- **Energy & the Environment (Fluid Mechanics)**

MACS @ UC Merced

Adam Binswanger

Anna Kucherova

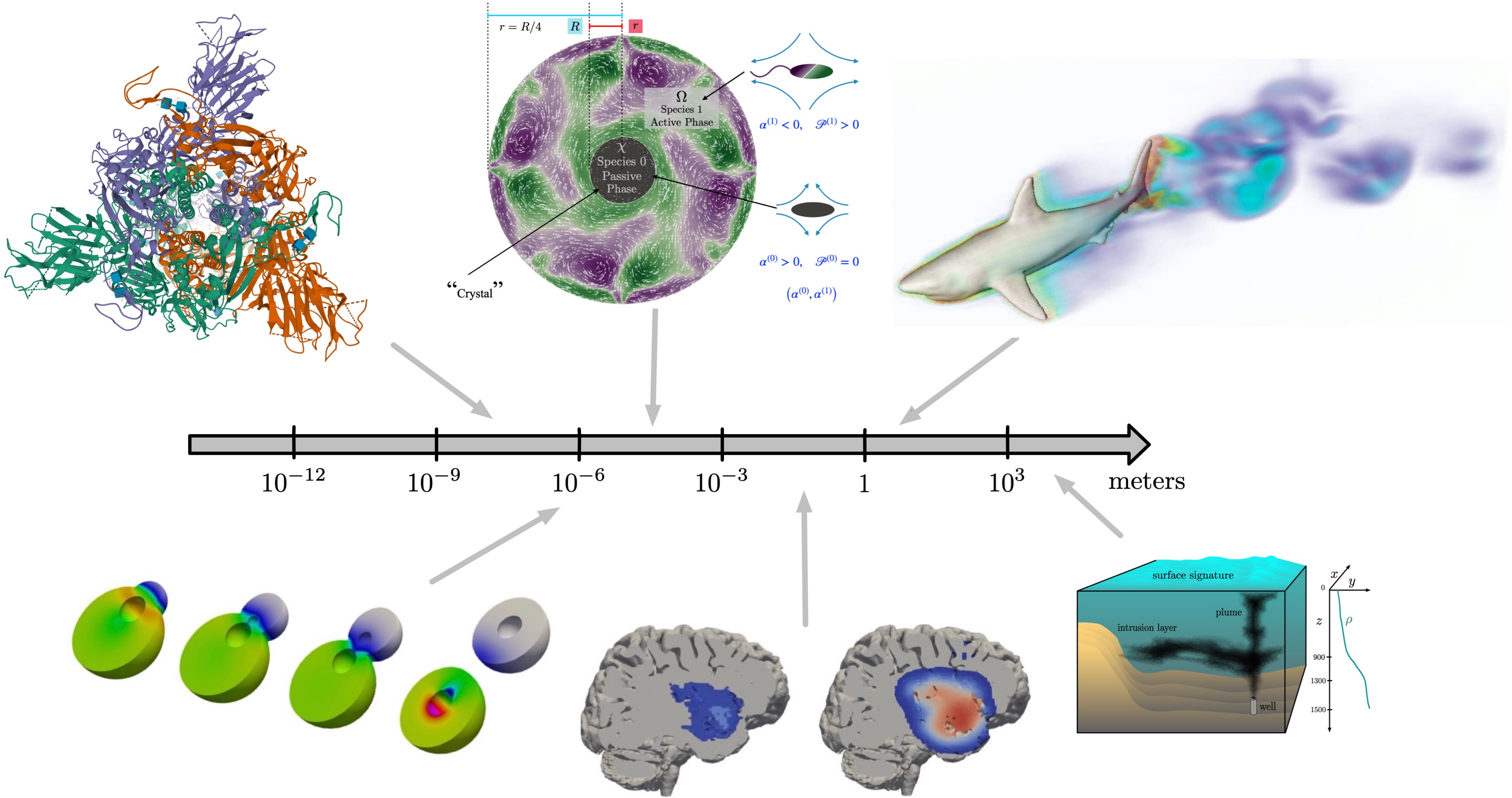


Cayce Fylling

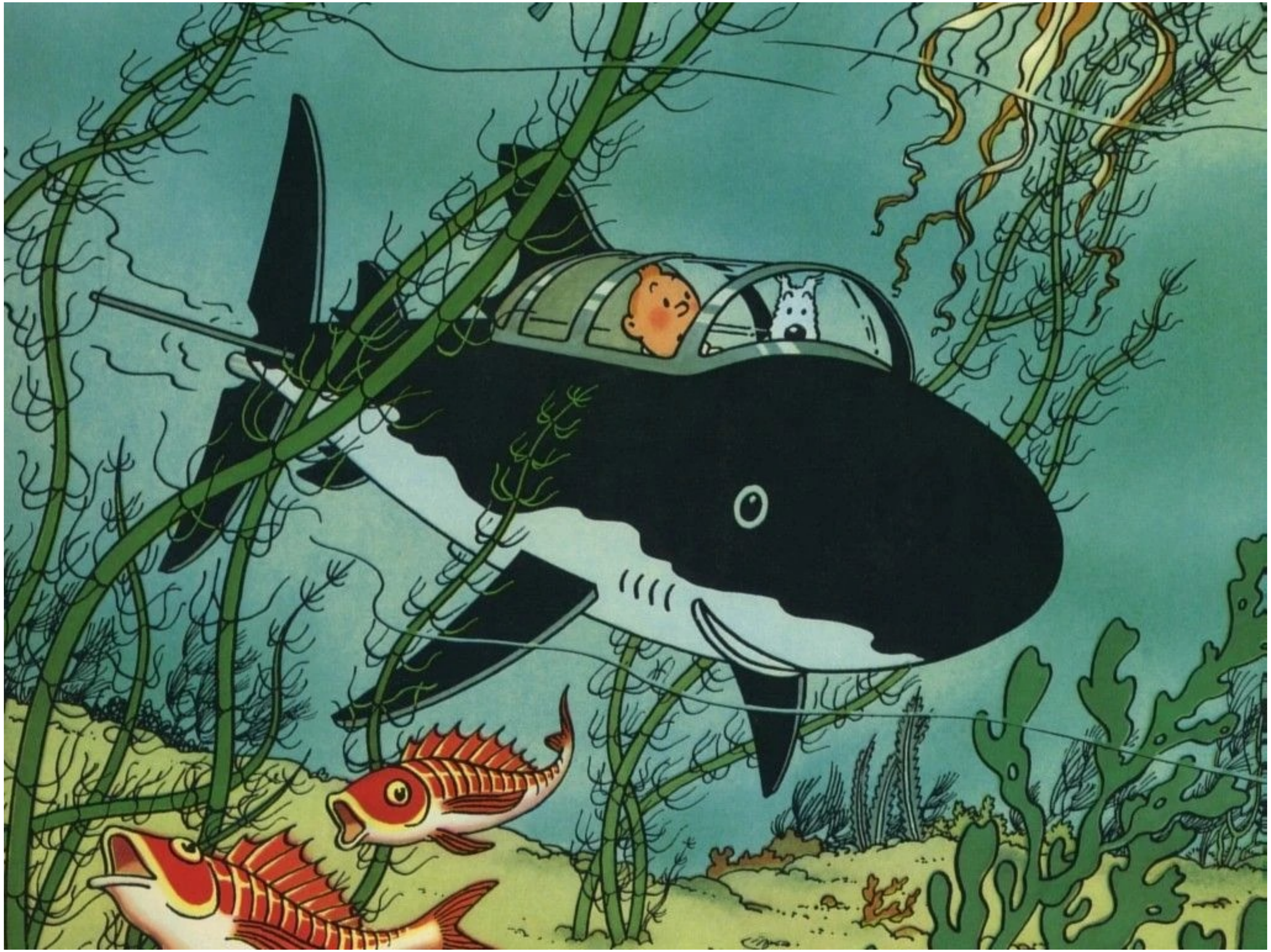
Matt Blomquist

Masato Terasaki

Scott West



MACS @ UC Merced



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Mathematical Modeling

$$\text{PDE:} \quad \frac{Du}{Dt} = \mu \triangle u - \nabla p f + \text{BC} \quad \forall x \in \Omega$$

$$\text{BC:} \quad u = g \quad \forall x \in \partial\Omega$$

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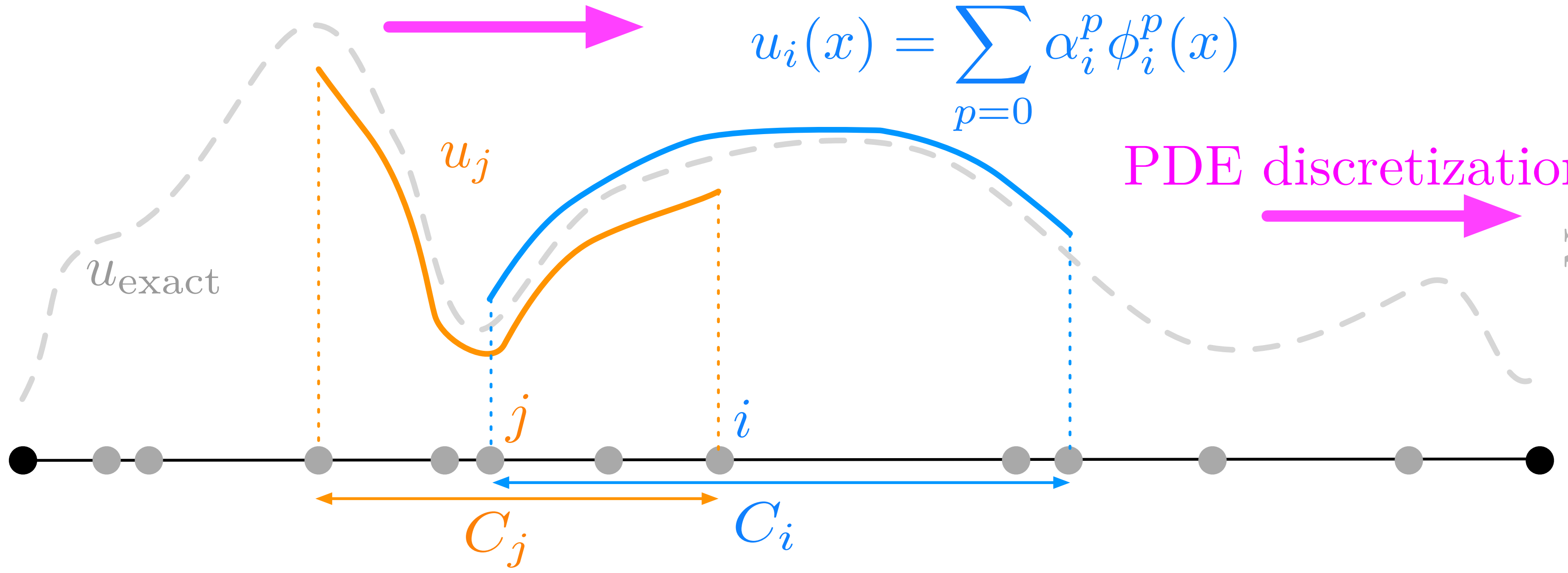
Mathematical Modeling

PDE: $\frac{Du}{Dt} = \mu \triangle u - \nabla p f + \text{BC} \quad \forall x \in \Omega$

BC: $u = g \quad \forall x \in \partial\Omega$

Solution representation

$$u_i(x) = \sum_{p=0}^{P} \alpha_i^p \phi_i^p(x)$$



PDE discretization

$P \times N$

N

$$\begin{bmatrix} \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots \\ & \vdots & \\ & \vdots & \\ \cdots & \cdots & \cdots \end{bmatrix} \begin{bmatrix} \alpha_1^1 \\ \alpha_1^2 \\ \vdots \\ \alpha_N^P \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ \vdots \\ b_N \end{bmatrix}$$

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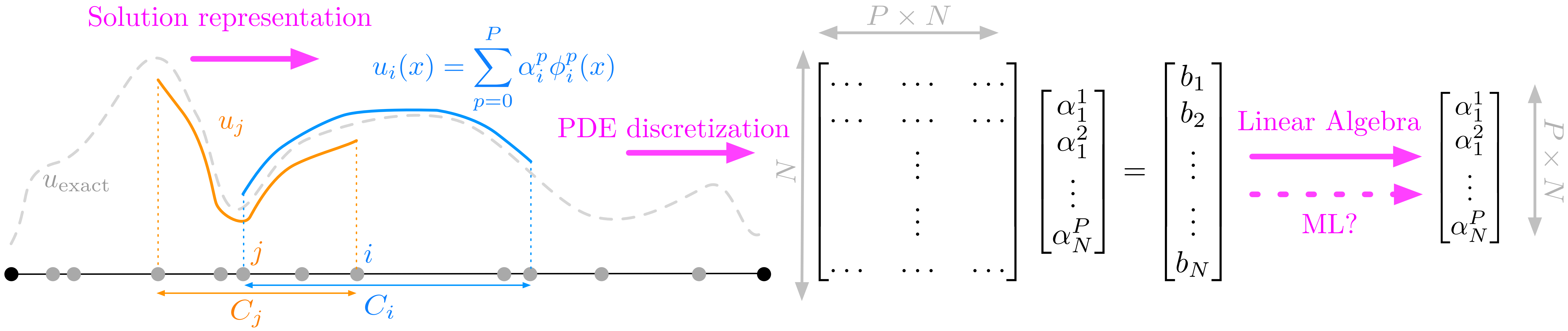
Mathematical Modeling

PDE: $$\frac{Du}{Dt} = \mu \triangle u - \nabla p f + \text{BC} \quad \forall x \in \Omega$$

BC: $$u = g \quad \forall x \in \partial\Omega$$



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Mathematical Modeling

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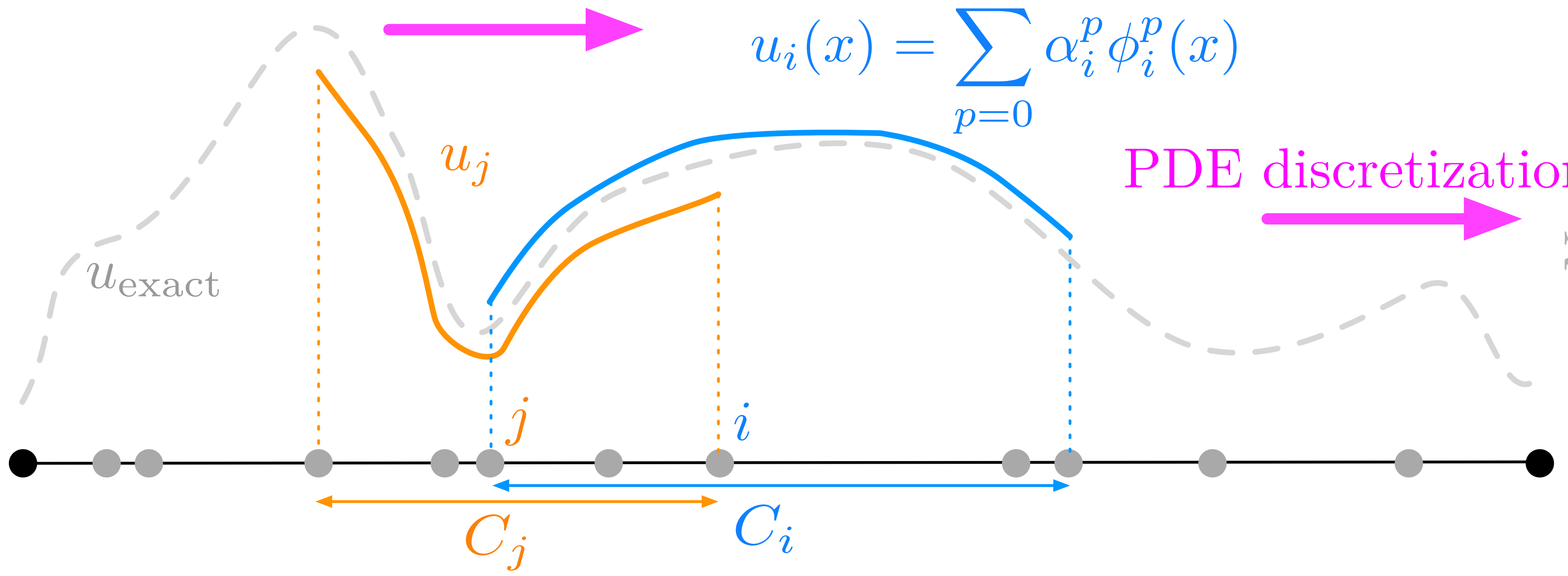

PDE discretization

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Linear Algebra

ML?

$$\begin{bmatrix} \alpha_1^1 \\ \alpha_1^2 \\ \vdots \\ \alpha_N^P \end{bmatrix}$$

$P \times N$

Visualization

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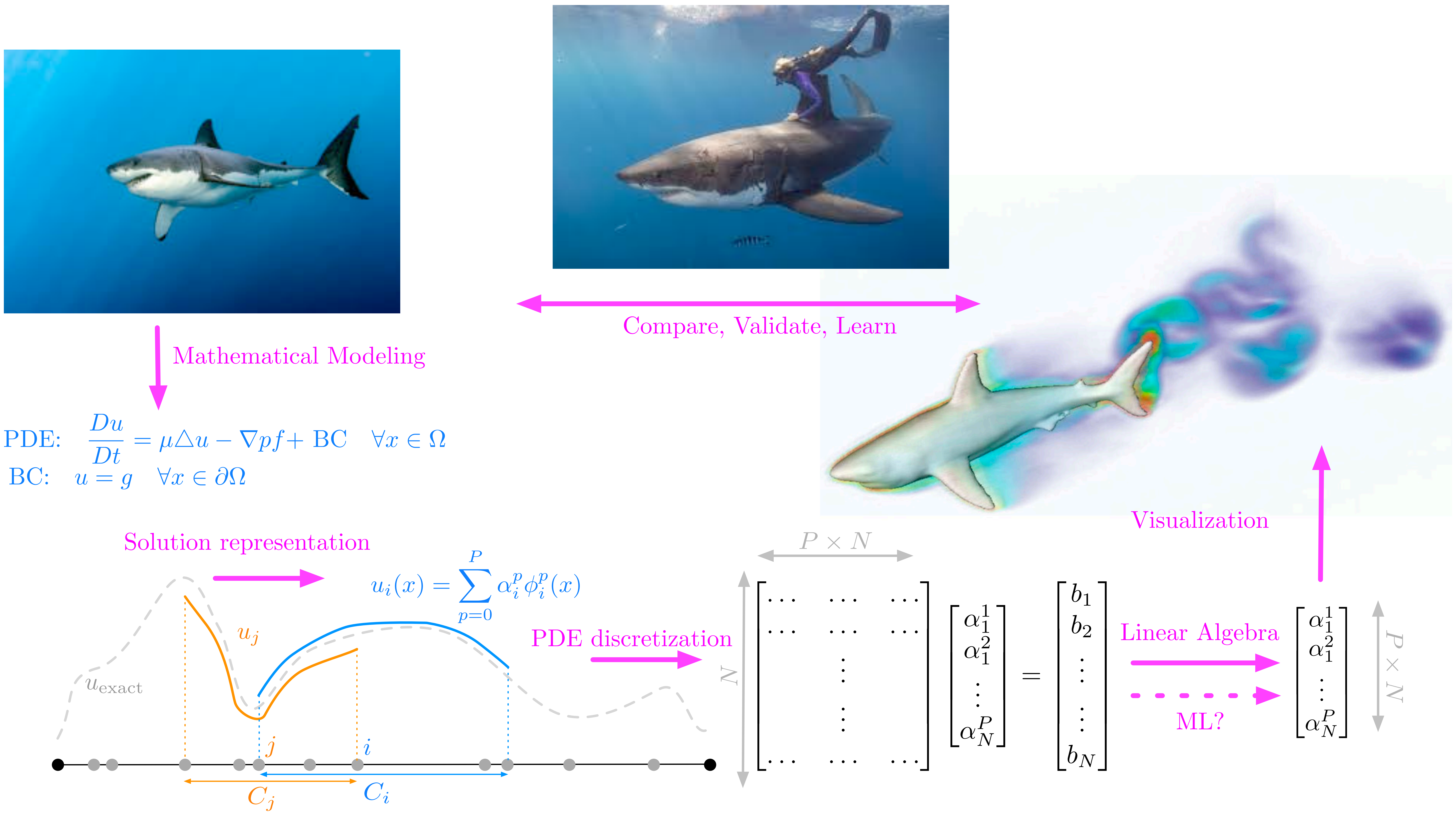

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Compare, Validate, Learn

Mathematical Modeling

PDE: $\frac{Du}{Dt} = \mu \Delta u - \nabla p f + \text{BC} \quad \forall x \in \Omega$

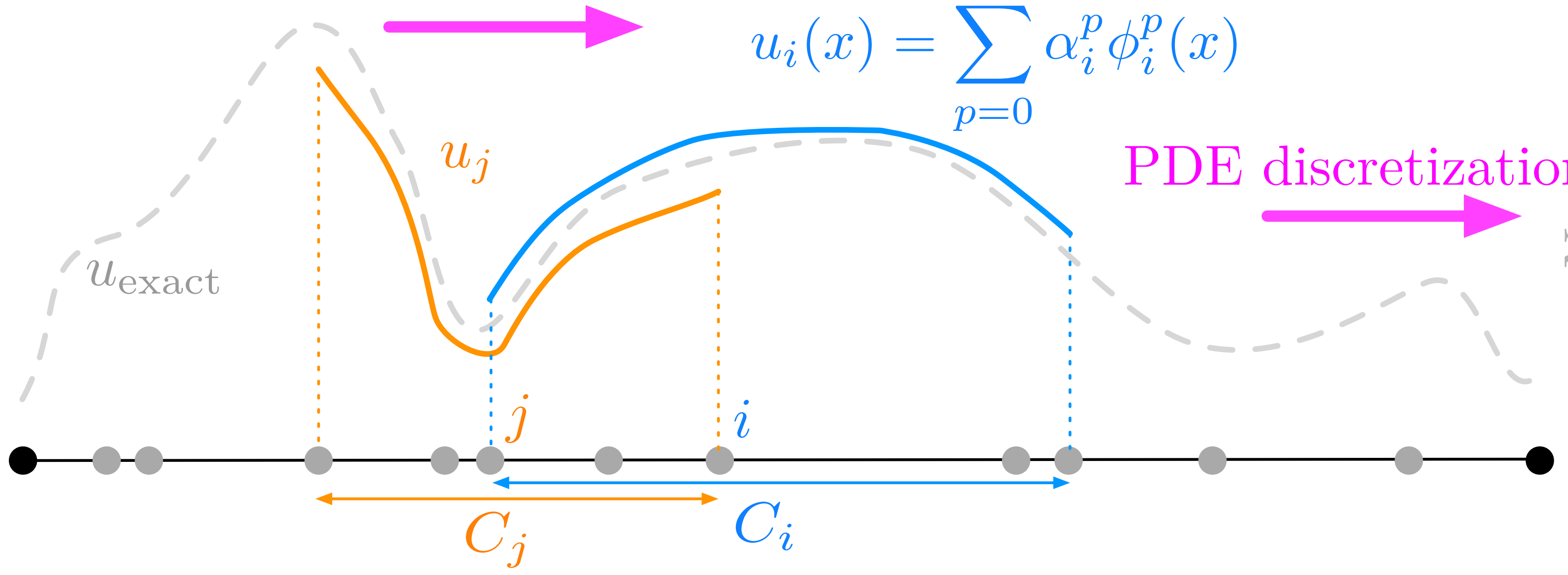
BC: $u = g \quad \forall x \in \partial\Omega$

bitbucket.org/casl_macs

Visualization

Solution representation

$$u_i(x) = \sum_{p=0}^{P} \alpha_i^p \phi_i^p(x)$$



PDE discretization

$P \times N$

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$$\begin{bmatrix} \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots \\ & \vdots & \\ & \vdots & \\ \cdots & \cdots & \cdots \end{bmatrix} \begin{bmatrix} \alpha_1^1 \\ \alpha_1^2 \\ \vdots \\ \alpha_N^P \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ \vdots \\ b_N \end{bmatrix}$$

Linear Algebra

ML?

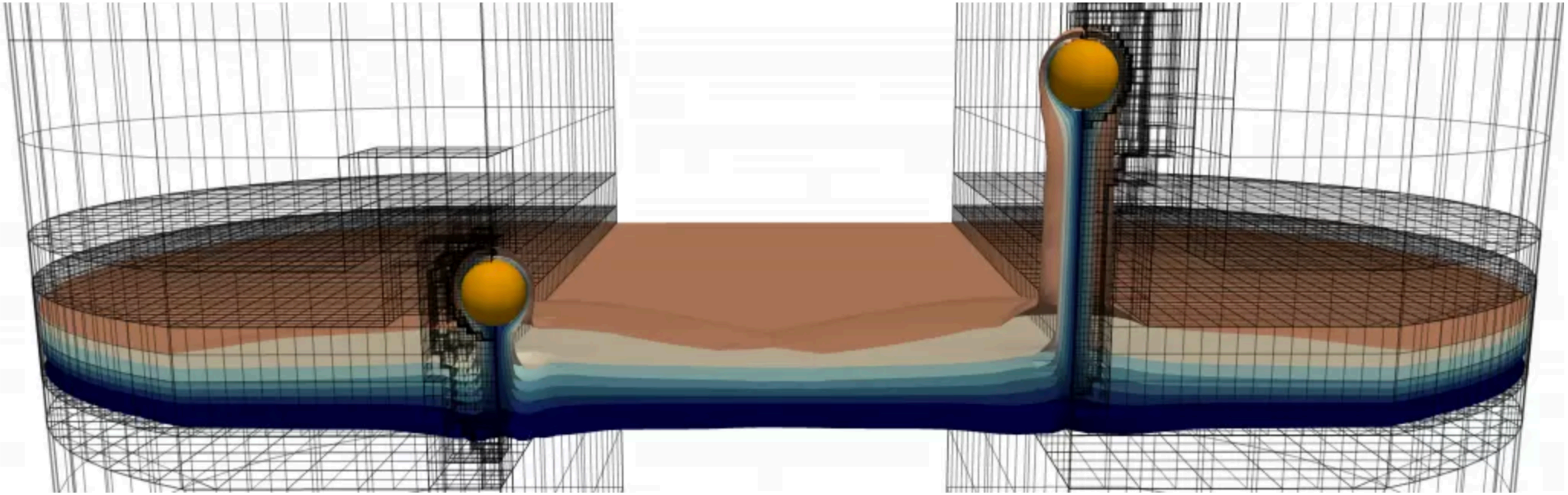
$$\begin{bmatrix} \alpha_1^1 \\ \alpha_1^2 \\ \vdots \\ \alpha_N^P \end{bmatrix}$$

$P \times N$

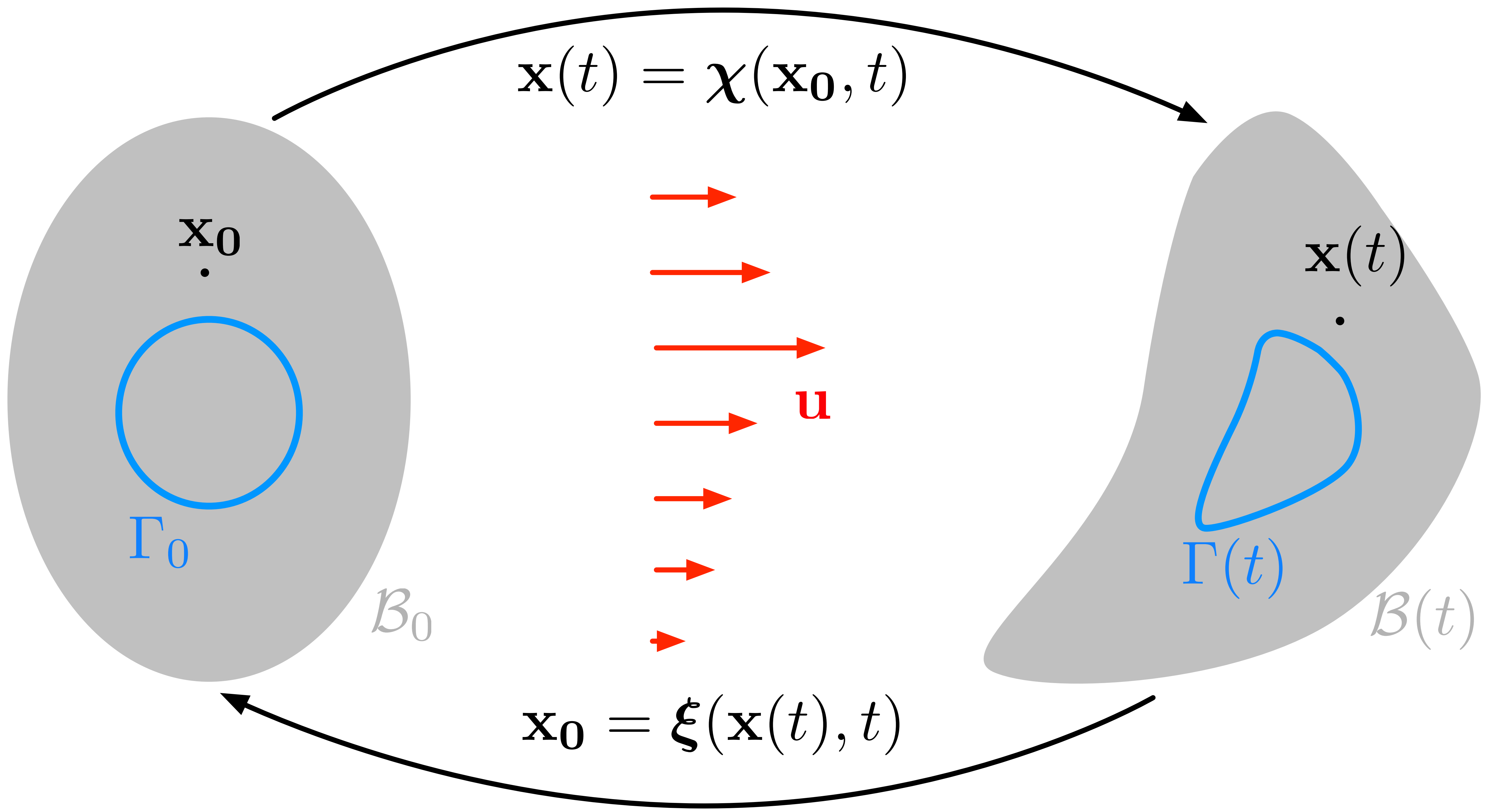
Scientific Library

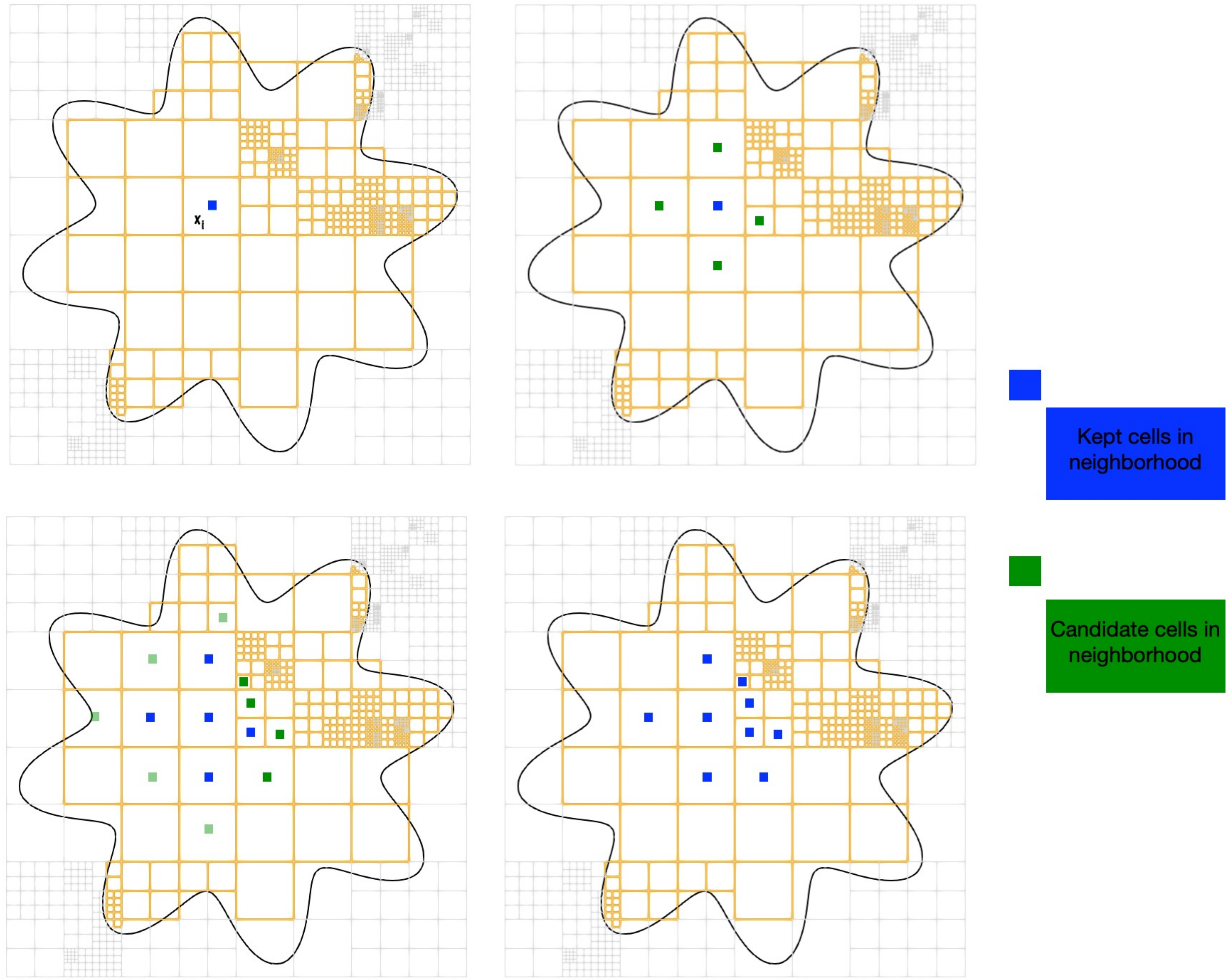
- Self-contained HPC library: **Mathematical Sandbox**
- C++, openMP
- (Non-graded) **Octree/Quadtree**
- Finite **Differences** and **Volumes**
- **Elliptic, parabolic, and hyperbolic** (advection, diffusion, reaction)
- **Sharp** Boundary conditions, **Complex/moving** interfaces
- More than 200K lines of code
- "User friendly"

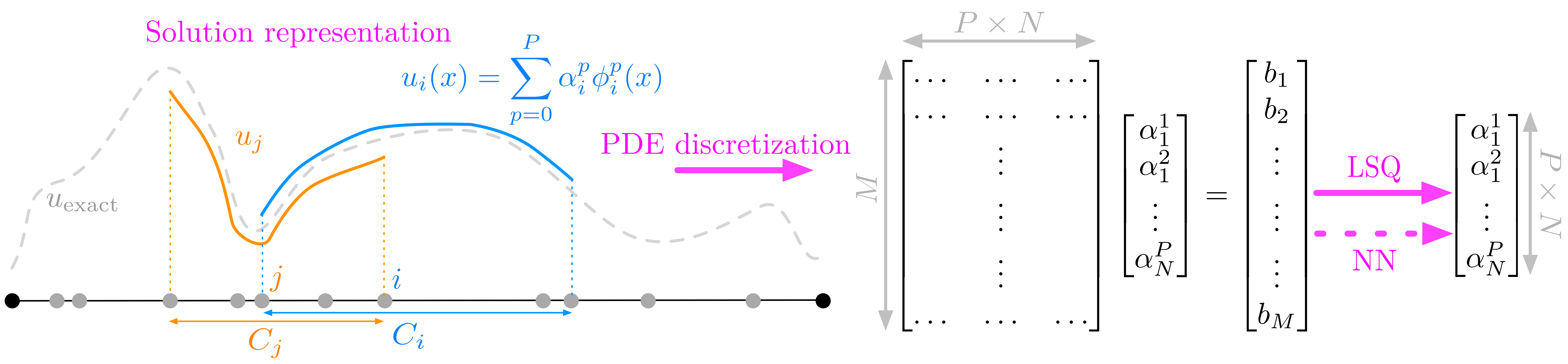
bitbucket.org/casl_macs



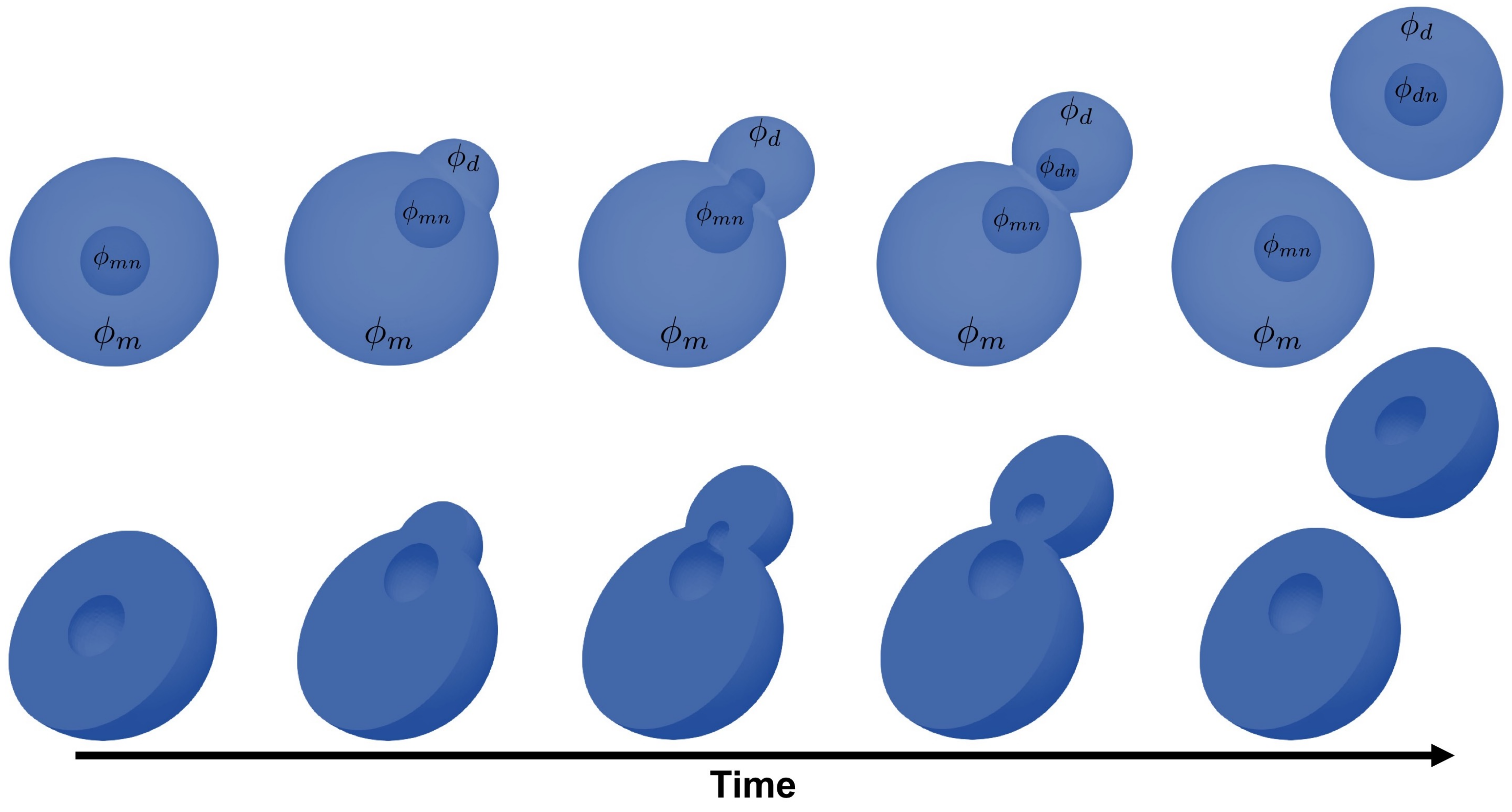
Scientific Computing





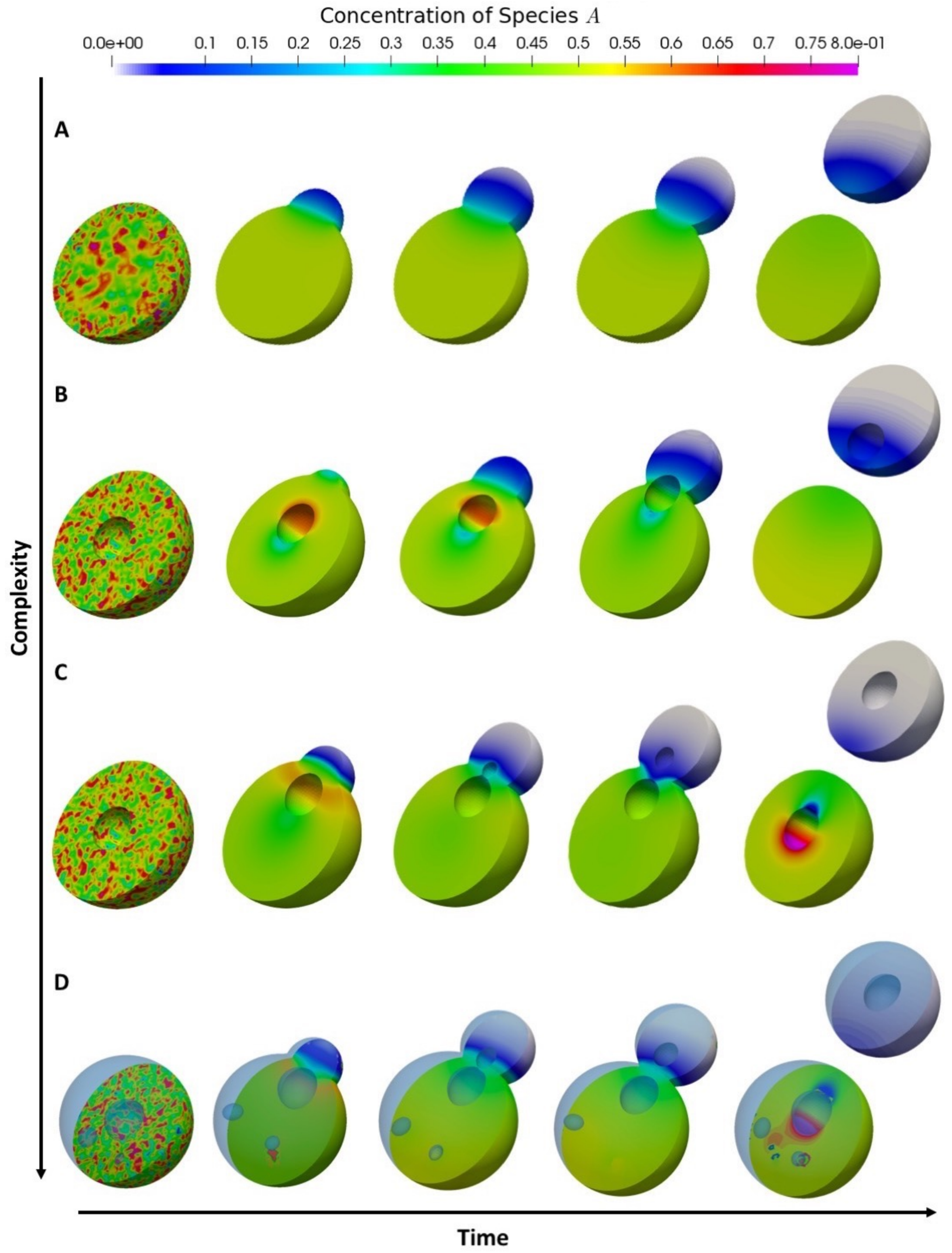


Prions aggregation in dividing yeast cells



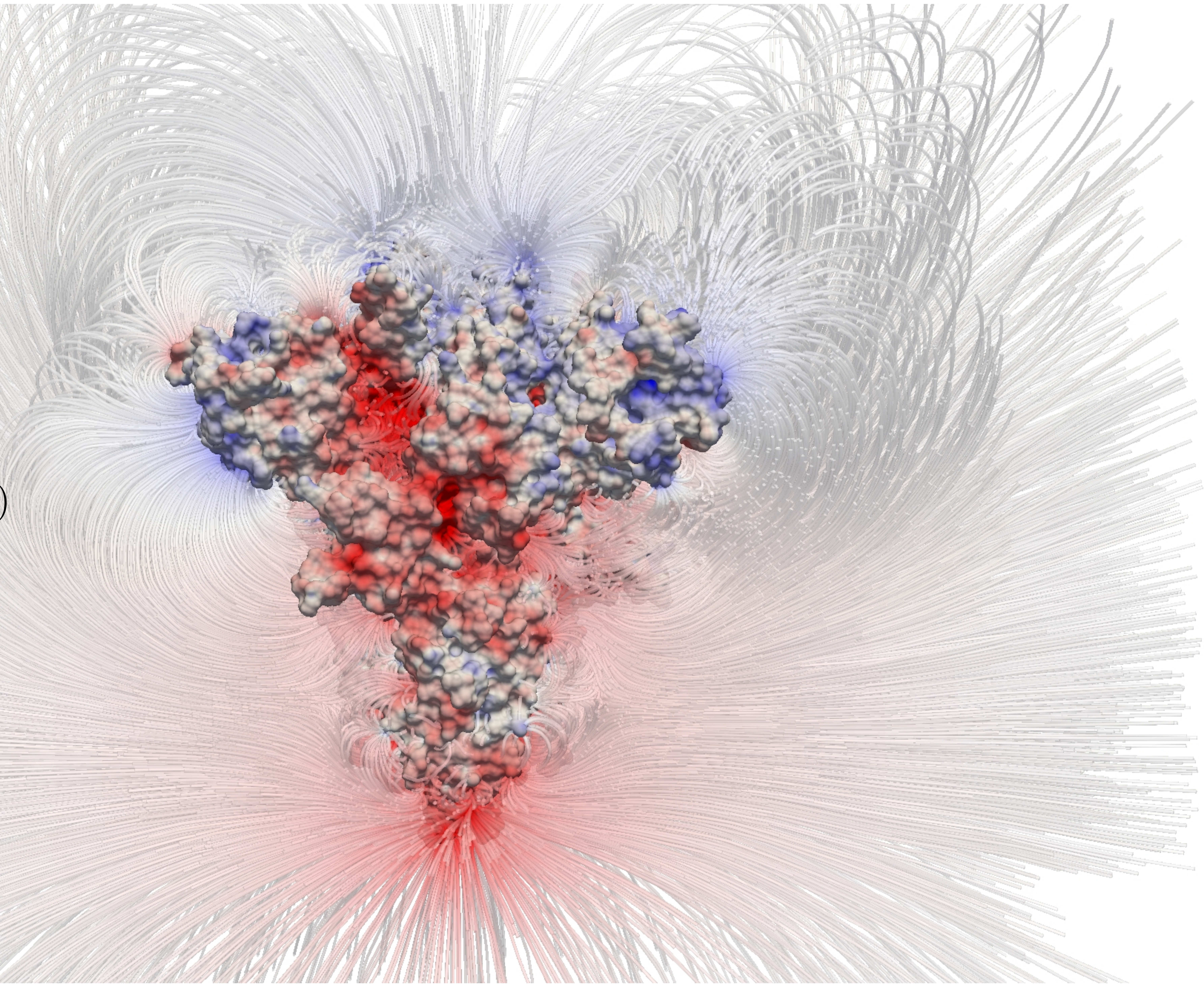
Diffusion reaction equations

$$
\begin{aligned}
\frac{\partial \psi_A}{\partial t} - D_A \Delta \psi_A &= 2\gamma_{BA}\psi_B - \gamma_{AB}\psi_A^2 \quad \forall \mathbf{x} \in \Omega(t), \\
\frac{\partial \psi_B}{\partial t} - D_B \Delta \psi_B &= \frac{1}{2}\gamma_{AB}\psi_A^2 - \gamma_{BA}\psi_B \quad \forall \mathbf{x} \in \Omega(t).
\end{aligned}
$$



Heydari et al. Journal of Computational Sciences (2021)

Electrostatic of folding proteins



Main quantities

potential: ψ Electric field: $\mathbf{E} = -\nabla\psi$

Poisson-Boltzmann

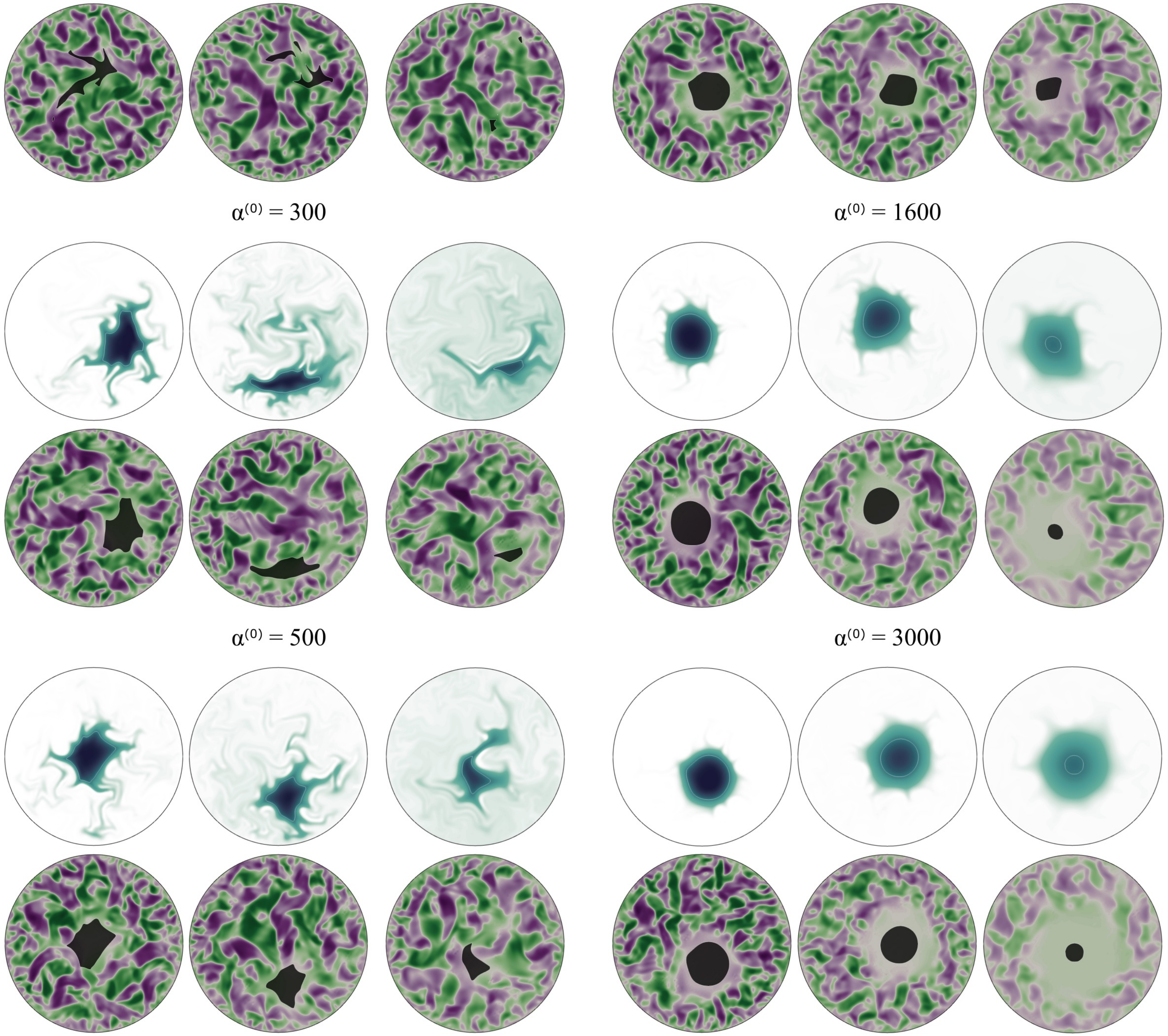
$$-\nabla \cdot (\epsilon \nabla \psi) + \kappa_D^2(\mathbf{x}) \sinh(\psi) = \sum_{i=1}^{N} \lambda_B z_i \delta(\mathbf{x} - \mathbf{x}_i)$$

Interface conditions

$$[\psi]_\Gamma = 0, \qquad [\epsilon \nabla \psi \cdot \mathbf{n}]_\Gamma = 0$$

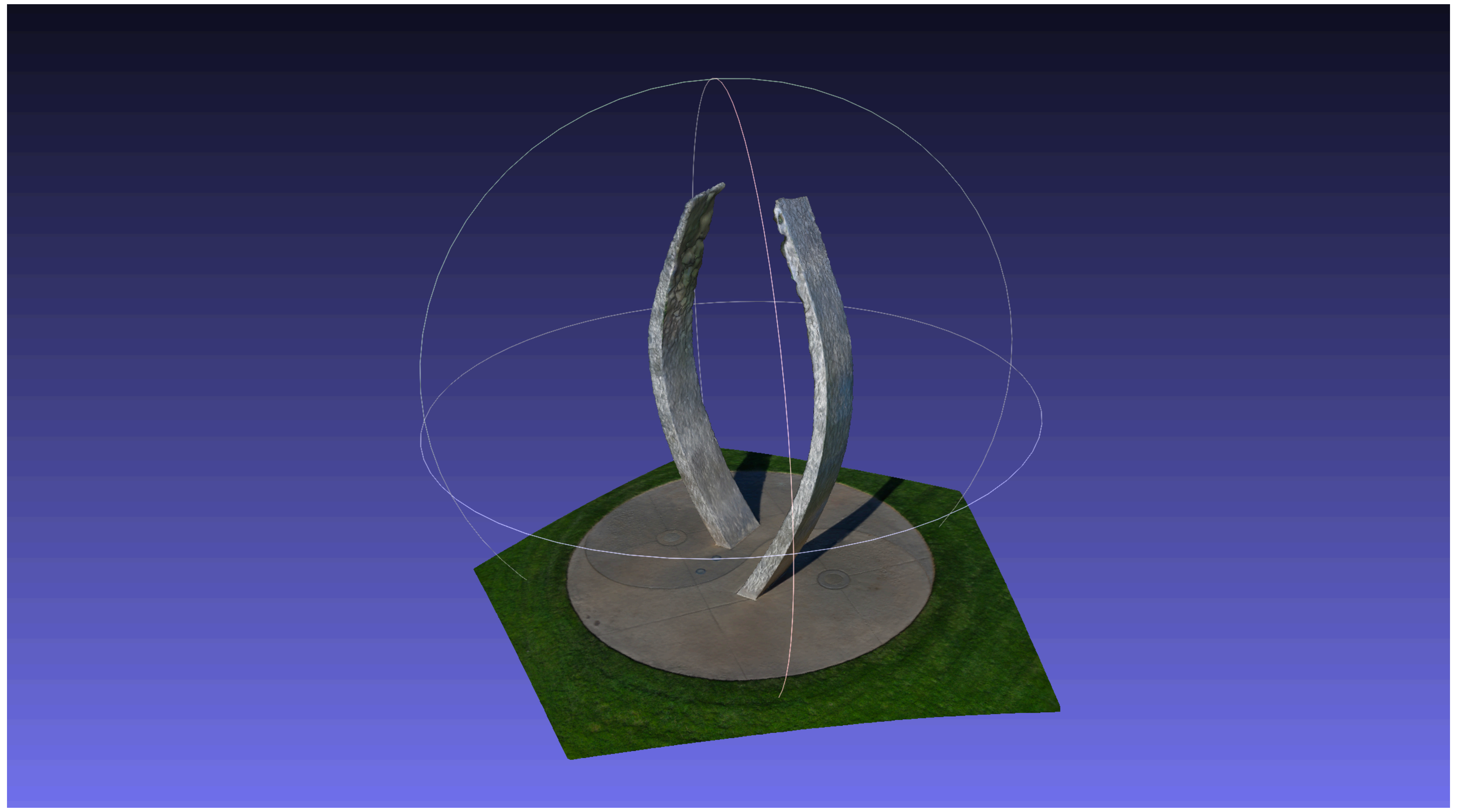
Kucherova et al. Journal of Computational Sciences (2020)

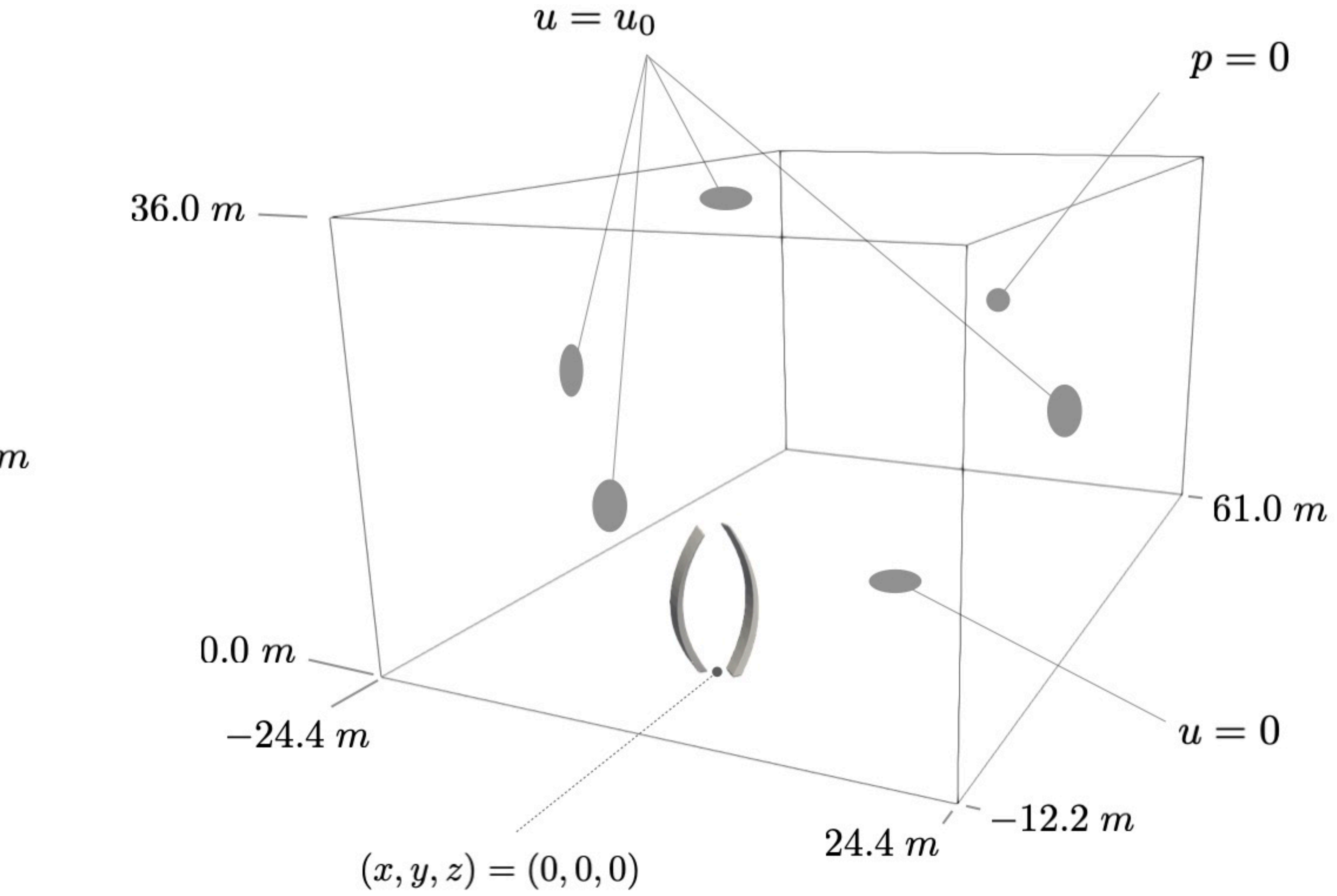
Active Biological Suspensions

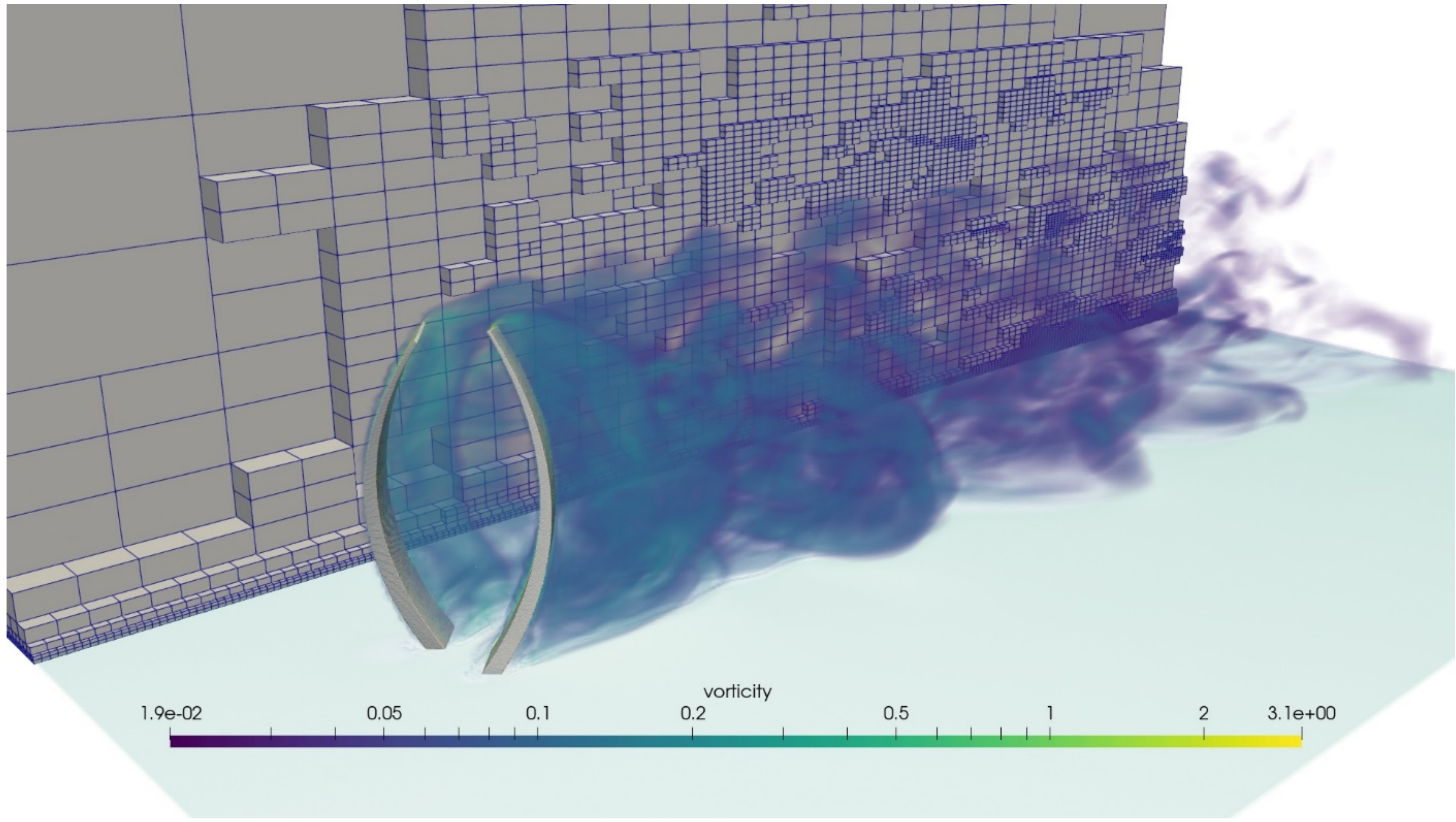


Fylling et al. SoftMatter 2023

Flows around urban structures





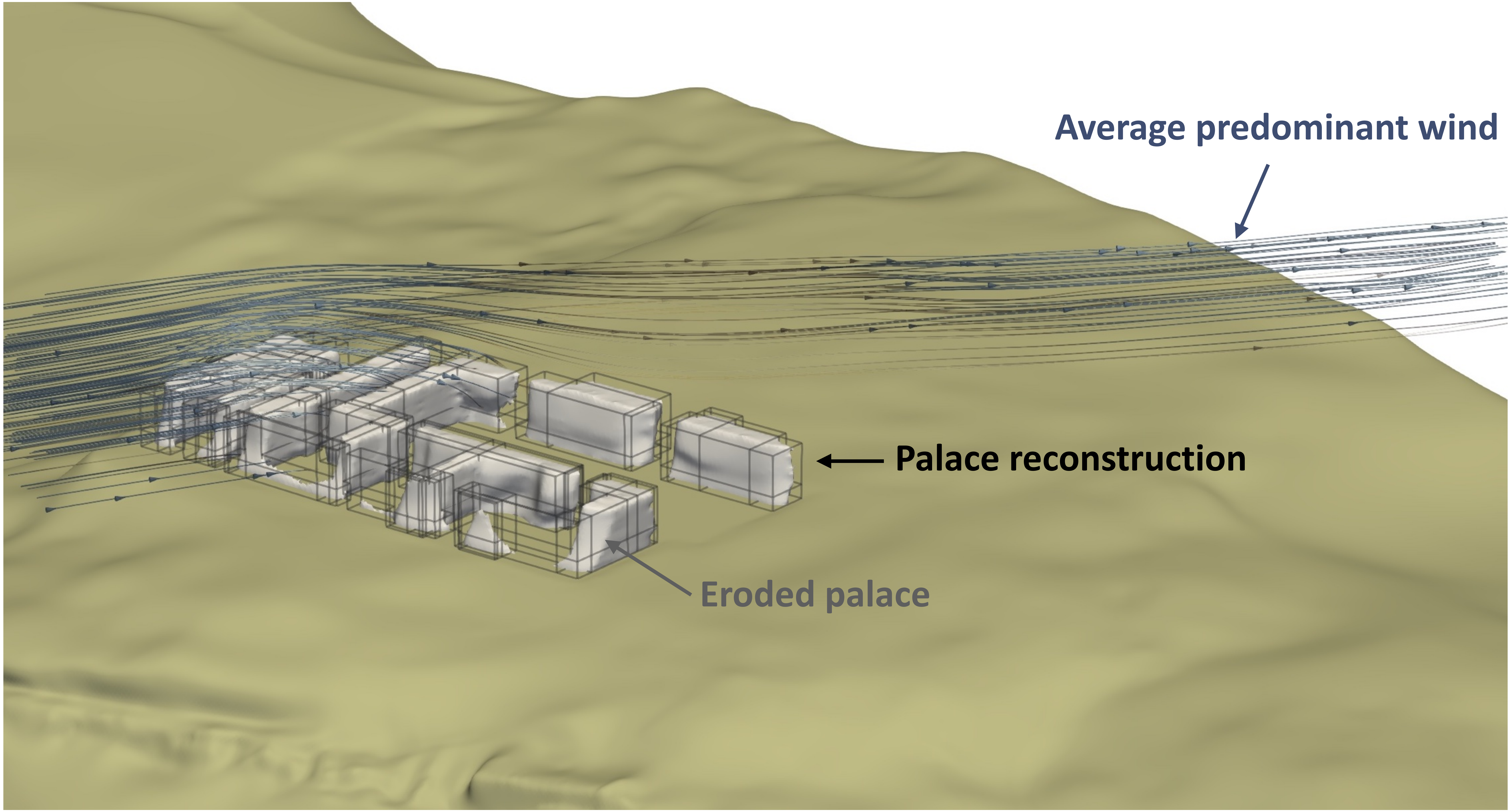


Flows around urban structures

$$CFL = 20$$

$$Re = 10^7$$

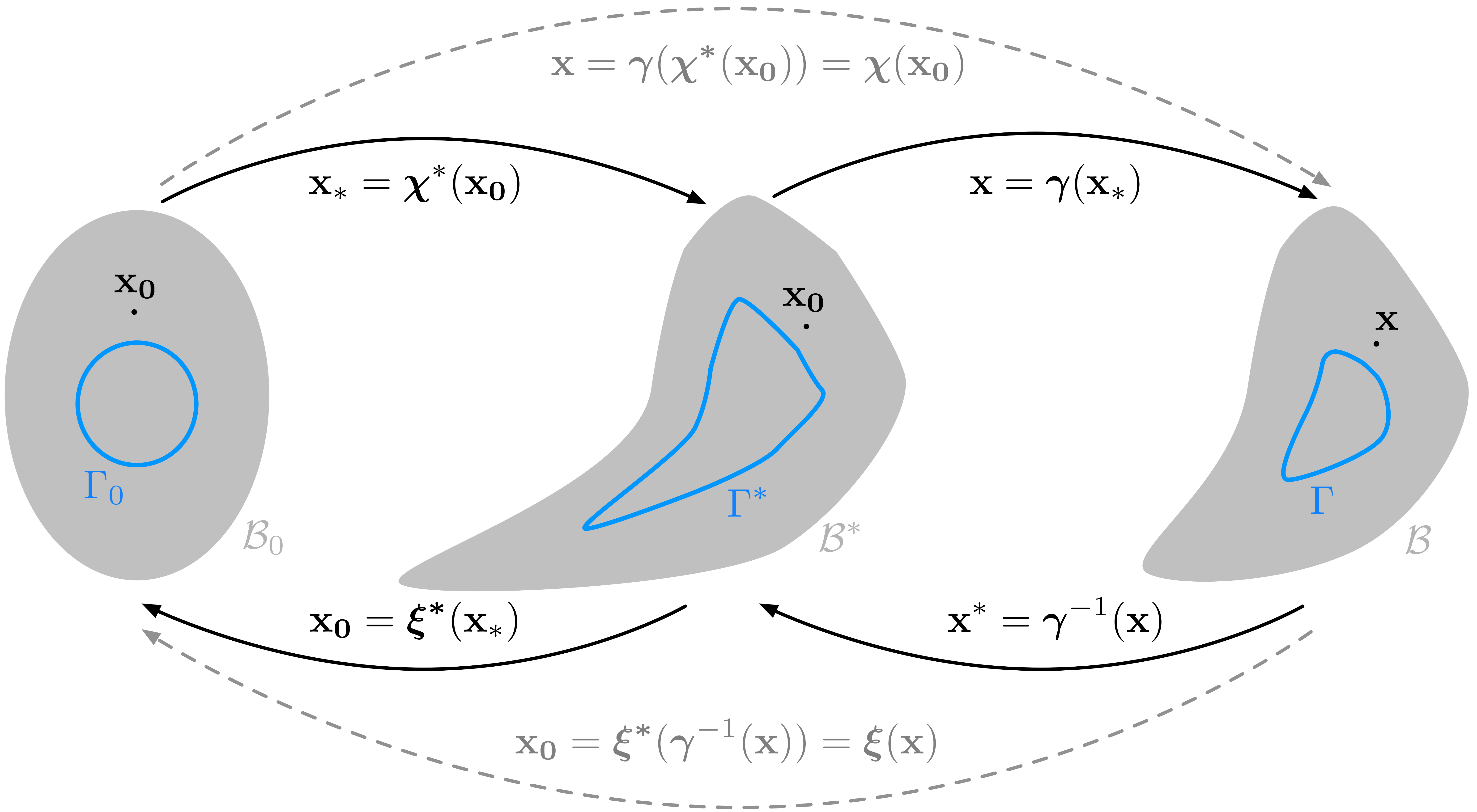
Flows Around Solid Objects - Erosion of an Assyrian Palace



Flows Around Solid Objects - Spining Windturbine

$CFL = 10$
$Re = 10^8$

A Volume-Preserving Reference Map Method for the Level Set Representation



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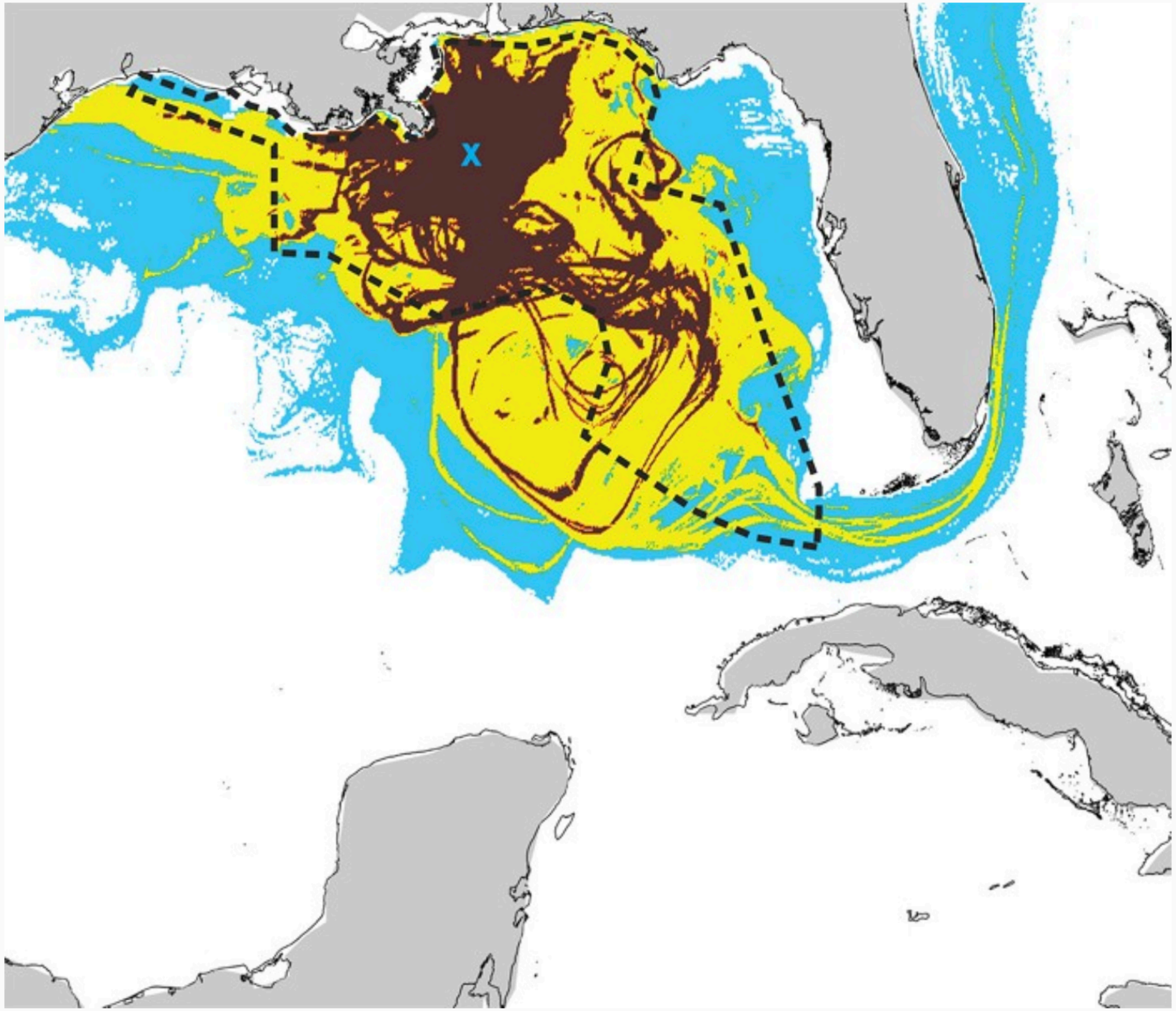
Motivations

Deep horizon oil spill (2010)

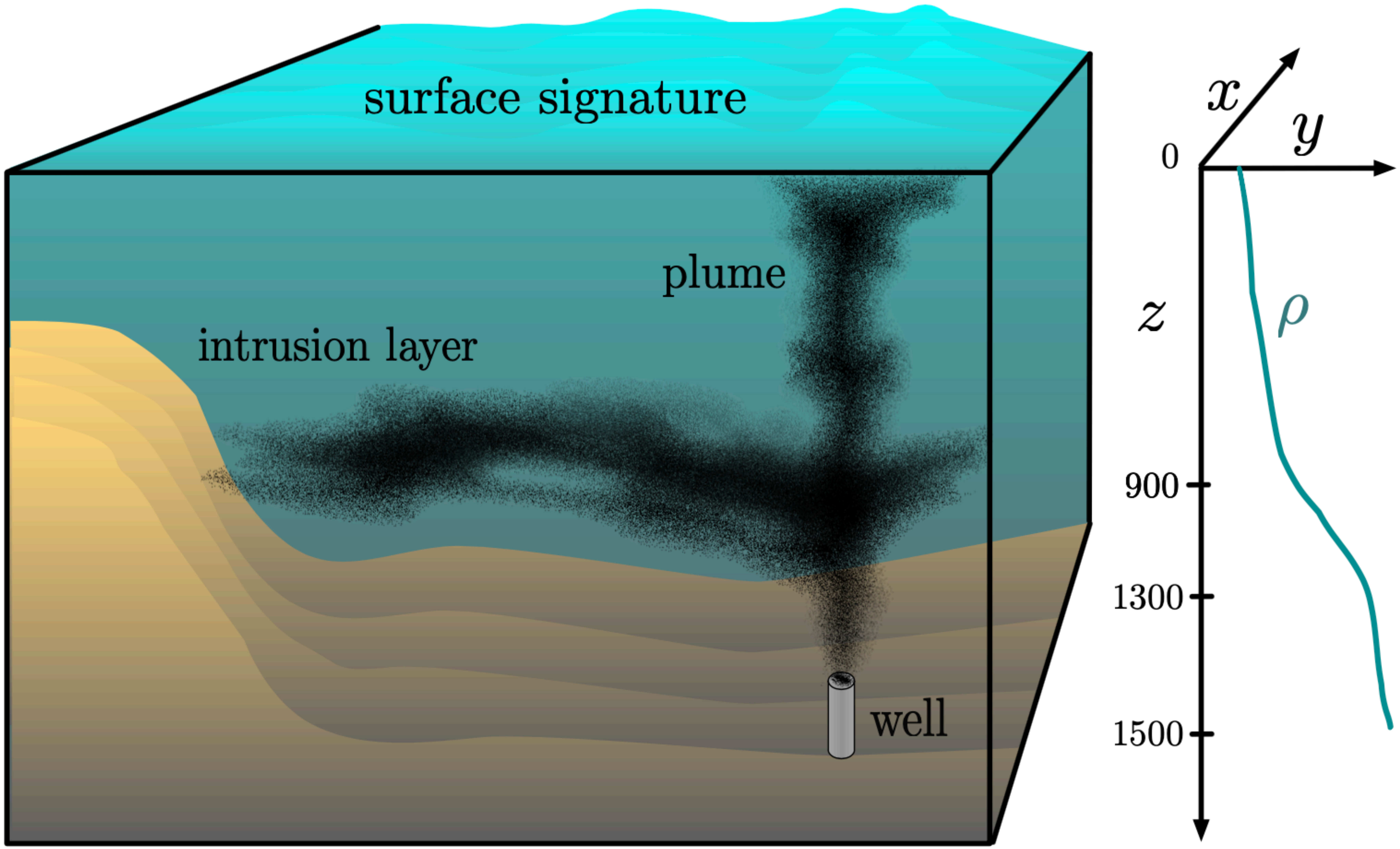
Motivations



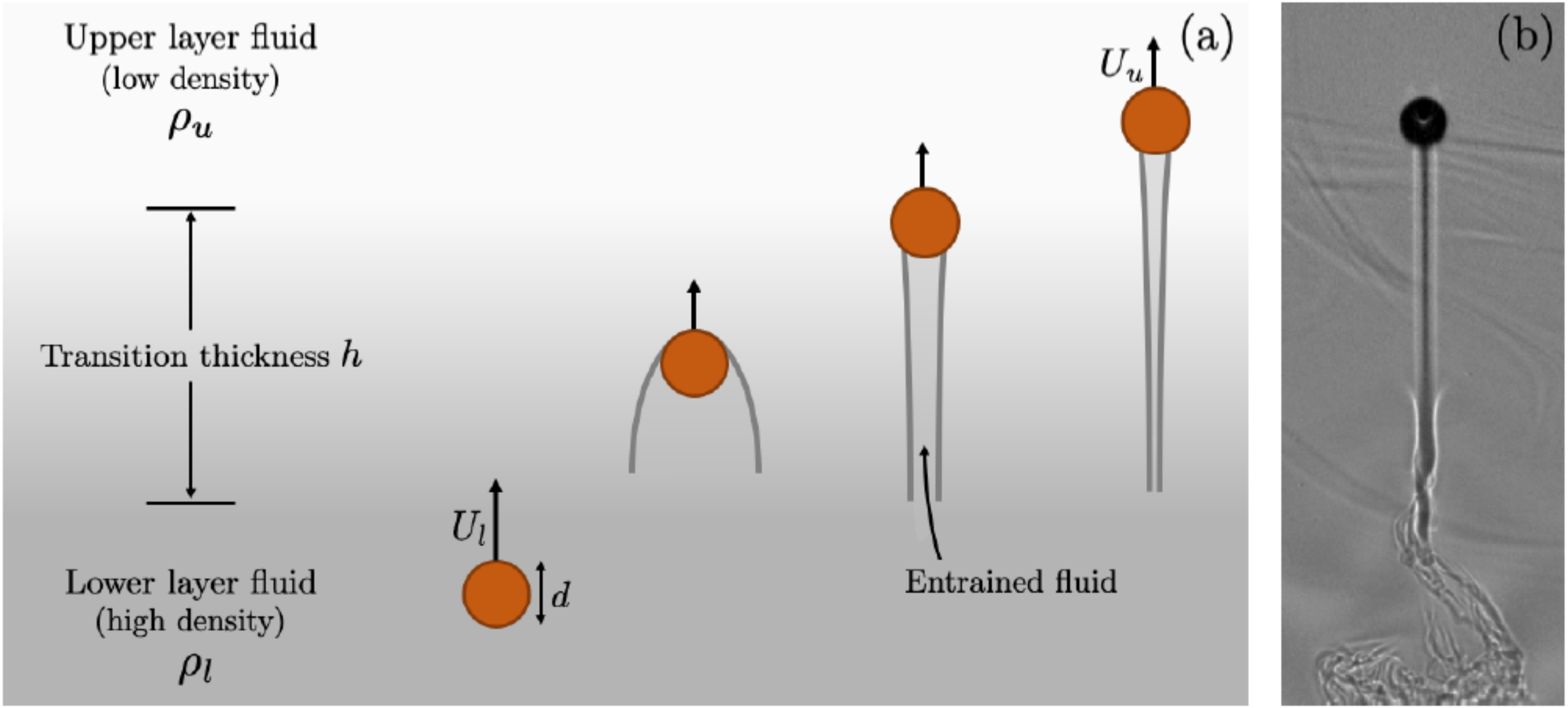
Credit: *Sci. Adv.*

Brown = extent of oil visible in satellite or aerial imagery; **yellow** = modeled extent of toxic oil compounds not seen by satellites; **cyan** = modeled extent of nontoxic oil compounds; **dashed line** = area closed to fishers to prevent contaminated catches

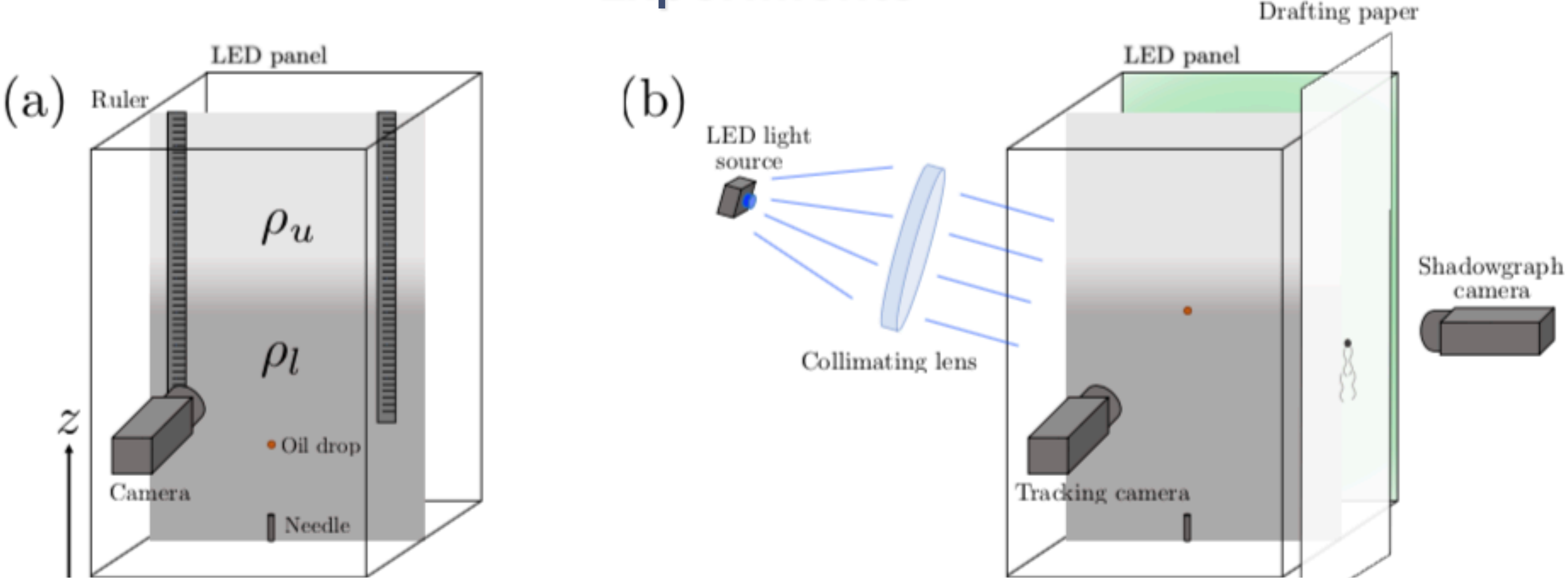
Oil droplets retention in oceanic plumes

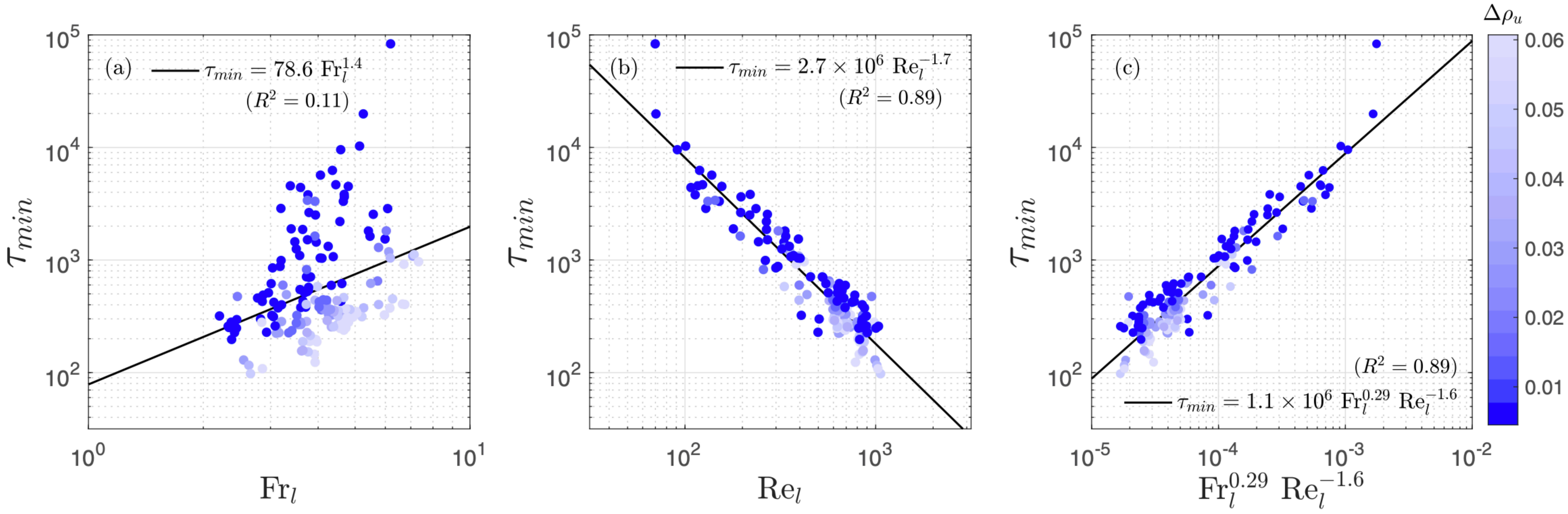


Oil droplets retention in stratified fluid

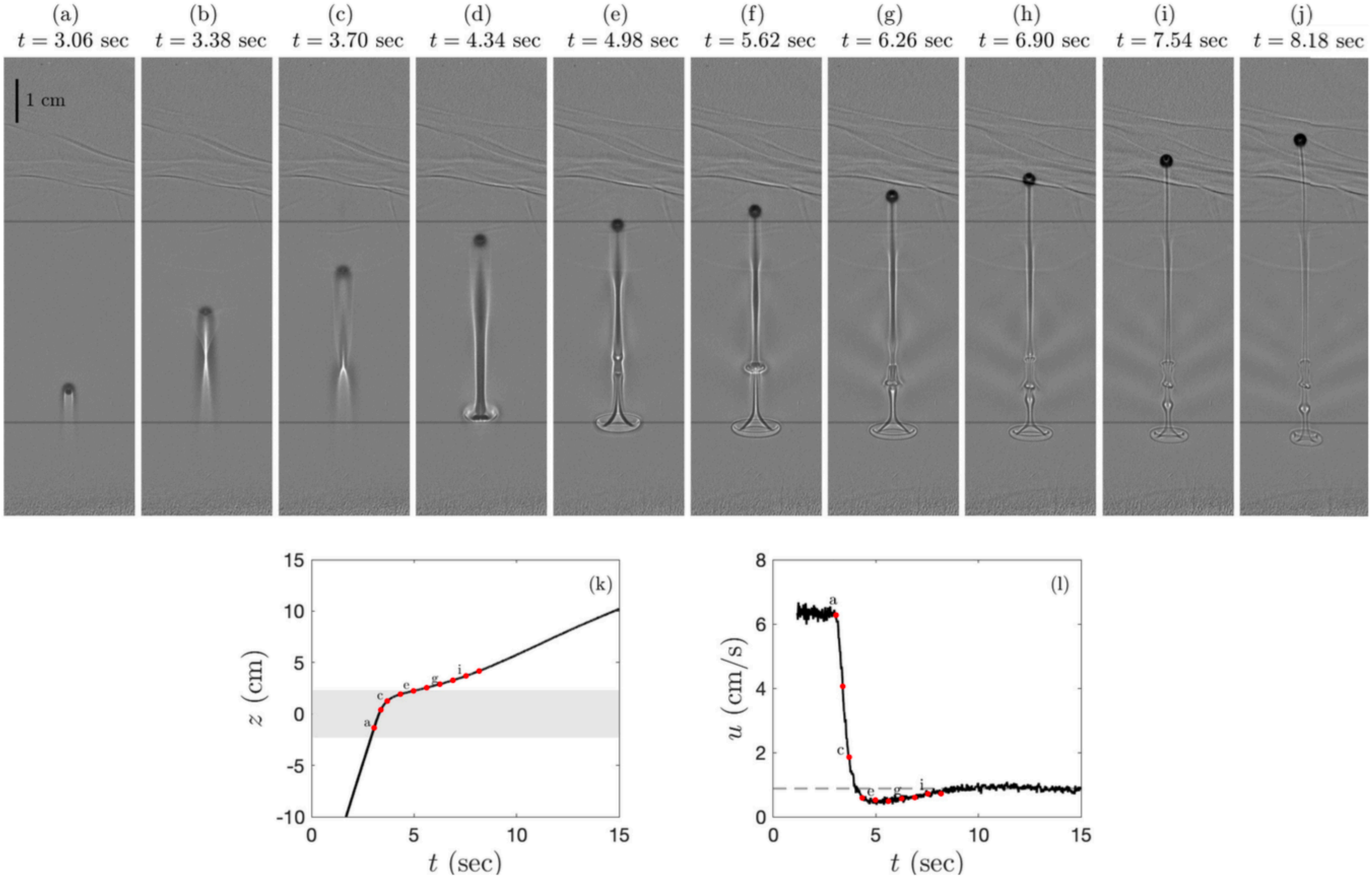


Experiments

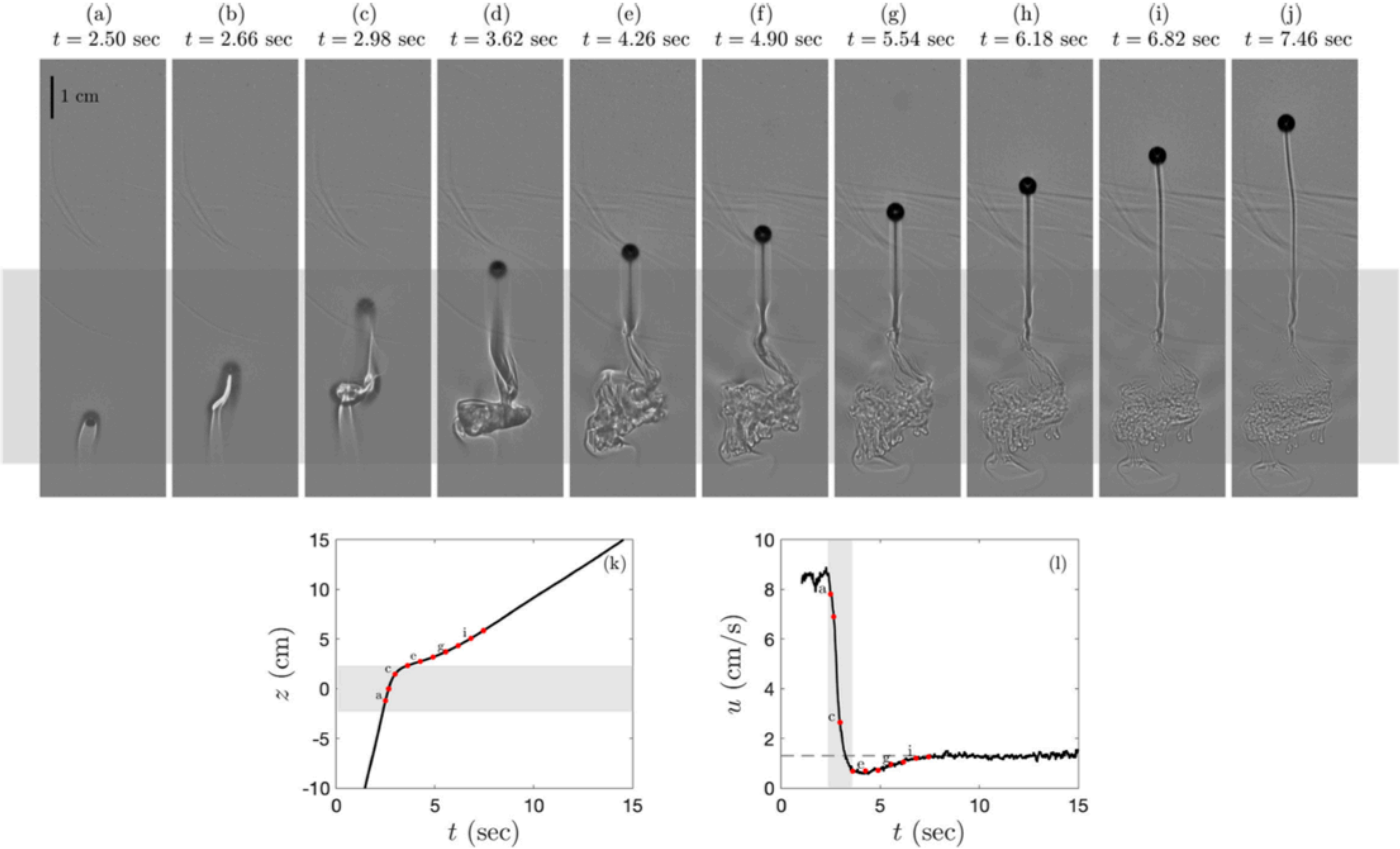




Experiments

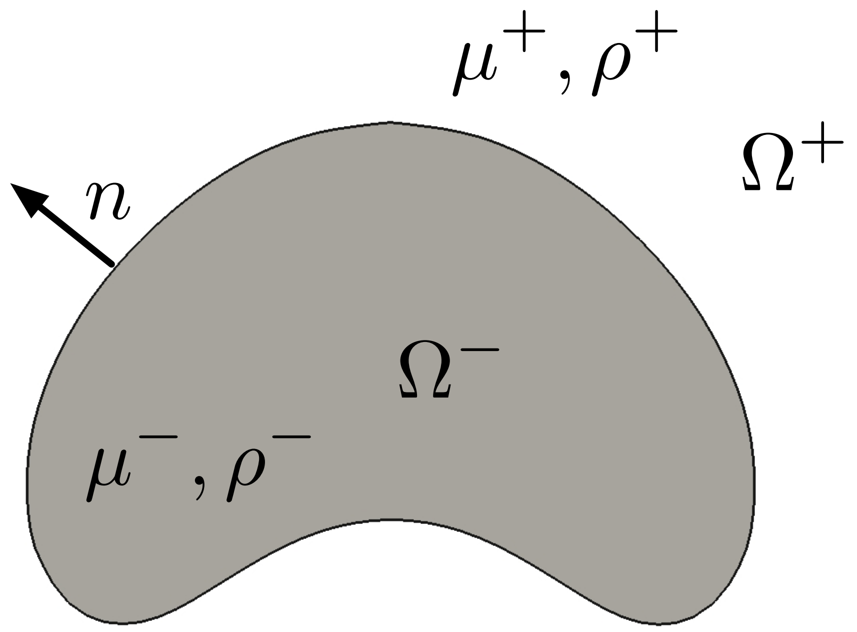


Experiments



Mathematical & numerical modeling

- **Problem**



  - incompressible NS in each phase

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla p + \mu\triangle\mathbf{u} + \mathbf{f}$$

$$\nabla\cdot\mathbf{u} = 0$$

  - continuity equations

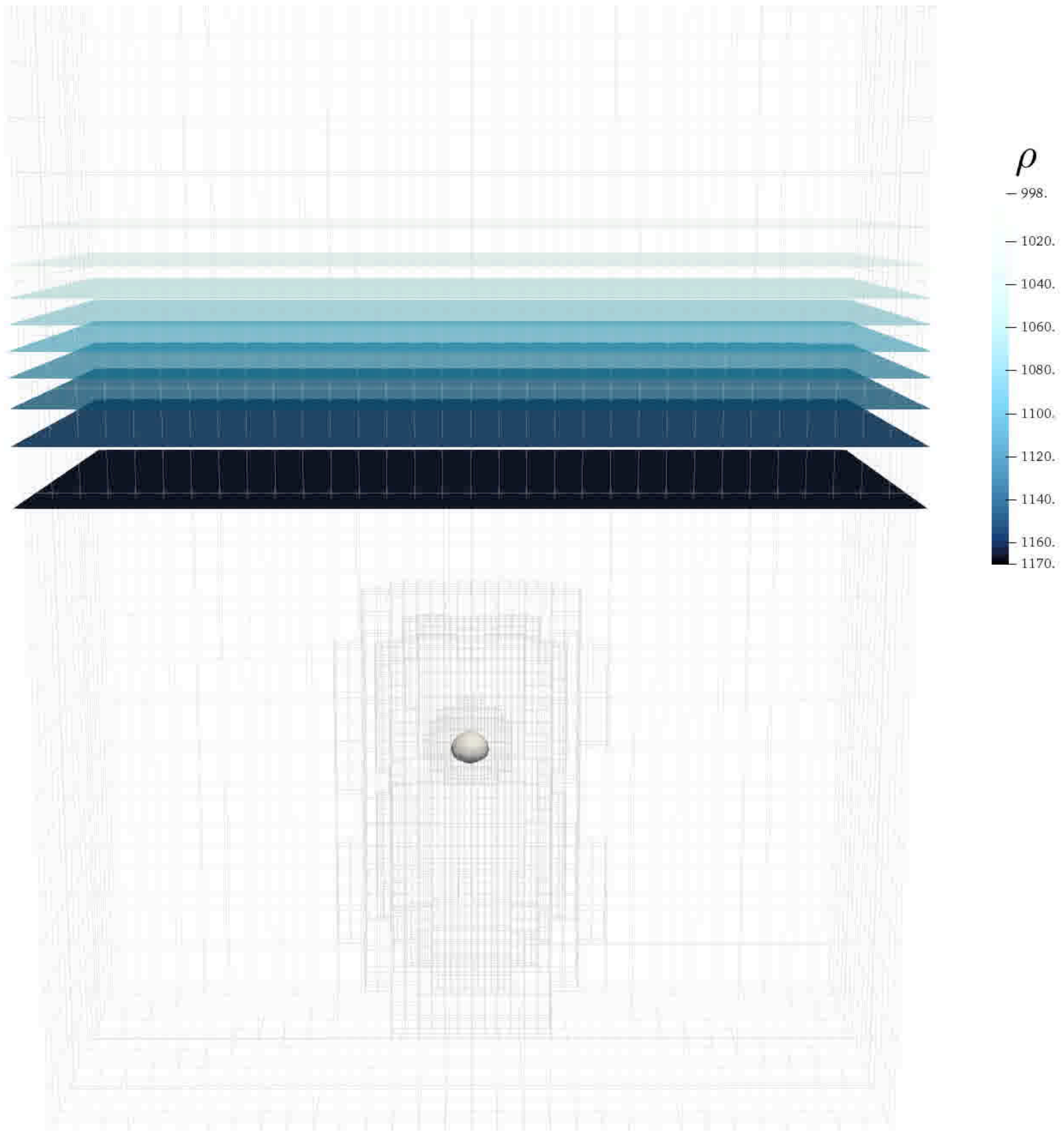
$$[\mathbf{u}] = 0$$

$$\left[\mu\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right)\cdot\mathbf{n} - p\mathbf{n}\right] = \gamma\kappa\mathbf{n}$$

  - Density advection

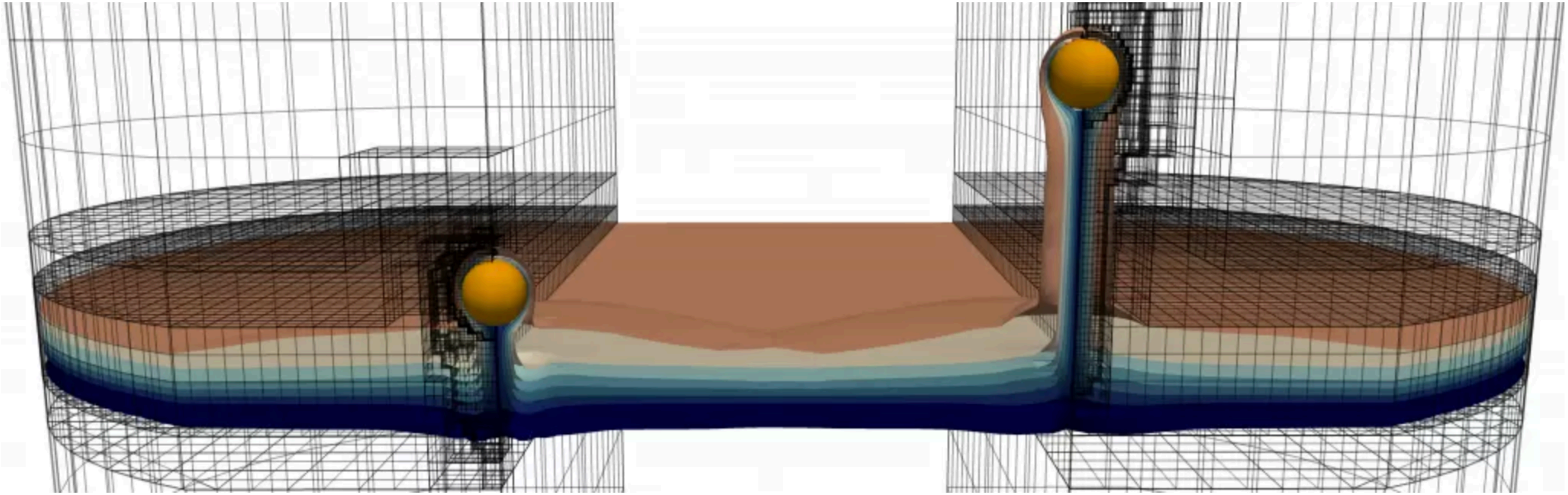
$$\frac{\partial \rho}{\partial t} + \mathbf{u}\cdot\nabla\rho = 0$$

  - Motion of the interface



- **Numerical tools:** *Finite Volume, projection method, level-set/reference map, adaptive octree grids, sharp discretization, OpenMP...*

Computational challenges

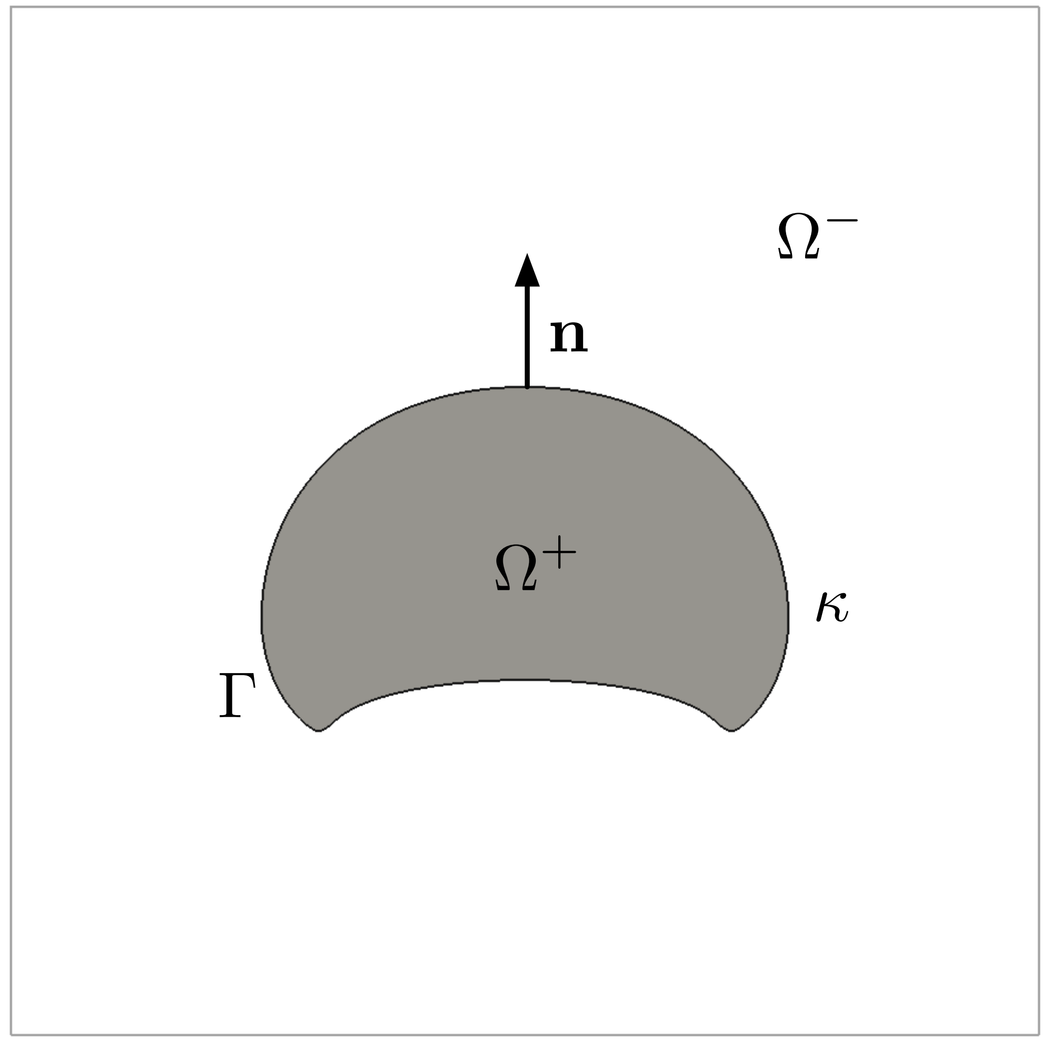


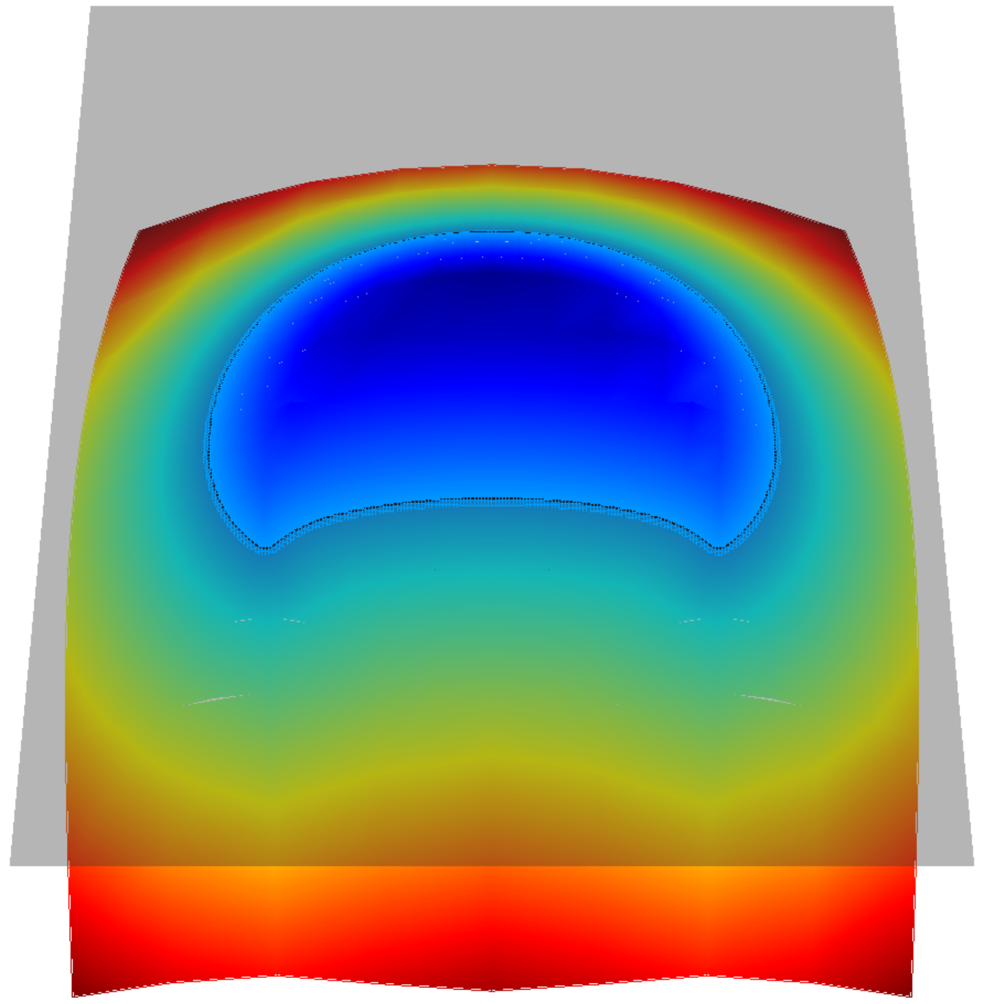
- Solve incompressible two-phase Navier-Stokes
- Coupling with the droplet interface
- Expensive simulations: long times, large domains....

$\Longrightarrow$ Significant mass loss

Interface representation

- **Level set method**





- Geometric quantities

$$\mathbf{n} = \frac{\nabla \phi}{|\nabla \phi|} \qquad \kappa = \nabla \cdot \left(\frac{\nabla \phi}{|\nabla \phi|} \right)$$

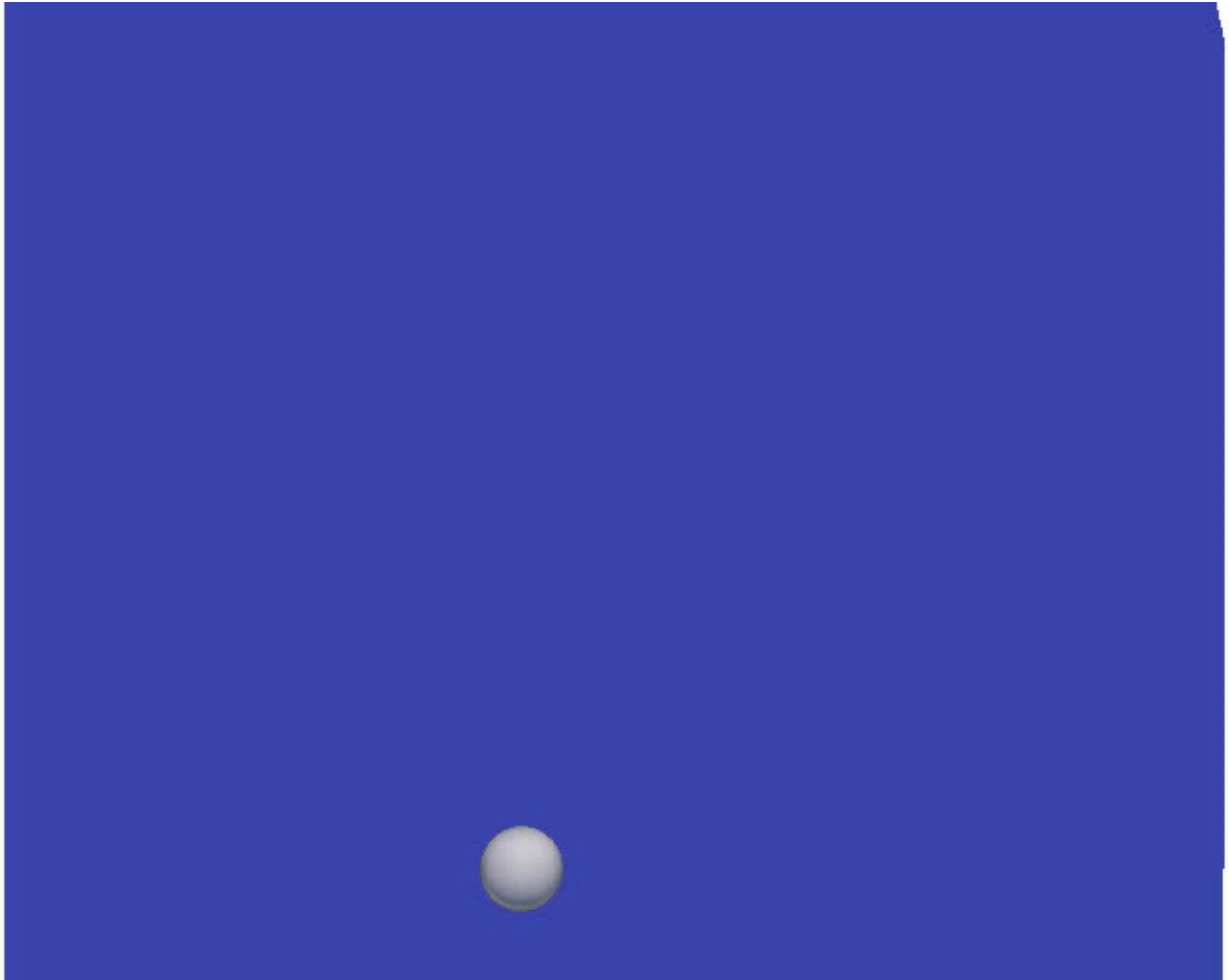
- Motion of the interface

$$\frac{\partial \phi}{\partial t} + V_n |\nabla \phi| = 0$$

- Reinitialization

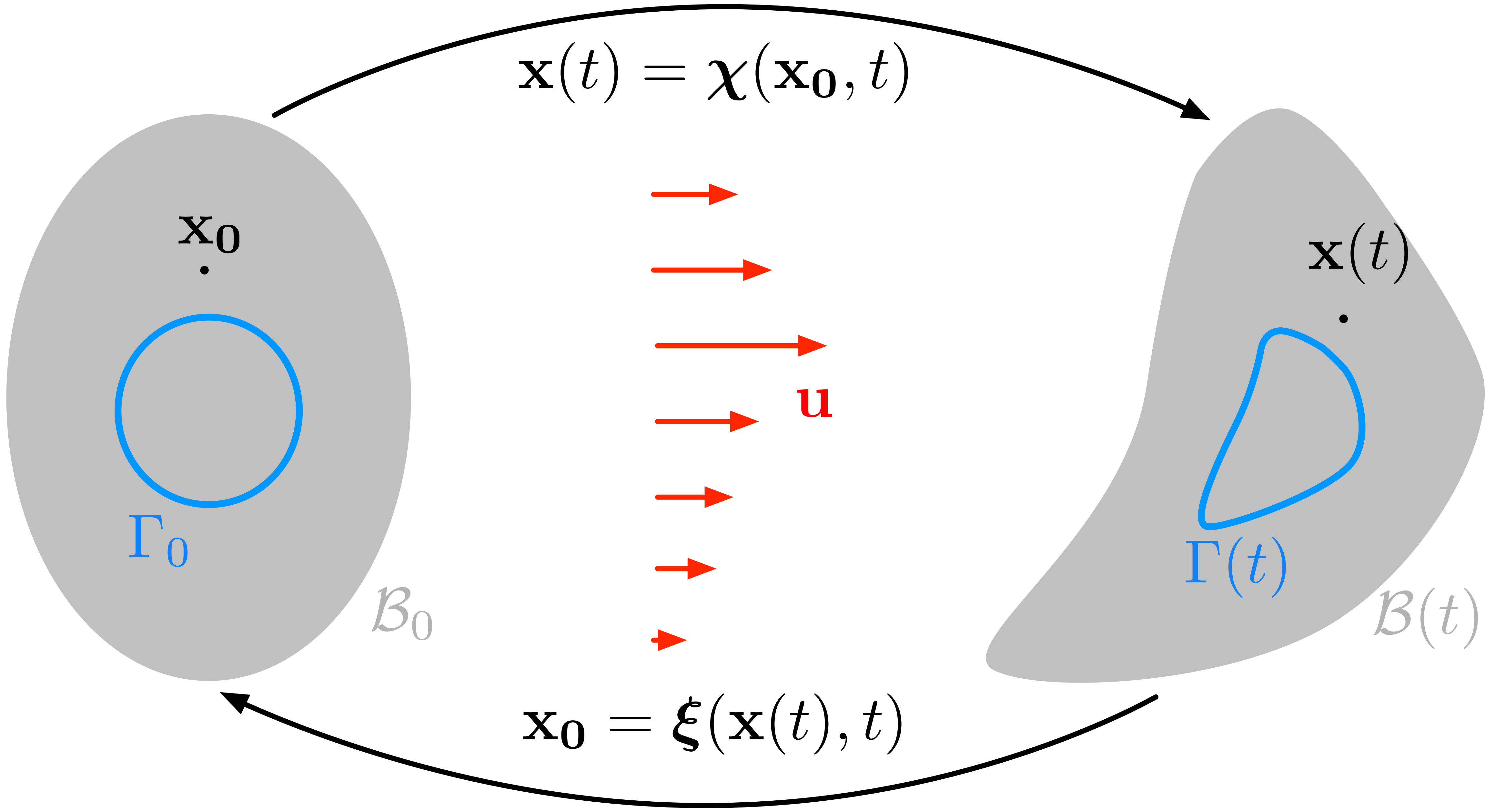
$$\frac{\partial \phi}{\partial \tau} + sign(\phi_0) \left(|\nabla \phi| - 1 \right) = 0$$

Level set method



Reference map

- **Reference map**



- Advection

$$\frac{\partial \boldsymbol{\xi}}{\partial t} + \mathbf{u} \cdot \nabla \boldsymbol{\xi} = 0$$

- Level-set reconstruction

$$\phi(t, \mathbf{x}) = \phi_0(\boldsymbol{\xi}(t, \mathbf{x}))$$

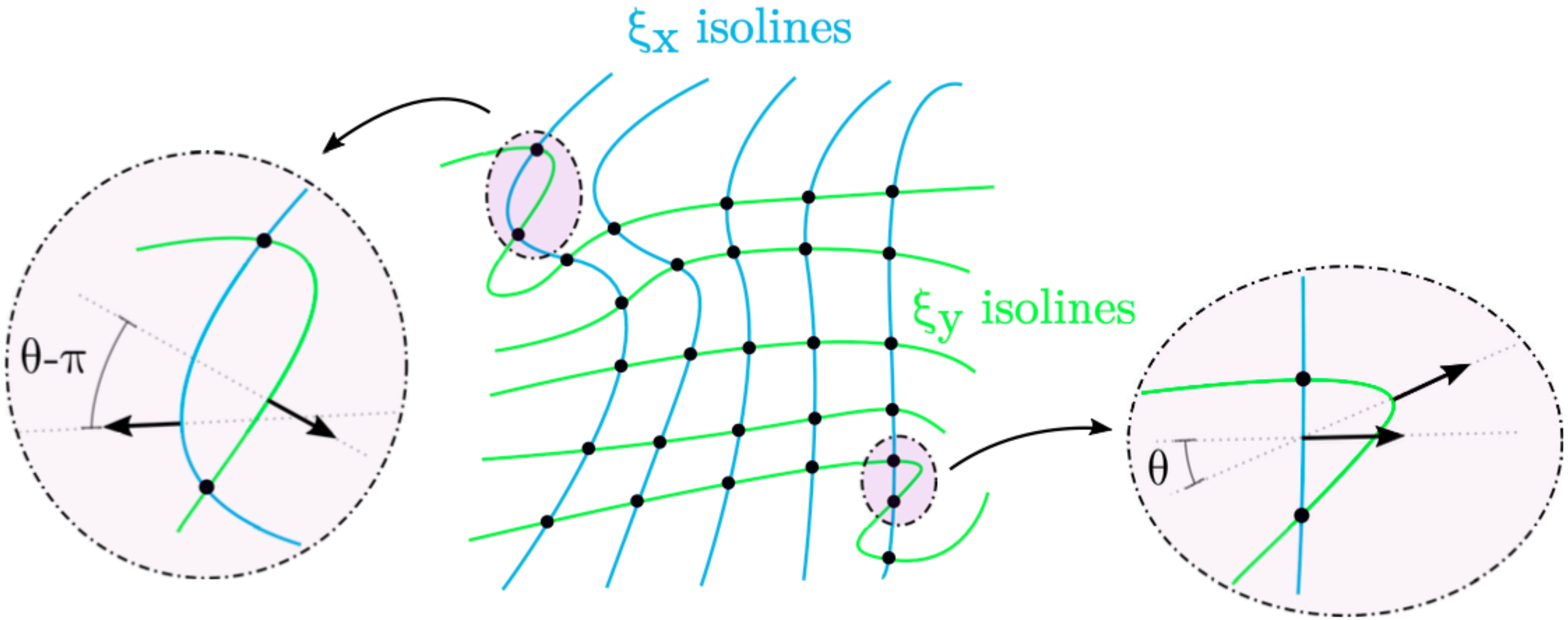
- Restart if needed to ensure

$$\det(\nabla \boldsymbol{\chi}) > 0.$$

. *A coupled level-set and reference-map method for interface representation, T. Bellotti, M. Theillard, JCP 2019*

Reference map

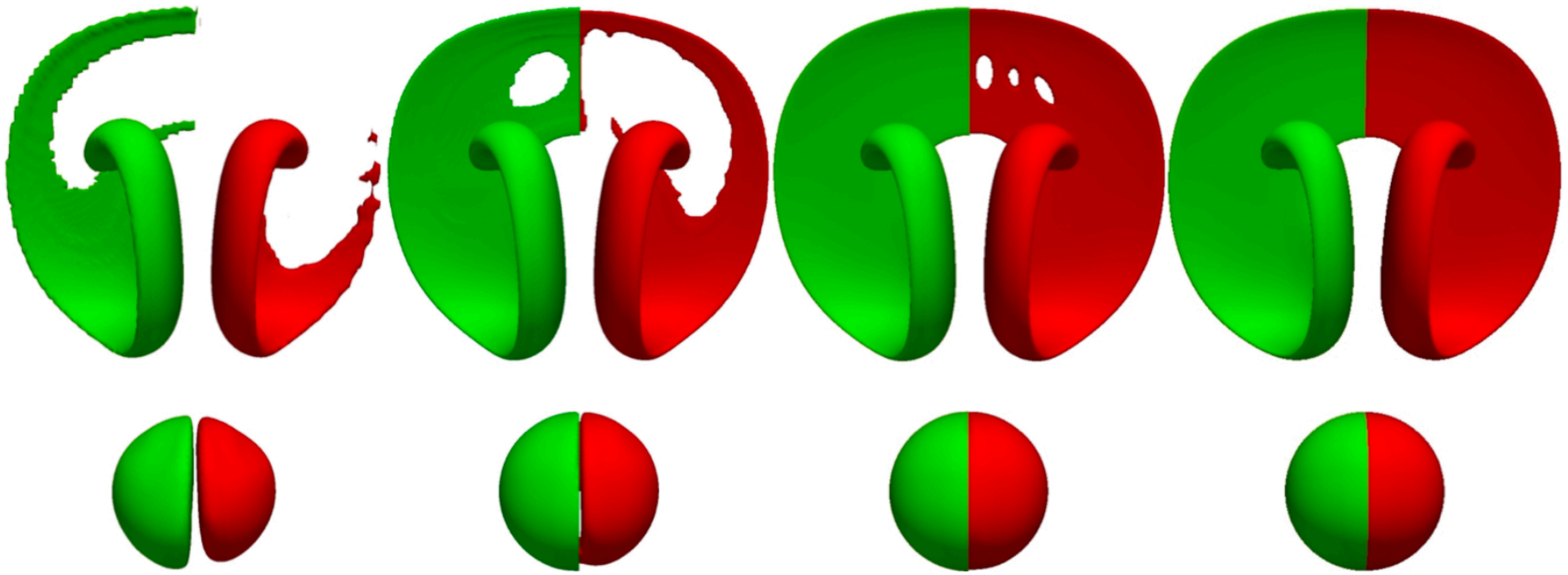
- **Restarting criteria**



$$\text{restart } \boldsymbol{\xi} \text{ if } \quad : \qquad \left\| \det\left(\frac{\nabla \xi_1}{\|\nabla \xi_1\|}, \dots, \frac{\nabla \xi_d}{\|\nabla \xi_d\|} \right) \right\|_{L^\infty(\mathcal{V})} < \sin(\theta_{crit}),$$

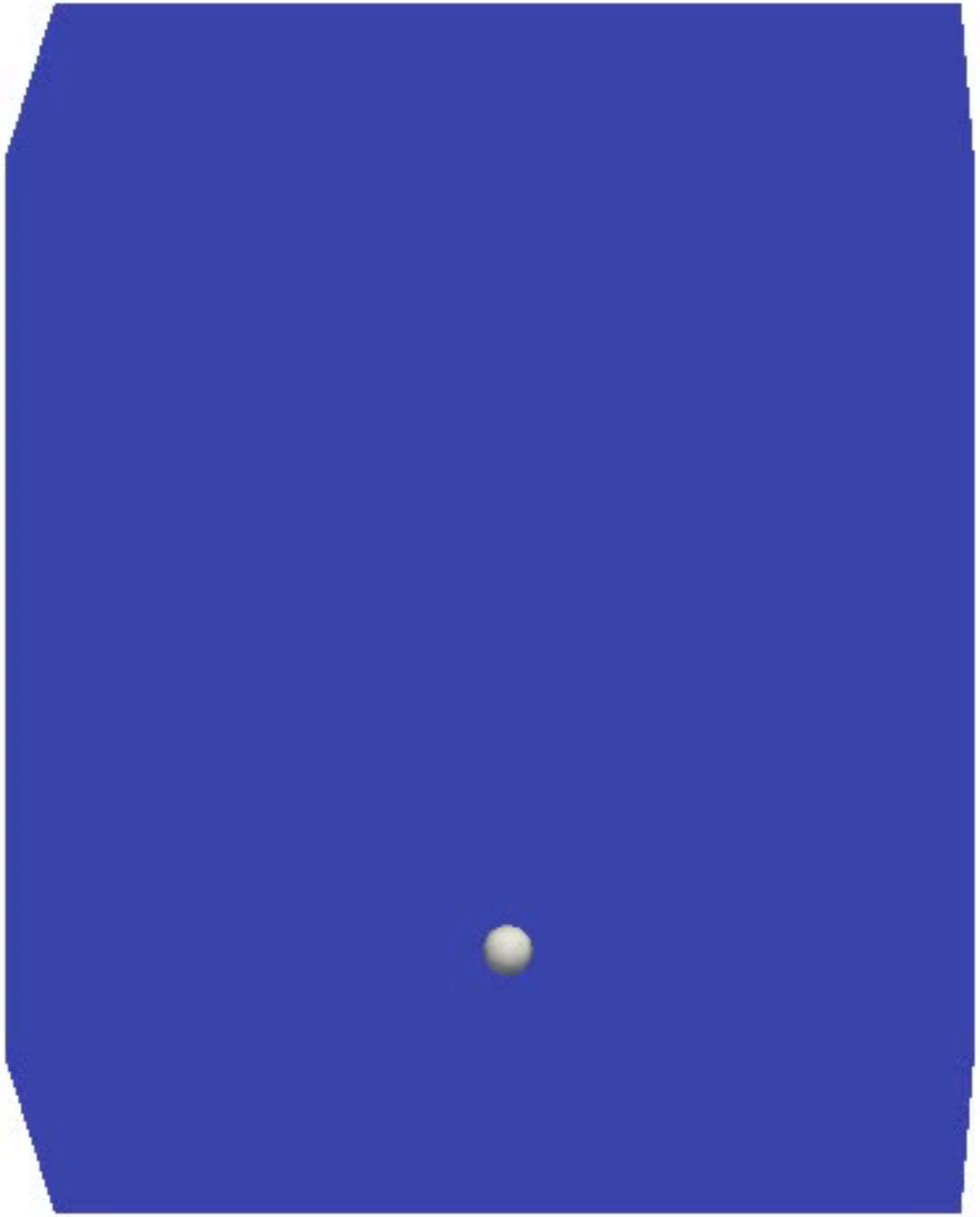
Reference map

Results: Enright's sphere

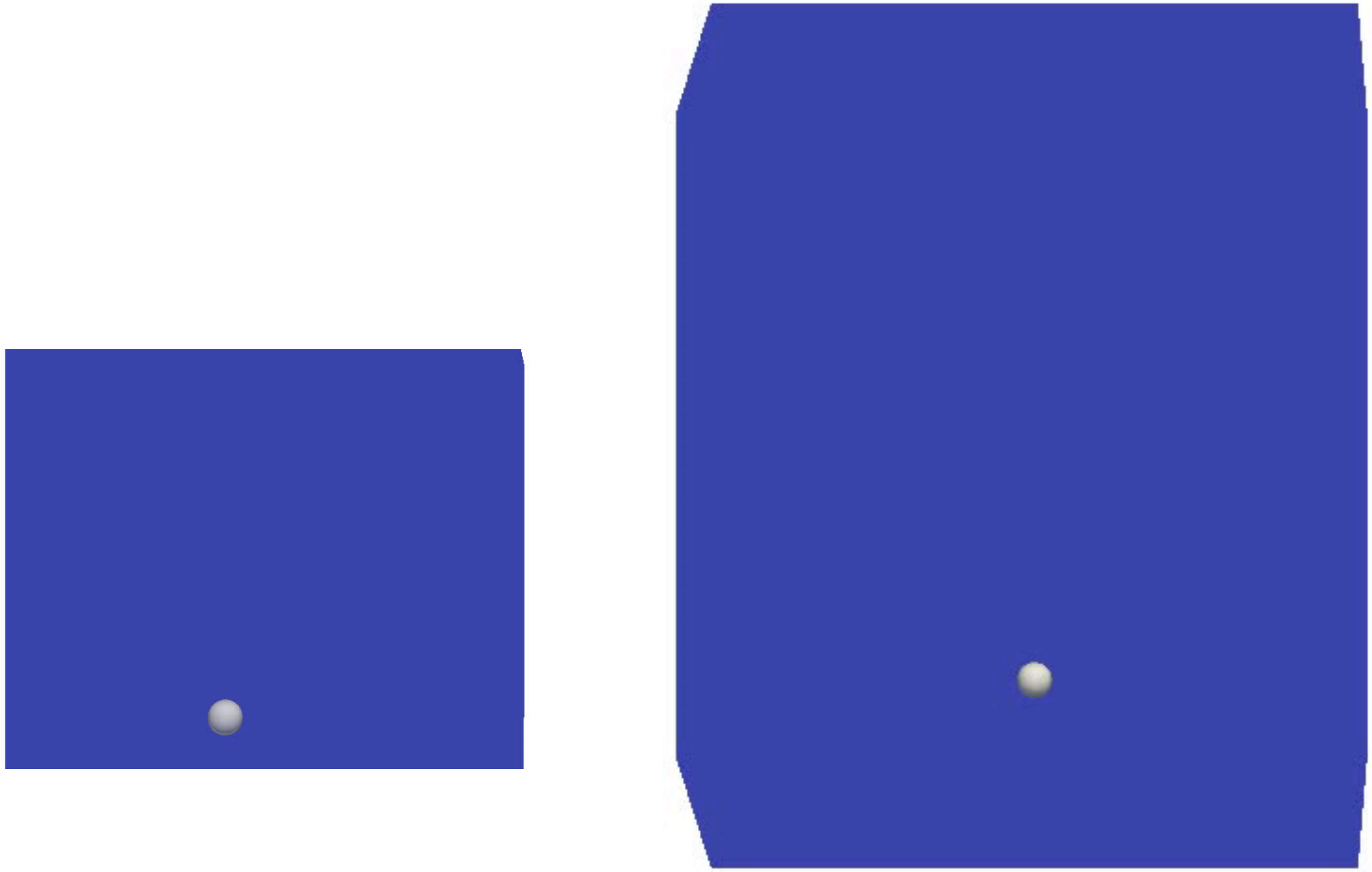


	levels	$d_{L^\infty}(\phi)$	order	$e_{L^\infty}(\phi)$	order	$d_{L^1}(\phi)$	order	$d_{L^2}(\phi)$	order	mass loss (%)	order
CLSRM	1:7	$1.46 \cdot 10^{-1}$	-	$1.48 \cdot 10^{-1}$	-	$5.54 \cdot 10^{-4}$	-	$1.56 \cdot 10^{-3}$	-	$1.11 \cdot 10^{1}$	-
	2:8	$9.70 \cdot 10^{-2}$	0.59	$1.46 \cdot 10^{-1}$	0.03	$1.54 \cdot 10^{-4}$	1.84	$4.22 \cdot 10^{-4}$	1.12	$1.12 \cdot 10^{0}$	3.31
	3:9	$3.13 \cdot 10^{-3}$	4.95	$9.00 \cdot 10^{-3}$	4.02	$2.57 \cdot 10^{-5}$	2.58	$7.41 \cdot 10^{-5}$	2.51	$1.06 \cdot 10^{-1}$	3.39
	4:10	$2.76 \cdot 10^{-4}$	3.49	$2.76 \cdot 10^{-4}$	5.02	$5.91 \cdot 10^{-6}$	2.12	$1.63 \cdot 10^{-5}$	2.18	$2.86 \cdot 10^{-2}$	1.89
level-set	1:7	$1.41 \cdot 10^{-1}$	-	$1.48 \cdot 10^{-1}$	-	$4.96 \cdot 10^{-4}$	-	$1.72 \cdot 10^{-3}$	-	$2.46 \cdot 10^{1}$	-
	2:8	$1.45 \cdot 10^{-1}$	-0.04	$1.50 \cdot 10^{-1}$	-0.01	$2.39 \cdot 10^{-4}$	1.05	$7.16 \cdot 10^{-4}$	1.26	$1.03 \cdot 10^{1}$	1.25
	3:9	$1.32 \cdot 10^{-1}$	0.13	$1.32 \cdot 10^{-1}$	0.18	$9.54 \cdot 10^{-5}$	1.32	$2.82 \cdot 10^{-4}$	1.34	$1.93 \cdot 10^{0}$	2.41
	4:10	$4.70 \cdot 10^{-3}$	4.81	$4.70 \cdot 10^{-3}$	4.81	$3.63 \cdot 10^{-5}$	1.39	$1.09 \cdot 10^{-4}$	1.37	$3.99 \cdot 10^{-1}$	2.27

Reference map



Level set VS reference map



Volume preserving method

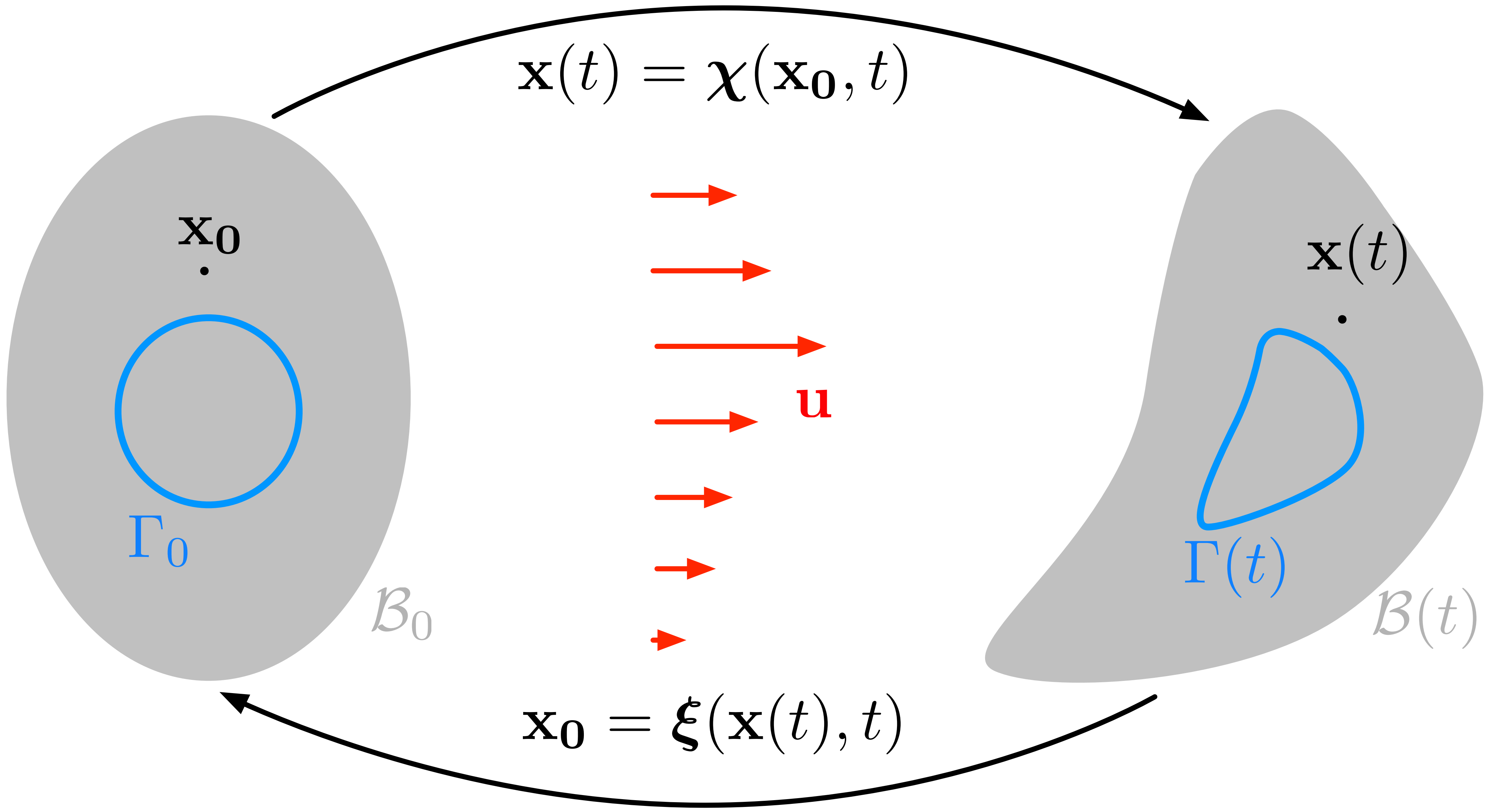
- **Mass conservation**
  - Assume divergence-free velocity
  - Level-set perspective

$$\Rightarrow \quad \int_{\Omega(t)} d\omega = |\Omega(t)| = |\Omega_0|.$$

  - Reference map perspective

$$\Rightarrow \quad \int_{\mathcal{D}(t)} d\omega = |\mathcal{D}(t)| = |\mathcal{D}_0|,$$

  - Change of variable

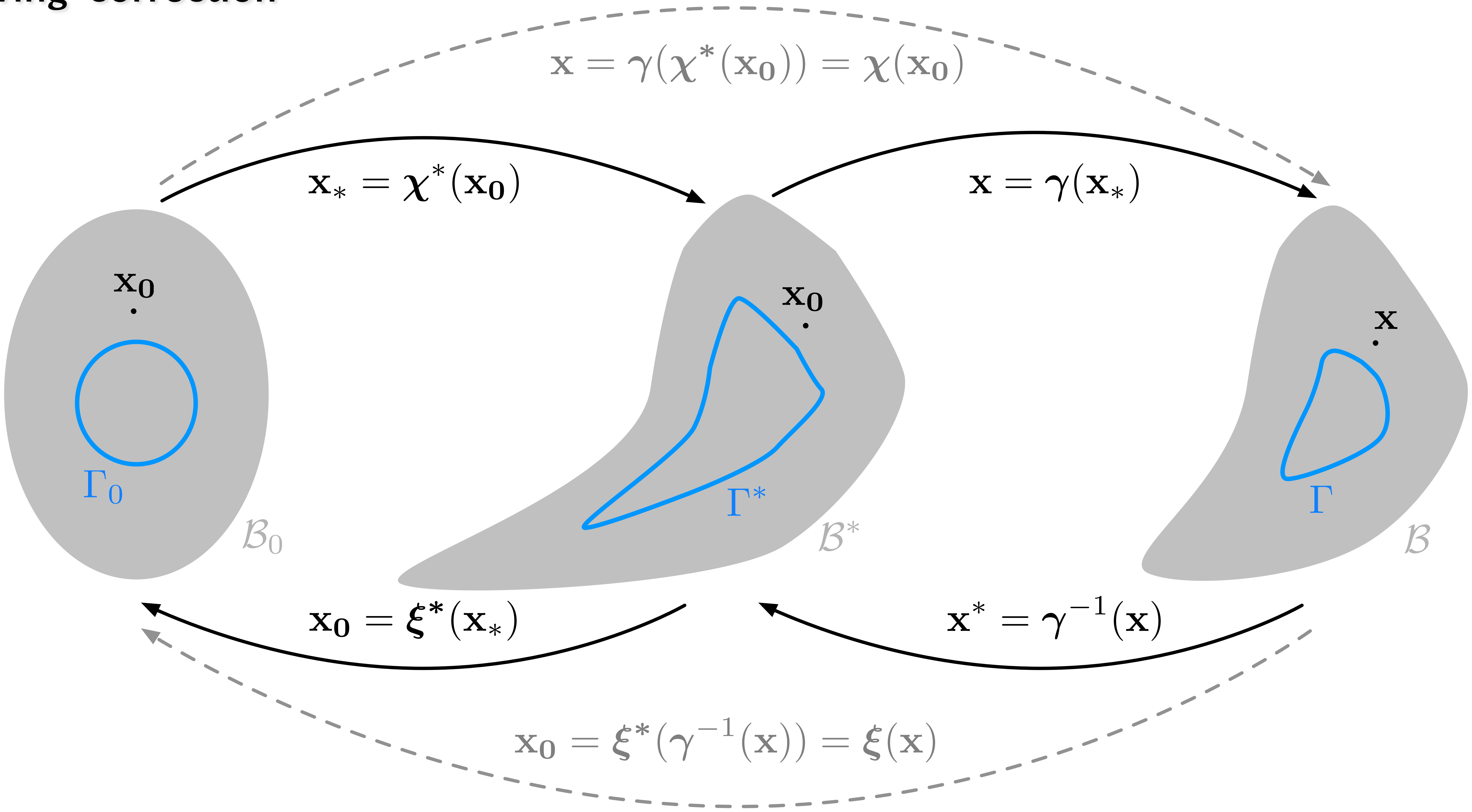


$$\Leftrightarrow \int_{\mathcal{D}(t)} d\omega - |\mathcal{D}_0| = \int_{\xi(\mathcal{D}(t))} |\det(\nabla \xi^{-1})| d\omega - |\mathcal{D}_0| = \int_{\mathcal{D}_0} (|\det(\nabla \chi)| - 1)\, d\omega$$

$$\Leftrightarrow \quad \det(\nabla \boldsymbol{\chi}(t, \mathbf{x_0})) = 1 \qquad \forall \mathbf{x_0} \in \mathcal{B}_0.$$

Volume preserving method

- **Volume-preserving correction**

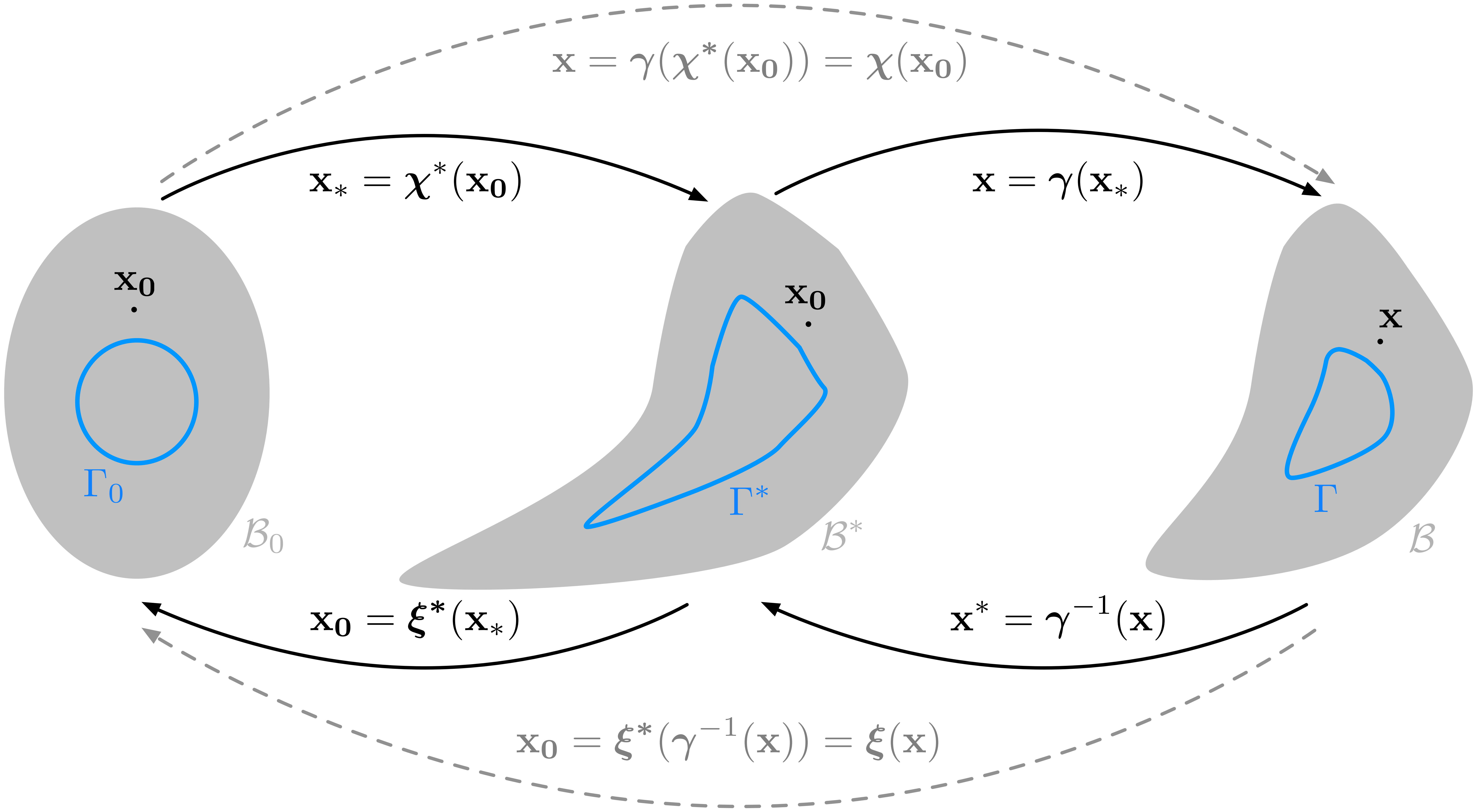


- Such that

$$\det \nabla \boldsymbol{\chi}(\mathbf{x_0}) = 1, \qquad \forall \mathbf{x_0} \in \mathcal{B}_0,$$
$$\det \nabla \boldsymbol{\xi}(\mathbf{x}) = 1, \qquad \forall \mathbf{x} \in \mathcal{B}.$$

Volume preserving method

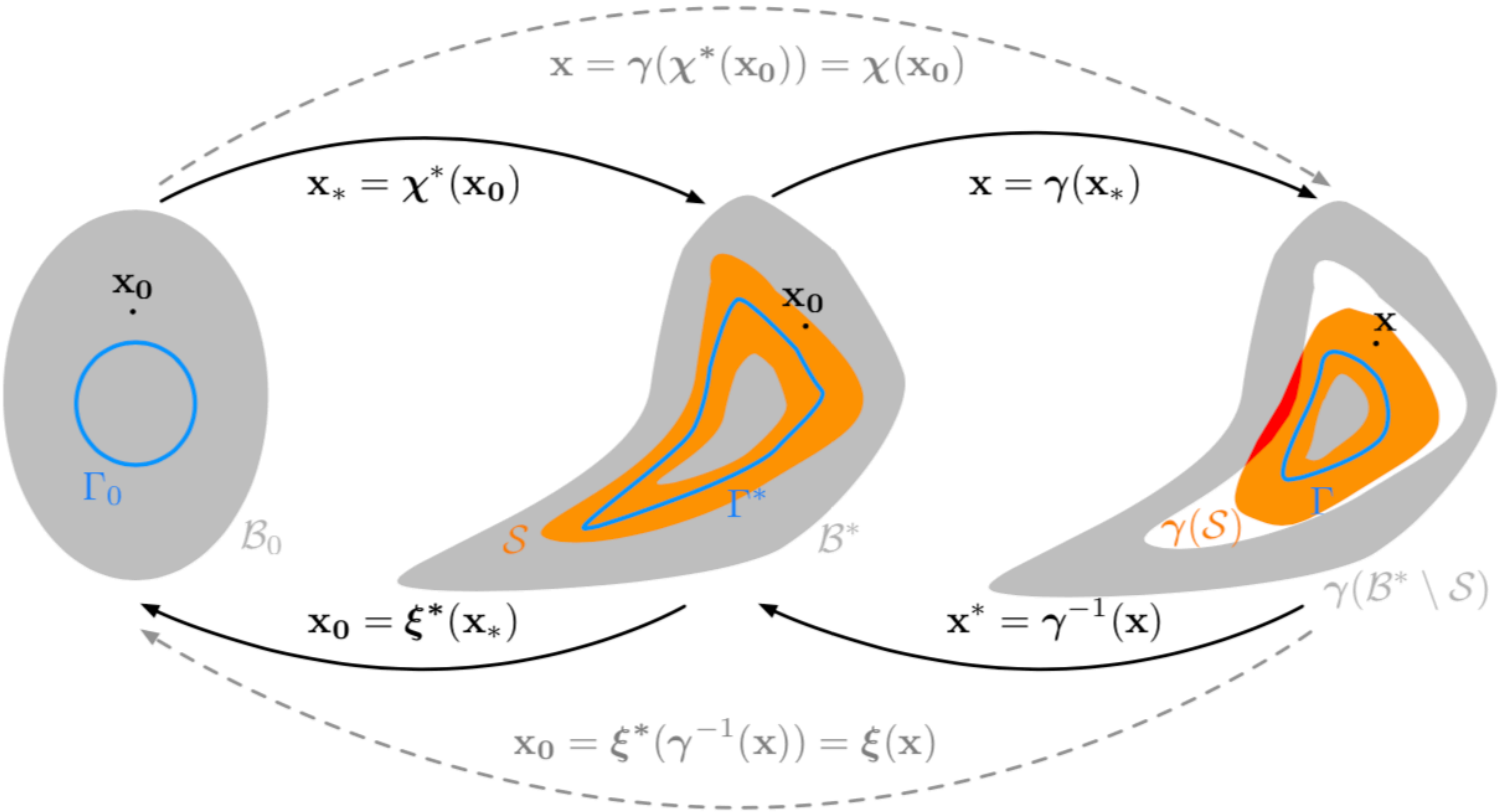
- **Properties**



- Stability $\quad \xi(\mathbf{x}) = \xi^*(\gamma^{-1}(\mathbf{x})) \quad \Longrightarrow \quad ||\xi||_{L^\infty(\mathcal{B})} \leq ||\xi^*||_{L^\infty(\mathcal{B}^*)}.$
- Accuracy $\quad \gamma(\mathbf{x}_*) = \mathbf{x}_* + \epsilon(\mathbf{x}_*), \quad \Longrightarrow \quad \chi(\mathbf{x_0}) = \chi^*(\mathbf{x_0}) + \epsilon(\chi^*(\mathbf{x_0}))$

Volume preserving method

- Shell only



- Potential issues: loss of bijectivity (red), loss of connectivity (white)
- Shell width?

Volume preserving method

- **Definition of the correction**
  - Linearization $\gamma(\mathbf{x}) = \mathbf{x} + \epsilon(\mathbf{x})$
  - We want $\det \nabla \boldsymbol{\xi}(\mathbf{x}) = 1$

$$\det(\nabla \boldsymbol{\xi}^*(\mathbf{x})) = \det(\mathcal{I} + \nabla \boldsymbol{\epsilon}(\mathbf{x})) \quad \forall \mathbf{x} \in \mathcal{S},$$

  - Small deviations from volume-preserving space

$$\Longrightarrow \det(\nabla \boldsymbol{\xi}^*(\mathbf{x})) = 1 + \mathrm{Tr}(\nabla \boldsymbol{\epsilon}(\mathbf{x})) = 1 + \nabla \cdot \boldsymbol{\epsilon}(\mathbf{x}) \quad \forall \mathbf{x} \in \mathcal{S},$$

  - Smallest possible correction

$$\min_{\boldsymbol{\epsilon}} \int_{\mathcal{S}} \frac{\boldsymbol{\epsilon} \cdot \boldsymbol{\epsilon}}{2}$$

  - Lagrangian saddle point $(\boldsymbol{\epsilon}, \lambda)$ of the Lagragian

$$\mathcal{L}(\boldsymbol{\mu}, \rho) = \int_{\mathcal{S}} \frac{\boldsymbol{\mu}(\mathbf{x}) \cdot \boldsymbol{\mu}(\mathbf{x})}{2} + \int_{\mathcal{S}} \left(\nabla \cdot \boldsymbol{\mu}(\mathbf{x}) + 1 - \det(\nabla \boldsymbol{\xi}^*(\mathbf{x}))\right) \rho(\mathbf{x})$$

Volume preserving method

- **Existence and Uniqueness of the correction**

Theorem 1. $\forall \mathcal{S} \subseteq \mathcal{B}^*$, *the Lagrangian* $\mathcal{L}(\boldsymbol{\mu}, \rho)$ *has a unique saddle point* $(\boldsymbol{\epsilon}, \lambda)$. *The adjoint* λ *is the unique solution of the following Poisson problem*

$$\begin{cases} -\triangle\lambda(\mathbf{x}) & = 1 - \det(\nabla\boldsymbol{\xi}^*(\mathbf{x})) \qquad \forall \mathbf{x} \in \mathcal{S}, \\ \lambda(\mathbf{x}) & = 0 \qquad \forall \mathbf{x} \in \partial\mathcal{S}, \end{cases}$$

and the correction $\boldsymbol{\epsilon}$ *is defined as*

$$\boldsymbol{\epsilon} = \boldsymbol{\nabla}\lambda \qquad \forall \mathbf{x} \in \mathcal{S}.$$

- **Proof**
  - Differentiate the Lagrangian
  - Express optimality conditions
  - Functional analysis

Volume preserving method

- **Proof**
  - Differentiate the Lagrangian

$$\left\langle \frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}}(\boldsymbol{\epsilon}, \lambda) \middle| \boldsymbol{\Theta} \right\rangle = 0 \qquad \forall \boldsymbol{\Theta} \in H^1(\mathcal{S})^2, \qquad\qquad \left\langle \frac{\partial \mathcal{L}}{\partial \rho}(\boldsymbol{\epsilon}, \lambda) \middle| \theta \right\rangle = 0 \qquad \forall \theta \in H^1(\mathcal{S}).$$

  - Express optimality conditions

$$\int_{\mathcal{S}} (\nabla \cdot \boldsymbol{\epsilon}(\mathbf{x}) + 1 - \det(\nabla \boldsymbol{\xi}^*(\mathbf{x})))\, \theta(\mathbf{x}) ds = 0 \qquad \forall \theta \in H^1(\mathcal{S}),$$

$$\int_{\mathcal{S}} \boldsymbol{\Theta}(\mathbf{x}) \cdot (\boldsymbol{\epsilon}(\mathbf{x}) - \nabla \lambda(\mathbf{x}))\, ds + \int_{\partial \mathcal{S}} \boldsymbol{\Theta}(\mathbf{x}) \cdot \boldsymbol{n} \lambda(\mathbf{x}) ds = 0 \qquad \forall \boldsymbol{\Theta} \in H^1(\mathcal{S})^2,$$

  - Functional analysis

$$\Longrightarrow \qquad \begin{aligned} \boldsymbol{\epsilon}(\mathbf{x}) &= \nabla \lambda(\mathbf{x}) && \forall \mathbf{x} \in \mathcal{S}. \\ \lambda(\mathbf{x}) &= 0 && \forall \mathbf{x} \in \partial \mathcal{S}. \\ -\Delta \lambda(\mathbf{x}) &= 1 - \det(\nabla \boldsymbol{\xi}^*(\mathbf{x})) && \forall \mathbf{x} \in \mathcal{S}. \end{aligned}$$

Volume preserving method

- **Algorithm**

(1) Advection of the reference map

Compute the intermediate reference map $\boldsymbol{\xi}^*$ by solving the advection equation

$$\begin{cases} \frac{\partial \boldsymbol{\xi}}{\partial t} + \mathbf{u} \cdot \nabla \boldsymbol{\xi} = 0 & \forall t \geq 0, \quad \forall \mathbf{x} \in \mathcal{B}(t), \\ \boldsymbol{\xi}(t = t_n, \mathbf{x}) = \boldsymbol{\xi}^n & \forall \mathbf{x} \in \mathcal{B}_0. \end{cases}$$

(2) Projection on the volume preserving space

Compute the adjoint λ in the shell $\mathcal{S}$ as the solution of

$$\begin{cases} -\triangle \lambda & = 1 - \det(\nabla \boldsymbol{\xi}^*) & \forall \mathbf{x} \in \mathcal{S}, \\ \lambda & = 0 & \forall \mathbf{x} \in \partial \mathcal{S}, \end{cases}$$

and compute the correction $\gamma^{-1}(\mathbf{x}) = \mathbf{x} - \nabla \lambda$.

(3) Correction and update

From the corrected reference-map

$$\boldsymbol{\xi}^{n+1}(\mathbf{x}) = \boldsymbol{\xi}^*(\boldsymbol{\gamma}^{-1}(\mathbf{x}))$$

we construct the updated the level-set function

$$\phi^{n+1}(\mathbf{x}) = \phi_0(\xi^{n+1}(\mathbf{x}))$$

(4) Restarting

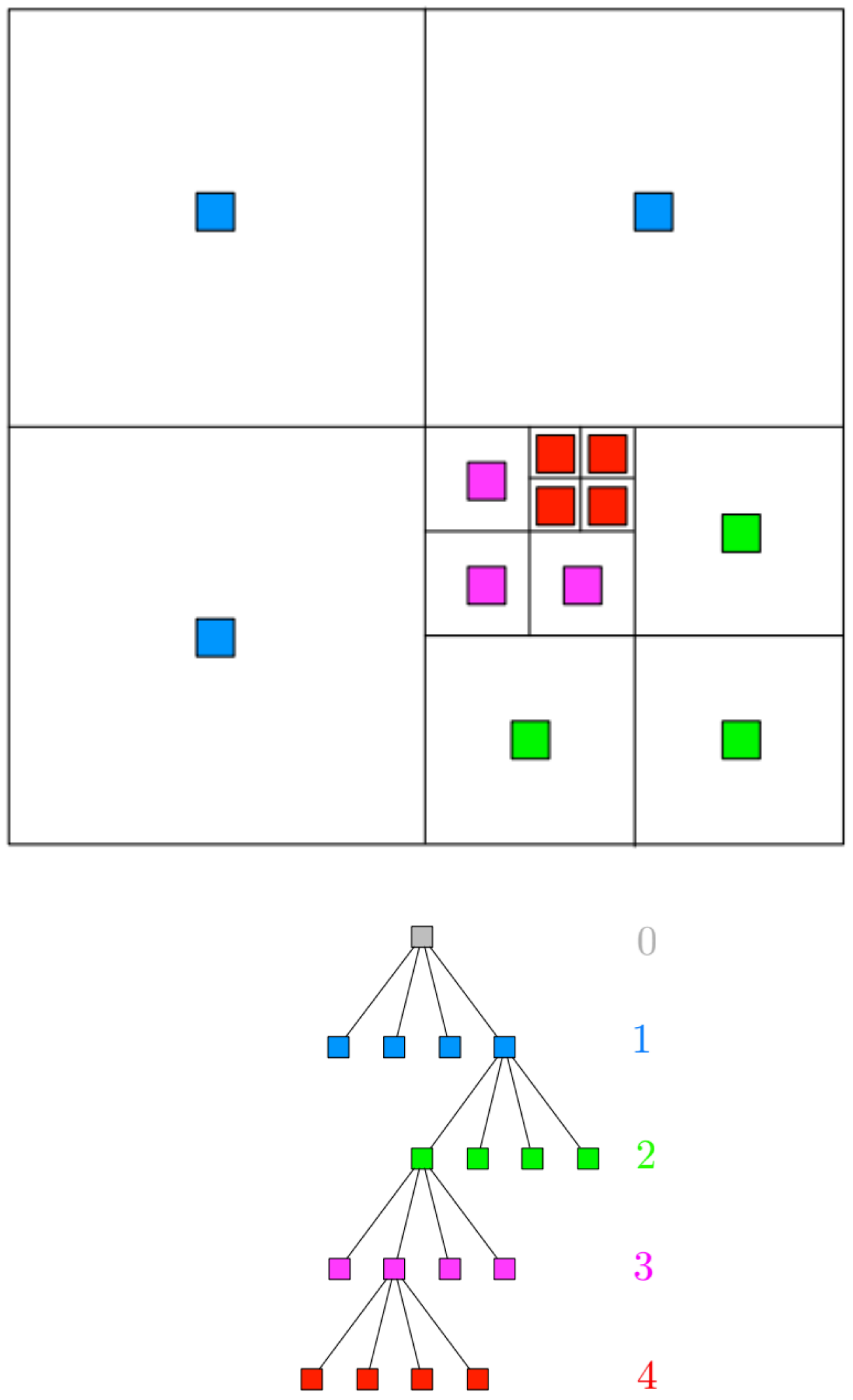
Evaluate the restarting criteria and perform restarting if needed.

(5) Mesh adaptation

Adapt the mesh to ϕ^{n+1} and update all the variables accordingly.

Volume preserving method

- **Implementation**
    - Quad/Octree grids
    - Adapted to the interface location
    - Advection: semi-Lagrangian
    - Poisson: Finite Difference
        - Supra convergenet
    - Interpolations: Quadratic WENO



Theoretical error analysis

- **Summary**

Quantity	Notation	Expression *	Value **
Magnitude of the compressible part	V	$\mathcal{O}\left(\Delta x^{\alpha}\right)$	$\mathcal{O}\left(\Delta x^2\right)$
Discretization errors	D	$\mathcal{O}\left(\Delta x^2\right)$	$\mathcal{O}\left(\Delta x^2\right)$
Linearization errors	L	$\mathcal{O}\left(\Delta x^3 + \Delta x^{2+\alpha} + \Delta x^{1+2\alpha}\right)$	$\mathcal{O}\left(\Delta x^3\right)$
Advection errors	A	$\mathcal{O}\left(\Delta x^2\right)$	
Reinitialization errors	R	$\mathcal{O}\left(\Delta x^2\right)$	
Error on interface position	E_{CLSRM}	$\mathcal{O}(A+V)$	$\mathcal{O}(\Delta x^2)$
	E_{VP}	$E_{CLSRM} + \mathcal{O}\left(\frac{A}{\Delta x} + V\right)$	$\mathcal{O}\left(\Delta x\right)$
Mass loss	M_{CLSRM}	$\mathcal{O}(A+V+R)$	$\mathcal{O}(\Delta x^2)$
	M_{VP}	$\mathcal{O}(D+L+R)$	$\mathcal{O}(\Delta x^2)$
Deviation from volume-preseving space	Δ_{CLSRM}	$\mathcal{O}(\frac{A}{\Delta x} + V)$	$\mathcal{O}(\Delta x)$
	Δ_{VP}	$\mathcal{O}\left(D+L\right)$	$\mathcal{O}(\Delta x^2)$

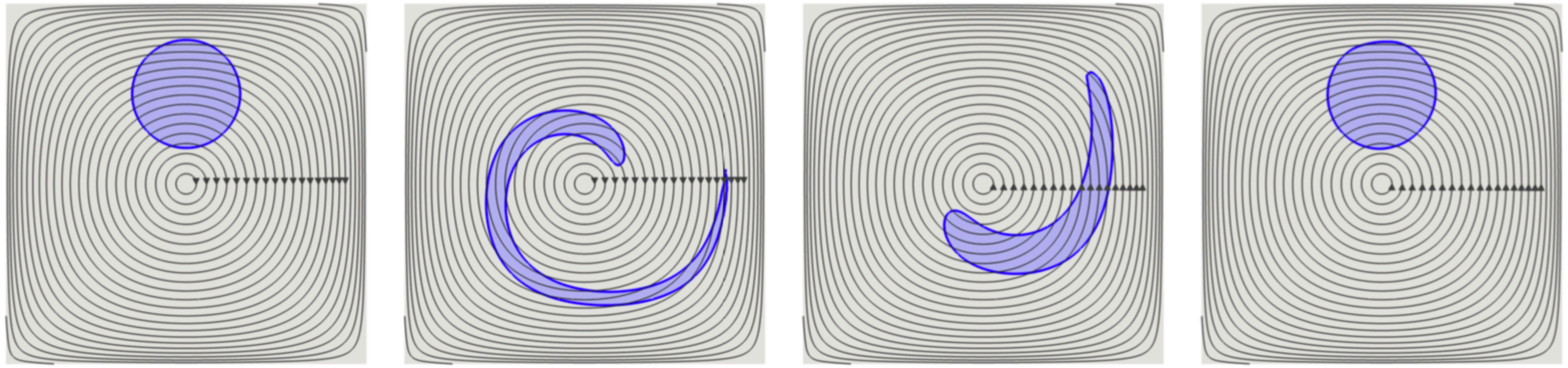
* *Using 2nd order discretization*

** *Assuming compressible velocity is* $\mathcal{O}(\Delta x)$

Analytic vortex

- **Velocity**

$$\mathbf{u}(x,y) = \left(-\sin^2(\pi x)\sin(2\pi y), \sin^2(\pi y)\sin(2\pi x)\right)$$



$t=0$ $t=1.57$ $t=5.69$ $t=6.28$

- **Errors**

$$\mathrm{e}_{L^1}(\phi) = \int_{\Gamma_{\text{exact}}} |\delta(\mathbf{x})|\, dl \qquad \mathrm{e}_{L^\infty}(\phi) = \max_{\mathbf{x}\in N(\phi)} |\delta(\mathbf{x}) - \delta_{\text{exact}}(\mathbf{x})|$$

$$\mathrm{d}_{VP}(\boldsymbol{\xi}) = \frac{1}{2\pi}\int_0^{2\pi}\int_{\Gamma_{\text{exact}}} |\det \nabla\boldsymbol{\xi} - 1|\, dl$$

Analytic vortex

- **Convergence**
  - Index by tree level
  - CFL = 5

CLSRM.

levels	$e_{L^\infty}(\phi)$	order	$e_{L^1}(\phi)$	order	mass loss (%)	order	$d_{VP}(\boldsymbol{\xi})$	order
6:2	$2.43 \cdot 10^{-2}$	-	$7.77 \cdot 10^{-4}$	-	$3.87 \cdot 10^{1}$	-	$1.28 \cdot 10^{-2}$	-
7:3	$1.30 \cdot 10^{-2}$	0.90	$1.39 \cdot 10^{-3}$	-0.83	$6.63 \cdot 10^{0}$	2.55	$2.92 \cdot 10^{-3}$	2.13
8:4	$6.90 \cdot 10^{-3}$	0.91	$6.19 \cdot 10^{-4}$	1.17	$7.92 \cdot 10^{-1}$	3.06	$6.43 \cdot 10^{-4}$	2.18
9:5	$1.91 \cdot 10^{-3}$	1.85	$1.34 \cdot 10^{-4}$	2.21	$1.20 \cdot 10^{-1}$	2.72	$1.51 \cdot 10^{-4}$	2.09
10:6	$5.15 \cdot 10^{-4}$	1.89	$2.28 \cdot 10^{-5}$	2.55	$1.80 \cdot 10^{-2}$	2.73	$3.83 \cdot 10^{-5}$	1.98
11:7	$1.22 \cdot 10^{-4}$	2.08	$3.57 \cdot 10^{-6}$	2.67	$2.71 \cdot 10^{-3}$	2.73	$1.76 \cdot 10^{-5}$	1.12
12:8	$3.69 \cdot 10^{-5}$	1.72	$7.12 \cdot 10^{-7}$	2.32	$4.83 \cdot 10^{-4}$	2.49	$2.29 \cdot 10^{-5}$	-0.37
average		1.56		1.68		2.71		1.52

VP using $|\mathcal{S}|/2 = 5\Delta x_{\min}$

levels	$e_{L^\infty}(\phi)$	order	$e_{L^1}(\phi)$	order	mass loss (%)	order	$d_{VP}(\boldsymbol{\xi})$	order
6:2	$2.44 \cdot 10^{-2}$	-	$1.01 \cdot 10^{-3}$	-	$5.01 \cdot 10^{1}$	-	$5.99 \cdot 10^{-4}$	-
7:3	$1.35 \cdot 10^{-2}$	0.86	$1.75 \cdot 10^{-3}$	-0.78	$5.34 \cdot 10^{0}$	3.23	$1.36 \cdot 10^{-4}$	2.14
8:4	$6.90 \cdot 10^{-3}$	0.96	$6.22 \cdot 10^{-4}$	1.49	$9.73 \cdot 10^{-1}$	2.46	$2.56 \cdot 10^{-5}$	2.41
9:5	$1.92 \cdot 10^{-3}$	1.85	$1.34 \cdot 10^{-4}$	2.21	$1.29 \cdot 10^{-1}$	2.92	$5.61 \cdot 10^{-6}$	2.19
10:6	$5.29 \cdot 10^{-4}$	1.86	$2.36 \cdot 10^{-5}$	2.51	$1.91 \cdot 10^{-2}$	2.75	$1.60 \cdot 10^{-6}$	1.81
11:7	$1.22 \cdot 10^{-4}$	2.12	$4.29 \cdot 10^{-6}$	2.46	$2.65 \cdot 10^{-3}$	2.84	$1.65 \cdot 10^{-6}$	-0.43
12:8	$3.68 \cdot 10^{-5}$	1.73	$1.85 \cdot 10^{-6}$	1.21	$2.74 \cdot 10^{-4}$	3.28	$2.78 \cdot 10^{-6}$	-0.75
average		1.56		1.21		2.91		1.23

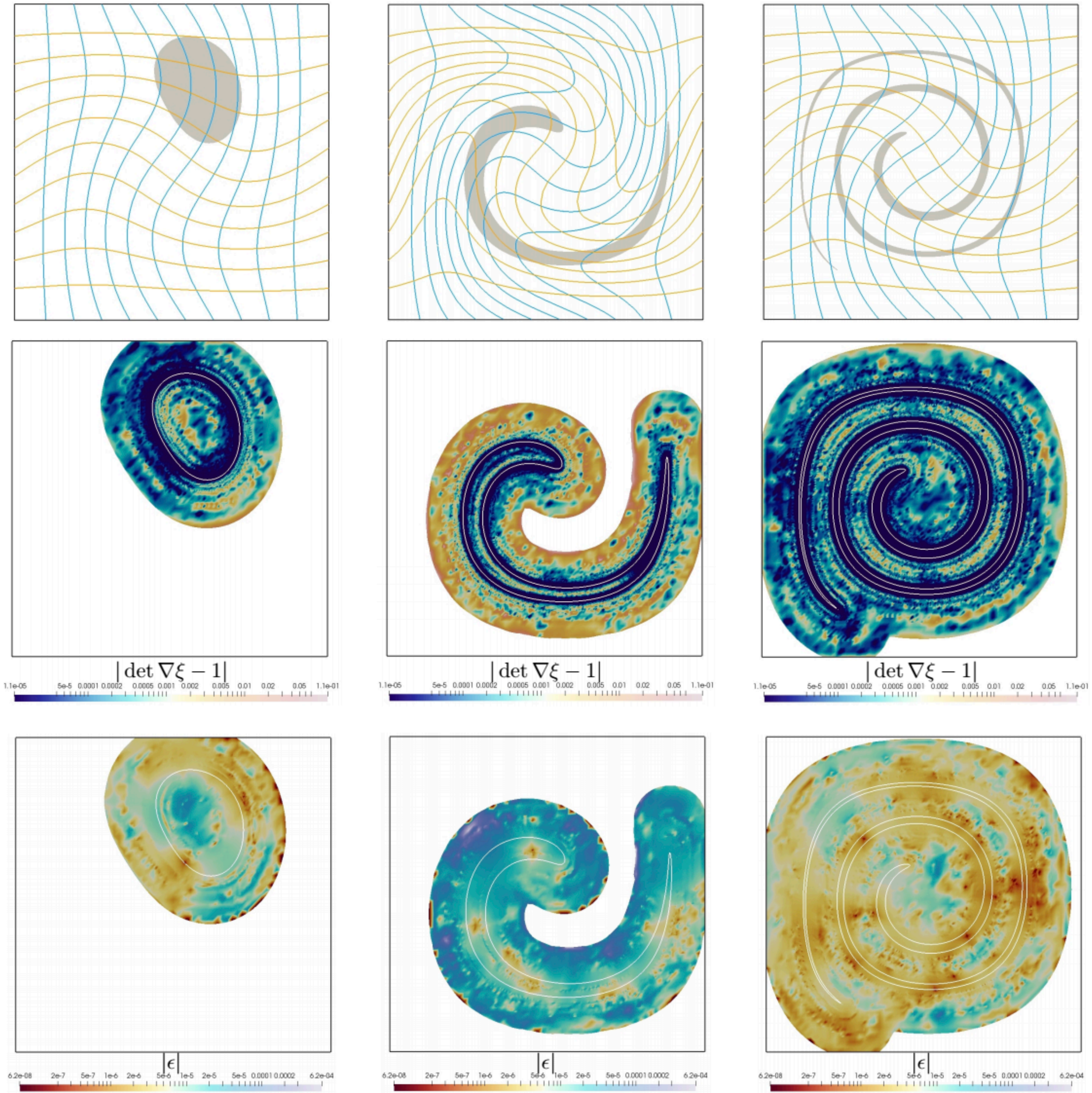
VP using $|\mathcal{S}|/2 = 2R$

levels	$e_{L^\infty}(\phi)$	order	$e_{L^1}(\phi)$	order	mass loss (%)	order	$d_{VP}(\boldsymbol{\xi})$	order
6:2	$2.29 \cdot 10^{-2}$	-	$1.92 \cdot 10^{-3}$	-	$5.14 \cdot 10^{1}$	-	$2.38 \cdot 10^{-4}$	-
7:3	$1.48 \cdot 10^{-2}$	0.63	$1.03 \cdot 10^{-3}$	0.89	$8.10 \cdot 10^{0}$	2.67	$5.26 \cdot 10^{-5}$	2.18
8:4	$7.06 \cdot 10^{-3}$	1.07	$4.62 \cdot 10^{-4}$	1.16	$1.19 \cdot 10^{0}$	2.76	$9.50 \cdot 10^{-6}$	2.47
9:5	$3.32 \cdot 10^{-3}$	1.09	$1.99 \cdot 10^{-4}$	1.21	$2.31 \cdot 10^{-1}$	2.37	$1.87 \cdot 10^{-6}$	2.34
10:6	$1.69 \cdot 10^{-3}$	0.97	$7.61 \cdot 10^{-5}$	1.39	$6.59 \cdot 10^{-2}$	1.81	$6.58 \cdot 10^{-7}$	1.51
11:7	$8.24 \cdot 10^{-4}$	1.04	$4.15 \cdot 10^{-5}$	0.88	$5.54 \cdot 10^{-2}$	0.25	$4.01 \cdot 10^{-7}$	-0.75
12:8	$4.62 \cdot 10^{-4}$	0.83	$2.49 \cdot 10^{-5}$	0.74	$3.85 \cdot 10^{-2}$	0.52	$2.84 \cdot 10^{-7}$	0.50
average		0.94		1.04		1.73		1.37

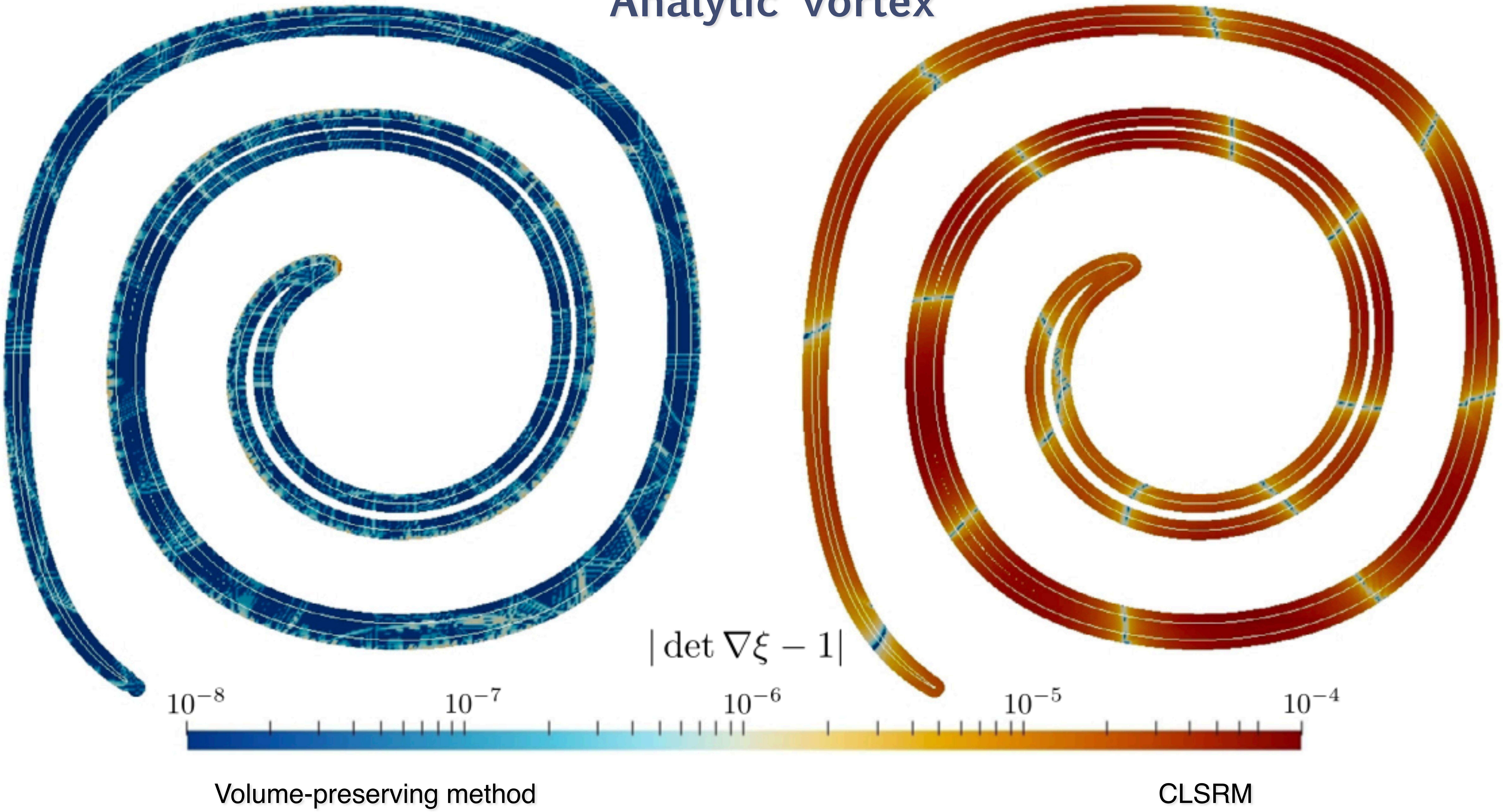
VP using $|\mathcal{S}|/2 = \infty$

levels	$e_{L^\infty}(\phi)$	order	$e_{L^1}(\phi)$	order	mass loss (%)	order	$d_{VP}(\boldsymbol{\xi})$	order
6:2	$2.44 \cdot 10^{-2}$	-	$2.07 \cdot 10^{-3}$	-	$5.03 \cdot 10^{1}$	-	$2.39 \cdot 10^{-4}$	-
7:3	$1.31 \cdot 10^{-2}$	0.89	$1.12 \cdot 10^{-3}$	0.85	$7.97 \cdot 10^{0}$	2.66	$5.27 \cdot 10^{-5}$	2.18
8:4	$6.15 \cdot 10^{-3}$	1.09	$4.04 \cdot 10^{-4}$	1.47	$1.21 \cdot 10^{0}$	2.71	$9.53 \cdot 10^{-6}$	2.47
9:5	$3.38 \cdot 10^{-3}$	0.86	$4.82 \cdot 10^{-5}$	3.07	$1.71 \cdot 10^{-1}$	2.83	$1.87 \cdot 10^{-6}$	2.35
10:6	$1.81 \cdot 10^{-3}$	0.89	$3.33 \cdot 10^{-5}$	0.53	$6.24 \cdot 10^{-2}$	1.45	$6.55 \cdot 10^{-7}$	1.51
11:7	$8.69 \cdot 10^{-4}$	1.06	$4.44 \cdot 10^{-5}$	-0.41	$5.60 \cdot 10^{-2}$	0.15	$4.00 \cdot 10^{-7}$	0.73
12:8	$4.25 \cdot 10^{-4}$	1.03	$2.33 \cdot 10^{-5}$	0.93	$4.08 \cdot 10^{-2}$	0.46	$2.83 \cdot 10^{-7}$	0.49
average		0.97		1.07		1.71		1.62

Analytic vortex



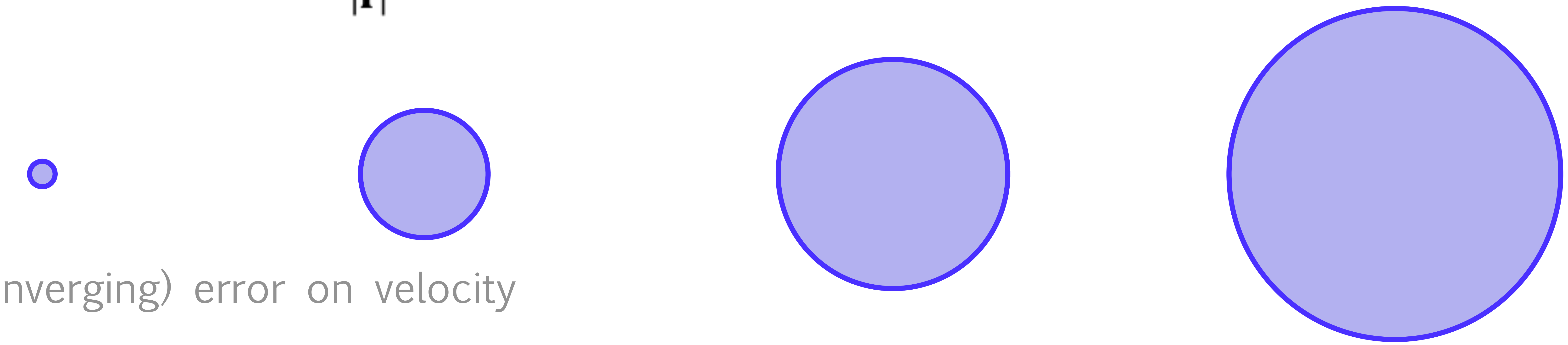
Analytic vortex



Artificial Expansion

- **Velocity field**

$$\mathbf{u}(x,y) = 0.1 \cdot \Delta x^{\alpha} \frac{\mathbf{r}}{|\mathbf{r}|}, \qquad \mathbf{r} = (x-0.5,\, y-0.5), \qquad \alpha \in [0.01, 1], \qquad \forall t \in [0, 2\pi],$$



  - Mimic (converging) error on velocity

- **Errors**

VP using $|\mathcal{S}|/2 = R$

Levels	$\Delta x^{1.5}$		Δx^{1}		$\Delta x^{0.6}$		$\Delta x^{0.25}$		$\Delta x^{0.1}$	
	Mass loss (%)	Order	Mass loss (%)	Order	Mass loss (%)	Order	Mass loss (%)	Order	Mass loss (%)	Order
6:2	$1.02 \cdot 10^{-2}$	-	$9.92 \cdot 10^{-2}$	-	$2.69 \cdot 10^{-2}$	-	$4.75 \cdot 10^{1}$	-	$1.45 \cdot 10^{2}$	-
7:3	$1.25 \cdot 10^{-3}$	3.16	$4.39 \cdot 10^{-3}$	2.46	$2.11 \cdot 10^{-3}$	3.67	$1.35 \cdot 10^{1}$	1.82	$1.48 \cdot 10^{2}$	-0.03
8:4	$1.87 \cdot 10^{-4}$	2.74	$1.79 \cdot 10^{-4}$	1.80	$9.83 \cdot 10^{-4}$	1.10	$1.68 \cdot 10^{0}$	3.01	$1.15 \cdot 10^{2}$	0.36
9:5	$3.83 \cdot 10^{-5}$	2.29	$1.27 \cdot 10^{-4}$	0.53	$1.63 \cdot 10^{-3}$	-0.73	$1.68 \cdot 10^{-1}$	3.31	$5.41 \cdot 10^{-1}$	4.77
10:6	$8.17 \cdot 10^{-5}$	2.23	$6.58 \cdot 10^{-4}$	1.12	$7.93 \cdot 10^{-4}$	1.04	$2.18 \cdot 10^{-2}$	2.95	$5.31 \cdot 10^{-1}$	0.02
11:7	$4.23 \cdot 10^{-5}$	4.27	$1.37 \cdot 10^{-7}$	9.32	$4.43 \cdot 10^{-5}$	4.16	$2.76 \cdot 10^{-1}$	-3.67	$1.12 \cdot 10^{0}$	-1.07
12:8	$6.68 \cdot 10^{-6}$	2.66	$1.02 \cdot 10^{-6}$	-1.96	$8.00 \cdot 10^{-6}$	2.47	$2.98 \cdot 10^{-2}$	3.21	$2.37 \cdot 10^{-1}$	2.24
average		2.89		2.22		1.95		1.77		1.04

CLSRM

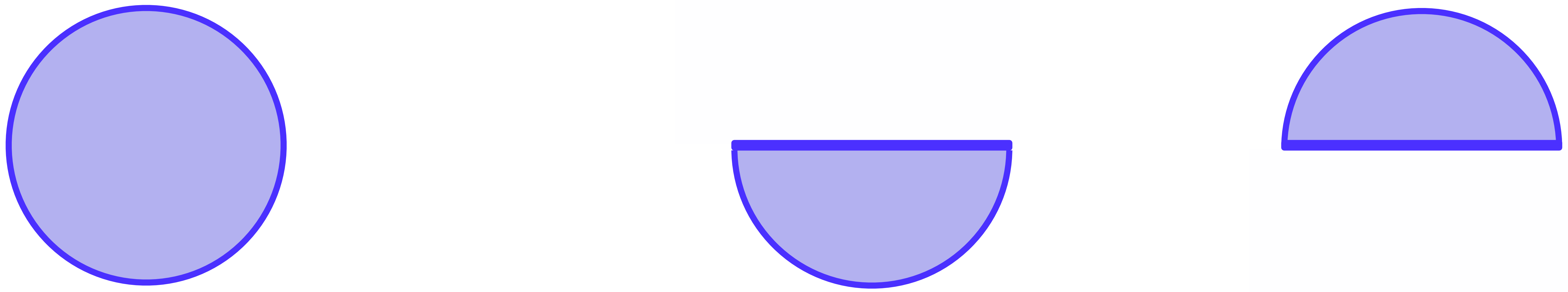
Levels	$\Delta x^{1.5}$		Δx^{1}		$\Delta x^{0.6}$		$\Delta x^{0.25}$		$\Delta x^{0.1}$	
	Mass loss (%)	Order	Mass loss (%)	Order	Mass loss (%)	Order	Mass loss (%)	Order	Mass loss (%)	Order
6:2	$8.10 \cdot 10^{-1}$	-	$6.65 \cdot 10^{1}$	-	$3.76 \cdot 10^{1}$	-	$2.03 \cdot 10^{2}$	-	$4.68 \cdot 10^{2}$	-
7:3	$2.89 \cdot 10^{-1}$	1.50	$3.30 \cdot 10^{1}$	1.01	$2.41 \cdot 10^{1}$	0.64	$1.63 \cdot 10^{2}$	0.31	$4.24 \cdot 10^{2}$	0.14
8:4	$1.02 \cdot 10^{-1}$	1.50	$1.64 \cdot 10^{1}$	1.01	$1.56 \cdot 10^{1}$	0.63	$1.32 \cdot 10^{2}$	0.30	$3.85 \cdot 10^{2}$	0.13
9:5	$3.61 \cdot 10^{-2}$	1.50	$8.20 \cdot 10^{-1}$	1.00	$1.02 \cdot 10^{1}$	0.62	$1.07 \cdot 10^{2}$	0.30	$3.50 \cdot 10^{2}$	0.13
10:6	$1.28 \cdot 10^{-2}$	1.50	$4.09 \cdot 10^{-1}$	1.00	$6.65 \cdot 10^{0}$	0.61	$8.78 \cdot 10^{1}$	0.29	$3.19 \cdot 10^{2}$	0.13
11:7	$4.52 \cdot 10^{-3}$	1.50	$2.05 \cdot 10^{-1}$	1.00	$4.36 \cdot 10^{0}$	0.61	$7.20 \cdot 10^{1}$	0.28	$2.91 \cdot 10^{2}$	0.13
12:8	$1.60 \cdot 10^{-3}$	1.50	$1.02 \cdot 10^{-1}$	1.00	$2.87 \cdot 10^{0}$	0.61	$5.92 \cdot 10^{1}$	0.28	$2.65 \cdot 10^{2}$	0.13
average		1.50		1.00		0.62		0.29		0.13

Split in two

- **Velocity field**

$$\mathbf{u}(x,y)=\begin{cases}(0.1,0) & \text{if} \quad y>0.4\\(-0.1,0) & \text{elsewhere}\end{cases}$$

$$\phi_{exact}(x,y)=\begin{cases}\phi_0(x-0.1\pi,y) & \text{if} \quad y>0.4\\ \phi_0(x+0.1\pi,y) & \text{elsewhere}\end{cases}.$$



- **Errors**

CLSRM

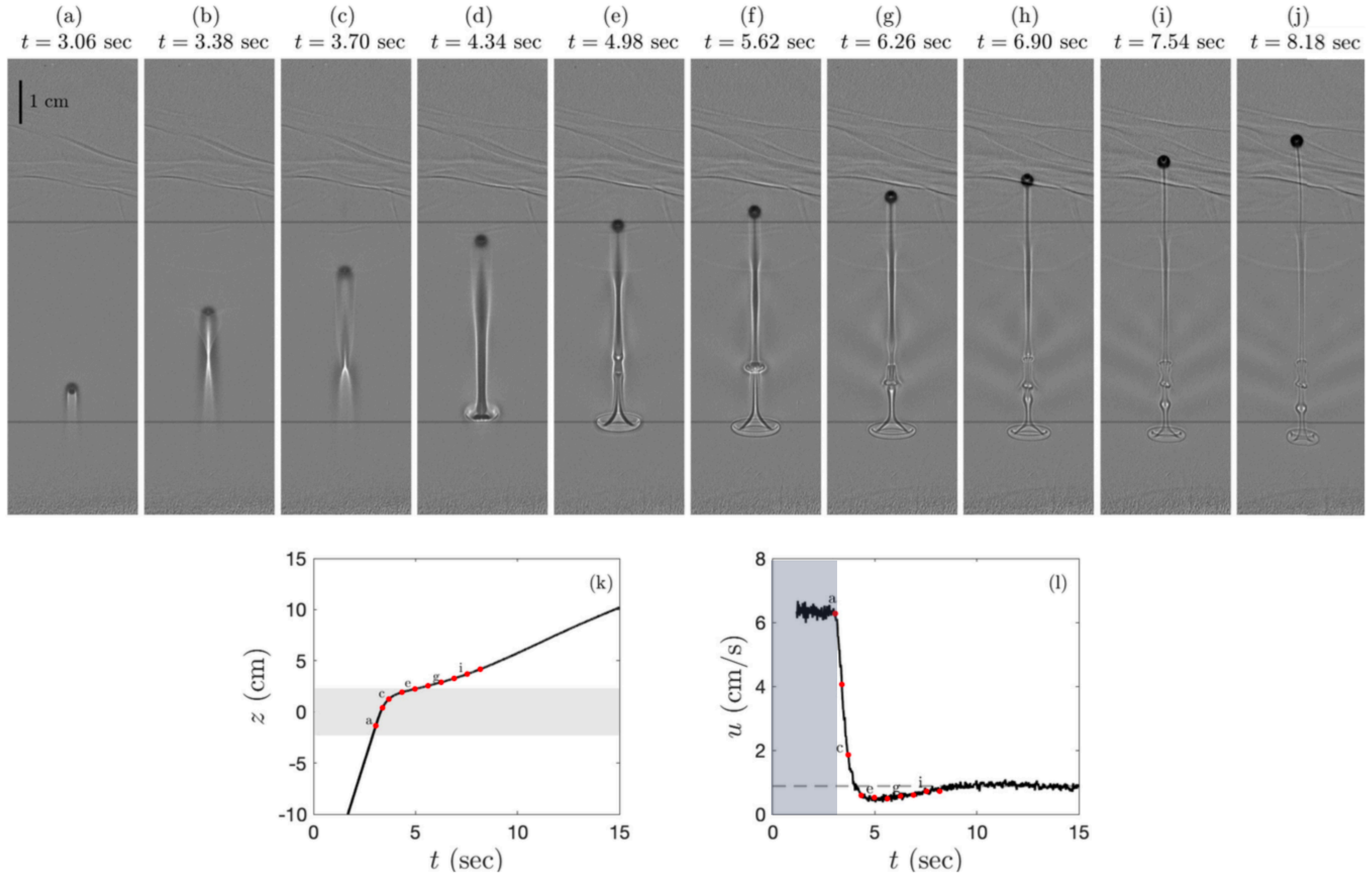
Levels	$e_{L^\infty}(\phi)$	Order	$e_{L^1}(\phi)$	Order	Mass loss (%)	Order	Time (s)
6:2	$1.78\cdot10^{-2}$	-	$1.01\cdot10^{-3}$	-	$4.59\cdot10^{0}$	-	$1.72\cdot10^{-1}$
7:3	$7.54\cdot10^{-3}$	1.24	$3.26\cdot10^{-4}$	1.64	$1.93\cdot10^{0}$	1.25	$7.95\cdot10^{-1}$
8:4	$3.27\cdot10^{-3}$	1.21	$6.53\cdot10^{-5}$	2.32	$8.51\cdot10^{-1}$	1.18	$2.95\cdot10^{0}$
9:5	$1.95\cdot10^{-3}$	0.74	$2.19\cdot10^{-5}$	1.58	$4.12\cdot10^{-1}$	1.05	$1.21\cdot10^{1}$
10:6	$1.19\cdot10^{-3}$	0.72	$5.68\cdot10^{-6}$	1.95	$2.05\cdot10^{-1}$	1.01	$4.87\cdot10^{1}$
11:7	$4.33\cdot10^{-4}$	1.46	$1.70\cdot10^{-6}$	1.74	$1.01\cdot10^{-1}$	1.02	$2.12\cdot10^{2}$
12:8	$2.52\cdot10^{-4}$	0.78	$4.05\cdot10^{-7}$	2.07	$5.00\cdot10^{-2}$	1.02	$1.00\cdot10^{3}$
average		1.02		1.88		1.09	

VP using $|\mathcal{S}|/2=R$

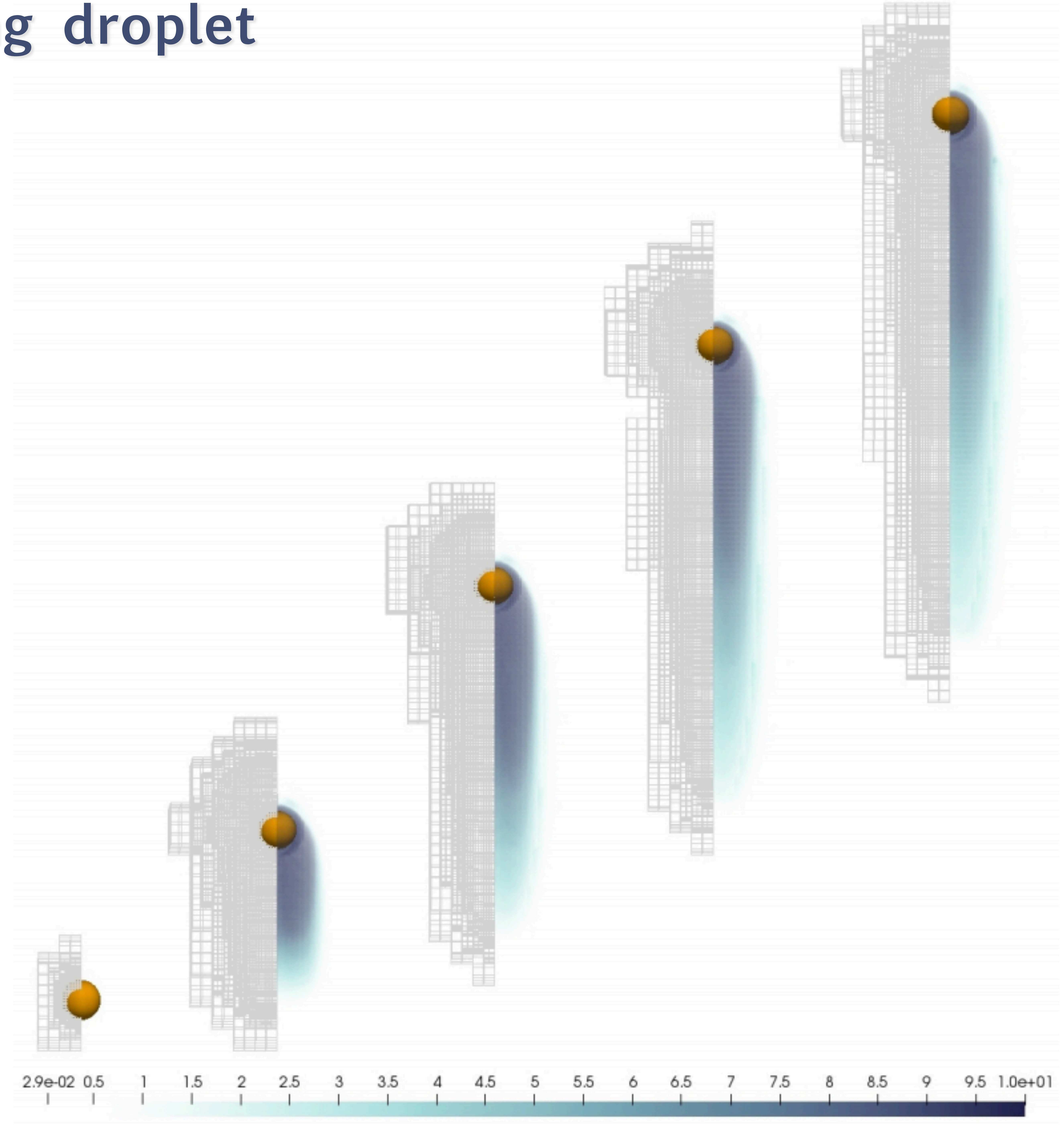
Levels	$e_{L^\infty}(\phi)$	Order	$e_{L^1}(\phi)$	Order	Mass loss (%)	Order	Time (s)
6:2	$1.78\cdot10^{-2}$	-	$1.02\cdot10^{-3}$	-	$4.59\cdot10^{0}$	-	$2.48\cdot10^{-1}$
7:3	$1.25\cdot10^{-2}$	0.51	$3.95\cdot10^{-4}$	1.36	$1.90\cdot10^{0}$	1.28	$1.25\cdot10^{0}$
8:4	$4.99\cdot10^{-3}$	1.33	$2.30\cdot10^{-4}$	0.78	$9.92\cdot10^{-1}$	0.94	$7.01\cdot10^{0}$
9:5	$2.59\cdot10^{-3}$	0.94	$2.53\cdot10^{-4}$	-0.14	$4.01\cdot10^{-1}$	1.31	$3.43\cdot10^{1}$
10:6	$1.70\cdot10^{-3}$	0.61	$1.18\cdot10^{-4}$	1.11	$2.25\cdot10^{-1}$	0.83	$1.50\cdot10^{2}$
11:7	$9.47\cdot10^{-4}$	0.84	$3.88\cdot10^{-5}$	1.60	$1.19\cdot10^{-1}$	0.91	$6.15\cdot10^{2}$
12:8	$4.33\cdot10^{-4}$	1.13	$3.07\cdot10^{-5}$	0.34	$3.29\cdot10^{-2}$	1.85	$2.55\cdot10^{3}$
average		0.89		0.84		1.18	

Rising droplet

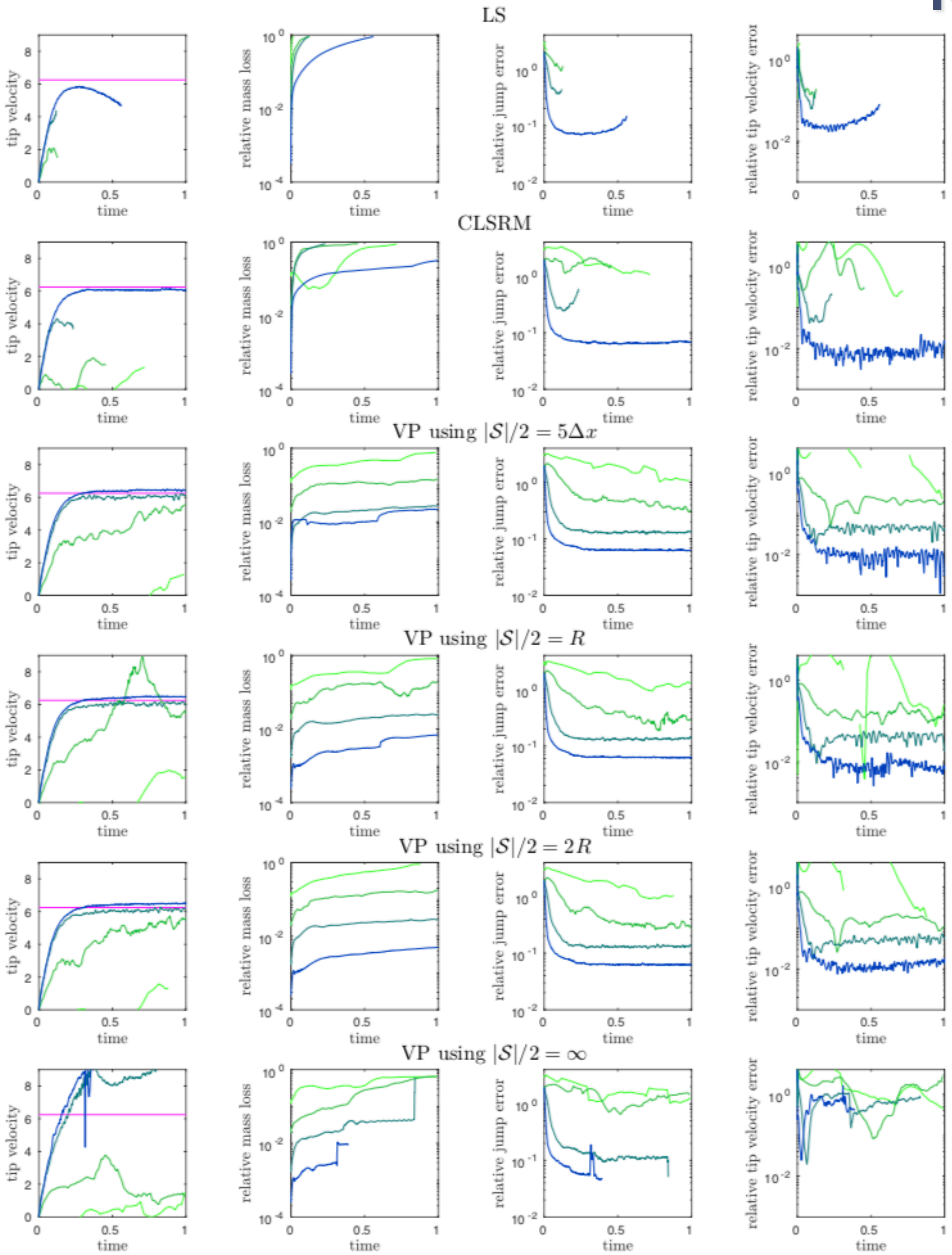
- **Experimental parameters**
  - Uniform density (lower/heavier fluid)
  - Full NS

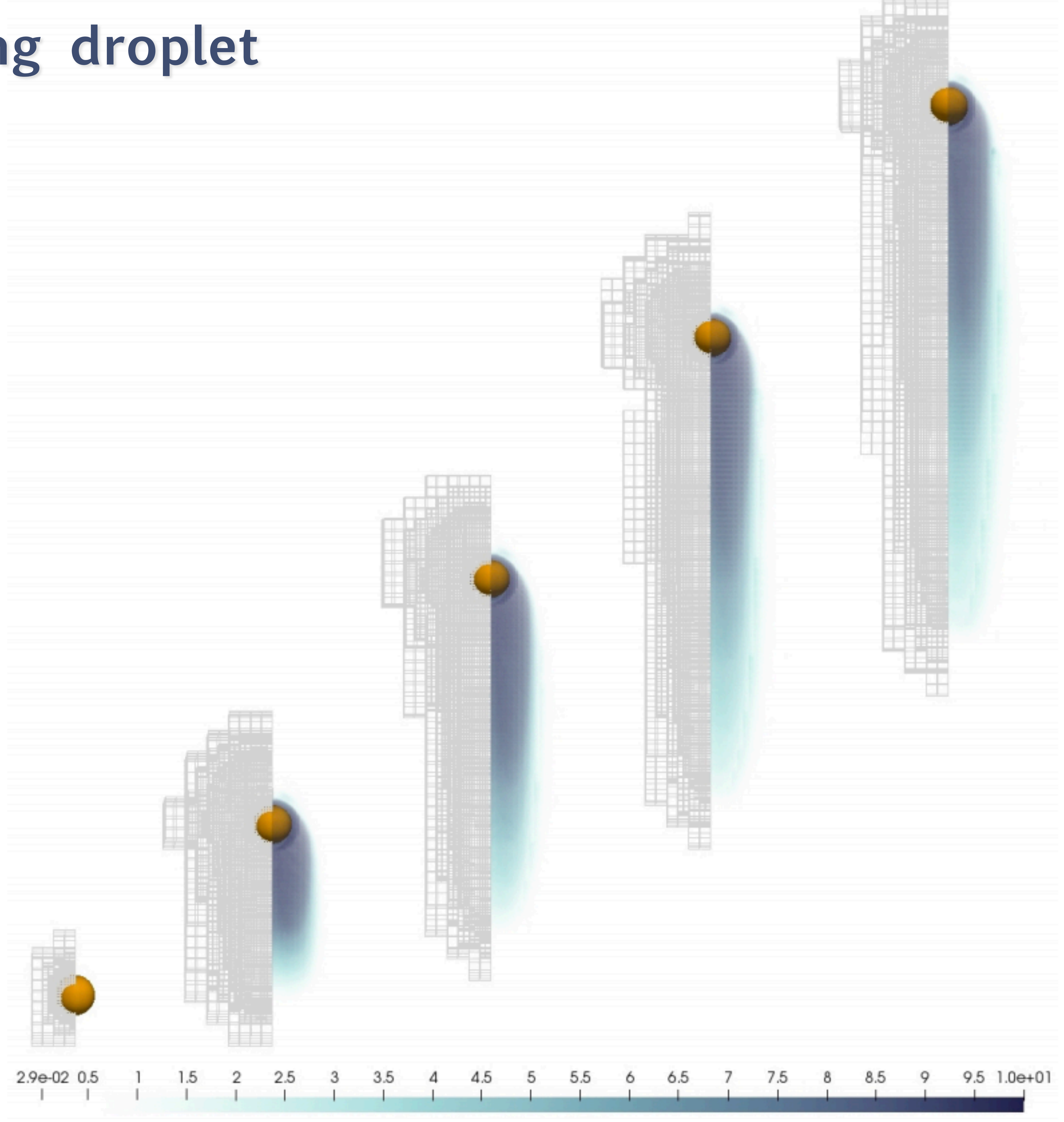


. *Retention of oil droplets in density stratification, T. Mandel et al., PRF 2020*

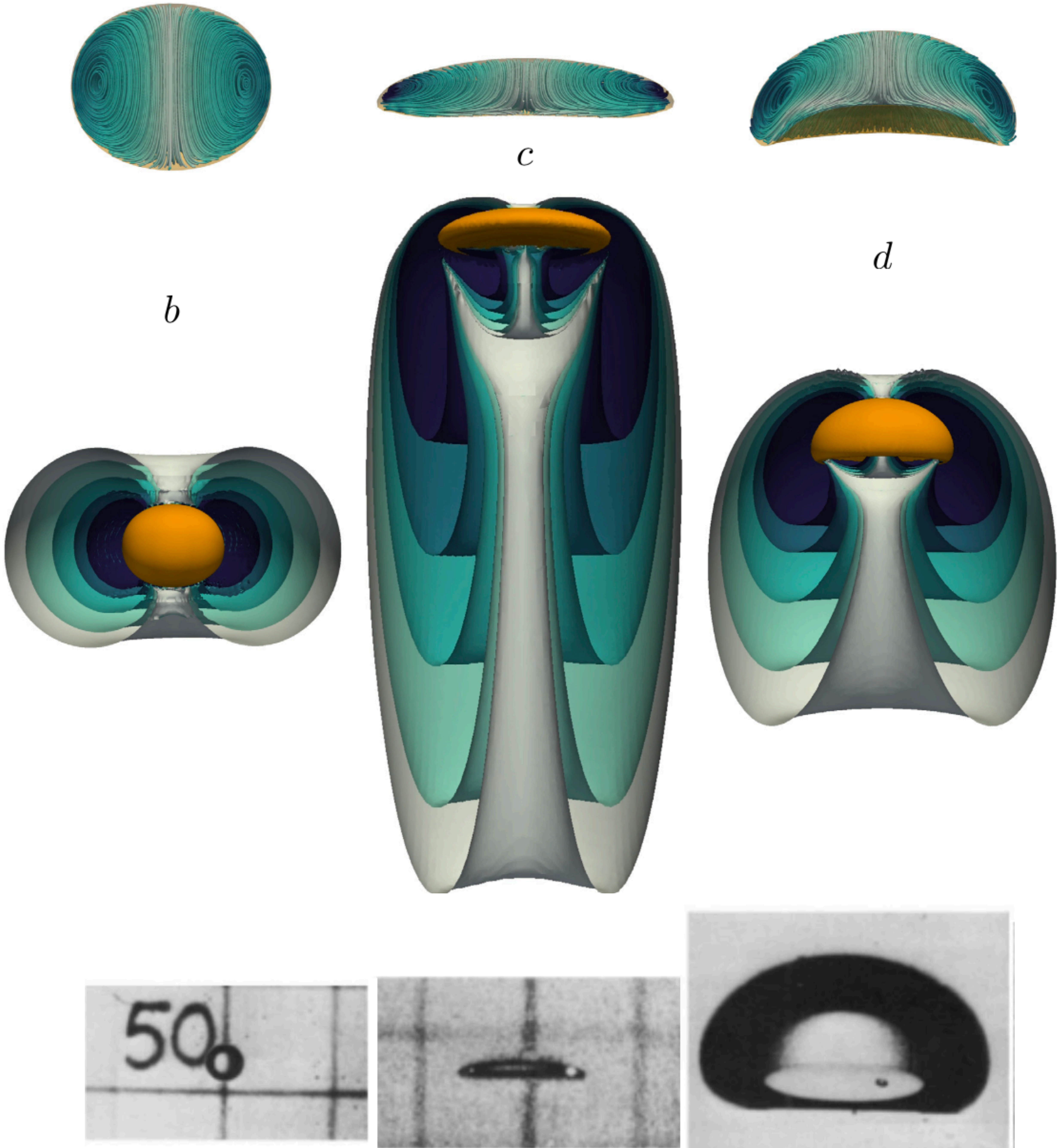


Rising droplet

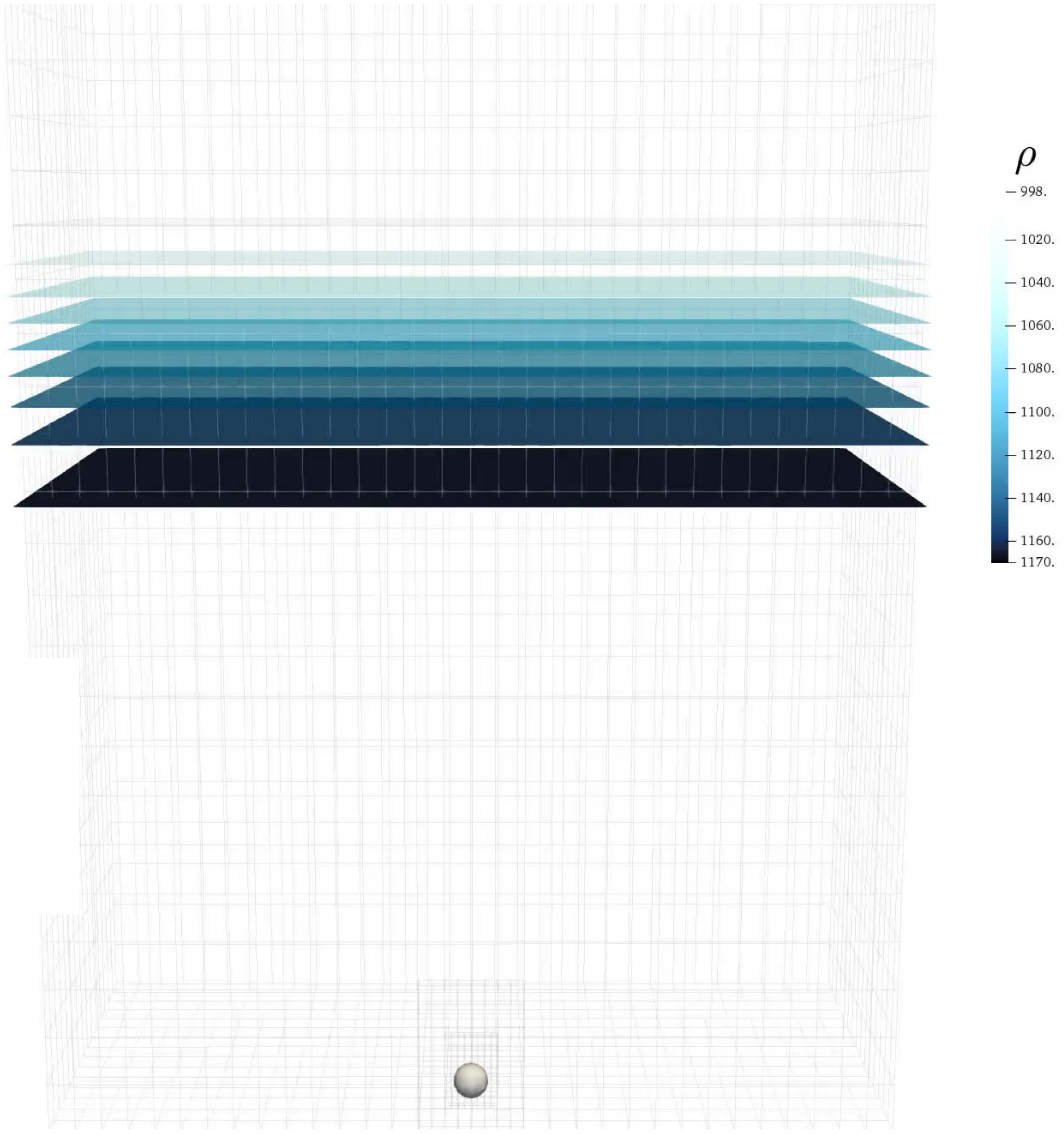


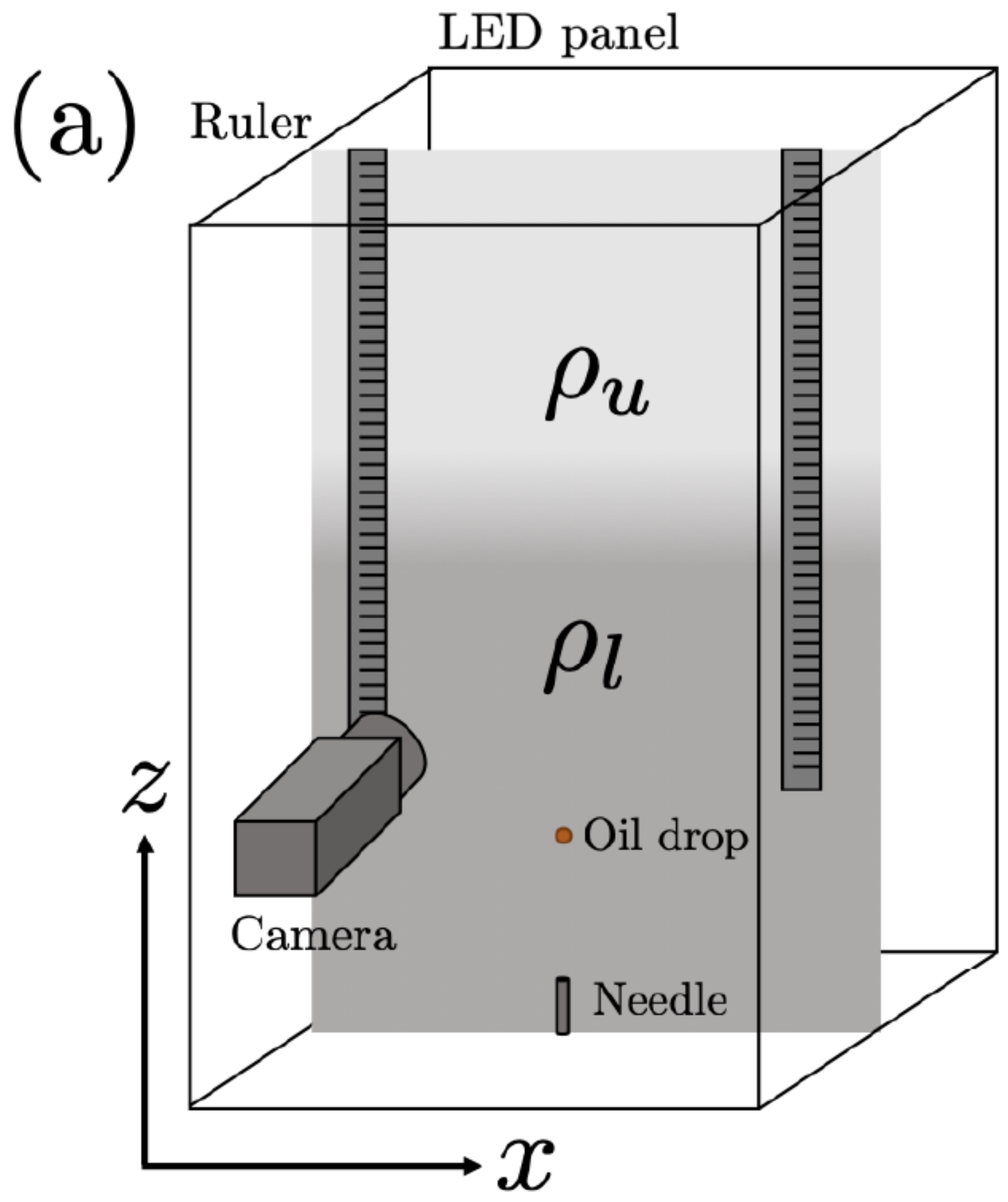


Rising droplet (Bhaga & Weber 1981)

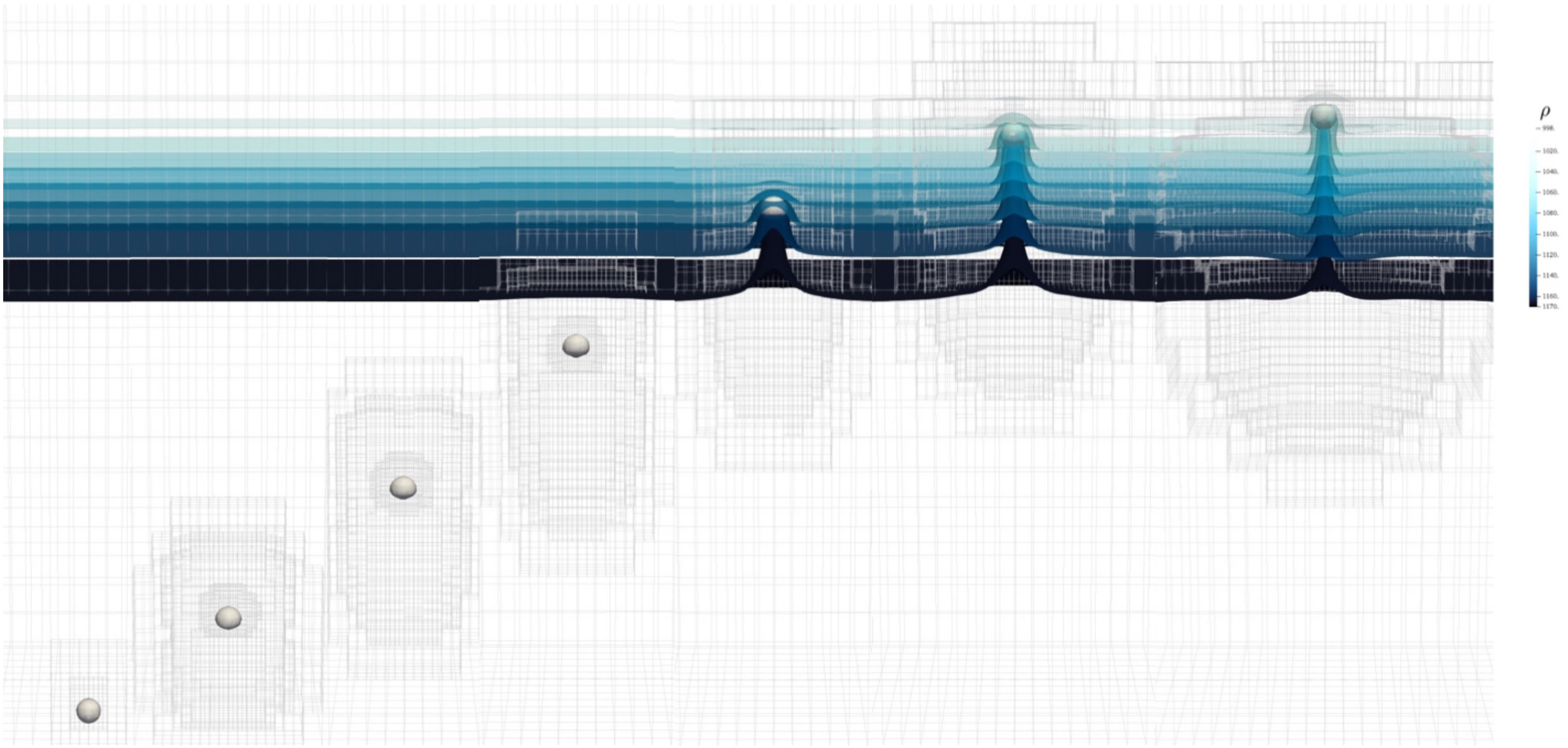


Rising droplet in stratified flows

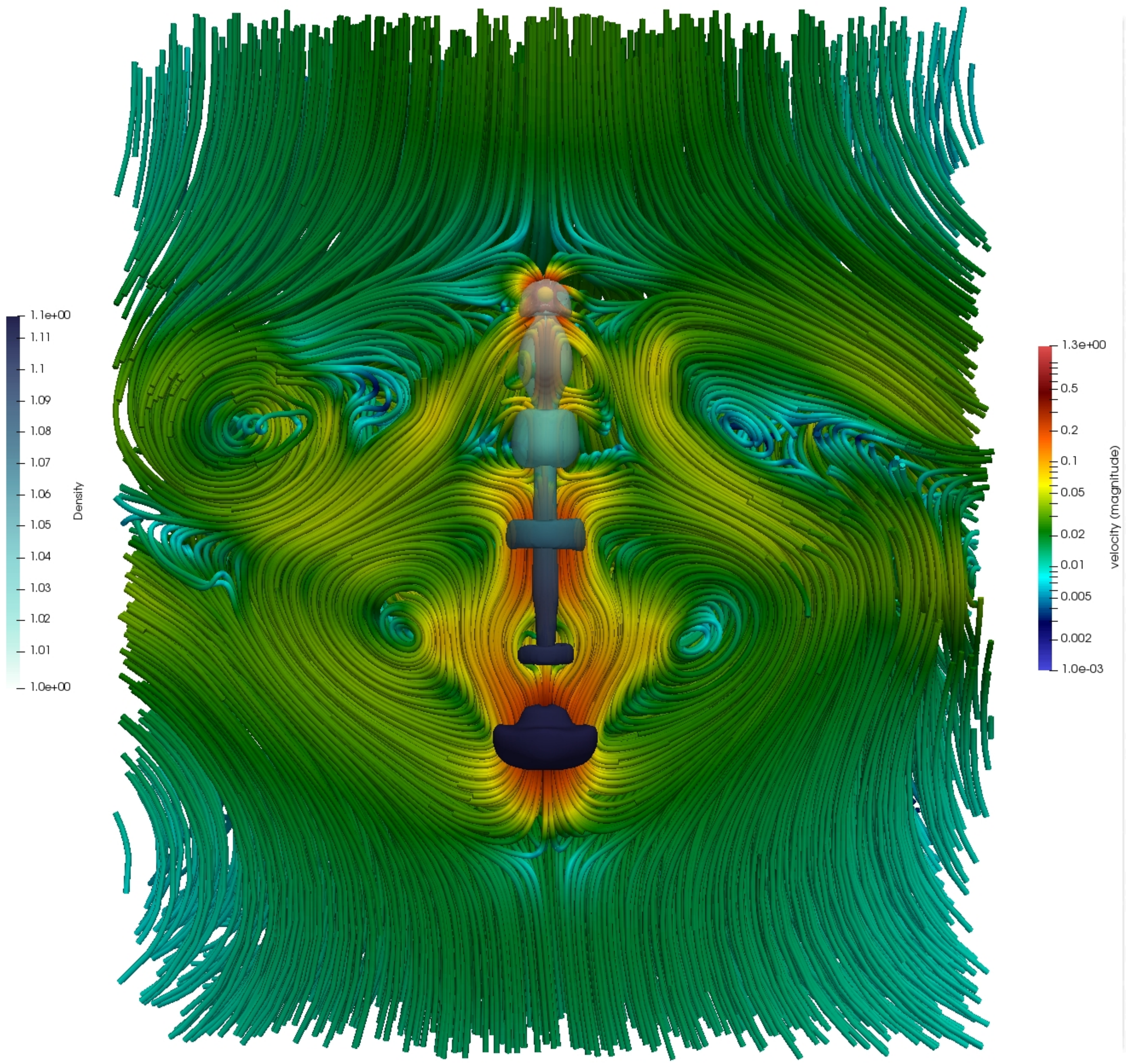


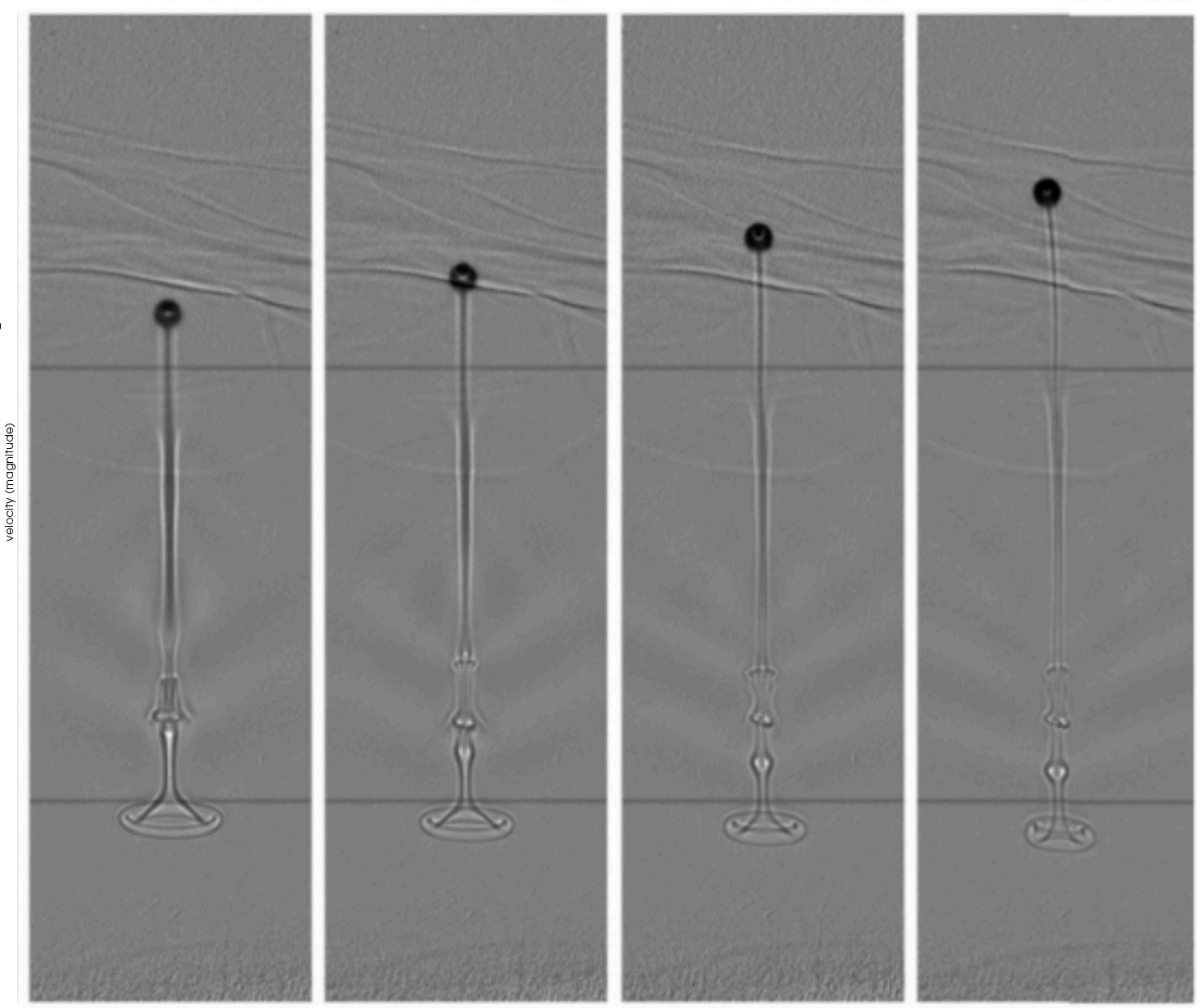


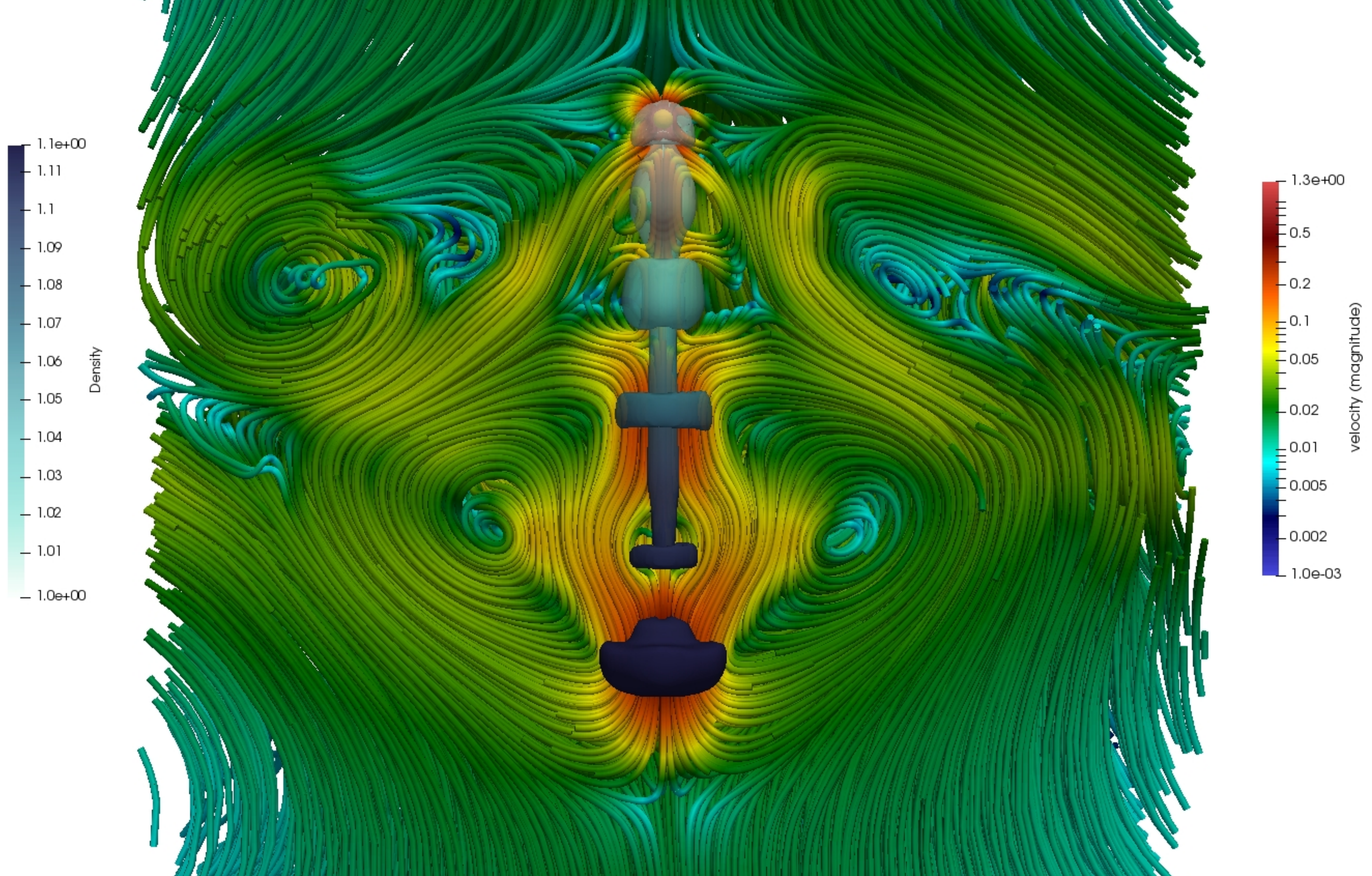
Rising droplet in stratified flows



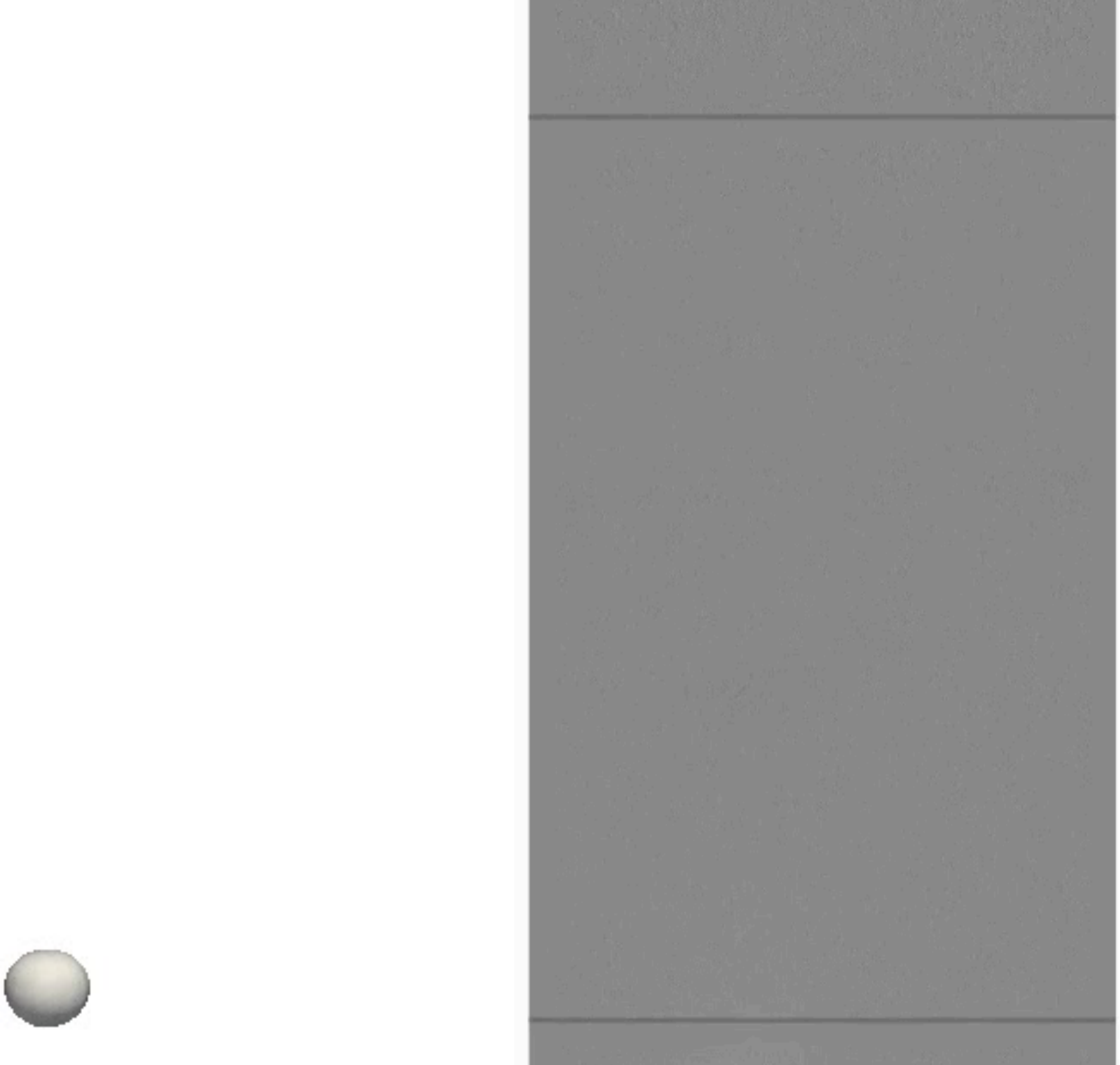
Rising droplet in stratified flows





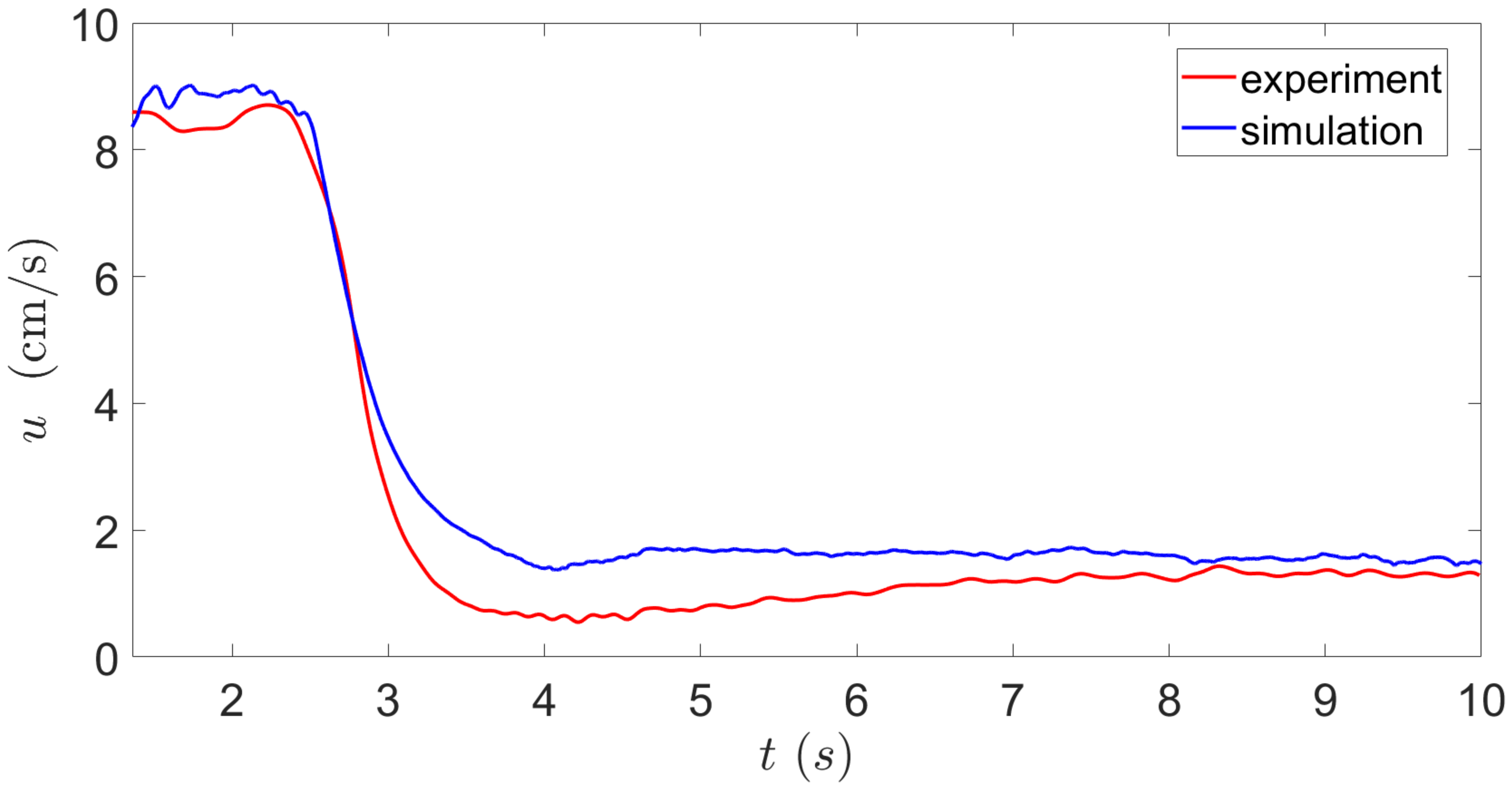


1.1e+00
1.11
1.1
1.09
1.08
1.07
1.06
1.05
1.04
1.03
1.02
1.01
1.0e+00
Density
1.3e+00
0.5
0.2
0.1
0.05
0.02
0.01
0.005
0.002
1.0e-03
velocity (magnitude)



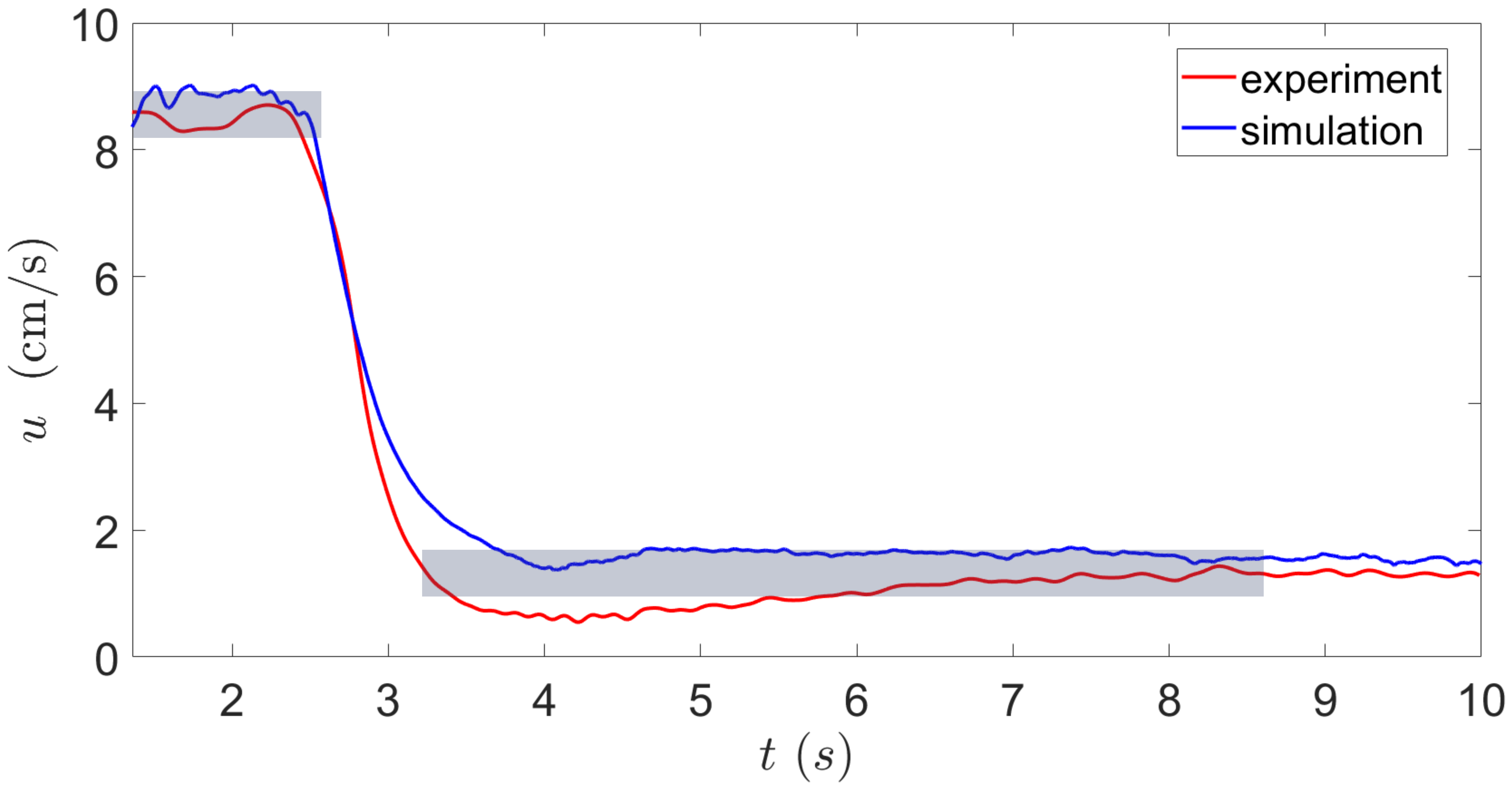
Rising droplet in stratified flows

- Rising velocity



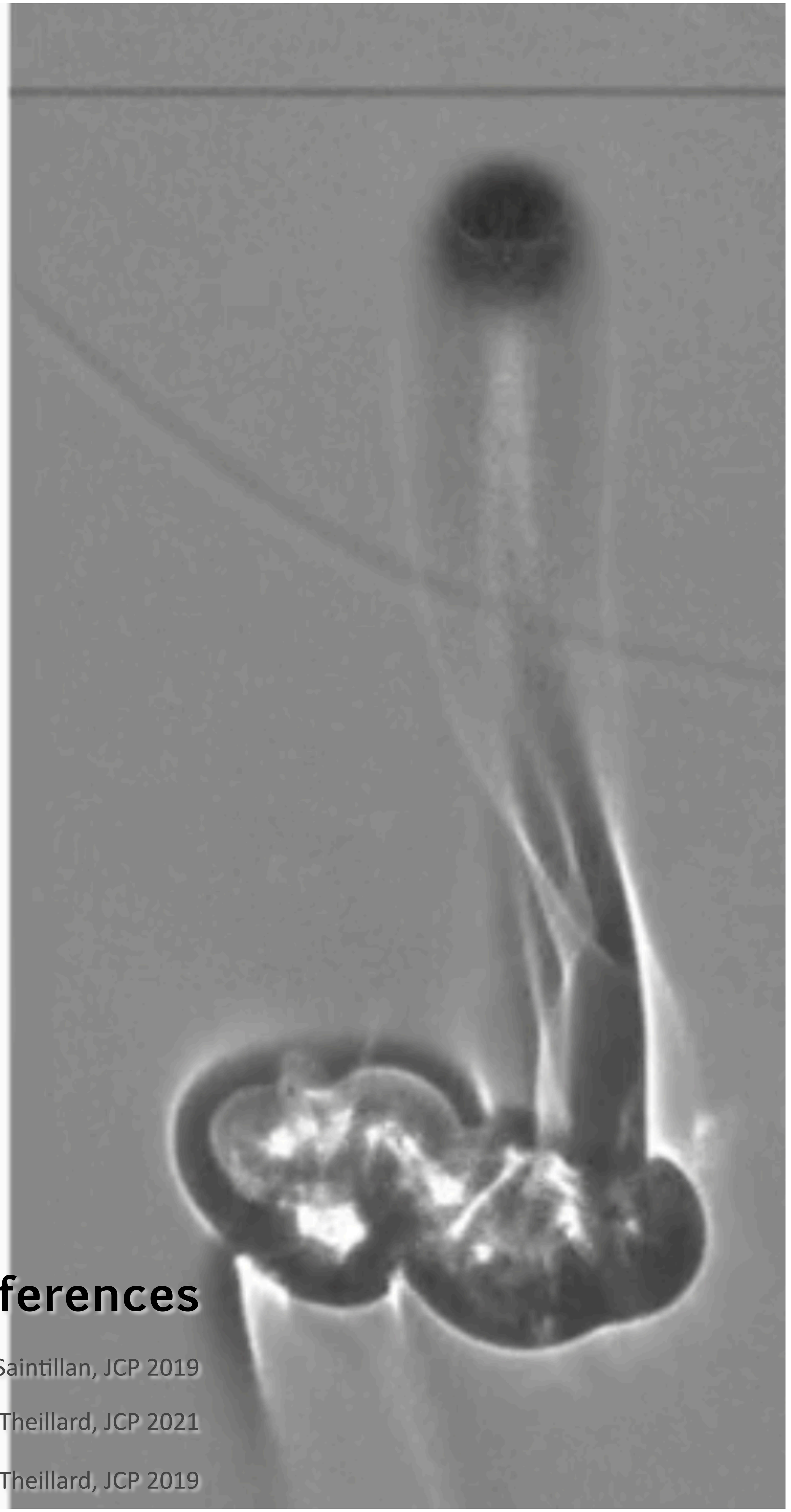
Rising droplet in stratified flows

- Rising velocity



Marangoni forces due to surfactants?

Conclusions



Novel volume-preserving reference map method

- Projection on the volume-preserving space
- Improved but inexact mass conservation
- Substantial mass loss reduction

Future directions

- Generalization to other advection problems
- Iterative method for the non-linear constraint
- Compressible case ?

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- UW Madison - Chris Rycroft
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- UCM - Dustin Kleckner, Shilpa Khatri
- UNH - Tracy Mandel
- UCM - Adam Binswanger, Matt Blomquist, De Zhen Zhou

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