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Schrödinger's Smoke

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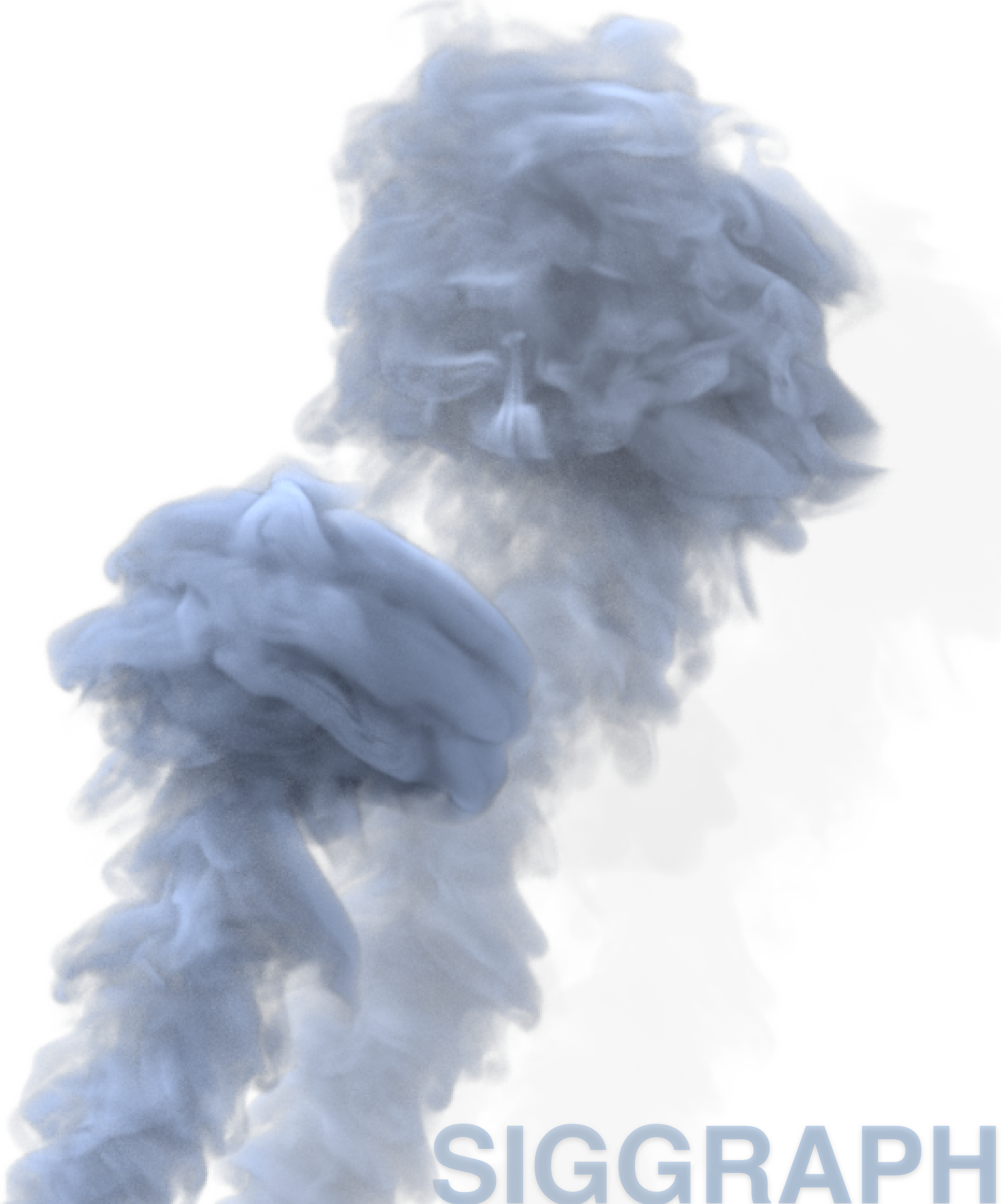
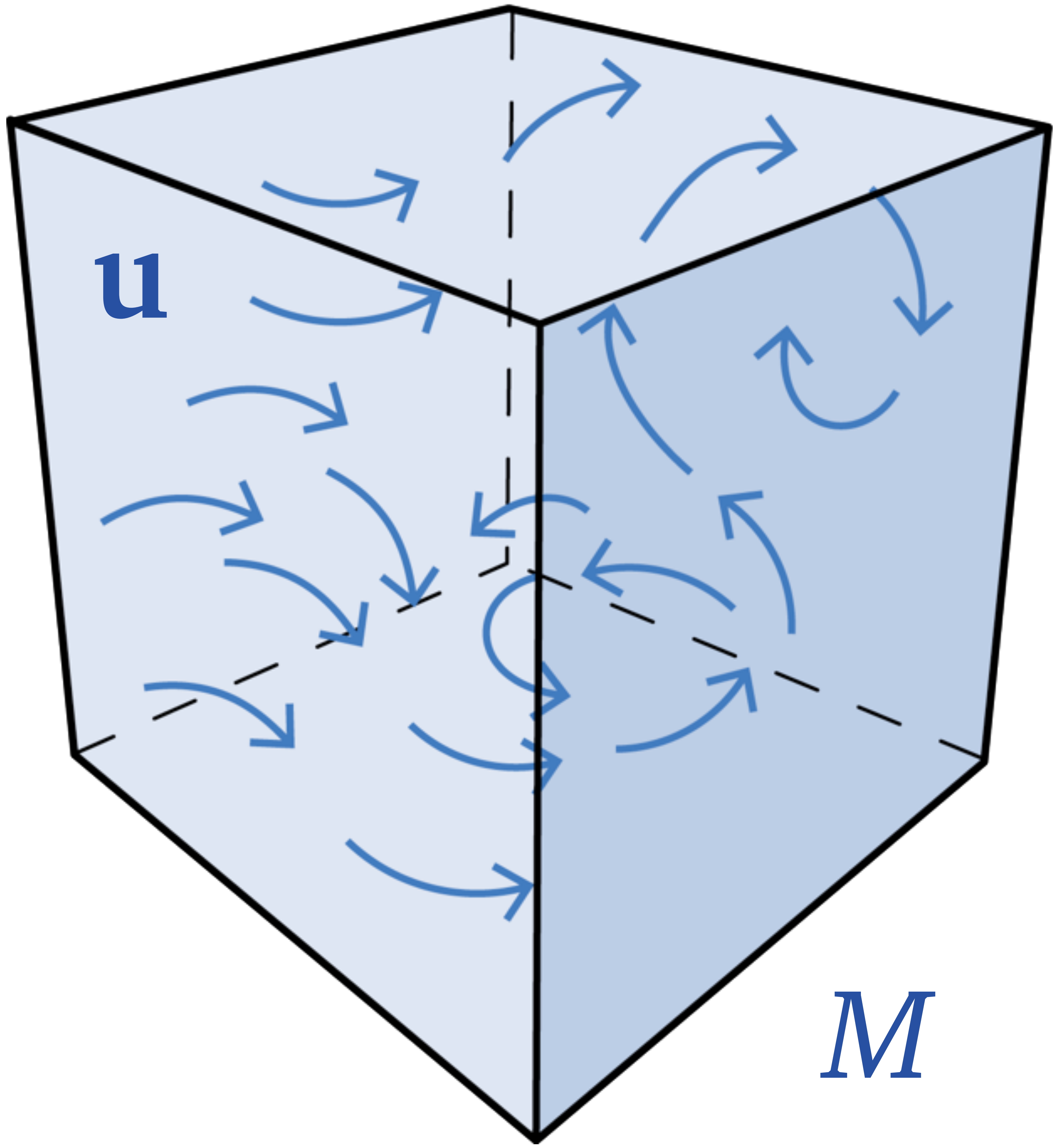


Fluids

The state of fluid is described by

- **density field**
  $\rho : M \to \mathbb{R}^+$
- **velocity field**
  $\mathbf{u} : M \to \mathbb{R}^3$



Fluids

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

(conservation of mass)

$$\frac{\partial}{\partial t}\mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{\nabla p}{\rho}$$

(conservation of momentum)

$$p = p(\rho)$$

—*Compressible* Euler equation

Fluids

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

$$\frac{\partial}{\partial t}\mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{\nabla p}{\rho}$$

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

Fluids

$$\rho = 1$$

$$\begin{cases} \frac{\partial}{\partial t}\mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

— *Incompressible* Euler equation

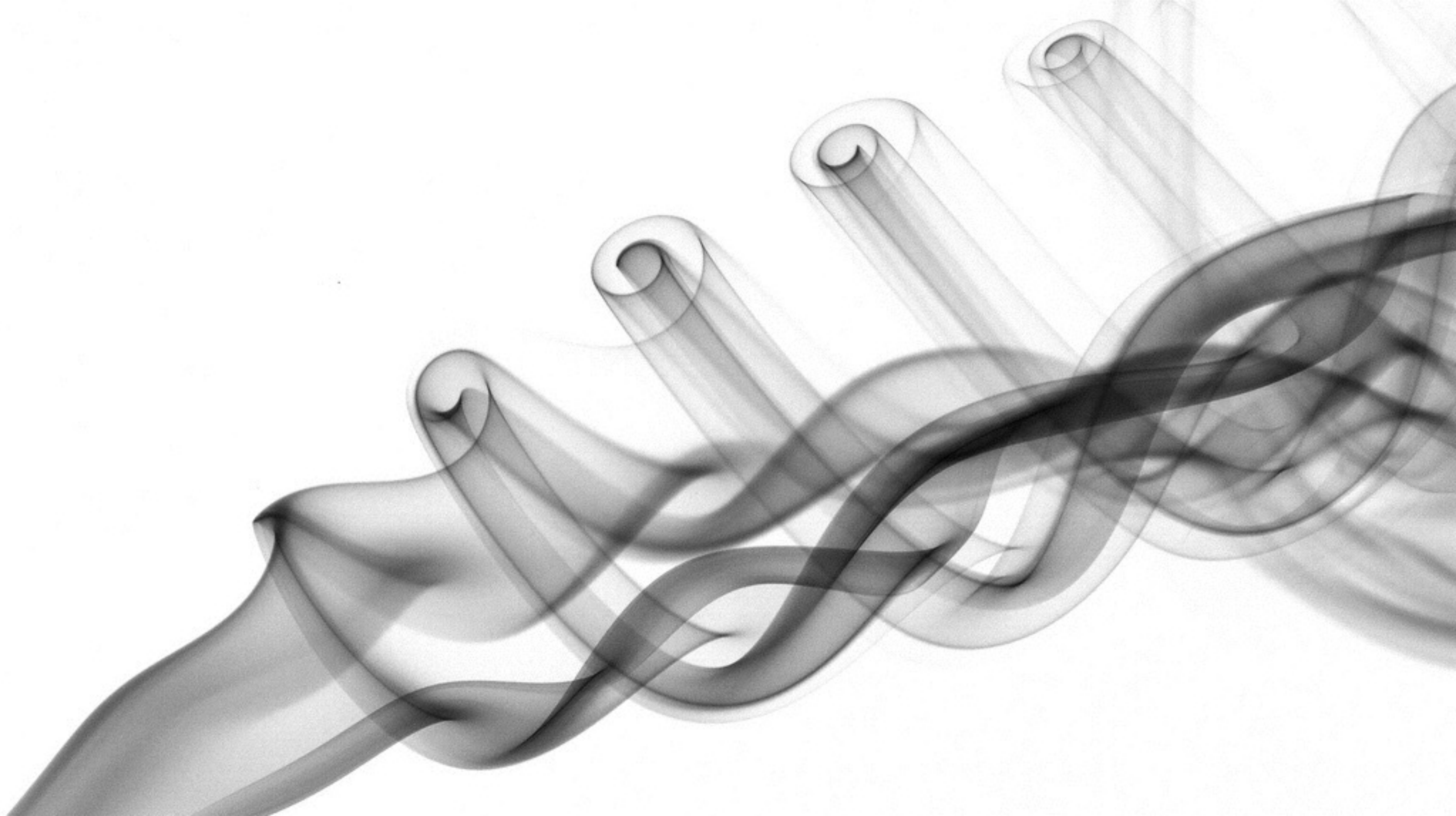
Vorticity

Vorticity $\omega = \nabla \times \mathbf{u}$

originates in boundary layers and shear layers.

Vorticity concentrates in 2D vortex sheets.

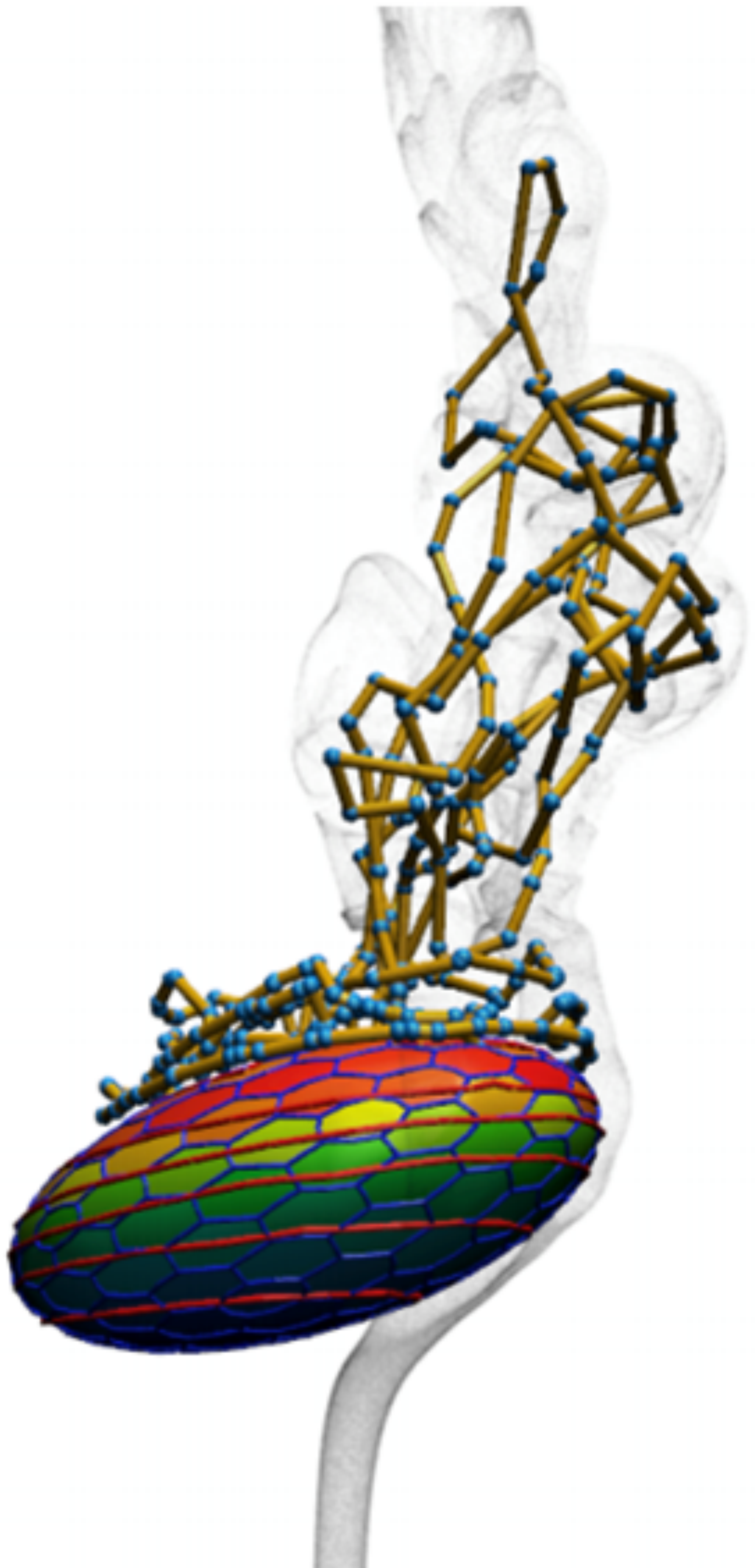
Sheets roll up into filaments



Capturing Vorticity

Most interesting flows are dominated by **thin vortices**.

Capturing vorticity



Vorticity based

[Elcott et al. 2007] [Zhang et al. 2015] …

Lagrangian

[Rosenhead 1931] [Leonard 1980]

[Cottet and Koumoutsakos 2000]

[Park and Kim 2005] [Angelidis and Neyret 2005]

[Stock et al. 2008] [Weißmann and Pinkall 2010]

[Brochu et al. 2012] …

Hybrid

[Selle et al. 2005] [Koumoutsakos et al. 2008] [Kim et al. 2009]

[Pfaff et al. 2012] [Jiang et al. 2015] …

Our approach

- Simple algorithm.
- On a modestly sized grid

  (e.g. 64 x 64 x 64)
- Captures thin vortex dynamics.
- *No advection* is needed.

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

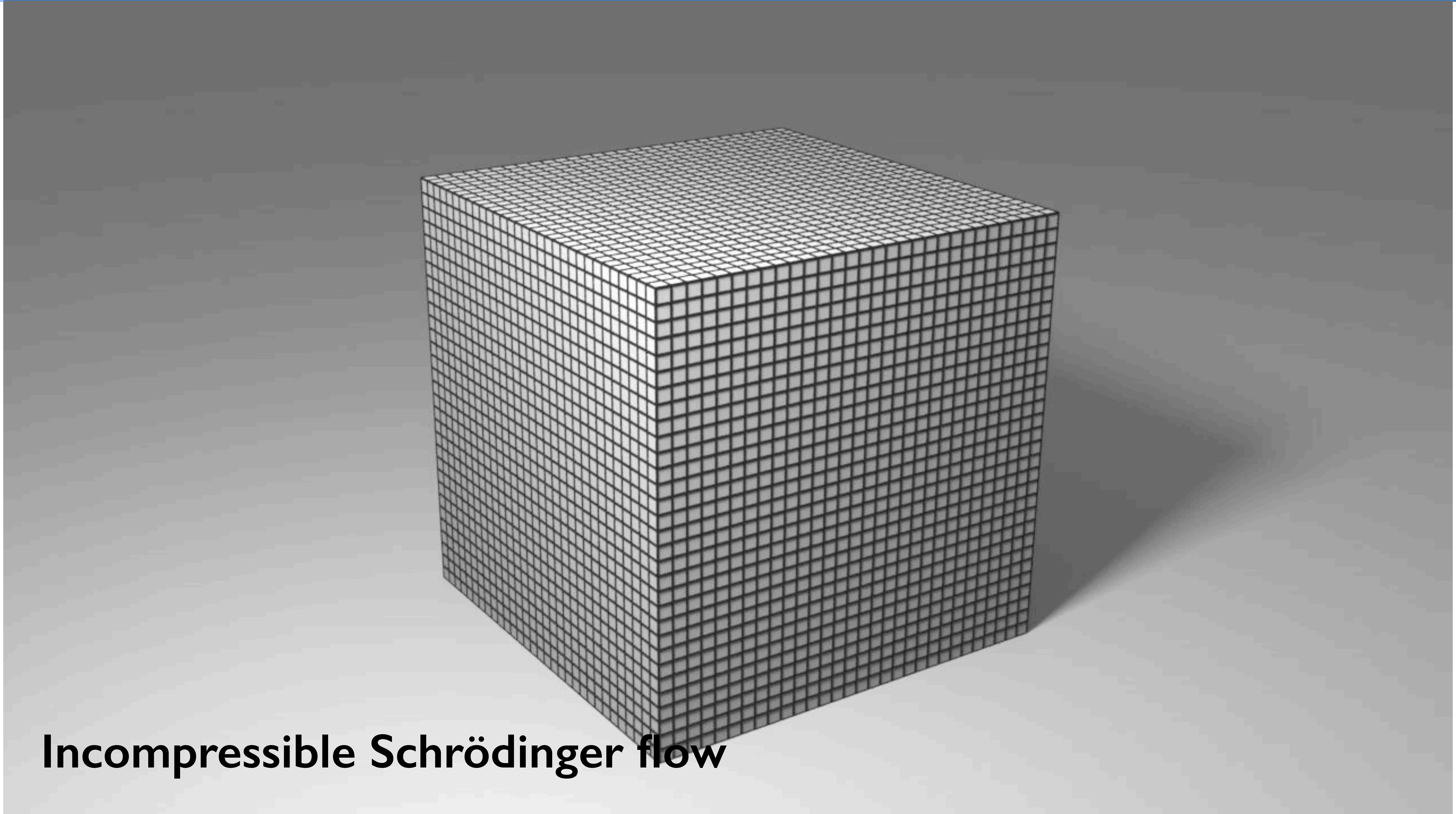
$$\nabla \times (\mathbf{u} \times \omega)$$

$$\mathcal{L}_{\mathbf{u}} \mathbf{u}^{\flat}$$

$$\mathbf{u} \times \omega$$

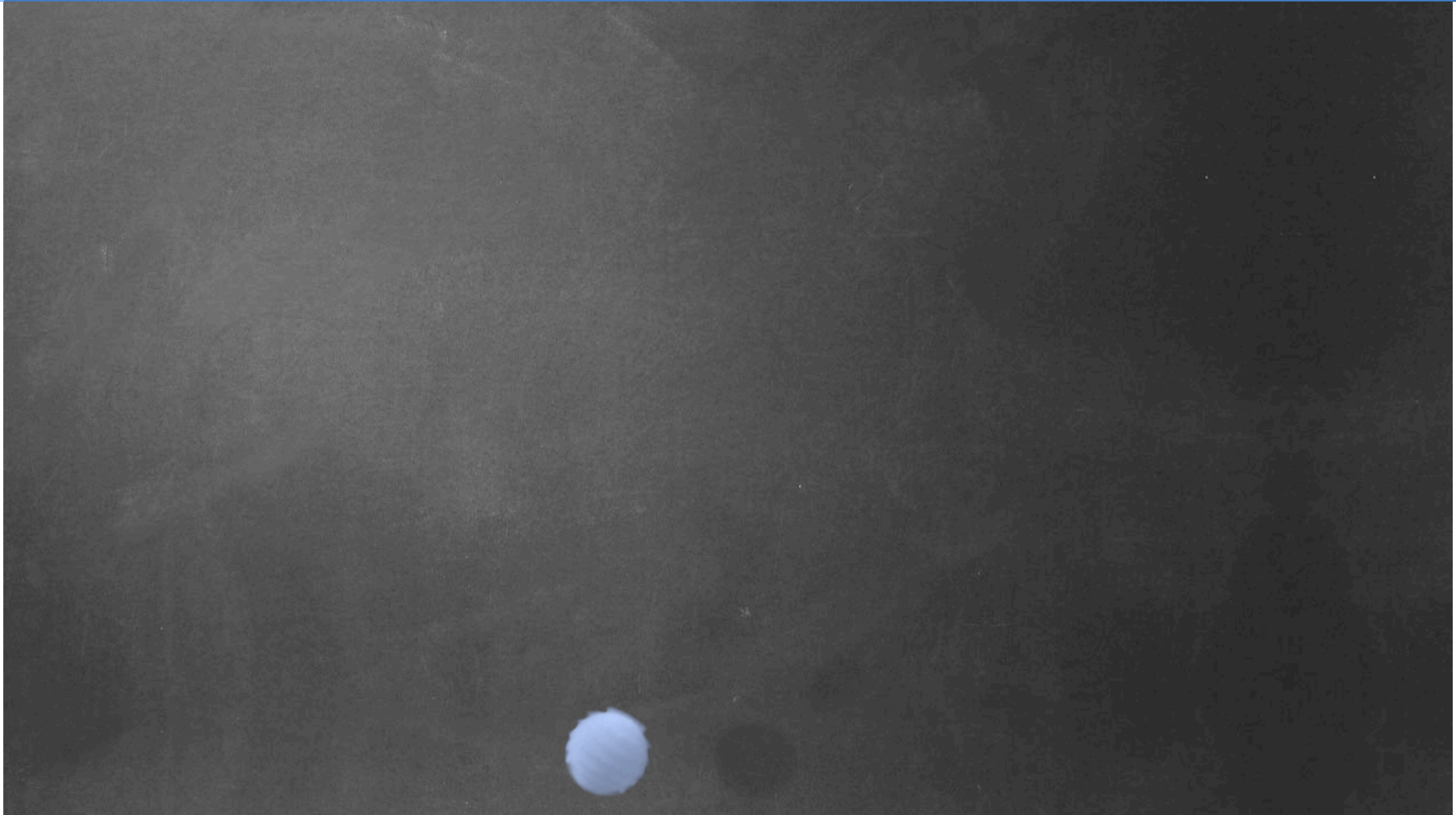
$$\mathbf{u} \cdot \nabla \omega - \omega \cdot \nabla \mathbf{u}$$

Use 2 complex-valued functions



Incompressible Schrödinger flow

Velocity inferred from complex functions



Schrödinger equation

Schrödinger equation?

Schrödinger equation (1925)

Wave-function $\varphi : M \to \mathbb{C}$

Planck constant

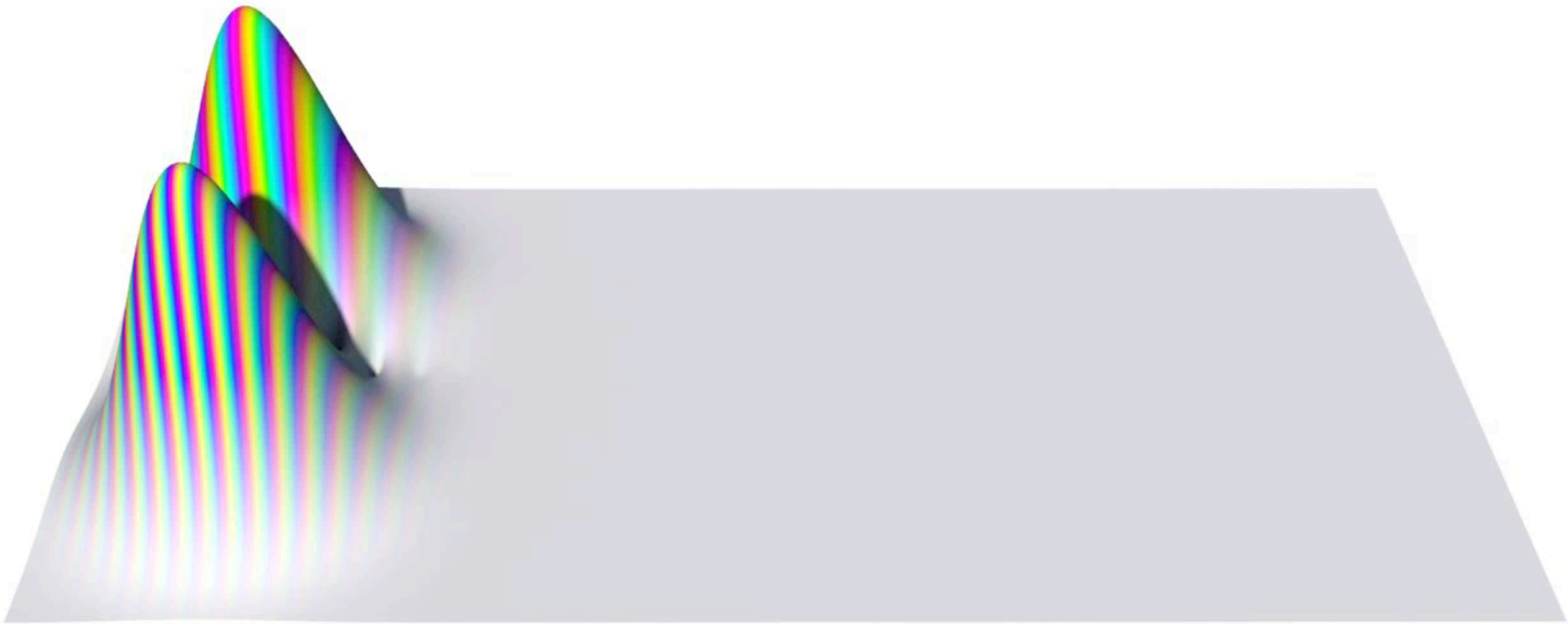
$$\frac{\partial}{\partial t}\varphi = \boxed{\mathbf{i}}\frac{\boxed{\hbar}}{2}\Delta\varphi$$

$\sqrt{-1}$

Schrödinger equation (1925)

$$\varphi = r e^{\mathbf{i}\theta}$$

Wave speed (group velocity) $= \hbar \nabla \theta$



Madelung transform (1926)

$$\rho := |\varphi|^2$$

$$\mathbf{u} := \hbar \nabla \theta$$

$$\frac{\partial}{\partial t}\varphi = \mathbf{i}\,\frac{\hbar}{2}\Delta\varphi$$

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

$$\frac{\partial}{\partial t}\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla Q$$

$$Q(\rho) = \frac{\hbar^2}{2}\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}$$

(Compressible) quantum Euler equation

Hydrodynamics interpretation of Q.M.

Quantentheorie in hydrodynamischer Form.

Von **E. Madelung** in Frankfurt a. M.

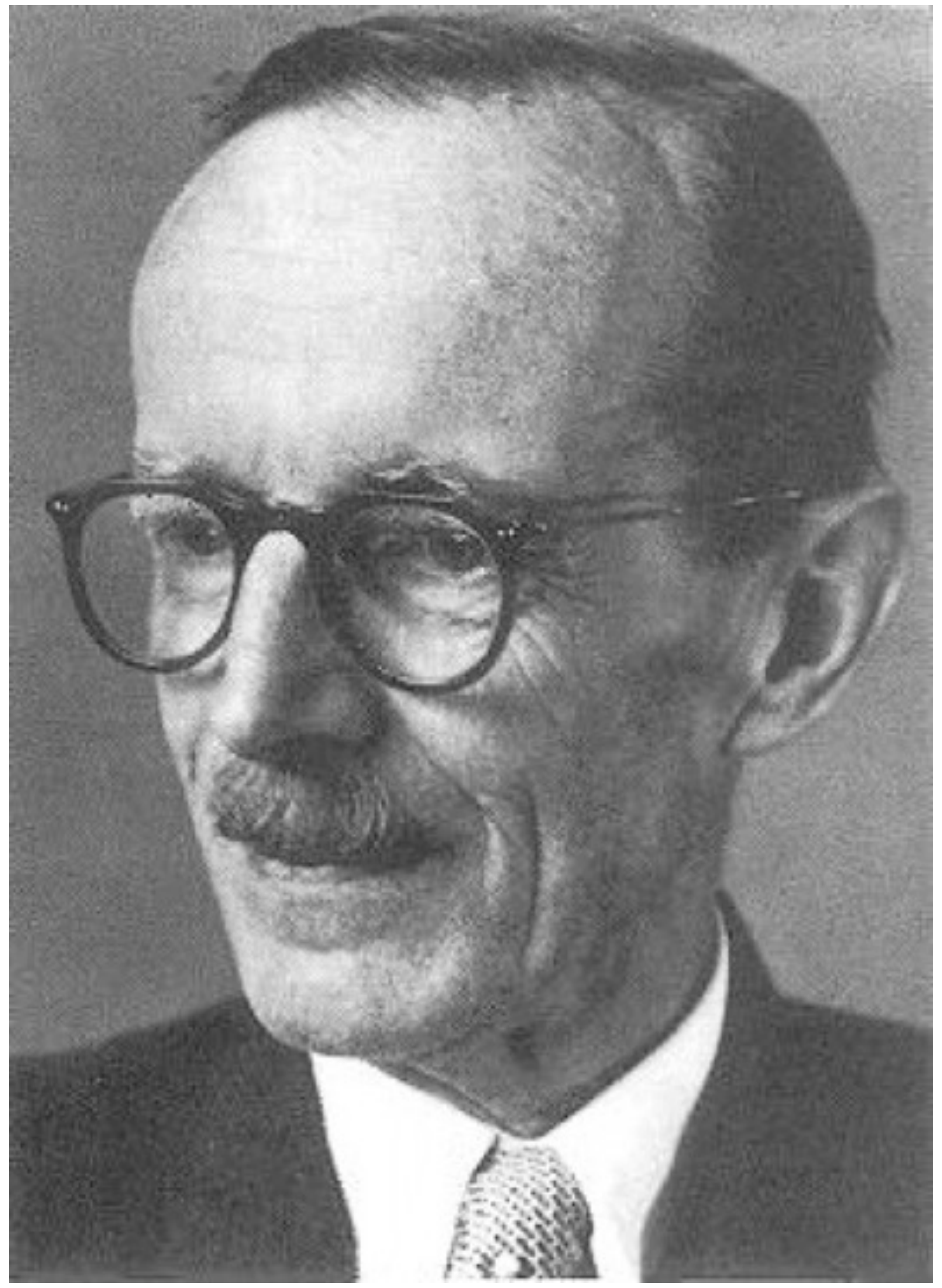
(Eingegangen am 25. Oktober 1926.)

Es wird gezeigt, daß man die Schrödingersche Gleichung des Einelektronenproblems in die Form der hydrodynamischen Gleichungen transformieren kann.

Nach E. Schrödinger[1]) wird die Quantentheorie des Einelektronenproblems beherrscht von der „Amplitudengleichung“:

$$\varDelta \psi_0 + \frac{8\pi^2 m}{h^2}(W - U)\psi_0 = 0, \qquad \psi = \psi_0 e^{i 2\pi \frac{W}{h} t}. \qquad (1)$$

Hierin bedeutet W die Energie des Systems, U die potentielle Energie als Funktion des Ortes des Elektrons, m dessen Masse. Man suche eine Lösung, die überall endlich und stetig ist. Das ist nur für gewisse Werte von W möglich. Diese „Eigenwerte“ W_i sollen dann die Energien sein, die das System in seinen „Quantenzuständen“ besitzt. Sie sind bekanntlich spektroskopisch festzustellen. Der Vergleich zwischen Theorie und Erfahrung spricht durchaus für die Brauchbarkeit der hiermit festgelegten Rechenmethode.



Erwin Madelung

[Madelung 1926]
[Madelung 1927]

Simulate fluid via Schrödinger equation

- Schrödinger equation corresponds to a *compressible* fluid…

- The velocity is a gradient $\mathbf{u} := \hbar\nabla\theta$

no vorticity…

2-component wave-function

Multicomponent Schrödinger system (physics: spin-$\frac{n-1}{2}$ particles)

$$\psi = \begin{bmatrix} \varphi_1 \\ \varphi_2 \end{bmatrix} : M \to \mathbb{C}^2, \qquad \frac{\partial}{\partial t}\psi = \mathbf{i}\,\frac{\hbar}{2}\Delta\psi$$

2-component wave-function

Madelung transform for $\psi = \begin{bmatrix} \varphi_1 \\ \varphi_2 \end{bmatrix}$ is given by

[Schönberg 1954]
[Sorokin 2001]

$$\rho = |\psi|^2 \qquad = \rho_1 + \rho_2$$

$$\rho\mathbf{u} = \hbar \boxed{\langle \nabla\psi, \mathbf{i}\psi \rangle_{\mathbb{R}}} = \rho_1\mathbf{u}_1 + \rho_2\mathbf{u}_2$$

non-trivial **vorticity** and **helicity**

$\langle .,. \rangle_{\mathbb{R}}$ — inner product for $\mathbb{C}^2 \cong \mathbb{R}^4$

Simulate fluid via Schrödinger equation

- Schrödinger equation corresponds to a *compressible* fluid…

- The velocity is a gradient $\mathbf{u} := \hbar \nabla \theta$

  no vorticity…

Incompressible constraints

$$\rho = 1$$
$$\nabla \cdot \mathbf{u} = 0$$

$$|\psi|^2 = 1$$
$$\langle \Delta\psi, \mathbf{i}\psi \rangle_{\mathbb{R}} = 0$$

Classical pressure projection

Given any vector field $\tilde{\mathbf{u}}$

$$\downarrow$$

$$\mathbf{u} = \tilde{\mathbf{u}} - \nabla q$$ is divergence-free.

The scalar function q is found by a Poisson equation:

$$\Delta q = \nabla \cdot \tilde{\mathbf{u}}$$

For wave-functions

$$
\begin{tikzcd}
\tilde{\psi} \arrow[r, bend left] \arrow[d, mapsto, "\text{phase shift}"'] & \tilde{\mathbf{u}} \\
\psi = e^{-\mathbf{i}q}\,\tilde{\psi} \arrow[r, bend left] & \mathbf{u} = \tilde{\mathbf{u}} - \hbar \nabla q
\end{tikzcd}
$$

Pressure projection

Given any vector field $\widetilde{\mathbf{u}}$

$$\downarrow$$

$$\mathbf{u} = \widetilde{\mathbf{u}} - \nabla q$$ is divergence-free.

The scalar function q is found by a Poisson equation:

$$\Delta q = \nabla \cdot \widetilde{\mathbf{u}}$$

Pressure projection

Given any wave func. $\tilde{\psi}$

$$\downarrow$$

$$\psi = e^{-\mathbf{i}q}\,\tilde{\psi}$$ is divergence-free.

$$\langle \Delta\psi, \mathbf{i}\psi\rangle_{\mathbb{R}} = 0$$

The scalar function q is found by a Poisson equation:

$$\Delta q = \frac{1}{\hbar}\nabla\cdot\tilde{\mathbf{u}}$$

To impose incompressible constraint

$$\frac{\partial}{\partial t}\psi = \mathbf{i}\,\frac{\hbar}{2}\Delta\psi - \mathbf{i}\,p\psi$$

$$\langle \Delta\psi, \mathbf{i}\psi \rangle_{\mathbb{R}} = 0$$

Incompressible Schrödinger equation

Incompressible Schrödinger flow (**ISF**)

$$\begin{cases} \frac{\partial}{\partial t}\psi = \mathbf{i}\,\frac{\hbar}{2}\Delta\psi - \mathbf{i}\,p\psi \\ \langle \Delta\psi, \mathbf{i}\psi\rangle_{\mathbb{R}} = 0 \end{cases}$$

Note that $|\psi|^2 = 1$ at all time.

Time splitting

$$\begin{cases} \frac{\partial}{\partial t}\psi = \mathbf{i}\,\frac{\hbar}{2}\Delta\psi - \mathbf{i}\,p\psi \\ \langle \Delta\psi, \mathbf{i}\psi\rangle_{\mathbb{R}} = 0 \end{cases}$$

Time splitting

$$\begin{cases} \frac{\partial}{\partial t}\psi = \mathbf{i}\,\frac{\hbar}{2}\Delta\psi - \mathbf{i}\,p\psi \\ \langle \Delta\psi, \mathbf{i}\psi\rangle_{\mathbb{R}} = 0 \end{cases}$$

① Linear Schrödinger equation

(on a regular grid, use FFT)

Time splitting

$$\begin{cases} \frac{\partial}{\partial t}\psi = \mathbf{i}\,\frac{\hbar}{2}\Delta\psi - \mathbf{i}\,p\psi \\ \langle \Delta\psi, \mathbf{i}\psi \rangle_{\mathbb{R}} = 0 \end{cases}$$

② Pressure projection

(on a regular grid, use FFT)

Algorithm

Algorithm 1 Basic ISF

Input: $\psi^{(0)}, dt, \hbar$ ▷ Initial state and parameters

1: **for** $j \leftarrow 0, 1, 2, \ldots$ **do**

2: $\quad \psi^{\text{tmp}} \leftarrow \textsc{Schrödinger}(\psi^{(j)}, dt, \hbar)$

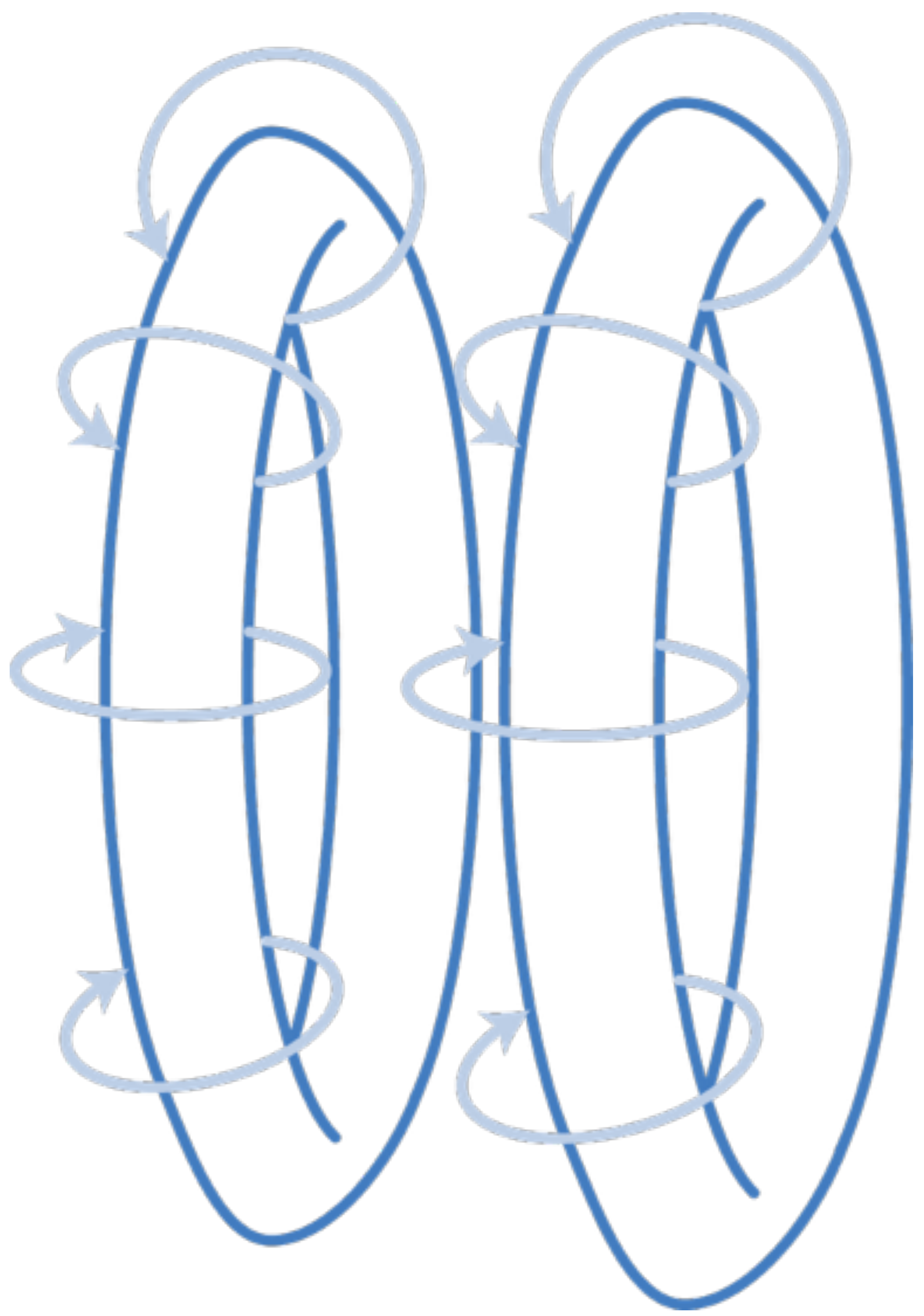
3: $\quad \psi^{\text{tmp}} \leftarrow \psi^{\text{tmp}} / |\psi^{\text{tmp}}|$ ▷ Normalization

4: $\quad \psi^{(j+1)} \leftarrow \textsc{PressureProject}(\psi^{\text{tmp}})$

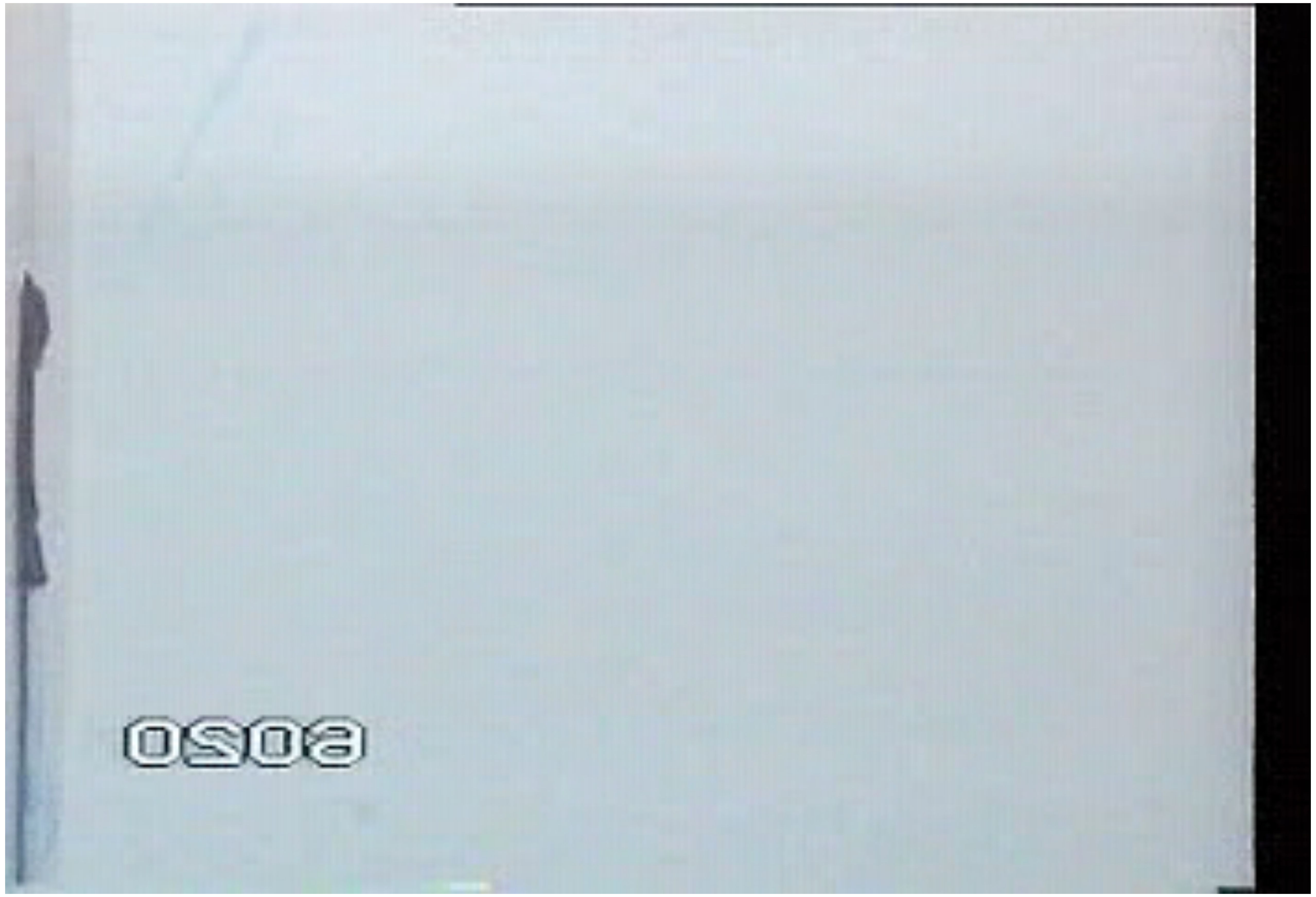
5: **end for**

- Simple to implement
- Efficient
- Unconditionally stable

Leapfrogging Vortex Rings



Leapfrogging Vortex Rings



Video courtesy T.T. Lim

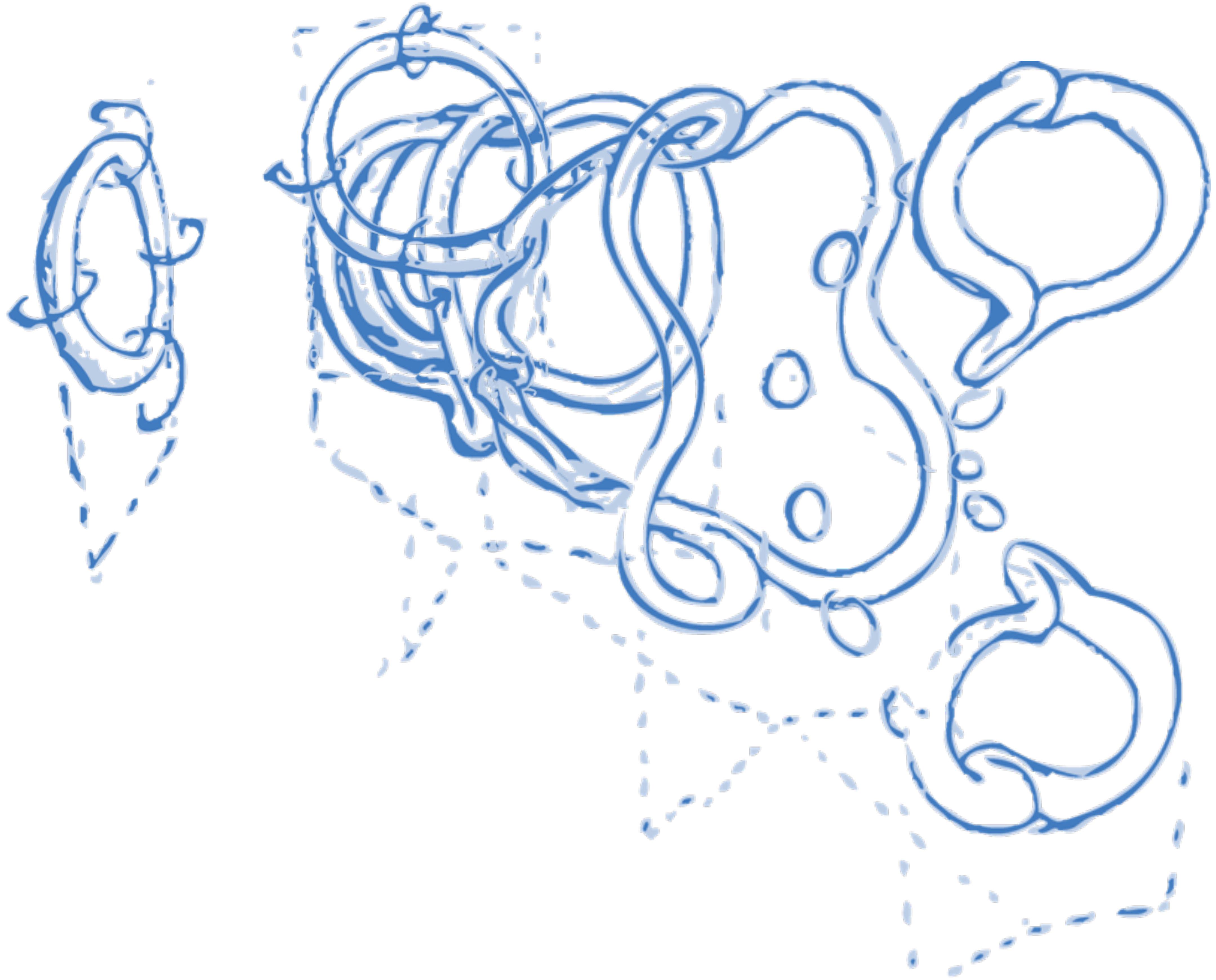
Leapfrogging Vortex Rings

HJWENO/MacCormack

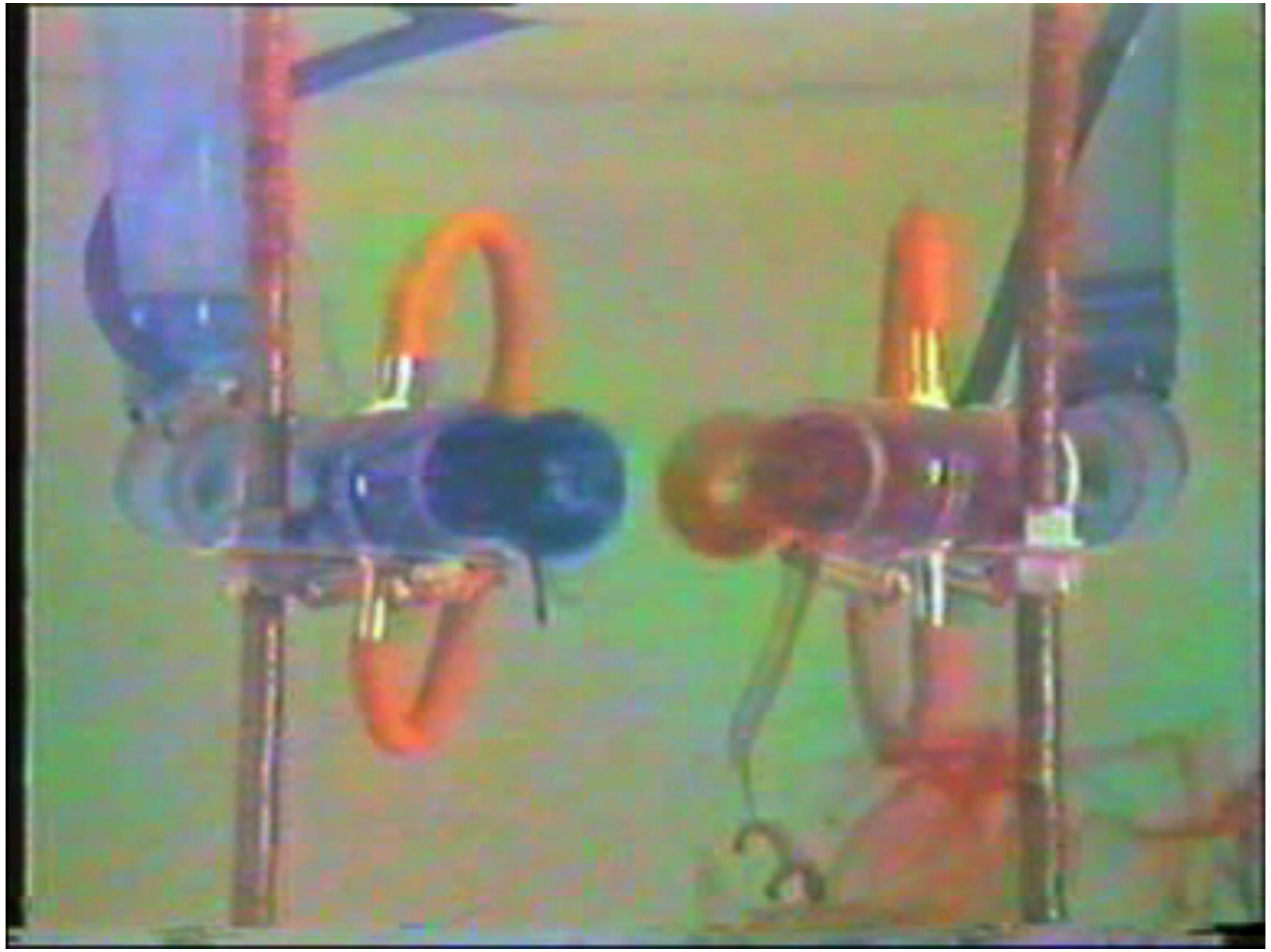
Incompressible Schrödinger Flow

Grid size: 64x64x128

Vortex Reconnection



Vortex Reconnection



Video courtesy T.T. Lim

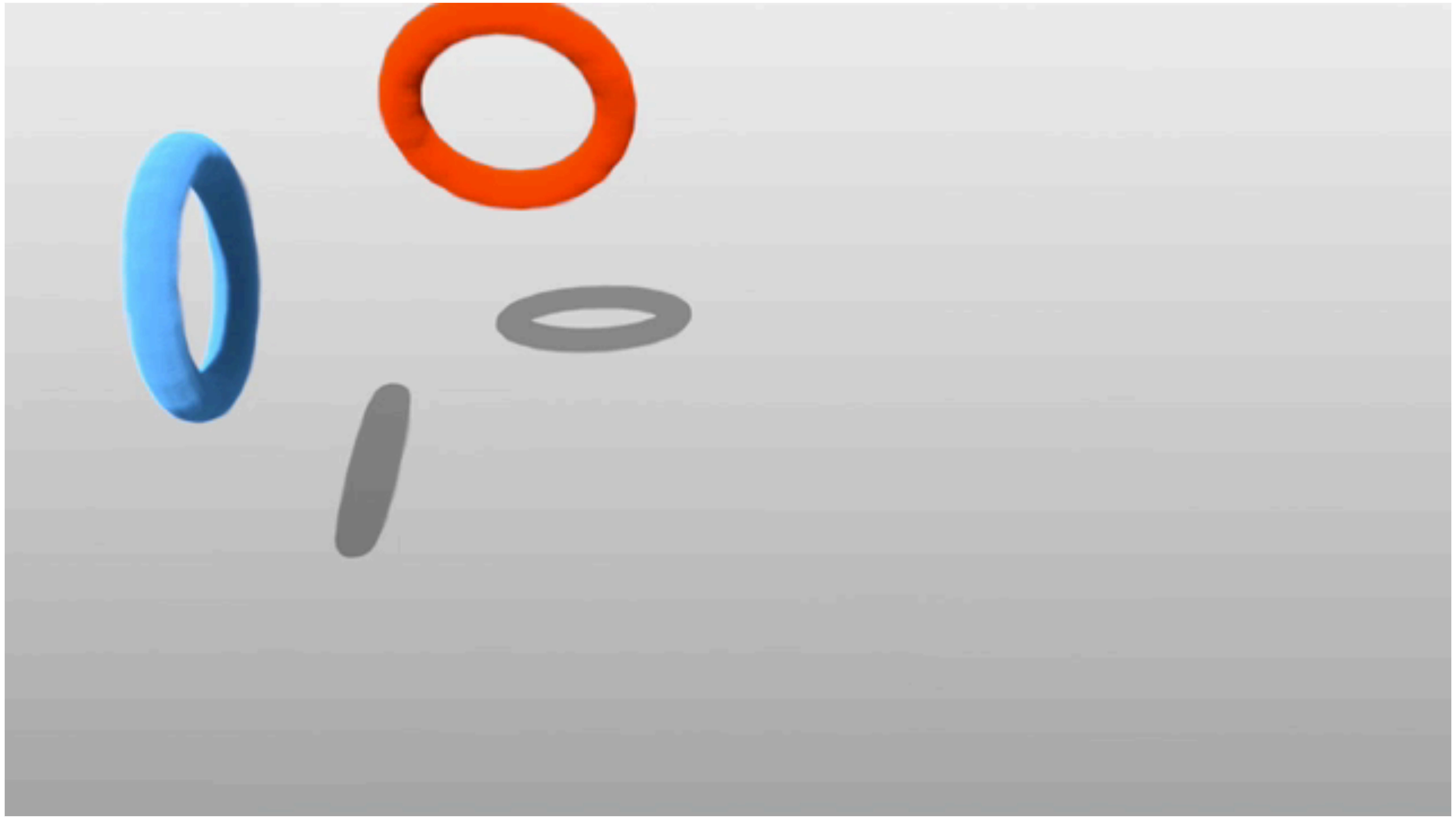
Vortex Reconnection

Euler's Equation, HJWENO/MacCormack scheme

Grid size: 64x64x64

Vortex Reconnection

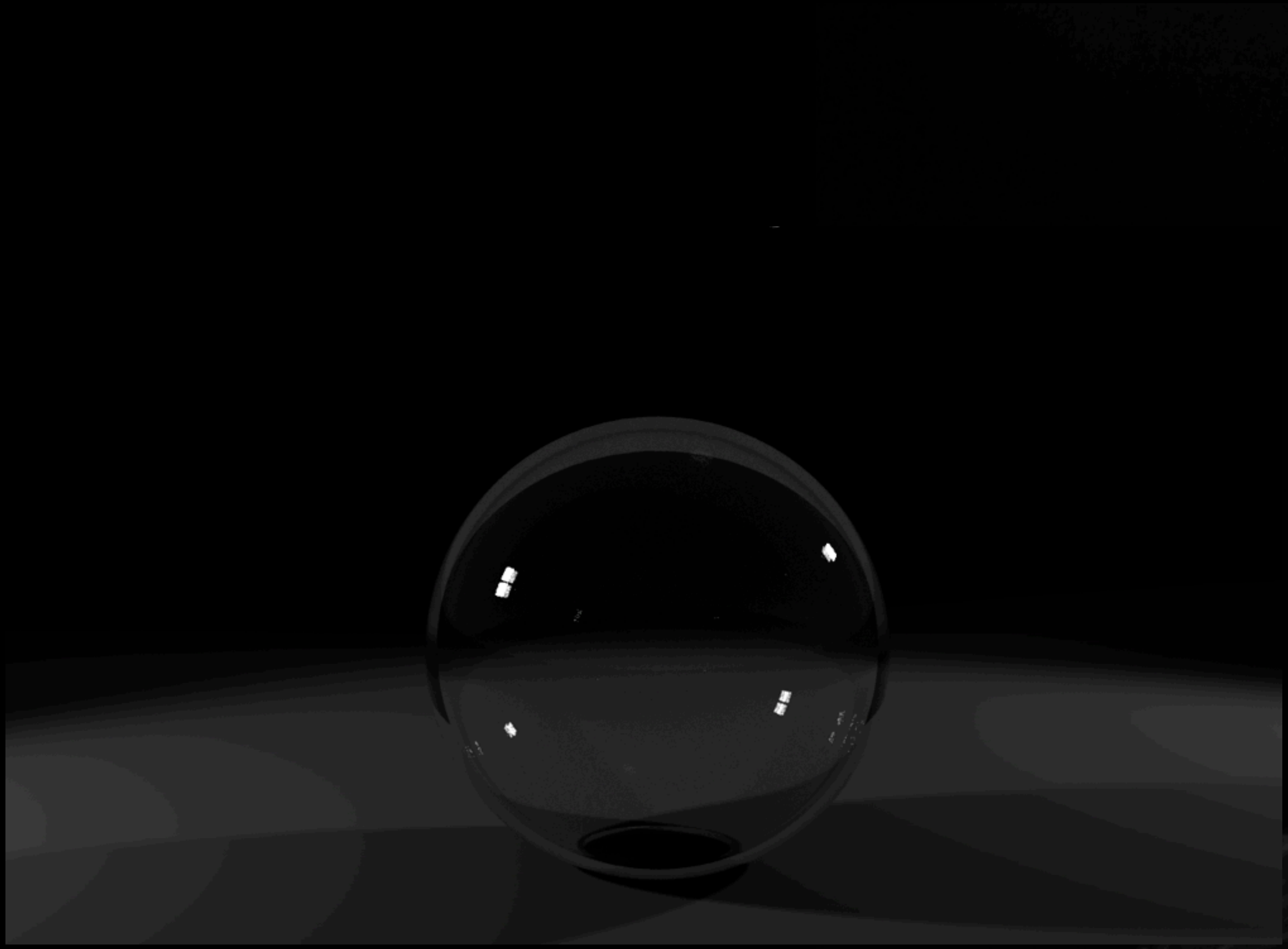
Incompressible Schrödinger Equation



Grid size: 64x64x64

Jet

Dry ice vapor



simulation

experiment footage

How does it work?

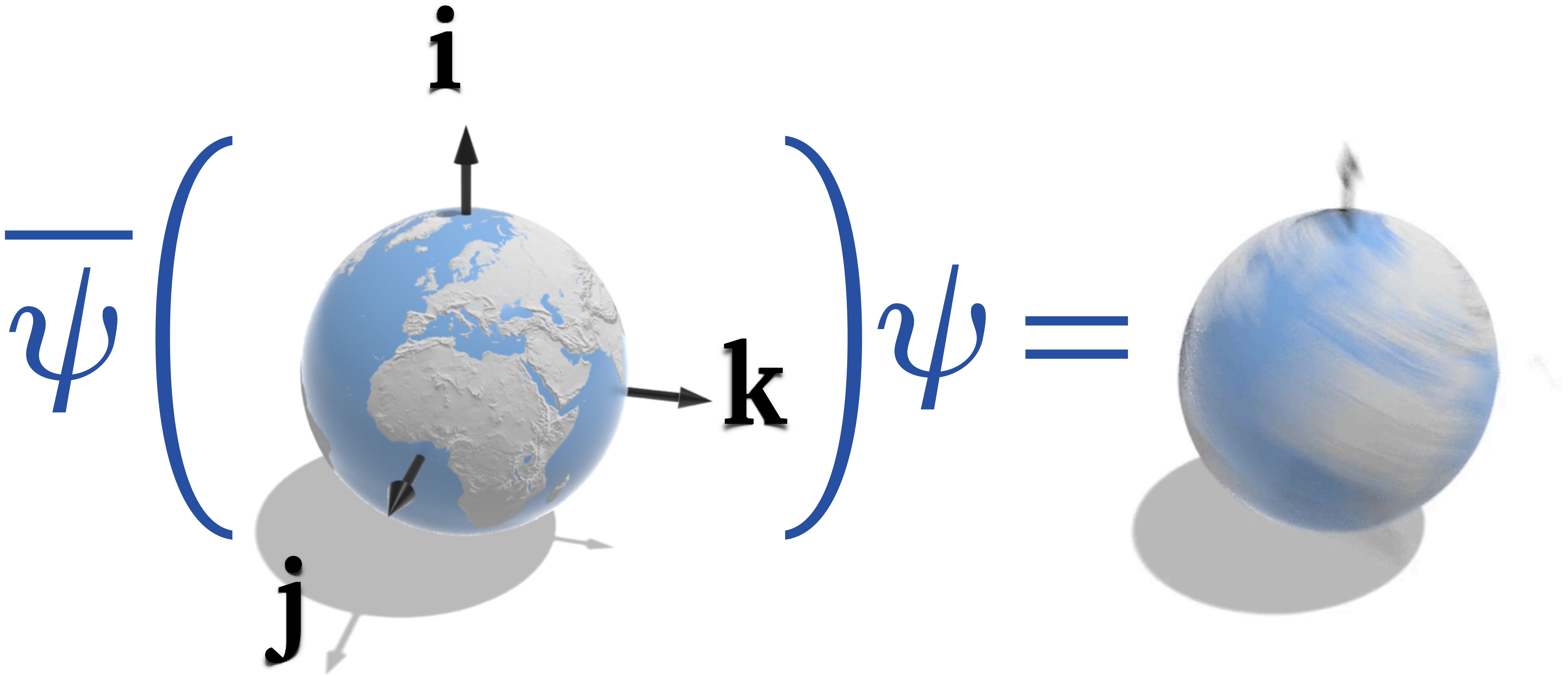
Geometric picture of ISF

$\mathbb{C}^2$-values of our wave-function can be viewed as **unit quaternions**

$$\psi = \begin{bmatrix} a + b\mathbf{i} \\ c + d\mathbf{i} \end{bmatrix} \quad \longleftrightarrow \quad a + b\mathbf{i} + c\mathbf{j} + d\mathbf{k}$$

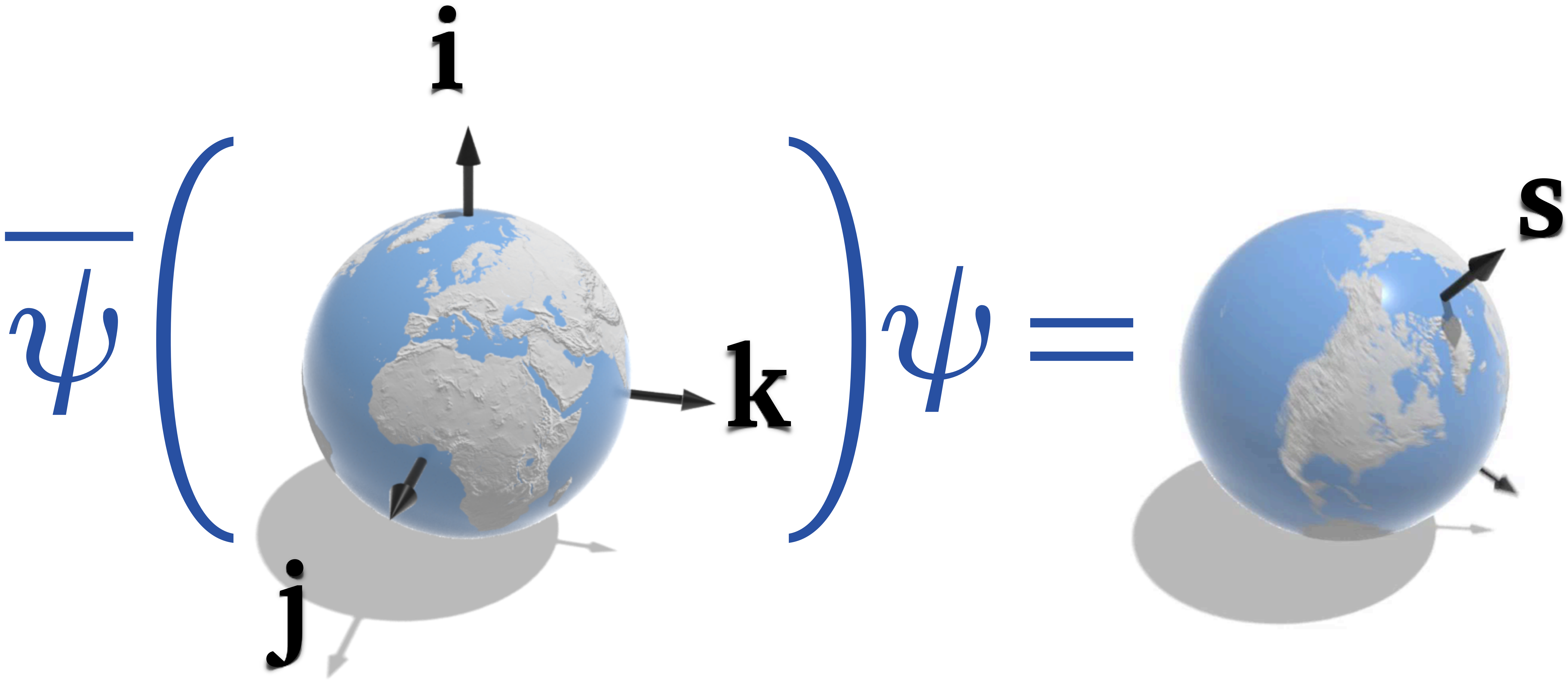
which represent **3D rotations**.

Geometric picture of ISF



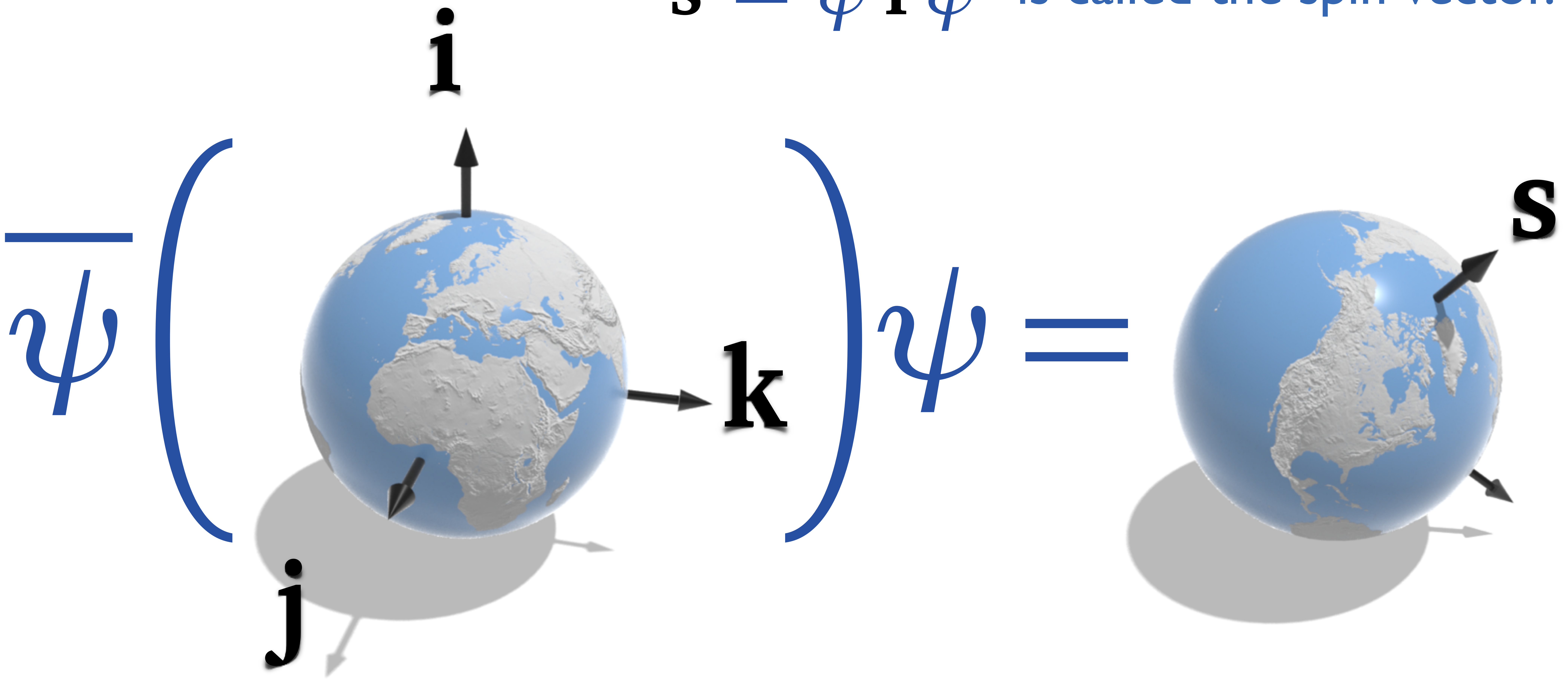
Phase change

$$\psi \mapsto e^{-\mathbf{i}q}\psi$$



Spin vector

$\mathbf{s} = \overline{\psi}\,\mathbf{i}\,\psi$ is called the spin vector.

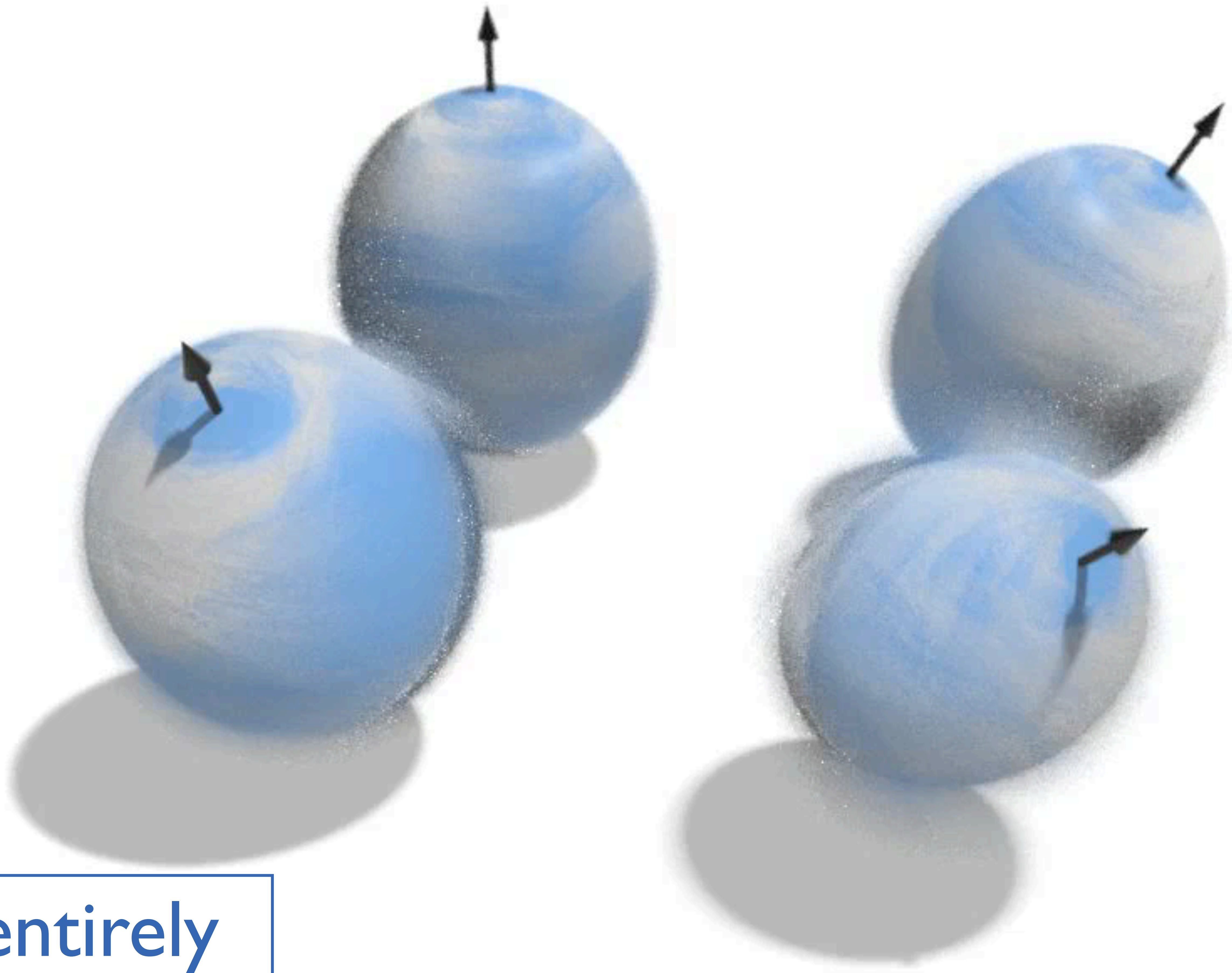


Pressure projection

Recall pressure projection applies a phase change

$$\psi = e^{-\mathbf{i}q}\widetilde{\psi}$$

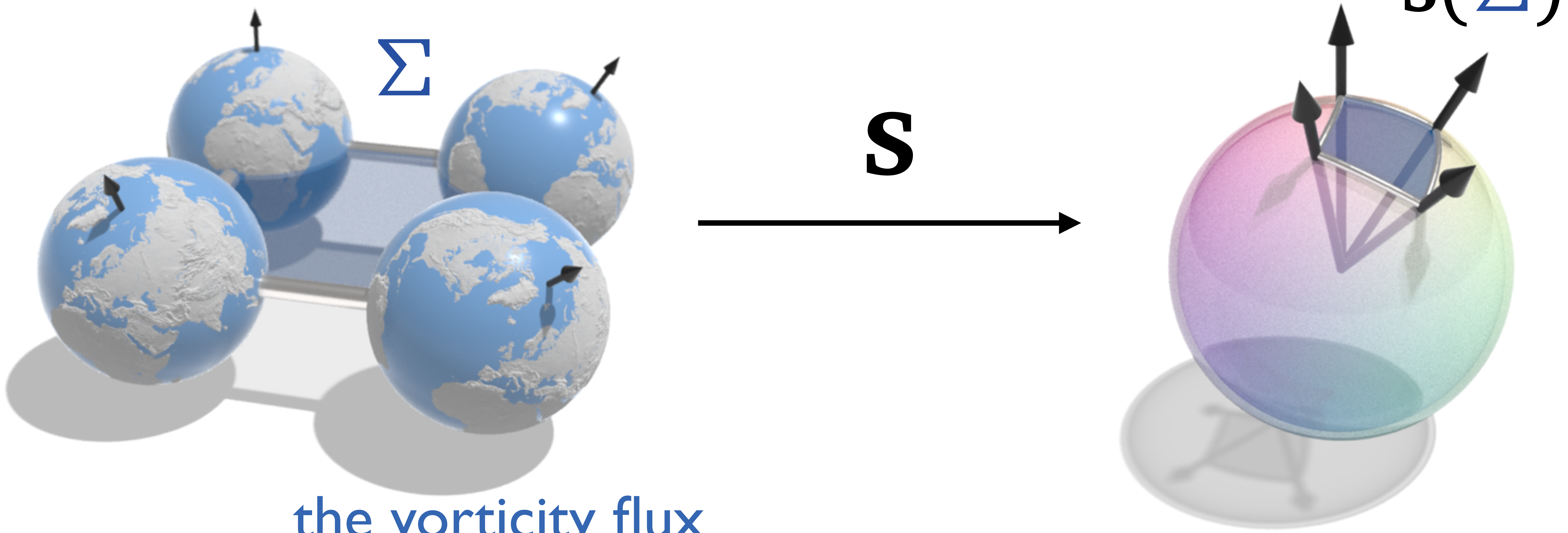
to the wave-function.



The fluid state is described entirely by the spin vector $\boldsymbol{s}$.

Spin vector and vorticity

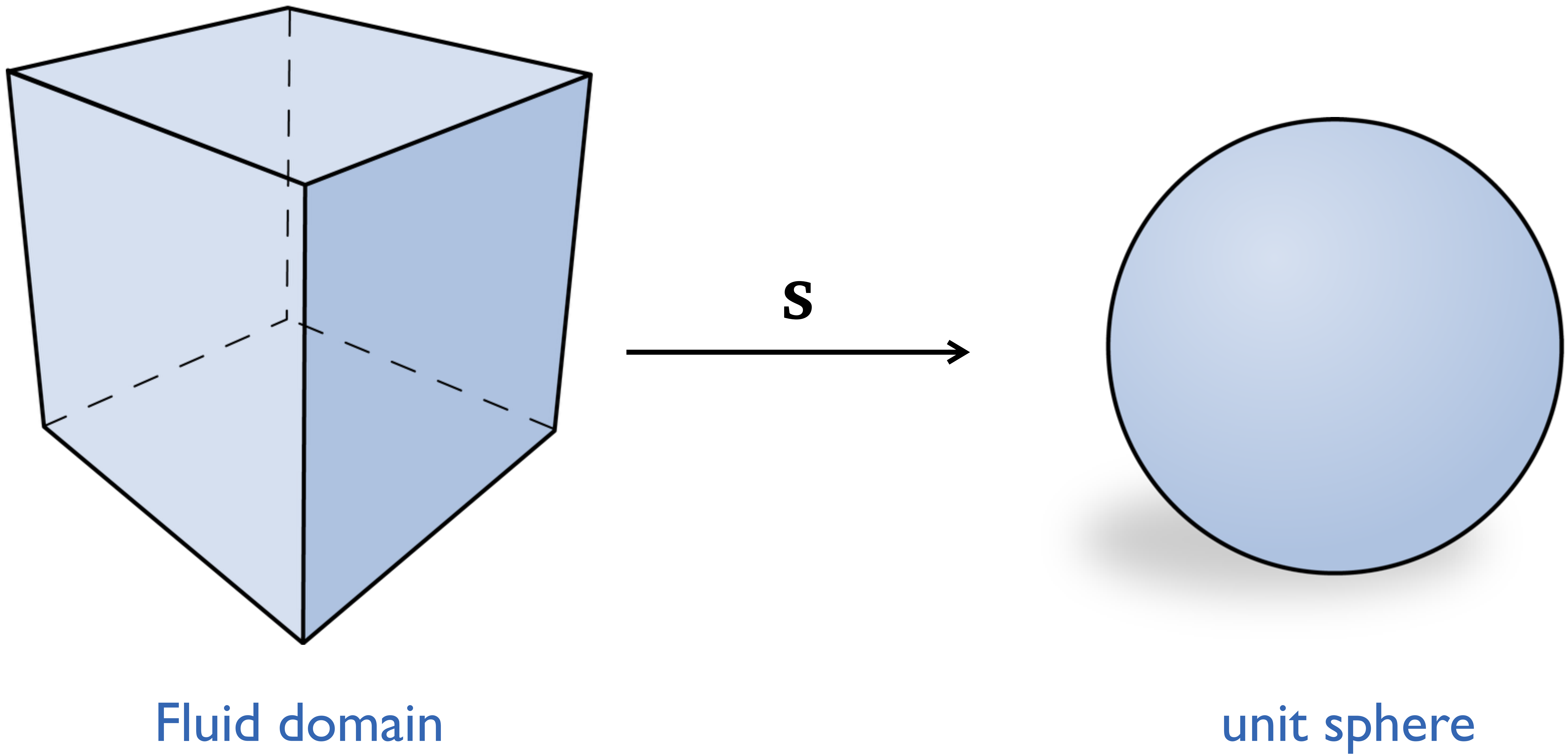
For any oriented surface $\Sigma \subset$ fluid domain,



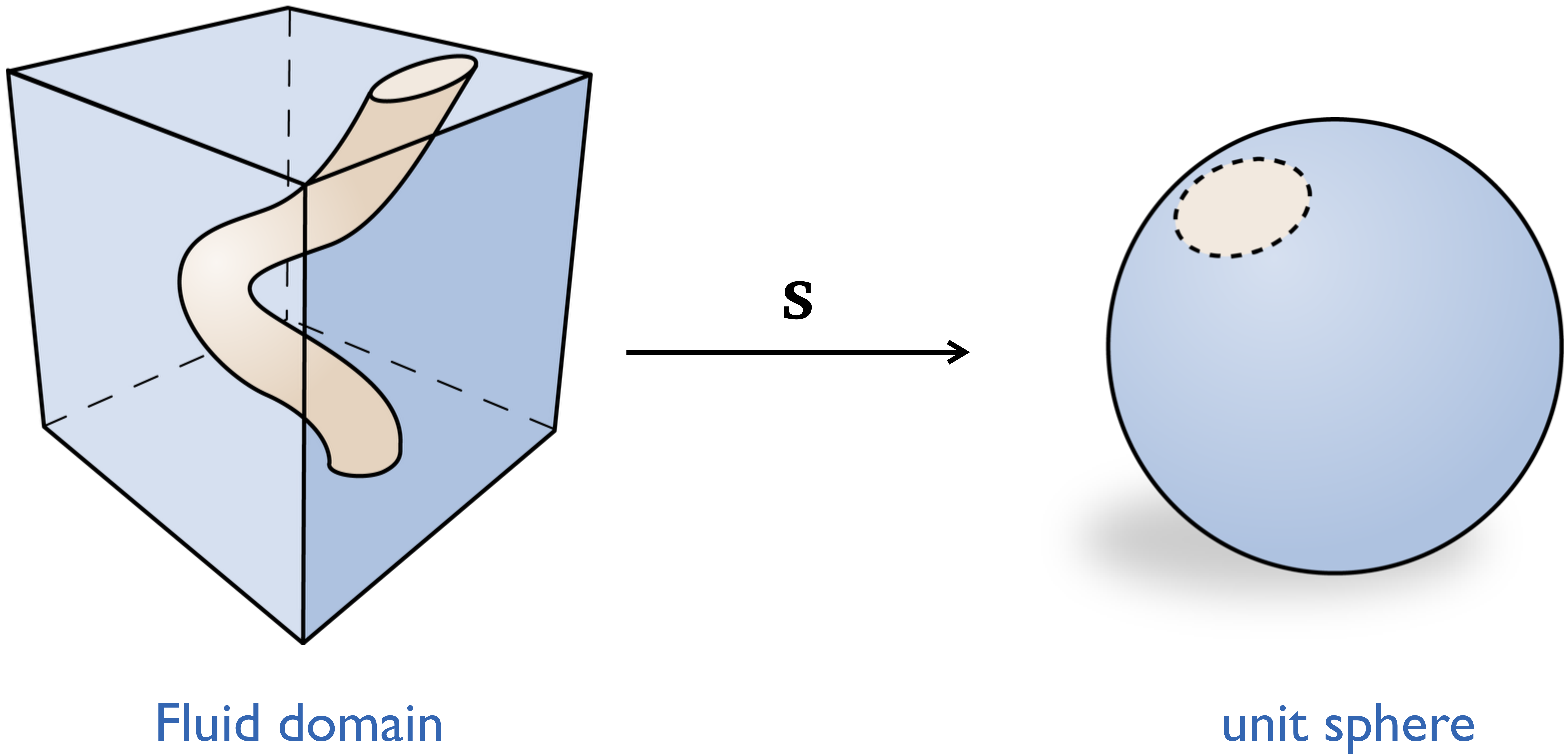
the vorticity flux

$$\boxed{\iint_\Sigma \omega \cdot \mathbf{n}\, dA = \frac{\hbar}{2} \operatorname{Area}\left[\mathbf{s}(\Sigma)\right]}$$

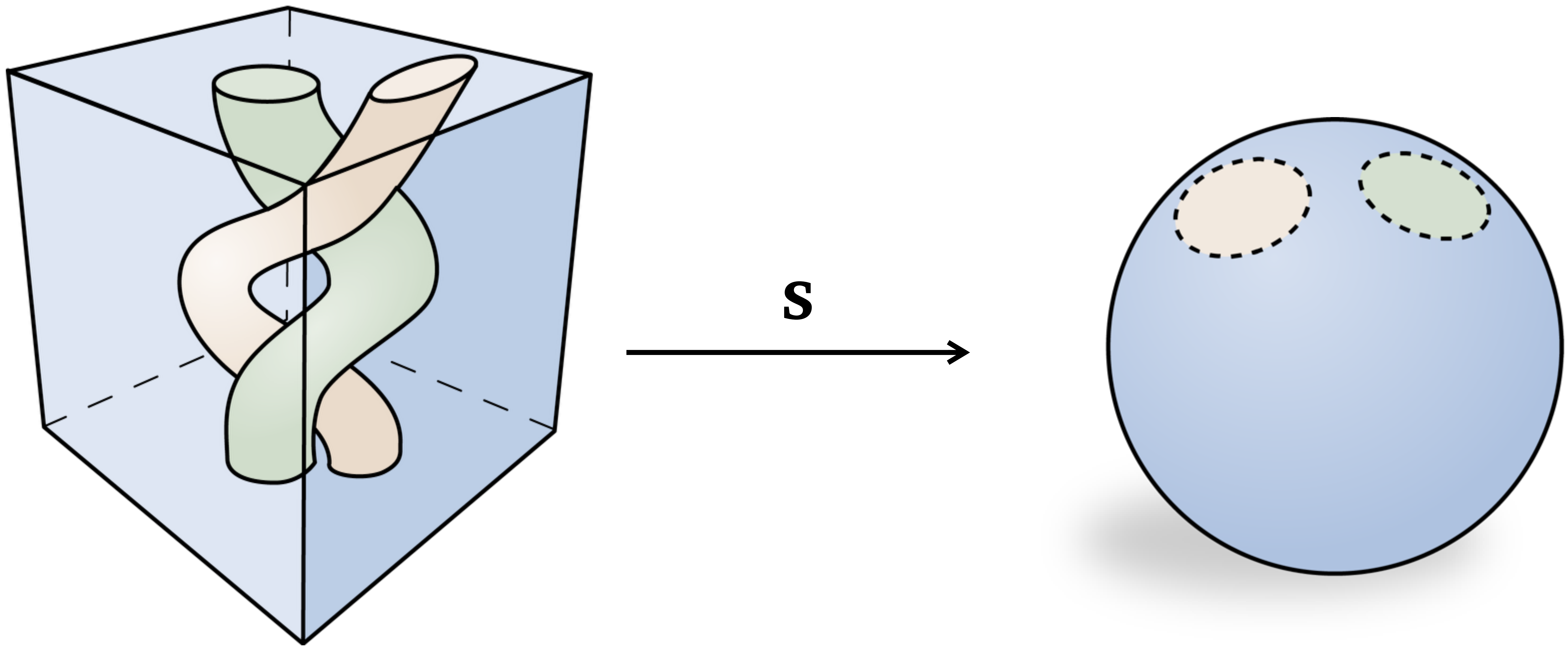
Vortex tube visualization



Vortex tube visualization



Vortex tube visualization

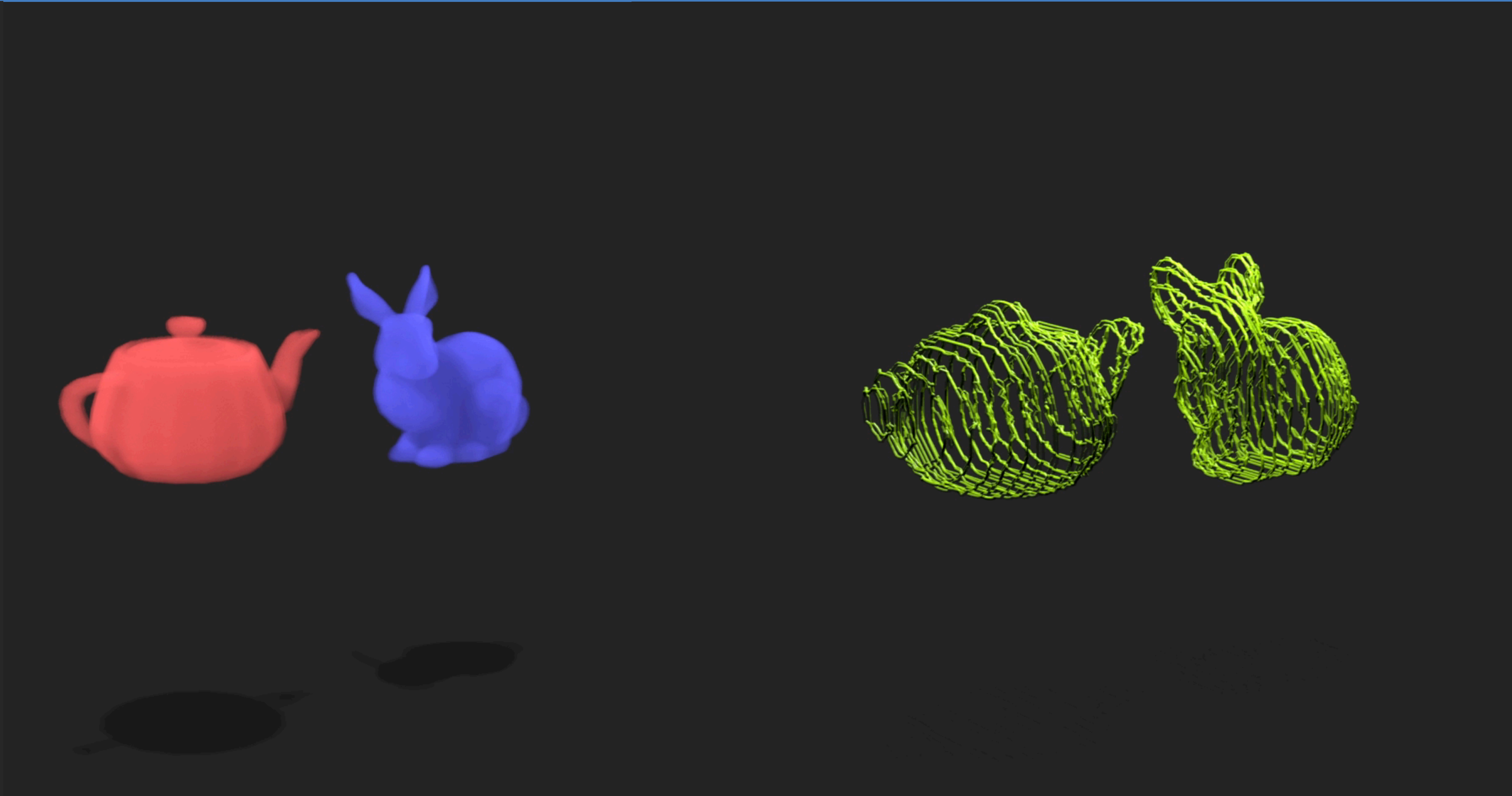


Fluid domain

unit sphere

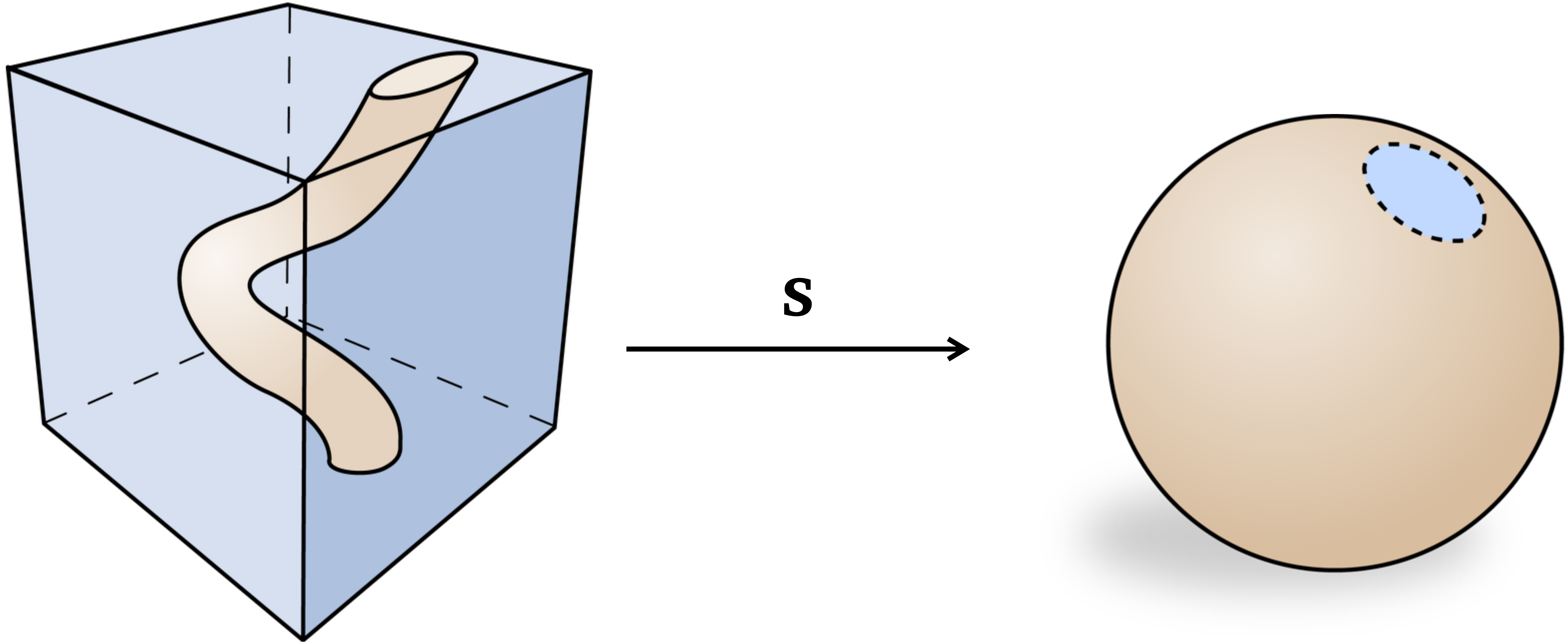
Vortex tube visualization

Vortex tube visualization

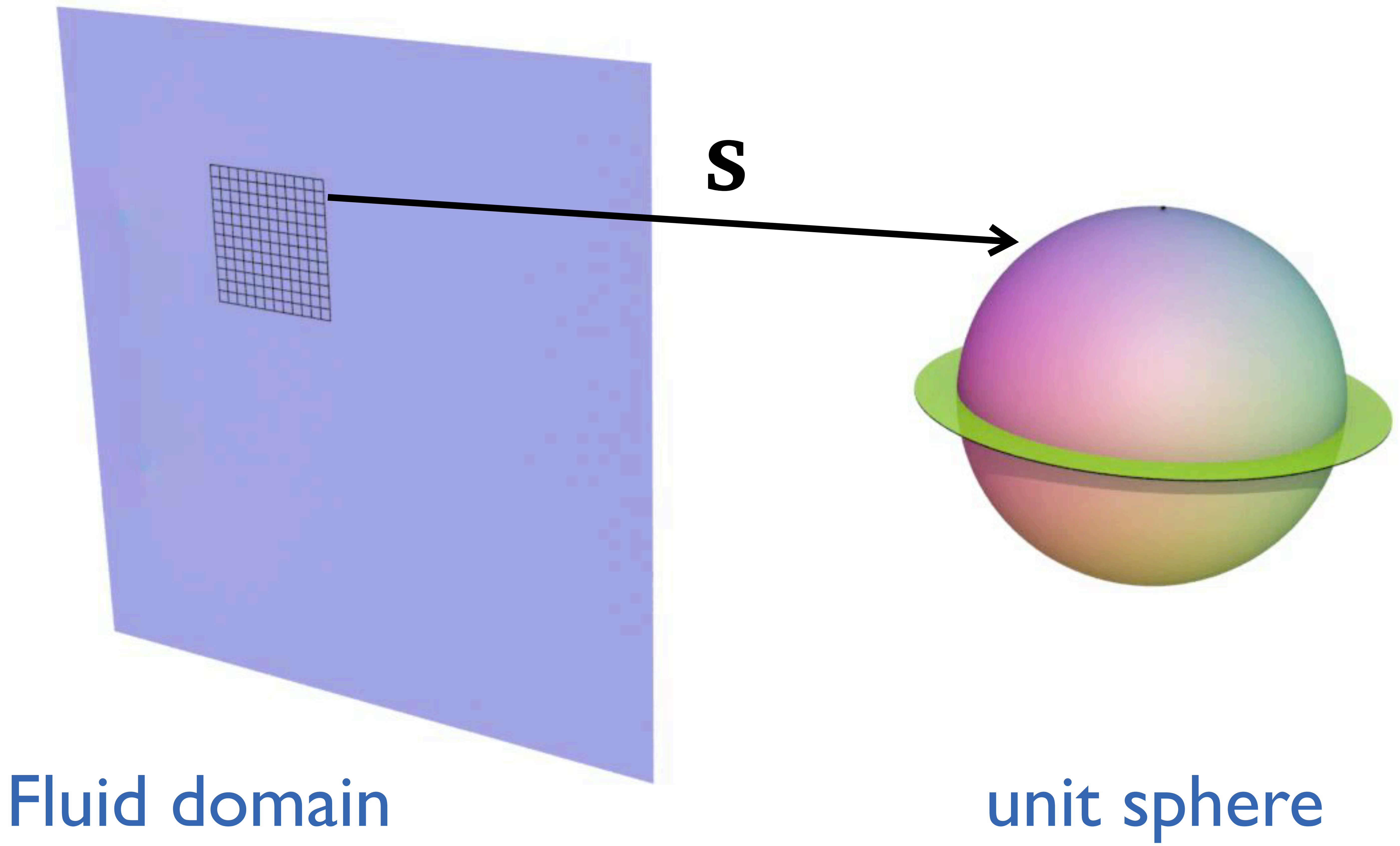


Concentrated vorticity

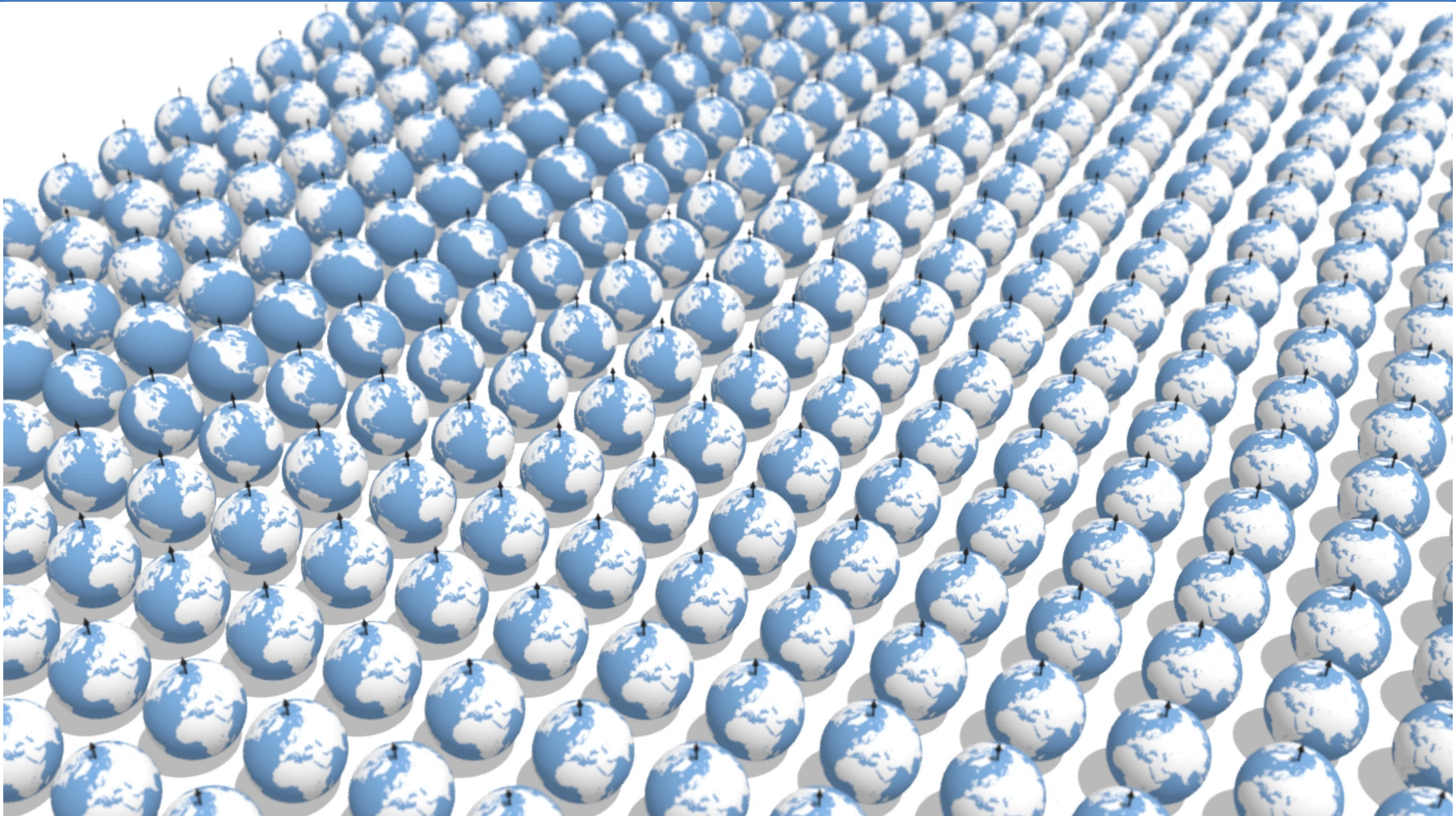
$\mathbf{S}$ sweeps over the entire sphere in a small region



Spin sweeps over the entire sphere



Spin sweeps over the entire sphere



Stable vortex unit

$$\boxed{\iint_\Sigma \omega \cdot \mathbf{n}\, dA \;=\; \frac{\hbar}{2}\,\mathrm{Area}\Big[\mathbf{s}(\Sigma)\Big]}$$

Stable vortex has quantized vorticity $2\pi\hbar$

Tuning $\hbar$

Large $\hbar$ Small $\hbar$

Dynamics of the spins

ISF in terms of spin:

$$\boxed{\frac{\partial}{\partial t}\mathbf{s}}\boxed{+\,\mathbf{u}\cdot\nabla\mathbf{s}} = \boxed{\frac{\hbar}{2}\mathbf{s}\times\Delta\mathbf{s}}$$

Spin is transported by the velocity

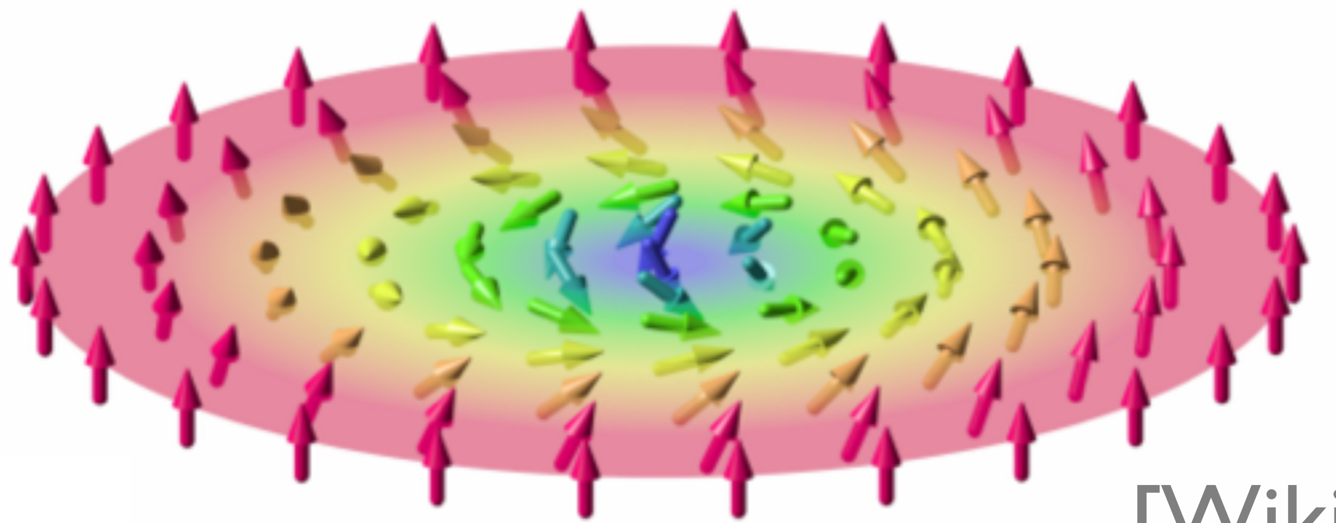
$\Downarrow$

Vortex lines are transported by the vel

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

Local interaction between spins in vortex core

(Ferromagnetic Landau-Lifshitz equation)



[Wikipedia: Magnetic skyrmion]

Dynamics of the spins

ISF in terms of spin:

$$\boxed{\frac{\partial}{\partial t}\mathbf{s} + \mathbf{u} \cdot \nabla \mathbf{s}} = \frac{\hbar}{2}\mathbf{s} \times \Delta \mathbf{s}$$

Kinetics is easily lost on coarse grid

Dynamics of the spins

ISF in terms of spin:

$$\boxed{\frac{\partial}{\partial t}\mathbf{s}} + \mathbf{u}\cdot\nabla\mathbf{s} = \boxed{\frac{\hbar}{2}\mathbf{s}\times\Delta\mathbf{s}}$$

Restore dynamics of vortices ***below grid resolution***

Final Remarks

We propose Incompressible Schrödinger Flow for fluid simulation.

- Simple, stable, no nonlinear advection term.
- A hidden spin vector $\boldsymbol{s}$ gives a new viewpoint in vorticity.
- ISF is a Landau-Lifshitz-modified Euler fluid flow, restoring sub-grid dynamics.
- ISF needs only a Laplacian.

Final Remarks

$$\begin{cases} \dfrac{\partial}{\partial t}\psi = \mathbf{i}\,\dfrac{\hbar}{2}\Delta\psi - \mathbf{i}\,p\psi \\ \langle \Delta\psi, \mathbf{i}\psi \rangle_{\mathbb{R}} = 0 \end{cases}$$

Final Remarks

Thank you

- YouTube search: **Schrödinger's Smoke**
- **Houdini** files
- **MATLAB** codes