

Computational Fluid Dynamics Simulation of Dipolar Gases in the Hydrodynamic Regime

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PHYSICAL REVIEW A **106**, 023319 (2022)

Thermal conductivity of an ultracold paramagnetic Bose gas

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Editors' Suggestion

Anisotropic acoustics in dipolar Fermi gases

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Theory

Hydrodynamic Equations & Anisotropic Viscosity Tensor

The Hydrodynamic Regime

- Hydrodynamic collisions result in fast local thermalization.
- Nonequilibrium thermodynamics is overshadowed by long wavelength scale fluid motion.
- Governing equations: **Continuity**, **Navier-Stokes** and **temperature balance**
- Re-equilibration processes are encapsulated by the transport tensors of **viscosity** and **thermal conductivity**.

Continuous field variables:

Mass density ρ

Flow velocity \mathbf{U}

Kinetic temperature T

$$\frac{\partial \rho}{\partial t} + \partial_j(\rho U_j) = 0,$$

$$\frac{\partial(\rho U_i)}{\partial t} + \partial_j(\rho U_j U_i) = \partial_j \tau_{ij} - \partial_i P - \frac{\rho}{m} \partial_i V(\mathbf{r}, t),$$

$$\frac{\partial(\rho T)}{\partial t} + \partial_j(\rho T U_j) = \frac{2m}{3k_B} [(\tau_{ij} - P\delta_{ij})\partial_j U_i - \kappa_{ij}\partial_i\partial_j T],$$

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CFD Simulations: COMSOL

COMSOL

Equation

Show equation assuming:

Study 3D Time Dependent, Time Dependent

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mathbf{K}] + \mathbf{F}$$

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

$$\mathbf{K} = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}$$

$$K_{ij} = \tau_{ij} = \mu_{ijnm} \partial_m u_n$$

(Newtonian Fluid)

! need to adapt to dipolar collisions!

Model Input

Fluid Properties

Density:

ρ From material

$\rho = \rho(p_A, T)$

Constitutive relation

Specify dynamic viscosity

μ From material

ρ is the density (SI unit: kg/m³)

\mathbf{u} is the velocity vector (SI unit: m/s)

p is pressure (SI unit: Pa)

\mathbf{I} is the identity matrix (unitless)

\mathbf{K} is the viscous stress tensor (SI unit: Pa)

\mathbf{F} is the volume force vector (SI unit: N/m³)

[COMSOL Documentation](#)

Continuous field variables:

Mass density ρ

Flow velocity \mathbf{U}

Kinetic temperature T

$$\frac{\partial \rho}{\partial t} + \partial_j(\rho U_j) = 0,$$

no dipolar mean field interaction

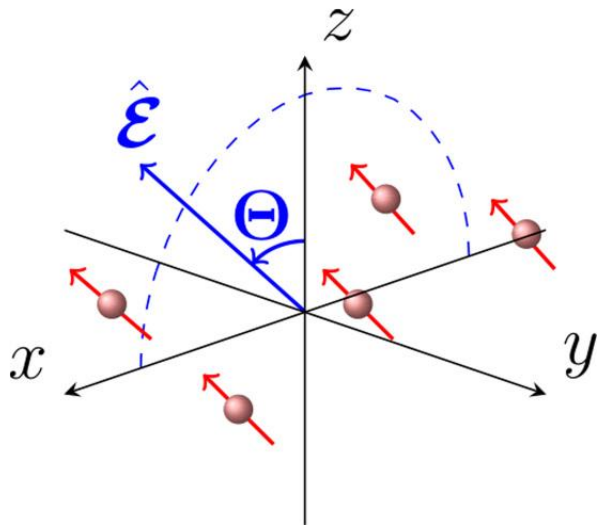
$$\frac{\partial(\rho U_i)}{\partial t} + \partial_j(\rho U_j U_i) = \partial_j \tau_{ij} - \partial_i P - \frac{\rho}{m} \dot{\mathbf{r}}(\mathbf{r}, t),$$

no heat transfer for the moment

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Anisotropic Viscosity Tensor from Dipolar Collisions

$$V_{dd}(\mathbf{r}) = \frac{d^2}{4\pi\epsilon_0} \frac{1 - 3(\hat{\mathbf{r}}^T \hat{\boldsymbol{\epsilon}})^2}{r^3}$$



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Wang & Bohn
using
Chapman and
Enskog procedure

Wang & Bohn
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Here: Non-degenerate, polar fermionic molecules.

$$\mu_{1111} = \frac{\mu_d}{512} (117 \cos(4\Theta) + 84 \cos(2\Theta) + 415),$$

$$\mu_{1113} = -\frac{3\mu_d}{512} (39 \sin(4\Theta) + 14 \sin(2\Theta)),$$

$$\mu_{1122} = -\frac{7\mu_d}{128} (3 \cos(2\Theta) + 11),$$

$$\mu_{1133} = -\frac{\mu_d}{512} (117 \cos(4\Theta) + 107),$$

$$\mu_{1212} = \frac{9\mu_d}{128} (5 \cos(2\Theta) + 9),$$

$$\mu_{1223} = -\frac{45\mu_d}{128} \sin(2\Theta),$$

$$\mu_{1313} = -\frac{9\mu_d}{512} (13 \cos(4\Theta) - 29),$$

$$\mu_{1322} = \frac{21\mu_d}{128} \sin(2\Theta),$$

$$\mu_{1333} = \frac{3\mu_d}{512} (39 \sin(4\Theta) - 14 \sin(2\Theta)),$$

$$\mu_{2222} = 77\mu_d,$$

$$\mu_{2233} = \frac{7\mu_d}{128} (3 \cos(2\Theta) - 11),$$

$$\mu_{2323} = -\frac{9\mu_d}{128} (5 \cos(2\Theta) - 9),$$

$$\mu_{3333} = \frac{\mu_d}{512} (117 \cos(4\Theta) - 84 \cos(2\Theta) + 415).$$

Symmetries:

- $\mu_{ijmn} = \mu_{jimn},$
- $\mu_{ijmn} = \mu_{jinm},$
- $\mu_{ijmn} = \mu_{mnij},$
- $\mu_{ijmn}\delta_{ij} = \mu_{ijmn}\delta_{mn} = \mu_{ijmn}\delta_{ijmn} = 0$

Viscosity Tensor (for Fermions)

rank-4 viscosity tensor

$$\left(\begin{array}{ccc} \left(\begin{array}{ccc} \mu_{1111} & \mu_{1112} & \mu_{1113} \\ \mu_{1121} & \mu_{1122} & \mu_{1123} \\ \mu_{1131} & \mu_{1132} & \mu_{1133} \end{array} \right) & \left(\begin{array}{ccc} \mu_{1211} & \mu_{1212} & \mu_{1213} \\ \mu_{1221} & \mu_{1222} & \mu_{1223} \\ \mu_{1231} & \mu_{1232} & \mu_{1233} \end{array} \right) & \left(\begin{array}{ccc} \mu_{1311} & \mu_{1312} & \mu_{1313} \\ \mu_{1321} & \mu_{1322} & \mu_{1323} \\ \mu_{1331} & \mu_{1332} & \mu_{1333} \end{array} \right) \\ \left(\begin{array}{ccc} \mu_{2111} & \mu_{2112} & \mu_{2113} \\ \mu_{2121} & \mu_{2122} & \mu_{2123} \\ \mu_{2131} & \mu_{2132} & \mu_{2133} \end{array} \right) & \left(\begin{array}{ccc} \mu_{2211} & \mu_{2212} & \mu_{2213} \\ \mu_{2221} & \mu_{2222} & \mu_{2223} \\ \mu_{2231} & \mu_{2232} & \mu_{2233} \end{array} \right) & \left(\begin{array}{ccc} \mu_{2311} & \mu_{2312} & \mu_{2313} \\ \mu_{2321} & \mu_{2322} & \mu_{2323} \\ \mu_{2331} & \mu_{2332} & \mu_{2333} \end{array} \right) \\ \left(\begin{array}{ccc} \mu_{3111} & \mu_{3112} & \mu_{3113} \\ \mu_{3121} & \mu_{3122} & \mu_{3123} \\ \mu_{3131} & \mu_{3132} & \mu_{3133} \end{array} \right) & \left(\begin{array}{ccc} \mu_{3211} & \mu_{3212} & \mu_{3213} \\ \mu_{3221} & \mu_{3222} & \mu_{3223} \\ \mu_{3231} & \mu_{3232} & \mu_{3233} \end{array} \right) & \left(\begin{array}{ccc} \mu_{3311} & \mu_{3312} & \mu_{3313} \\ \mu_{3321} & \mu_{3322} & \mu_{3323} \\ \mu_{3331} & \mu_{3332} & \mu_{3333} \end{array} \right) \end{array} \right)$$

color-coded magnitude



analytical expression

$$\left(\begin{array}{ccc} \left(\begin{array}{ccc} \frac{1}{8} \mu\theta (415 + 84 \cos[2\theta] + 117 \cos[4\theta]) & 0 & -\frac{3}{8} \mu\theta (14 \sin[2\theta] + 39 \sin[4\theta]) \\ 0 & -\frac{7}{2} \mu\theta (11 + 3 \cos[2\theta]) & 0 \\ -\frac{3}{8} \mu\theta (14 \sin[2\theta] + 39 \sin[4\theta]) & 0 & -\frac{1}{8} \mu\theta (107 + 117 \cos[4\theta]) \end{array} \right) & \left(\begin{array}{ccc} 0 & \frac{9}{2} \mu\theta (9 + 5 \cos[2\theta]) & 0 \\ \frac{9}{2} \mu\theta (9 + 5 \cos[2\theta]) & 0 & -\frac{45}{2} \mu\theta \sin[2\theta] \\ 0 & -\frac{45}{2} \mu\theta \sin[2\theta] & 0 \end{array} \right) & \left(\begin{array}{ccc} -\frac{3}{8} \mu\theta (14 \sin[2\theta] + 39 \sin[4\theta]) & 0 & -\frac{9}{8} \mu\theta (-29 + 13 \cos[4\theta]) \\ 0 & \frac{21}{2} \mu\theta \sin[2\theta] & 0 \\ -\frac{9}{8} \mu\theta (-29 + 13 \cos[4\theta]) & 0 & \frac{3}{8} \mu\theta (-14 \sin[2\theta] + 39 \sin[4\theta]) \end{array} \right) \\ \left(\begin{array}{ccc} 0 & \frac{9}{2} \mu\theta (9 + 5 \cos[2\theta]) & 0 \\ \frac{9}{2} \mu\theta (9 + 5 \cos[2\theta]) & 0 & -\frac{45}{2} \mu\theta \sin[2\theta] \\ 0 & -\frac{45}{2} \mu\theta \sin[2\theta] & 0 \end{array} \right) & \left(\begin{array}{ccc} -\frac{7}{2} \mu\theta (11 + 3 \cos[2\theta]) & 0 & \frac{21}{2} \mu\theta \sin[2\theta] \\ 0 & 77 \mu\theta & 0 \\ \frac{21}{2} \mu\theta \sin[2\theta] & 0 & \frac{7}{2} \mu\theta (-11 + 3 \cos[2\theta]) \end{array} \right) & \left(\begin{array}{ccc} -\frac{45}{2} \mu\theta \sin[2\theta] & 0 & -\frac{9}{2} \mu\theta (-9 + 5 \cos[2\theta]) \\ -\frac{45}{2} \mu\theta \sin[2\theta] & 0 & -\frac{9}{2} \mu\theta (-9 + 5 \cos[2\theta]) \\ 0 & -\frac{9}{2} \mu\theta (-9 + 5 \cos[2\theta]) & 0 \end{array} \right) \\ \left(\begin{array}{ccc} -\frac{3}{8} \mu\theta (14 \sin[2\theta] + 39 \sin[4\theta]) & 0 & -\frac{9}{8} \mu\theta (-29 + 13 \cos[4\theta]) \\ 0 & \frac{21}{2} \mu\theta \sin[2\theta] & 0 \\ -\frac{9}{8} \mu\theta (-29 + 13 \cos[4\theta]) & 0 & \frac{3}{8} \mu\theta (-14 \sin[2\theta] + 39 \sin[4\theta]) \end{array} \right) & \left(\begin{array}{ccc} 0 & -\frac{45}{2} \mu\theta \sin[2\theta] & 0 \\ -\frac{45}{2} \mu\theta \sin[2\theta] & 0 & -\frac{9}{2} \mu\theta (-9 + 5 \cos[2\theta]) \\ 0 & -\frac{9}{2} \mu\theta (-9 + 5 \cos[2\theta]) & 0 \end{array} \right) & \left(\begin{array}{ccc} -\frac{1}{8} \mu\theta (107 + 117 \cos[4\theta]) & 0 & \frac{3}{8} \mu\theta (-14 \sin[2\theta] + 39 \sin[4\theta]) \\ 0 & \frac{7}{2} \mu\theta (-11 + 3 \cos[2\theta]) & 0 \\ \frac{3}{8} \mu\theta (-14 \sin[2\theta] + 39 \sin[4\theta]) & 0 & \frac{1}{8} \mu\theta (415 - 84 \cos[2\theta] + 117 \cos[4\theta]) \end{array} \right) \end{array} \right)$$

General Viscosity Tensor in COMSOL

$$\begin{aligned}
 K_{xx} &= \mu_{1111} \partial_x u + \mu_{1121} \partial_x v + \mu_{1131} \partial_x w \\
 &+ \mu_{1112} \partial_y u + \mu_{1122} \partial_y v + \mu_{1132} \partial_y w \\
 &+ \mu_{1113} \partial_z u + \mu_{1123} \partial_z v + \mu_{1133} \partial_z w \\
 &= \mu_{1111} \cdot u_x + \mu_{1121} \cdot v_x + \mu_{1131} \cdot w_x \\
 &+ \mu_{1112} \cdot u_y + \mu_{1122} \cdot v_y + \mu_{1132} \cdot w_y \\
 &+ \mu_{1113} \cdot u_z + \mu_{1123} \cdot v_z + \mu_{1133} \cdot w_z
 \end{aligned}$$

Settings Properties x

Equation View

Study

Show equation view assuming:

Study 3D Time Dependent, Time Dependent

e.g. ↗

Variables

Name	Expression	Unit	Description
spf.K_stress_tensorxx	K_stress_tensor_tuning*(mu1111*ux+mu1112*uy+mu1113*uz+mu1121*vx+mu1122*vy+mu1123*vz+mu1131*wx+mu1132*wy+mu1133*wz)	N/m ²	Viscous stress tensor, xx-component
spf.K_stress_tensoryx	K_stress_tensor_tuning*(mu2111*ux+mu2112*uy+mu2113*uz+mu2121*vx+mu2122*vy+mu2123*vz+mu2131*wx+mu2132*wy+mu2133*wz)	N/m ²	Viscous stress tensor, yx-component
spf.K_stress_tensorzx	K_stress_tensor_tuning*(mu3111*ux+mu3112*uy+mu3113*uz+mu3121*vx+mu3122*vy+mu3123*vz+mu3131*wx+mu3132*wy+mu3133*wz)	N/m ²	Viscous stress tensor, zx-component
spf.K_stress_tensoryy	K_stress_tensor_tuning*(mu2211*ux+mu2212*uy+mu2213*uz+mu2221*vx+mu2222*vy+mu2223*vz+mu2231*wx+mu2232*wy+mu2233*wz)	N/m ²	Viscous stress tensor, yy-component
spf.K_stress_tensorzy	K_stress_tensor_tuning*(mu3211*ux+mu3212*uy+mu3213*uz+mu3221*vx+mu3222*vy+mu3223*vz+mu3231*wx+mu3232*wy+mu3233*wz)	N/m ²	Viscous stress tensor, zy-component
spf.K_stress_tensorxz	K_stress_tensor_tuning*(mu1311*ux+mu1312*uy+mu1313*uz+mu1321*vx+mu1322*vy+mu1323*vz+mu1331*wx+mu1332*wy+mu1333*wz)	N/m ²	Viscous stress tensor, xz-component
spf.K_stress_tensoryz	K_stress_tensor_tuning*(mu2311*ux+mu2312*uy+mu2313*uz+mu2321*vx+mu2322*vy+mu2323*vz+mu2331*wx+mu2332*wy+mu2333*wz)	N/m ²	Viscous stress tensor, yz-component
spf.K_stress_tensorzz	K_stress_tensor_tuning*(mu3311*ux+mu3312*uy+mu3313*uz+mu3321*vx+mu3322*vy+mu3323*vz+mu3331*wx+mu3332*wy+mu3333*wz)	N/m ²	Viscous stress tensor, zz-component

↑

$$K_{ij} = \tau_{ij} = \mu_{ijnm} \partial_m u_n$$

(Newtonian Fluid)

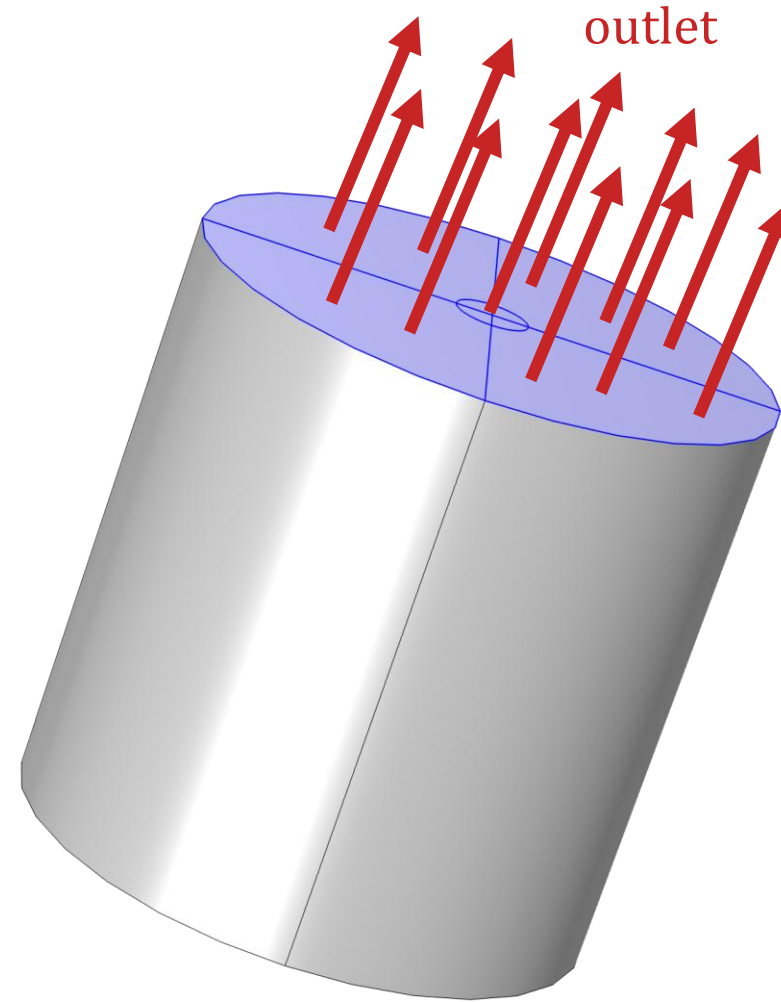
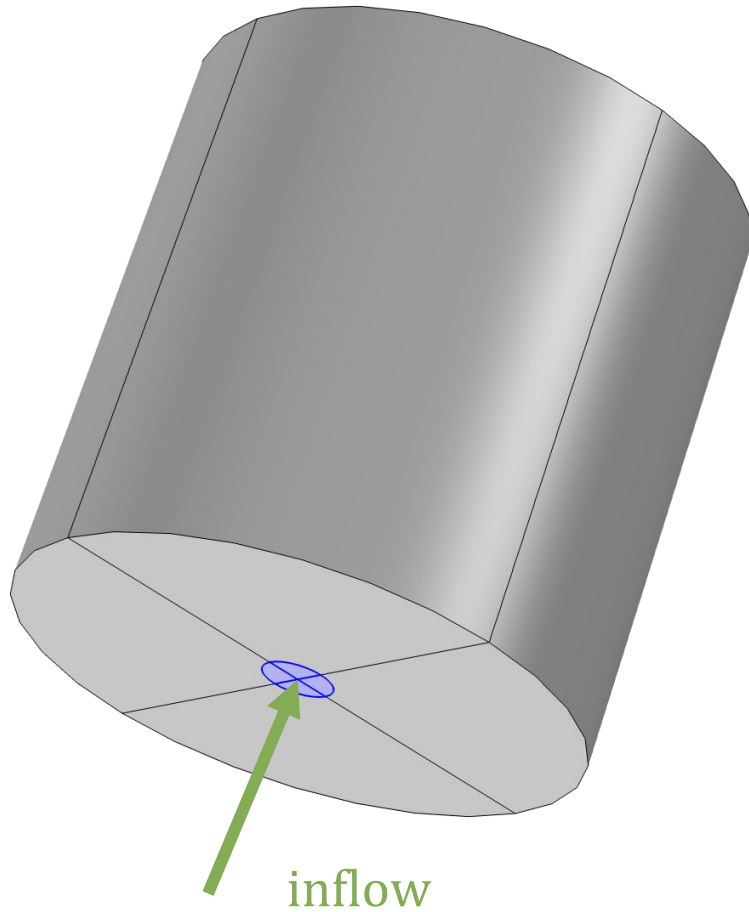
Simulation Results

Two Preliminary Examples

Flow through Orifice

ohm

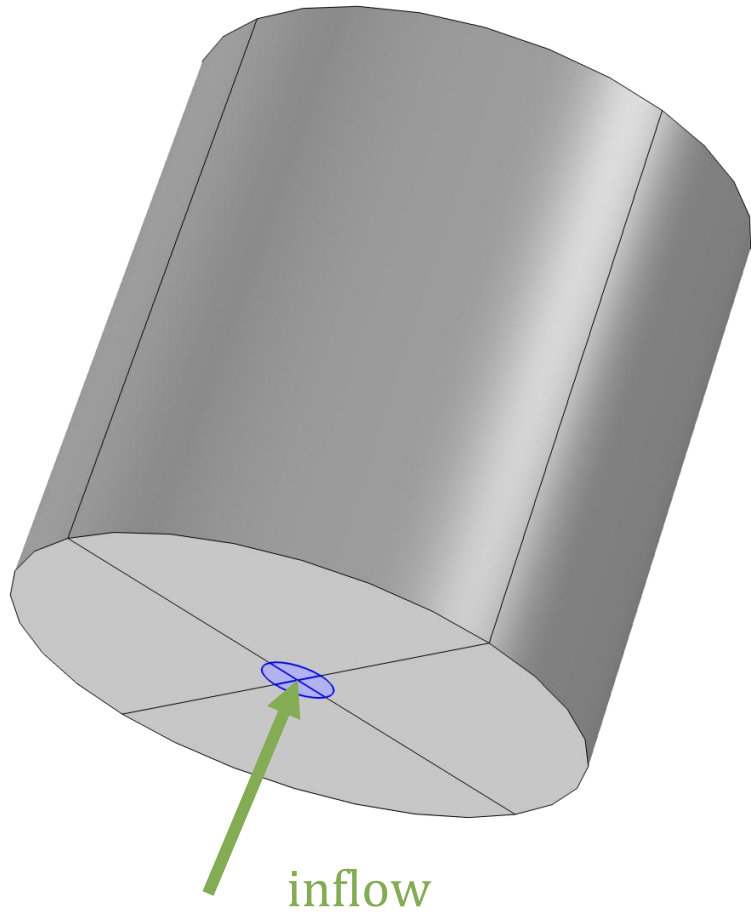
Flow through Orifice



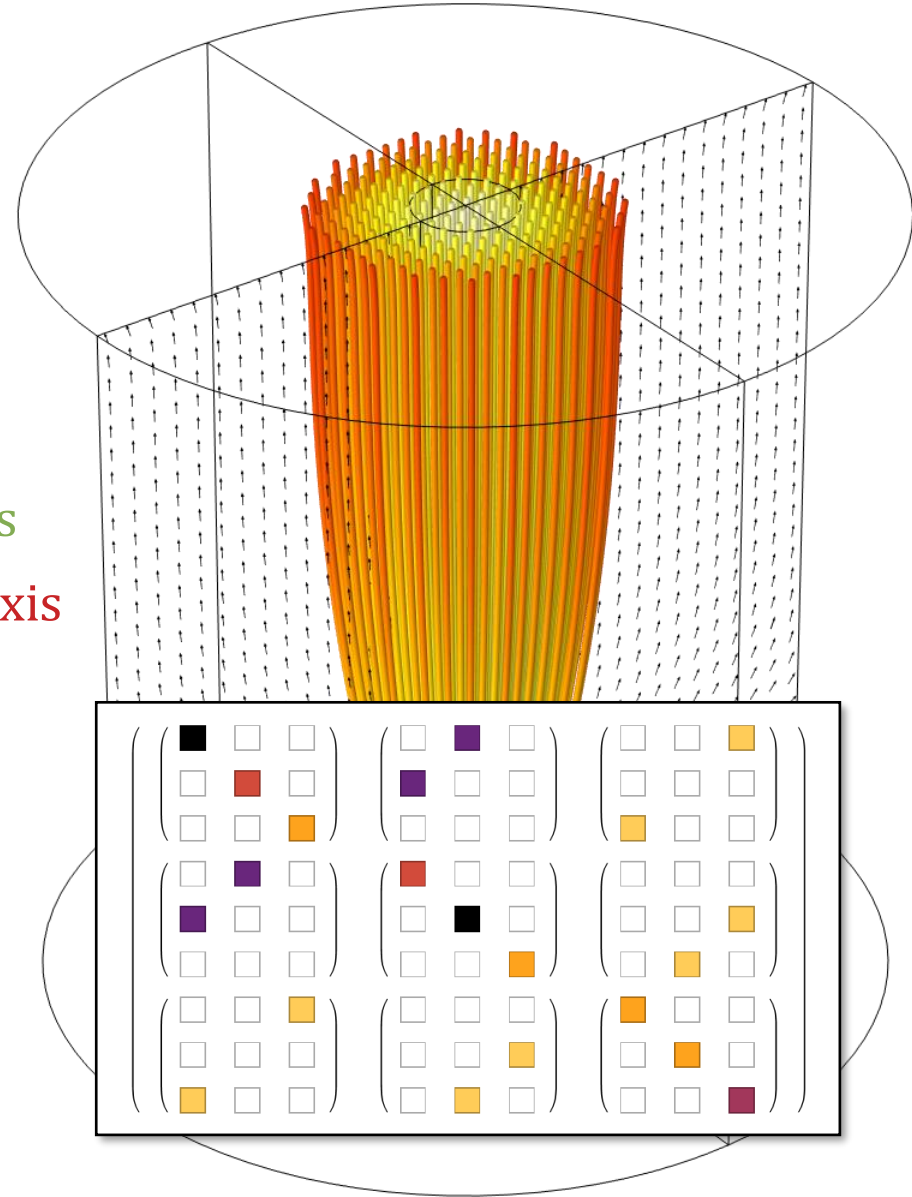
Fermionic $^{23}\text{Na}^{40}\text{K}$ parameters from PRA **108**, 013322 (2023)

ohm

Flow through Orifice

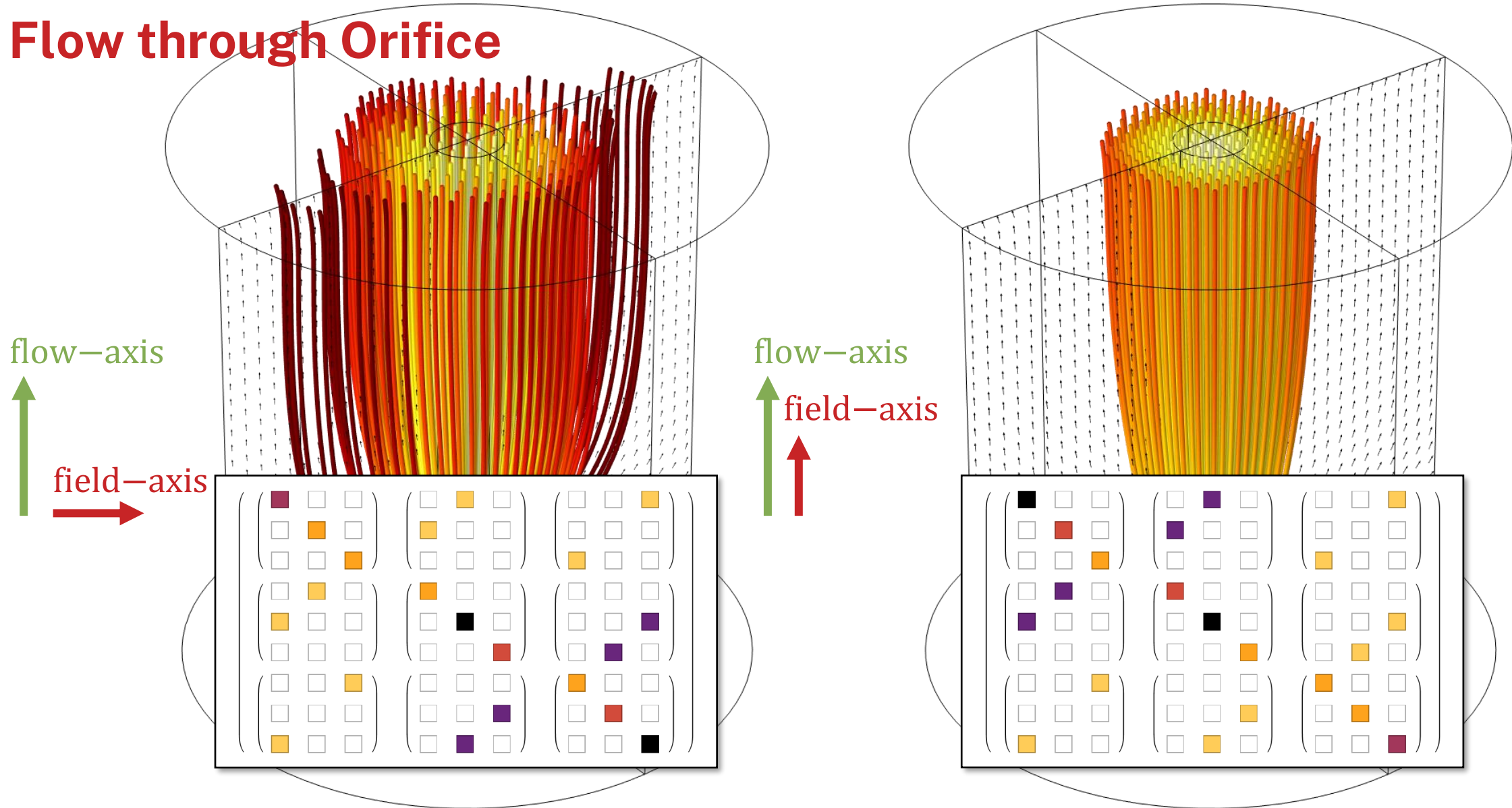


flow-axis
↑
field-axis
↑



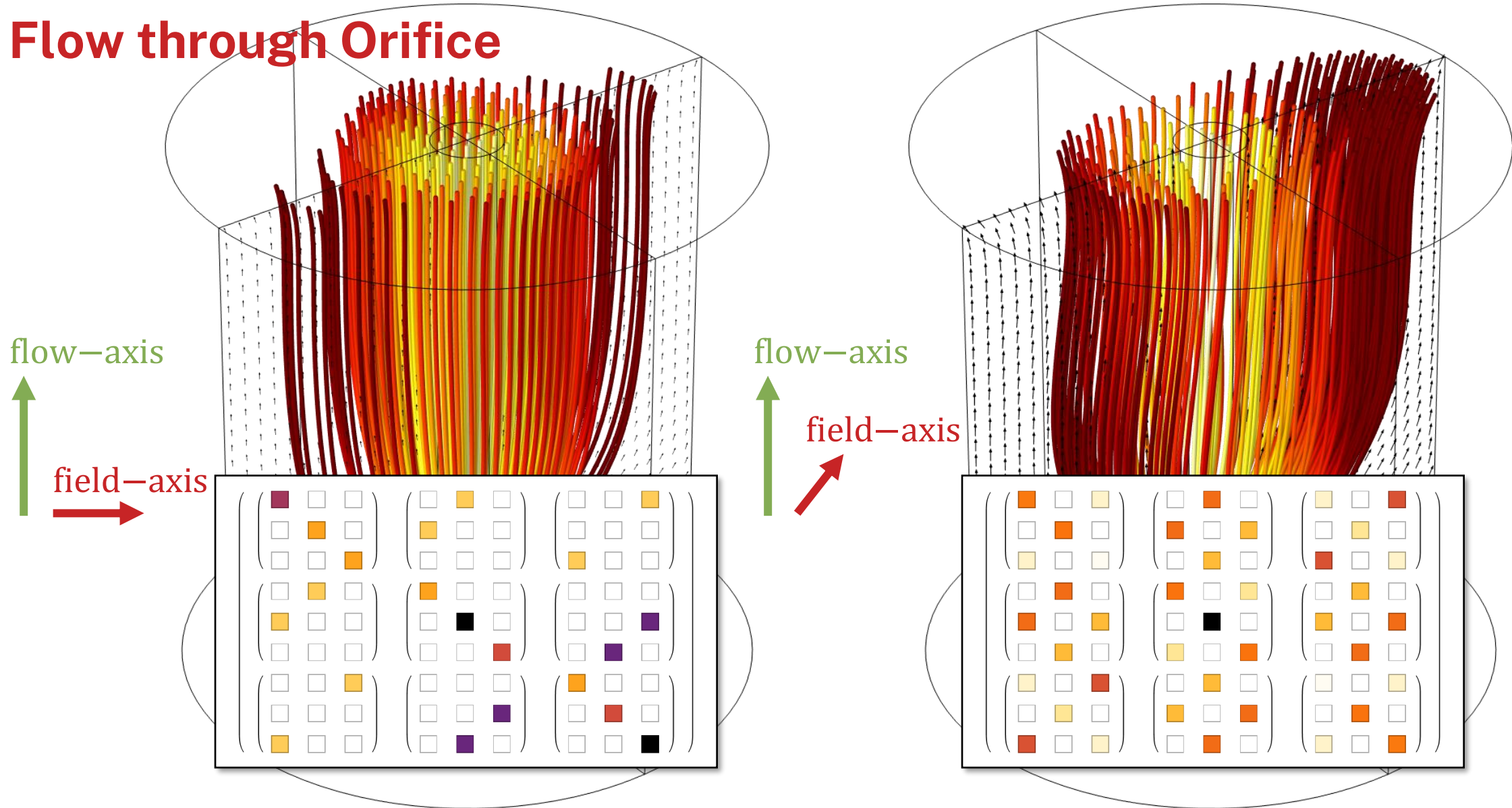
ohm

Flow through Orifice



ohm

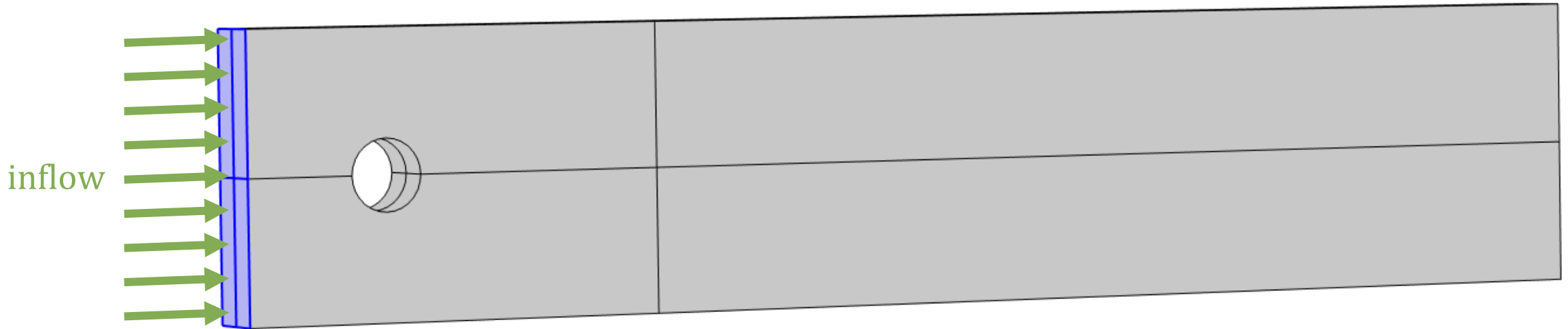
Flow through Orifice



Vortex Shedding

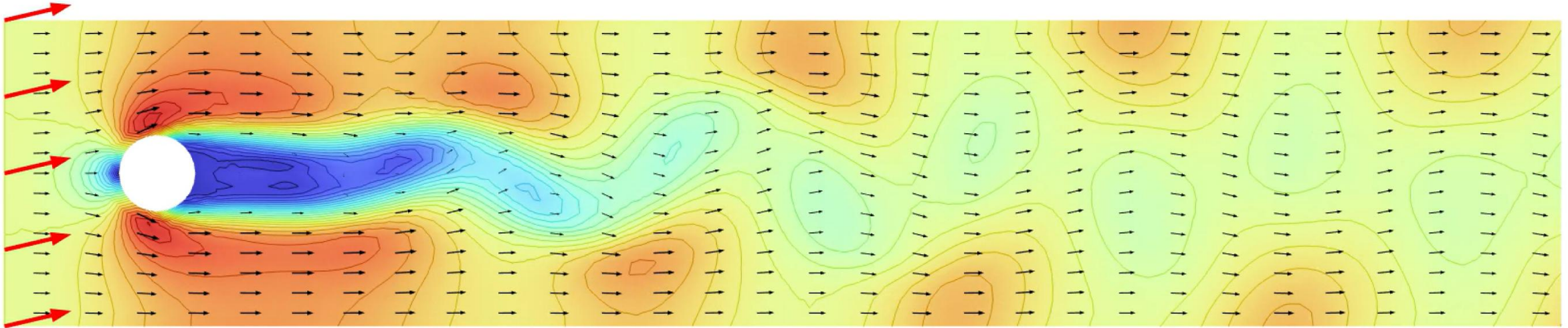
Vortex-Shedding

Dipole moment $\mu'_0 = \mu_0/25$ to show critical behavior.

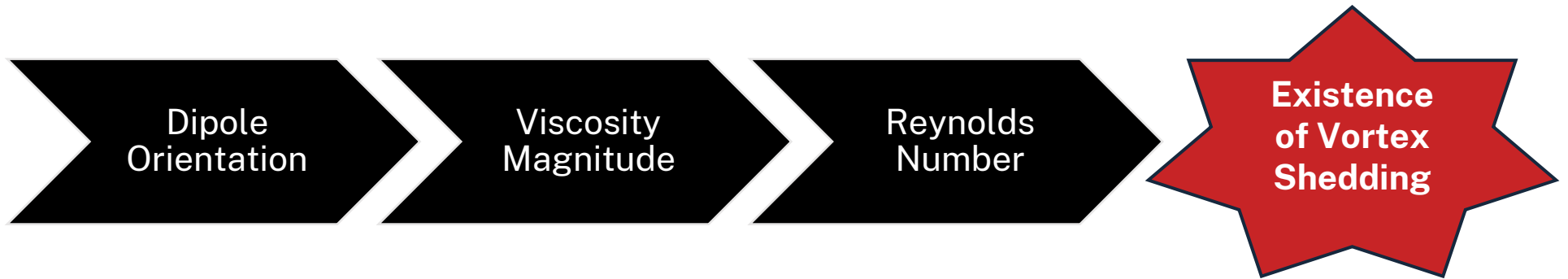


Vortex-Shedding

Dipole moment $\mu'_0 = \mu_0/25$ to show critical behavior.



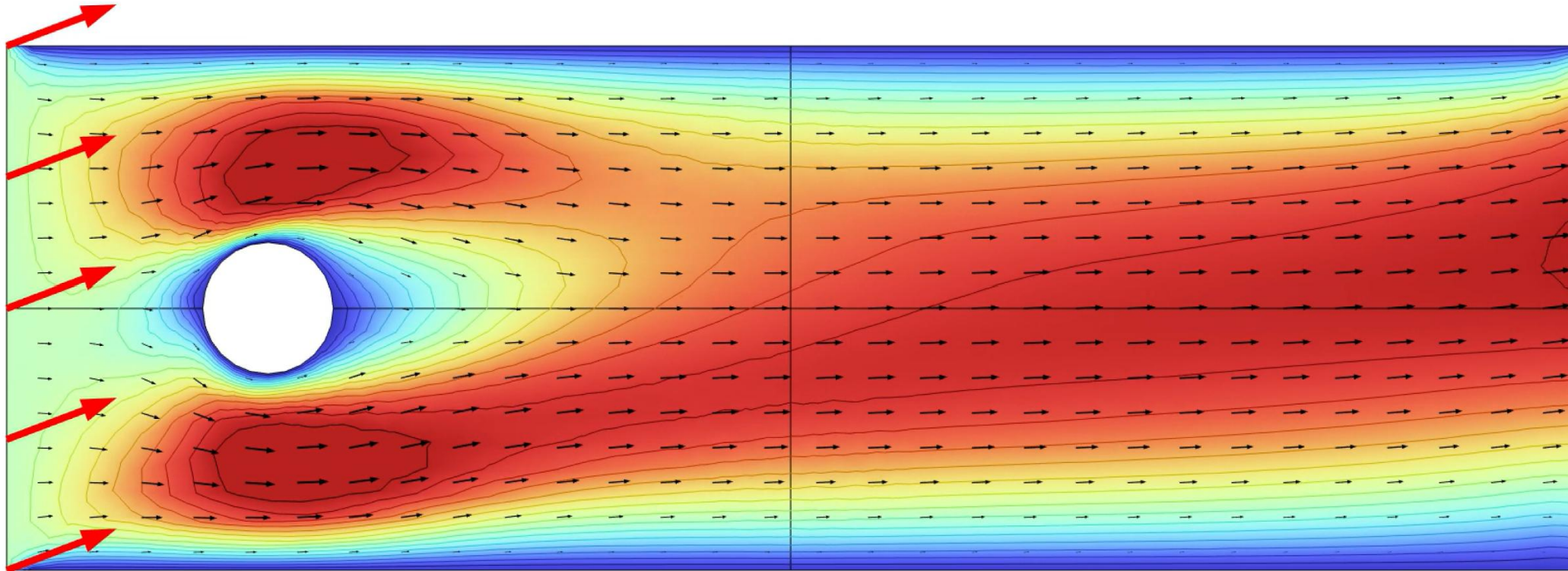
dipole orientation



ohm

No-Vortex-Shedding

Dipole moment μ_0 from Phys. Rev. A 108, 013322 (2023)



dipole orientation

THANK YOU!

Prof. Dr. Michael Mayle

Computational Physics for Sensor Technologies

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