Dynamics of moving bodies and boundaries in active and natural convective flows

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PhD Thesis Defense

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NYU

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Many others!

The Courant community, especially my PhD cohort

Part I: Morphology of melting ice

1. Anomalous natural convective sculpting of melting ice
2. Capsize dynamics of laboratory icebergs

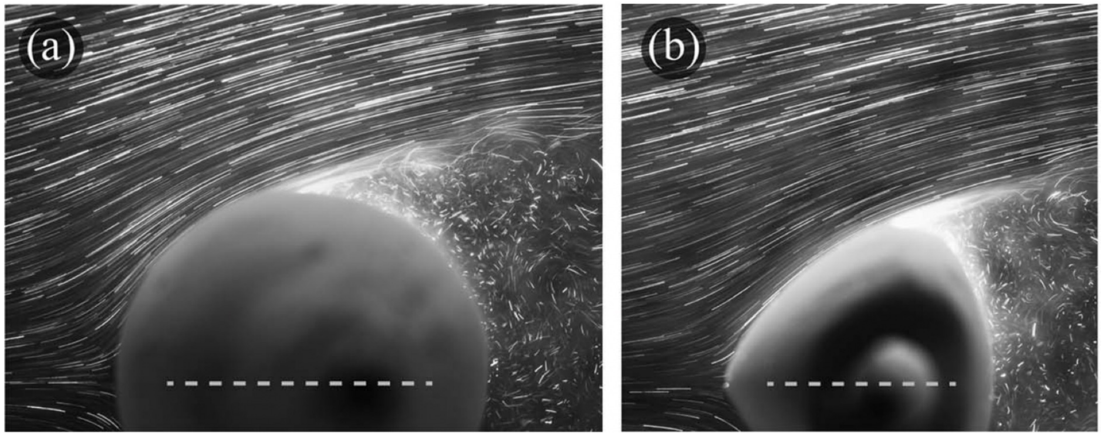
Part II: Continuum modeling of active fluids

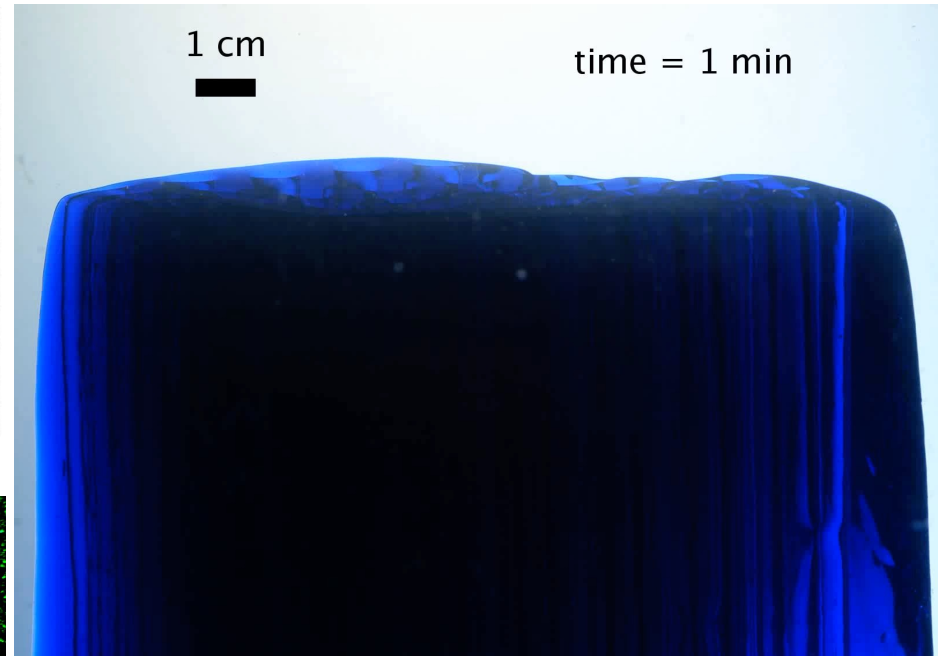
3. Coarse-graining kinetic theories of microswimmer suspensions
4. Numerical methods

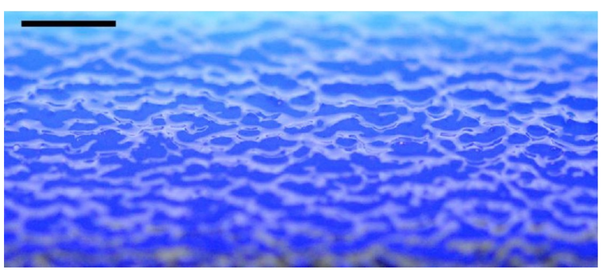
Part I
Morphology of melting ice

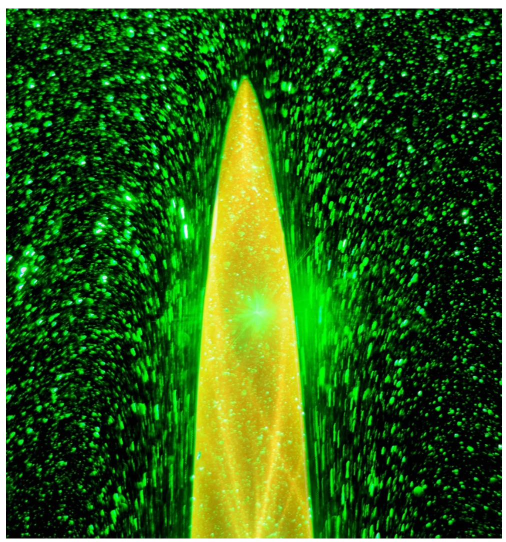
Geomorphology

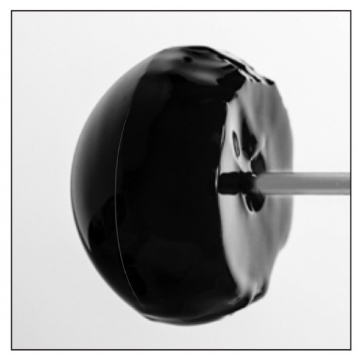
Table-top geophysics

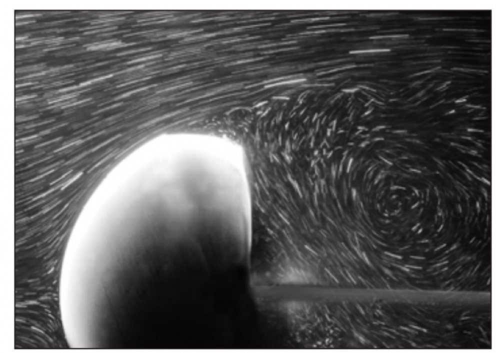












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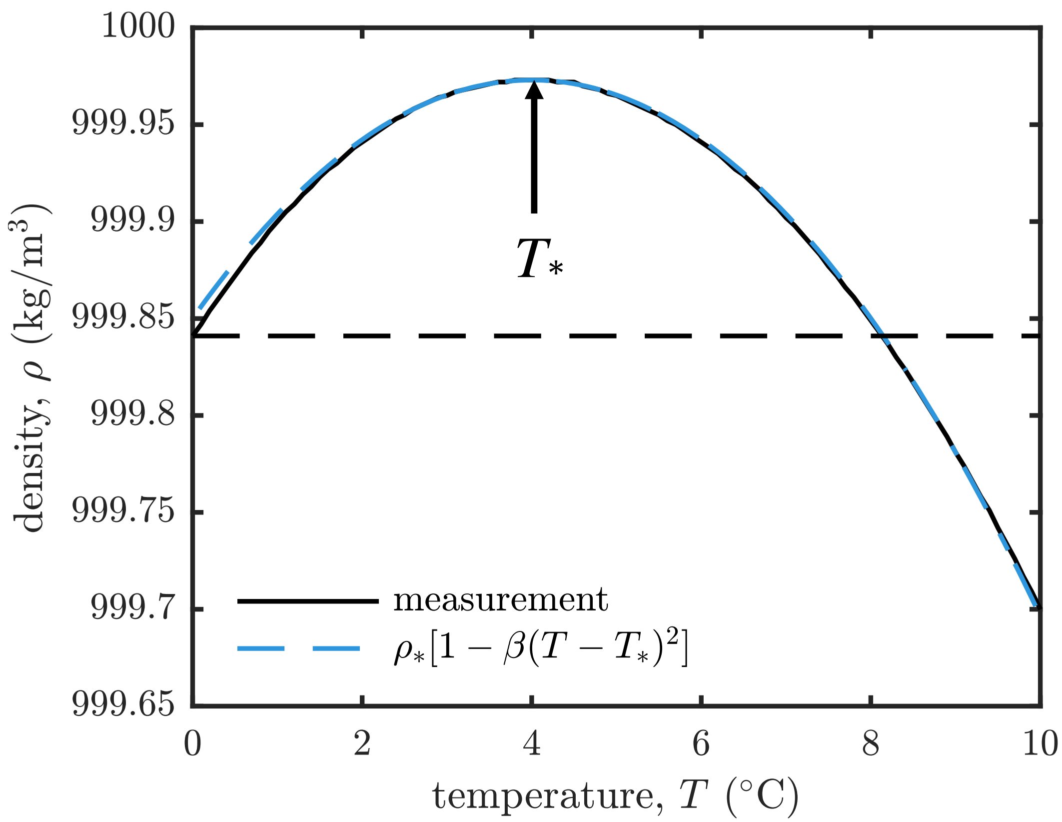
The density anomaly

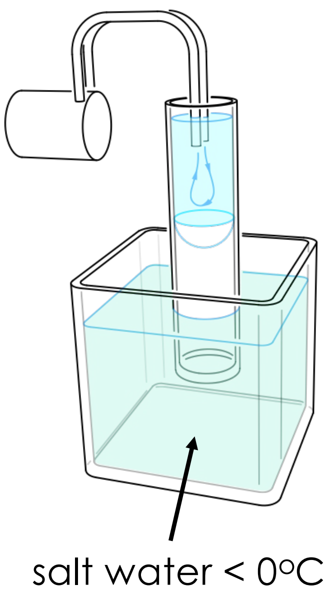


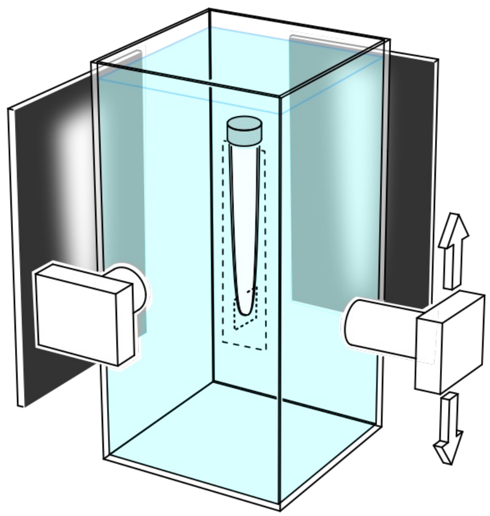
- Unlike most fluids, water is densest *above* its freezing point
- In some cases, against intuition, cold fluid may rise

How does the density anomaly influence shape?

Ice making and experimental system

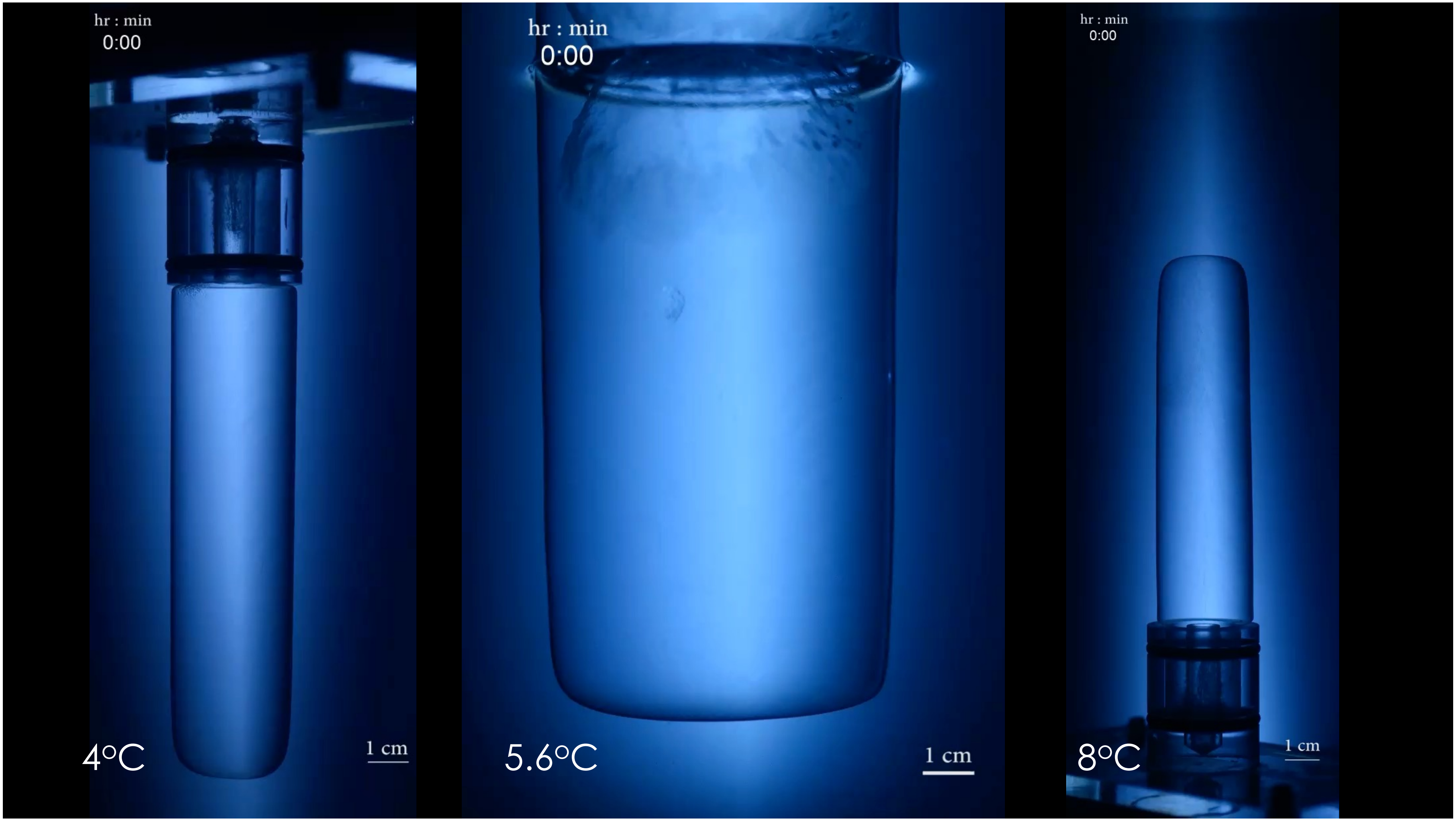
- Manufacture clear ice cylinders using directional freezing
- Ice is supported at its base -- not subject to gravity
- Experiments are conducted in a “cold” room to set far-field temperature





uniform lighting

gradient lighting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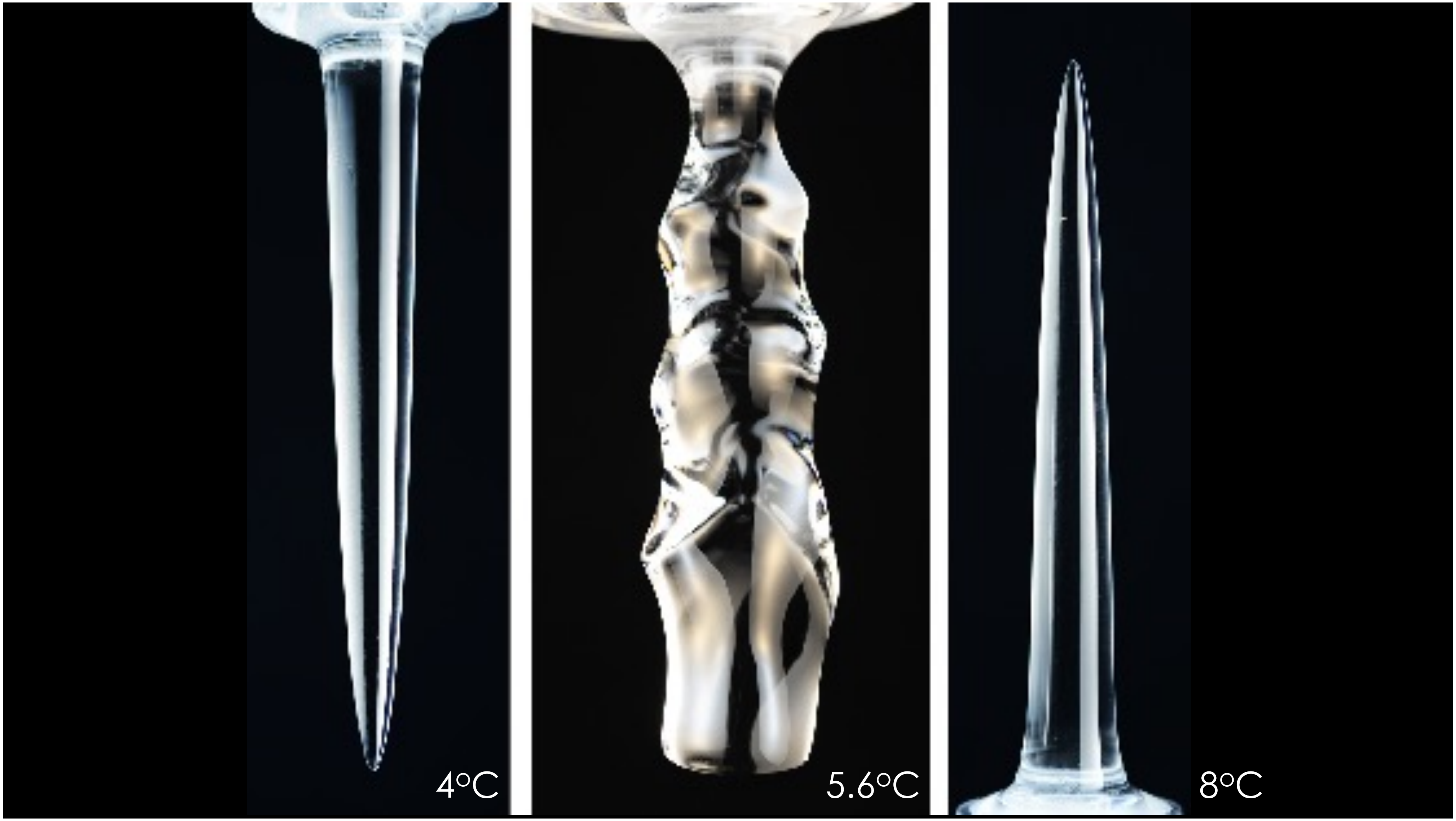
0:00
4°C
1 cm
hr : min
0:00
5.6°C
1 cm
hr : min
0:00
8°C
1 cm


4°C
5.6°C
8°C

Hydrodynamics and the Boussinesq approximation

- Density is approximated by a quadratic equation of state

$$\rho(T) = \rho_*[1 - \beta(T - T_*)^2]$$

- Fluid satisfies Navier-Stokes equation with coupled temperature field

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = \mathrm{Pr}\big(-\nabla p + \Delta \boldsymbol{u} + \boxed{\mathrm{Ra}\theta^2 \hat{\boldsymbol{z}}\big)}$$

$$\frac{\partial \theta}{\partial t} + \boldsymbol{u} \cdot \nabla\theta = \Delta\theta$$

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

Stefan condition: $V_n = \mathrm{St}\dfrac{\partial \theta}{\partial n}$

Dimensionless parameters

$$\mathrm{Ra} = \frac{g\beta(T_\infty - T_0)^2 H^3}{\nu D}$$

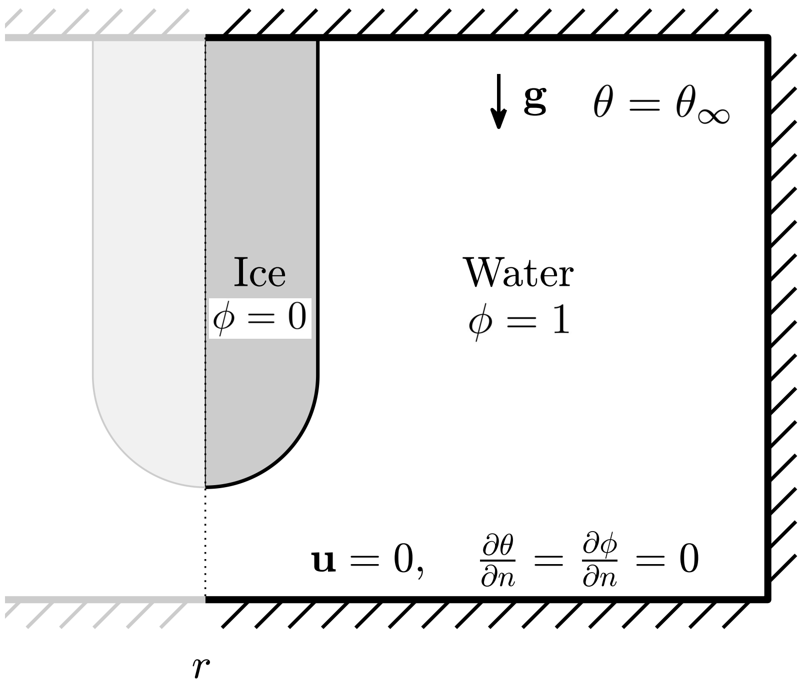
$$\mathrm{Pr} = \frac{\nu}{D}$$

$$\mathrm{St} = \frac{c_p(T_\infty - T_0)}{\mathcal{L}}$$

$$\theta(\boldsymbol{x}, t) = \frac{T(\boldsymbol{x}, t) - T_*}{T_\infty - T_0}$$

Phase-field model of melting ice

- Ice/water represented by continuous phase parameter $\phi(\boldsymbol{x}, t)$
- Fluid-structure interaction modeled by Brinkman penalization

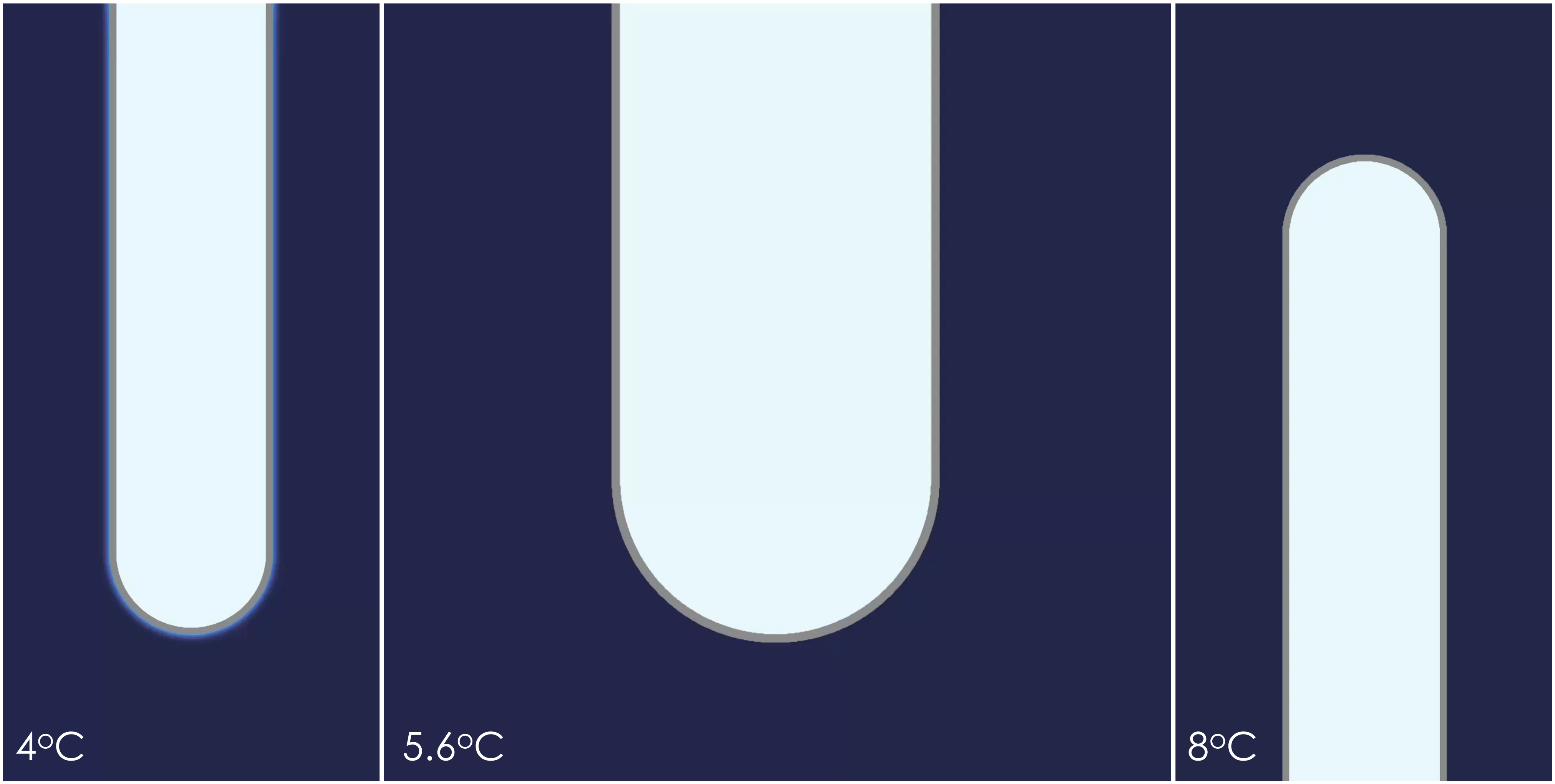


$$\frac{D\boldsymbol{u}}{Dt} = \mathrm{Pr}\left(-\nabla p + \Delta \boldsymbol{u} + \mathrm{Ra}\theta^2 \hat{\boldsymbol{z}}\right) - \eta(1-\phi)^2 \boldsymbol{u},$$

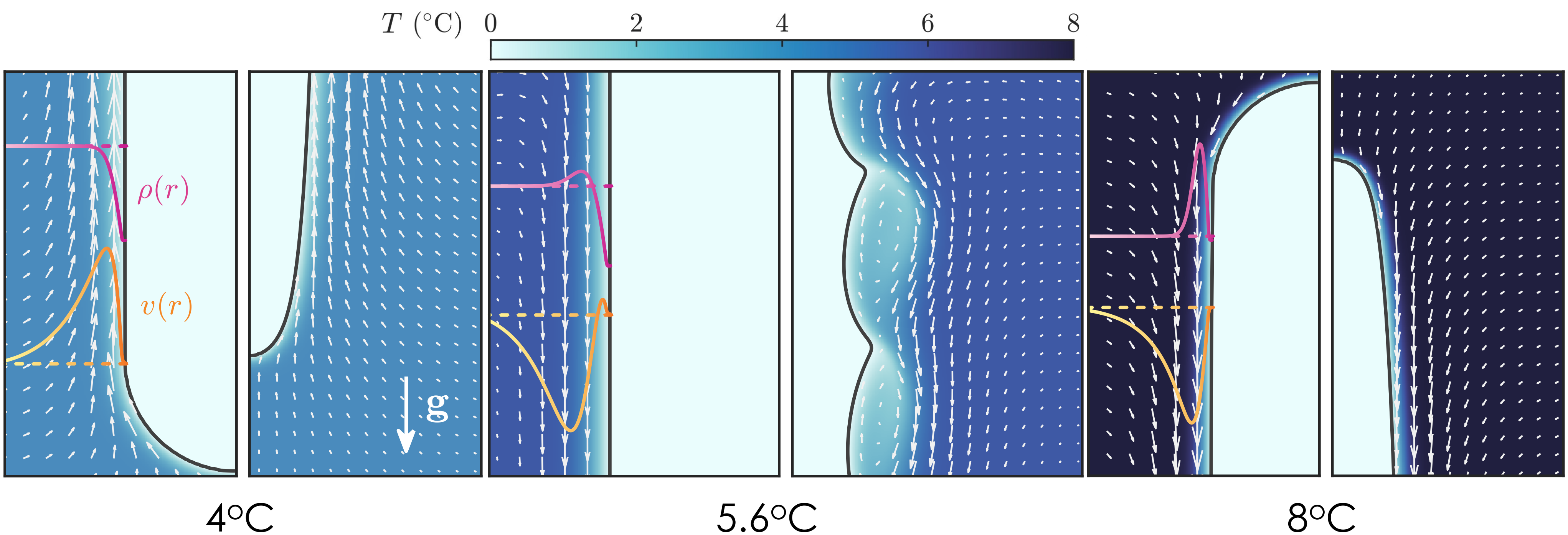
$$\frac{D\theta}{Dt} = \Delta\theta - \frac{1}{\mathrm{St}} \frac{df}{d\phi} \frac{\partial \phi}{\partial t},$$

$$\frac{\partial \phi}{\partial t} = m\Delta\phi + \frac{m(\theta - \theta_0)}{\delta^2} \frac{df}{d\phi} - \frac{m}{4\delta^2} \frac{dg}{d\phi},$$

$$\nabla \cdot \boldsymbol{u} = 0.$$


4°C
5.6°C
8°C

Simulated flow and temperature fields



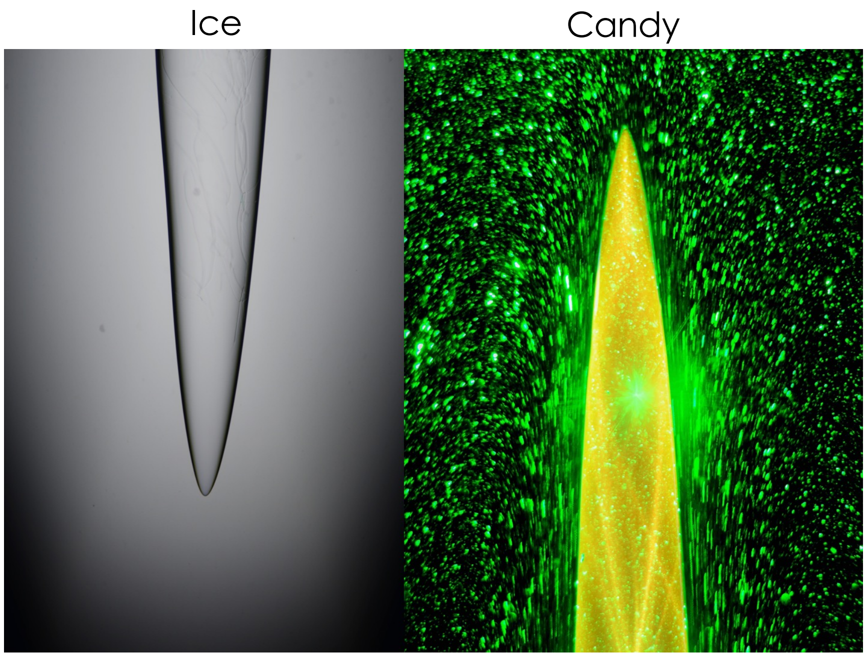
- Stable boundary layer flows occur at 4°C and 8°C
- A shear flow occurs at 5.6°C that rolls up into wall-bound vortices

Pinnacle formation: connections to dissolution

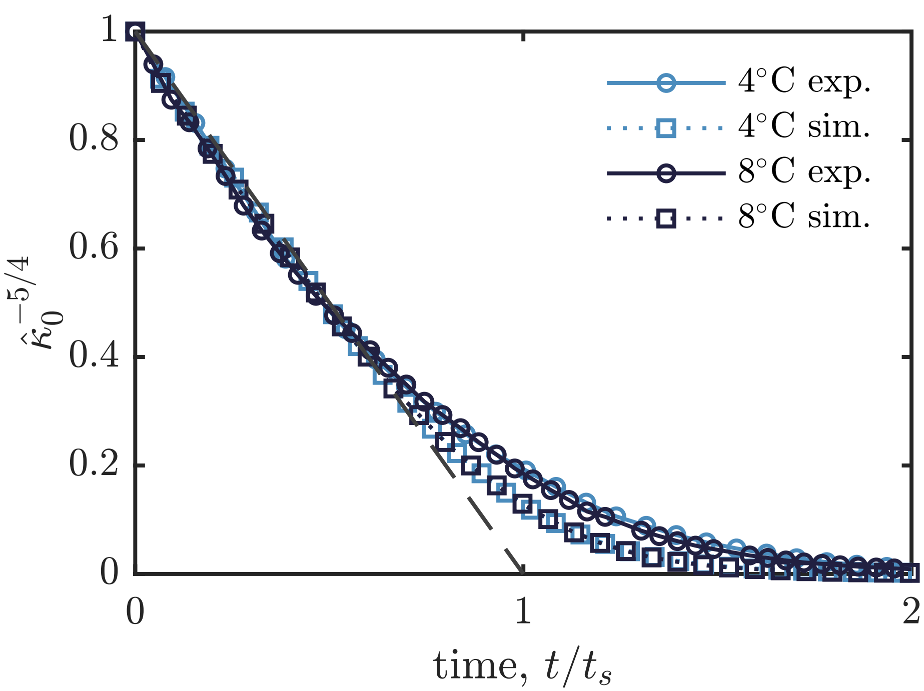
- Boundary layer analysis predicts finite time singularity in tip curvature

$$V_n(s,t) = -\mathrm{St}\frac{r^{1/3}(s,t)\cos^{1/3}\theta(s,t)}{\left[\int_0^s r^{4/3}(s',t)\cos^{1/3}\theta(s',t)ds'\right]^{1/4}}$$

$$\kappa_0(t) = \kappa_0(0)\left(1 - \frac{t}{t_s}\right)^{-4/5}$$



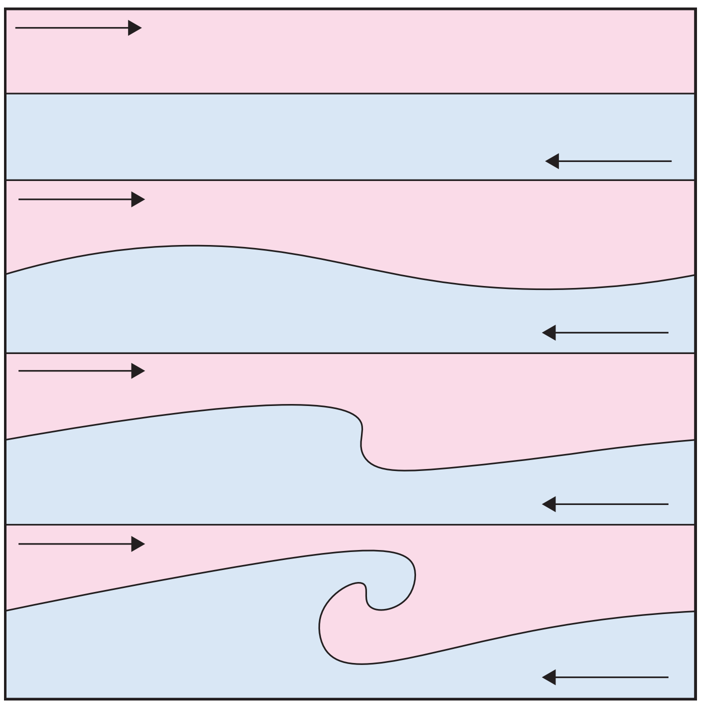
Huang et al., *PNAS* (2020)

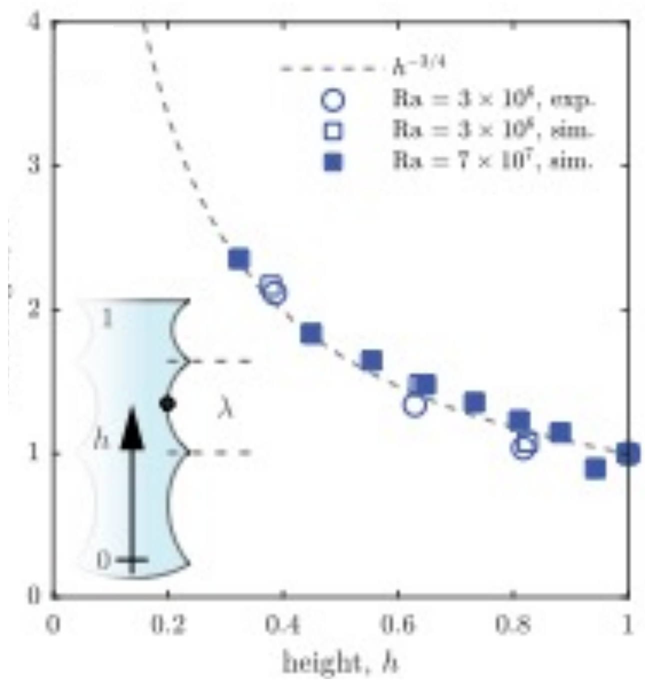


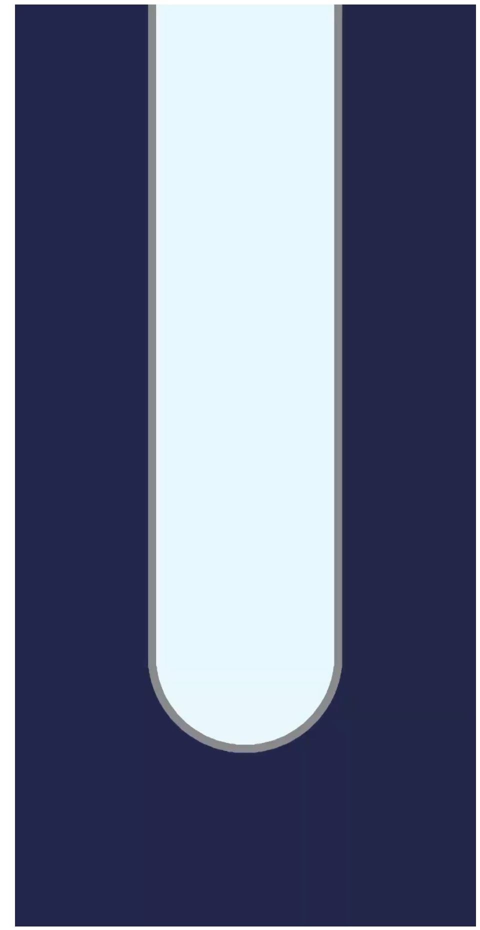
Scallop formation: the Kelvin-Helmholtz instability

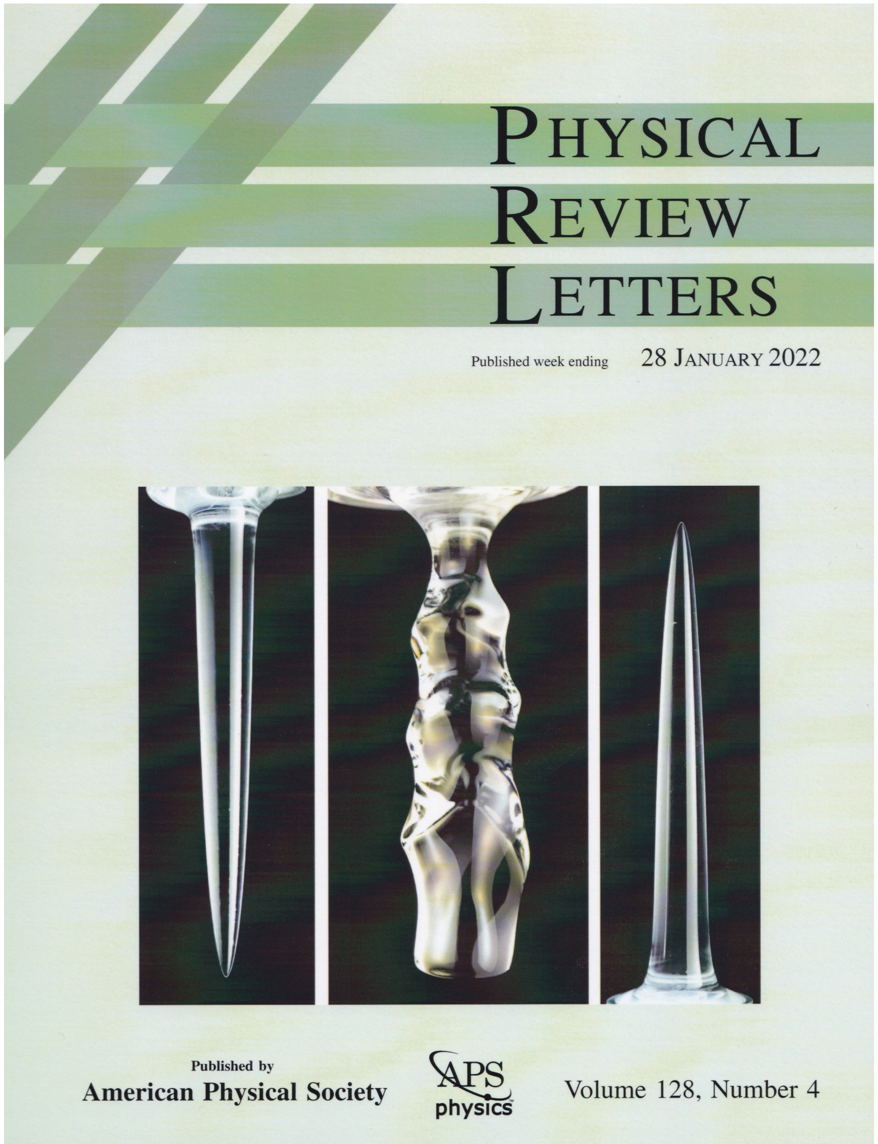
- Most unstable wavelength: $\lambda \propto \mathrm{Re}^{-1/2}$
- Experiments: $\mathrm{Re} \propto \mathrm{Ra}^{1/2}$
- Non-dimensionalization: $\mathrm{Ra} \propto h^3$

$$\lambda \propto h^{-3/4}$$









PHYSICAL REVIEW LETTERS **128,** 044502 (2022)

Featured in Physics

Anomalous Convective Flows Carve Pinnacles and Scallops in Melting Ice

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We report on the shape dynamics of ice suspended in cold fresh water and subject to the natural convective flows generated during melting. Experiments reveal shape motifs for increasing far-field temperature: Sharp pinnacles directed downward at low temperatures, scalloped waves for intermediate temperatures between 5 °C and 7 °C, and upward pointing pinnacles at higher temperatures. Phase-field simulations reproduce these morphologies, which are closely linked to the anomalous density-temperature profile of liquid water. Boundary layer flows yield pinnacles that sharpen with accelerating growth of tip curvature while scallops emerge from a Kelvin-Helmholtz–like instability caused by counterflowing currents that roll up to form vortex arrays. By linking the molecular-scale effects underlying water's density anomaly to the macroscale flows that imprint the surface, these results show that the morphology of melted ice is a sensitive indicator of ambient temperature.

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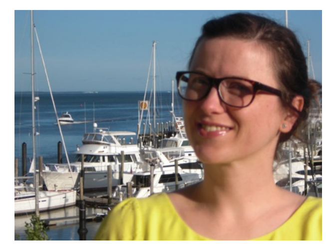
Questions?

Josh Tong



Alexandra Zidovska

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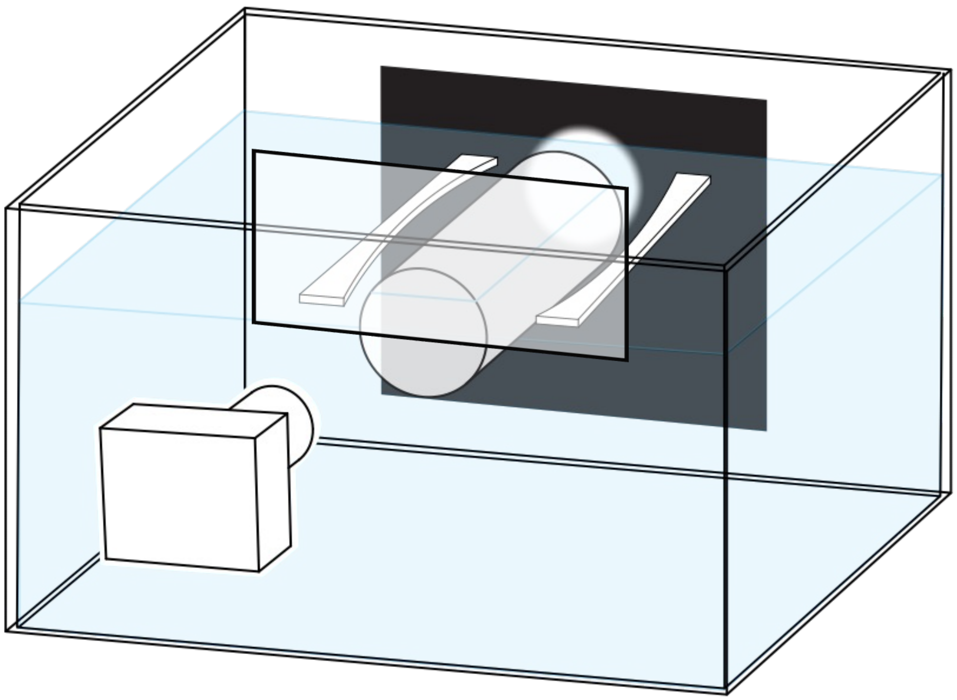
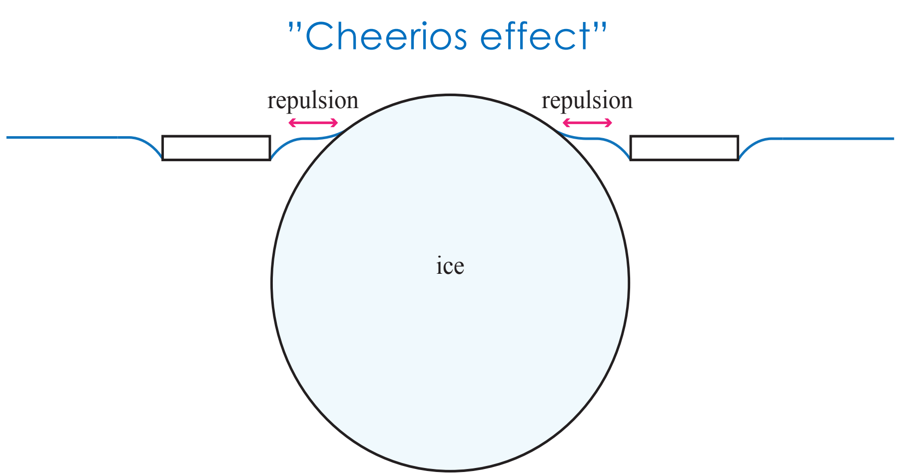
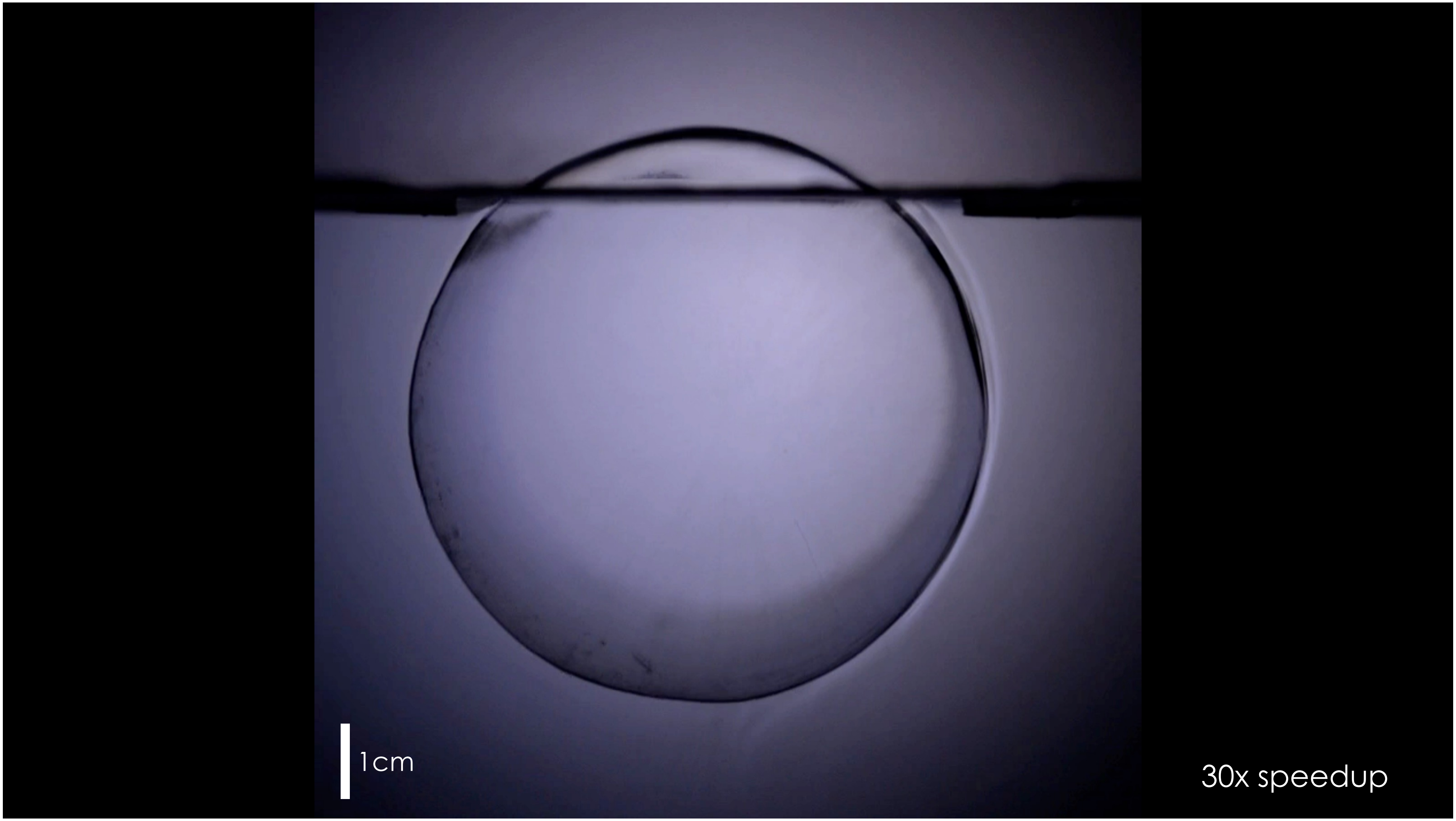
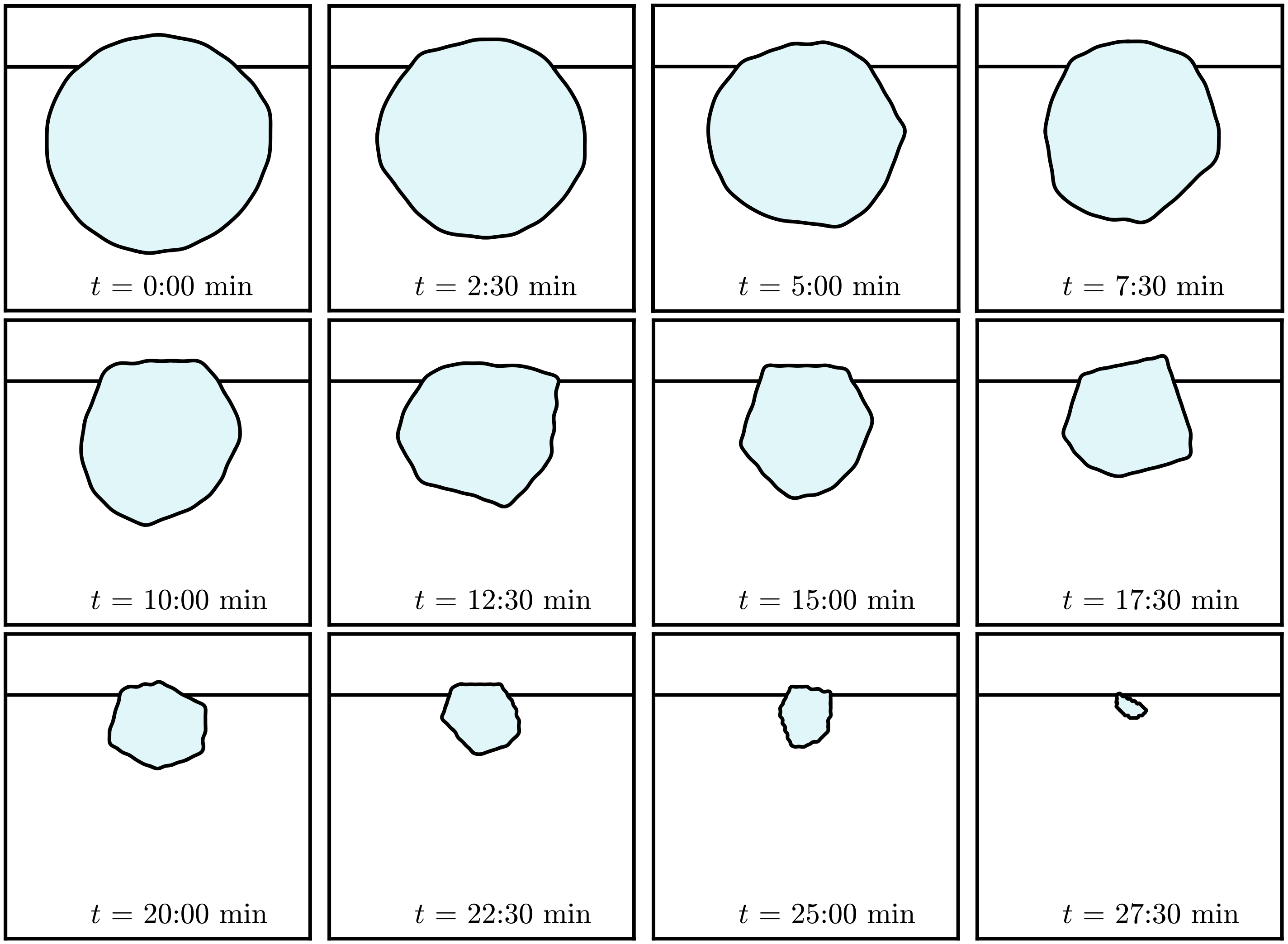
Laboratory icebergs

- Quasi two-dimensional geometry
- Ice floats and rolls due to buoyancy
- Low friction surface tension trap holds ice in camera view






1cm
30x speedup



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t = 7:30 min
t = 10:00 min
t = 12:30 min
t = 15:00 min
t = 17:30 min
t = 20:00 min
t = 22:30 min
t = 25:00 min
t = 27:30 min

Simulations: quasi-static model

- Represent interface in terms of tangent angle and total arclength

$$\frac{\partial \boldsymbol{X}}{\partial t} = V_n \hat{\boldsymbol{n}} + V_s \hat{\boldsymbol{s}} \qquad \frac{\partial \boldsymbol{X}}{\partial s} = L(\cos\theta, \sin\theta)^T$$

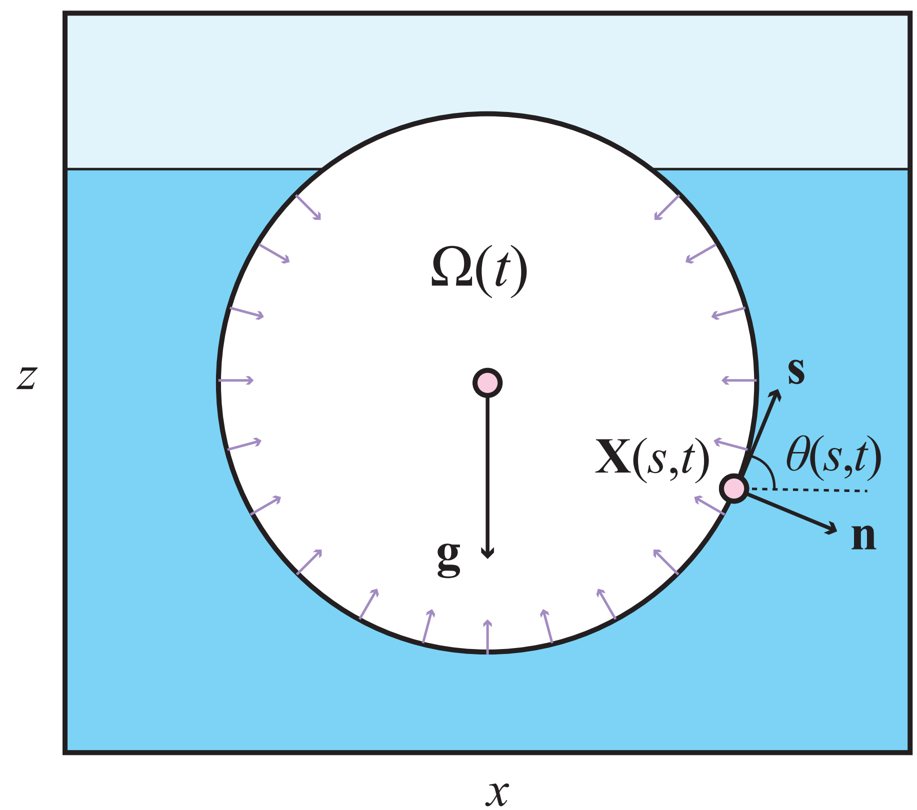
$$\frac{\partial \theta}{\partial t} = \frac{1}{L}\left(\frac{\partial V_n}{\partial s} + V_s \frac{\partial \theta}{\partial s}\right)$$

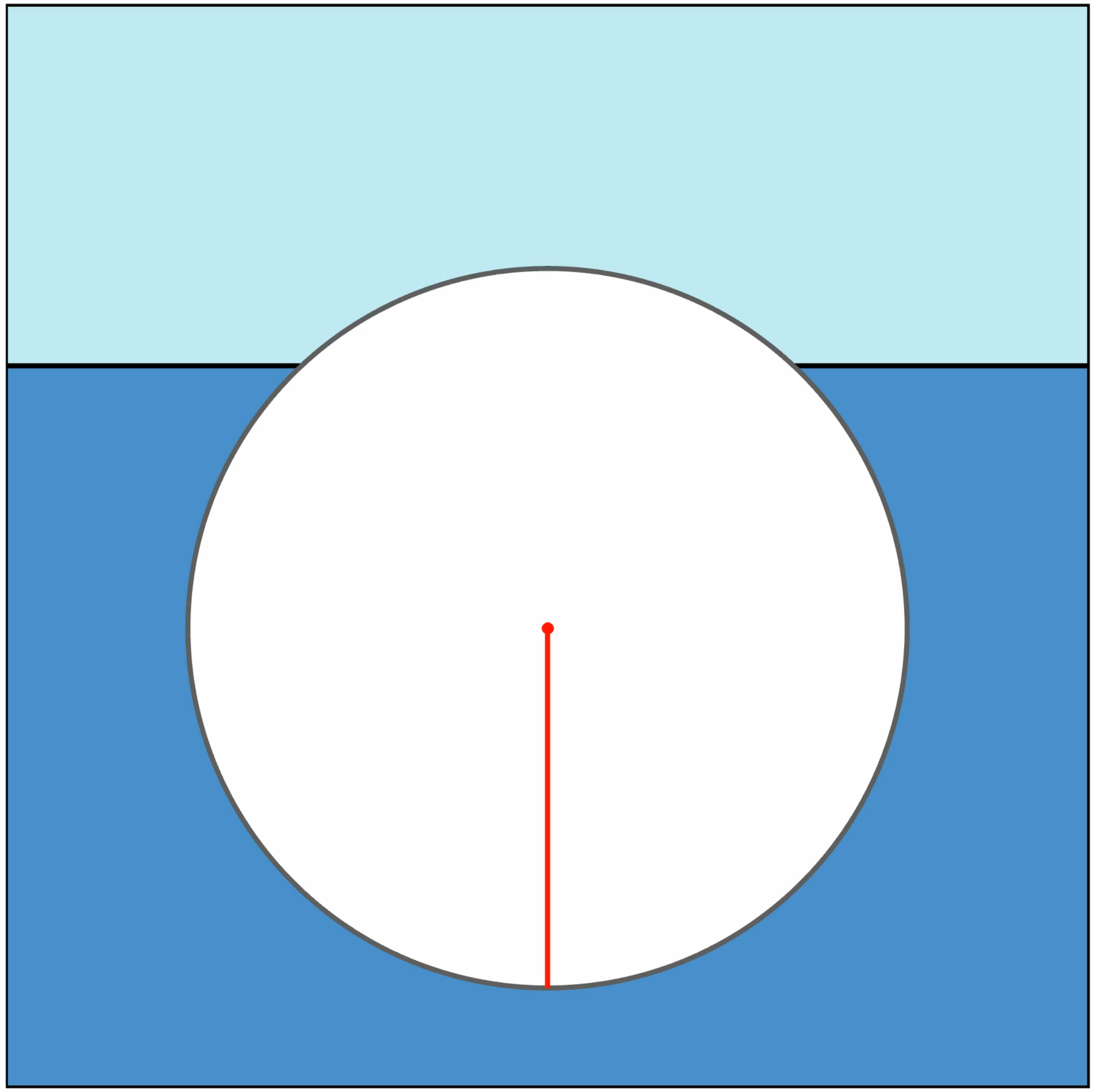
$$\frac{dL}{dt} = -\int_0^1 \kappa(s,t) V_n(s)\, ds$$

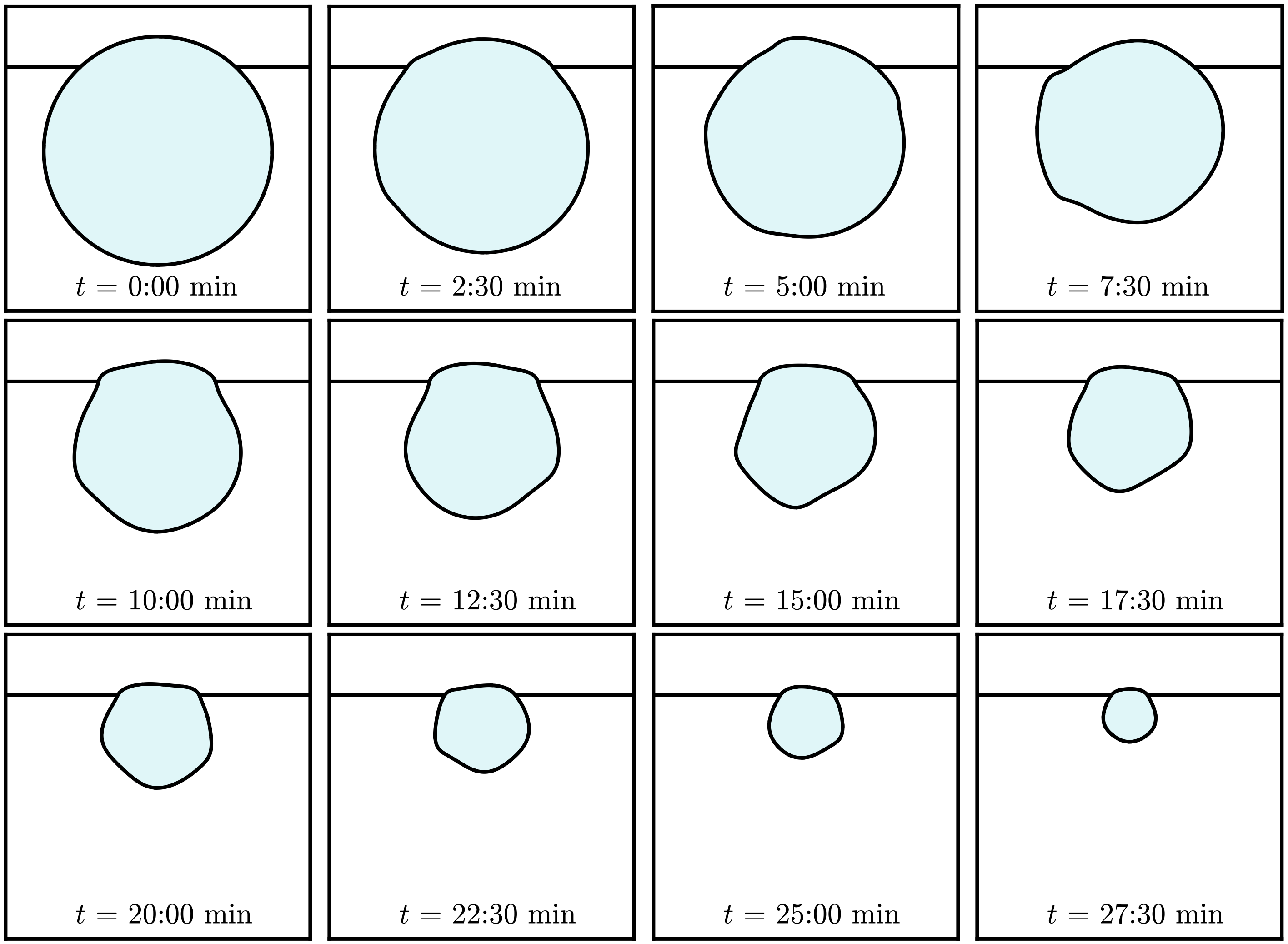
- Assume uniform melt rate below surface with boundary layer scaling

$$V_n = \begin{cases} \beta(L_0/L)^{1/4} & z < H \\ 0 & z \geq H \end{cases}$$

- Quasi-static center of mass dynamics follow Newton's laws







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t = 27:30 min

Discussion and future directions

- Ice persistently capsizes, no gravitationally stable terminal state
- Tends towards a polygonal geometry, is this attracting?
- What happens at low temperatures where the density anomaly plays a role?

Questions?

<u>Collaborators</u>
Bobae Johnson
Steven Zhang

Part II
Continuum modeling of active fluids

Swimming at low Reynolds number

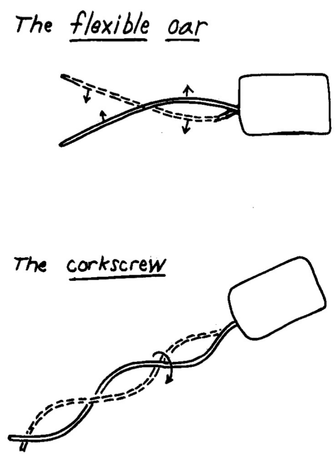
- At small scales, inertia is negligible

$$-\Delta \boldsymbol{u} + \nabla q = \nabla \cdot \boldsymbol{\Sigma} \qquad \mathrm{Re} = \frac{UL}{\nu} \ll 1$$

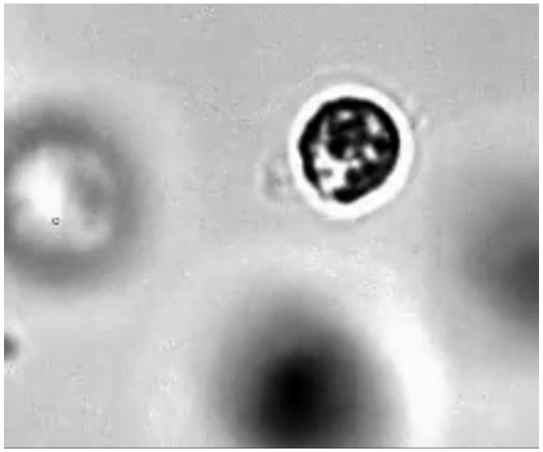
$$\nabla \cdot \boldsymbol{u} = 0$$

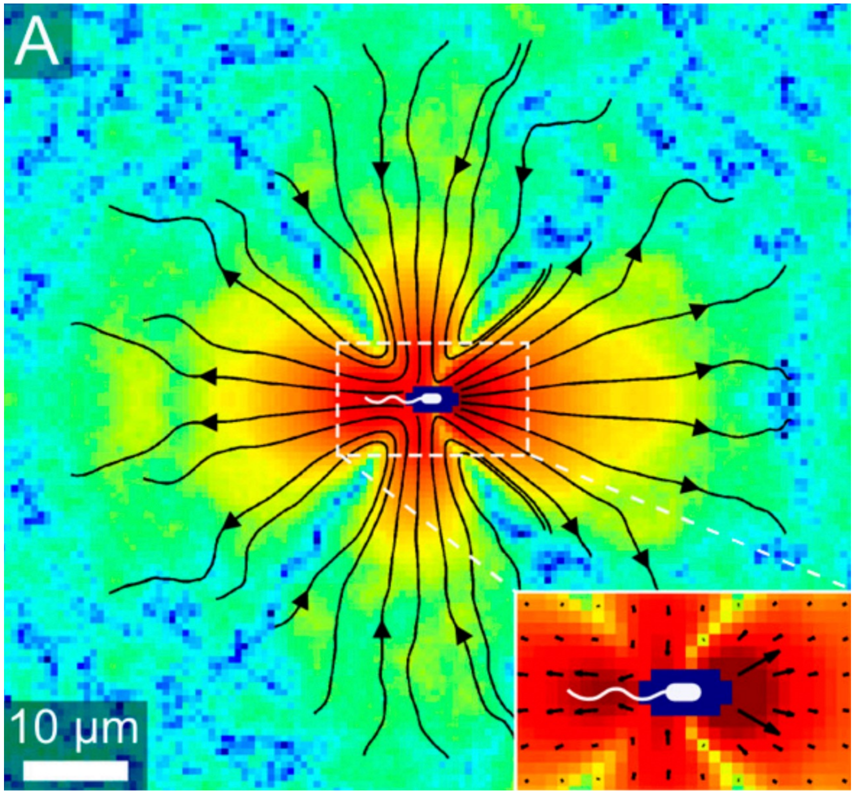
Stokes equations

- Linear, elliptic, time reversible – reciprocal strokes yield no net motion



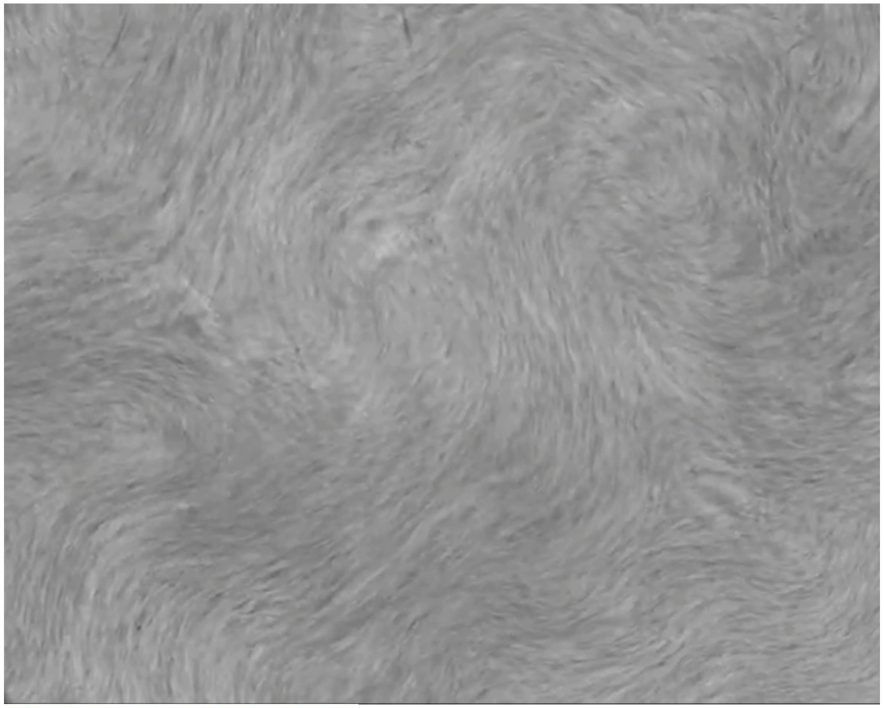
Purcell, *AIP* (1976)

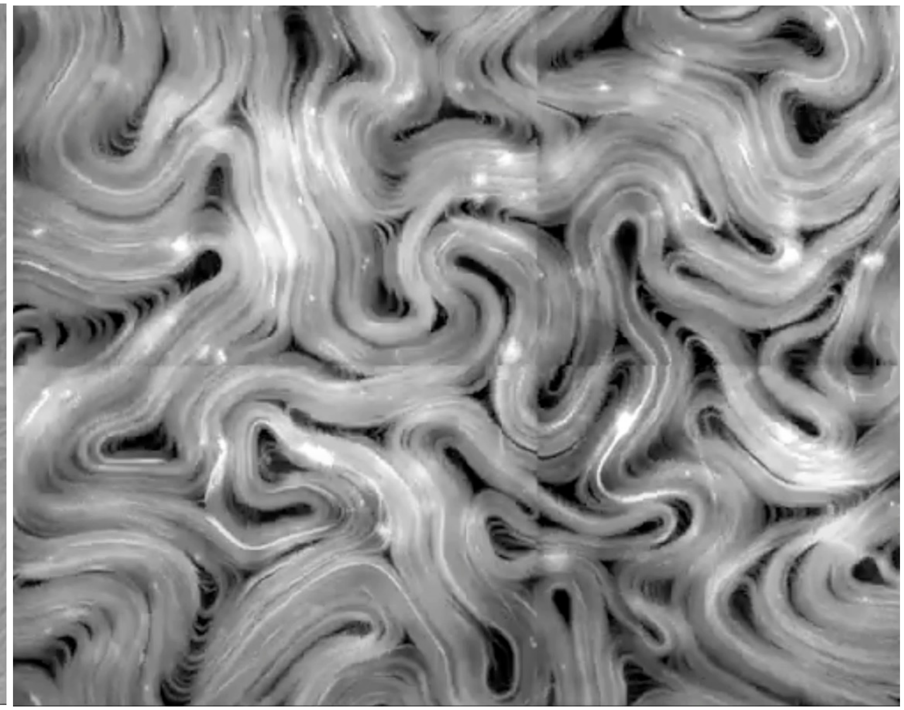


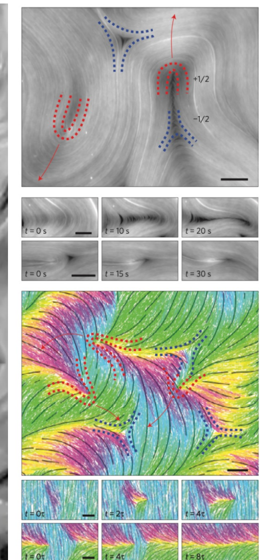


Drescher et al., *PNAS* (2011)

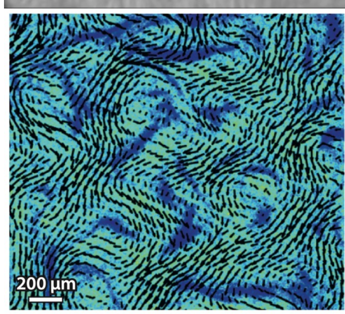
Collective flows of microswimmer suspensions



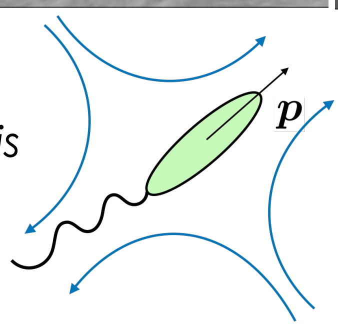




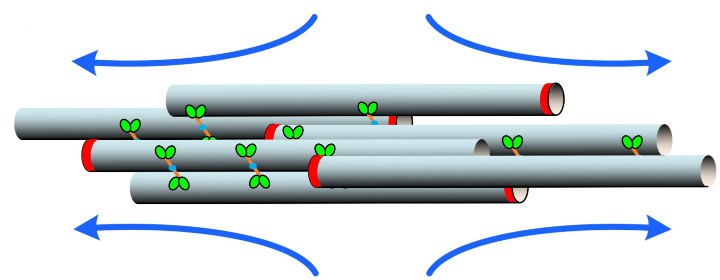
Dogic lab



B. Subtilis



Microtubules +
kinesin motors



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Doi-Saintillan-Shelley kinetic theory

- Particle position and orientation are represented by a continuous distribution function $\Psi(\boldsymbol{x}, \boldsymbol{p}, t)$

Microscopic model

$$\dot{\boldsymbol{x}} = v_s \boldsymbol{p} + \boldsymbol{u} - d_T \nabla_x \log \Psi$$

$$\dot{\boldsymbol{p}} = (\boldsymbol{I} - \boldsymbol{p}\boldsymbol{p}) \cdot \nabla \boldsymbol{u} \cdot \boldsymbol{p} - d_R \nabla_p \log \Psi$$

Conservation of particles

$$\frac{\partial \Psi}{\partial t} + \nabla_x \cdot (\dot{\boldsymbol{x}} \Psi) + \nabla_p \cdot (\dot{\boldsymbol{p}} \Psi) = 0$$

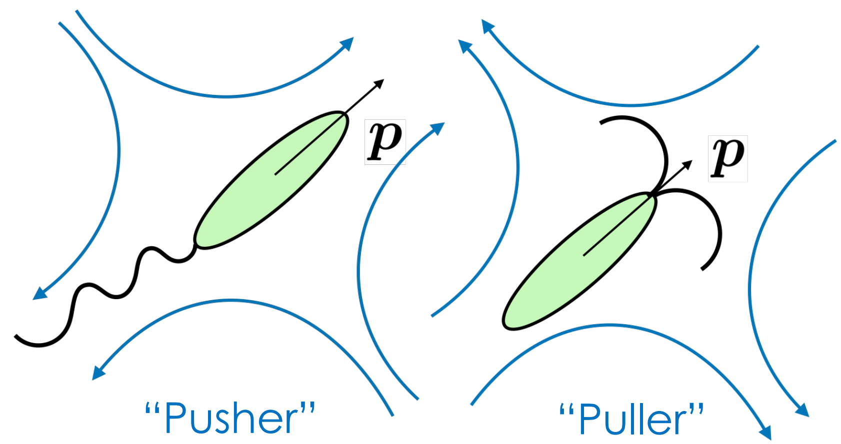
Conservation of momentum

$$-\Delta \boldsymbol{u} + \nabla q = \nabla \cdot \boldsymbol{\Sigma}$$

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

Active stress

$$\boldsymbol{\Sigma} = \alpha c \boldsymbol{Q}$$



"Pusher"
$\alpha < 0$

"Puller"
$\alpha > 0$

$$c(\boldsymbol{x}, t) = \int_{|\boldsymbol{p}|=1} \Psi \, d\boldsymbol{p}$$

$$\boldsymbol{Q}(\boldsymbol{x}, t) = (1/c) \int_{|\boldsymbol{p}|=1} \boldsymbol{p}\boldsymbol{p}\Psi \, d\boldsymbol{p}$$

Mean-field equations and the closure problem

- Kinetic theory has 2*d*-1degrees of freedom
- Evolve low-order orientational moments/order parameters

concentration: $c(\boldsymbol{x},t) = \langle 1 \rangle$

polar order: $\boldsymbol{n}(\boldsymbol{x},t) = \langle \boldsymbol{p} \rangle / c$

nematic order: $\boldsymbol{Q}(\boldsymbol{x},t) = \langle \boldsymbol{pp} \rangle / c$

$$\boldsymbol{R}(\boldsymbol{x},t) = \langle \boldsymbol{ppp} \rangle / c$$

$$\boldsymbol{S}(\boldsymbol{x},t) = \langle \boldsymbol{pppp} \rangle / c$$

$$\frac{Dc}{Dt} = -v_s \nabla \cdot (c\boldsymbol{n}) + H_c$$

$$(c\boldsymbol{n})^{\nabla} + c\boxed{\boldsymbol{R}} : \boldsymbol{E} = -v_s \nabla \cdot (c\boldsymbol{Q}) + \boldsymbol{H_n}$$

$$(c\boldsymbol{Q})^{\nabla} + 2c\boxed{\boldsymbol{S}} : \boldsymbol{E} = -v_s \nabla \cdot (c\boxed{\boldsymbol{R}}) + \boldsymbol{H_Q}$$

kinematic

swimming

diffusion, steric interactions

equations are not closed!

Quasi-equilibrium closure

- Seek a distribution function that minimizes the *conformational entropy*

$$\mathcal{S}(t) = \int_V \int_{|\boldsymbol{p}|=1} \left(\frac{\Psi}{\Psi_0}\right) \log\left(\frac{\Psi}{\Psi_0}\right) \, d\boldsymbol{p} d\boldsymbol{x}$$

- "Maximum entropy" distribution, analogous to Gibbs-Boltzmann

$$\boxed{\Psi_B(\boldsymbol{x}, \boldsymbol{p}, t) = Z^{-1}(\boldsymbol{x}, t) e^{\boldsymbol{B}(\boldsymbol{x},t):\boldsymbol{pp}+\boldsymbol{a}(\boldsymbol{x},t)\cdot\boldsymbol{p}}}$$

- Solve for this distribution constrained to known moments, then integrate to obtain higher moments

$$(c, \boldsymbol{n}, \boldsymbol{Q}) \mapsto (Z, \boldsymbol{a}, \boldsymbol{B}) \mapsto \begin{array}{l} \boldsymbol{R}_B = \langle \boldsymbol{ppp} \rangle_B / c \\ \boldsymbol{S}_B = \langle \boldsymbol{pppp} \rangle_B / c \end{array}$$

"*B*-model"

Thermodynamic consistency

- Quasi-equilibrium distribution preserves balance of entropy production and dissipation

$$\mathcal{S}'(t) = \mathcal{P}(t) - \mathcal{D}(t)$$

$$\mathcal{S}(t) = \int_V \int_{|\boldsymbol{p}|=1} \left(\frac{\Psi}{\Psi_0}\right) \log\left(\frac{\Psi}{\Psi_0}\right) \, d\boldsymbol{p} d\boldsymbol{x}$$

$$\mathcal{P}(t) = -\frac{2d}{\alpha} \int_V \boldsymbol{E} : \boldsymbol{E} \, d\boldsymbol{x}$$

$$\mathcal{D}(t) = \int_V \int_{|\boldsymbol{p}|=1} (d_T |\nabla_x \log \Psi|^2 + d_R |\nabla_p \log \Psi|^2) \Psi \, d\boldsymbol{p} d\boldsymbol{x}$$

- Analogous to fundamental thermodynamic relation out of equilibrium

Linear theory of the isotropic base state

- Homogeneous steady state:

$$\Psi_0 = 1/4\pi$$

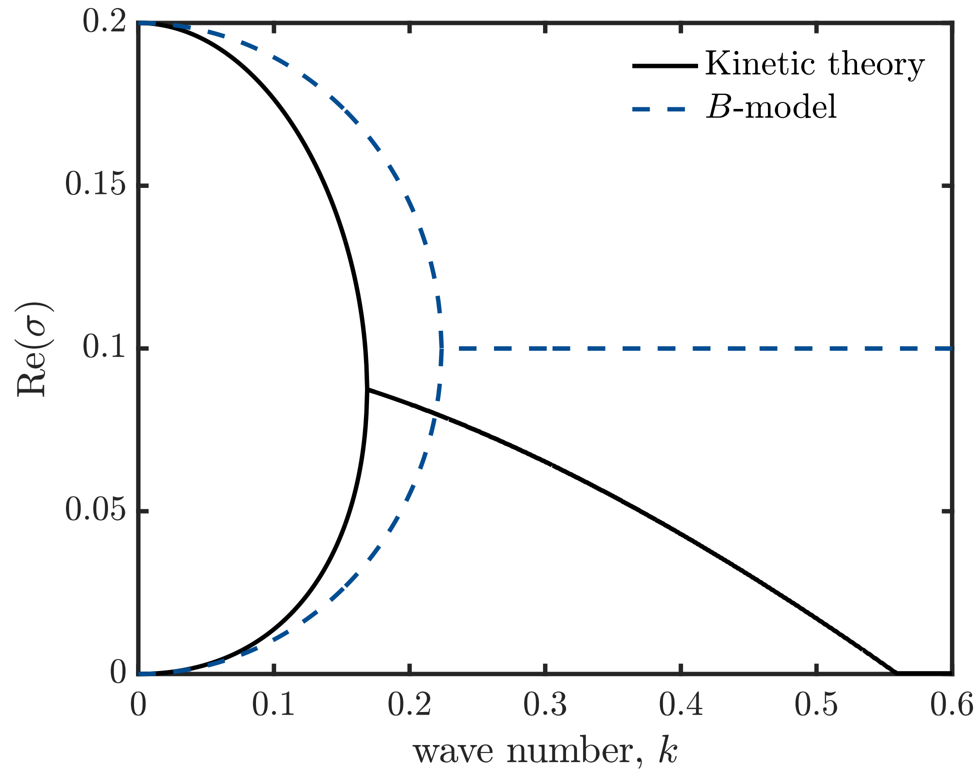
- Linearized distribution:

$$\Psi'_B = Z'^{-1}(1 + a_d \boldsymbol{n}' \cdot \boldsymbol{p} + b_d \boldsymbol{Q}' : \boldsymbol{pp})$$

- Consider plane-wave perturbations

$$\phi = \tilde{\phi}(\boldsymbol{k}) e^{\sigma t + i\boldsymbol{k}\cdot\boldsymbol{x}}$$

$$\sigma_\pm = -\frac{\alpha}{10} \pm \frac{1}{10}\left(\alpha^2 - 20k^2\right)^{1/2}$$



$\alpha < 0$ unstable

$\alpha > 0$ stable

Linear theory of the polar aligned base state

- Base state:

$$\Psi_0 = \lim_{\gamma \to \infty} Z^{-1} e^{\gamma \cos \phi}$$

- Linearized equations

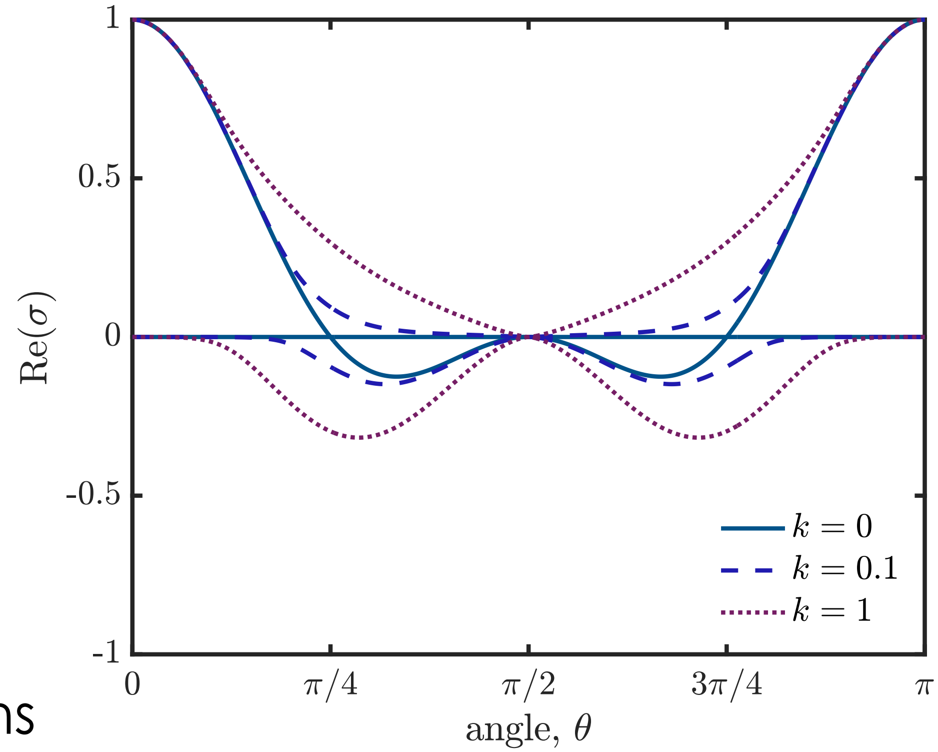
$$\frac{\partial c'}{\partial t} + \hat{\boldsymbol{z}} \cdot \nabla c' + \nabla \cdot \boldsymbol{n}' = 0$$

$$\frac{\partial \boldsymbol{n}'}{\partial t} + \hat{\boldsymbol{z}} \cdot \nabla \boldsymbol{n}' - (\boldsymbol{I} - \hat{\boldsymbol{z}}\hat{\boldsymbol{z}}) \cdot \nabla \boldsymbol{u}' \cdot \hat{\boldsymbol{z}} = 0$$

$$-\Delta \boldsymbol{u}' + \nabla q' = \alpha \nabla \cdot (c' \hat{\boldsymbol{z}}\hat{\boldsymbol{z}} + \hat{\boldsymbol{z}} \boldsymbol{n}' + \boldsymbol{n}' \hat{\boldsymbol{z}})$$

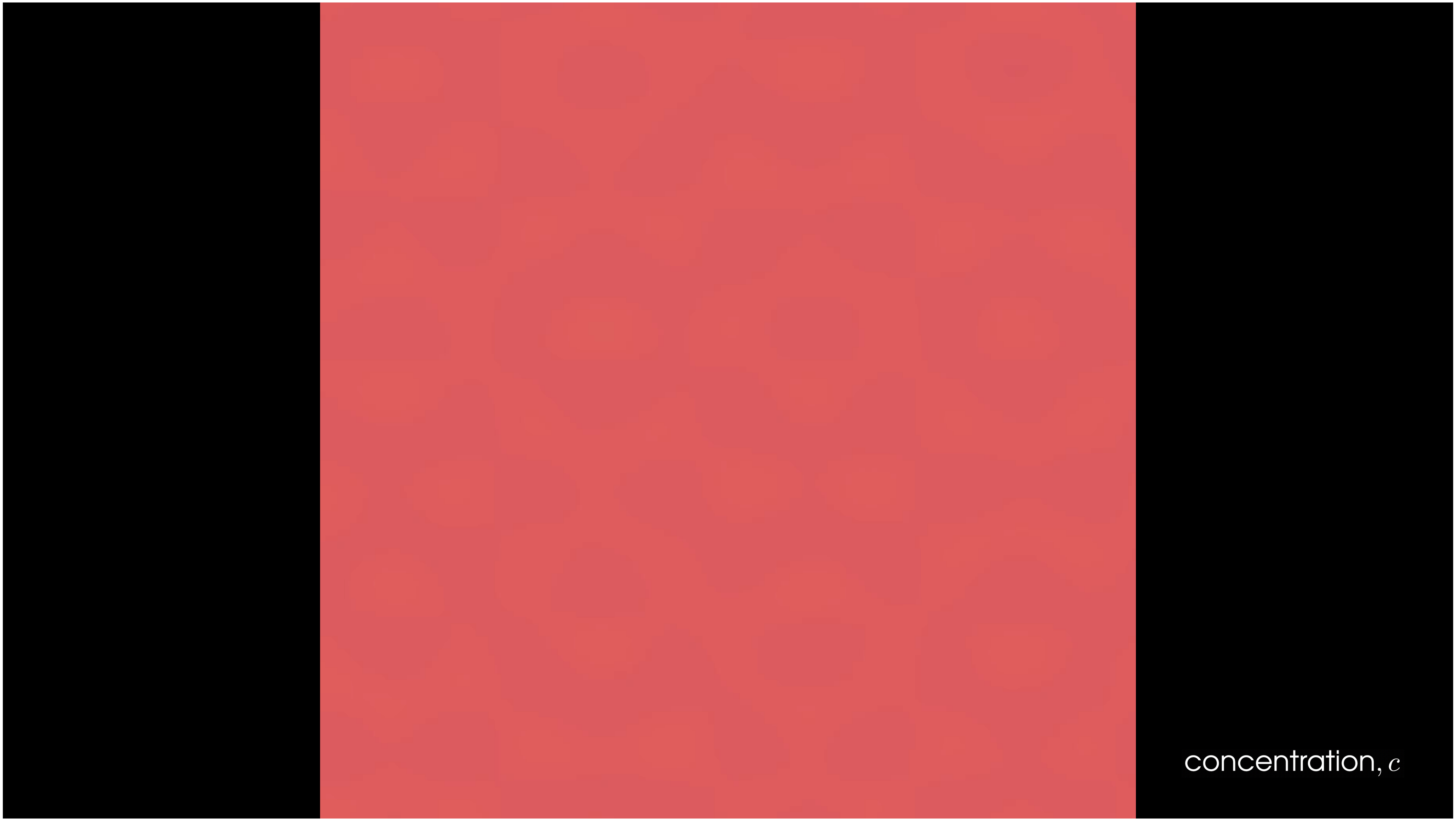
$$\nabla \cdot \boldsymbol{u}' = 0$$

- Consider plane-wave perturbations

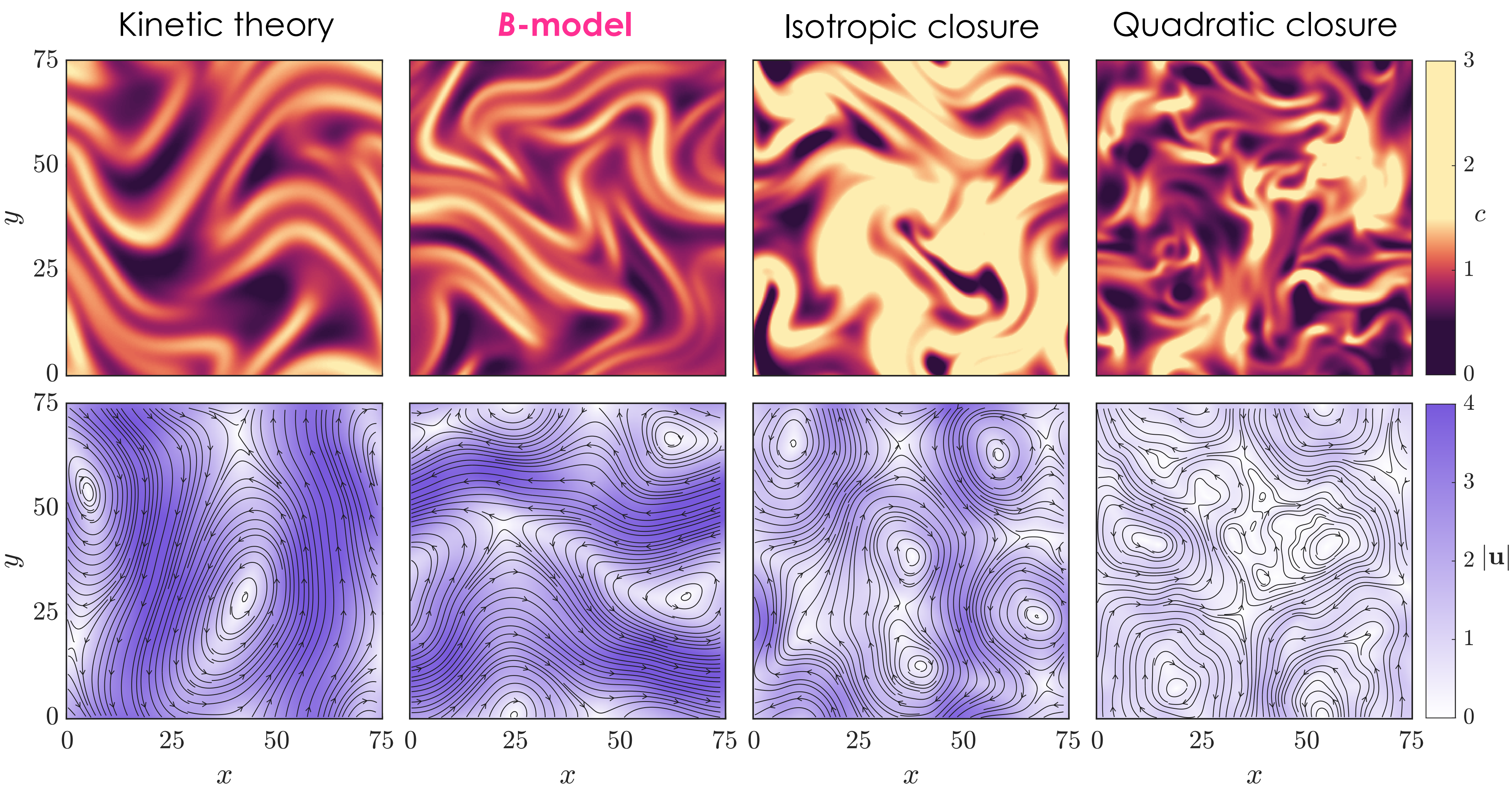


$$\sigma_{\pm} = \frac{1}{2} f(\theta) \cos 2\theta \left[1 \pm \left(1 - \frac{4ik}{\alpha} \frac{\sin^2 \theta \cos \theta}{f(\theta) \cos^2 2\theta} \right)^{1/2} \right] - ik \cos \theta$$

always unstable


concentration, c

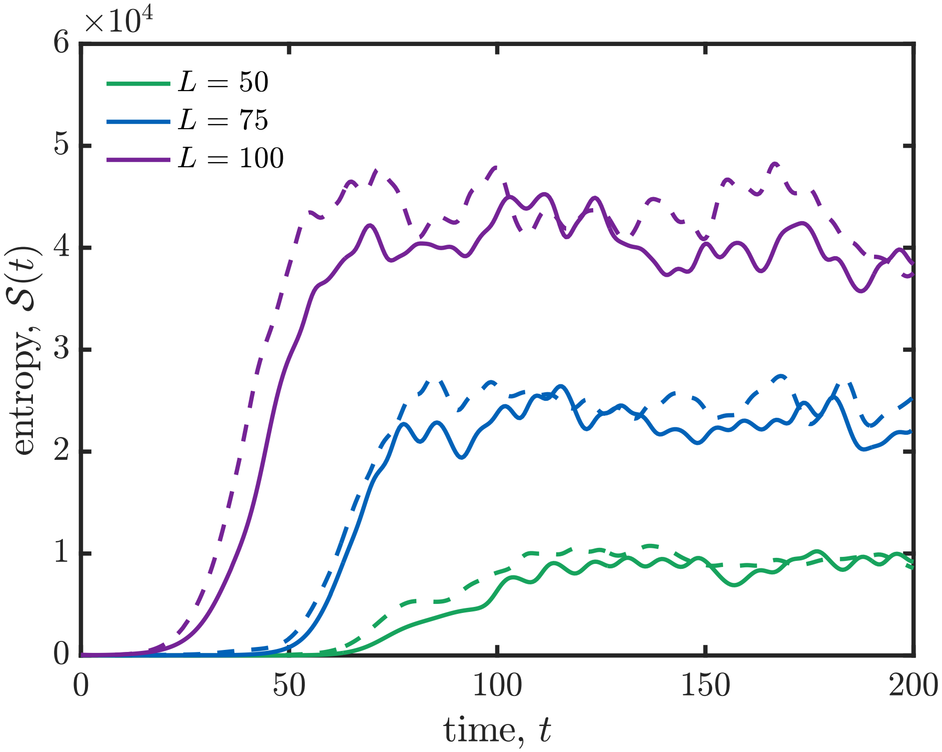
Nonlinear simulations

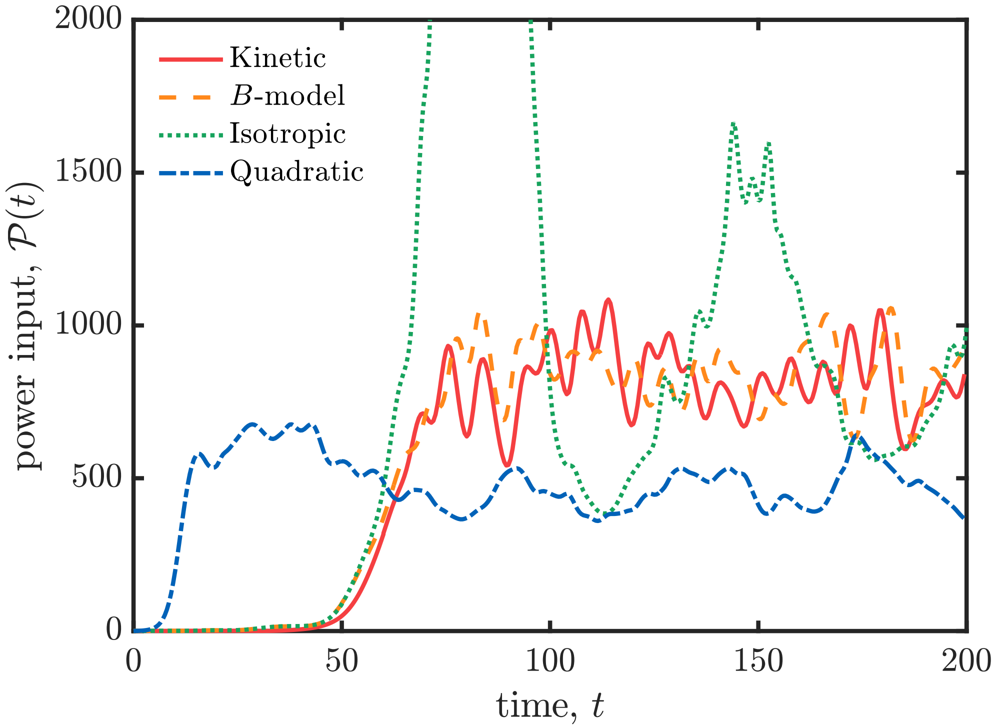


Entropy and fluctuations

$$\mathcal{S}(t) = \int_V \int_{|\boldsymbol{p}|=1} \left(\frac{\Psi}{\Psi_0}\right) \log\left(\frac{\Psi}{\Psi_0}\right) \, d\boldsymbol{p} d\boldsymbol{x}$$

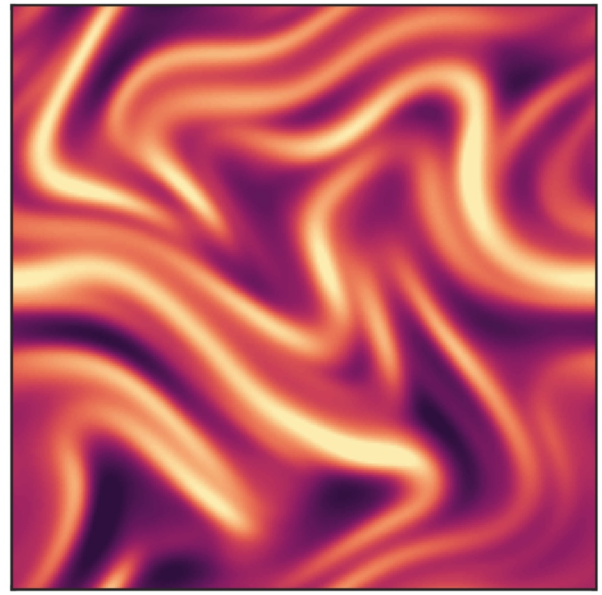
$$\mathcal{S}'(t) = \underline{\mathcal{P}(t)} - \mathcal{D}(t)$$





Discussion & conclusions

- Captures linear instabilities of the kinetic theory
- Preserves balance of conformational entropy production and dissipation – "thermodynamically consistent"
- Accurately reproduces nonlinear dynamics and nonequilibrium statistics



Questions?

David Stein

S. Weady, D.B. Stein, M.J. Shelley, "Thermodynamically consistent coarse-graining of polar active fluids," *Phys. Rev. Fluids* (2022)

Part I: Morphology of melting ice

1. Anomalous natural convective sculpting of melting ice
2. Capsize dynamics of laboratory icebergs

Part II: Continuum modeling of active fluids

3. Coarse-graining kinetic theories of microswimmer suspensions
4. Numerical methods

Inverse problem for the quasi-equilibrium distribution

- The *B*-model consists of a mapping

$$(c, \boldsymbol{n}, \boldsymbol{Q}) \mapsto (\boldsymbol{R}_B, \boldsymbol{S}_B)$$

- Need to solve for the distribution function to match known moments

Constraints

$$c = \int_{|\boldsymbol{p}|=1} \Psi_B \, d\boldsymbol{p}$$

$$\boldsymbol{n} = (1/c) \int_{|\boldsymbol{p}|=1} \boldsymbol{p} \Psi_B \, d\boldsymbol{p}$$

$$\boldsymbol{Q} = (1/c) \int_{|\boldsymbol{p}|=1} \boldsymbol{p}\boldsymbol{p} \Psi_B \, d\boldsymbol{p}$$

$$\Psi_B(\boldsymbol{x}, \boldsymbol{p}, t) = \underline{Z}^{-1}(\boldsymbol{x}, t) e^{\underline{\boldsymbol{B}(\boldsymbol{x},t)}:\boldsymbol{p}\boldsymbol{p} + \underline{\boldsymbol{a}(\boldsymbol{x},t)}\cdot\boldsymbol{p}}$$

$$\boldsymbol{R}_B = \langle \boldsymbol{p}\boldsymbol{p}\boldsymbol{p} \rangle_B, \boldsymbol{S}_B = \langle \boldsymbol{p}\boldsymbol{p}\boldsymbol{p}\boldsymbol{p} \rangle_B$$

5 (2D) or 8 (3D) dimensional nonlinear system – **interpolate**

Interpolation in the nematic frame

- Define $\tilde{\boldsymbol{n}} = \boldsymbol{\Omega}^T \boldsymbol{n}, \tilde{\boldsymbol{Q}} = \boldsymbol{\Omega}^T \boldsymbol{Q} \boldsymbol{\Omega}$ where $\tilde{\boldsymbol{Q}} = \mathrm{diag}\{\mu_1, \ldots, \mu_d\}$
- Reparametrize the unit sphere by $\tilde{\boldsymbol{p}} = \boldsymbol{\Omega}^T \boldsymbol{p}$

$$\tilde{\boldsymbol{n}} = \frac{\int_{|\tilde{\boldsymbol{p}}|=1} \tilde{\boldsymbol{p}} e^{\tilde{\boldsymbol{B}}:\tilde{\boldsymbol{p}}\tilde{\boldsymbol{p}}+\tilde{\boldsymbol{a}}\cdot\tilde{\boldsymbol{p}}} \, d\tilde{\boldsymbol{p}}}{\int_{|\tilde{\boldsymbol{p}}|=1} e^{\tilde{\boldsymbol{B}}:\tilde{\boldsymbol{p}}\tilde{\boldsymbol{p}}+\tilde{\boldsymbol{a}}\cdot\tilde{\boldsymbol{p}}} \, d\tilde{\boldsymbol{p}}}$$

d d.o.f

$$\tilde{\boldsymbol{Q}} = \frac{\int_{|\tilde{\boldsymbol{p}}|=1} \tilde{\boldsymbol{p}}\tilde{\boldsymbol{p}} e^{\tilde{\boldsymbol{B}}:\tilde{\boldsymbol{p}}\tilde{\boldsymbol{p}}+\tilde{\boldsymbol{a}}\cdot\tilde{\boldsymbol{p}}} \, d\tilde{\boldsymbol{p}}}{\int_{|\tilde{\boldsymbol{p}}|=1} e^{\tilde{\boldsymbol{B}}:\tilde{\boldsymbol{p}}\tilde{\boldsymbol{p}}+\tilde{\boldsymbol{a}}\cdot\tilde{\boldsymbol{p}}} \, d\tilde{\boldsymbol{p}}}$$

(d-1) d.o.f

$$(\tilde{\boldsymbol{n}}, \tilde{\boldsymbol{Q}}) \mapsto (\tilde{\boldsymbol{R}}_B, \tilde{\boldsymbol{S}}_B)$$

3 (2D) or 5 (3D) degrees of freedom

Apolar suspensions: the Bingham closure

- For apolar states, $\boldsymbol{n} = 0$, distribution is invariant under $\boldsymbol{p} \mapsto -\boldsymbol{p}$
- Reduces to a (*d*-1)-dimensional system of equations

$$\tilde{\boldsymbol{Q}} = \frac{\int_{|\boldsymbol{p}|=1} \boldsymbol{p}\boldsymbol{p} e^{\tilde{\boldsymbol{B}}:\boldsymbol{p}\boldsymbol{p}}\, d\boldsymbol{p}}{\int_{|\boldsymbol{p}|=1} e^{\tilde{\boldsymbol{B}}:\boldsymbol{p}\boldsymbol{p}}\, d\boldsymbol{p}}$$

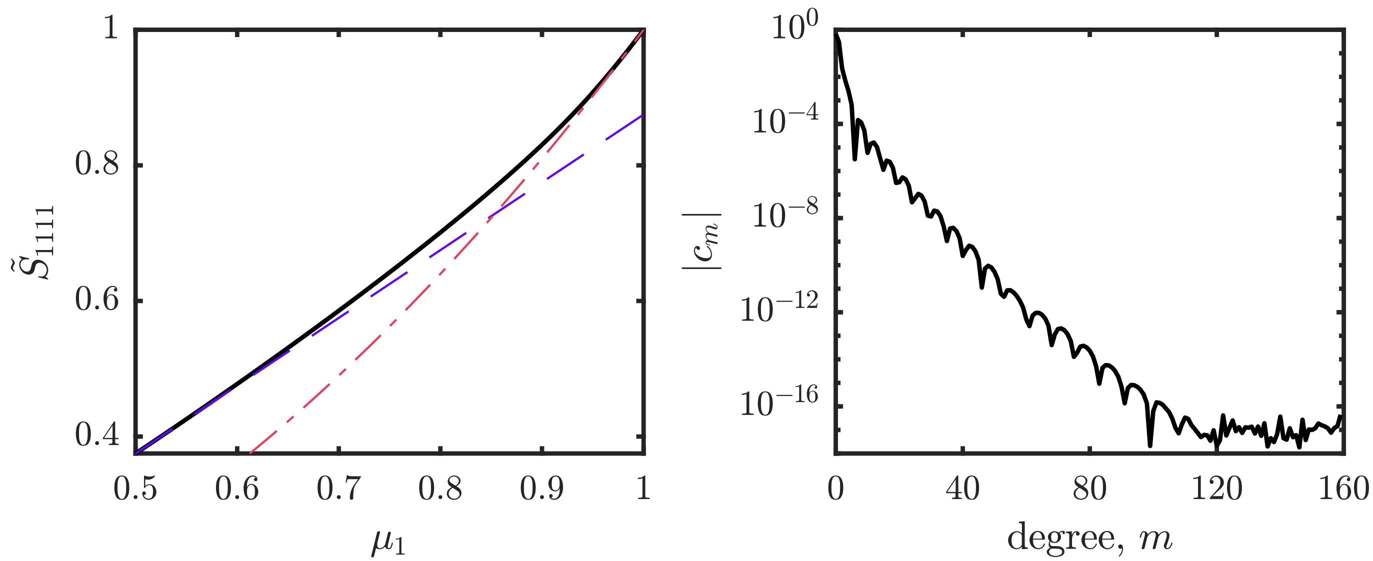
- Map from (*d*-1) eigenvalues of $\tilde{\boldsymbol{Q}}$ to diagonal components of $\tilde{\boldsymbol{S}}_B$

C. Chaubal & L.G. Leal, *Journal of Rheology* (1998)

Apolar suspensions: two dimensions

$$\mu_1 = \frac{\int_0^{2\pi} \cos^2 \theta e^{\lambda \cos 2\theta} \, d\theta}{\int_0^{2\pi} e^{\lambda \cos 2\theta} \, d\theta} \longrightarrow \tilde{S}_{1111} = \frac{\int_0^{2\pi} \cos^4 \theta e^{\lambda \cos 2\theta} \, d\theta}{\int_0^{2\pi} e^{\lambda \cos 2\theta} \, d\theta}$$

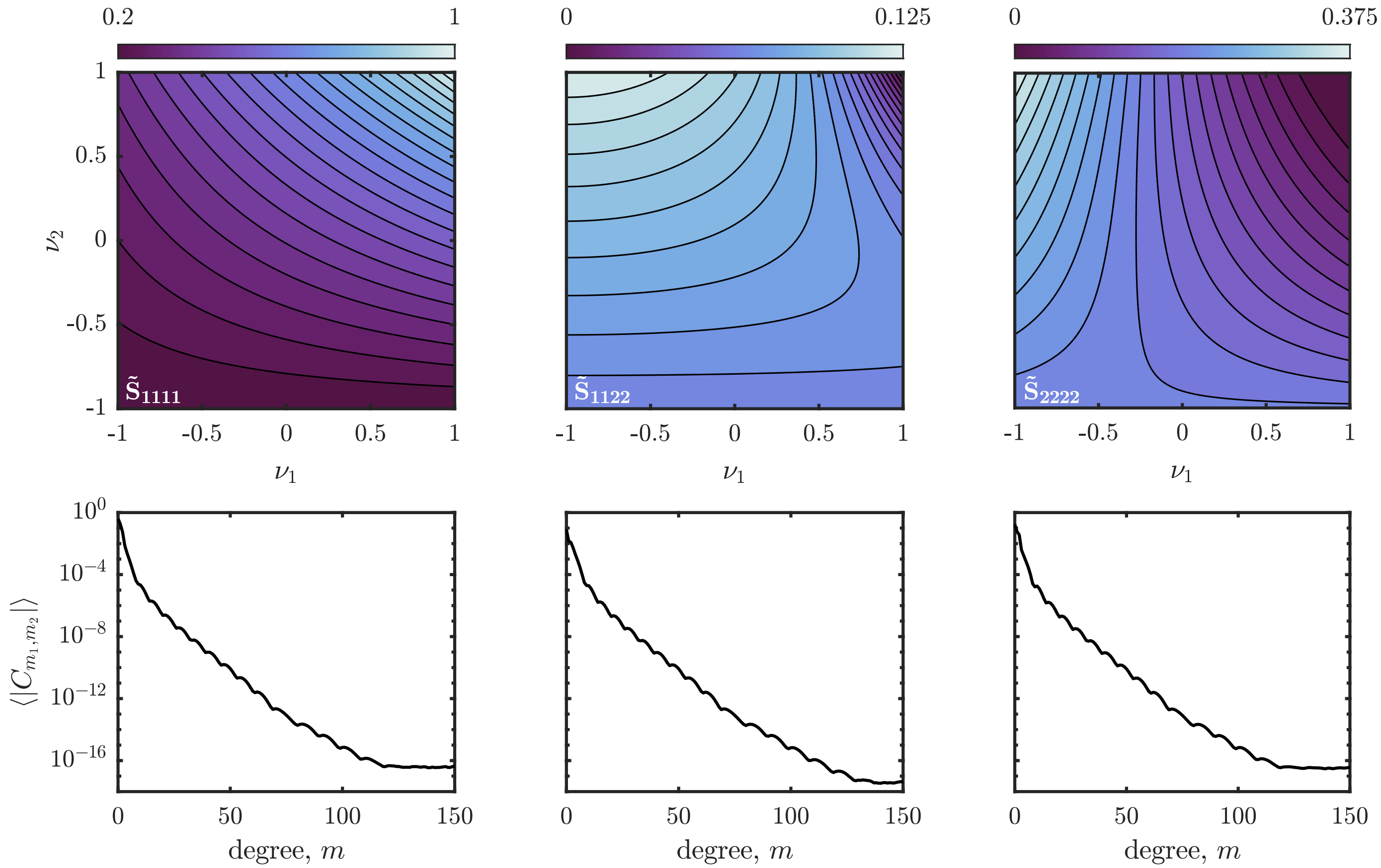
Expand in Chebyshev basis: $\tilde{S}_{1111}(\mu_1) \approx \sum_{m=0}^{M} c_m T_m(4\mu_1 - 3)$



Apolar suspensions: three dimensions

$$\mu_1 = \langle p_1^2 \rangle / \langle 1 \rangle$$
$$\mu_2 = \langle p_2^2 \rangle / \langle 1 \rangle$$

$$\tilde{S}_{1111} = \langle p_1^4 \rangle / \langle 1 \rangle$$
$$\tilde{S}_{1122} = \langle p_1^2 p_2^2 \rangle / \langle 1 \rangle$$
$$\tilde{S}_{2222} = \langle p_2^4 \rangle / \langle 1 \rangle$$



Expand in separable Chebyshev basis: $\tilde{S}_{iijj} = \sum_{m+n \leq M} C_{mn}^{ij} T_m(\nu_1) T_n(\nu_2)$

Polar suspensions

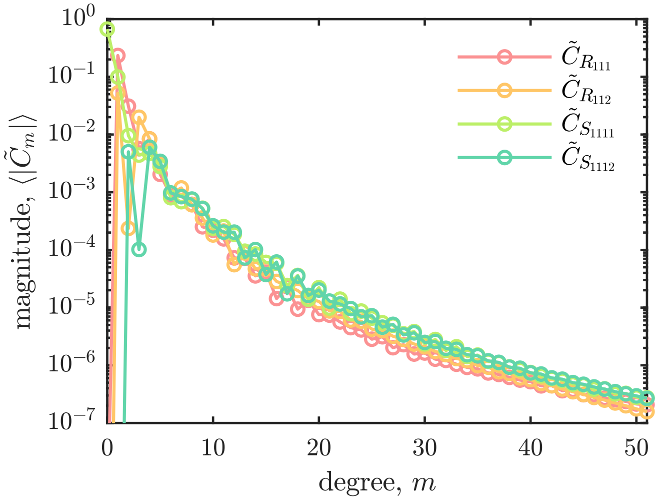
- Now need the full map $(\tilde{\boldsymbol{n}}, \tilde{\boldsymbol{Q}}) \mapsto (\tilde{\boldsymbol{R}}_B, \tilde{\boldsymbol{S}}_B)$
- Transform domain of moment constraints to hypercube, expand in Chebyshev basis

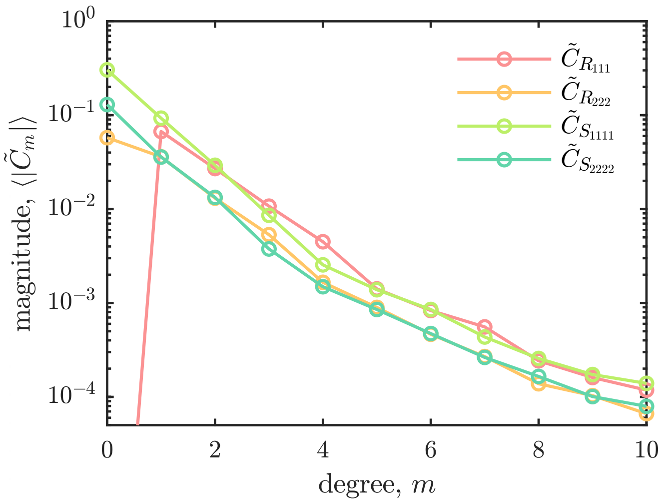
$$\tilde{\boldsymbol{R}}_B = \sum_{\ell+m+n} \boldsymbol{C}^R_{\ell mn} T_\ell(x) T_m(y) T_n(u)$$

$$\tilde{\boldsymbol{S}}_B = \sum_{\ell+m+n} \boldsymbol{C}^S_{\ell mn} T_\ell(x) T_m(y) T_n(u)$$

$$\tilde{\boldsymbol{R}}_B = \sum_{\ell+m+n+p+q} \boldsymbol{C}^R_{\ell mnpq} T_\ell(x) T_m(y) T_n(z) T_p(u) T_q(v)$$

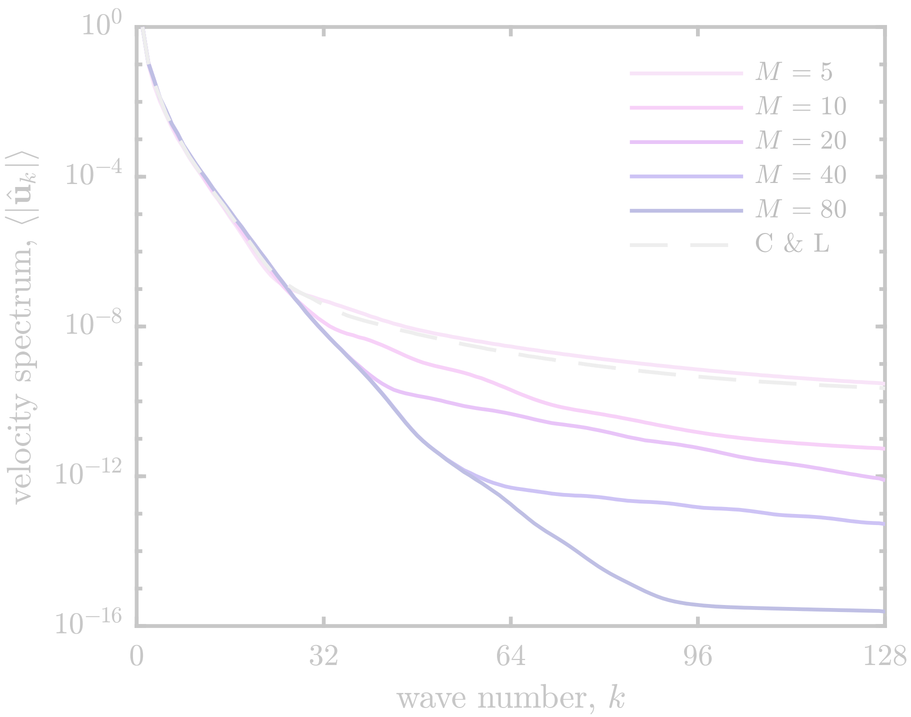
$$\tilde{\boldsymbol{S}}_B = \sum_{\ell+m+n+p+q} \boldsymbol{C}^S_{\ell mnpq} T_\ell(x) T_m(y) T_n(z) T_p(u) T_q(v)$$

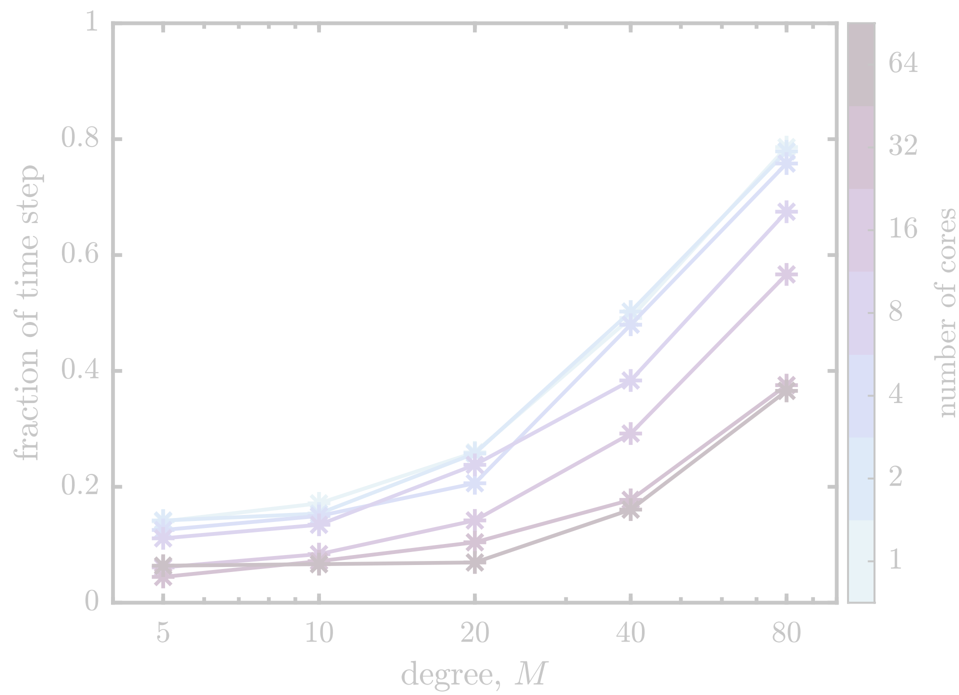




Cost and convergence (3D)

- Low accuracy in closure map limits spatial accuracy
- Execution time of interpolants is comparable to FFTs



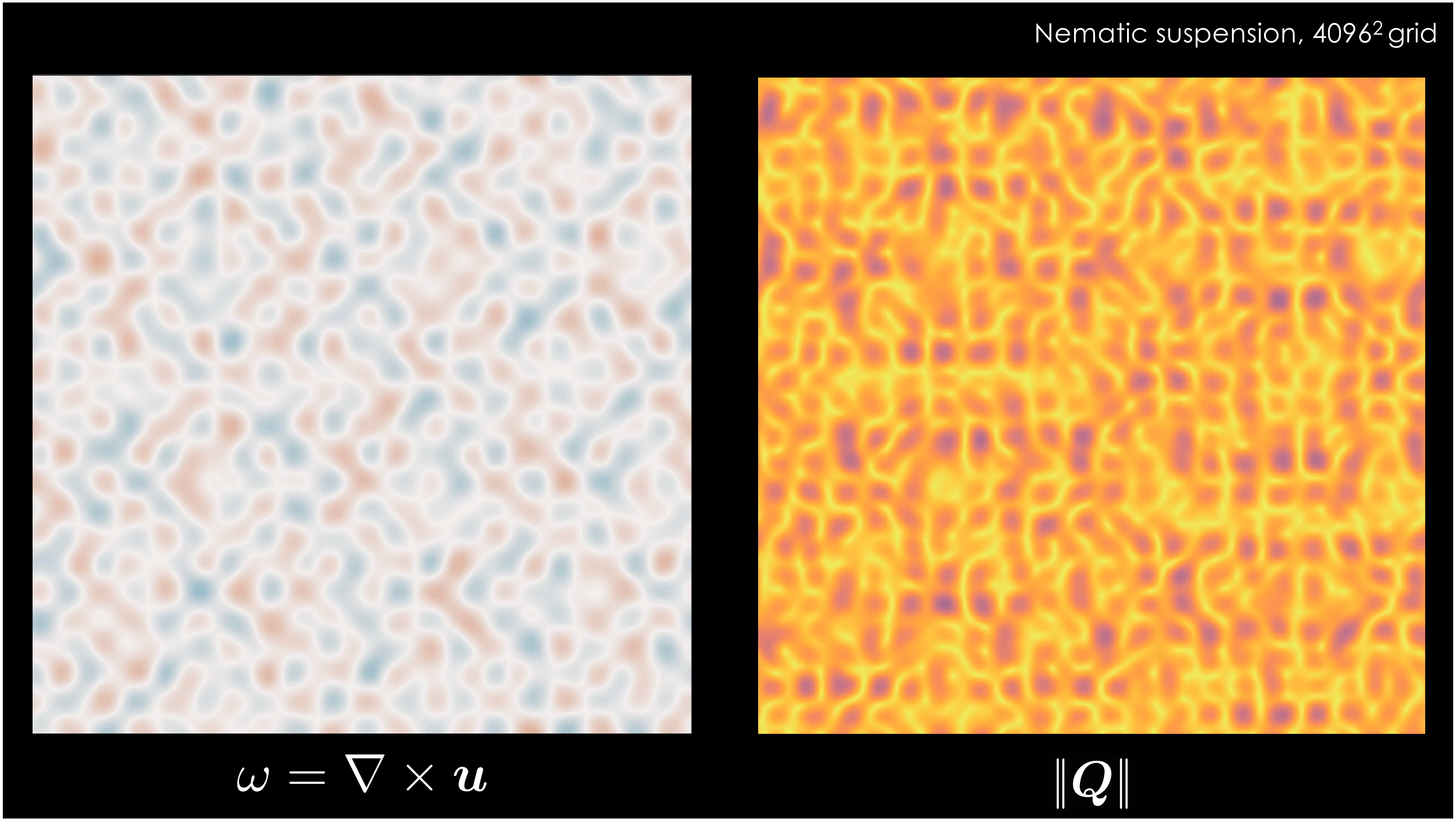


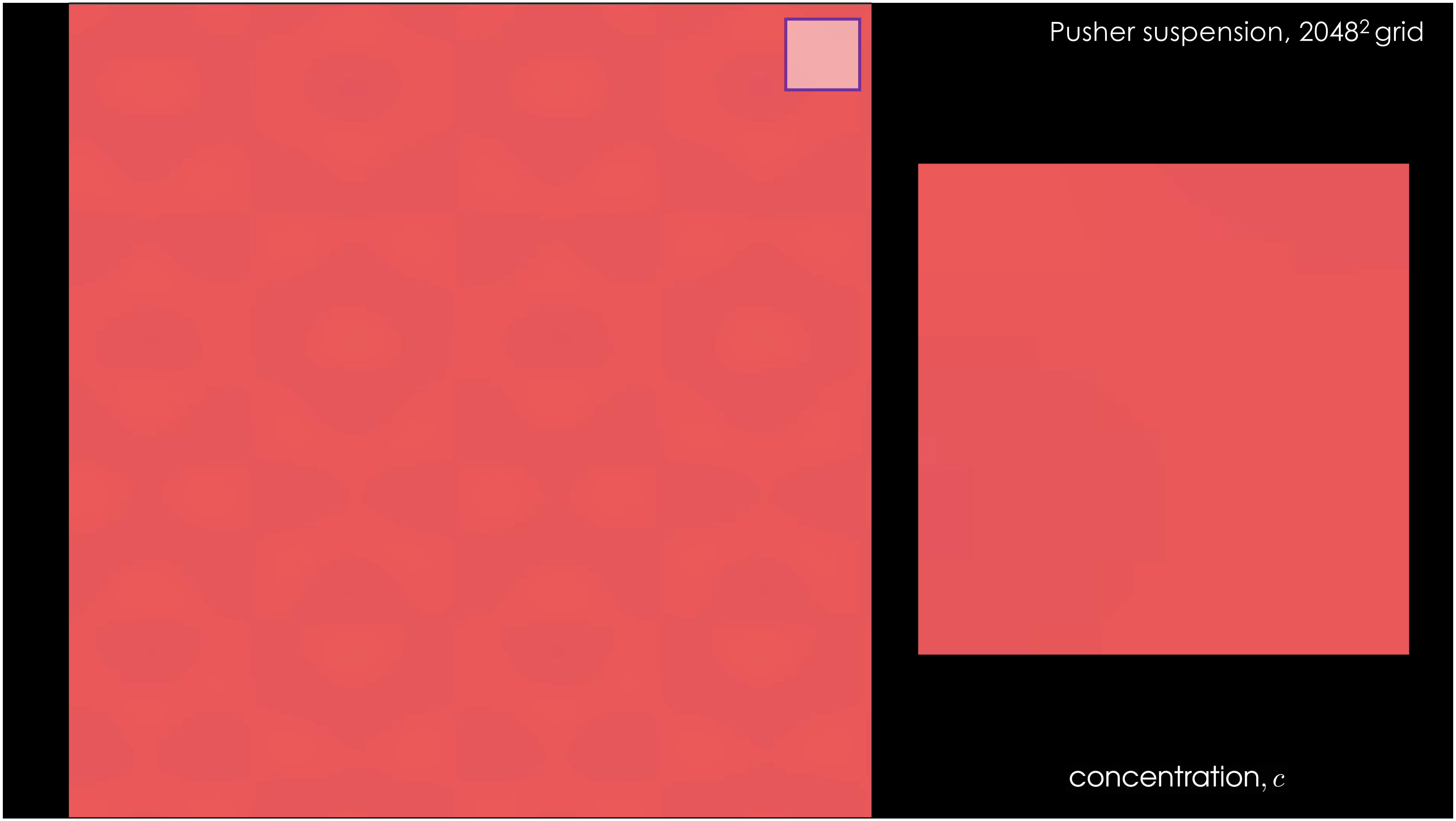
Discussion & conclusions

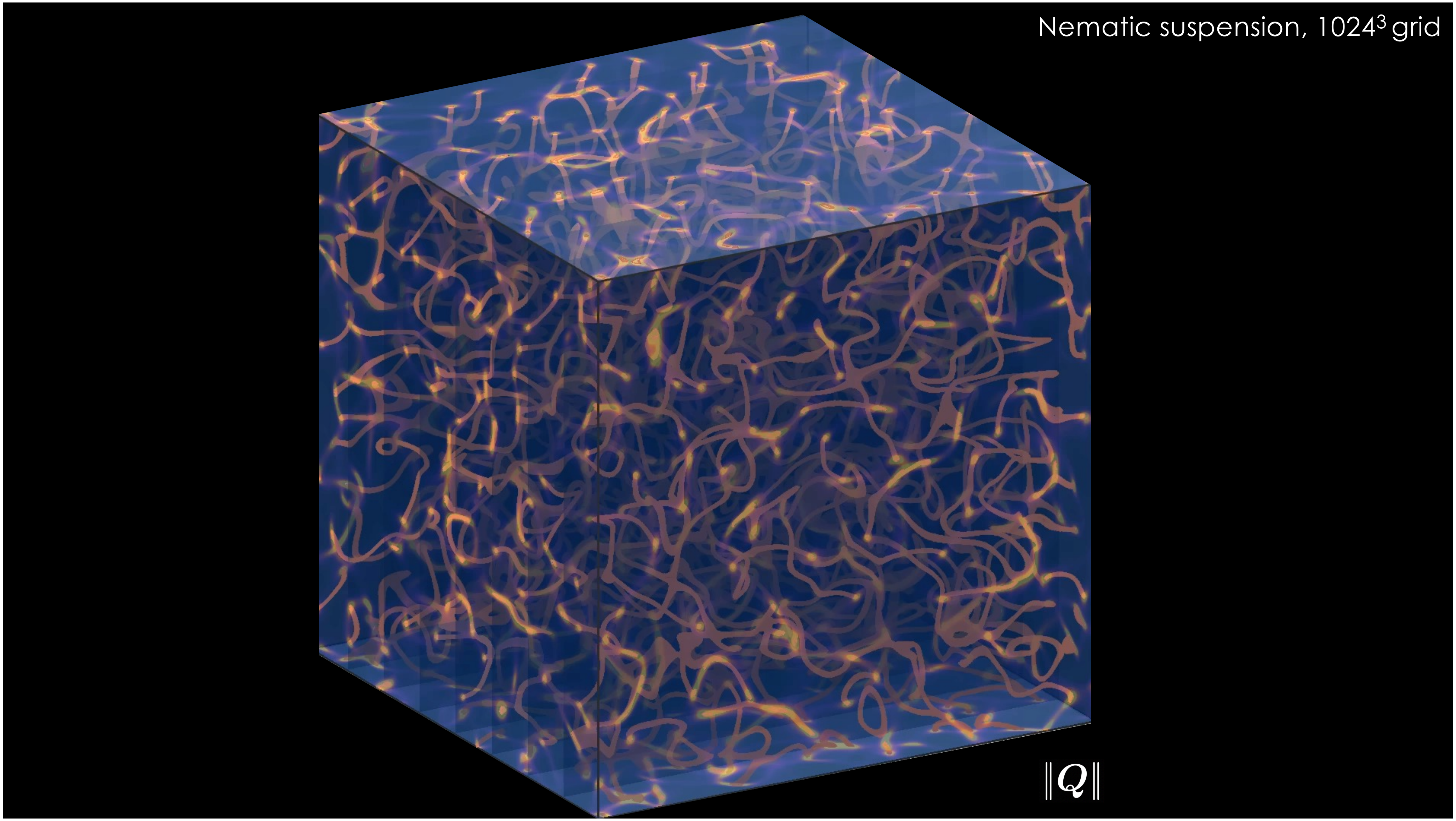
- Chebyshev interpolation preserves accuracy of nonlinear solve at low cost
- Inaccurate interpolation results in slow decay in Fourier coefficients of mean-field variables
- Rotation-based framework extends to polar suspensions, but cost is high – further approximations may be needed

S. Weady, M.J. Shelley, D.B. Stein, "A fast Chebyshev method for the Bingham closure with application to active nematic suspensions," *J. Comp. Phys.* (2022)

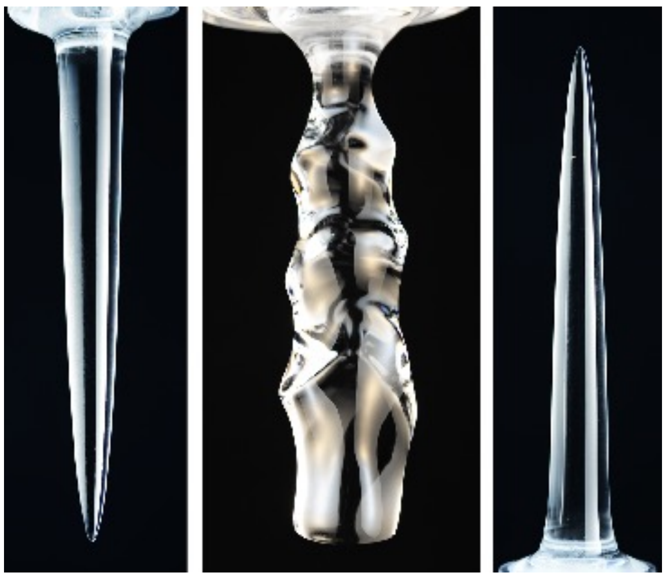
David Stein

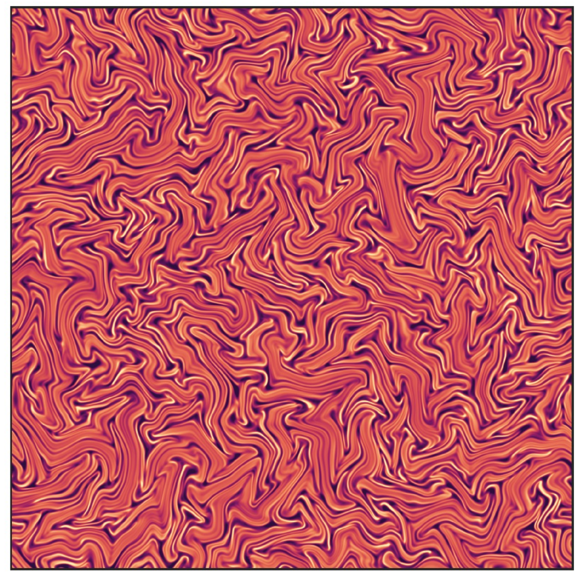

Nematic suspension, 4096² grid
$\omega = \nabla \times \boldsymbol{u}$
$\|\boldsymbol{Q}\|$

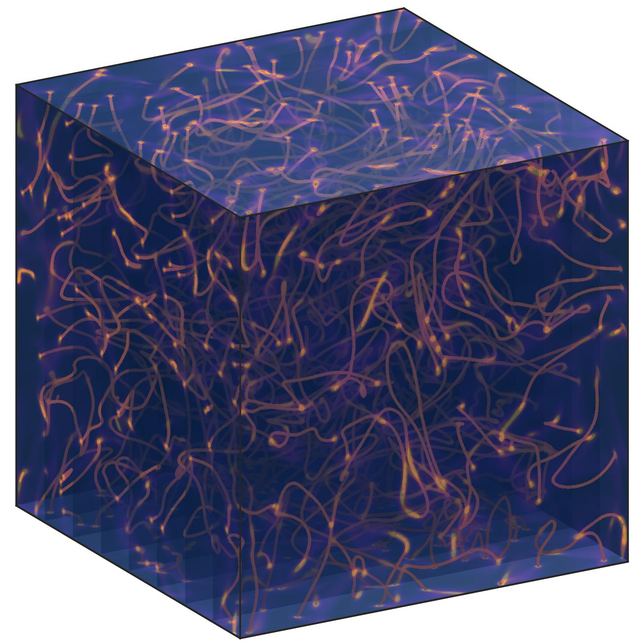

Pusher suspension, 2048^2 grid
concentration, c


Nematic suspension, 1024^3 grid
$\|Q\|$

Thanks! Questions?







References:

- S. Weady, J. Tong, A. Zidovska, L. Ristroph, "Anomalous convective flows carve pinnacles and scallops in melting ice," *Phys. Rev. Letters* (2022)
- S. Weady, D.B. Stein, M.J. Shelley, "Thermodynamically consistent coarse-graining of polar active fluids," *Phys. Rev. Fluids* (2022)
- S. Weady, M.J. Shelley, D.B. Stein, "A fast Chebyshev method for the Bingham closure with application to active nematic suspensions," *J. Comp. Phys.* (2022)