Hydrodynamics beyond Navier-Stokes:

Nanofluidic transport through the lens of the numerical model

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Blue Waters Symposium
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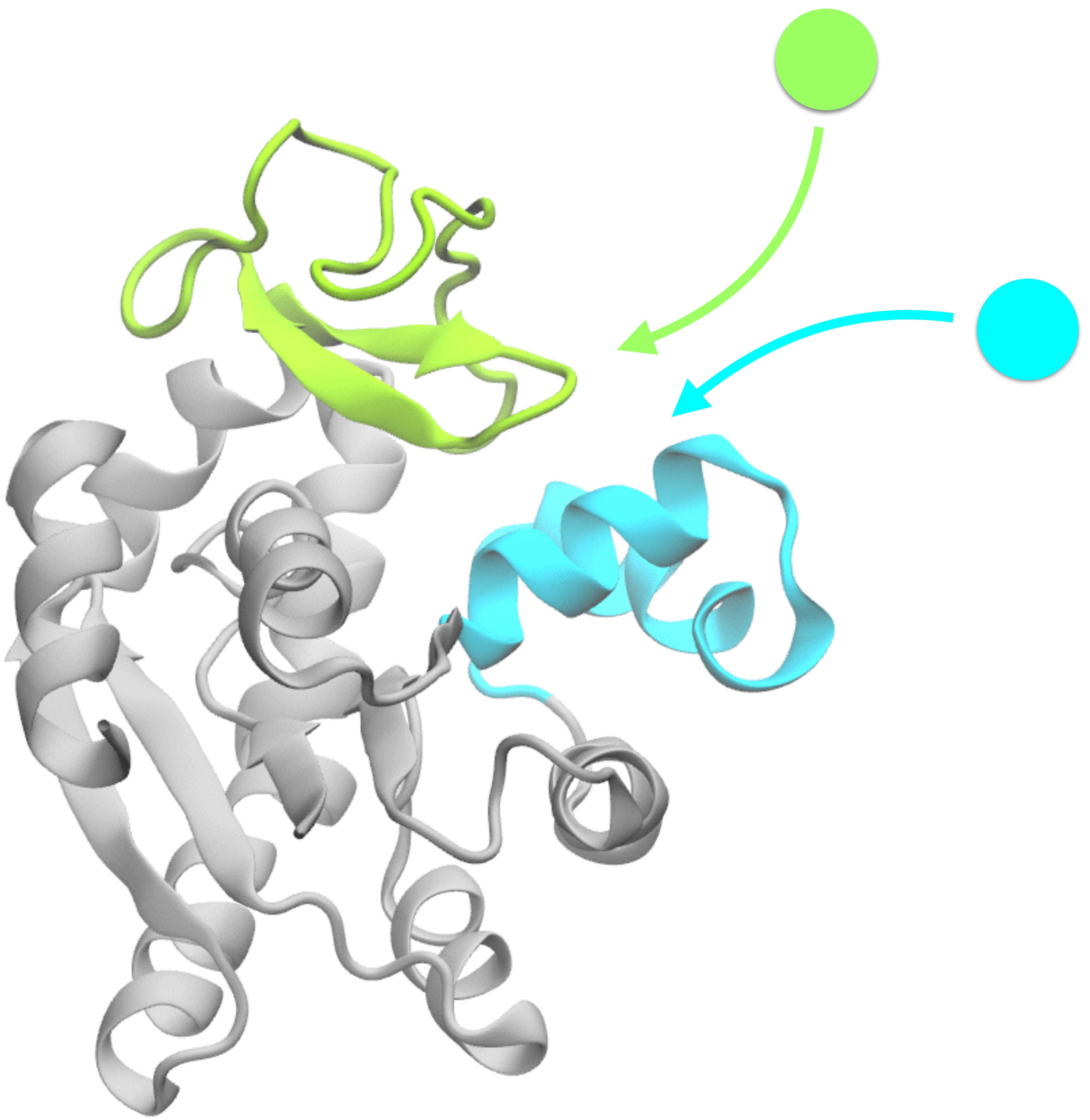
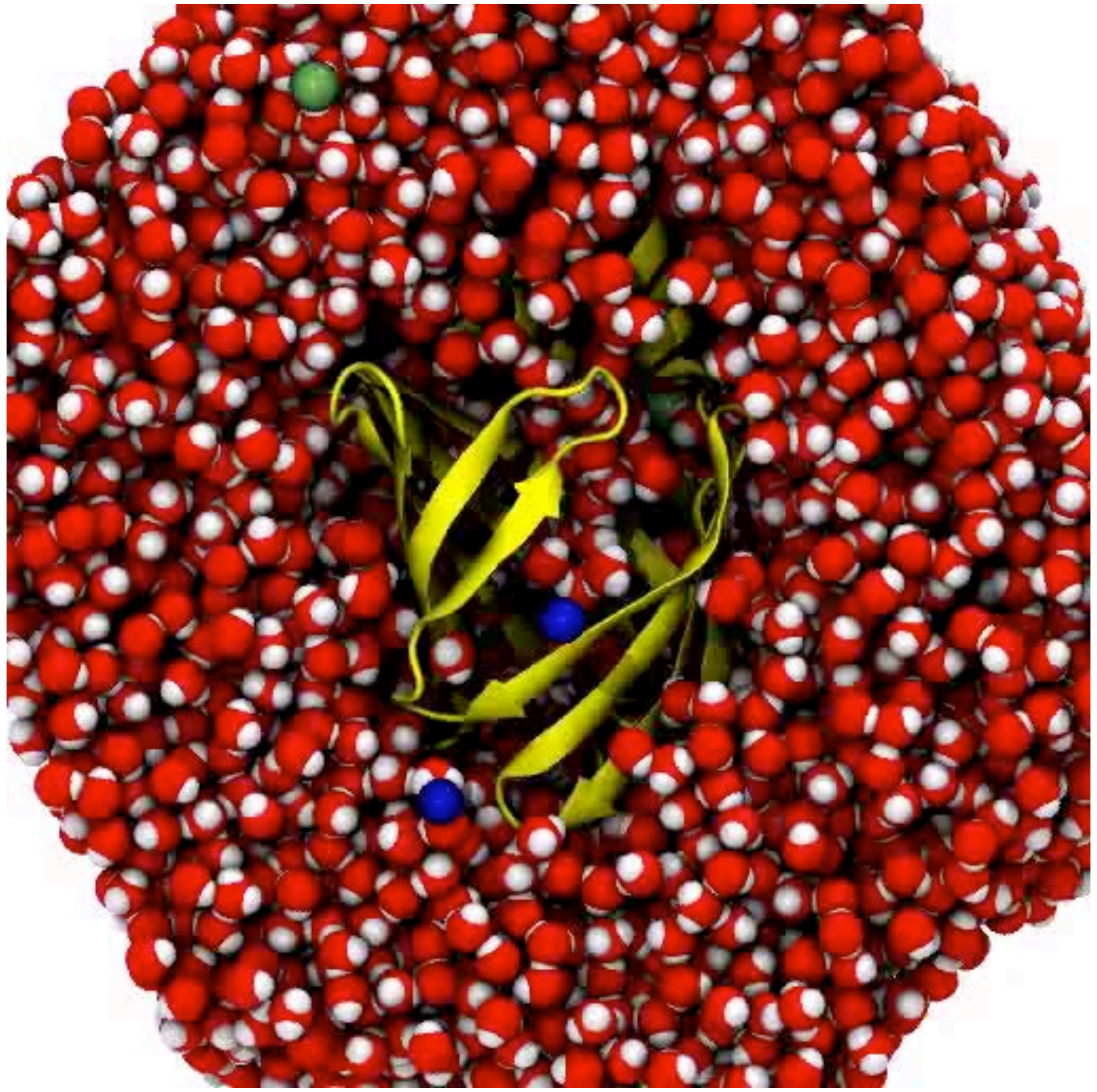
Structure-function connection

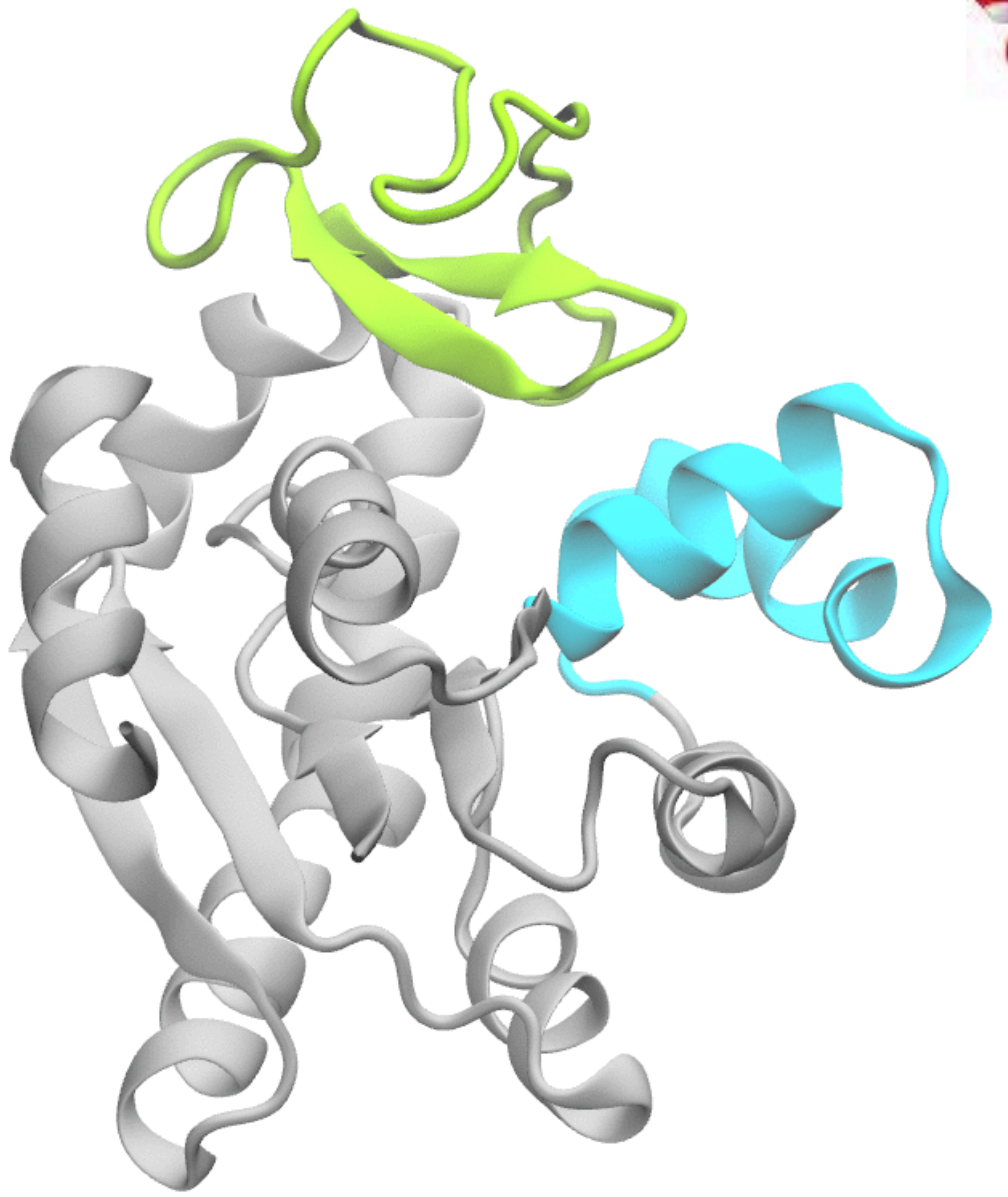


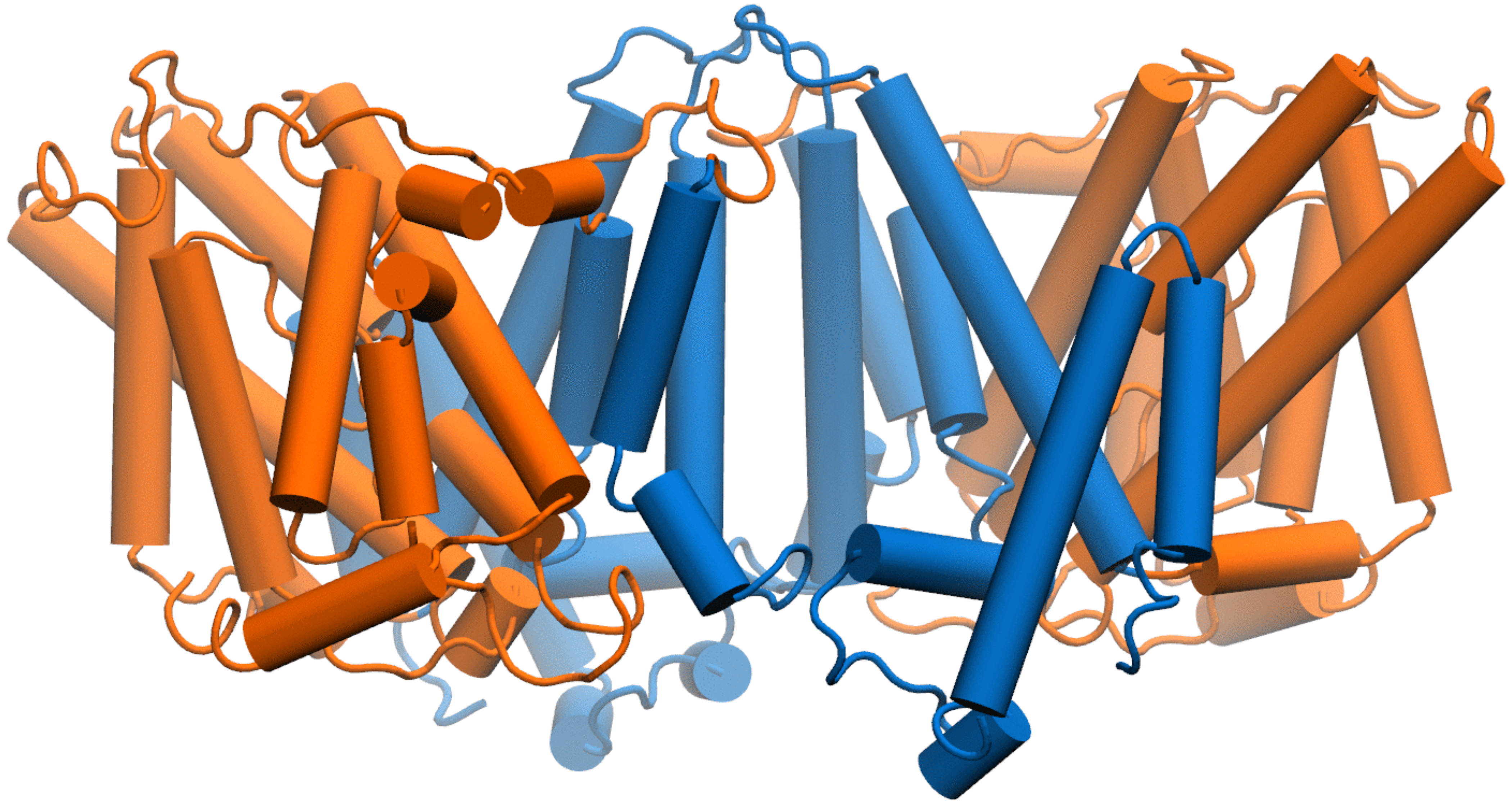
Structure-function connection

What about the solvent bath?



Timescales of interest:
micro- to milliseconds+



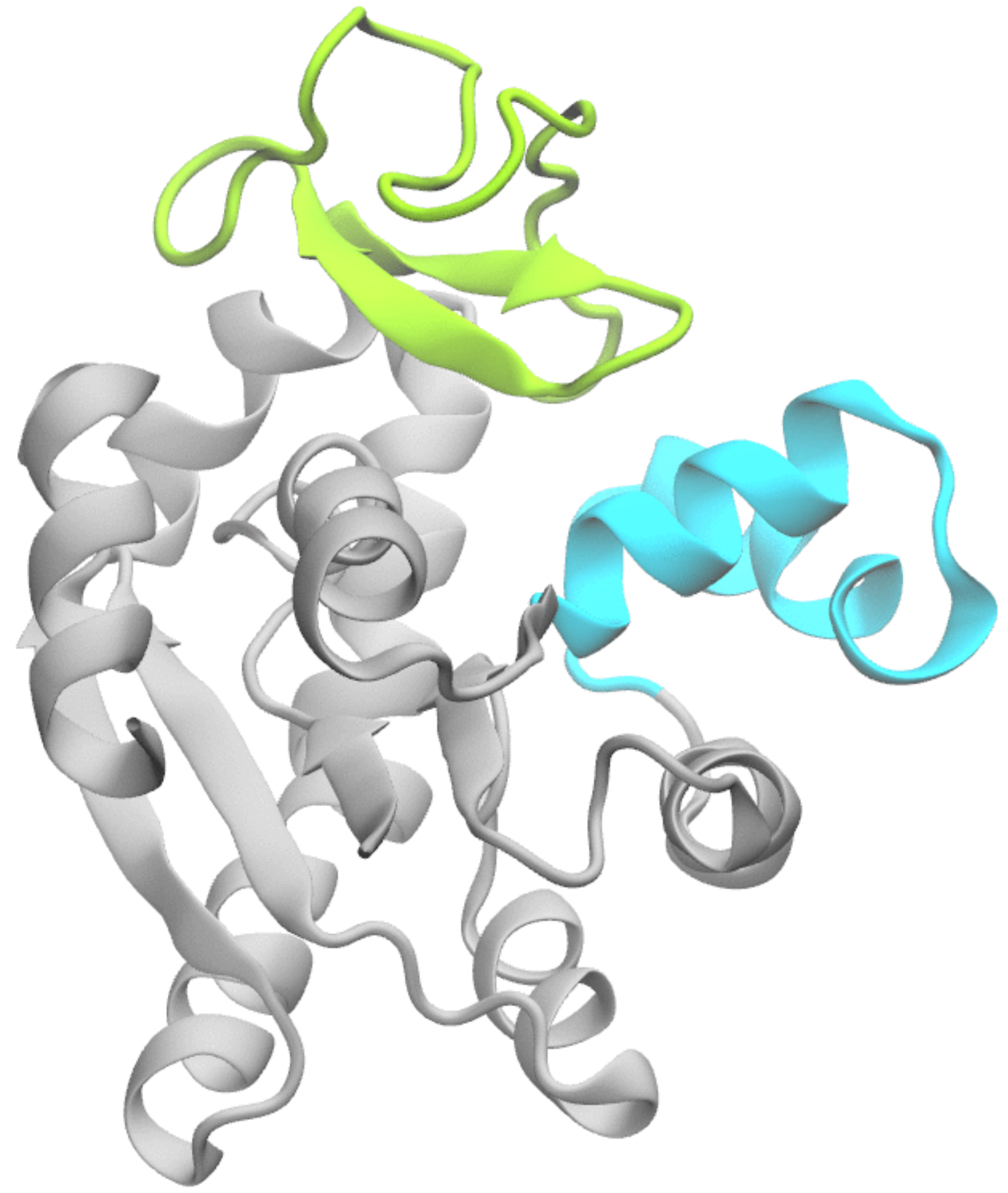


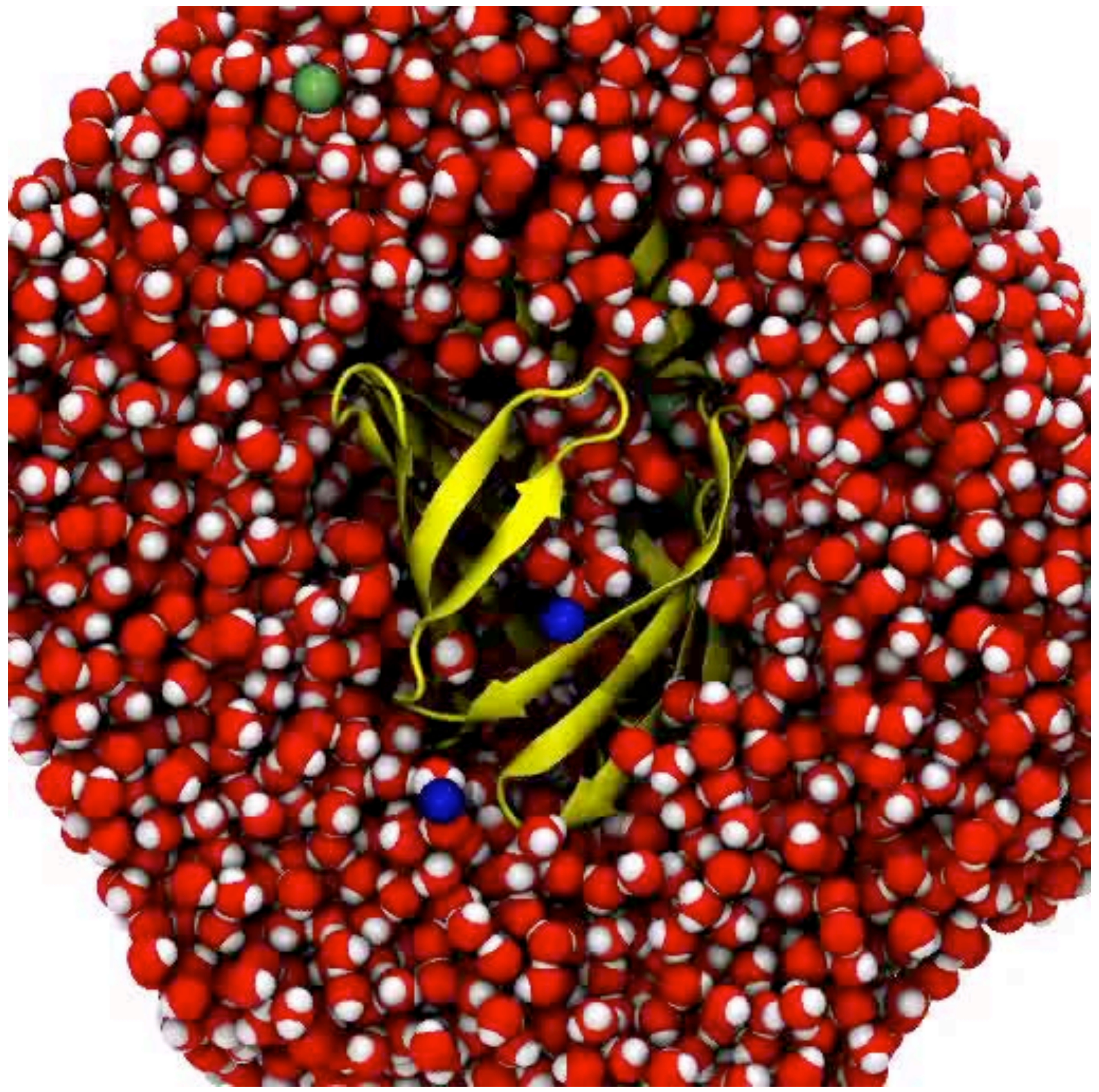
Fully atomistic simulations are *really expensive*

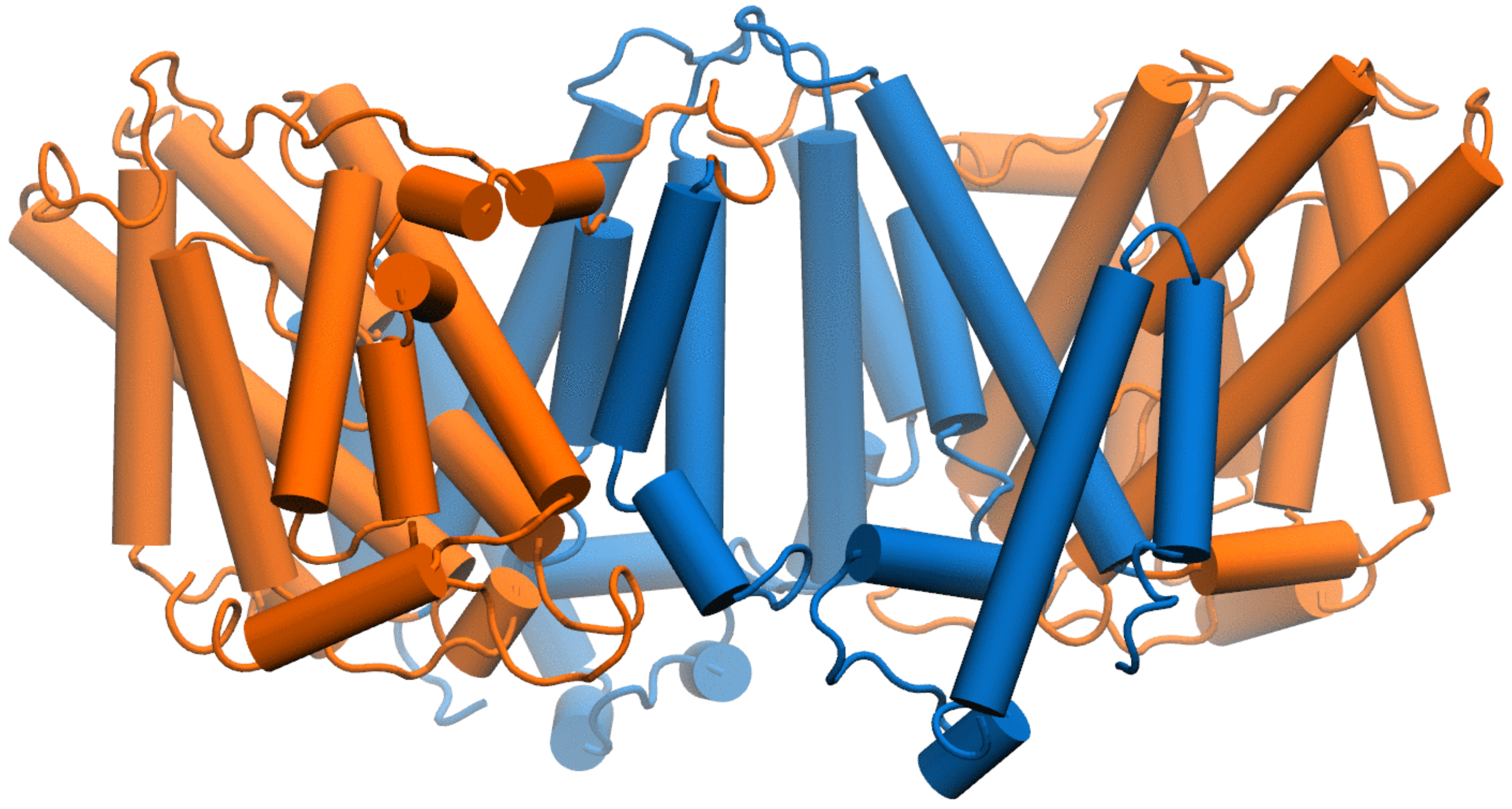
Timesteps:
femtoseconds

→ Billions to trillions of steps →

Timescales of interest:
micro- to milliseconds+

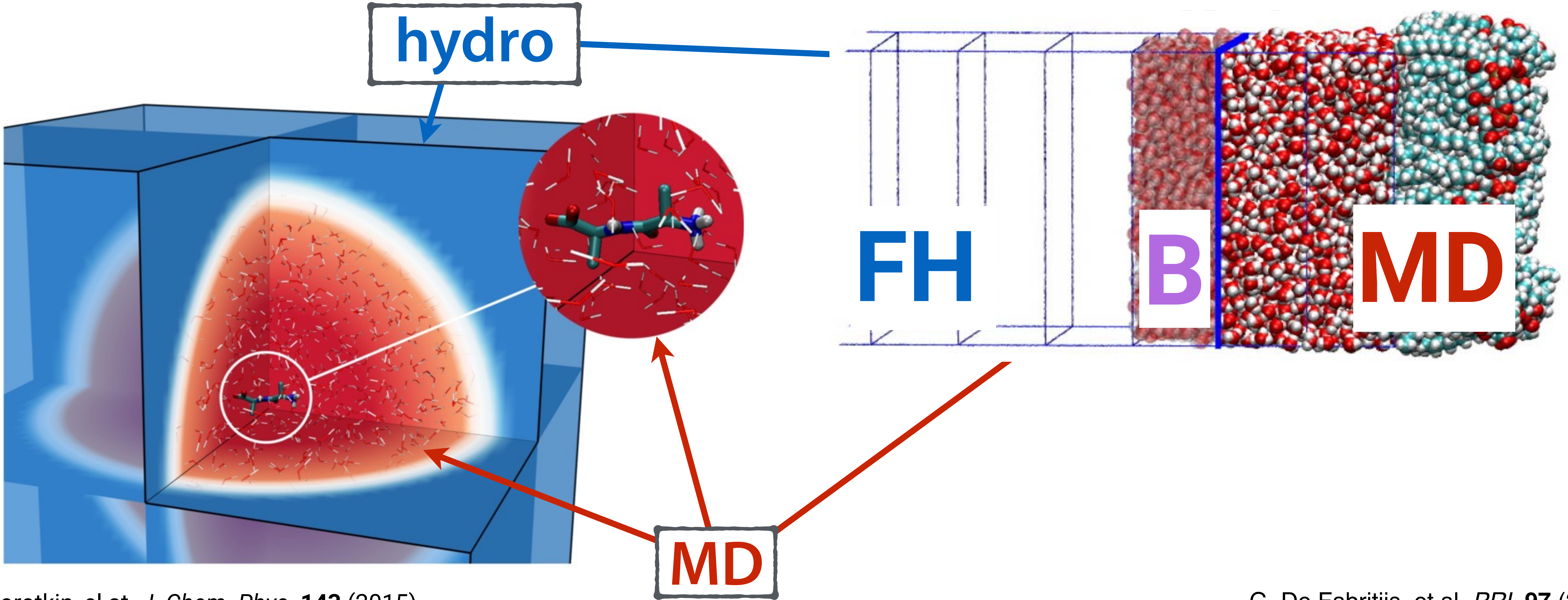






Can a hybrid atomistic-continuum approach help?

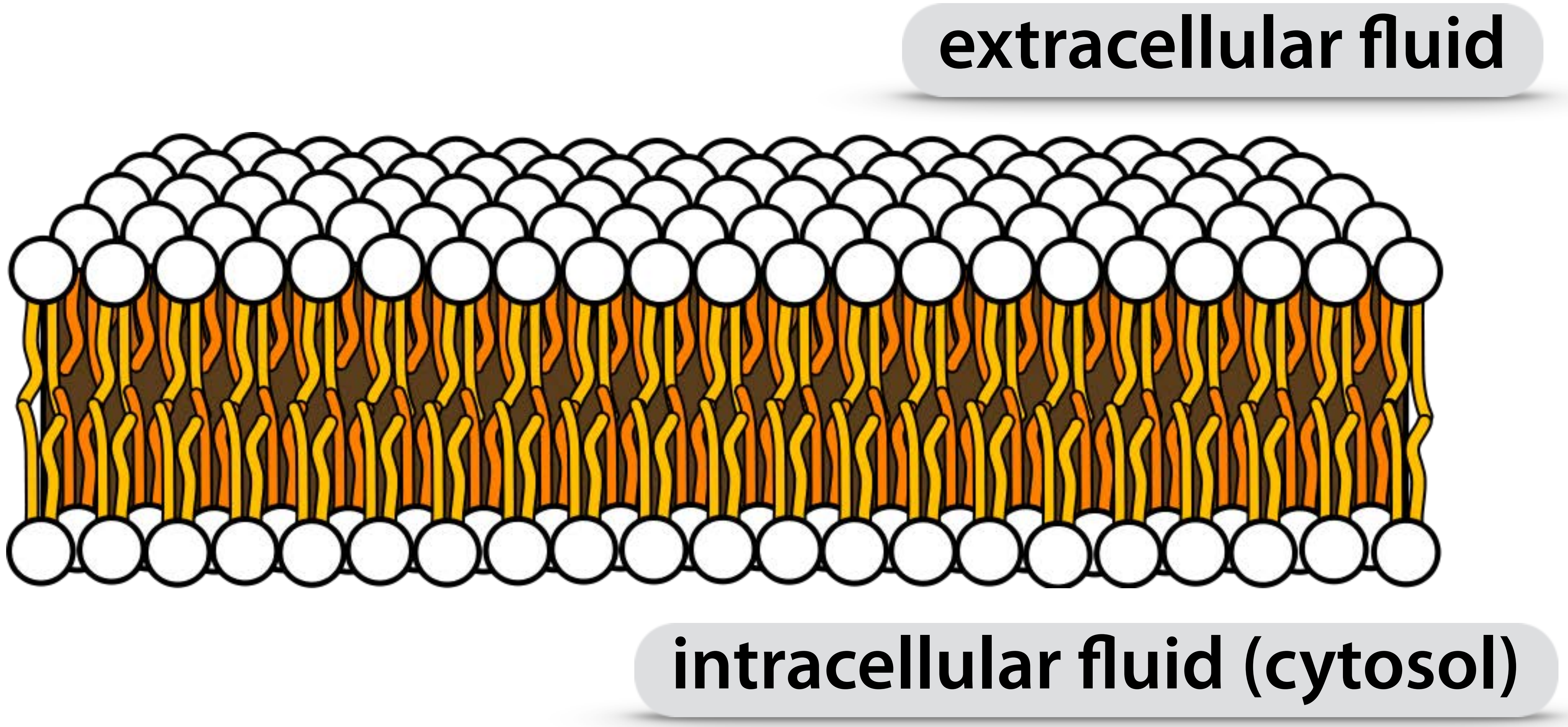
- All-atom **MD** in *restricted subdomain…*
- **Fluctuating HydroDynamics (FHD)** for surrounding *solvent*

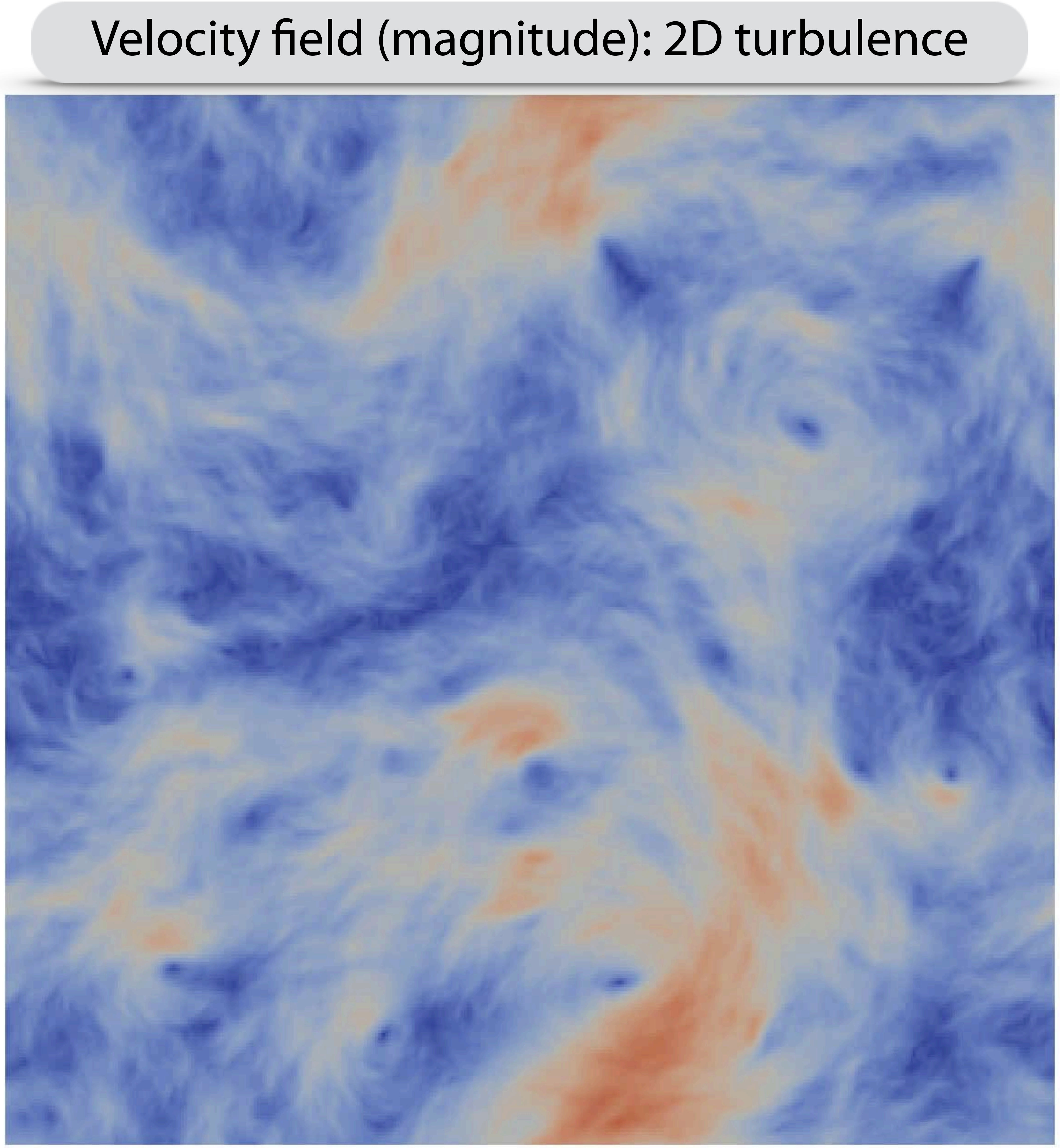


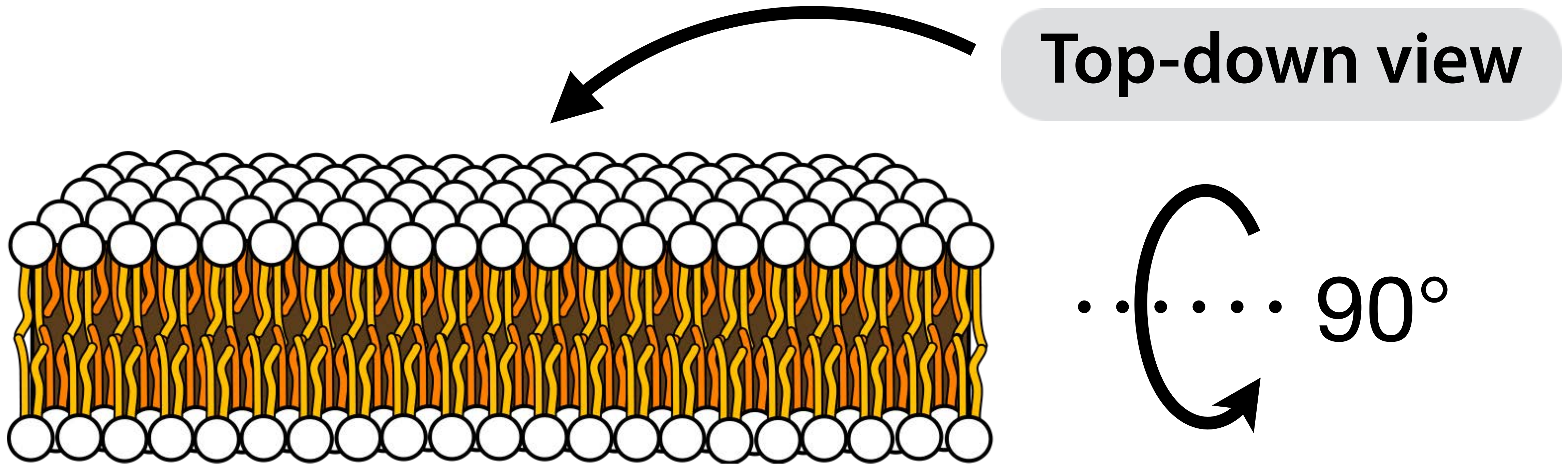
I. Korotkin, el at. *J. Chem. Phys.* **143** (2015).

G. De Fabritiis, et al. *PRL* **97** (2006)

Hydrodynamics is relevant at shorter length scales than expected

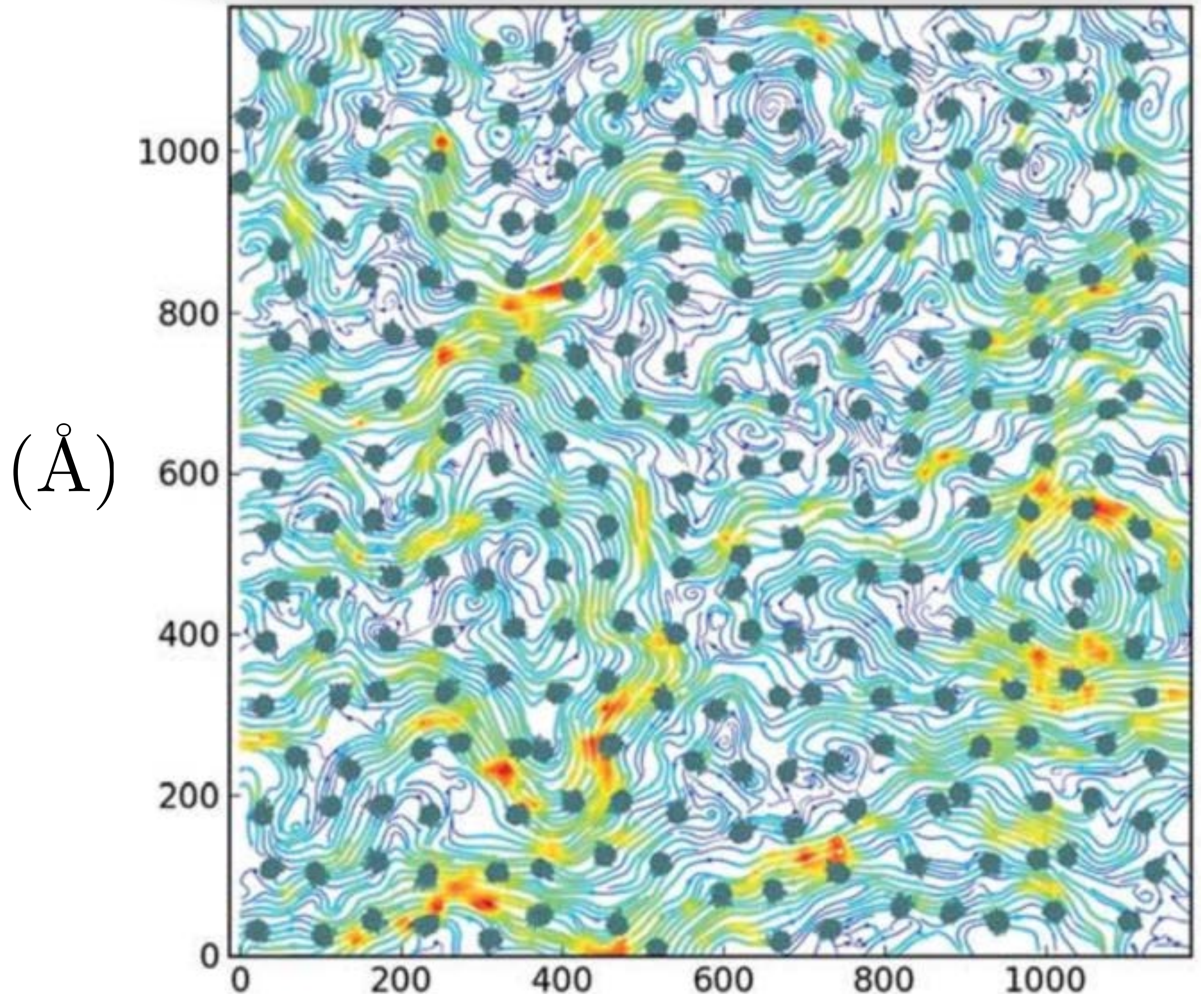




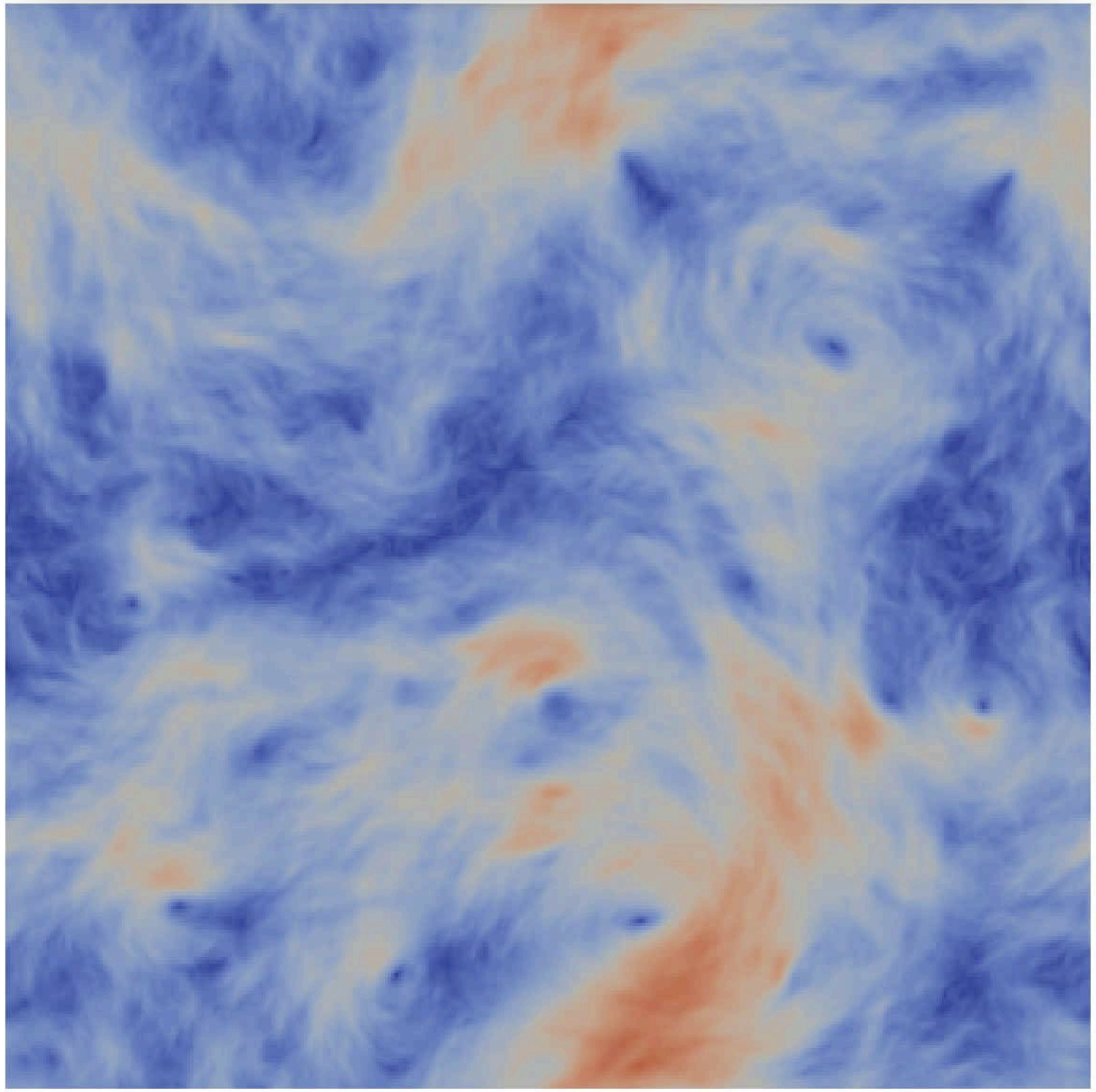


Hydrodynamics is relevant at shorter length scales than expected

Streamlines: planar lipid membrane†



Velocity field (magnitude): 2D turbulence



†M. Chavent et al. *Faraday Discussions* **169**, 455 (2014)

Hydrodynamic equation in conservation form

$$\partial_t \phi + \boldsymbol{\nabla} \cdot (\phi \mathbf{u}) = S(\phi)$$

Mass

$$\phi \longrightarrow \rho \qquad \partial_t \rho + \boldsymbol{\nabla} \cdot (\rho \mathbf{u}) = 0$$

Momentum

$$\phi \longrightarrow \rho \mathbf{u} \qquad \partial_t (\rho \mathbf{u}) + \boldsymbol{\nabla} \cdot \left(\rho \mathbf{u}\mathbf{u} + p \vec{\vec{I}} + \vec{\vec{\sigma}} \right) = 0$$

Energy

$$\phi \longrightarrow \mathcal{E} \qquad \partial_t \mathcal{E} + \boldsymbol{\nabla} \cdot \left[\mathbf{u}(\mathcal{E} + p) + \mathbf{u} \cdot \vec{\vec{\sigma}} \right] = 0$$

Stress-strain $\Longrightarrow$ Navier-Stokes (Newtonian fluid)

$$\vec{\vec{\sigma}} = -\eta \left(\boldsymbol{\nabla}\mathbf{u} + (\boldsymbol{\nabla}\mathbf{u})^{\mathsf{T}} - \frac{2}{3} (\boldsymbol{\nabla} \cdot \mathbf{u}) \vec{\vec{I}} \right)$$

Hydrodynamic equation in conservation form

$$\partial_t \phi + \boldsymbol{\nabla} \cdot (\phi \mathbf{u}) = S(\phi)$$

Account for *thermal fluctuations* in **stress** and heat flux (not shown)†

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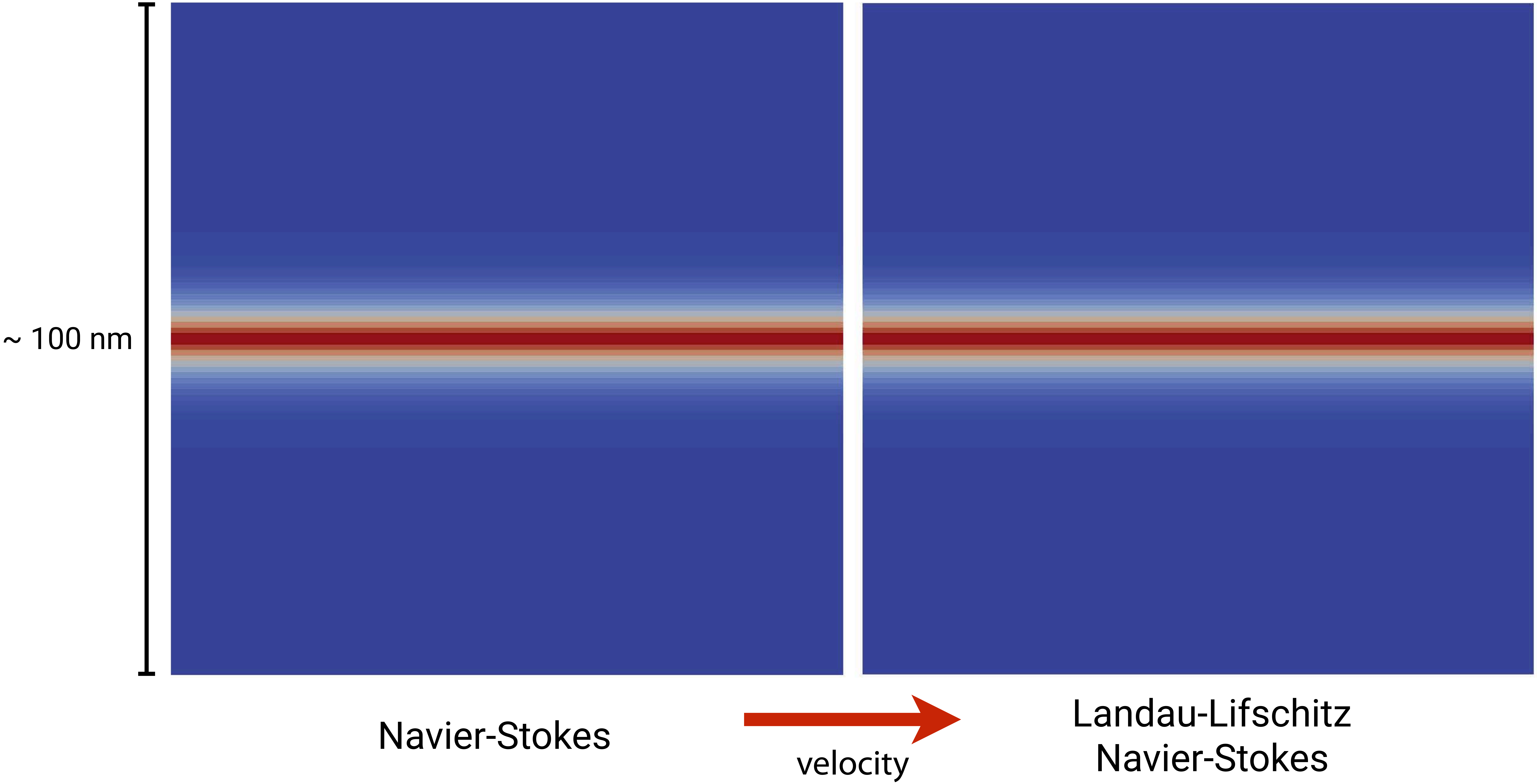
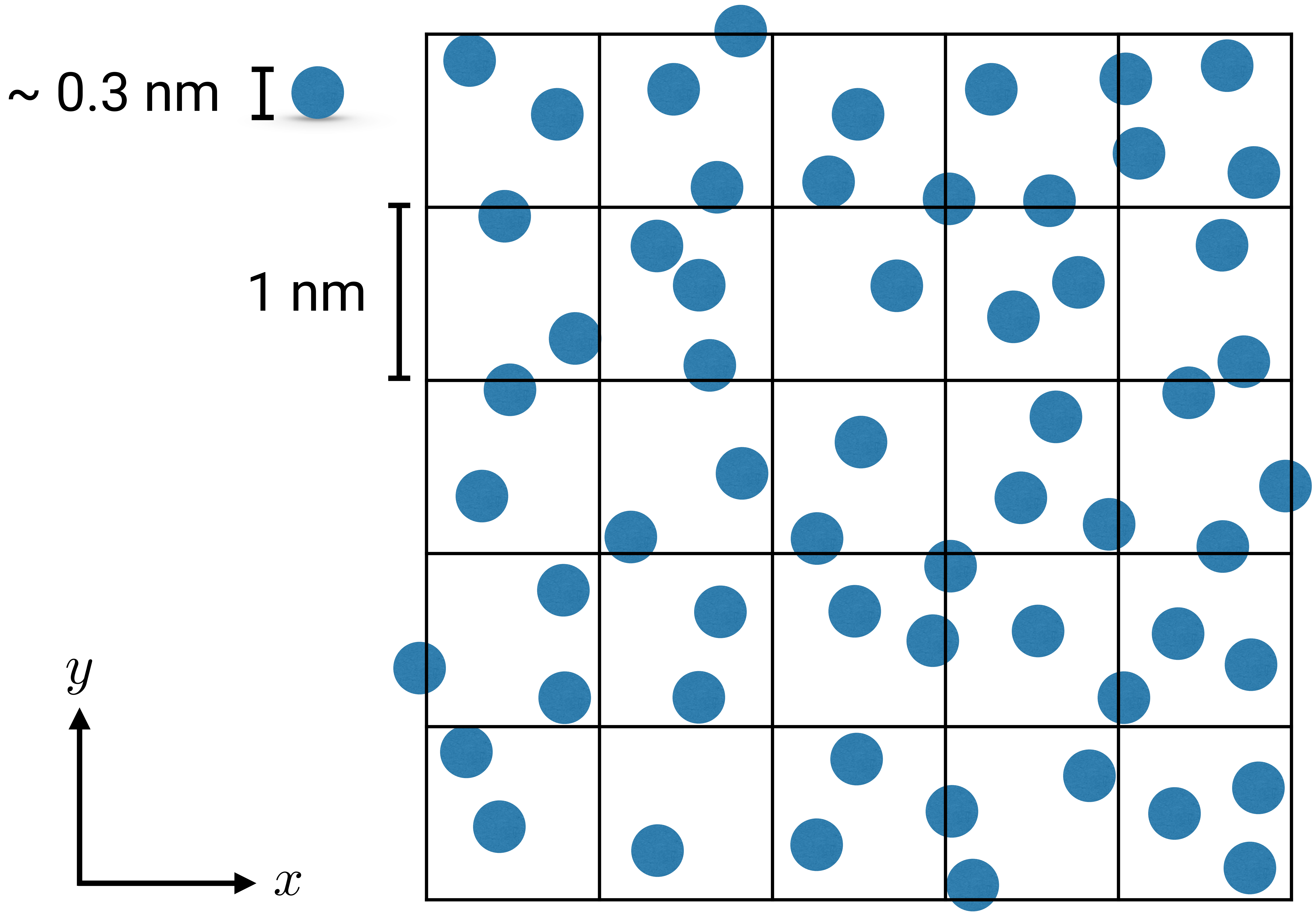
†L. D. Landau & E. M. Lifschitz, *Fluid Mechanics*, third ed. (1966).

Hydrodynamic instabilities show that fluctuations matter

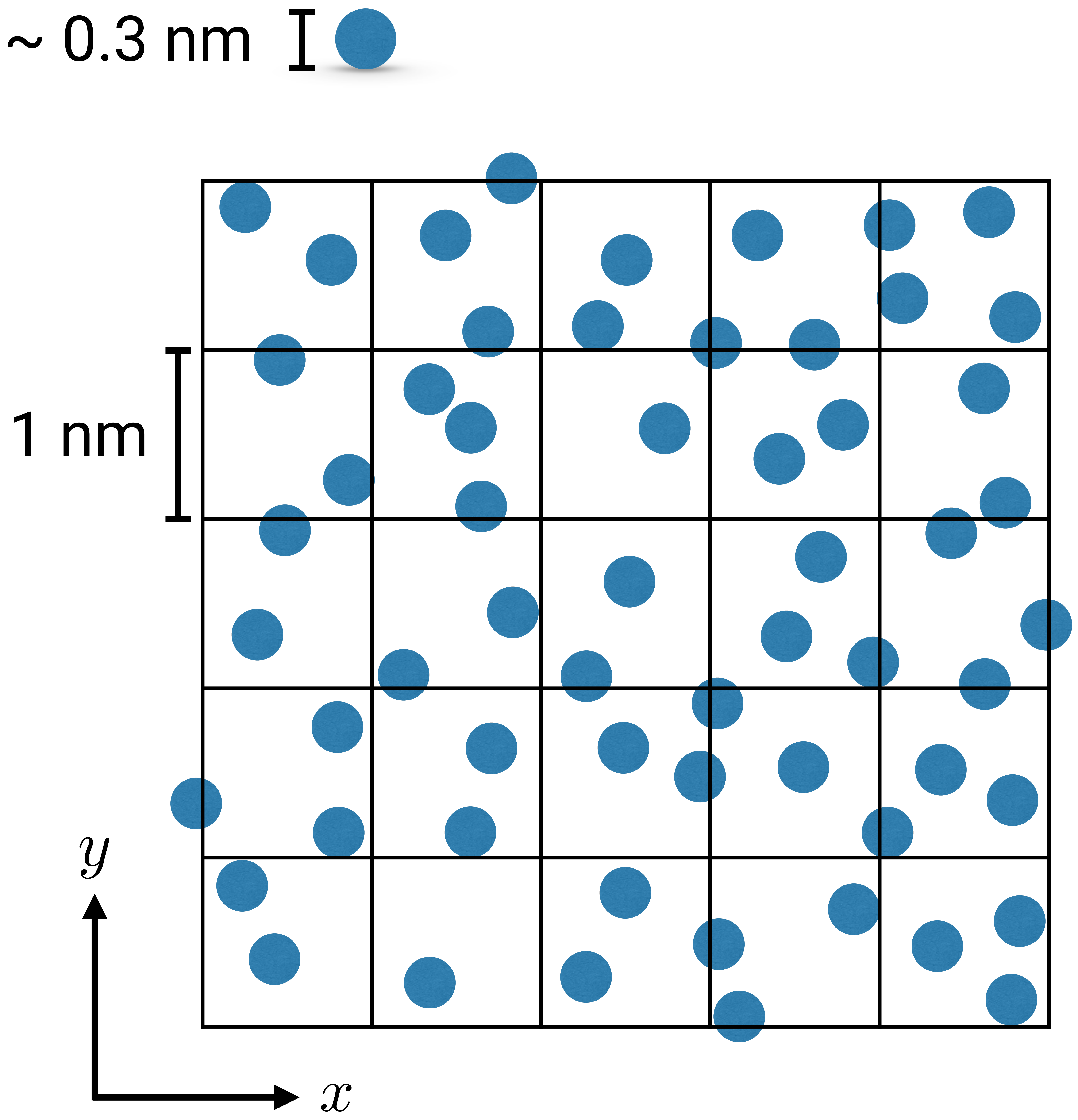


Nanojet breakup: snapshots in time

What if grid cells are comparable in size to a fluid particle?



What if grid cells are comparable in size to a fluid particle?



Fluctuations $\propto \sqrt{\dfrac{1}{\Delta V \Delta t}}$

Spatial resolution ~ mean free path

Temporal resolution ~ collision time

Stress *instantaneously* proportional to rate of strain?

Hydrodynamic equation in conservation form

$$\partial_t \phi + \nabla \cdot (\phi \mathbf{u}) = S(\phi)$$

Account for *thermal fluctuations* in **stress** and heat flux (not shown)†

Mass

$$\phi \longrightarrow \rho \qquad \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0$$

Momentum

$$\phi \longrightarrow \rho \mathbf{u} \qquad \partial_t (\rho \mathbf{u}) + \nabla \cdot \left(\rho \mathbf{u}\mathbf{u} + p \overleftrightarrow{I} + \overleftrightarrow{\sigma} + \overleftrightarrow{\mathcal{S}} \right) = 0$$

Energy

$$\phi \longrightarrow \mathcal{E} \qquad \partial_t \mathcal{E} + \nabla \cdot \left[\mathbf{u}(\mathcal{E} + p) + \mathbf{u} \cdot (\overleftrightarrow{\sigma} + \overleftrightarrow{\mathcal{S}}) \right] = 0$$

Stress-strain $\Longrightarrow$ Navier-Stokes (Newtonian fluid)

$$\overleftrightarrow{\sigma} = -\eta \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathsf{T}} - \frac{2}{3} (\nabla \cdot \mathbf{u}) \overleftrightarrow{I} \right)$$

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Hydrodynamic equation in conservation form

$$\partial_t \phi + \boldsymbol{\nabla} \cdot (\phi \mathbf{u}) = S(\phi)$$

Account for *thermal fluctuations* in **stress** and heat flux (not shown)†

Account for *time dependent* **stress** and heat flux (not shown)‡

Mass

$$\phi \longrightarrow \rho \qquad \partial_t \rho + \boldsymbol{\nabla} \cdot (\rho \mathbf{u}) = 0$$

Momentum

$$\phi \longrightarrow \rho \mathbf{u} \qquad \partial_t (\rho \mathbf{u}) + \boldsymbol{\nabla} \cdot \left(\rho \mathbf{u}\mathbf{u} + p \vec{\vec{I}} + \vec{\vec{\sigma}} + \vec{\vec{\mathcal{S}}} \right) = 0$$

Energy

$$\phi \longrightarrow \mathcal{E} \qquad \partial_t \mathcal{E} + \boldsymbol{\nabla} \cdot \left[\mathbf{u}(\mathcal{E} + p) + \mathbf{u} \cdot (\vec{\vec{\sigma}} + \vec{\vec{\mathcal{S}}}) \right] = 0$$

Time-dependent stress $\Longrightarrow$ linearized form of higher-order moments

$$\frac{\partial \vec{\vec{\sigma}}}{\partial t} + \frac{\eta}{\tau} \left(\boldsymbol{\nabla} \mathbf{u} + (\boldsymbol{\nabla} \mathbf{u})^{\mathsf{T}} - \frac{2}{3} (\boldsymbol{\nabla} \cdot \mathbf{u}) \vec{\vec{I}} \right) = -\frac{\vec{\vec{\sigma}}}{\tau}$$

microscopic collision time

†L. D. Landau & E. M. Lifschitz, *Fluid Mechanics*, third ed. (1966).

‡H. Grad. *Comm. Pure Appl. Math.* **2**, 331 (1949).

Fluctuating hydrodynamics: *10-moment approximation*

Mass	$\partial_t \rho + \boldsymbol{\nabla} \cdot (\rho \mathbf{u}) = 0$	1
Momentum	$\partial_t (\rho \mathbf{u}) + \boldsymbol{\nabla} \cdot \left(\rho \mathbf{u}\mathbf{u} + p \vec{\vec{I}} + \vec{\vec{\sigma}} + \vec{\vec{\mathcal{S}}} \right) = 0$	3
Energy	$\partial_t \mathcal{E} + \boldsymbol{\nabla} \cdot \left[\mathbf{u}(\mathcal{E} + p) + \mathbf{u} \cdot \left(\vec{\vec{\sigma}} + \vec{\vec{\mathcal{S}}} \right) \right] = 0$	1
Stress	$\dfrac{\partial \vec{\vec{\sigma}}}{\partial t} + \dfrac{\eta}{\tau} \left(\boldsymbol{\nabla} \mathbf{u} + (\boldsymbol{\nabla} \mathbf{u})^{\mathsf{T}} - \dfrac{2}{3} (\boldsymbol{\nabla} \cdot \mathbf{u}) \vec{\vec{I}} \right) = -\dfrac{\vec{\vec{\sigma}}}{\tau}$	5

H. Grad. *Comm. Pure Appl. Math.* **2**, 331 (1949).

S. L. Seyler, C. E. Seyler & O. Beckstein, *In preparation.*

Navier-Stokes from slow observations

$$\frac{\partial \vec{\vec{\sigma}}}{\partial t} + \frac{\eta}{\tau}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathsf{T}} - \frac{2}{3}(\nabla\cdot\mathbf{u})\vec{\vec{I}}\right) = -\frac{\vec{\vec{\sigma}}}{\tau}$$

$$\vec{\vec{\sigma}}^{n+1} = \frac{1}{1+\frac{\Delta t}{\tau}}\vec{\vec{\sigma}}^{n} - \frac{\frac{\Delta t}{\tau}}{1+\frac{\Delta t}{\tau}}\eta\left(\nabla\mathbf{u}^{n+1} + (\nabla\mathbf{u}^{n+1})^{\mathsf{T}} - \frac{2}{3}(\nabla\cdot\mathbf{u}^{n+1})\right)$$

(annotations: the first term is struck through → **0**; the coefficient of the second term is struck through → **1**)

$$\frac{\Delta t}{\tau} \gg 1$$

$$\vec{\vec{\sigma}}^{n+1} = -\eta\left(\nabla\mathbf{u}^{n+1} + (\nabla\mathbf{u}^{n+1})^{\mathsf{T}} - \frac{2}{3}(\nabla\cdot\mathbf{u}^{n+1})\vec{\vec{I}}\right)$$

$$\vec{\vec{\sigma}} = -\eta\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathsf{T}} - \frac{2}{3}(\nabla\cdot\mathbf{u})\vec{\vec{I}}\right)$$

Fluctuating hydrodynamics: *10-moment approximation*

Mass	$\partial_t \rho + \boldsymbol{\nabla} \cdot (\rho \mathbf{u}) = 0$	1
Momentum	$\partial_t (\rho \mathbf{u}) + \boldsymbol{\nabla} \cdot \left(\rho \mathbf{u}\mathbf{u} + p \vec{\vec{I}} + \vec{\vec{\sigma}} + \vec{\vec{\mathcal{S}}} \right) = 0$	3
Energy	$\partial_t \mathcal{E} + \boldsymbol{\nabla} \cdot \left[\mathbf{u}(\mathcal{E} + p) + \mathbf{u} \cdot (\vec{\vec{\sigma}} + \vec{\vec{\mathcal{S}}}) \right] = 0$	1
Stress	$\partial_t \vec{\vec{\sigma}} + \frac{\eta}{\tau} \left(\boldsymbol{\nabla}\mathbf{u} + (\boldsymbol{\nabla}\mathbf{u})^{\mathsf{T}} - \frac{2}{3}(\boldsymbol{\nabla} \cdot \mathbf{u}) \vec{\vec{I}} \right) = -\frac{\vec{\vec{\sigma}}}{\tau} \left(\vec{\vec{\sigma}} + \vec{\vec{\mathcal{S}}} \right)$	5

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S. L. Seyler, C. E. Seyler & O. Beckstein, *In preparation.*

Fluctuating hydrodynamics: *13-moment approximation*

Mass	$\partial_t \rho + \boldsymbol{\nabla} \cdot (\rho \mathbf{u}) = 0$	1
Momentum	$\partial_t (\rho \mathbf{u}) + \boldsymbol{\nabla} \cdot \left(\rho \mathbf{u}\mathbf{u} + p \vec{\vec{I}} + \vec{\vec{\sigma}} \right) = 0$	3
Energy	$\partial_t \mathcal{E} + \boldsymbol{\nabla} \cdot \left[\mathbf{u}(\mathcal{E} + p) + \mathbf{u} \cdot \vec{\vec{\sigma}} + \mathbf{q} \right] = 0$	1
Stress (linearized)	$\partial_t \vec{\vec{\sigma}} + \frac{\eta}{\tau} \left(\boldsymbol{\nabla}\mathbf{u} + (\boldsymbol{\nabla}\mathbf{u})^{\mathsf{T}} - \frac{2}{3} (\boldsymbol{\nabla} \cdot \mathbf{u}) \vec{\vec{I}} \right) = -\frac{1}{\tau} \left(\vec{\vec{\sigma}} + \vec{\vec{\mathcal{S}}} \right)$	5
Heat flux (linearized)	$\partial_t \mathbf{q} + 2T_0 \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} + \frac{\kappa}{\tau} \boldsymbol{\nabla} T = -\frac{1}{\tau} \left(\mathbf{q} + \mathcal{Q} \right)$	3

H. Grad. *Comm. Pure Appl. Math.* **2**, 331 (1949).

S. L. Seyler, C. E. Seyler & O. Beckstein, *In preparation*.

HERMESHD†

***H**yp**E**rbolic **R**elaxation **M**odel for **E**xtended **S**ystems of **H**ydro**D**ynamics*

- **Nanoscale**: beyond Landau-Lifschitz Navier-Stokes
- **Physical**: finite-speed transport
- **Natural**: physics dictated by *timestep*
- **Accurate**: discontinuous Galerkin (avoids higher-order FV)
- **Fast**: no 2nd-order space-derivs, ***local*** in space *and* time
- *Python* **interface**; Fortran **backend**
- https://bitbucket.org/sseyler/hermeshd/

†PERSEUS XMHD code: X. Zhao, Y. Yang, & C. E. Seyler (2014) *J. Comput. Phys.* **278**

BLUE WATERS
SUSTAINED PETASCALE COMPUTING

Beckstein Lab
Computational Biophysics at Arizona State University

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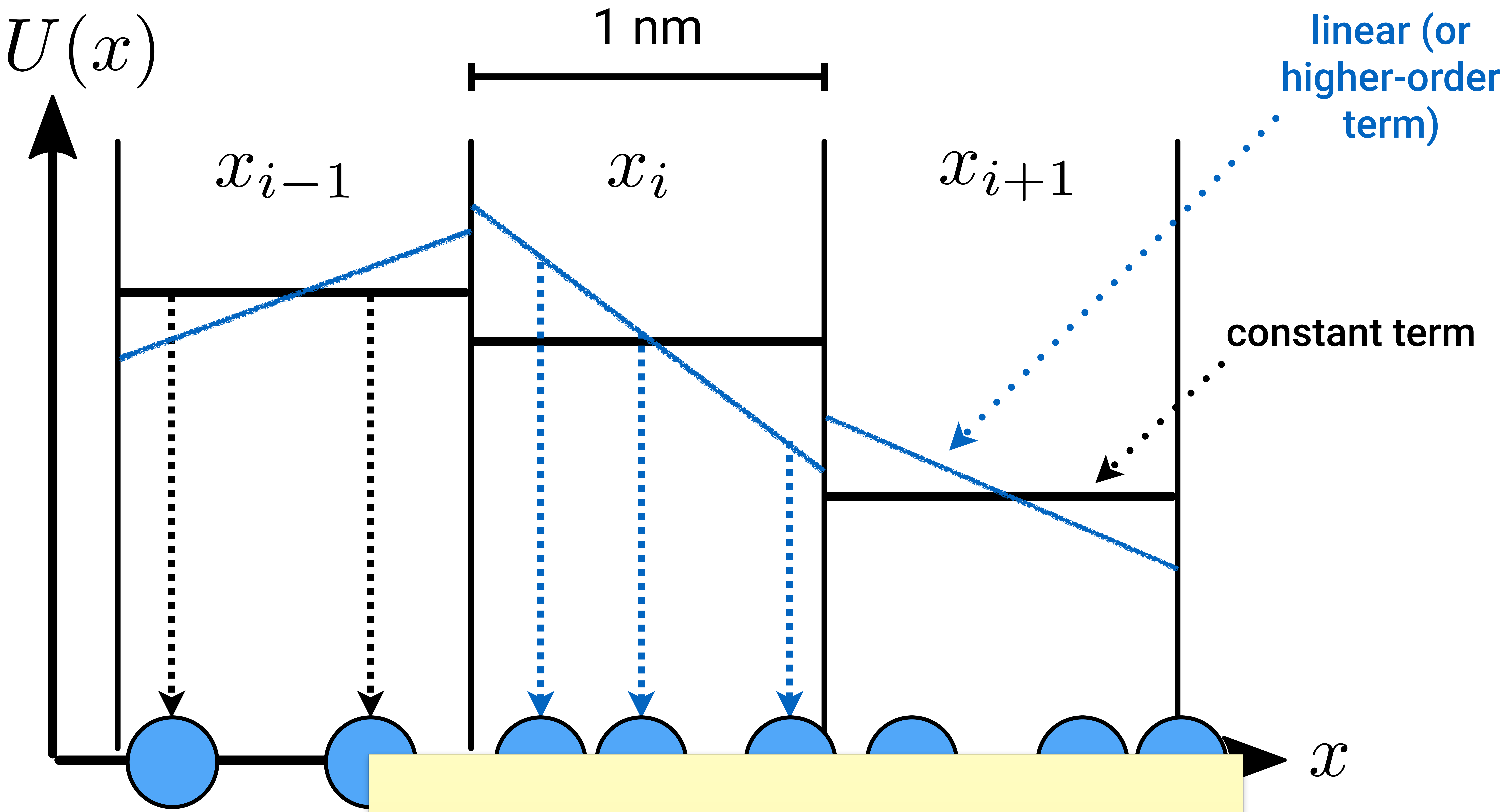
Arizona State University
Oliver Beckstein
Steve Pressé

Cornell Engineering
Charles E. Seyler

NCSA

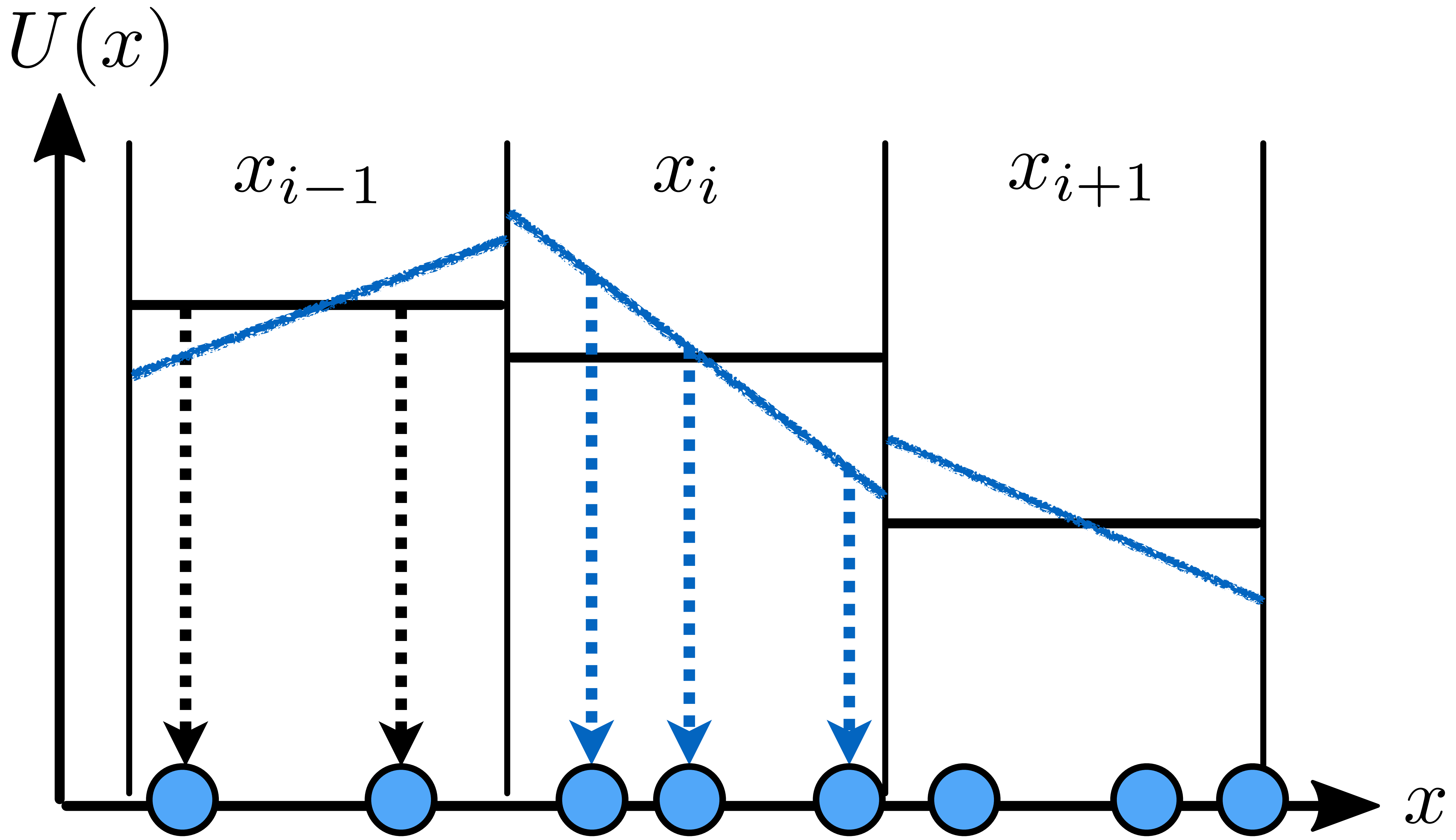
NSF

Why use a discontinuous Galerkin approach?



• Plan to release as open source under GPLv3 (GitHub)

Why use a discontinuous Galerkin approach?

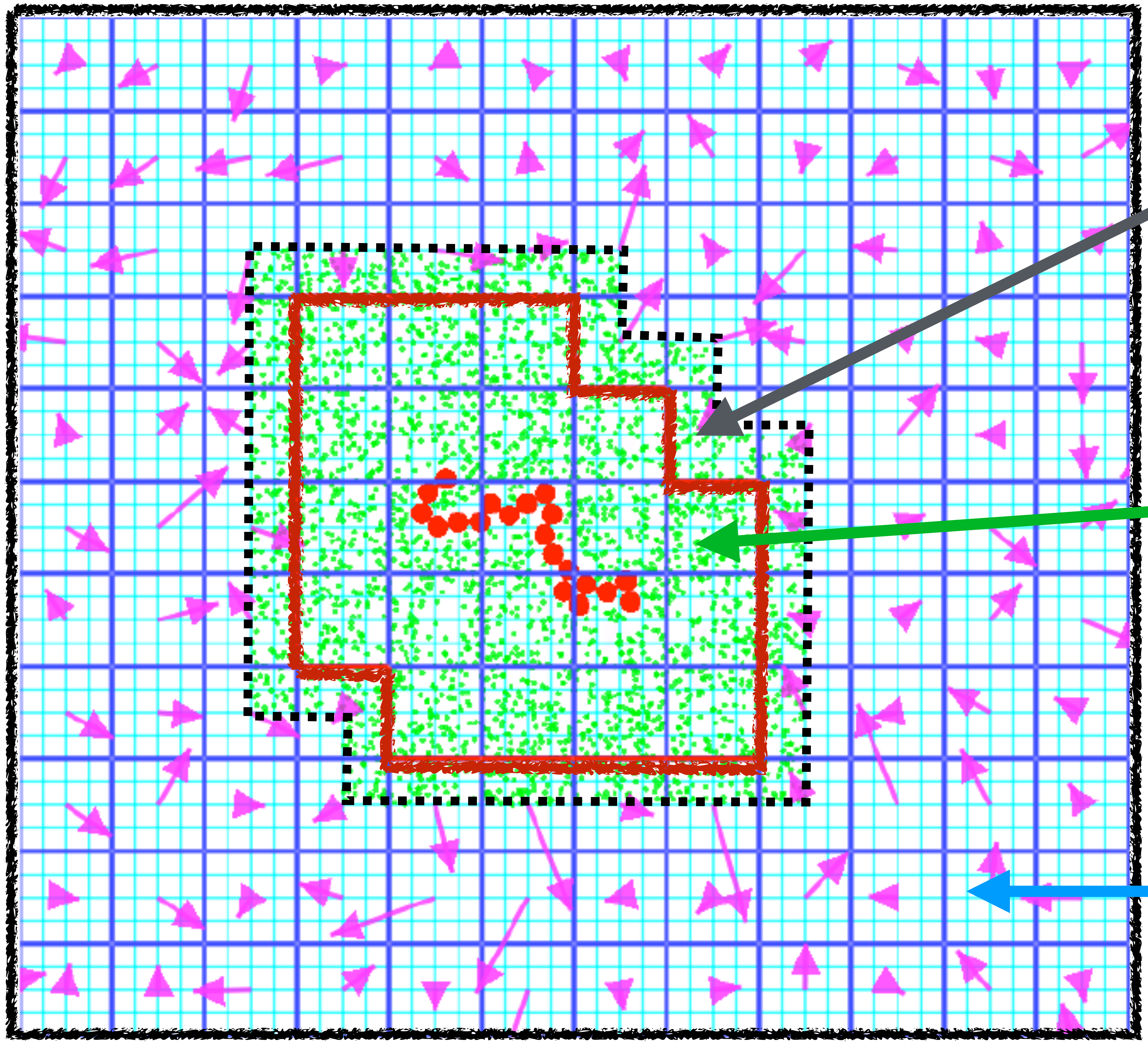


- Choosing grid cell size determines:
  - ➡ observation scale
  - ➡ magnitude of fluctuations

$$\text{Fluctuations} \propto \sqrt{\frac{1}{\Delta V \Delta t}}$$

- Interpolation: fields → particles
- spatial resolution and fluctuations *decouple*

What components are needed?



A. Donev, A. L. Garcia, J. B. Bell (2011) *Presentation at Center for Computational and Integrative Biology, Rutgers-Camden*.

Driver program

- Manage: communicate *boundary conditions*
- Run: MD (*N* steps) → *BCs* → FHD (*M* steps) → *BCs*

Molecular dynamics engine

- **LAMMPS***‡
  - Biomolecular force fields
  - Python interface

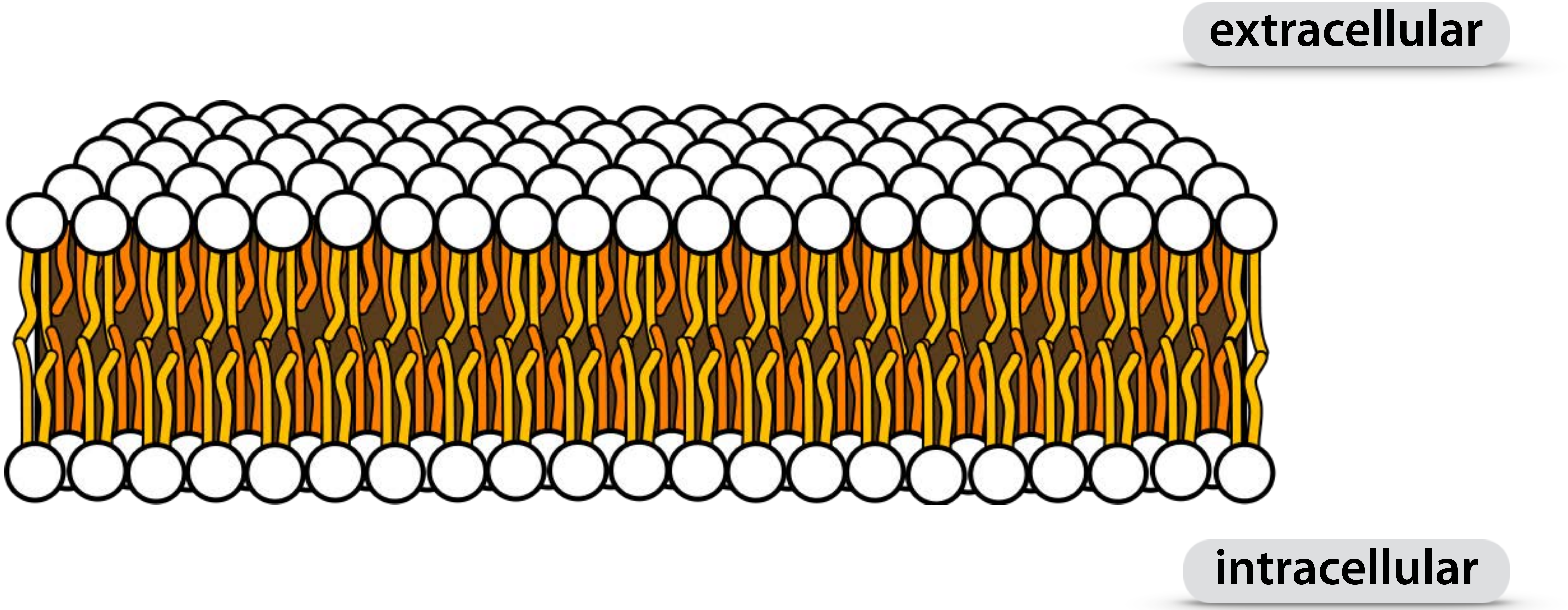
Fluctuating hydrodynamics solver†

- Compressible, dense fluids
- 3D Finite-volume-like (discontinuous Galerkin, or DG)

†PERSEUS XMHD code: X. Zhao, Y. Yang, & C. E. Seyler (2014) *J. Comput. Phys.* **278**

*S-H. Ko, et al. (2014) *J. Mech. Sci. Technol.* **28**
‡F. E. Mackay, et al. (2013) *Comput. Phys. Commun.* **184**

Hydrodynamics is relevant at shorter length scales than expected



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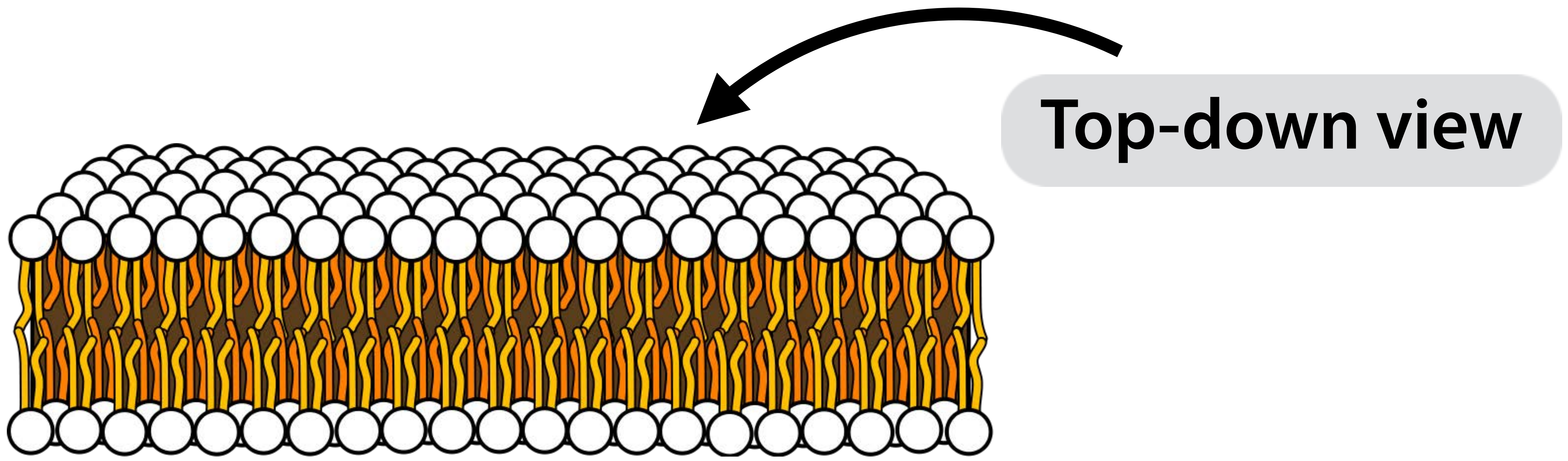
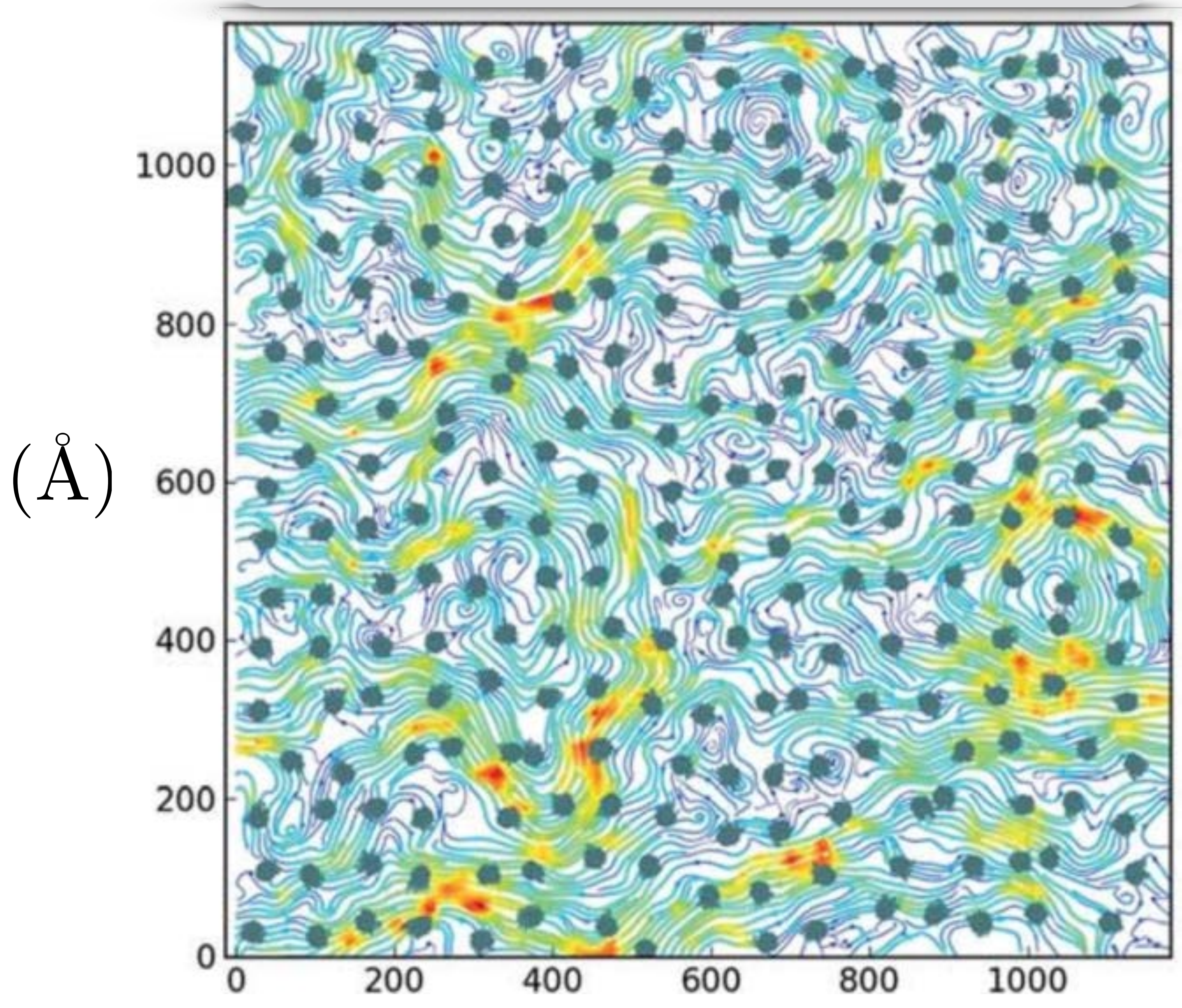
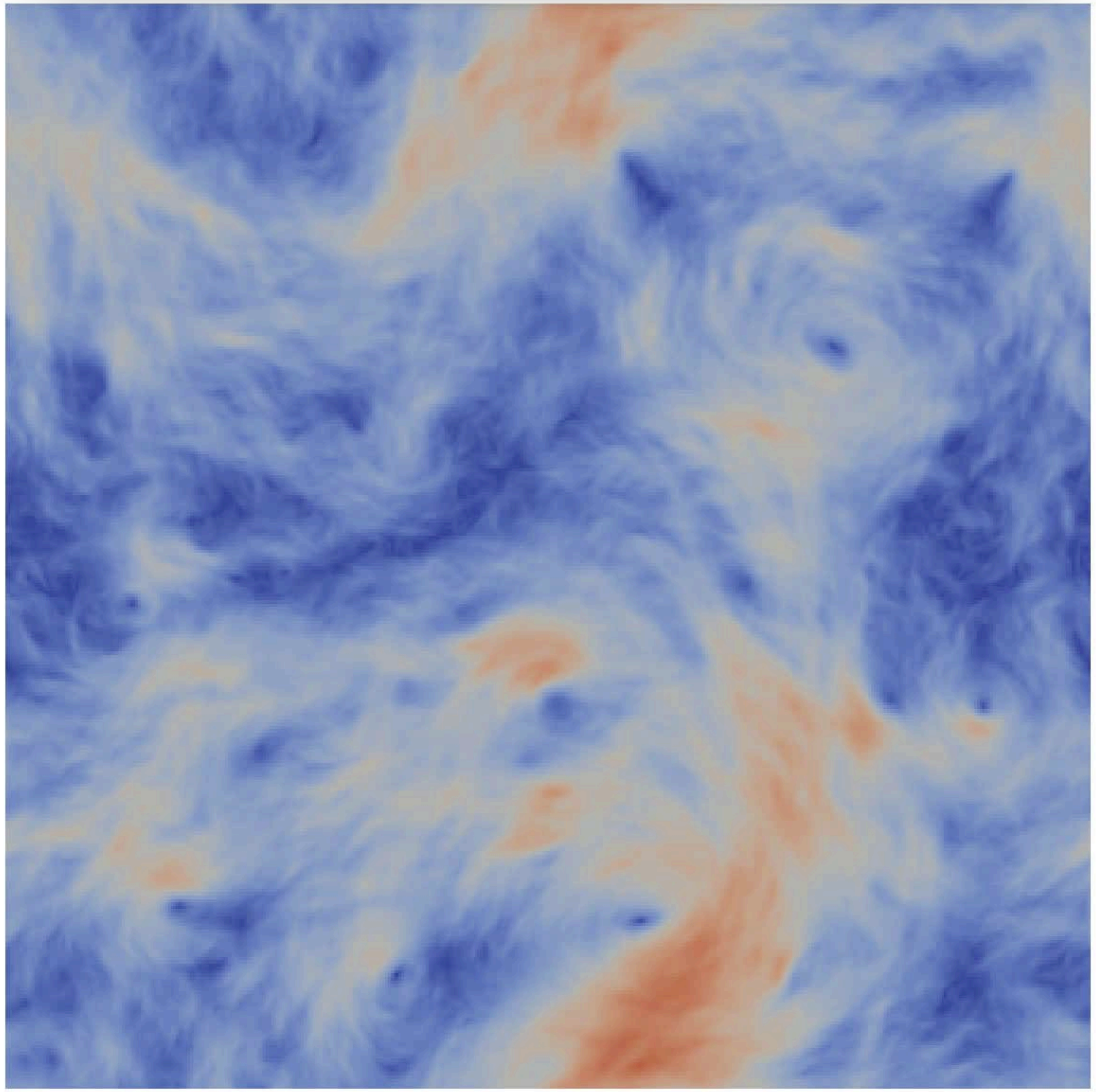


Streamlines: planar lipid membrane†



Velocity field (magnitude): 2D turbulence



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