TECHNISCHE UNIVERSITÄT WIEN
Vienna | Austria

COMETE kickoff

Simulation of turbulent bubbly flows

Gabriele Labanca

COMETE project

Advanced courses

TECHNICAL

Cross-topic training

Innovative methods

Unawareness about Multiphase Flows Methodologies

UNITARY FRAMEWORK

Contributions to ACADEMIA

Publications, conferences

Open Datasets

Dialogue with INDUSTRY

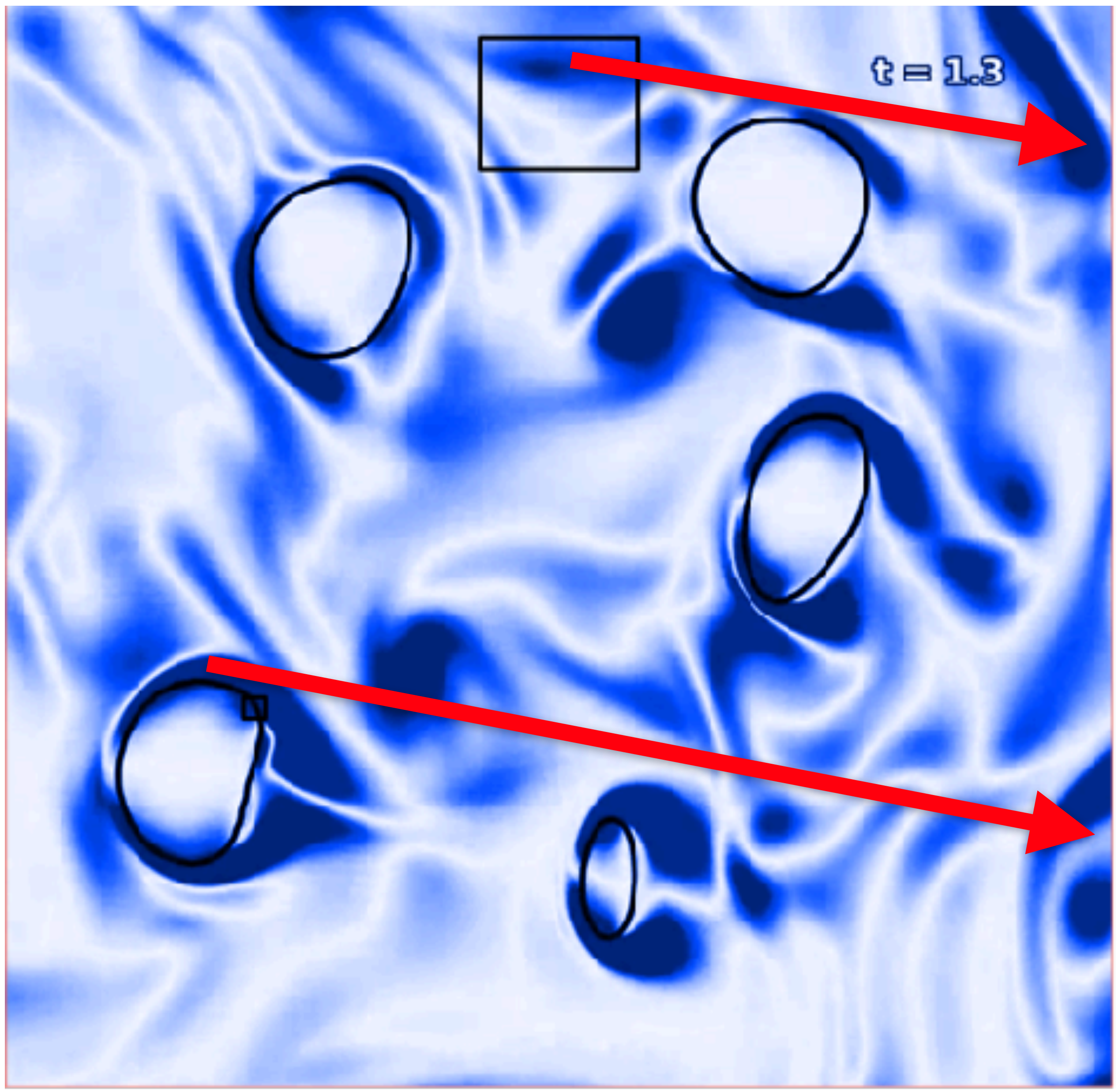
Interesting cases

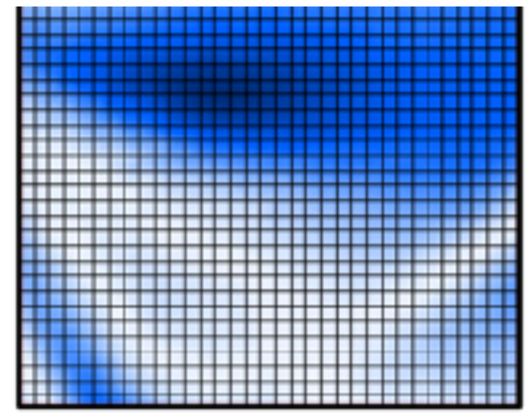
Best practices

COMMUNICATION

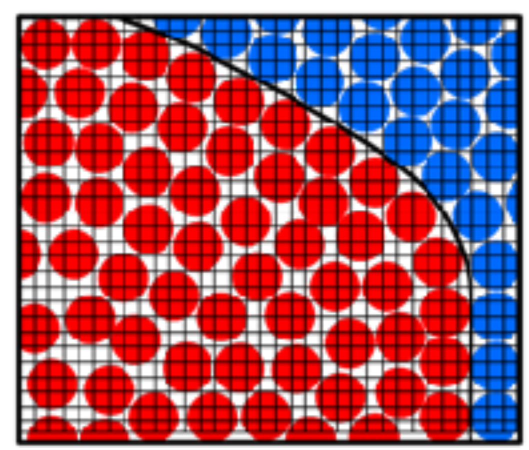
Computational effort

Homogeneous Isotropic Turbulence (HIT) in a cube of $1m^3$





Turbulence:
$Re_\lambda = 85$
$\Rightarrow$smallest scale $\simeq 10^{-3}m$
<u>3 orders of magnitude.</u>

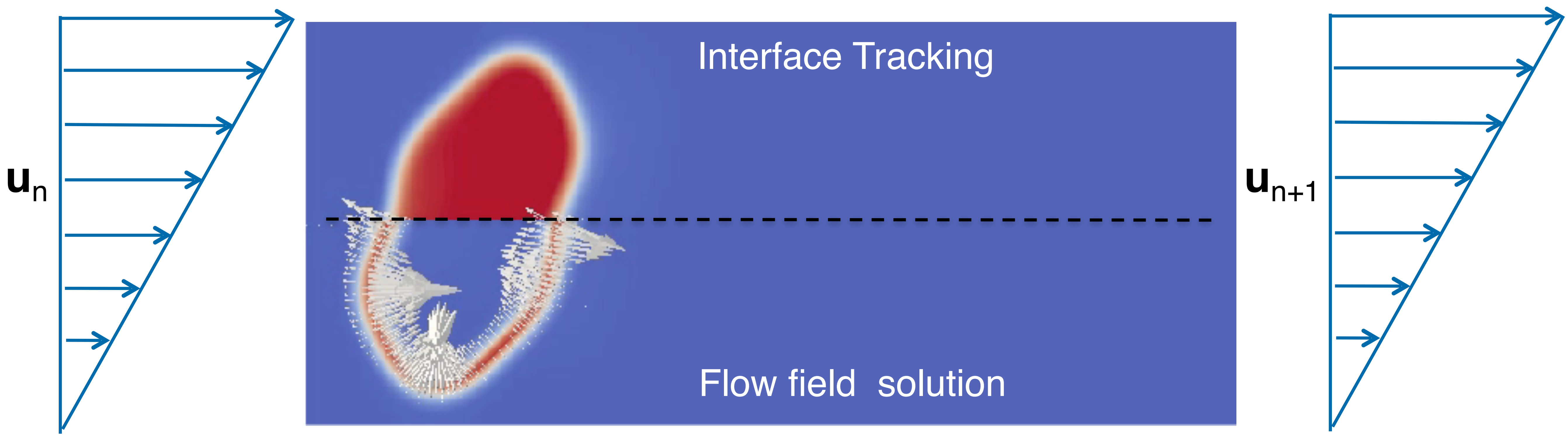


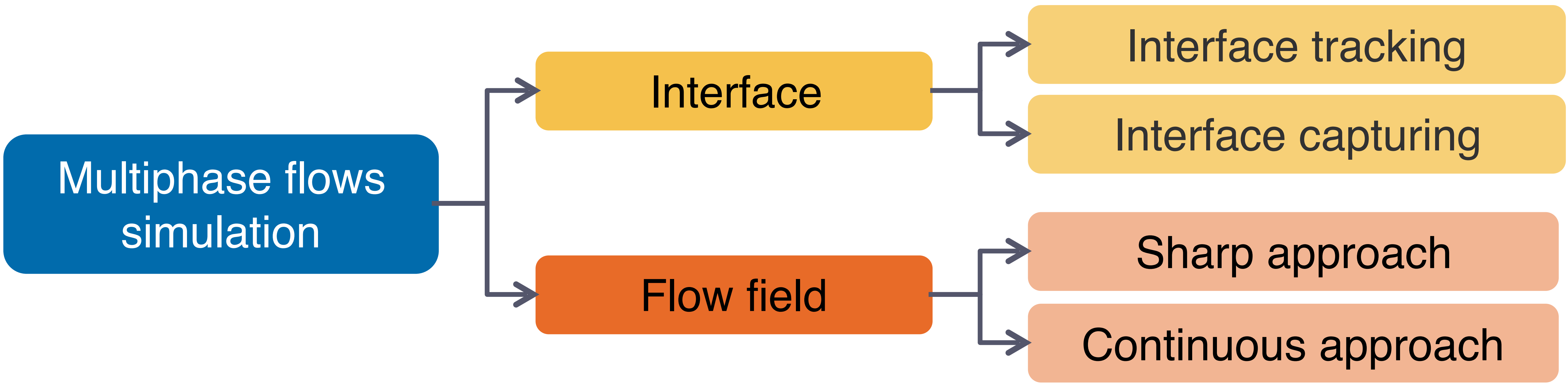
Interface:
smallest Scale $\simeq 10^{-9}m$
9 orders of magnitude.

$N_P \simeq (10^9)^3 = 10^{27}$!

M.S. Dodd and A. Ferrante, On the interaction of Taylor length scale size droplets and isotropic turbulence, JFM (2016)

Approaches to model the interface



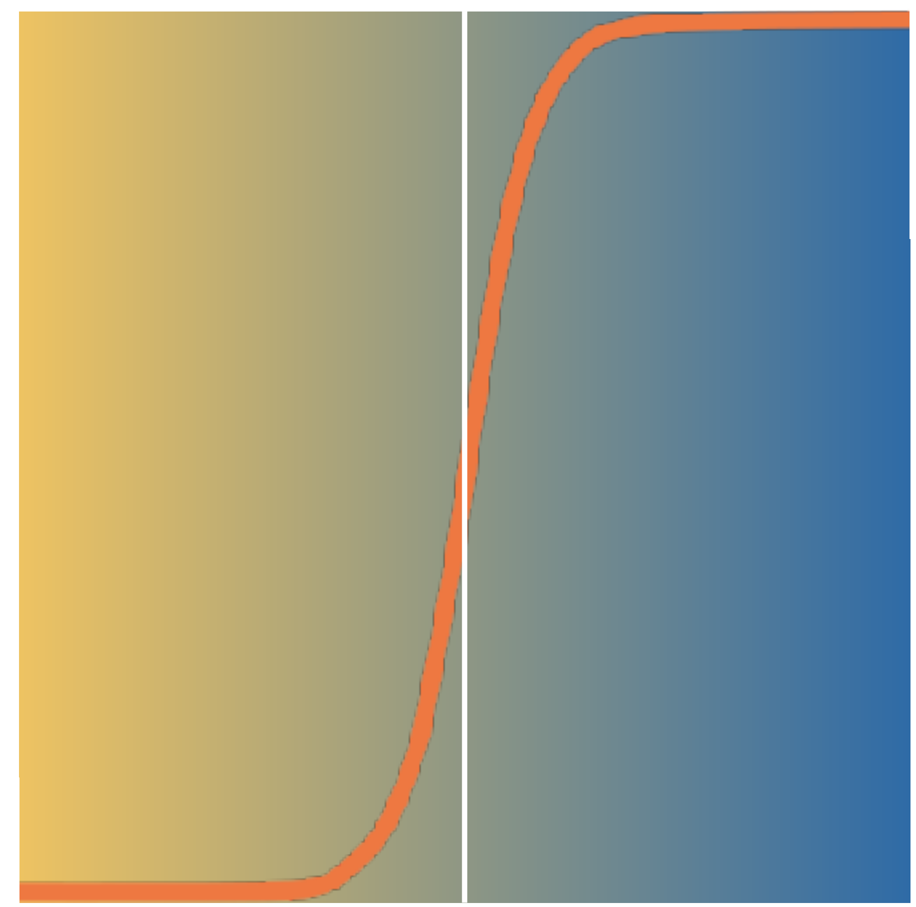


Interface tracking/capturing

INTERFACE TRACKING

Interface described by points
Lagrangian advection

INTERFACE CAPTURING



Scalar function:
phase characterised by its value

Cahn-Hilliard Equation

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \nabla \cdot \left(\mathcal{M}_\phi \nabla \mu_\phi \right) \;\cdots\cdots\blacktriangleright\; \frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \frac{1}{Pe_\phi} \nabla^2 \mu_\phi$$

Mobility parameter ($\mathcal{M}_\phi$)

Advection by flow ($\mathbf{u}$)

Diffusion by chemical potential (μ_ϕ)

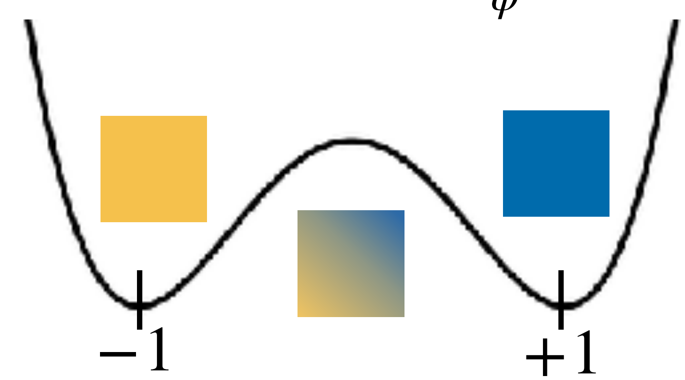
Peclet number: ratio between diffusive and convective time scales (Pe_ϕ)

$$\mu_\phi = \frac{\delta \mathcal{F}[\phi, \nabla \phi]}{\delta \phi}$$

$$\mathcal{F}[\phi, \nabla \phi] = \int_\Omega \left[f_0(\phi) + f_i(\nabla \phi) \right] \mathrm{d}\Omega$$

$$Pe_\phi = \frac{u_\tau h}{\mathcal{M}_\phi}$$

- $f_0(\phi) = \frac{1}{4}(\phi - 1)^2(\phi + 1)^2$ Phobic term



- $f_i(\nabla \phi) = \frac{Ch^2}{2} \left| \nabla \phi \right|^2$ Surface term

Cahn number: $Ch = \frac{\xi}{h}$

A. Roccon, M. De Paoli, F. Zonta, A. Soldati, Viscosity-modulated breakup and coalescence of large drops in bounded turbulence, *PRF*, 2017

Navier-Stokes Equations

Unique equation for both fluids: properties depending on phase field value

Ratio of viscosities: $\lambda = \frac{\eta_d}{\eta_c}$

Width of the interface

$$\rho(\phi)\left[\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right] = -\nabla\mathscr{P} + \frac{1}{Re_\tau}\nabla\cdot\left[\eta(\phi)\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right)\right] + \frac{3}{\sqrt{8}}\frac{Ch}{We}\nabla\cdot\tau_c$$

Weber number: ratio of inertial over surface forces

$$We = \frac{\rho U^2 h}{\sigma}$$

Density dependent on phase field

Korteweg stress tensor: capillary force due to surface tension

$$\tau_c = \left|\nabla\phi\right|^2\mathbf{I} - \nabla\phi\otimes\nabla\phi$$

A. Roccon, M. De Paoli, F. Zonta, A. Soldati, Viscosity-modulated breakup and coalescence of large drops in bounded turbulence, *PRF,* 2017

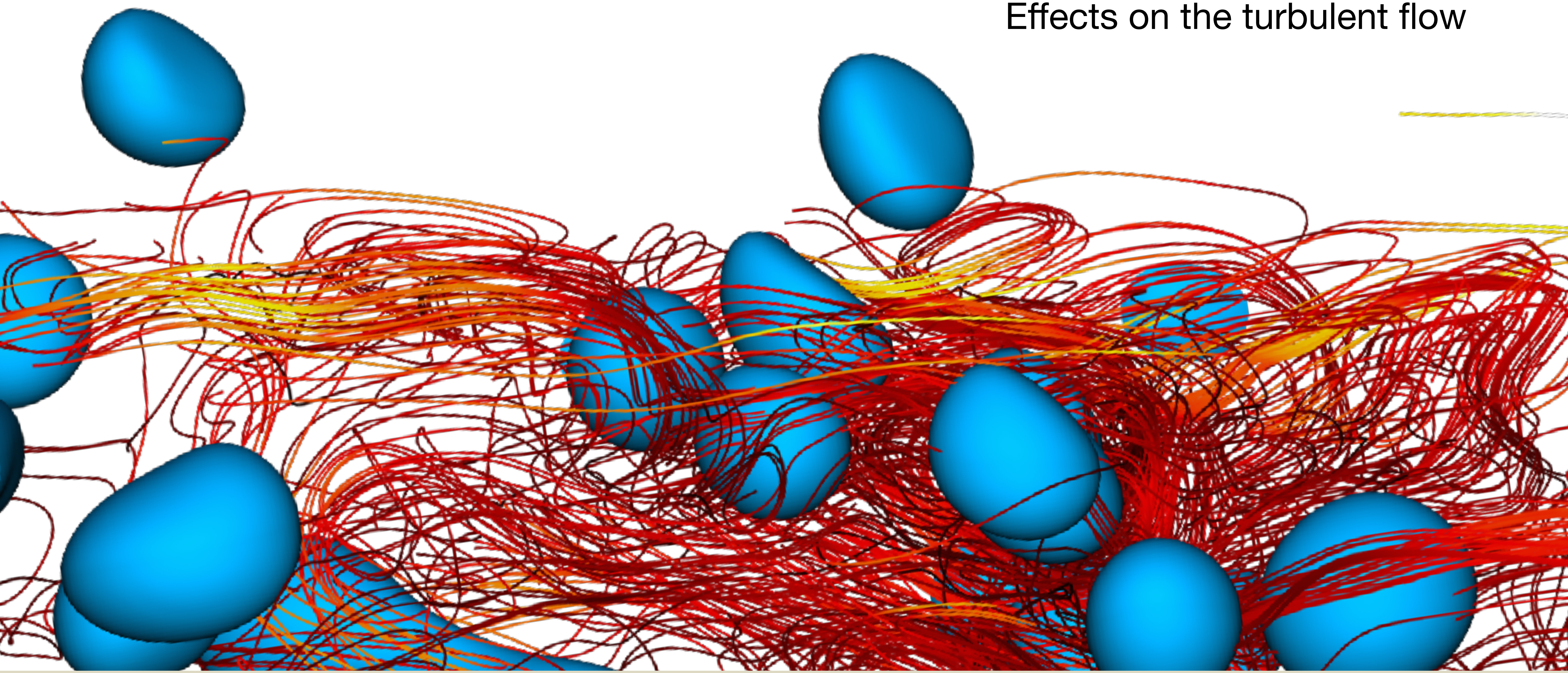
Goals of simulations

Different values of viscosity and density ratios →

Study of droplet-droplet interactions

Droplet statistics

Effects on the turbulent flow



Relevant Parameters

Reynolds number: inertial over viscous

$$Re_\tau = \frac{\rho u_\tau h}{\eta_c}$$

Weber number: ratio between inertial and surface forces

$$We = \frac{\rho u_\tau^2 h}{\sigma}$$

	Viscosity ($Pa \cdot s$)	Density ($kg \cdot m^{-3}$)
Air	10^{-5}	1
Water	10^{-3}	10^3
Butane	10^{-5}	600

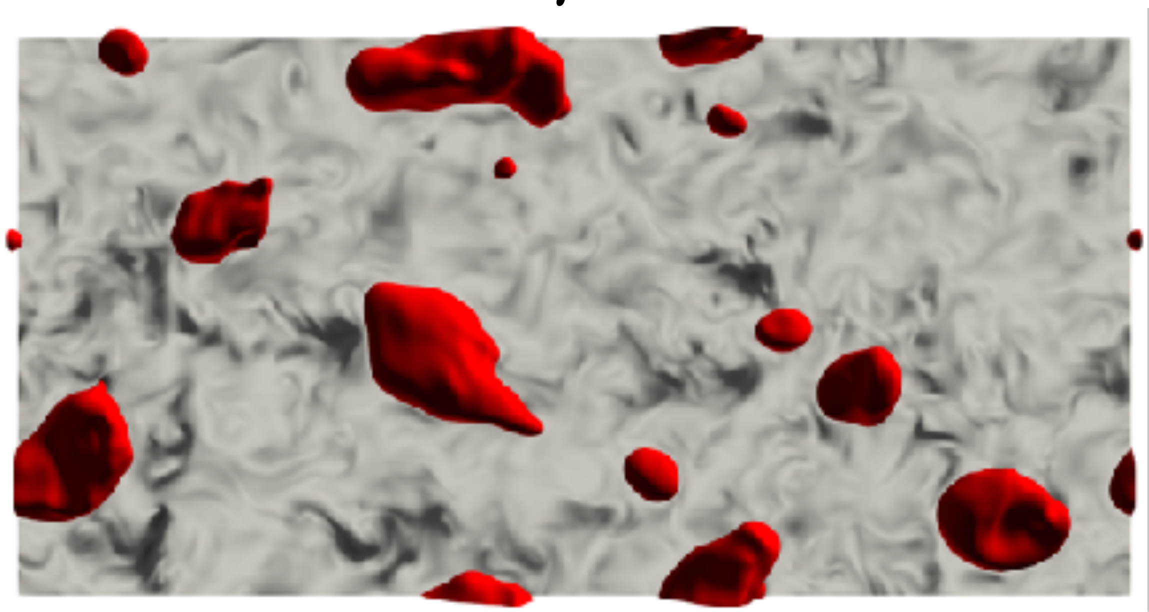
Viscosity ratio: $\lambda = \frac{\eta_d}{\eta_c} = 0.01 \div 100$

Density ratio: $\gamma = \frac{\rho_d}{\rho_c} = 0.001 \div 1$

γ \ λ	0.01	1	100
0.001		X	
0.01		X	
0.1		X	
1	X	X	X

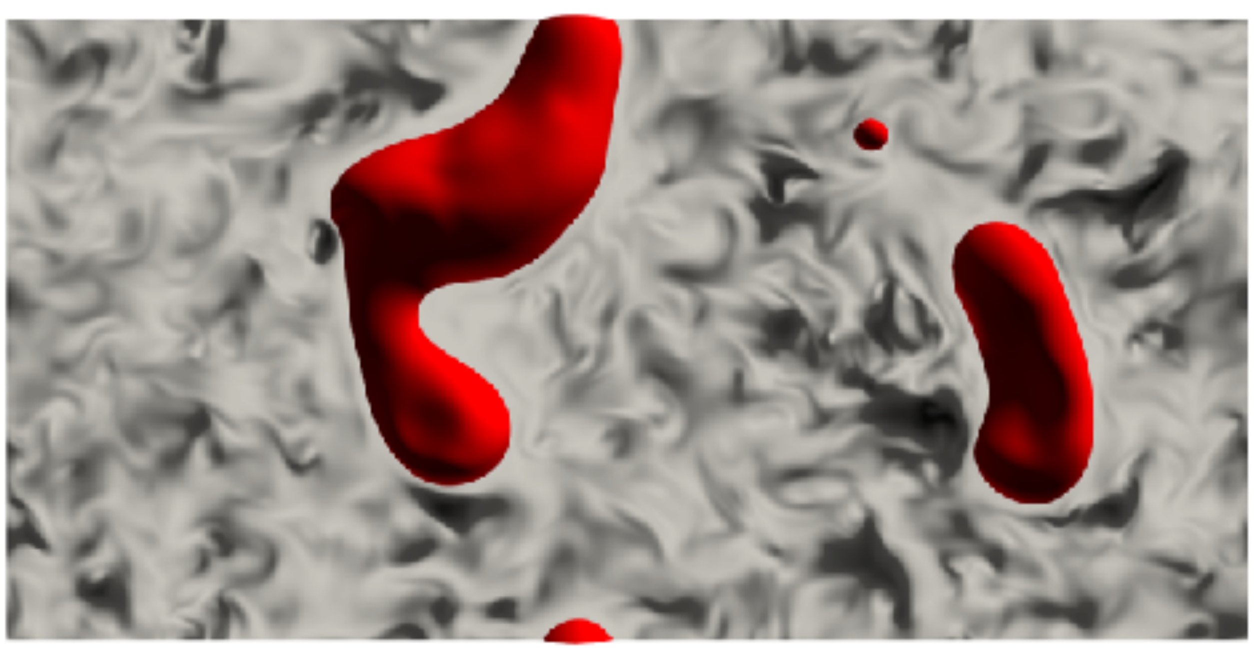
Results: qualitative differences

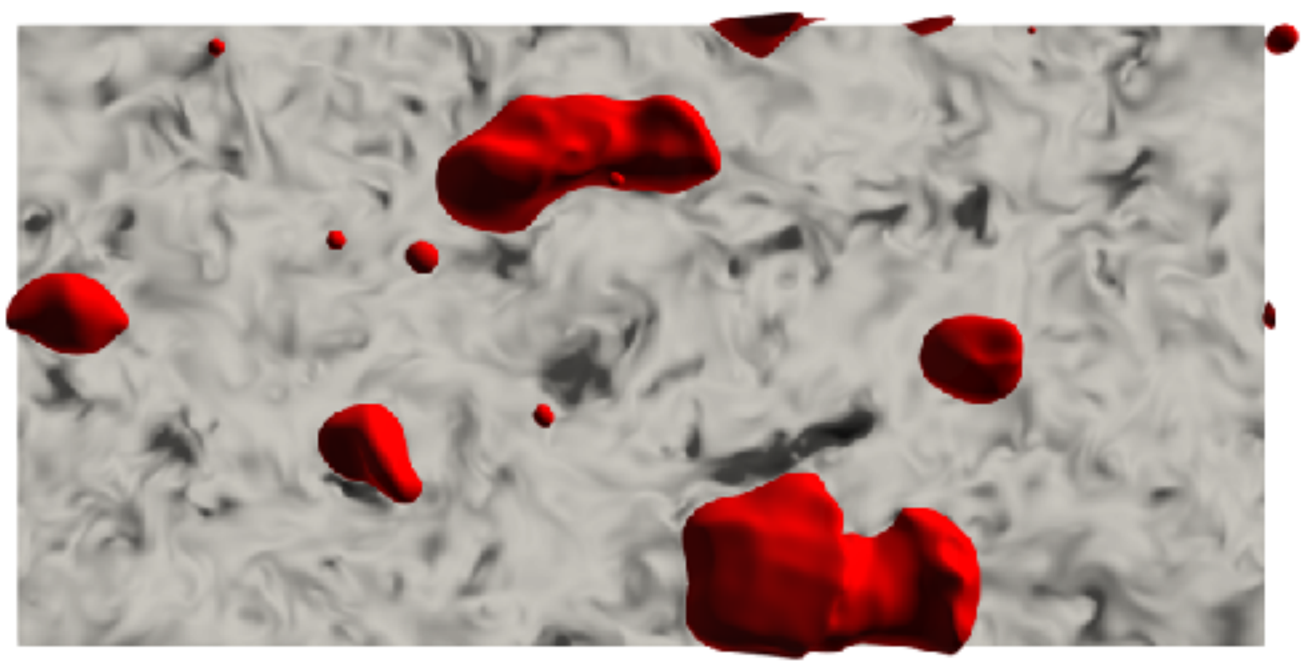
$\lambda = \gamma = 1$



Viscosity ratio $\lambda = 100$

Density ratio $\gamma = 0.001$





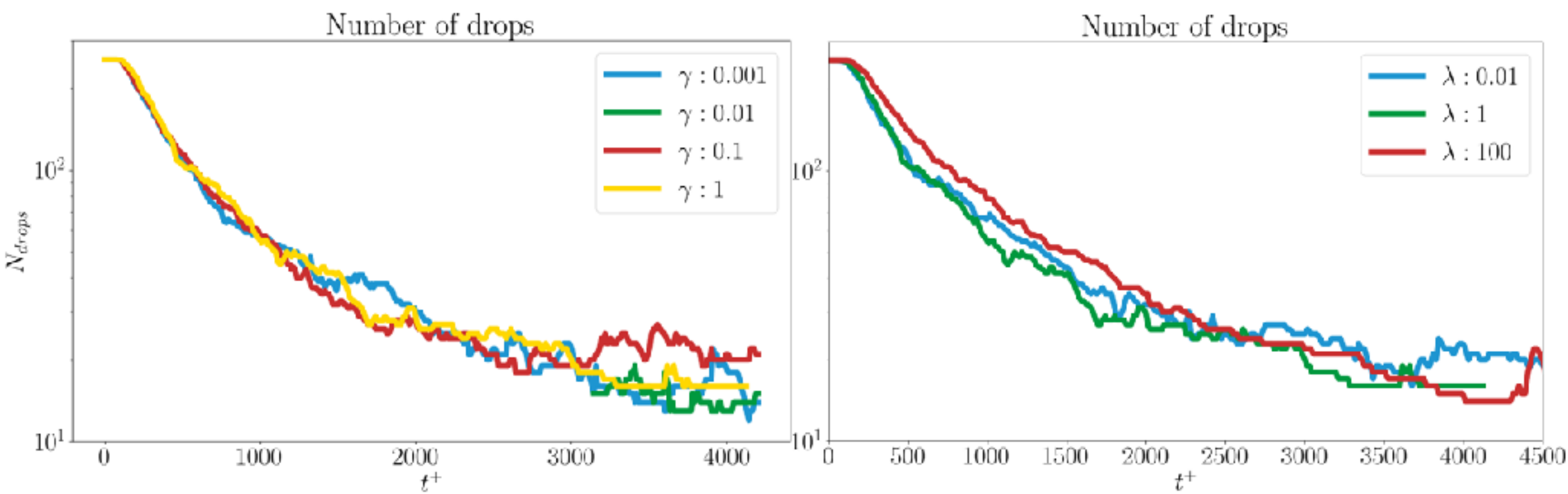
A. Roccon, M. De Paoli, F. Zonta, A. Soldati, Viscosity-modulated breakup and coalescence of large drops in bounded turbulence, *PRF,* 2017

Results: Number of drops

Higher viscosity leads to drops more resistant to breakage

↓

Dominance of coalescence events
leads to a lover number of drops



A. Roccon, M. De Paoli, F. Zonta, A. Soldati, Viscosity-modulated breakup and coalescence of large drops in bounded turbulence, *PRF,* 2017

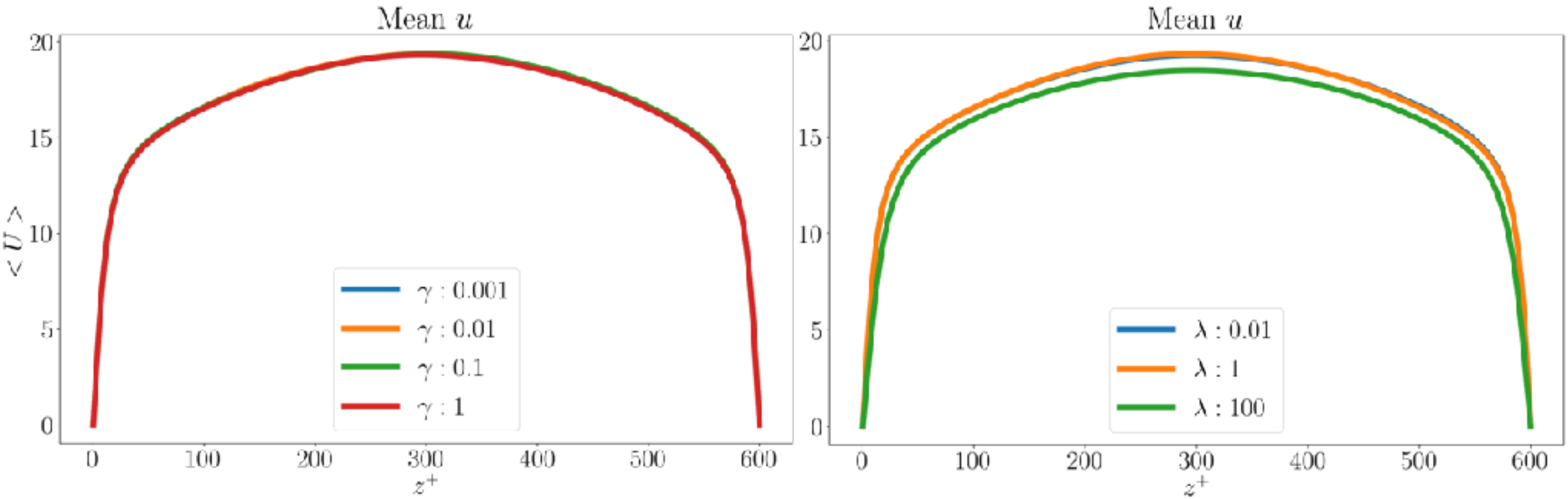
Results: Mean streamwise velocity

Streamwise component of velocity averaged over streamwise ($\hat{x}$) and span wise ($\hat{y}$) directions

Resistance to deformation damps the flow

No significative changes for different γ

Global reduction for $\lambda = 100$



Results: Effects on streaks

$\mathbf{u}' \cdot \mathbf{u}'$ evaluated at
10 w.u. from the wall

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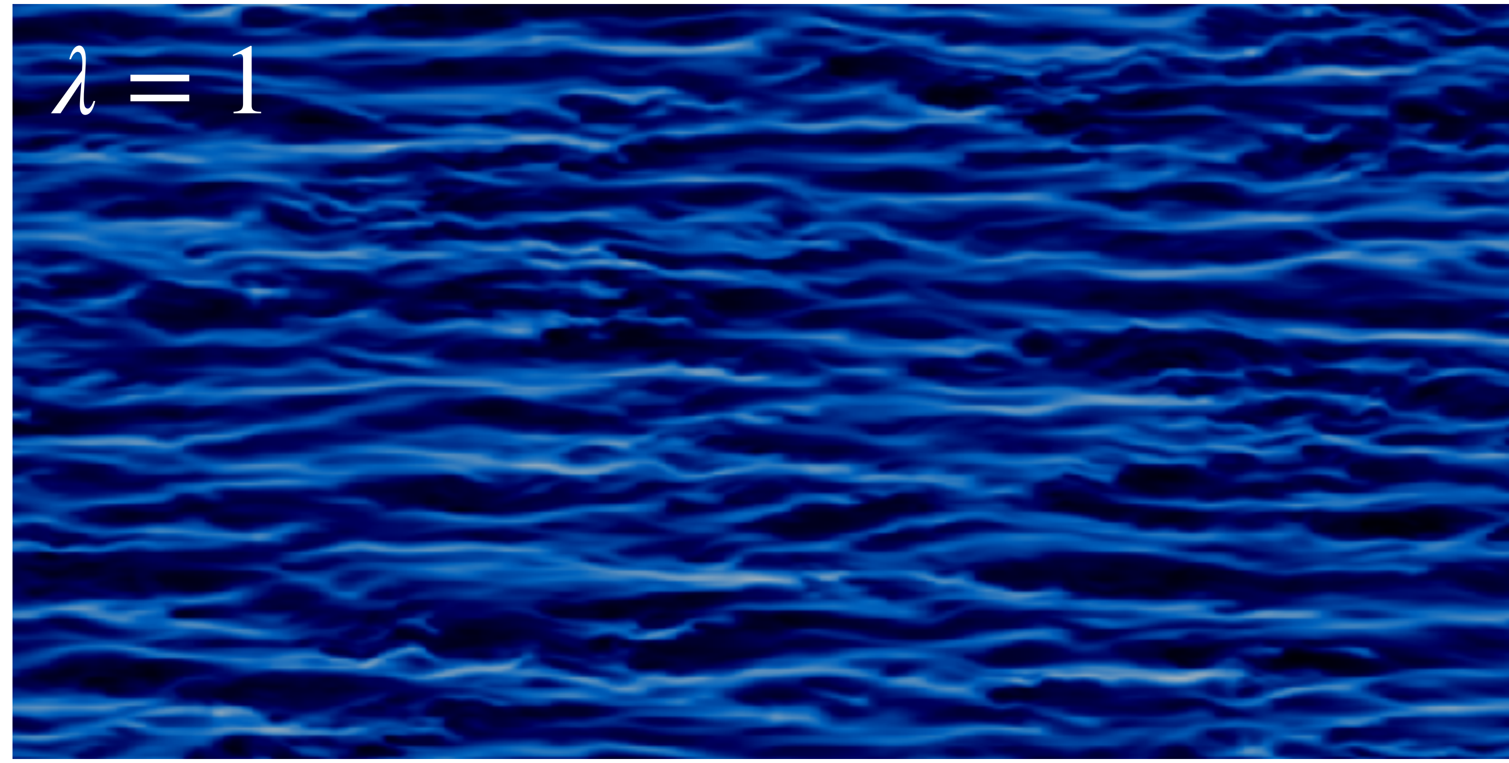
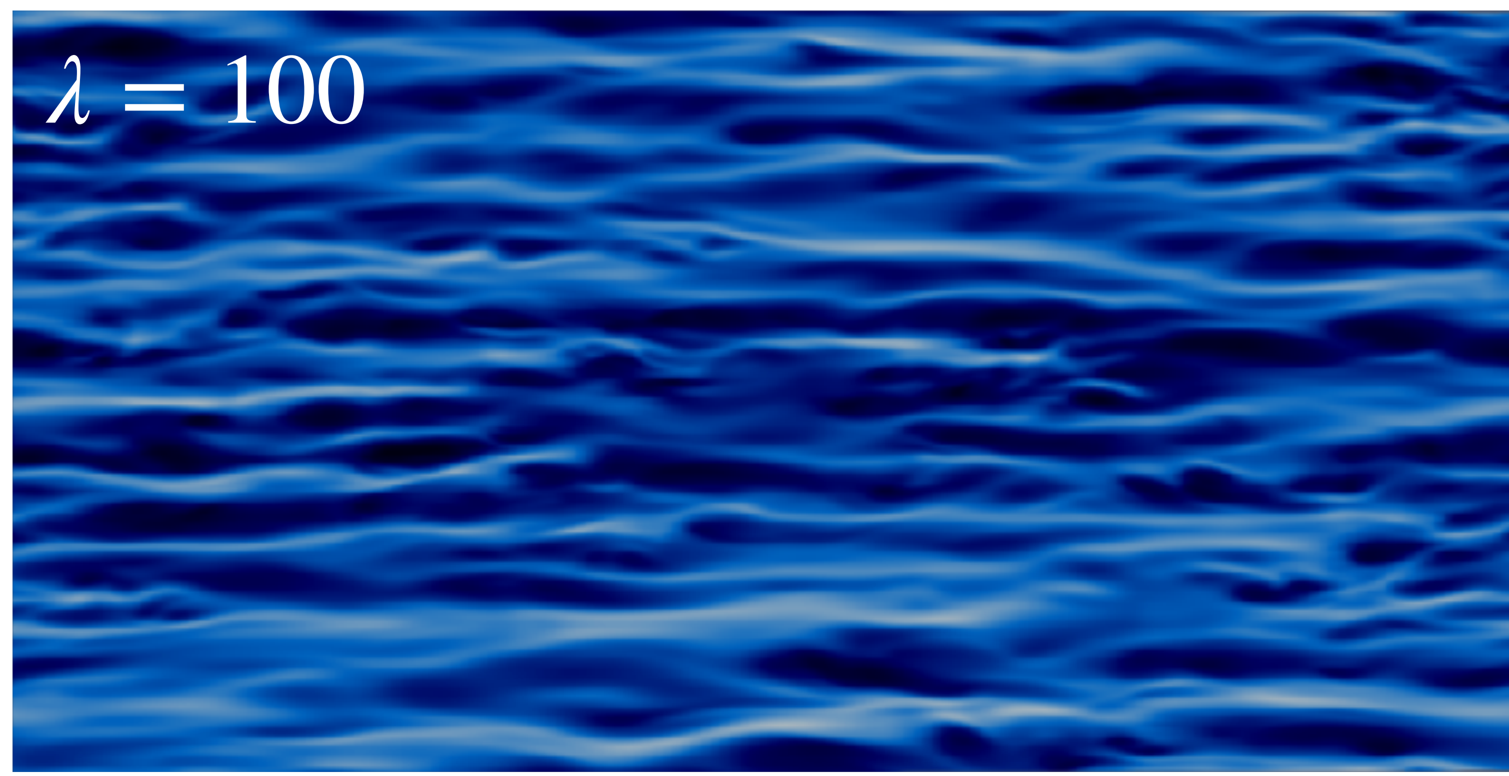
Structures aligned
with streamflow

At higher λ, the bubbles
resist more to deformations

↓

Less streaks, bigger timescales
Globally, higher fluctuations





A. Roccon, M. De Paoli, F. Zonta, A. Soldati, Viscosity-modulated breakup and coalescence of large drops in bounded turbulence, *PRF,* 2017

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Next steps

Continuation of the analysis

Widening of the range of parameters (FD wall-normal direction)

Conferences: ERCOFTAC, APS (november 2019)

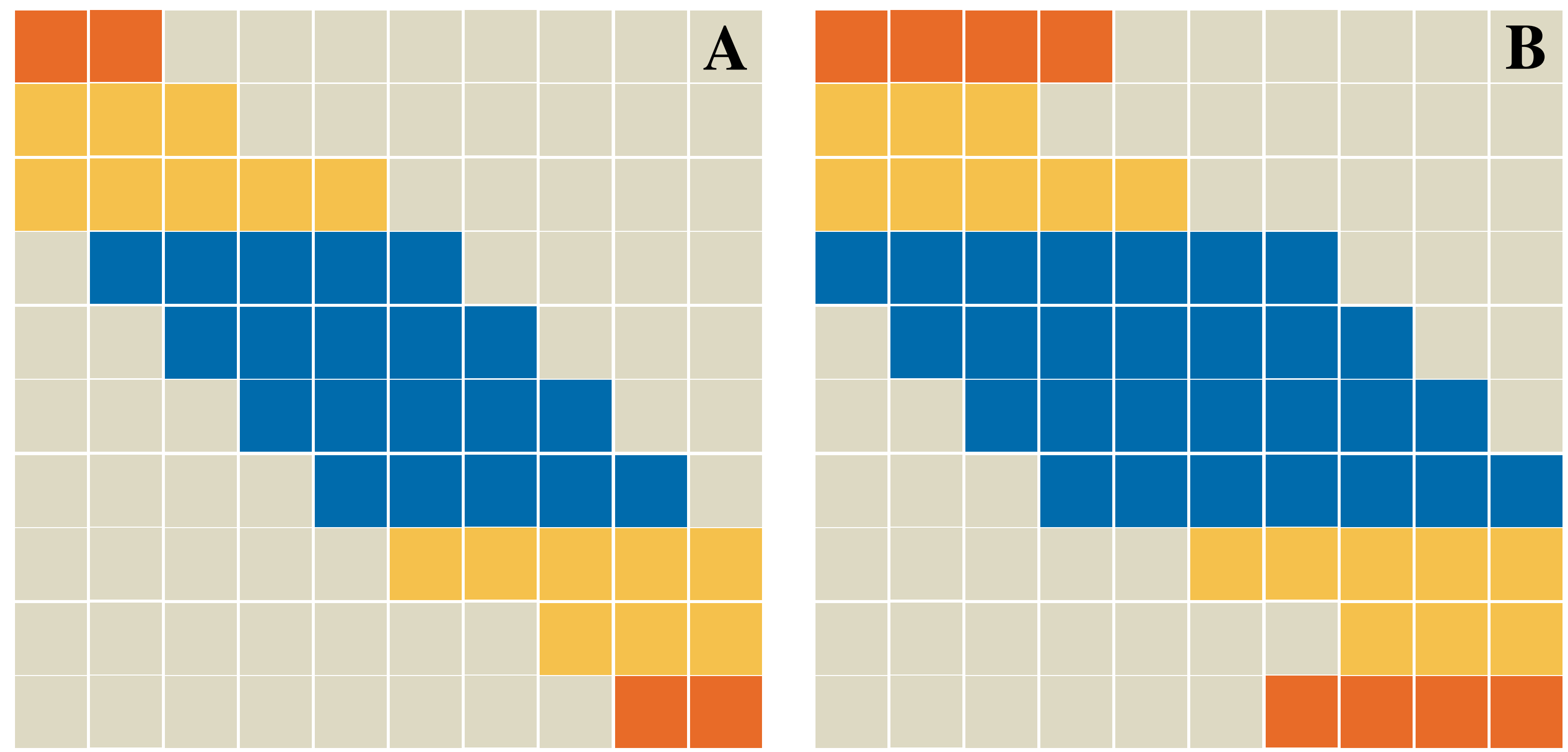
Finite Differences

Uniform grid

$$\beta f''_{i-2} + \alpha f''_{i-1} + f''_i + \alpha f''_{i+1} + \beta f''_{i+2} = c\frac{f_{i+3} - 2f_i + f_{i-3}}{9h^2} + b\frac{f_{i+2} - 2f_i + f_{i-2}}{4h^2} + a\frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}$$

Matching terms of Taylor series

$$\mathbf{A}\vec{f}'' = \mathbf{B}\vec{f}$$

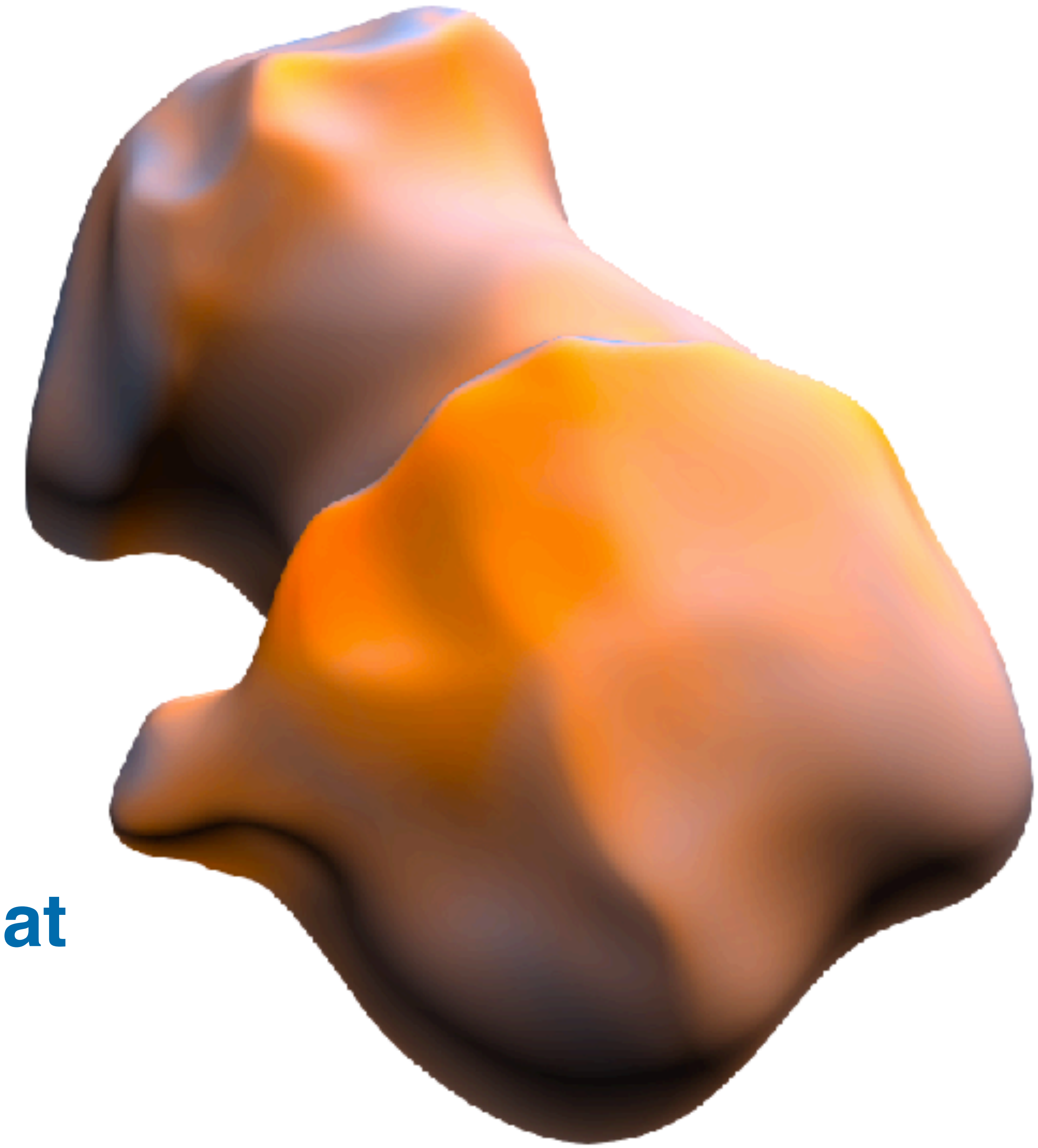


Non-uniform grid

General compact finite difference scheme: $u_i^{(p)} + \sum_{j \in J_n} a_j u_j^{(p)} = \sum_{j \in I_n} b_j u_j + \sum_{j \in J_m} b_j u_j$

The coefficients can be derived with polynomial interpolation and adapted to non-uniform grid (Chebyschev)

Badalassi et al., Computation of multiphase systems with phase model, *JCP* (2003)
Lele, S. K. "Compact finite difference schemes with spectral-like resolution." *J. Comput. Phys.* 103 (1991)
Shukla, Zhong. "Derivation of high-order compact finite difference schemes for non-uniform grid using polynomial interpolation." *J Comput Phys* 204.2 (2005)
Shukla,Tatineni, Zhong. "Very high-order compact finite difference schemes on non-uniform grids for incompressible Navier–Stokes equations." *J Comput Phys* 224.2 (2007)



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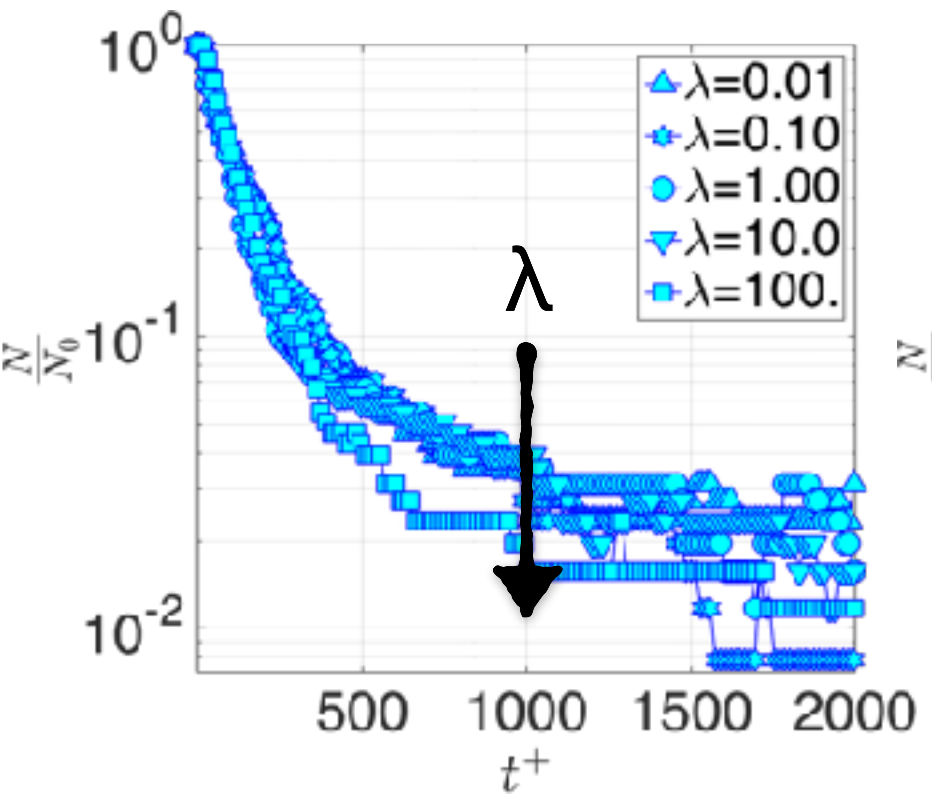
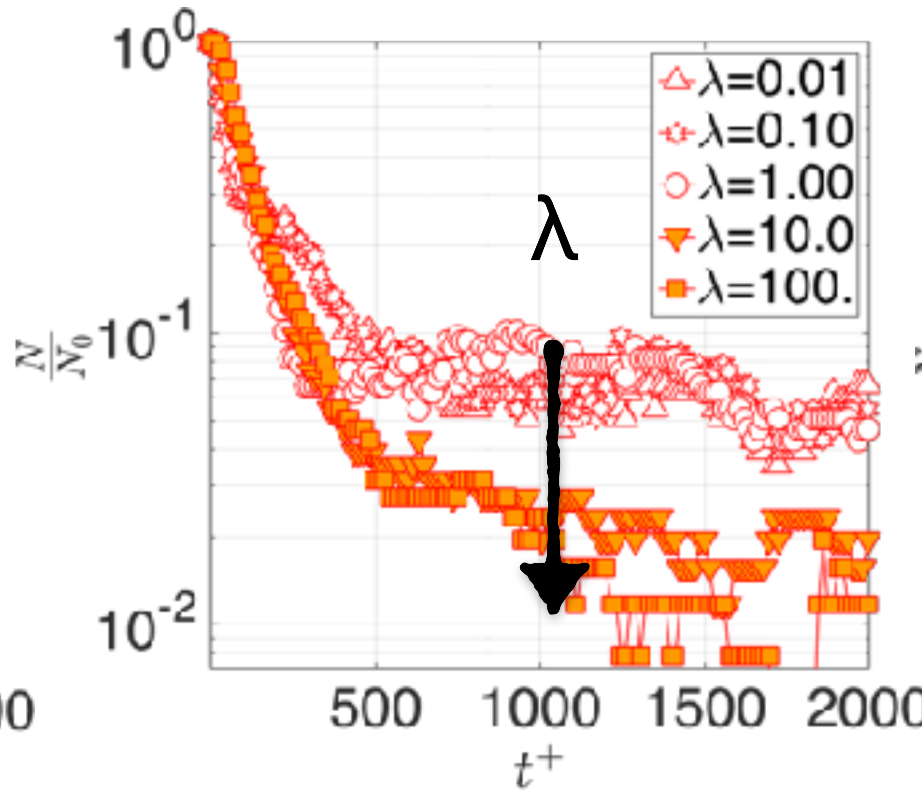
www.fluid.tuwien.ac.at

Collision/Coalescence/Break-up
Drops & Carrier Fluid w. different viscosity

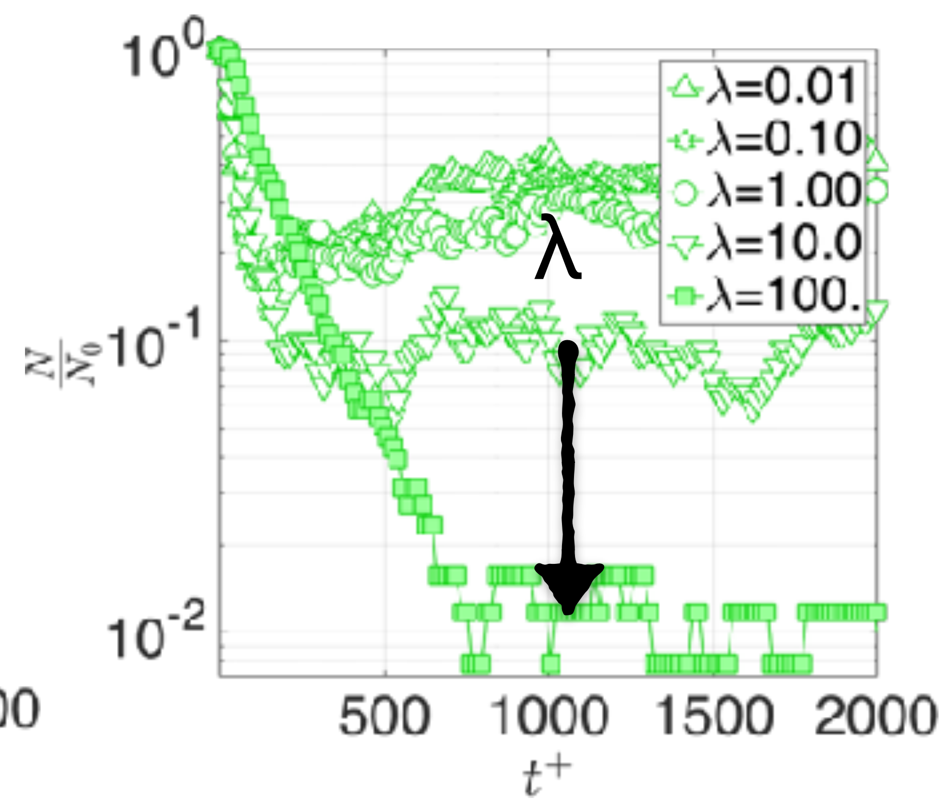
We=0.75



We=1.50



We=3.00



Coalescence Regime for every λ

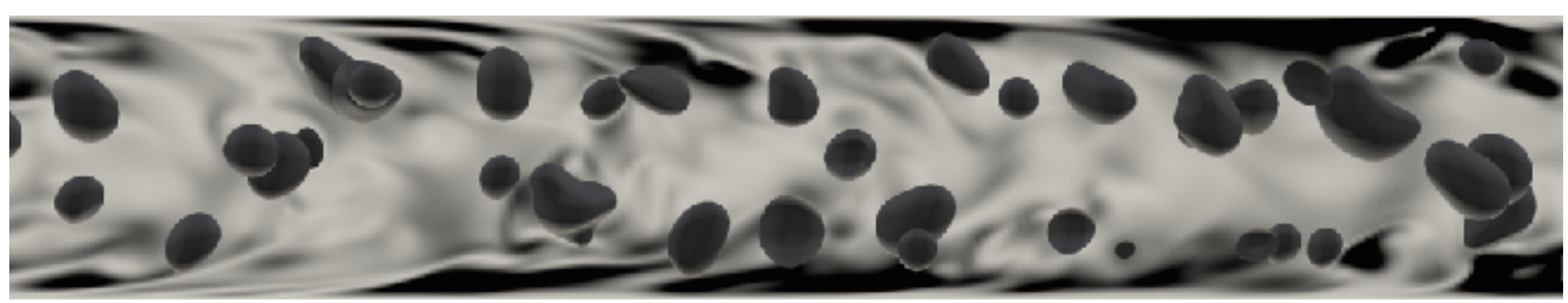
Coalescence Regime for λ < 1

Break-up Regime for λ > 1

Coalescence Regime for λ < 1

Break-up Regime for λ > 1

$$\lambda = \frac{\eta_d}{\eta_c} = \frac{\text{Drop Viscosity}}{\text{Continuous Viscosity}}$$



L. Scarbolo, A. Soldati et. al., Unified framework for a side-by-side comparison of different multicomponent algorithms , JCP. (2013)
A. Roccon, M. De Paoli, F. Zonta, A. Soldati, Viscosity-modulated breakup and coalescence of large drops in bounded turbulence, PRF (2017)

Surfactant Equations

$$\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi = \nabla \cdot \left[\psi(1-\psi)\nabla \mu_\psi\right] \qquad \mu_\phi = \frac{\delta \mathcal{F}[\phi, \nabla\phi, \psi]}{\delta \phi} \qquad \mu_\psi = \frac{\delta \mathcal{F}[\phi, \nabla\phi, \psi]}{\delta \psi}$$

$$\mathcal{F}[\phi, \nabla\phi, \psi] = \int_\Omega \left[f_0(\phi) + f_i(\nabla\phi) + f_\psi(\psi) + f_1(\phi,\psi) + f_b(\phi,\psi)\right] d\Omega$$

- $f_\psi(\psi) = Pi\left[\psi \log\psi + (1-\psi)\log(1-\psi)\right]$ Entropy term — Pi: diffusivity
- $f_1(\phi,\psi) = -\frac{1}{2}\psi\left(1-\phi^2\right)^2$ Adsorption term
- $f_b(\phi,\psi) = \frac{1}{2E_x}\phi^2\psi$ Solubility term — E_x: solubility

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla \mathcal{P} + \frac{1}{Re_\tau}\nabla \cdot \left[\frac{(\lambda-1)(\phi+1)}{2}\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right)\right] + \frac{3}{\sqrt{8}}\frac{Ch}{We}\nabla \cdot \left[\frac{\sigma(\psi)}{\sigma_0}\tau_c\right]$$

Variable surface tension → $\frac{\sigma(\psi)}{\sigma_0}$

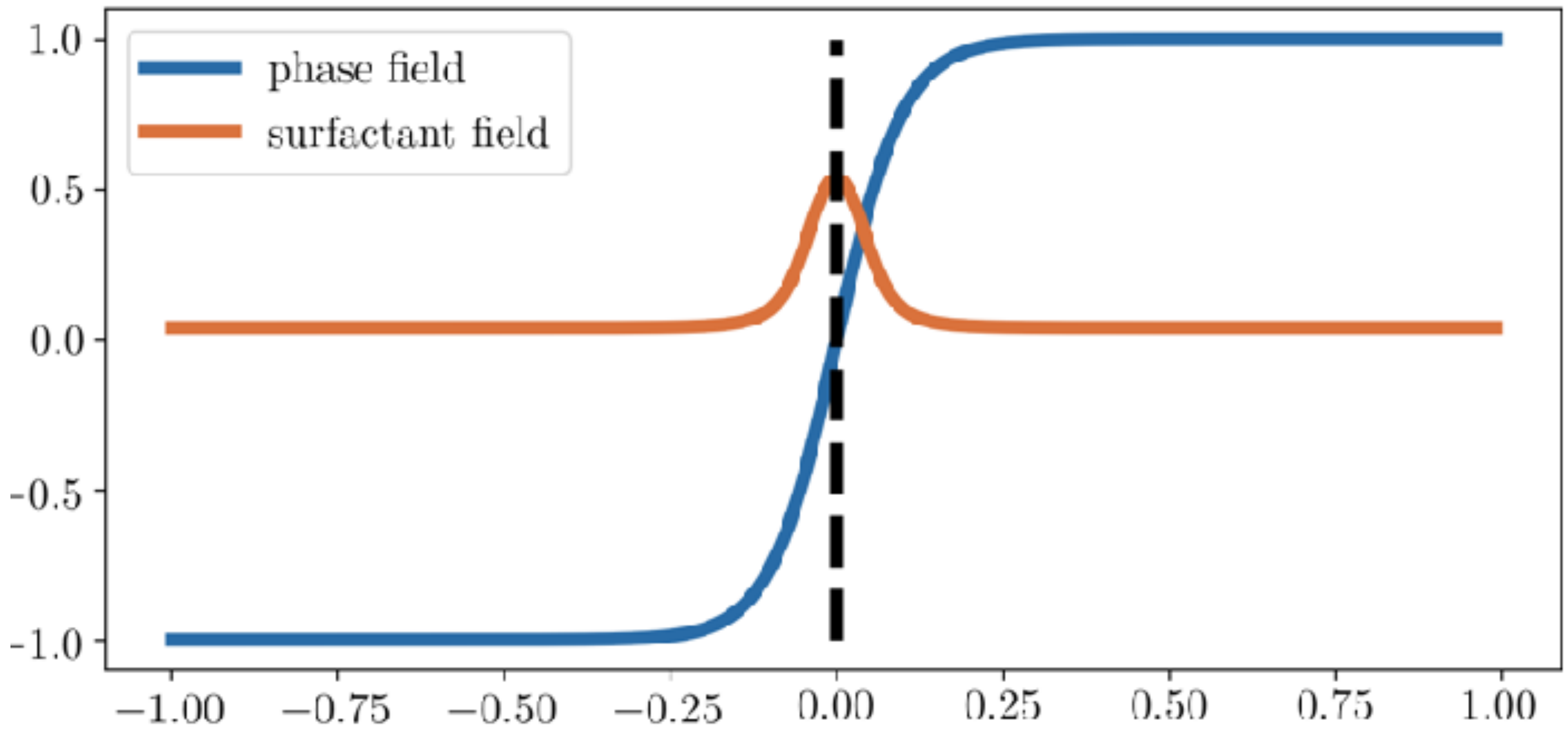
G. Soligo et al., Coalescence of surfactant-laden drops by Phase Field Method, *JCP*, 2019

Steady State of Field Variables

$$\phi(x) = \tanh\left(\frac{x}{\sqrt{2}Ch}\right)$$

$$\psi(x) = \frac{\psi_{bulk}}{\psi_{bulk} + \psi_c(\phi)(1 - \psi_{bulk})}$$

$$\psi_c(\phi) = \exp\left[-\frac{1-\phi^2}{2Pi}\left(1 - \phi^2 + \frac{1}{E_x}\right)\right]$$



Mass losses

Spontaneous shrinkage of droplets

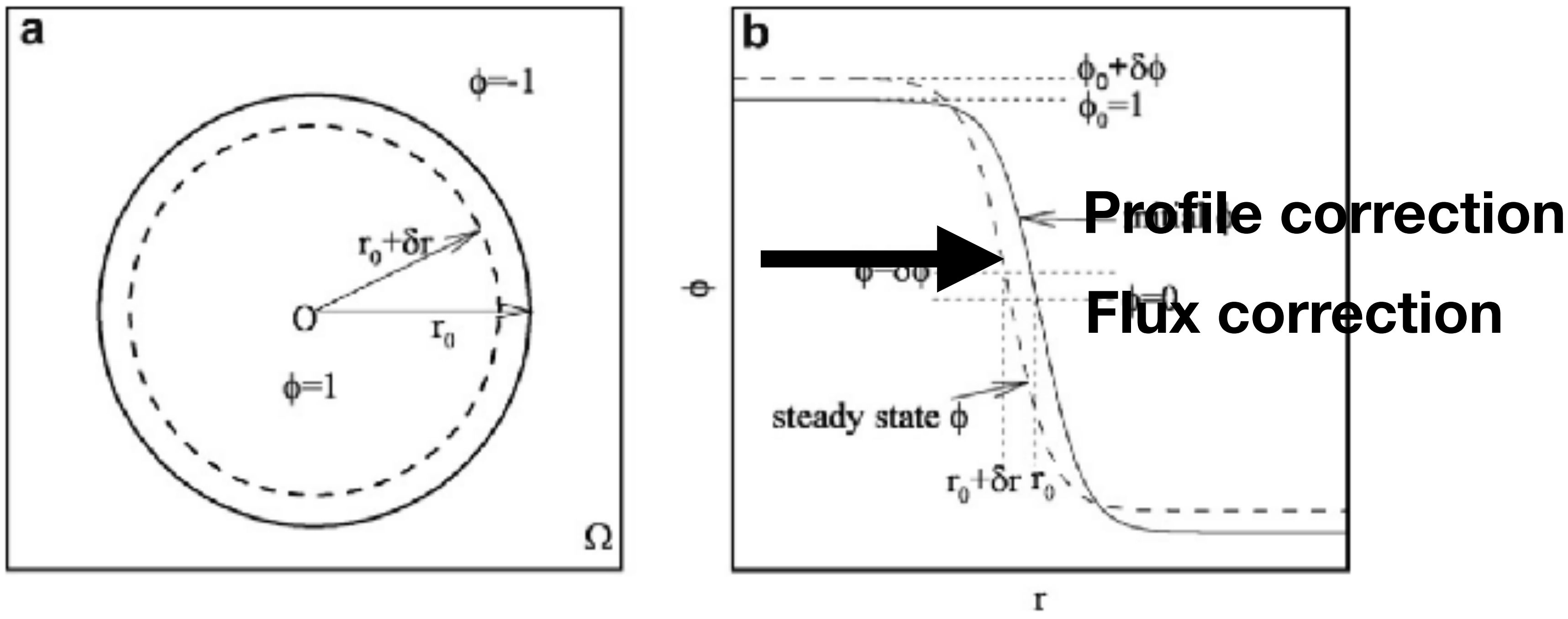
Reliability

$$\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} \leq 0$$

Total energy is lowered by drop shrinkage

$$\delta\mathscr{F} \propto \delta r$$

$$\left|\phi\right| > 1!$$



P. Yue et al., Spontaneous shrinkage of drops and mass conservation in phase-field simulations, *JCP* (2007)
G. Soligo et al., Mass-conservation-improved phase field methods for turbulent multiphase flow simulation, *Acta Mechanica* (2019)

Finite Differences: Uniform Grid

$$\beta f''_{i-2} + \alpha f''_{i-1} + f''_i + \alpha f''_{i+1} + \beta f''_{i+2}$$
$$= c\frac{f_{i+3} - 2f_i + f_{i-3}}{9h^2} + b\frac{f_{i+2} - 2f_i + f_{i-2}}{4h^2} + a\frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}$$

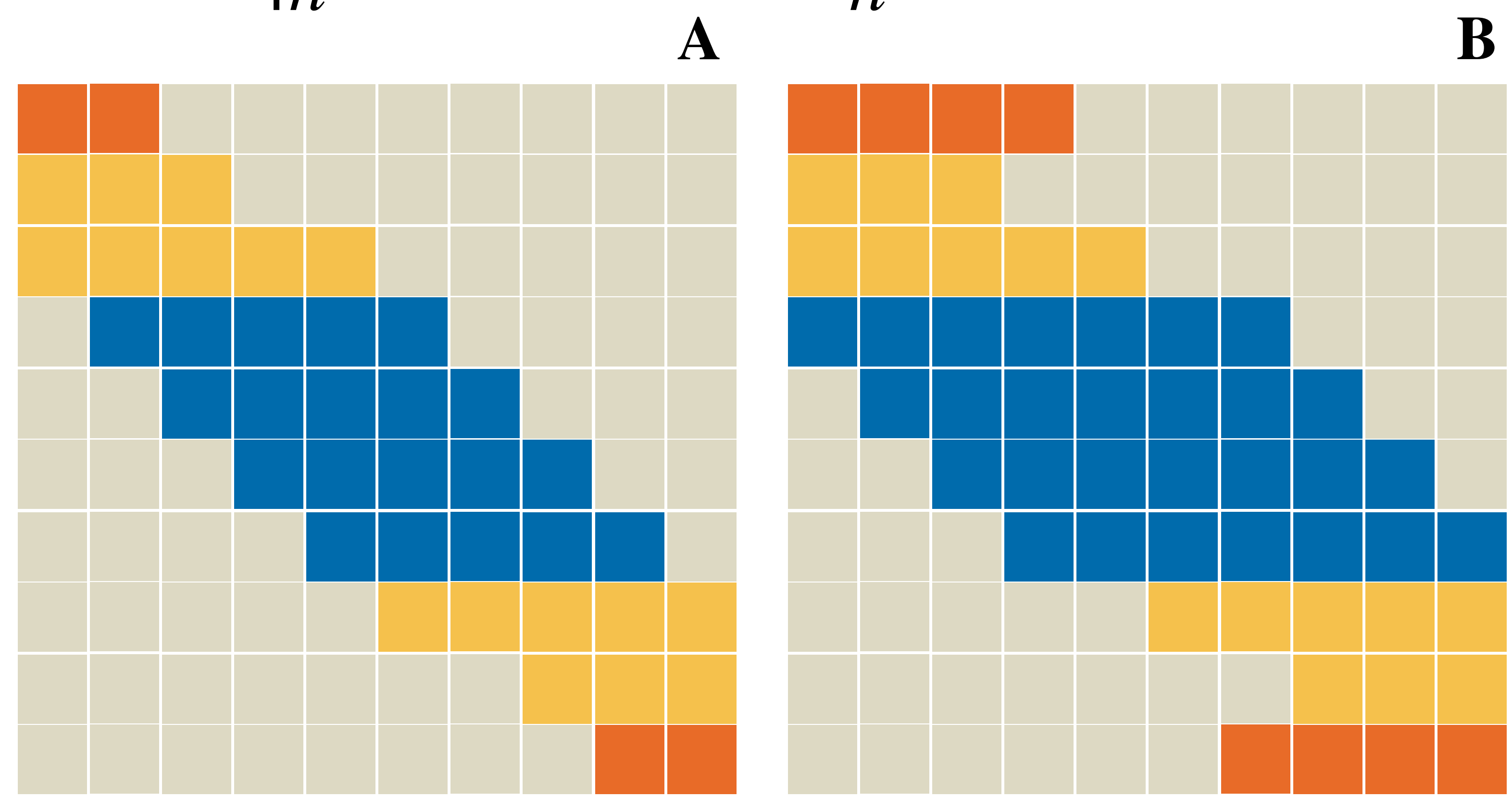
Matching terms of Taylor series

↓

α,β,a,b,c

↓

$\mathbf{A}\vec{f}'' = \mathbf{B}\vec{f}$



Helmholtz Equation: $P(x)f''(x) + Q(x)f(x) = R(x)$ → $\vec{P}\cdot\vec{f}'' + \vec{Q}\cdot\vec{f} = \vec{R}$

$$\underbrace{(\vec{P}\cdot\mathbf{A}^{-1}\mathbf{B} + \vec{Q})}_{\vec{M}}\cdot\vec{f} = \underbrace{\vec{R}}_{\vec{K}}$$

Badalassi et al., Computation of multiphase systems with phase model, *JCP* (2003)
Lele, S. K. "Compact finite difference schemes with spectral-like resolution." *J. Comput. Phys.* 103 (1991)
Shukla, Zhong. "Derivation of high-order compact finite difference schemes for non-uniform grid using polynomial interpolation." *J Comput Phys* 204.2 (2005)
Shukla,Tatineni, Zhong. "Very high-order compact finite difference schemes on non-uniform grids for incompressible Navier–Stokes equations." *J Comput Phys* 224.2 (2007)

Finite Differences: Adapted Grid

General compact finite difference scheme: $u_i^{(p)} + \sum_{j\in J_n} a_j u_j^{(p)} = \sum_{j\in I_n} b_j u_j + \sum_{j\in J_m} b_j u_j$

$$u(x) = \sum_{i\in I_n} u_i \rho_i(x) + \sum_{i\in I_n} u_i'' q_i(x) + \sum_{i\in I_m} u_i r_i(x)$$

Conditions on ρ_i, q_i, r_i

$$\rho_i(x_j) = \delta_{ij} \quad \forall i \in I_n, \forall j \in I_n \cup I_m$$
$$\rho_i''(x_j) = 0 \quad \forall i \in I_n, \forall j \in I_n$$

↓

Guess of the form

$$\rho_i(x) = \frac{\prod_m(x)}{\prod_m(x_i)} l_i^n(x) \left(1 + \sum_{r=1}^{n} A_r (x - x_i)^r\right), \quad i \in I_n$$

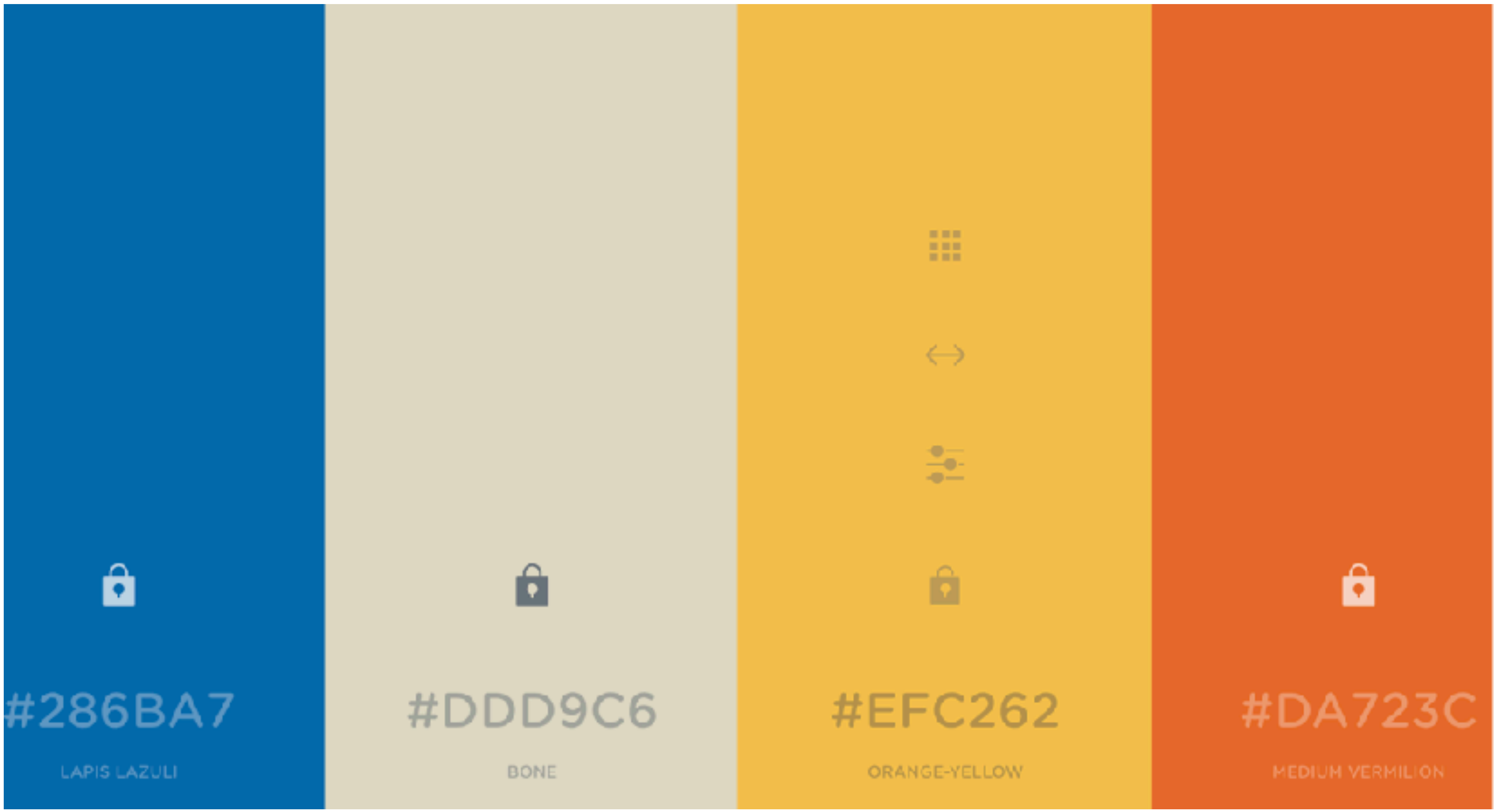
↓

Differentiating and using the condition gives n equations in n unknowns $A_1, A_2, \ldots A_n$

The coefficients can be adapted to non-uniform grid (Chebyschev)

Shukla, Zhong. "Derivation of high-order compact finite difference schemes for non-uniform grid using polynomial interpolation." *J Comput Phys* 204.2 (2005)
Shukla,Tatineni, Zhong. "Very high-order compact finite difference schemes on non-uniform grids for incompressible Navier–Stokes equations." *J Comput Phys* 224.2 (2007)

END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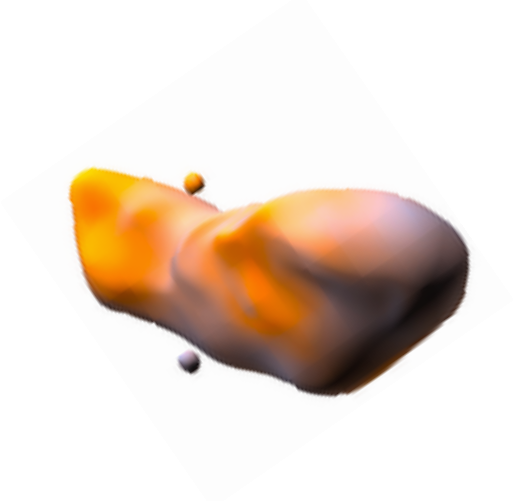
LAPIS LAZULI
#DDD9C6
BONE
#EFC262
ORANGE-YELLOW
#DA723C
MEDIUM VERMILION

Advanced courses

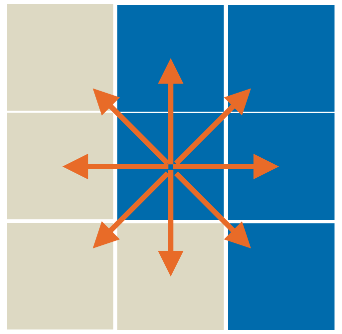
Cross-topic training

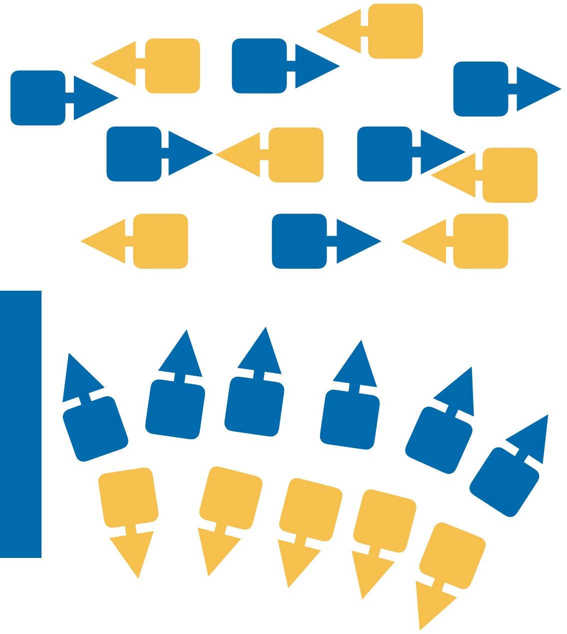
Innovative methods



$$\left.\frac{\partial(\delta \mathscr{F})}{\partial(\delta r)}\right|_{\delta r=0} > 0$$

Drops are identified with the **flood fill algorithm**



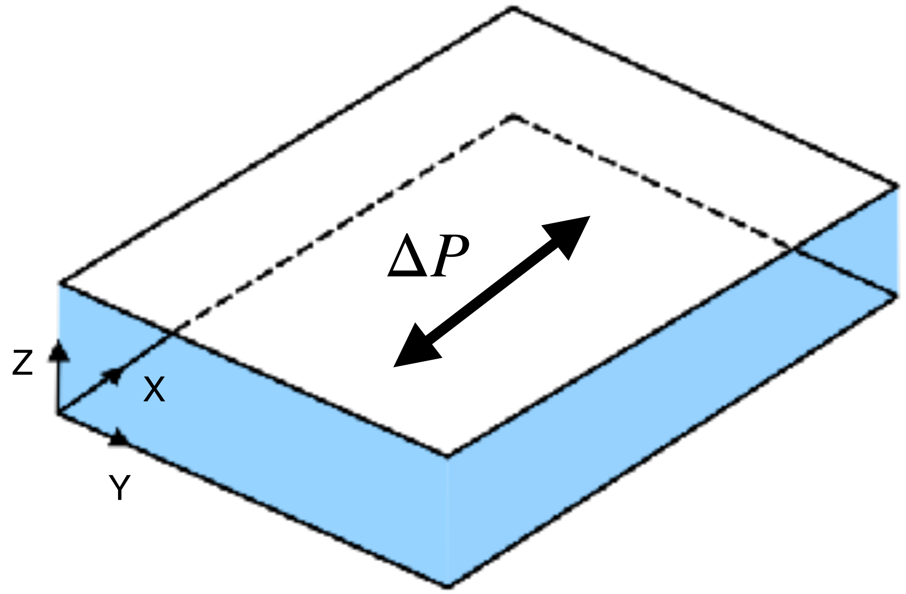


Implementation and testing of finite-differences method

Numerical Method

Direct Numerical Solution (DNS) coupled CH and NS equations, no models used.

Computational Domain



Solver NS (Vorticity-Velocity Formulation)

Curl of NS (Vorticity):

$$\frac{d\omega}{dt} = \nabla \times \mathbf{S} + \frac{1}{Re_\tau}\nabla^2\omega$$

Double Curl of NS (Vorticity)

$$\frac{d\nabla^2\mathbf{u}}{dt} = \nabla^2\mathbf{S} - \nabla(\nabla\cdot\mathbf{S}) + \frac{1}{Re_\tau}\nabla^4\mathbf{u}$$

CH (Same formulation)

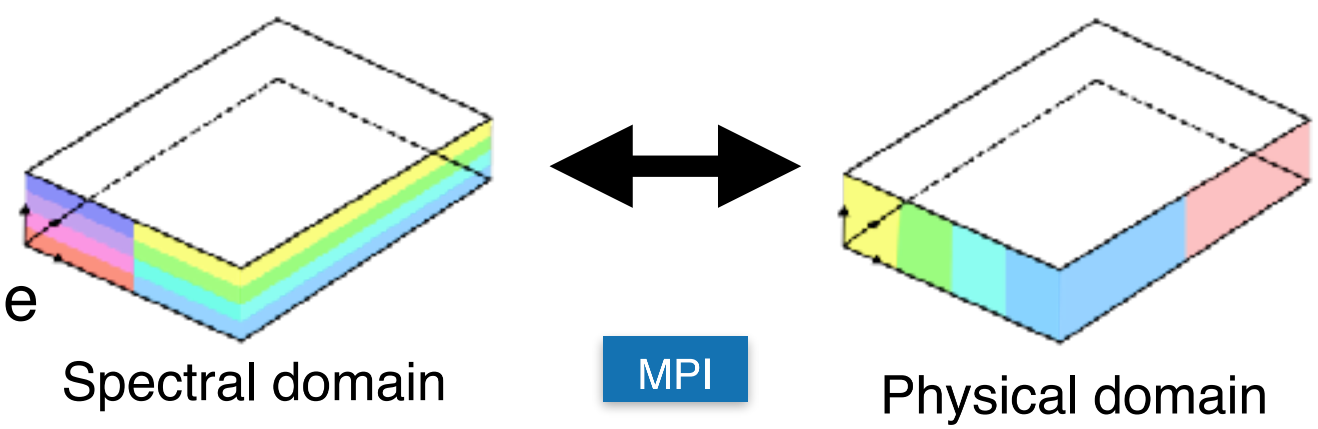
$$\frac{d\phi}{dt} = S_\phi + \frac{sCh^2}{Pe}\nabla^2\phi - \frac{Ch^2}{Pe}\nabla^4\phi$$

Space Discretisation:

- X Periodic direction (Fourier)
- Y Periodic direction (Fourier)
- Z Wall-normal (Chebyshev-Tau)

Time Discretisation:

- N-S: Crank-Nicolson/Adams-Bashforth scheme
- C-H: Crank-Nicolson/Euler scheme



Guidelines

TECHNICAL

- **Reliability**
- **Scaling**
- **Realistic parameters**

COMMUNICATION

- **Publications**
- **Ease of use** ⟷ **ESTECO**
- **Conferences**