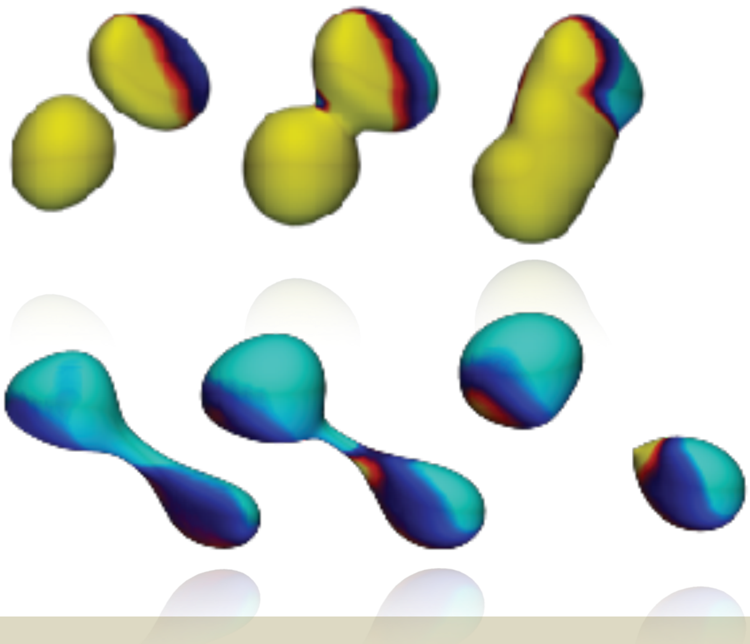
Simulations of interfaces in Turbulent Flows with Breakage, Coalescence and Drop Size Distribution - Phase Field & DNS



Alfredo Soldati and Francesco Zonta
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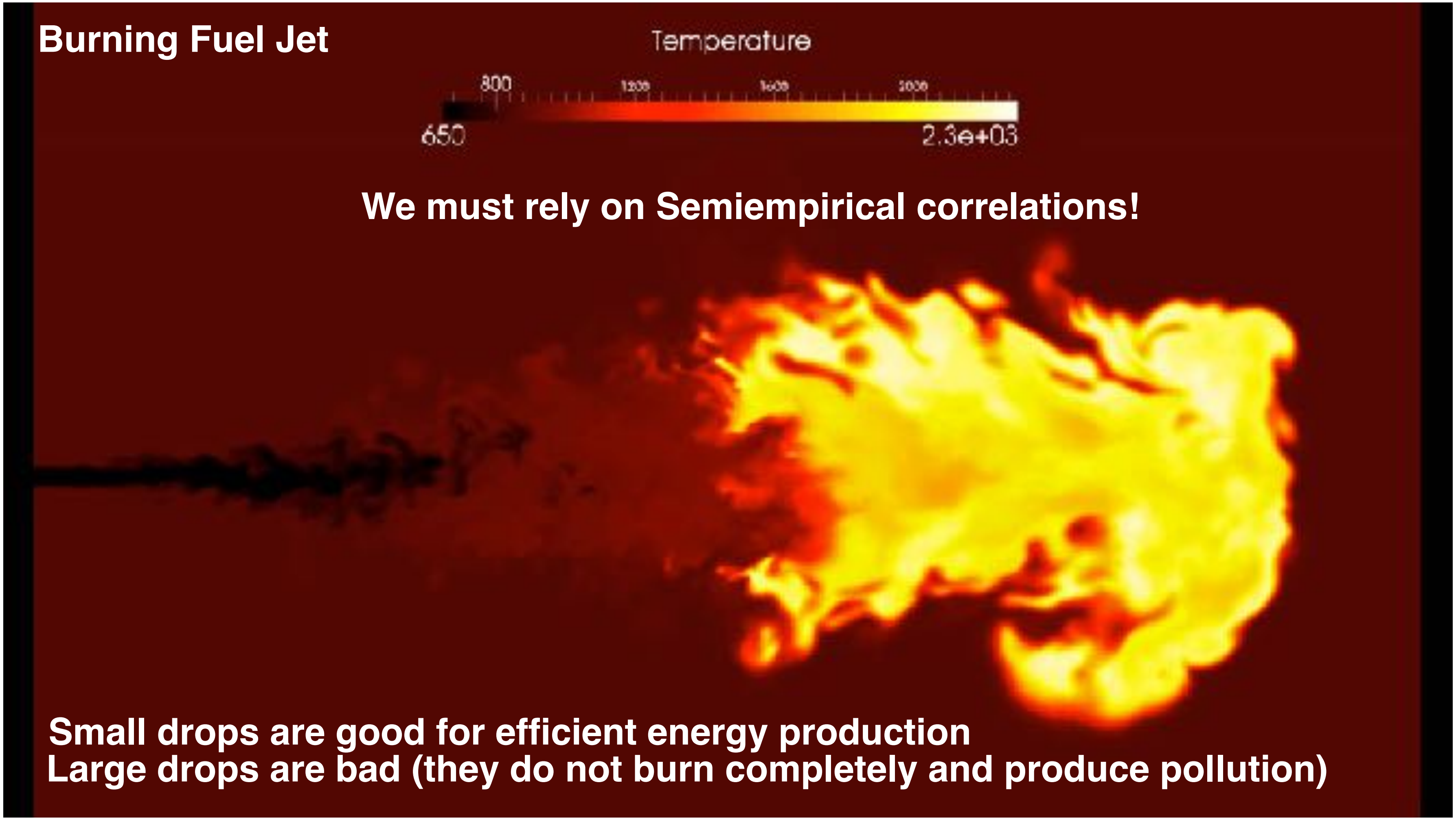
(also with DPIA University of Udine, Italy)

Fil Rouge

1. Historical Perspective, modelling and computational issues
2. A short story on droplets in turbulence (influence of viscosity/density contrast)
3. A short story on oil transport
4. A short story on drop coalescence/break-up (influence of surfactant)

Clean energy production … drops size makes the difference

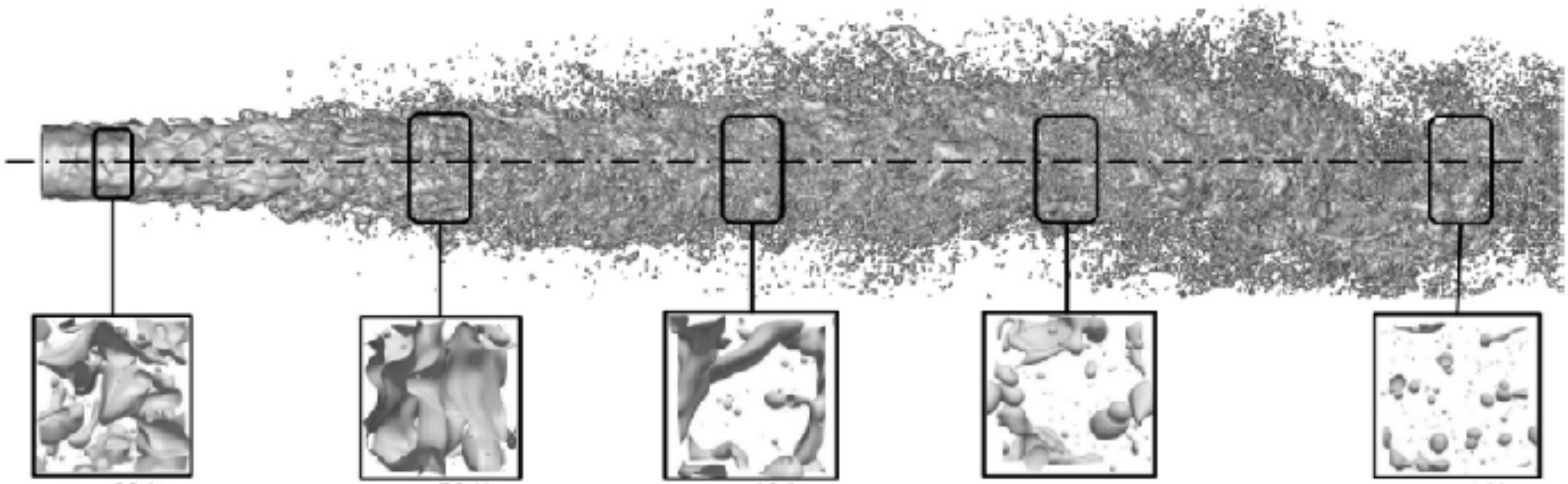


We must rely on Semiempirical correlations!

Small drops are good for efficient energy production
Large drops are bad (they do not burn completely and produce pollution)

Greenhouse effect … many small drops influence CO2 absorption by the Ocean

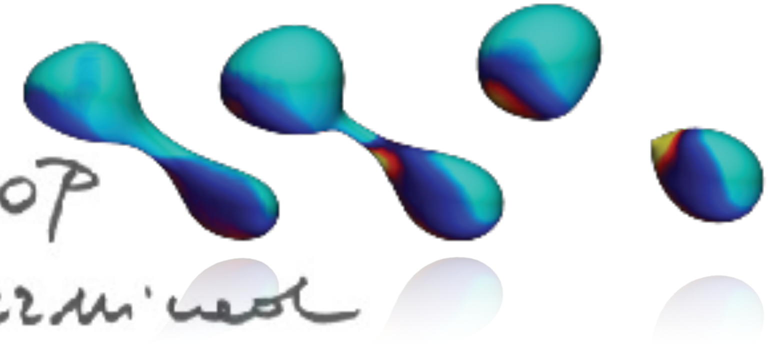
What establishes the different drop sizes?



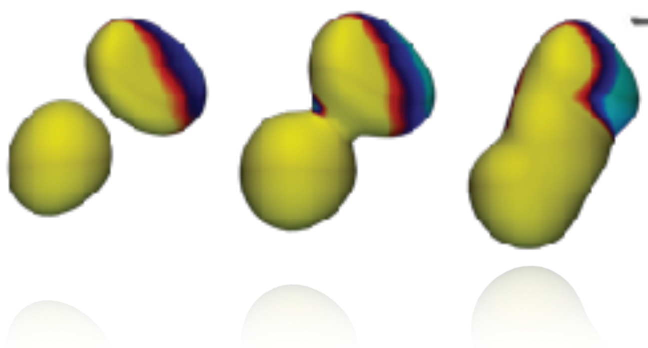
Drops break, collide, coalesce and evolve into a drop population

R. Canu et al., Where does the droplet size distribution come from? IJMF (2018)

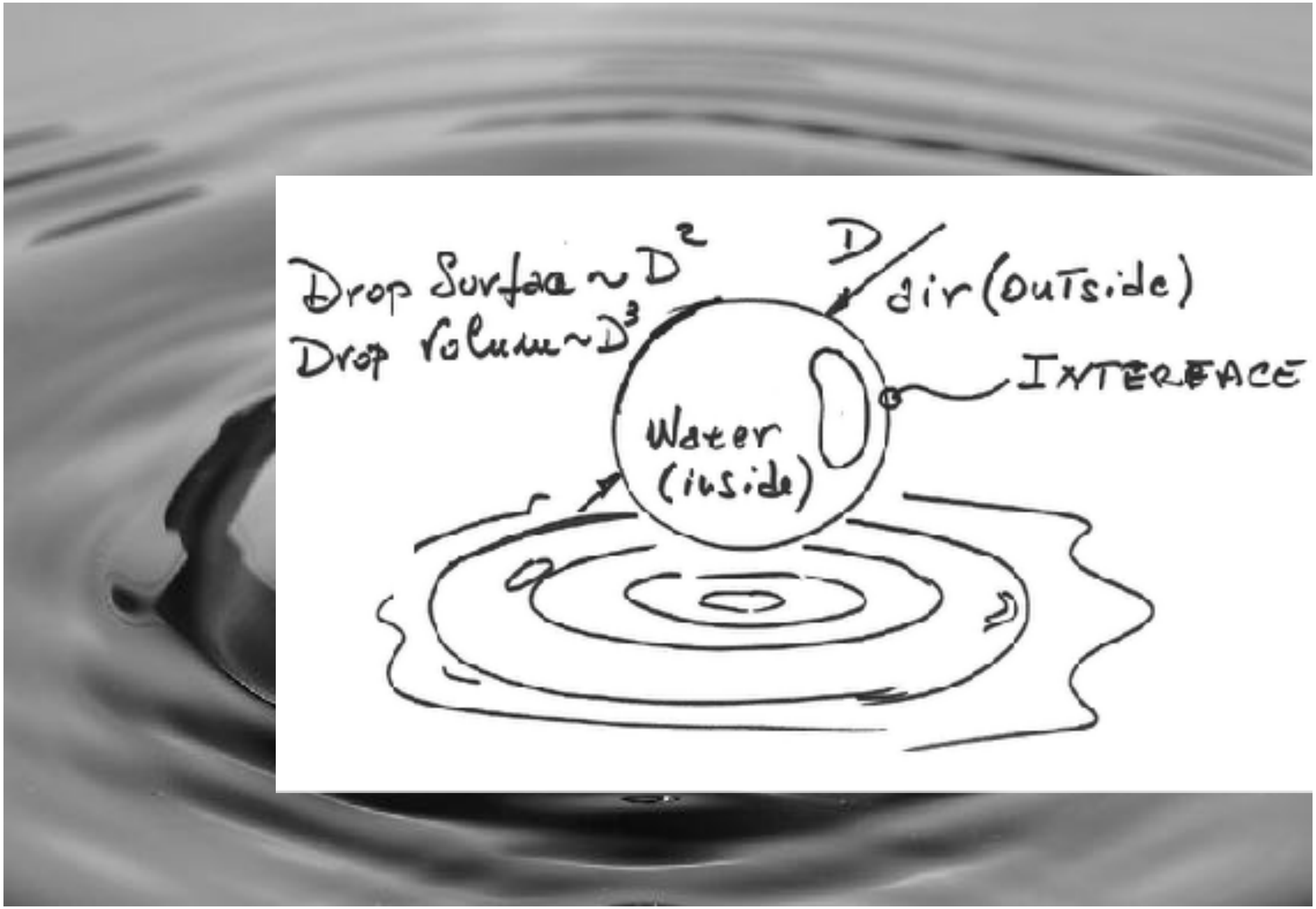
Break-up and Coalescence: This is what we want to know (model/compute)



The evolution of a drop population is determined by the competition between BREAK-UP and COALESCENCE



if "Manners *makyth* man" ….
Interface *makyth* drops …



Interface is conventionally defined (a model) and we assign a property to the interface: surface tension!

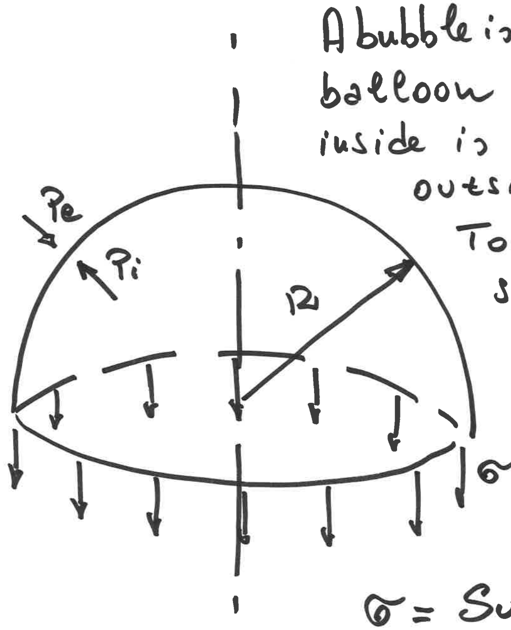
Surface tension

From Wikipedia, the free encyclopedia

For the short story by James I

Surface tension is the elastic ten
possible. Surface tension allows i
on a water surface.

At liquid–air interfaces, surface te
(due to cohesion) than to the mol
surface that causes the liquid to b
Thus, the surface becomes under
"surface tension" came from.[1] Be
through a web of hydrogen bonds
20 °C) compared to that of most c
capillarity.



A bubble is like a small balloon: pressure inside is larger than outside. Necessary to maintain the shape.

$$(P_i - P_e) = \frac{2\sigma}{R}$$

$$\sigma = \frac{P_i - P_e}{2} R$$

σ = Surface Tension

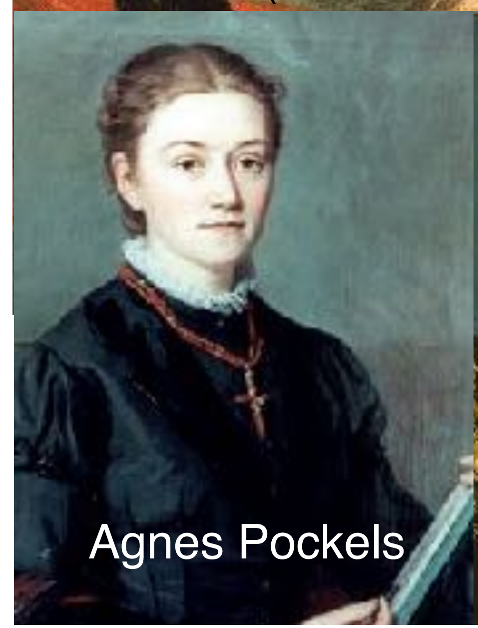
Alfredo Soldati and Francesco Zonta

Introduction:
Thickness of Interface and role of surfactants

In 1757, Franklin was sent by the American House of Assembly of Philadelphia to Great Britain to petition King George II against the policies and activity of the Penn family, the proprietors of Pennsylvania. Soon after leaving New York harbour, the fleet of 96 ships encountered windy weather, sending them ferociously rocking over the waves. Franklin noticed that <u>two of the ships in the fleet were sailing much more smoothly than the rest.</u>

Benjamin Franklin

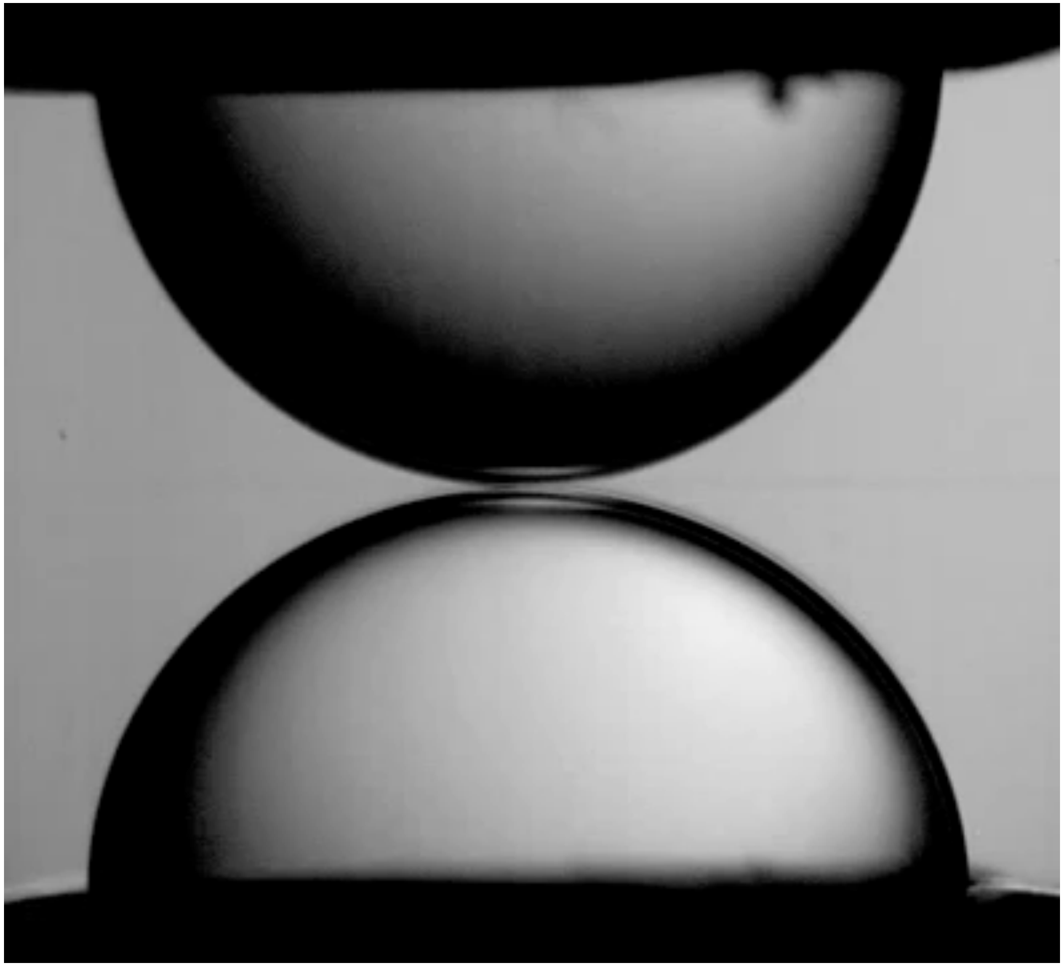
1.63×10^{-9} m (Rayleigh)
1.3×10^{-9} m (Pockels kitchen)



Agnes Pockels

Wang D.N. et al., Benjamin Franklin, Philadelphia's favourite son, was a membrane biophysicist, BJ (2013)
L. Rayleigh, Measurements of the Amount of Oil Necessary in Order to Check the Motions of Camphor upon Water, PRSL (1890)
A. Pockels, Surface Tension, Nature (1891)
A. Pockels., On the Relative Contamination of the Water-Surface by Equal Quantities of Different Substances, Nature (1892)

Droplet interactions in controlled cases 1.
Coalescence of two quiescent drops



Courtesy of
Nicole Sharp, FYFD.

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Droplet interactions in controlled cases 2.
Head-on drop collisions/coalescence/break-up

Accurate Experiments

023303-12 Lycett-Brown et al. Phys. Fluids 26, 023303 (2014)

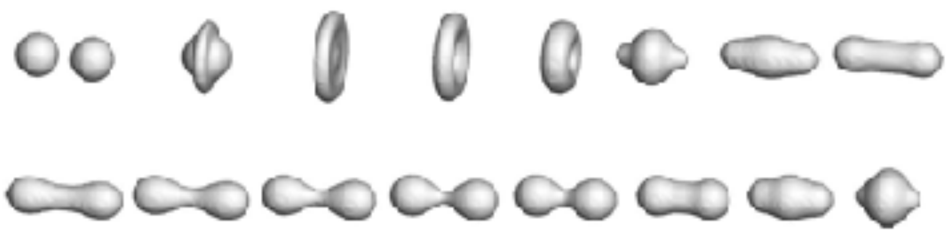


FIG. 6. Head-on coalescence of equal sized droplets. We = 61.5, Re = 238.

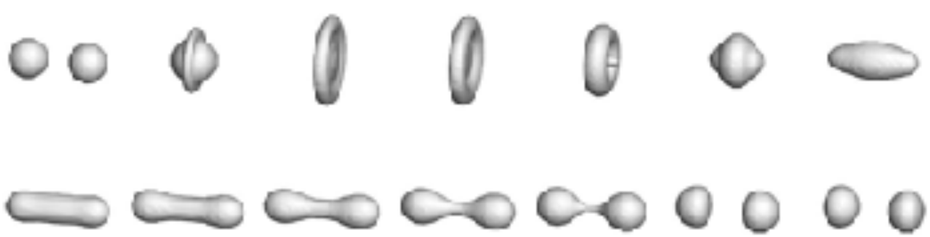


FIG. 7. Head-on separation of equal sized droplets. We = 83.5, Re = 277.

Ashgriz and J. Y. Poo, "Coalescence and separation in binary collisions of liquid drops," J. Fluid Mech. 221, 183 1990.
Qian and C. K. Law, "Regions of coalescence and separation in droplet collision," J. Fluid Mech. 331, 59 1997.

Accurate Simulations

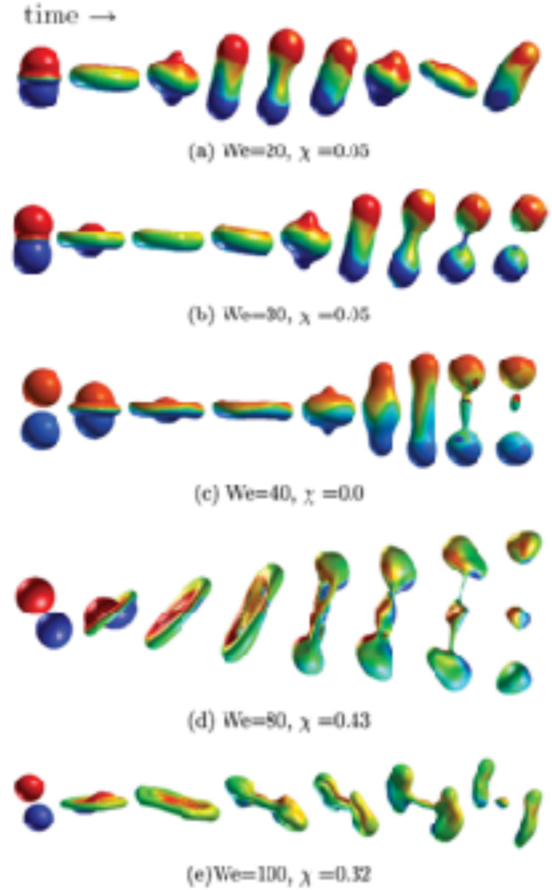
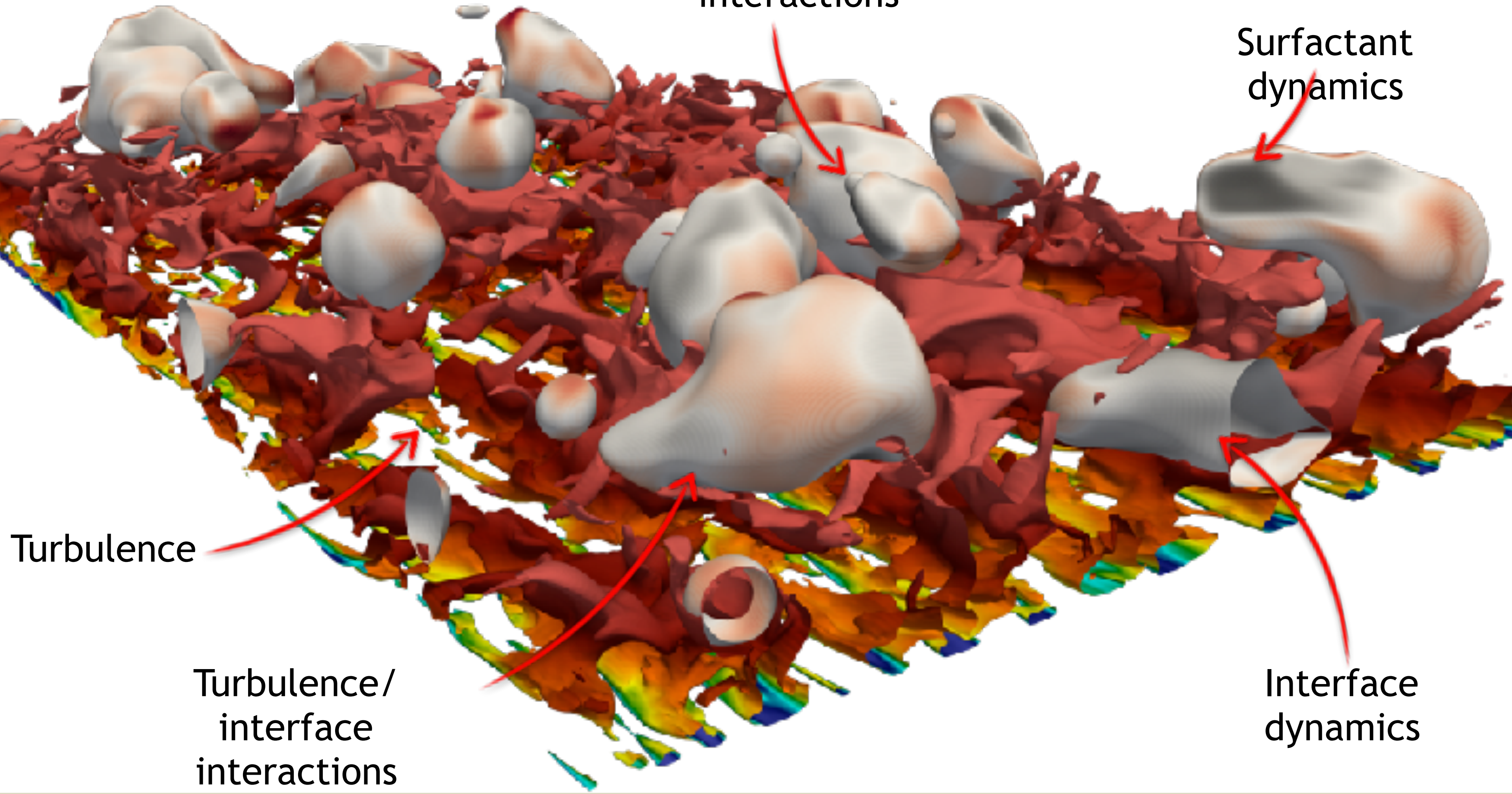


FIG. 13. (Color). Collision process of water drops in air at various Weber numbers and impact parameters.

Turbulence, Interface, Surfactant
A coupled problem



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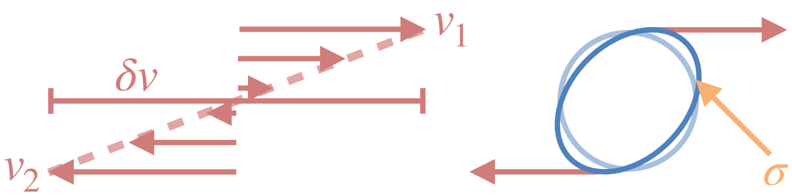
Drop/Bubble size distribution from Scaling Laws

Bubbles/Drops break if stresses win over restoring surface tens



Hinze Critical radius

$$r_H \propto \left(\frac{\rho}{\sigma}\right) \varepsilon^{-2/5} \propto We^{-3/5} \varepsilon^{-2/5}$$

$$We = \rho u_\tau^2 h/\sigma_0$$

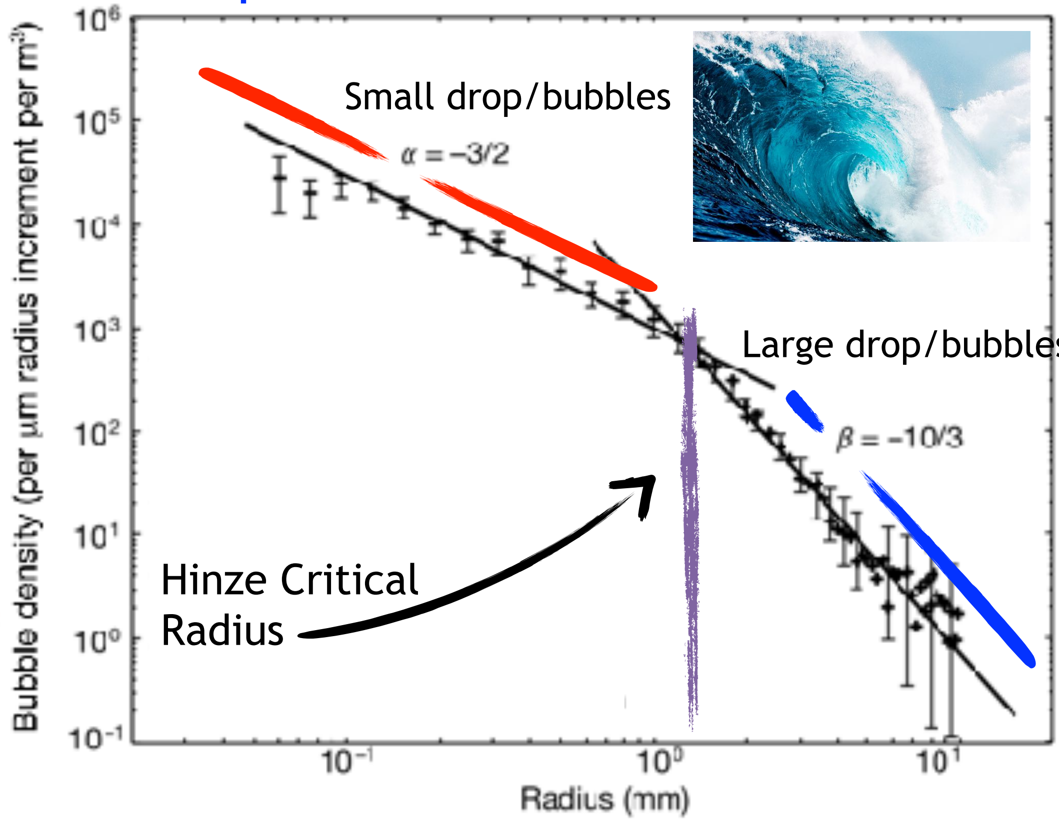
Small drops/bubbles

$$N(r) \propto Q \left(\frac{\sigma}{\rho}\right)^{-3/2} u^2 r^{-3/2}$$

Large drops/bubbles

$$N(r) \propto Q \varepsilon^{-1/3} r^{-10/3}$$

Experiments from Deane and Stokes



r : bubble radius
Q : rate of entrainment
u : flow velocity scale
ε : dissipation rate
σ : surface tension
ρ : fluid density

J.O. Hinze, Fundamentals of the hydrodynamic mechanism of splitting in dispersion processes, AIChE Journal (1955).
C. Garrett, M. Li, D. Farmer, The connection between bubble size spectra and energy dissipation rates in the upper ocean, J. Phys. Oceanogr. (2000).
G. B. Deane and M. Dale Stokes, Scale dependence of bubble creation mechanisms in breaking waves, Nature (2002)

Multiphase Flow Simulation .3
Approaches to Model the Interface ?

Flow Field Solution

Sharp approach

Ghost Fluid Method – GFM
Fedkiw *et al.*, JCP (2001)

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\right]=\eta\nabla^2\mathbf{u}-\nabla p$$

$$p=p^G\pm\sigma k \qquad u=u^G\pm\Delta u$$

Continuous approach

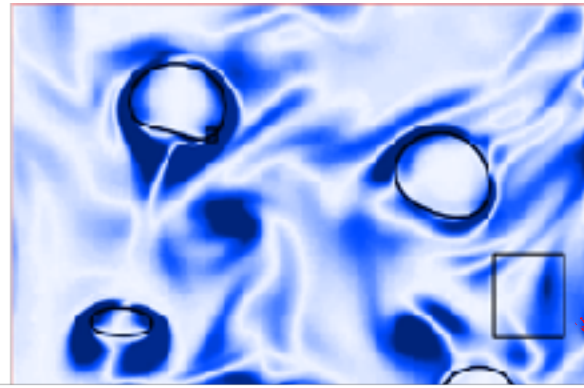
Force Coupling
Tryggvason *et al.*, JCP (2001)

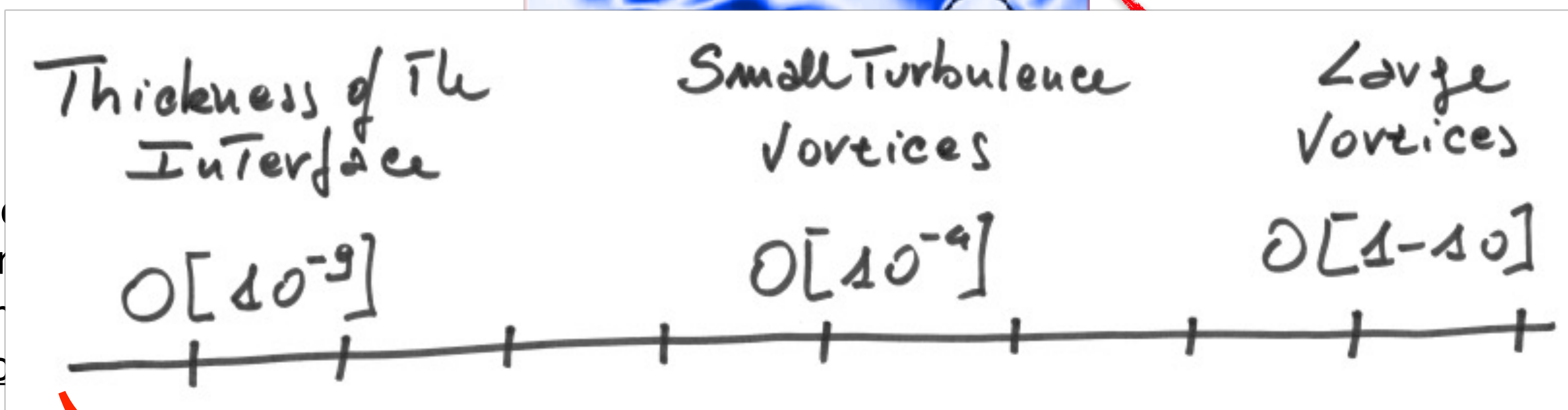
$$\rho\left[\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\right]=\eta\nabla^2\mathbf{u}-\nabla p+\sigma k\mathbf{n}\delta(\mathbf{x})$$

Phase Field Model

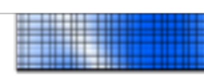
$$\rho\left[\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\right]=\eta\nabla^2\mathbf{u}-\nabla p+\mu\nabla\phi$$

But still …
we have an issue with the Resolution





Int
Lar
Sm … m
9 c
NP=10 …
NP=10 … =10^9



*for a 3D Cube (Reλ=85):

3-4 Orders of magnitude
with Largest Supercomputers

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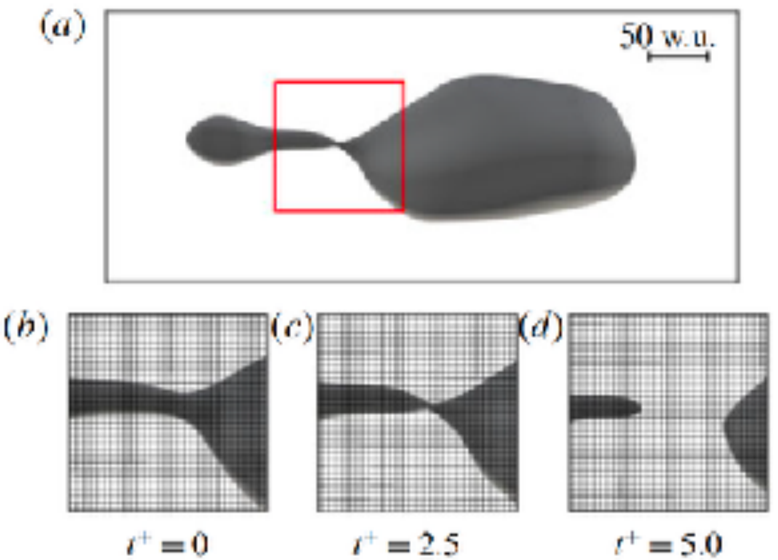
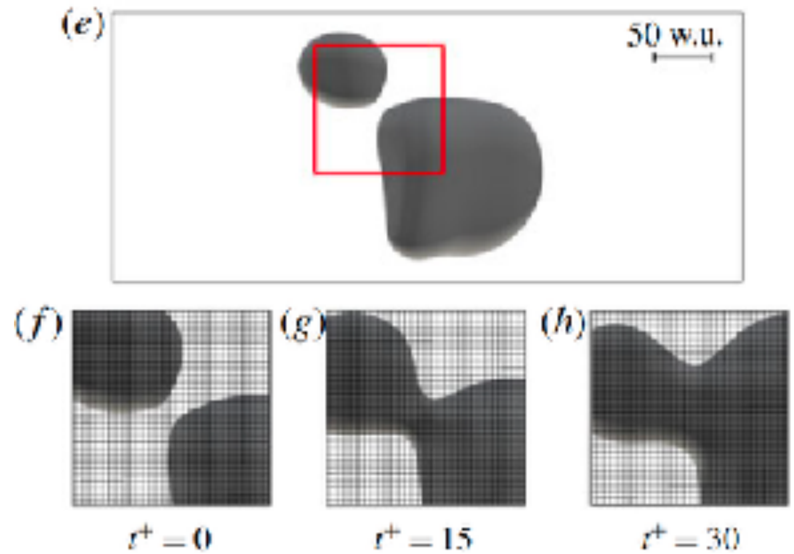
Physics and Simulation (?) of Coalescence and Breakup Processes

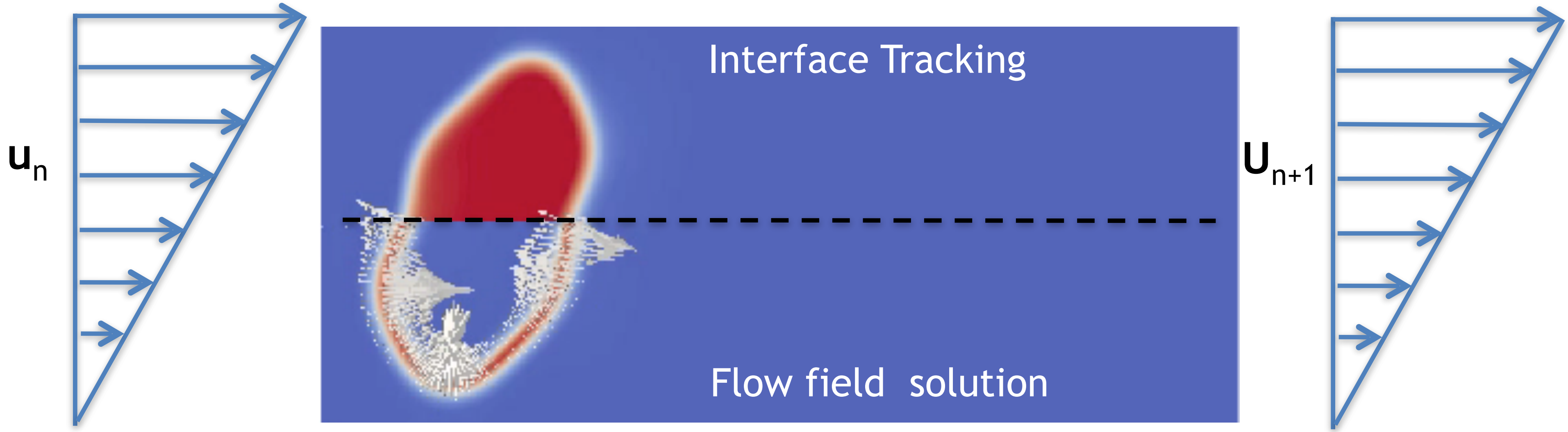


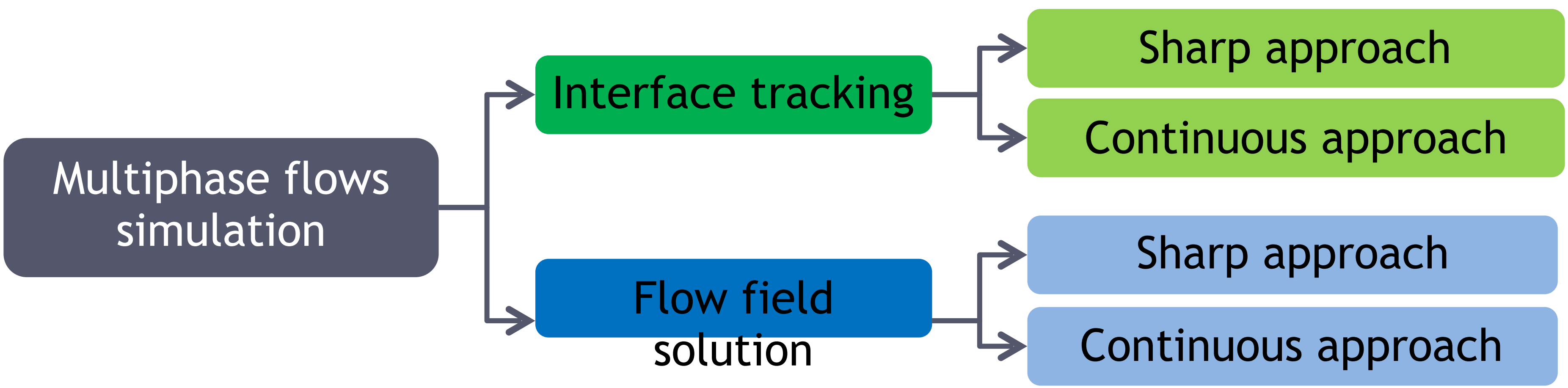
Breakage event: the thin thread becomes progressively thinner (b,c) and subsequently breaks (e).



Coalescence event: after the initial approach (f), the thin liquid film drains, a bridge is formed and the two droplets merge (g); finally surface tension forces reshape the droplet (h).

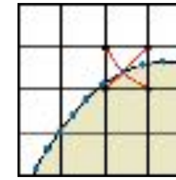
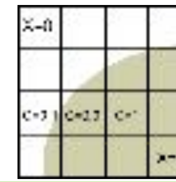
Multiphase Flow Simulation .1
Approaches to Model the Interface ?





Multiphase Flow Simulation .2
Approaches to Model the Interface ?

Interface Tracking

- **Sharp approach**
  - **Front - Capturing**
    Tryggvason *et al.*, JCP (2001)
    
  - **Volume Of Fluid (VOF)**
    Scardovelli & Zaleski, Ann. Rev. Fluid Mec. (1999)
    
- **Continuous approach**
  - **Level - Set**
    Sussmann *et al.*, JCP (2001)
    
    $$\frac{\partial \phi}{\partial t} + (\mathbf{u}\cdot\nabla)\phi = 0 \qquad \frac{\partial \phi}{\partial t} = sign(\phi_0)(1-|\nabla\phi|)$$
  - **Phase Field Model - Cahn Hilliard**
    $$\frac{\partial \phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = \nabla\cdot(M(\phi)\nabla\mu)$$
    

Sharp Interface Approach: We prescribe the interface and we assign properties to it. Properties are models

Phase Field Approach: We prescribe the properties of the two fluids and we define the interface to be in a conventional place. Properties of the two fluids at contact are prescribed according to physico-chemical laws.

Surface Tension $= \sigma$

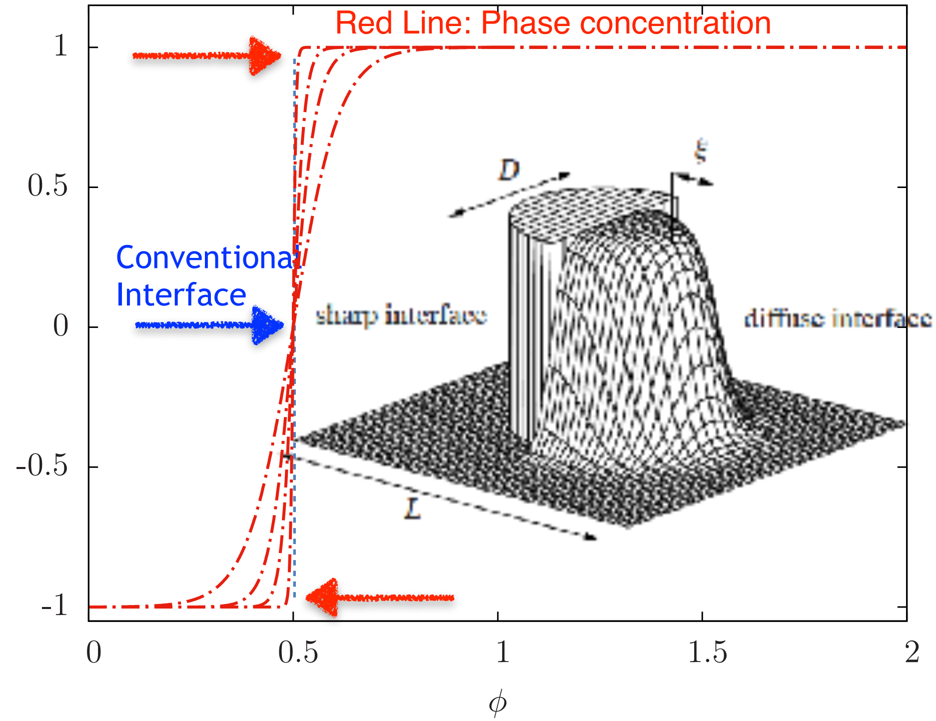
Interface $= \xi \ll H$

Mobilit $= M$

$$Ch = \frac{\xi}{H} \qquad Pe = \frac{u_\tau H}{M\beta}$$

$$Ch = \mathcal{O}(10^{-9}) \qquad Pe = \mathcal{O}(10^{9})$$

To reduce the computational effort, the interface must be fictitiously enlarged!! How much? To the point that it becomes computationally tractable

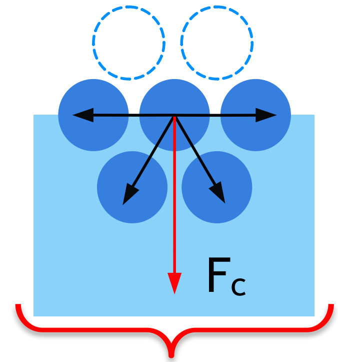


D. Jaqmin,Calculation of Two-Phase Navier–Stokes Flows Using Phase-Field Modeling, JCP (1999)
J.W. Cahn and J.E. Hilliard ,Free energy of a non-uniform system I, Interfacial free energy, JCP (1958)

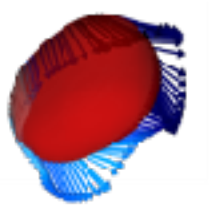
Assumptions:

- Matched density
- Matched viscosity
- Constant surface tension

Surface tension forces:



Flow:



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

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{Re_\tau} \nabla^2 \mathbf{u} + \frac{3}{\sqrt{8}} \frac{Ch}{We} \nabla \cdot \tau_c$$

Interface:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \frac{1}{Pe_\phi} \nabla^2 \mu_\phi$$

D. Jaqmin, Calculation of Two-Phase Navier–Stokes Flows Using Phase-Field Modelling, JCP (1999)
J.W. Cahn and J.E. Hilliard ,Free energy of a non-uniform system I, Interfacial free energy, JCP (1958)

Fil Rouge

1. Historical Perspective, modelling and computational issues
2. A short story on droplets in turbulence (influence of viscosity/density contrast)
3. A short story on oil transport
4. A short story on drop coalescence/break-up (influence of surfactant)

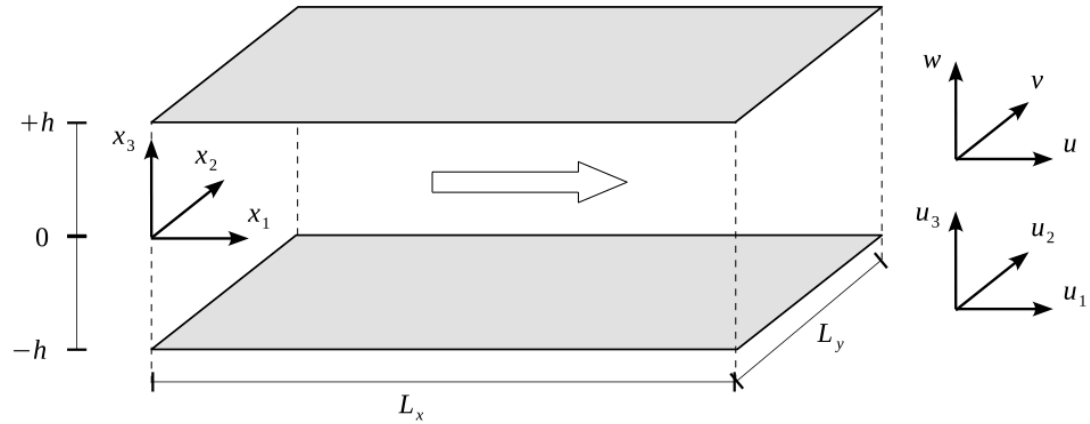
Numerical Implementation: Spectral & pseudo-spectral methods

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

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \frac{1}{Re_\tau} \nabla^2 \mathbf{u} + \frac{3}{\sqrt{8}} \frac{1}{WeCh} \mu \nabla \phi$$

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = + \frac{1}{Pe} \nabla^2 \mu$$

$$\mu = \phi^3 - \phi - Ch^2 \nabla^2 \phi$$



Vorticity-Velocity formulation
(curl+twice curl of NS+Vectorial identity)

$$\frac{\partial \omega}{\partial t} = -\nabla \times \mathbf{S} + \frac{1}{Re_\tau} \nabla^2 \omega$$

$$\nabla \times (\nabla \times \mathbf{u}) = \nabla (\nabla \cdot \mathbf{u}) - \nabla^2 \mathbf{u}$$

$$\frac{\partial \left(\nabla^2 \mathbf{u} \right)}{\partial t} = \nabla^2 \mathbf{S} - \nabla \left(\nabla \cdot \mathbf{S} \right) + \frac{1}{Re_\tau} \nabla^4 \mathbf{u}$$

$$\left(\mathbf{S} = -\mathbf{u} \cdot \nabla \mathbf{u} - \delta_{1,j} + \frac{3}{\sqrt{8}} \frac{1}{WeCh} \mu \nabla \phi \right)$$

This leads to the following system

$$\frac{\partial \omega_3}{\partial t} = \frac{\partial S_2}{\partial x_1} - \frac{\partial S_1}{\partial x_2} + \frac{1}{Re_\tau} \nabla^2 \omega_3$$

$$\frac{\partial \left(\nabla^2 \mathbf{u_3} \right)}{\partial t} = \nabla^2 \mathbf{S_3} - \frac{\partial}{\partial x_3} \frac{\partial S_j}{\partial x_j} + \frac{1}{Re_\tau} \nabla^4 \mathbf{u}$$

$$\frac{\partial \mathbf{u}_1}{\partial x_1} + \frac{\partial \mathbf{u}_2}{\partial x_2} = - \frac{\partial \mathbf{u}_3}{\partial x_3}$$

$$\left(\mathbf{S} = -\mathbf{u} \cdot \nabla \mathbf{u} - \delta_{1,j} + \frac{3}{\sqrt{8}} \frac{1}{WeCh} \mu \nabla \phi \right)$$

$$\frac{\partial \mathbf{u}_2}{\partial x_1} - \frac{\partial \mathbf{u}_1}{\partial x_2} = \omega_3$$

$$\frac{\partial \phi}{\partial t} = S_\phi + \frac{s}{Pe} \nabla^2 \phi - \frac{Ch^2}{Pe} \nabla^4 \phi$$

$$\left(\mathbf{S}_\phi = -\mathbf{u} \cdot \nabla \phi + \frac{1}{Pe} \nabla^2 \phi^3 - \frac{1+s}{Pe} \nabla^2 \phi ; s = \sqrt{\frac{4PeCh^2}{\Delta t}} \right)$$

Methods to discretize differential operators

- Idea: approximate a function (unknown, which satisfy PDE+BC), using a linear combination of test functions
- This tests functions are global

$$u(x) \simeq \tilde{u}(x) = \sum_{k=0}^{N} c_k \phi_k(x)$$

Common to Finite difference/ Finite elements methods

<u>For spectral methods</u>: global functions are defined in each node and are not zero

This brings some advantages for the representation of the derivatives

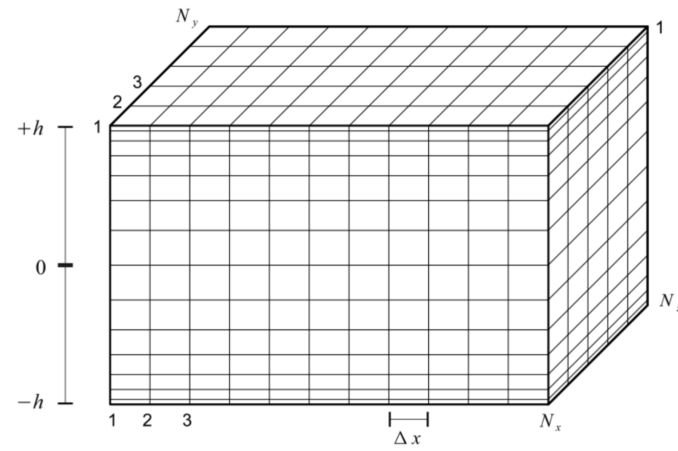
Numerical Implementation: Spectral & pseudo-spectral methods

Discrete geometry

$$x(i) = (i-1)\frac{L_x}{N_x - 1} \rightarrow i = 1,\ldots N_x$$

$$y(j) = (j-1)\frac{L_y}{N_y - 1} \rightarrow j = 1,\ldots N_y$$

$$z(k) = \cos\left(\frac{k-1}{N_z - 1}\pi\right) \rightarrow k = 1,\ldots N_z$$

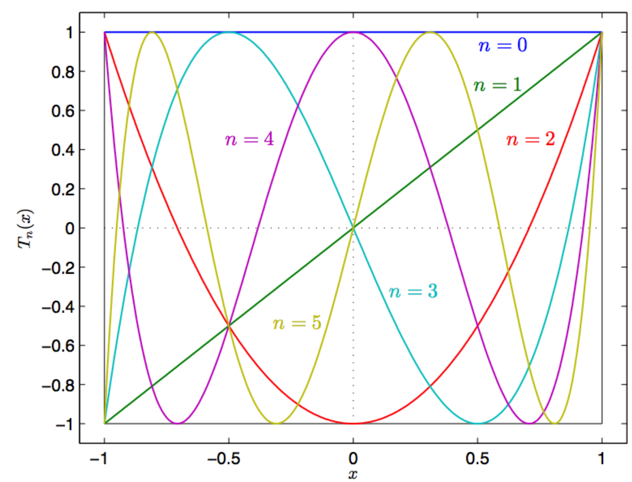


Spatial discretization of the solution (Fourier+Chebyshev)
Idea: approximate a function as the linear combination of test functions (which in this case are global)

$$f(x_1, x_2, x_3) = \sum_{n_1}\sum_{n_2}\sum_{n_3} \hat{f}\left(k_1, k_2, n_3\right) T_{n_3} e^{i\left(k_1 x_1 + k_2 x_2\right)}$$

$$k_1 = \frac{2\pi n_1}{L_x}; k_2 = \frac{2\pi n_2}{L_y} \qquad k^2 = k_1^2 + k_2^2$$

$$T_{n_3}(x_3) = cos\left[n_3 \cos^{-1}\left(x_3/h\right)\right]$$



$$ik_1\hat{u}_1 + ik_2\hat{u}_2 + \frac{\partial}{\partial x_3}\hat{u}_3 = 0$$

$$\hat{\omega}_3 = ik_1\hat{u}_2 - ik_2\hat{u}_1$$

$$\frac{\partial \hat{\omega}_3}{\partial t} = ik_1\hat{S}_2 - ik_2\hat{S}_1 + \frac{1}{Re_\tau}\left(\frac{\partial^2}{\partial x_3^2} - k^2\right)\hat{\omega}_3$$

$$\frac{\partial}{\partial t}\left(\frac{\partial^2 \hat{u}_3}{\partial x_3^2} - k^2\hat{u}_3\right) = -k^2\hat{S}_3 - ik_1\frac{\partial \hat{S}_1}{\partial x_3} - ik_2\frac{\partial \hat{S}_2}{\partial x_3} + \frac{1}{Re_\tau}\left(k^4\hat{u}_3 + \frac{\partial^4 \hat{u}_3}{\partial x_3^4} - 2k^2\frac{\partial^2 \hat{u}_3}{\partial x_3^2}\right)$$

$$\frac{\partial \hat{\phi}}{\partial t} = \hat{S}_\phi + \left(\frac{\partial^2}{\partial z^2} - k^2\right)\left[\frac{s}{Pe} - \frac{Ch^2}{Pe}\left(\frac{\partial^2}{\partial z^2} - k^2\right)\right]\hat{\phi}$$

Numerical Implementation: Spectral & pseudo-spectral methods

Introducing the ''historical'' terms H (lump together known functions);
Time splitting: viscous/diffusive term, Crank-Nicolson; convective term: Adams-Bashfort

$$\left(\frac{\partial^2}{\partial x_3^2} - \beta^2\right)\hat{\omega}_3^{\,n+1} = -\frac{ik_1 H_2^n - ik_2 H_1^n}{\gamma}$$

$$\gamma = \frac{\Delta t}{2Re_\tau}; \beta^2 = \frac{1+\gamma k^2}{\gamma}$$

$$\left(\frac{\partial^2}{\partial x_3^2} - \beta^2\right)\left(\frac{\partial^2}{\partial x_3^2} - k^2\right)\hat{u}_3^{\,n+1} = \frac{\hat{H}^n}{\gamma}$$

Helmholtz equations, solved by a Chebyshev-Tau method; Influence matrix method to solve the 4 order equations

$$ik_1\hat{u}_1 + ik_2\hat{u}_2 + \frac{\partial \hat{u}_3}{\partial x_3} = 0$$

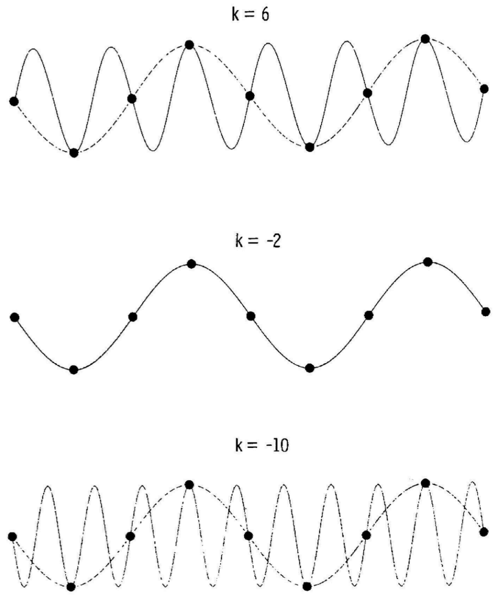
$$\hat{\omega}_3 = ik_1\hat{u}_2 - ik_2\hat{u}_1$$

$$\left(\frac{\partial^2}{\partial x_3^2} - k^2 - \frac{s}{2Ch}\right)\left(\frac{\partial^2}{\partial x_3^2} - k^2 - \frac{s}{2Ch}\right)\hat{\phi}^{n+1} = \frac{\hat{H}_\phi^{\;n}}{\gamma}$$

Numerical Implementation: Spectral & pseudo-spectral methods

Why pseudo-spectral?

- Performing products in modal space, $\mathcal{O}(N^2)$
- Transform into physical, multiply, back to modal, $\mathcal{O}(N \log_2 N)$
- Aliasing error (2/3 rule)



Aliasing of sin(-2x) by sin(6x) wave

Aliasing of sin(-2x) by sin(10x) wave [Canuto et al. (1988)]

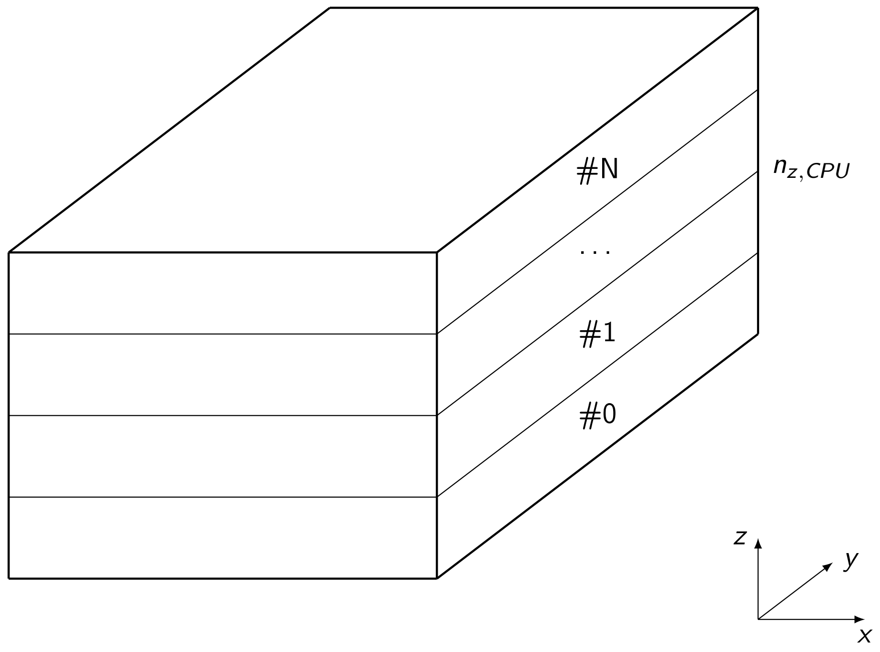
Pros & cons: Accuracy/Convergence; Good performances (FFTW)
Not easy to code; Less flexible

Performance of the code

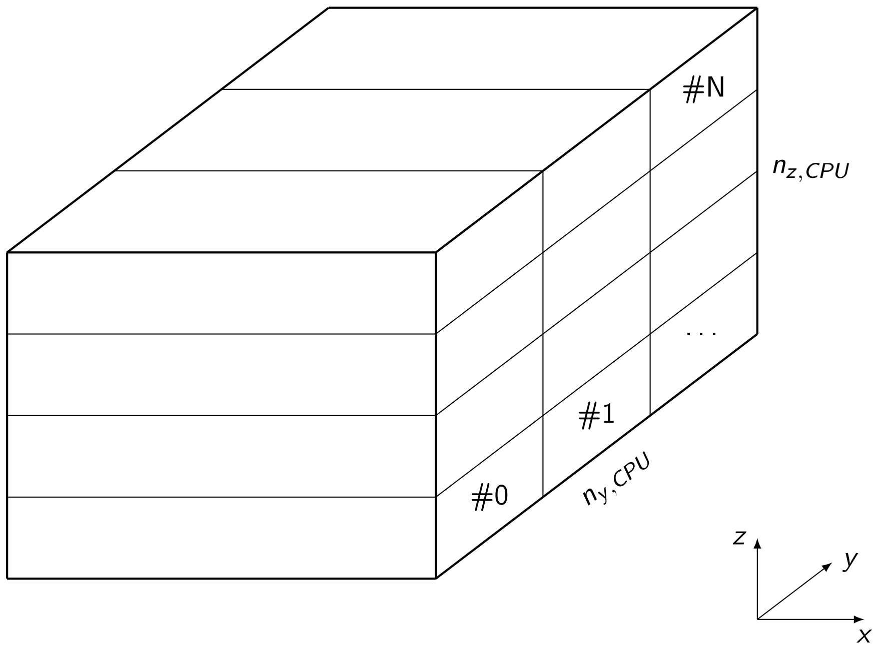
Machine	Centre	Processors	Frequency [GHz]	RAM/node [GB]
Marconi BDW	CINECA (Bologna, Italy)	2x18 cores Intel Xeon	2,3	128
Marconi KNL	CINECA (Bologna, Italy)	1x68 cores Intel Xeon Phi	1,4	16 MCDRAM + 96 DDR4
Vesta	ANL (Chicago, USA)	1x16 IBM PowerPC A2	1,6	16
VSC 3	VSC (Vienna, Austria)	2x16 Intel Xeon 2x20 Intel Xeon	2.6 2.2	64/128/256 64

Performance of the code

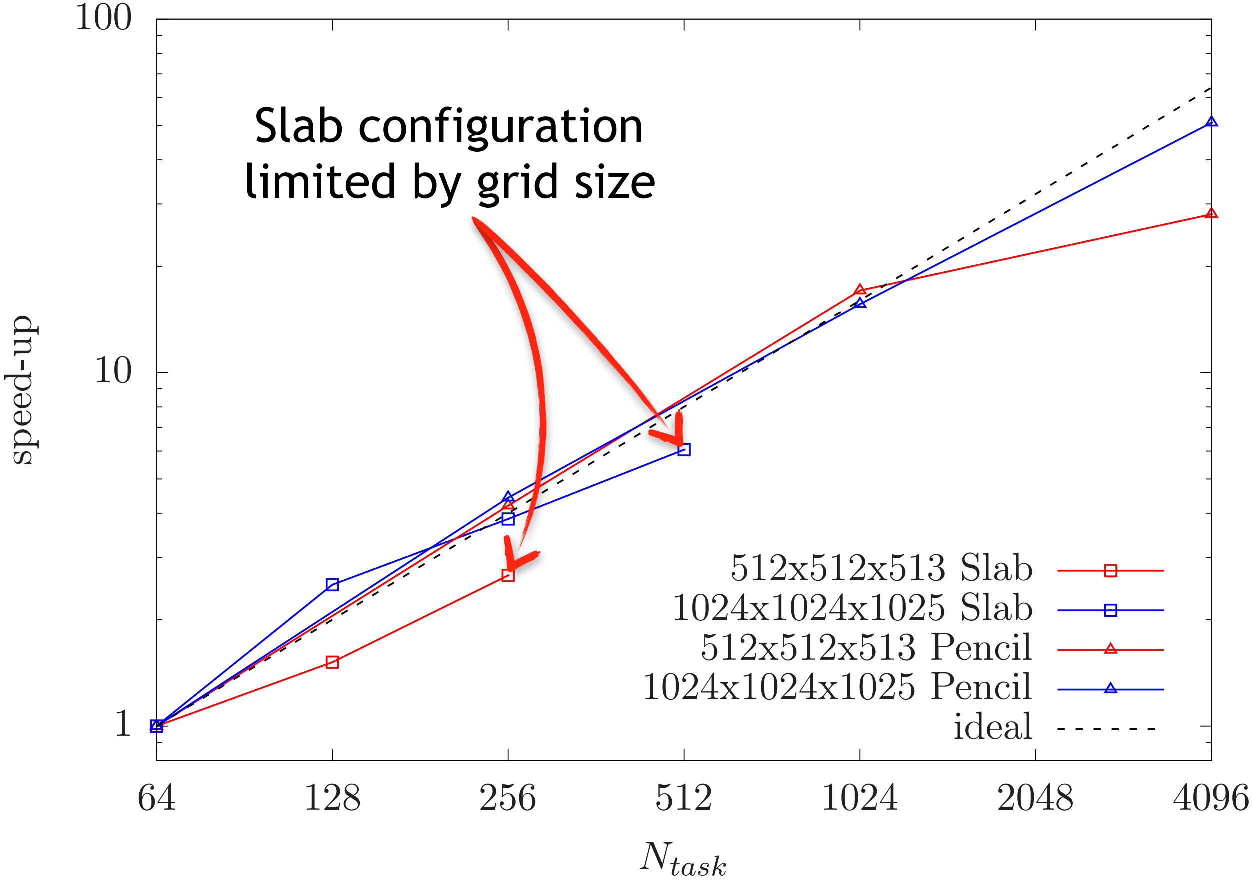
1D domain decomposition “Slab”



2D domain decomposition “Pencil”

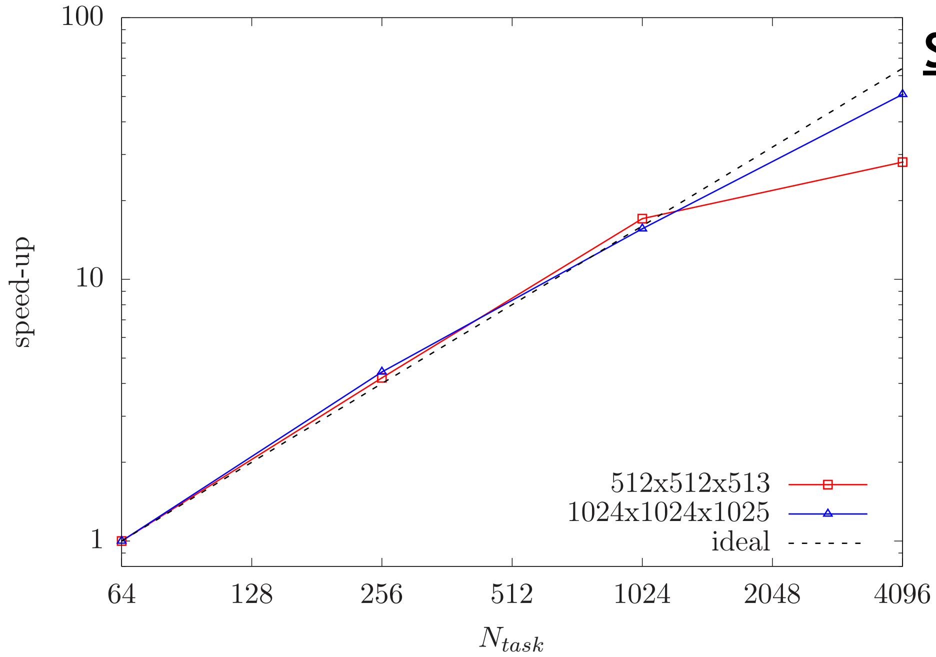


Performance of the code



Comparison Slab *vs* Pencil on Marconi BDW

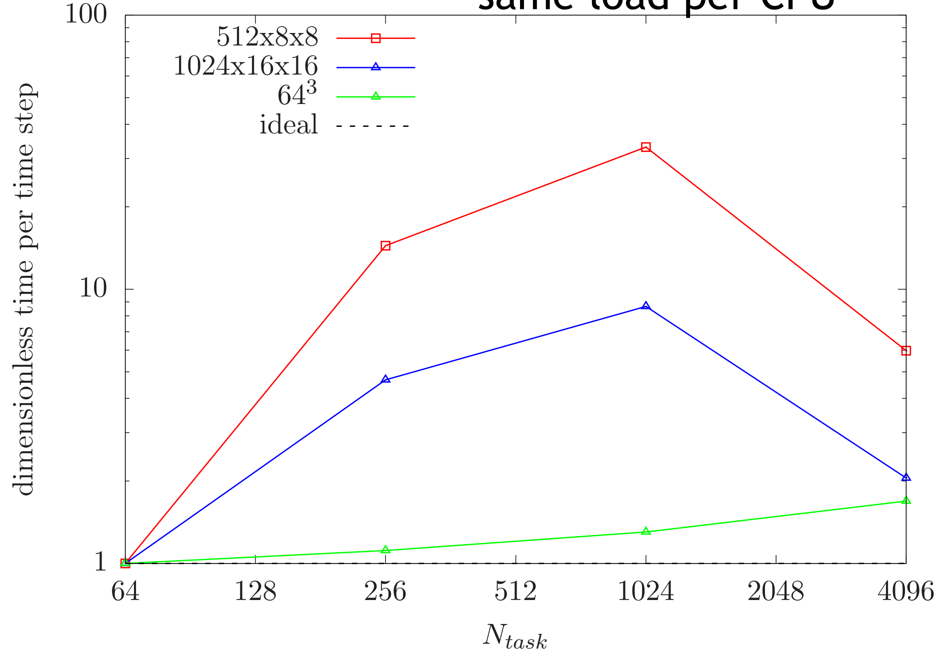
Performance of the code



Strong scaling

Marconi BDW

Different aspect ratios of the pencil for the same load per CPU

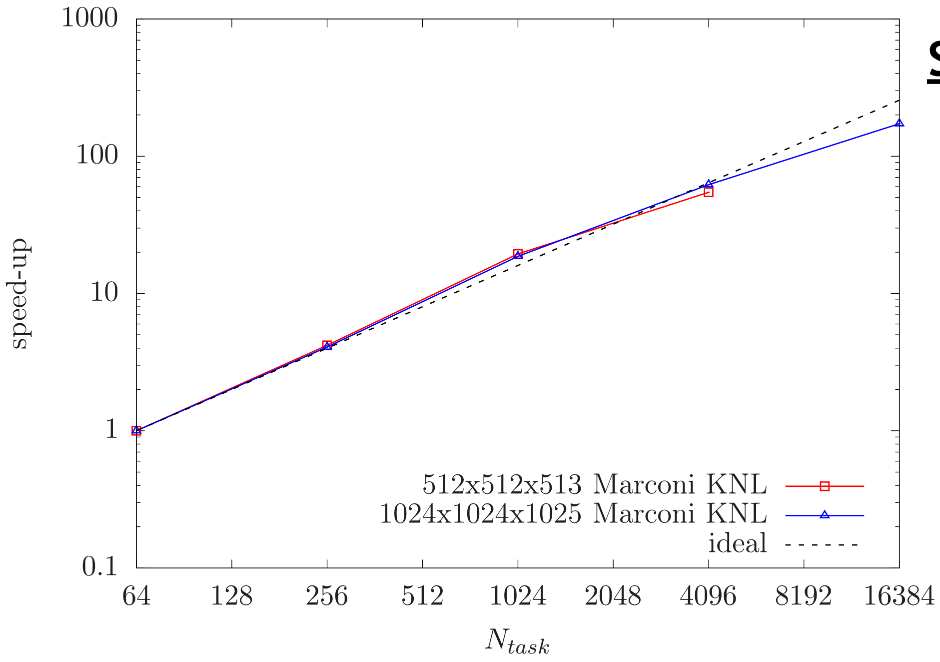


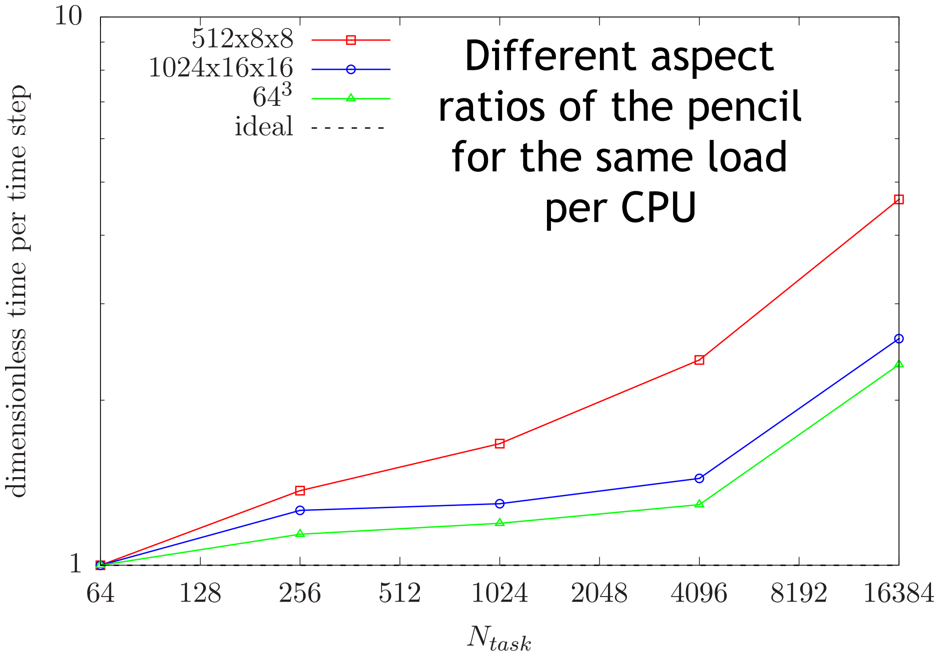
Weak scaling

Performance of the code

Strong scaling

Marconi KNL





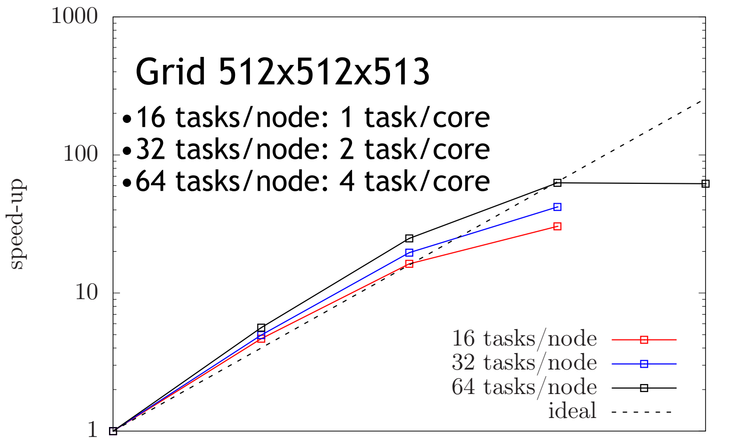
Different aspect ratios of the pencil for the same load per CPU

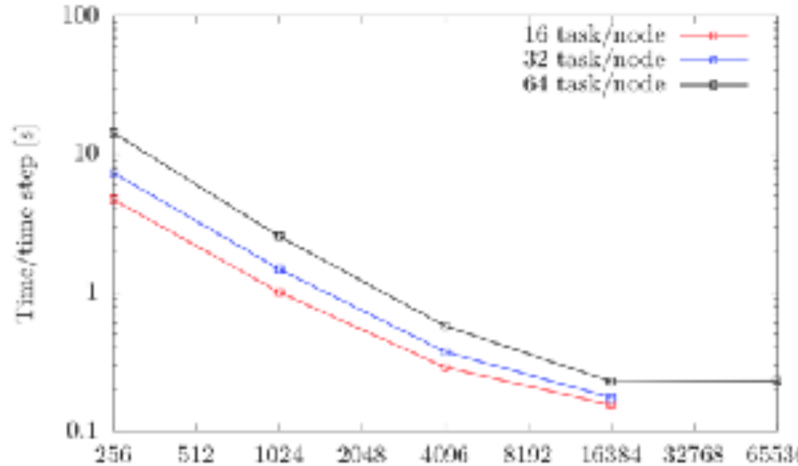
Weak scaling

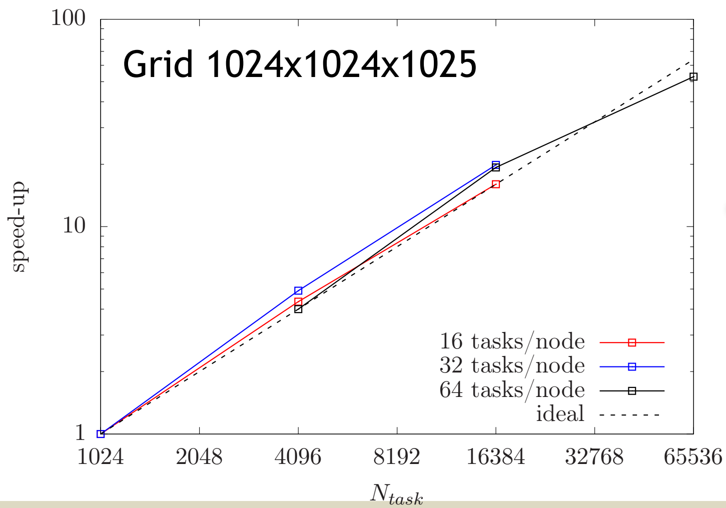
Performance of the code

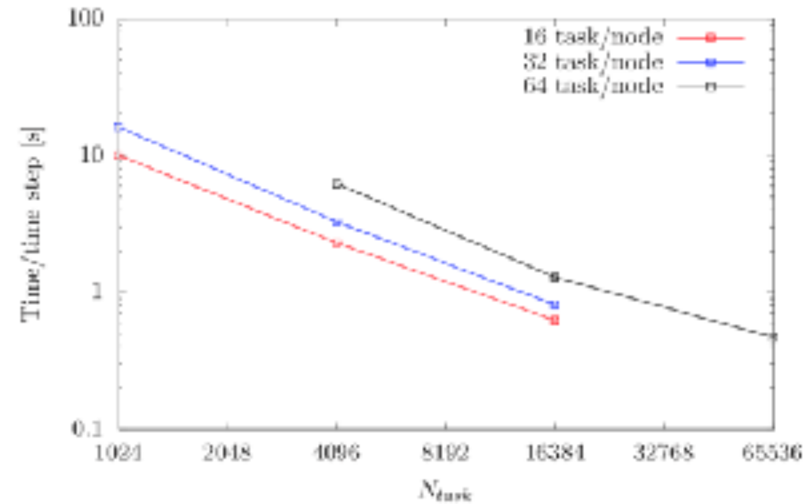
Strong scaling Vesta (ANL, Argonne)

Different multithreading option





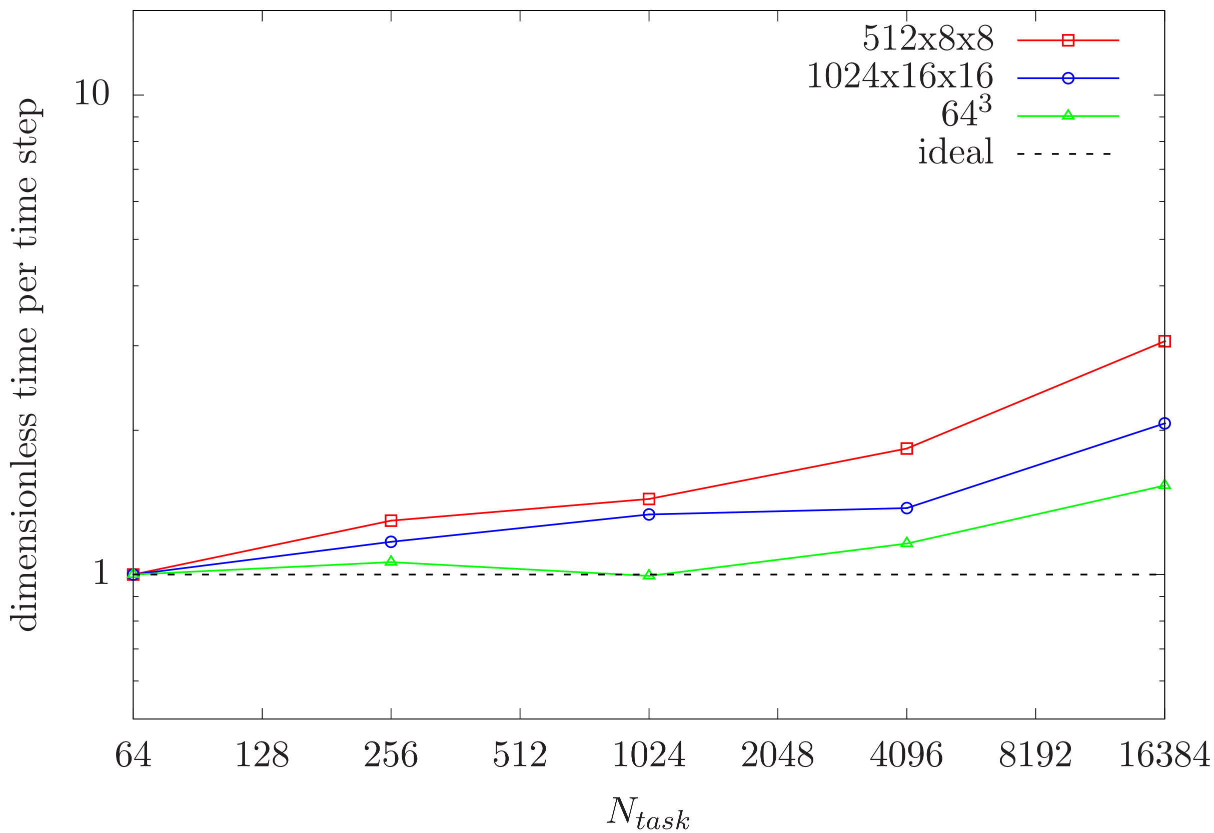




Performance of the code

Vesta (ANL, Argonne)

Weak scaling



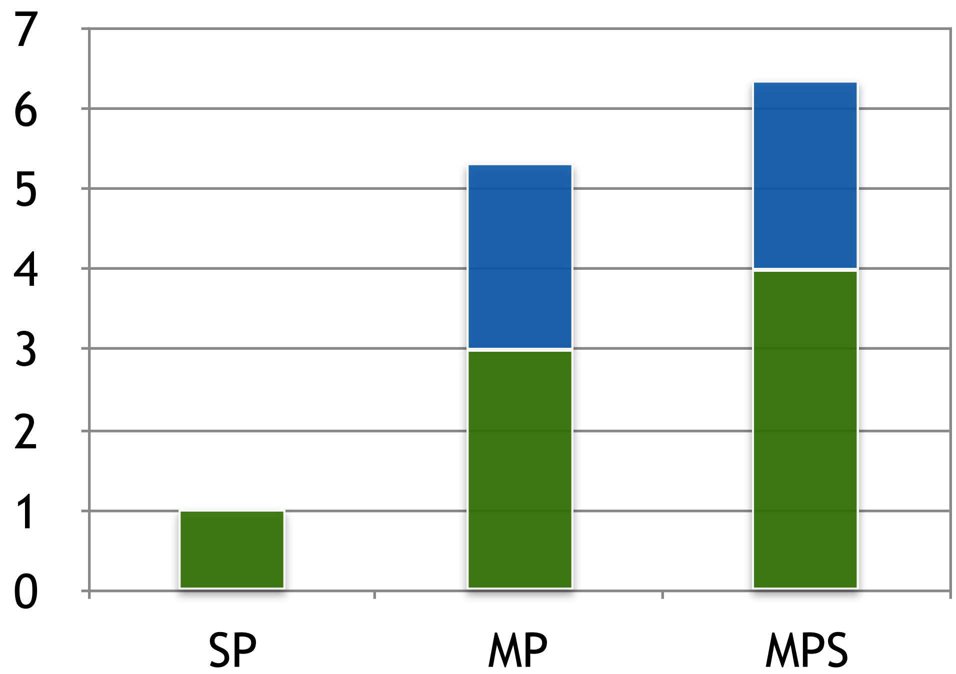
Testing different pencil aspect ratios for the same load per CPU

Multiphase Flow Simulation
Computational Cost

In the present example we refer to Pseudo-Spectral Method, where Computational effort is directly linked with the number of FFT and iFFT needed for each time step:

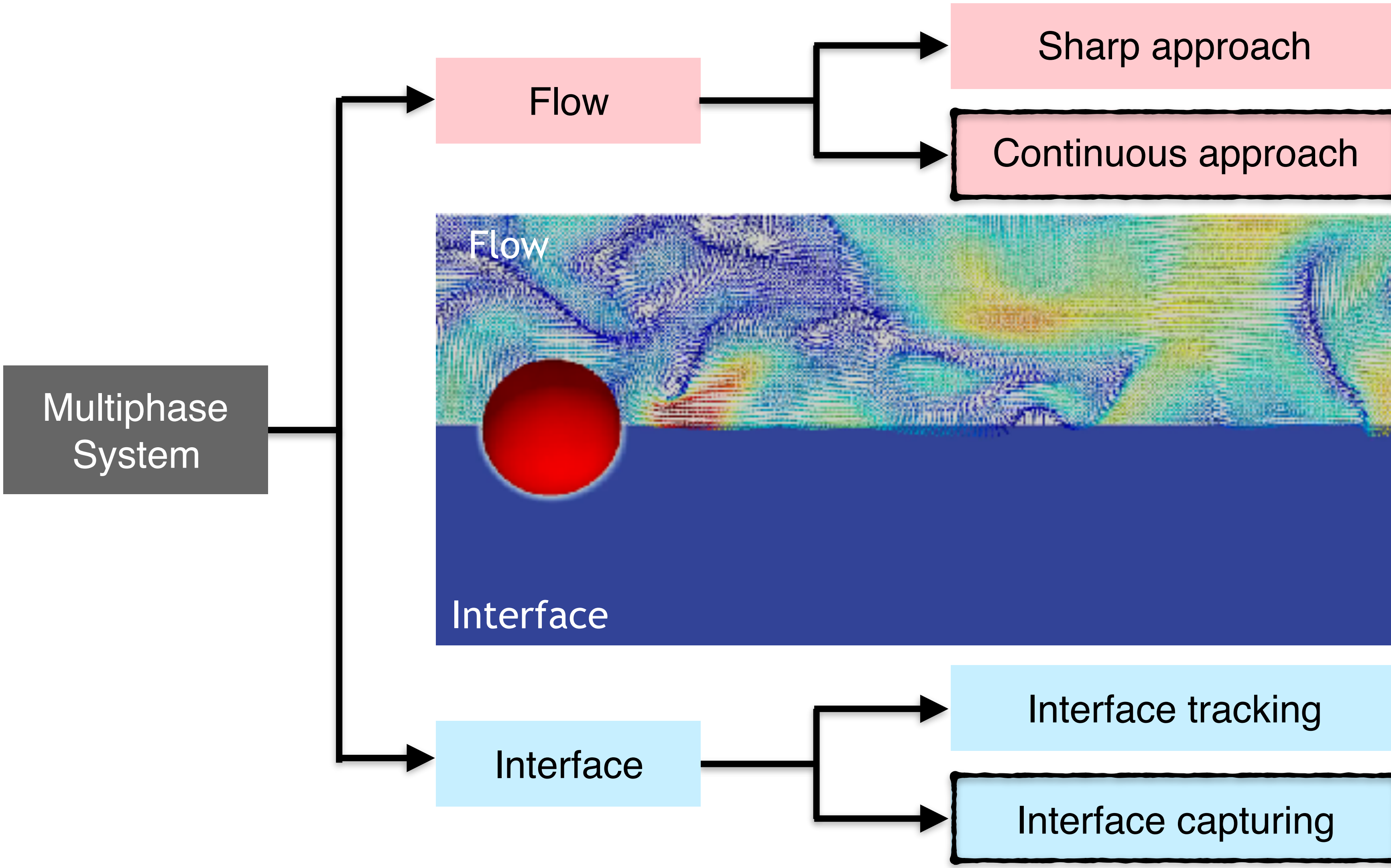
SP=Single Phase Flow
MP=Multiphase Flow
MPS=Multiphase Flow with surfactant

Comp. Effort/Comp. Effort(SP)



For MP and MPS cases, the efforts depends also on the density and viscosity ratio, lower when density and viscosity are matched, higher vice-versa.

Numerical method (Recap)

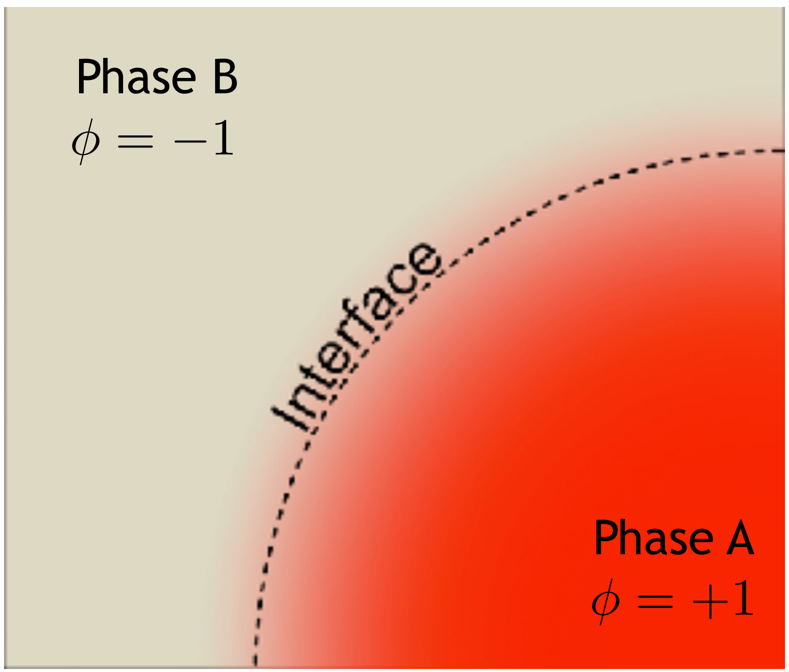


Numerical method (Recap)

Defining a concentration ϕ :

$$\phi = \frac{n_A - n_B}{n_A + n_B}$$

- $\phi = +1$ Phase A
- $\phi = 0$ Interface
- $\phi = -1$ Phase B



Cahn-Hilliard equation:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \frac{1}{Pe_\phi} \nabla^2 \mu_\phi$$

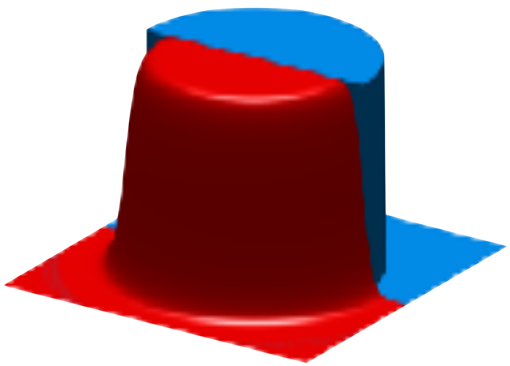
Chemical potential:

$$\mu_\phi = \frac{\delta \mathcal{F}}{\delta \phi} = \phi^3 - \phi - Ch^2 \nabla^2 \phi$$

At the equilibrium:

$$\mu_\phi = \mu_\phi^{eq}$$

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



Cahn and Hilliard, Free energy of a non-uniform system I, Interfacial free energy, JCP (1958)
Cahn and Hilliard, Free energy of a non-uniform system II, Thermodynamic Basis, JCP (1959)
Cahn and Hilliard, Free energy of a non-uniform system III, Nucleation in a Two-Component Incompressible Fluid, JCP (1959)

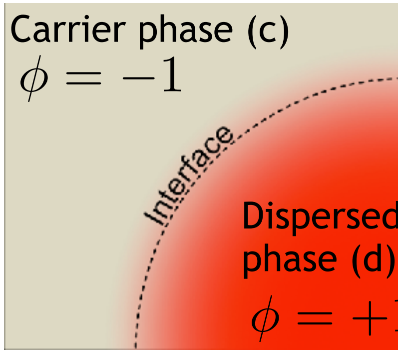
Numerical method (Recap)+ Additional features

<u>Assumptions:</u>

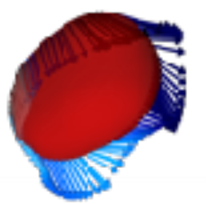
- Different density
- Different viscosity
- Constant surface tension

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

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



Flow:



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

$$\eta(\phi) = 1 + \frac{\lambda - 1}{2}(\phi + 1)$$

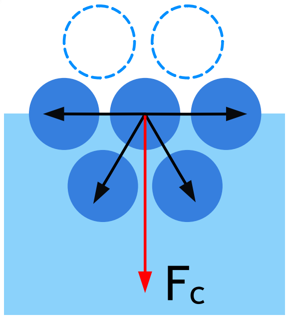
$$\rho(\phi)\left[\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right] = -\nabla p + \frac{1}{Re_\tau}\nabla \cdot \left[\eta(\phi)(\nabla \mathbf{u} + \nabla \mathbf{u}^T))\right] + \frac{3}{\sqrt{8}}\frac{Ch}{We}\nabla \cdot \tau_c$$

$$\rho(\phi) = 1 + \frac{\gamma - 1}{2}(\phi + 1)$$

Interface:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \frac{1}{Pe_\phi}\nabla^2 \mu_\phi$$

Interface

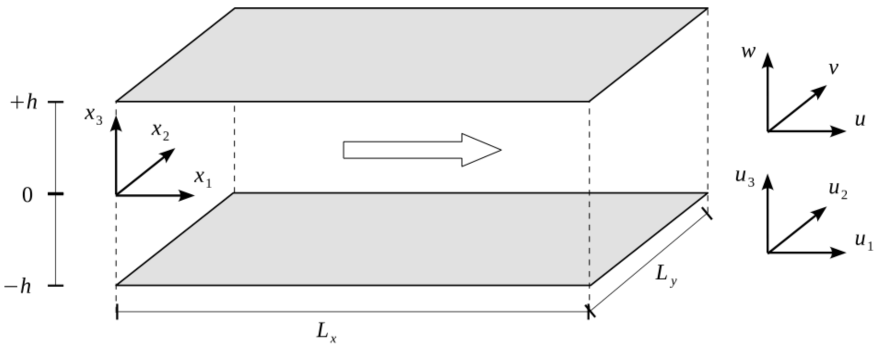


Jacqmin, Calculation of Two-Phase Navier–Stokes Flows Using Phase-Field Modelling, JCP (1999)
Badalassi et al., Computation of multiphase systems with phase model, JCP (2003)

Numerical method (Recap)

Method: Direct Numerical Solution (DNS) of NS and CH equations, no models used.

Computational Domain



Space Discretization:
- X Periodic direction (Fourier)
- Y Periodic direction (Fourier)
- Z Wall-normal (Chebychev-Tau)

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

Solver NS (Vorticity-Velocity Formulation):

Curl of NS (Vorticity)

$$\frac{\partial \omega_z}{\partial t} = \nabla \times \mathbf{S} + \frac{1}{Re_\tau}\nabla^2 \omega_z$$

Twice Curl of NS

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

CH:

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

C.Canuto and A. Quarteroni, Spectral and pseudo-spectral methods for parabolic problems with non periodic boundary condition.

Numerical method (Recap)

$$\frac{\partial \omega_z}{\partial t} = \nabla \times \mathbf{S} + \frac{1}{Re_\tau}\nabla^2 \omega_z$$

- Solve for the 3rd component of vorticity
- 2nd order PDE
- Single Helmotz solver

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

- Solve for the 3rd component of velocity
- 4th order PDE
- Double Helmotz solver, Influence Matrix Method

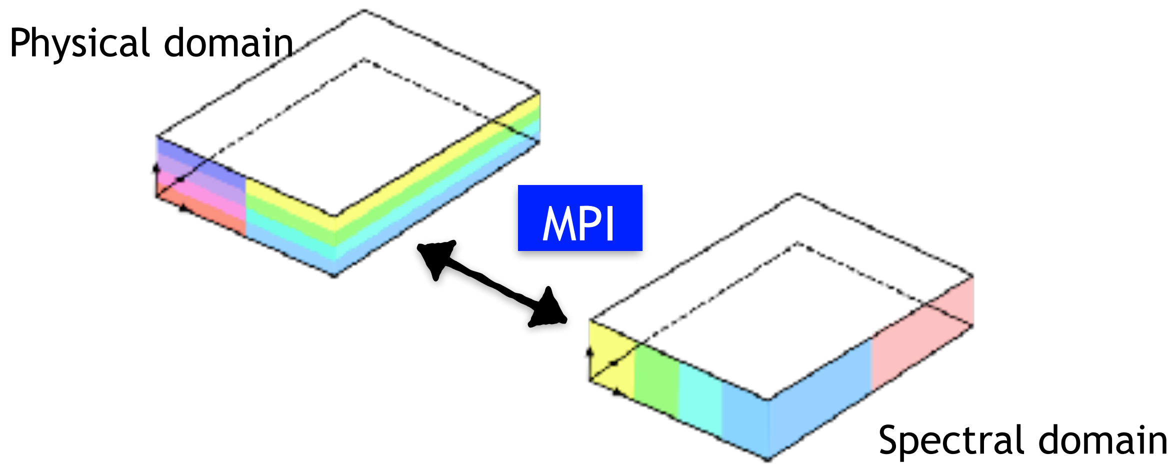
$$\frac{\partial \phi}{\partial t} = S_\phi + \frac{sCh^2}{Pe}\nabla^2 \phi - \frac{Ch^2}{Pe}\nabla^4 \phi$$

- Solve for phi
- 4th order PDE
- Double Helmotz solver

With no-flux BC ϕ is conserved.

$$\frac{\partial}{\partial t}\int_\Omega \phi \, d\Omega = 0$$

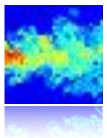
- MPI Paradigm, 2D Domain decomposition



C.Canuto and A. Quarteroni, Spectral and pseudo-spectral methods for parabolic problems with non periodic boundary condition.

Simulations Setup

Boundary Conditions:

FLOW FIELD 

PHASE FIELD 

NO SLIP AT THE WALLS

$$u_i(\pm h) = 0$$

90° CONTACT ANGLE

$$\frac{\partial \phi}{\partial z}(\pm h) = \frac{\partial^3 \phi}{\partial z^3}(\pm h) = 0$$

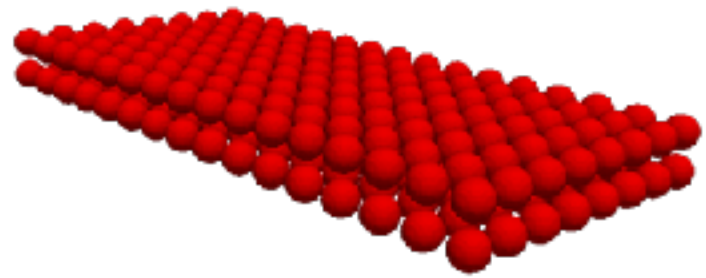
PERIODICITY ALONG X and Y

$$u_i(0) = u_i(L_x) \qquad \phi(0) = \phi(L_x)$$

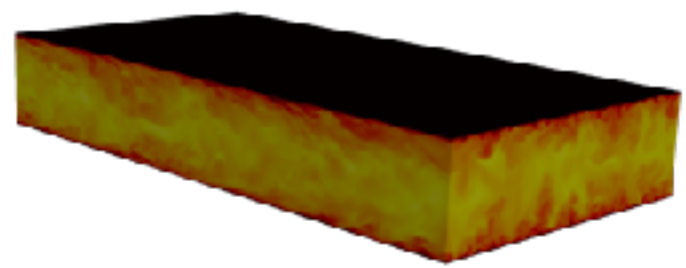
$$u_i(0) = u_i(L_y) \qquad \phi(0) = \phi(L_y)$$

Initial Conditions:

- Phase Field
  - 256 spherical drops



- Flow Field
  - Single Phase Flow Re=150.



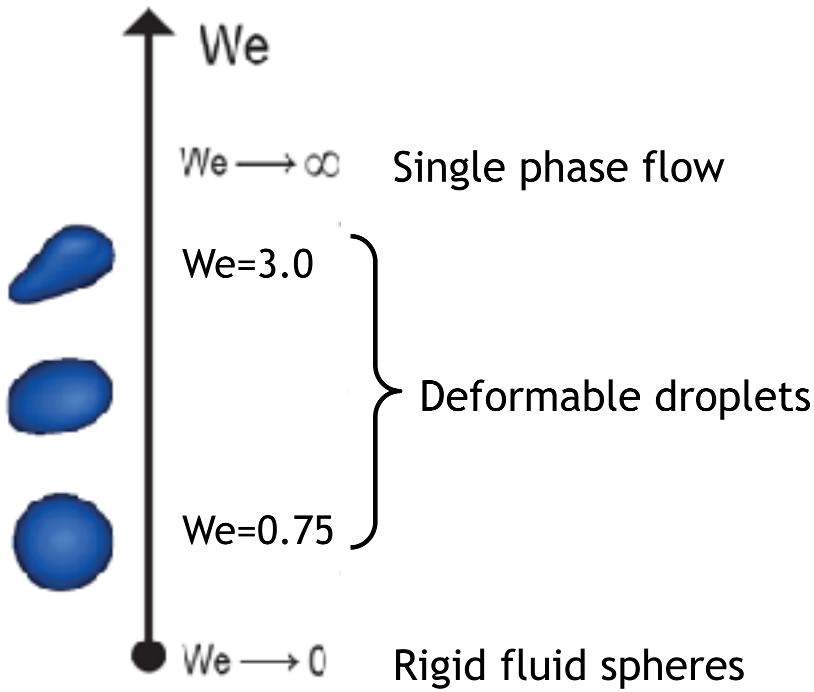
S. Ahmadi et al, Turbulent Drag Reduction by a Near Wall Surface Tension Active Interface, FTAC (2018)
S. Ahmadi et al, Turbulent drag reduction in channel flow with viscosity stratified fluids, CEF (2016)

Simulation Setup
Effect of Surface Tension and Viscosity

Effect of Surface Tension and Viscosity (matched density)

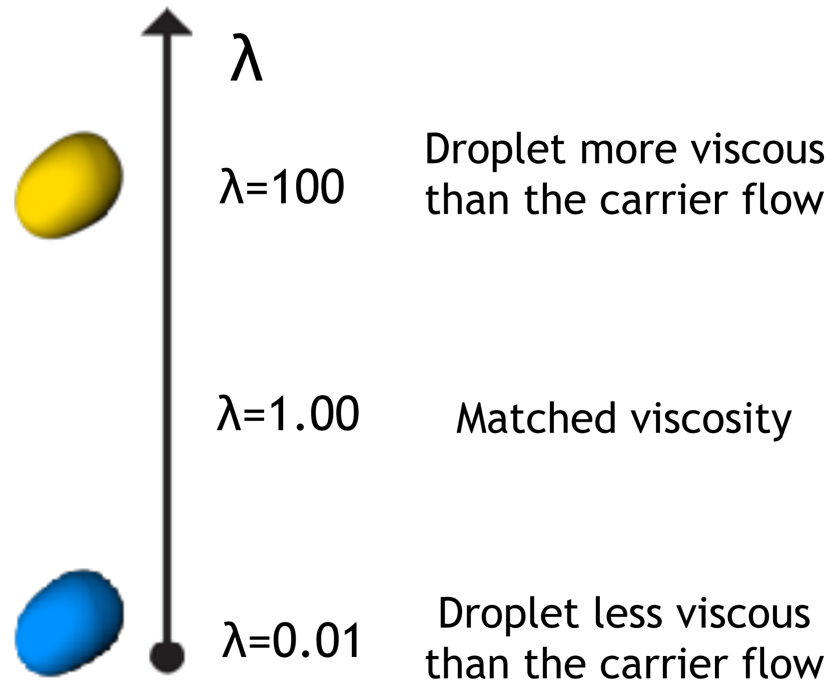
Weber number:

$$We = \frac{\rho u_\tau^2 h}{\sigma} = \frac{\text{Inertial Forces}}{\text{Surface Tension Forces}}$$



Viscosity Ratio:

$$\lambda = \frac{\eta_d}{\eta_c} = \frac{\text{Droplet Viscosity}}{\text{Carrier Viscosity}}$$



Scarbolo et al., Coalescence and breakup of large droplets in turbulent channel flow, PoF (2015)
Roccon et al., Viscosity-modulated breakup and coalescence of large drops in bounded turbulence, PRF (2017)

Physical parameters

Weber Number (We):

$$We = \frac{\rho u_\tau^2 h}{\sigma} = \frac{\text{Inertial Forces}}{\text{Surface Tension Forces}}$$

Low We

High We

Viscosity Ratio (λ):

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

Low λ
(Water+Hexane)

High λ
(Water+Oil)

Simulations setup

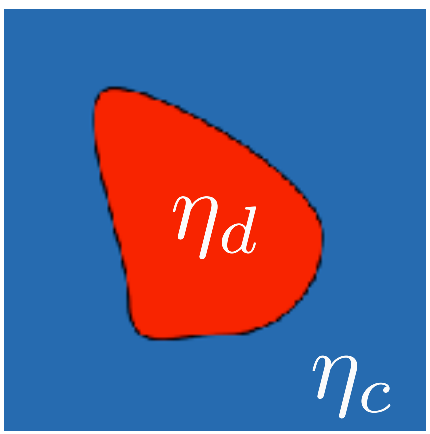
Fixed Parameters:

Reynolds number $Re_\tau=150$

Pe and Ch numerical parameters based on the grid resolution:

- Ch=0.0185
- Pe=162.20

Grid: up to 512 x 512 x 513 (N_x-N_y-N_z)
Size: 4πH x 2πH x 2H (L_x-L_y-L_z)

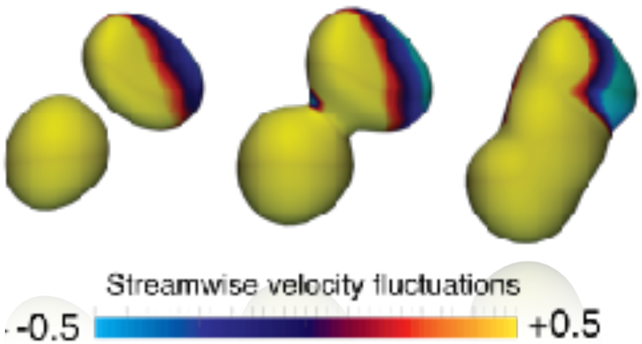


$$\lambda = \frac{\eta_d}{\eta_c}$$

#	We	λ
S1		0.01
S2		0.1
S3	0.75	1
S4		10
S5		100
S6		0.01
S7		0.1
S8	1.50	1
S9		10
S10		100
S11		0.01
S12		0.1
S13	3.00	1
S14		10
S15		100

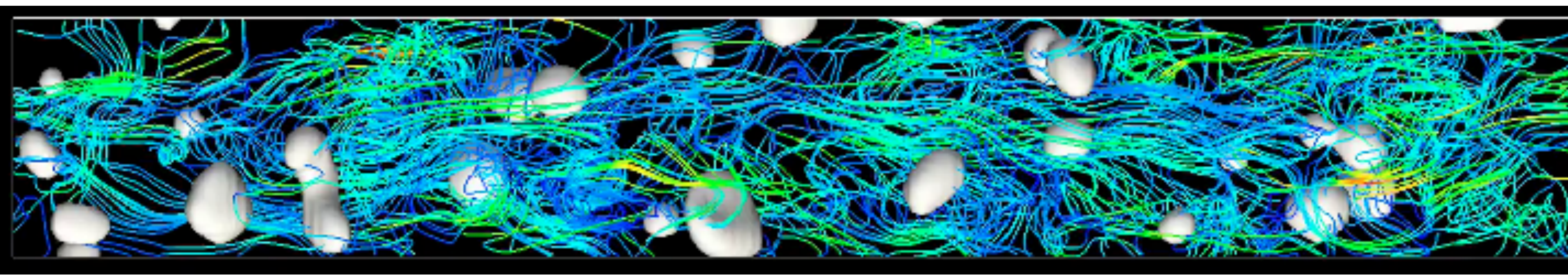
L. Scarbolo et. al., Unified framework for a side-by-side comparison of different multicomponent algorithms , JCP. (2013)
A. Roccon et al, Viscosity-modulated breakup and coalescence of large drops in bounded turbulence, PR Fluids (2017)

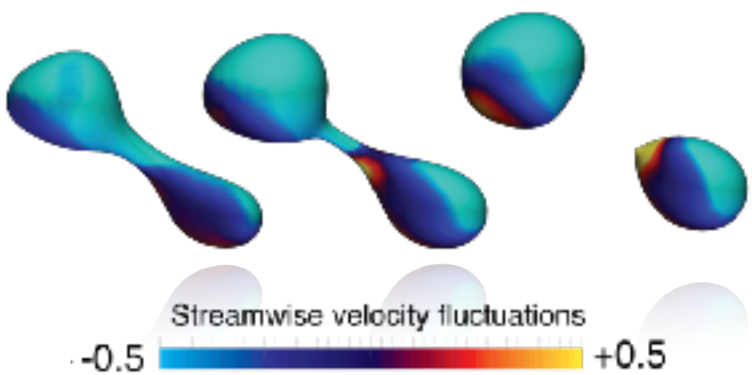
Drop-drop interaction



COALESCENCE

Two droplets come close and collide due to turbulence fluctuations. During the collision, a small bridge is initially formed; later, surface tension (which tends to reshape the droplet) comes into the picture and complete the coalescence process.



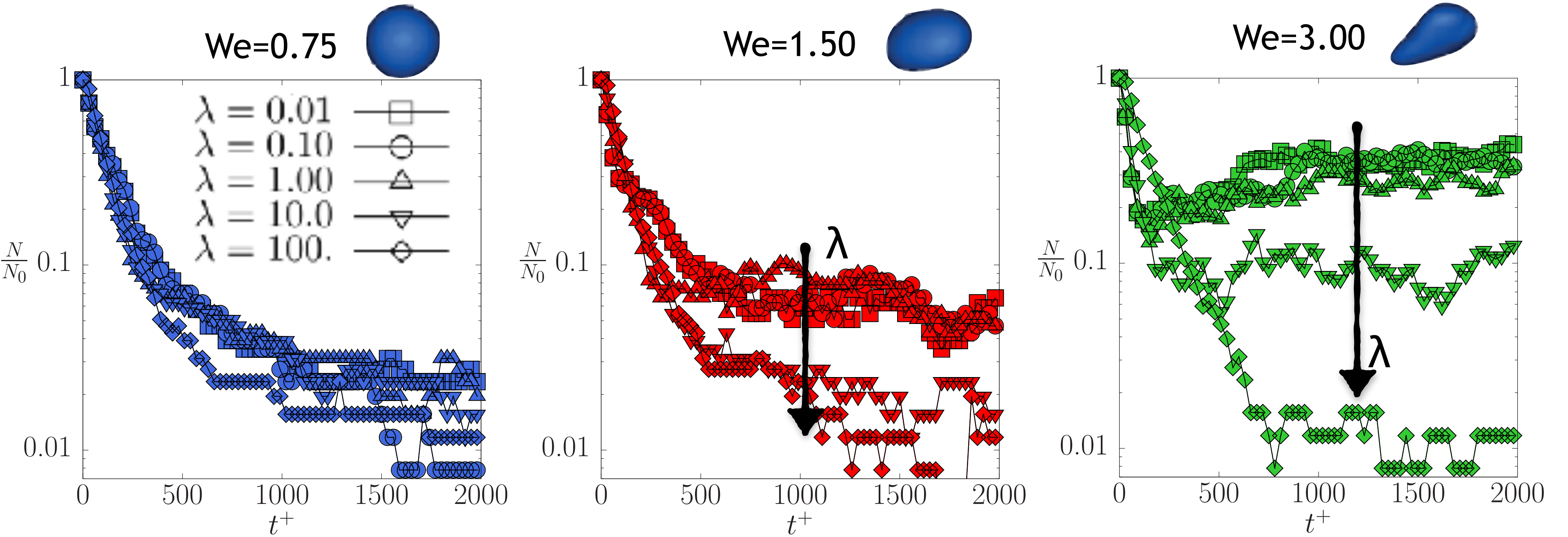


BREAK-UP

A droplet is subjected to a sufficient shear stress, such that it is deformed and stretched until the emerging thin liquid bridge is broken (due to surface tension that acts minimizing the energy stored at the interface).

Scarbolo et al., Coalescence and breakup of large droplets in turbulent channel flow, PoF (2015)
Roccon et al., Viscosity-modulated breakup and coalescence of large drops in bounded turbulence, PRF (2017)

Number of drops
Effect of viscosity



Coalescence Regime for every λ

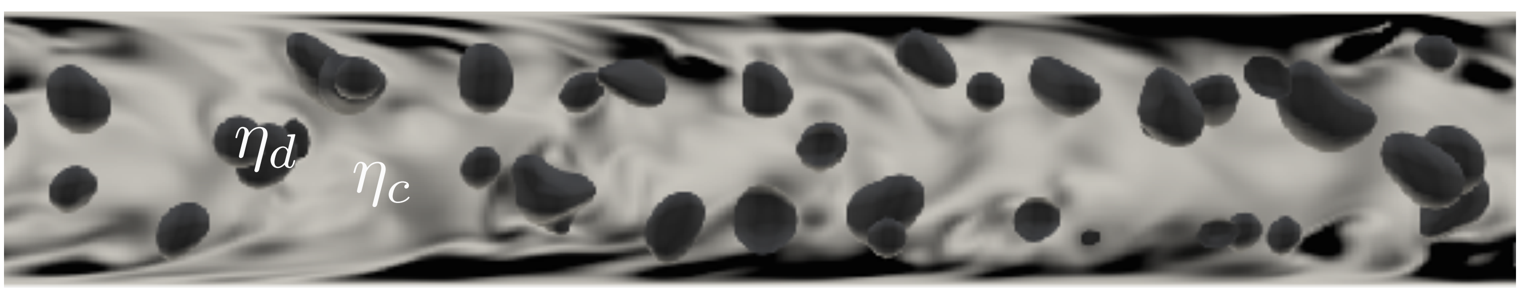
Coalescence Regime for λ > 1

Break-up Regime for λ < 1

Coalescence Regime for λ > 1

Break-up Regime for λ < 1

$$\lambda = \frac{\eta_d}{\eta_c}$$



Scarbolo et al., Coalescence and breakup of large droplets in turbulent channel flow, PoF (2015)

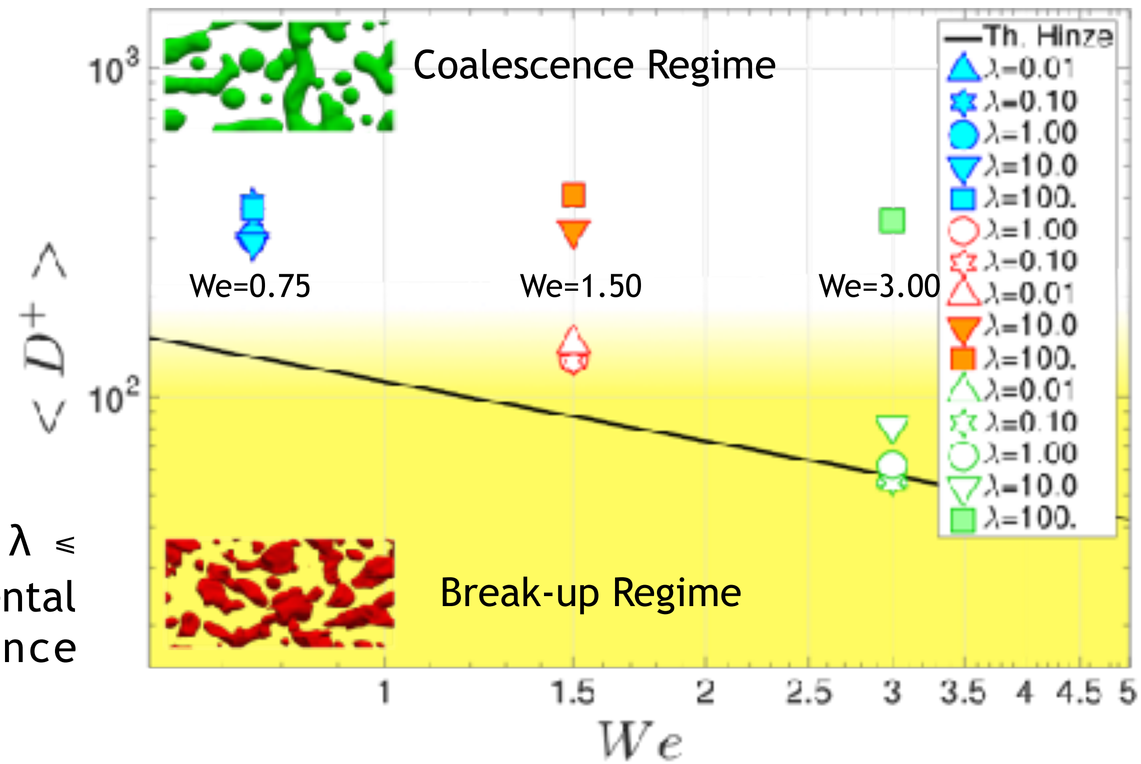
Roccon et al., Viscosity-modulated breakup and coalescence of large drops in bounded turbulence, PRF (2017)

Hinze theory

Comparison with maximum stable droplet dimension theory by Hinze (coalescence is neglected; correlates well exp. data). In turbulence, where breakups and coalescences are both important, we can replace D_{max} with <D>.

$$D_{max} = 0.725\left(\frac{\rho}{\sigma}\right)^{-3/5}\epsilon^{-2/5}$$

$$< D^+ > = 0.725\left(\frac{We}{Re_\tau}\right)^{-3/5}\varepsilon^{-2/5}$$



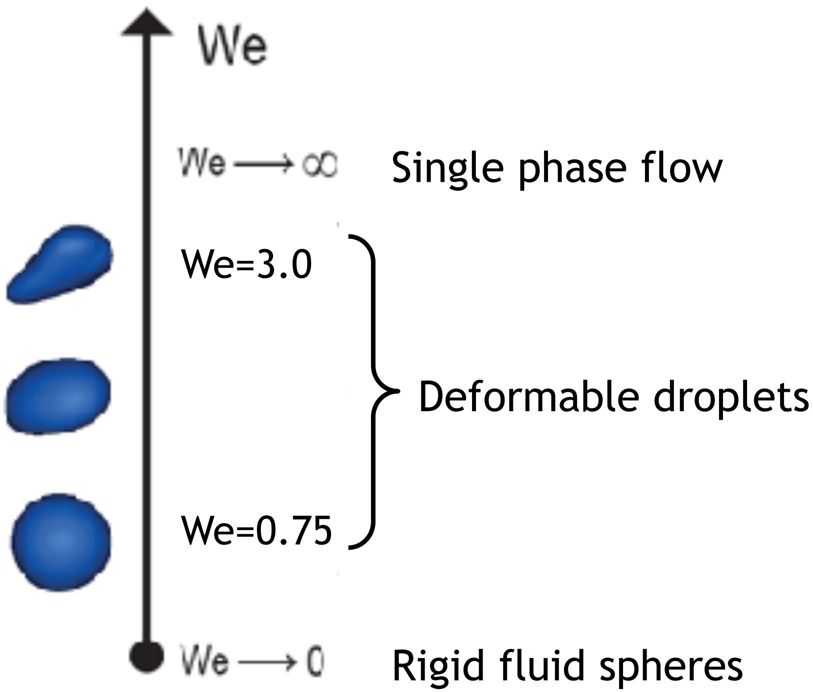
When a Breakups dominate (and λ ≤ 1), fair agreement with experimental results. Otherwise, coalescence cannot be neglected

J. O. Hinze, Fundamentals of the Hydrodynamic Mechanism of Splitting in Dispersion Processes, A.I.Ch.e Journal (1955)
P. Perlekar et al, Droplet size distribution in homogeneous isotropic turbulence, Physic of Fluids (2012)
A. Roccon et al, Viscosity-modulated breakup and coalescence of large drops in bounded turbulence, PR Fluids (2017)

Effect of Density and Surface Tension (matched viscosity)

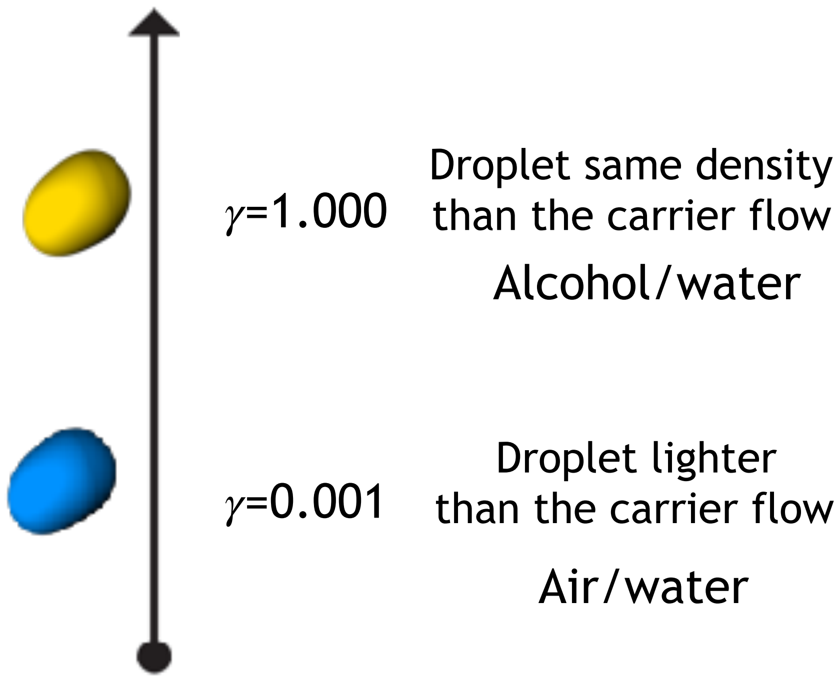
Weber number:

$$We = \frac{\rho u_\tau^2 h}{\sigma} = \frac{\text{Inertial Forces}}{\text{Surface Tension Forces}}$$

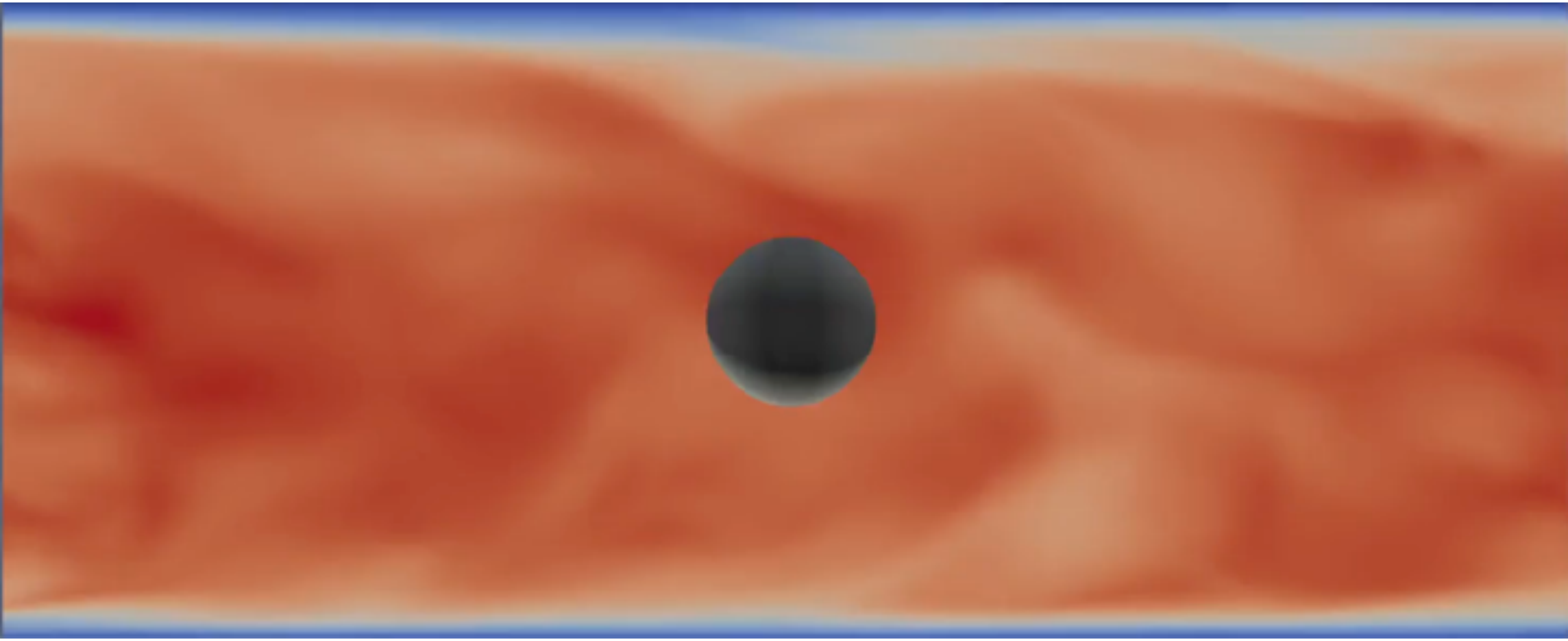


Density Ratio:

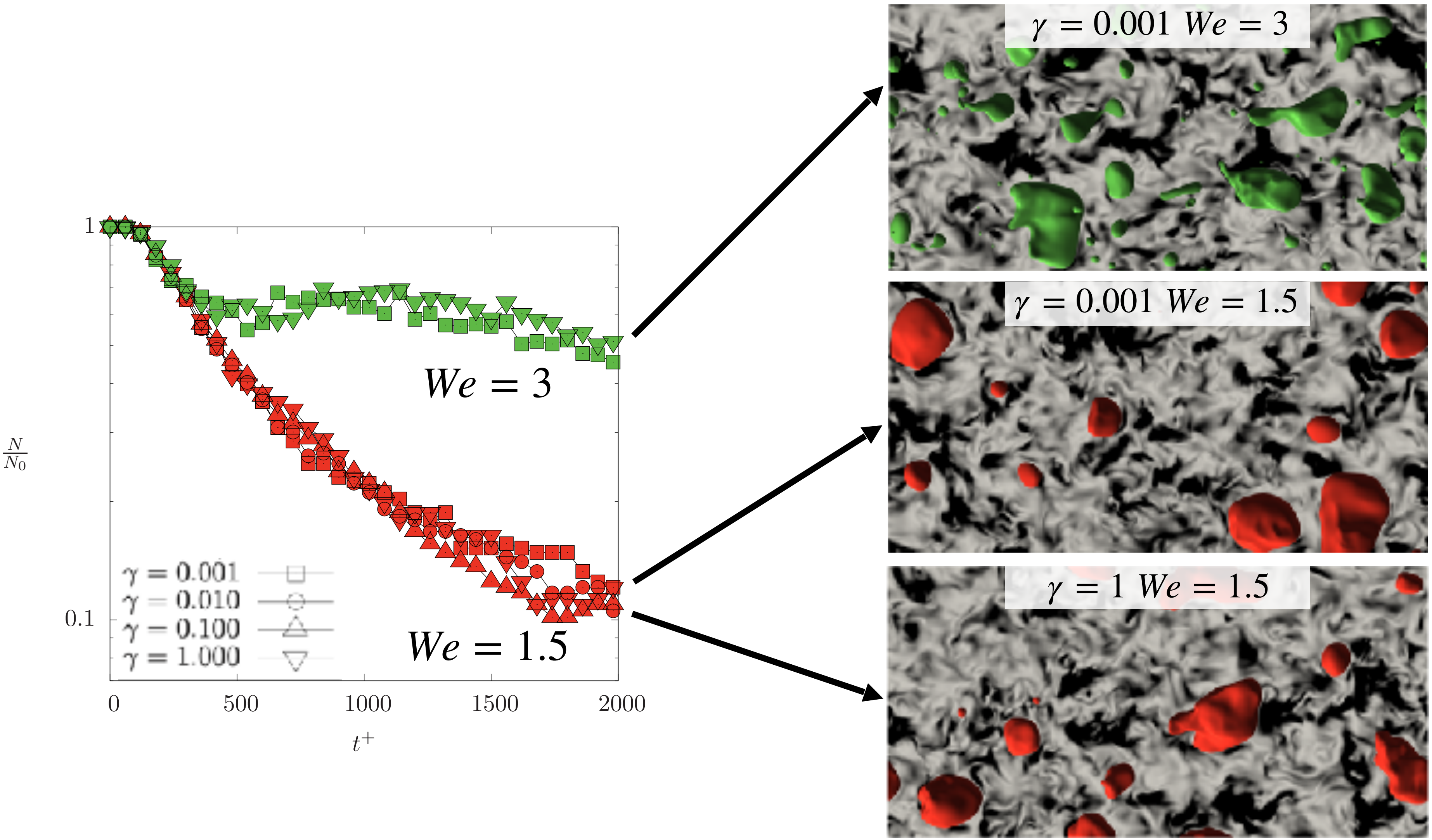
$$\gamma = \frac{\rho_d}{\rho_c} = \frac{\text{Droplet density}}{\text{Carrier density}}$$



Bubble dynamics: Qualitative behavior



Effect of density
Number of drops

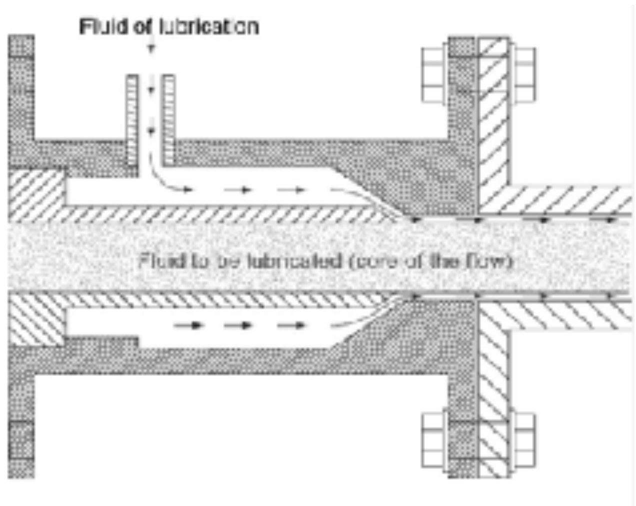


Fil Rouge

1. Historical Perspective, modelling and computational issues
2. A short story on droplets in turbulence (influence of viscosity/density contrast)
3. A short story on oil transport
4. A short story on drop coalescence/break-up (influence of surfactant)

Inspiration: Core Annular Flow (D.D. Joseph)

Method and apparatus for measuring characteristics of core-annular flow
US PATENT 20050033545 A1
Abstract
An apparatus and method are disclosed […] core-annular flow (CAF) in a pipe […] the CAF may be developed from a lubricating fluid, such as water, and a fluid to be transported, such as oil, where the fluid to be transported forms the core region and the lubricating fluid forms the annular region.



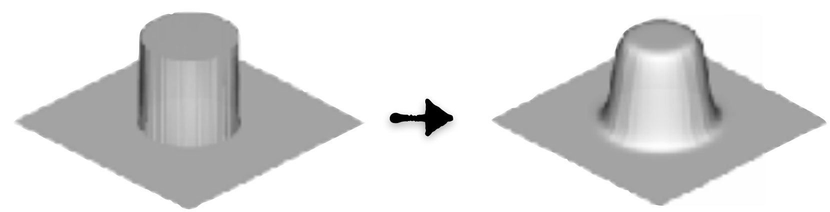
Credit: ALFA Research Group

"There is a strong tendency for two fluids to arrange themselves so that the low-viscosity constituent is in the region of high shear.
This gives rise to a kind of a gift of nature in which the lubricated flows are stable, and it opens up very interesting possibilities for technological applications in which one fluid is used to lubricate another "

Explore the effect of surface tension

Hypothesis:
-Matched density and incompressible flow.
-Different viscosity of the two phases.

Phase Field Method (PFM)



$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \frac{1}{Pe} \nabla^2 (\phi^3 - \phi - Ch^2 \nabla^2 \phi)$$

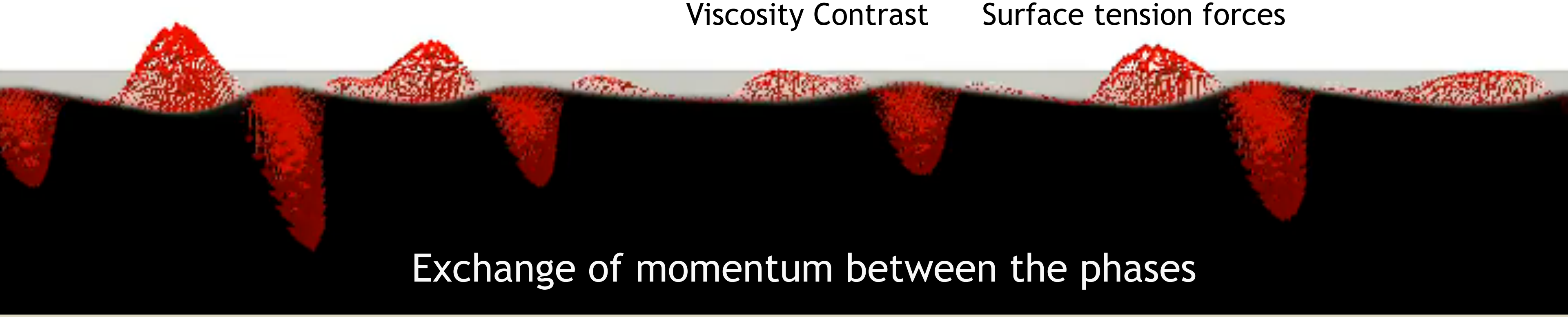
$$\nabla \cdot \mathbf{u} = 0$$

Flow driven by a constant mean pressure gradient

$$\frac{\partial \mathbf{u}}{\partial t} = -\mathbf{u} \cdot \nabla \mathbf{u} - \nabla p' + \Pi + \frac{1}{Re_\tau} \nabla \cdot (r(\phi, \lambda)(\nabla \mathbf{u} + \nabla \mathbf{u}^\mathbf{T})) + \frac{3}{\sqrt{8}} \frac{Ch}{We} \nabla \cdot \tau_c$$

Viscosity Contrast

Surface tension forces

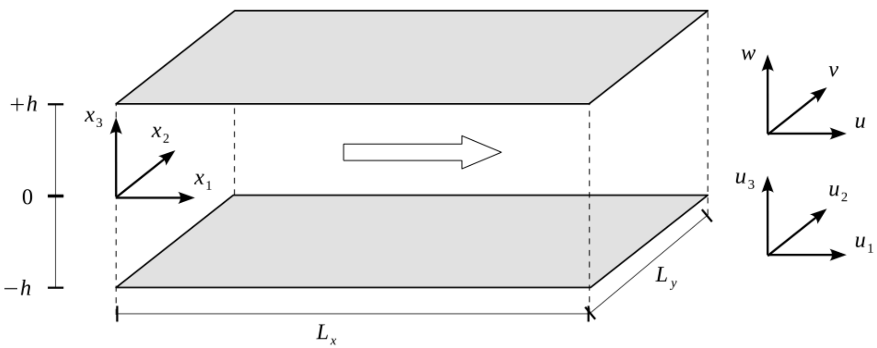


Jacqmin,Calculation of Two-Phase Navier-Stokes Flows Using Phase-Field Modeling, JCP (1999)
Badalassi et al. ,Computation of multiphase systems with phase field models, JCP (2003)
Yue et al, A diffuse-interface method for simulating two-phase flows of complex fluids, JFM (2004)
Kim, A continuous surface tension force formulation for diffuse-interface models, JCP (2005)

Numerical method (Recap)

Method: Direct Numerical Solution (DNS) of NS and CH equations, no models used.

Computational Domain



Space Discretization:
- X Periodic direction (Fourier)
- Y Periodic direction (Fourier)
- Z Wall-normal (Chebychev-Tau)

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

Solver NS (Vorticity-Velocity Formulation):

Curl of NS (Vorticity)

$$\frac{\partial \omega_z}{\partial t} = \nabla \times \mathbf{S} + \frac{1}{Re_\tau}\nabla^2 \omega_z$$

Twice Curl of NS

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

CH:

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

C.Canuto and A. Quarteroni, Spectral and pseudo-spectral methods for parabolic problems with non periodic boundary condition.

Numerical method (Recap)

$$\frac{\partial \omega_z}{\partial t} = \nabla \times \mathbf{S} + \frac{1}{Re_\tau}\nabla^2 \omega_z$$

- Solve for the 3rd component of vorticity
- 2nd order PDE
- Single Helmotz solver

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

- Solve for the 3rd component of velocity
- 4th order PDE
- Double Helmotz solver, Influence Matrix Method

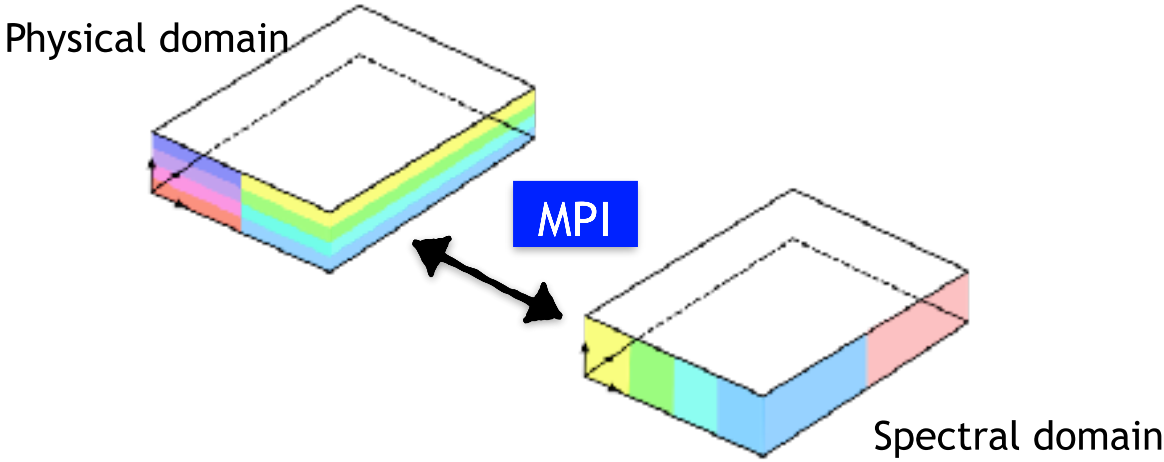
$$\frac{\partial \phi}{\partial t} = S_\phi + \frac{sCh^2}{Pe}\nabla^2 \phi - \frac{Ch^2}{Pe}\nabla^4 \phi$$

- Solve for phi
- 4th order PDE
- Double Helmotz solver

With no-flux BC ϕ is conserved.

$$\frac{\partial}{\partial t}\int_\Omega \phi d\Omega = 0$$

- MPI Paradigm, 2D Domain decomposition

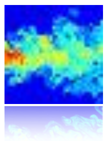


C.Canuto and A. Quarteroni, Spectral and pseudo-spectral methods for parabolic problems with non periodic boundary condition.

Simulations Setup

Boundary Conditions:

FLOW FIELD



PHASE FIELD

NO SLIP AT THE WALLS

$$u_i(\pm h) = 0$$

90° CONTACT ANGLE

$$\frac{\partial \phi}{\partial z}(\pm h) = \frac{\partial^3 \phi}{\partial z^3}(\pm h) = 0$$

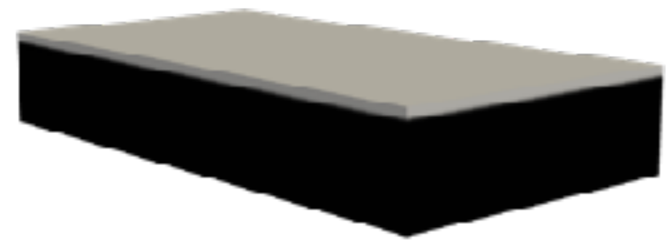
PERIODICITY ALONG X and Y

$$u_i(0) = u_i(L_x) \qquad \phi(0) = \phi(L_x)$$

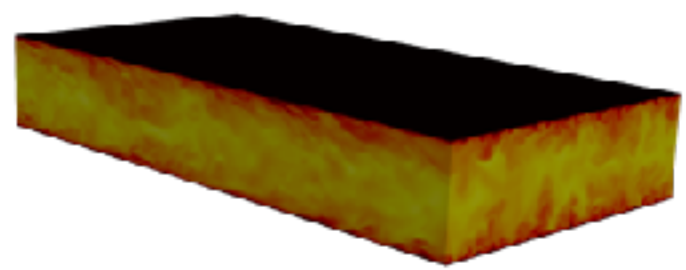
$$u_i(0) = u_i(L_y) \qquad \phi(0) = \phi(L_y)$$

Initial Conditions:

- Phase Field
  - Flat Interface
  - Layer Thickness 45 w.u.
  - Total height 600 w.u.



- Flow Field
  - Single Phase Flow Re=300.



S. Ahmadi et al, Turbulent Drag Reduction by a Near Wall Surface Tension Active Interface, FTAC (2018)
S. Ahmadi et al, Turbulent drag reduction in channel flow with viscosity stratified fluids, CEF (2016)

Simulations Setup

Flow parameters:

- Weber Number, inertia over interfacial tension, considering oil/water:

$$We = \frac{\rho u_\tau^2 h}{\sigma} = 0.5$$

- Reference shear Reynolds number (oil):

$$Re_\tau = \frac{\rho u_\tau h}{\eta_o} = 300$$

Phase field parameters:

- Peclet number (interface relaxation time):
-

$$Pe = 150$$

- Cahn number (interfacial layer thickness):

$$Ch = 0.02$$

We consider 3 different viscosity ratio λ :
(ratio between the viscosity of the two phases)

$$\lambda = \frac{\eta_w}{\eta_o} = \frac{\text{Water Viscosity}}{\text{Oil Viscosity}}$$

#	λ	Grid (N_x x N_y x N_z)
SP	-	512 x 256 x 257
S1	1,000	512 x 256 x 257
S3	0,500	512 x 256 x 513
S4	0,250	1024 x 512 x 513

S. Ahmadi et al, Turbulent Drag Reduction by a Near Wall Surface Tension Active Interface, FTAC (2018)
S. Ahmadi et al, Turbulent drag reduction in channel flow with viscosity stratified fluids, CEF (2016)

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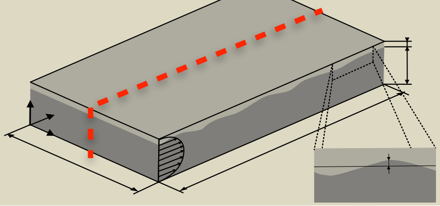
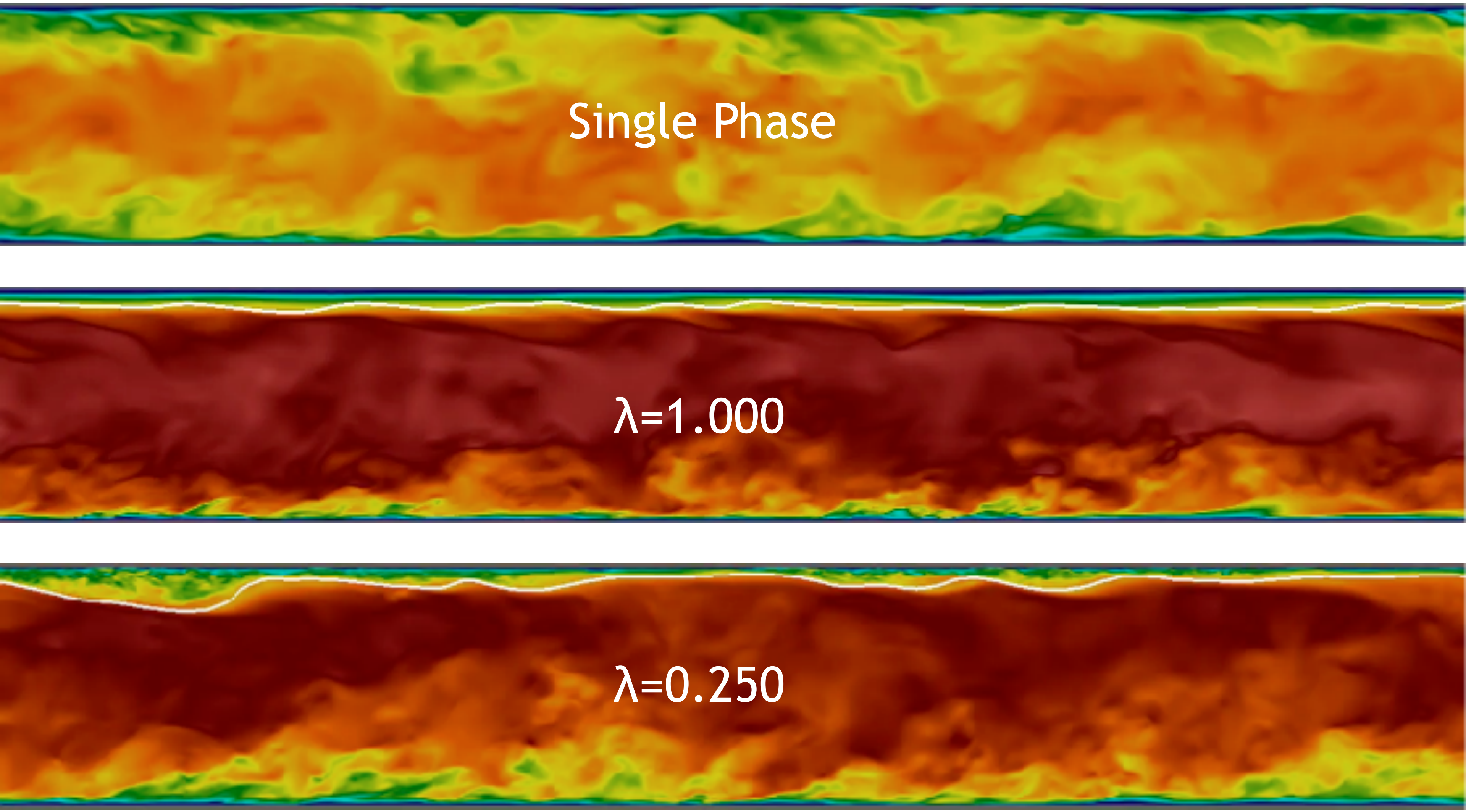
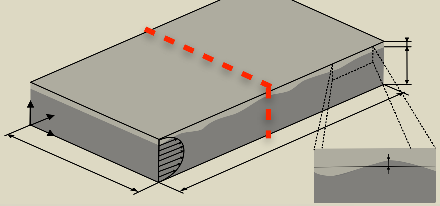
Visualization

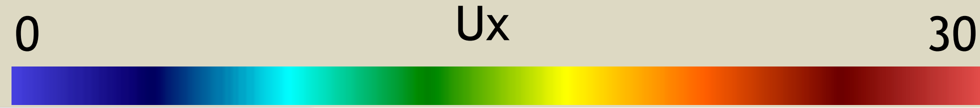


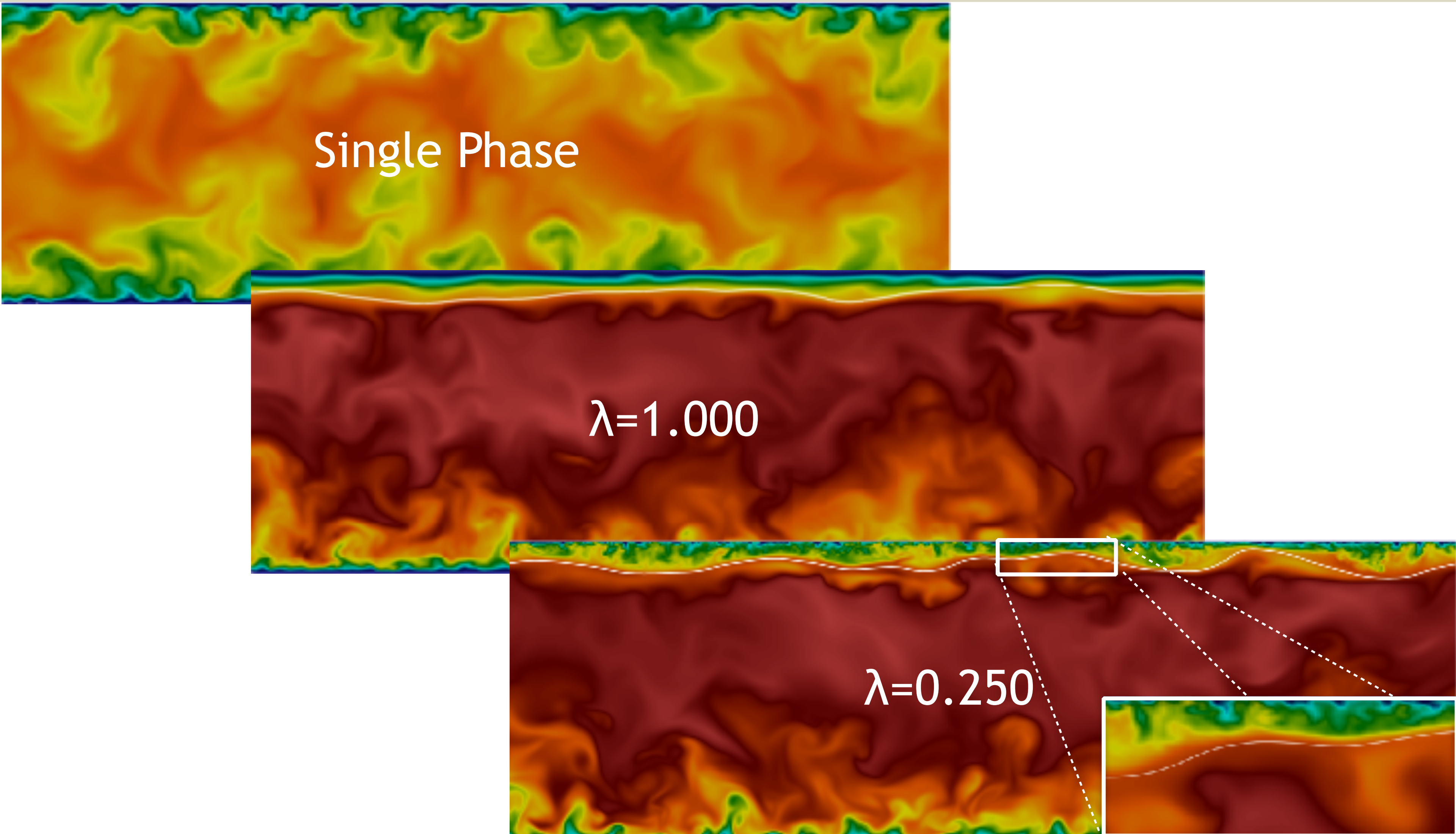


Visualization

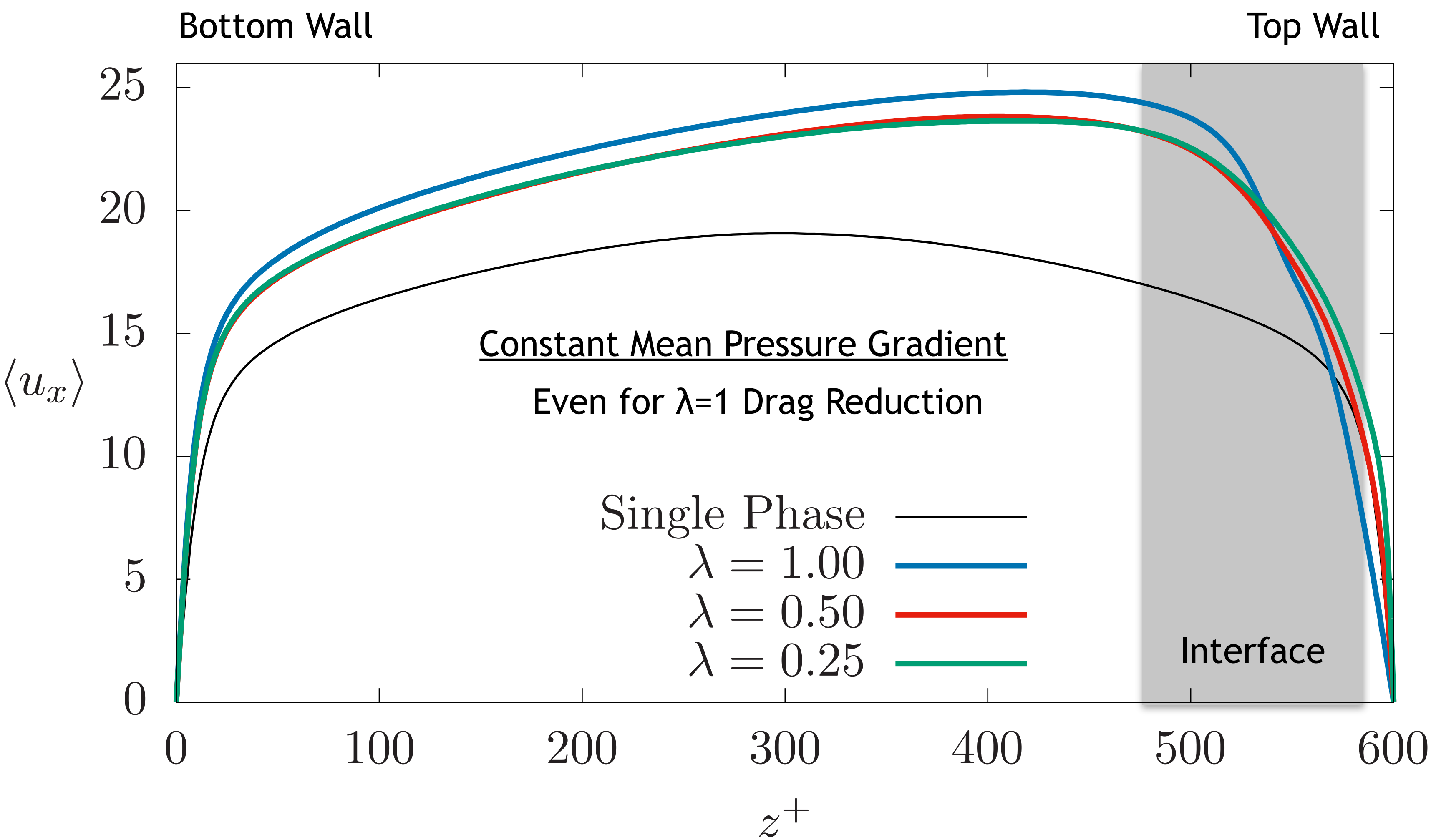
TECHNISCHE UNIVERSITÄT WIEN
Vienna | Austria



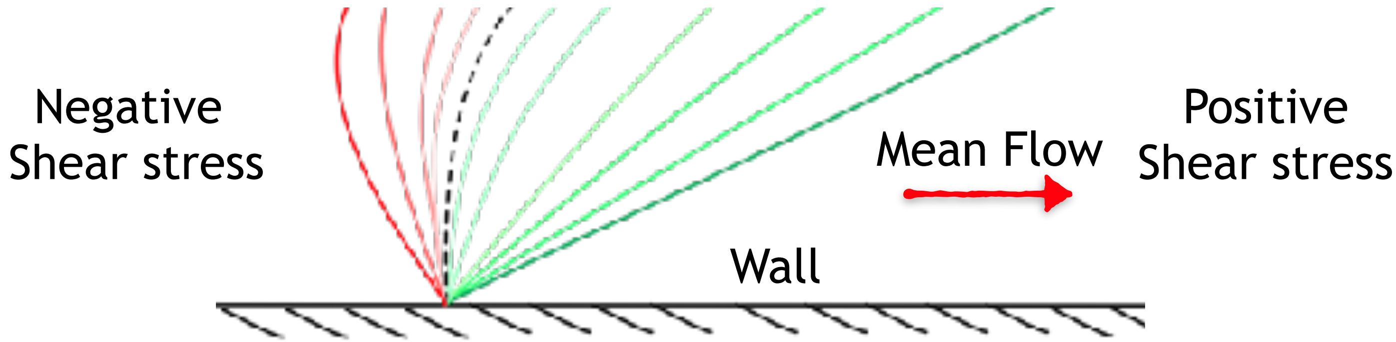




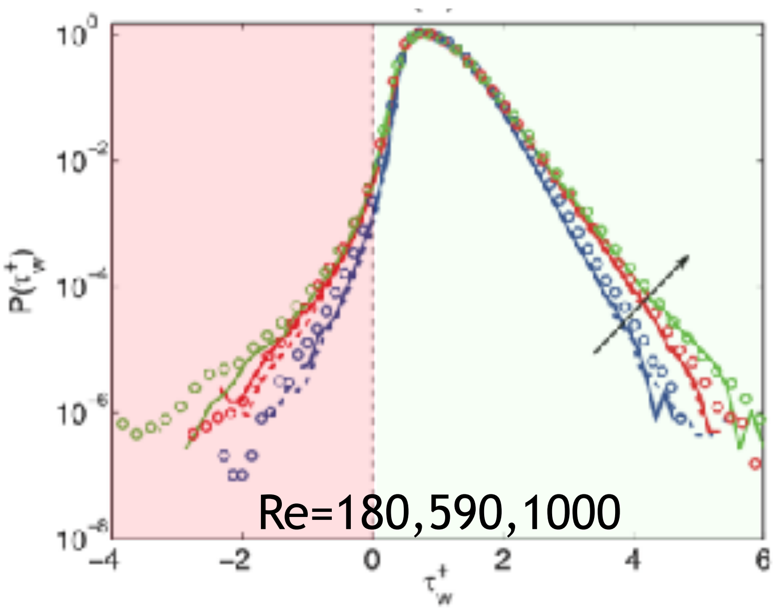
Mean Velocity Profile

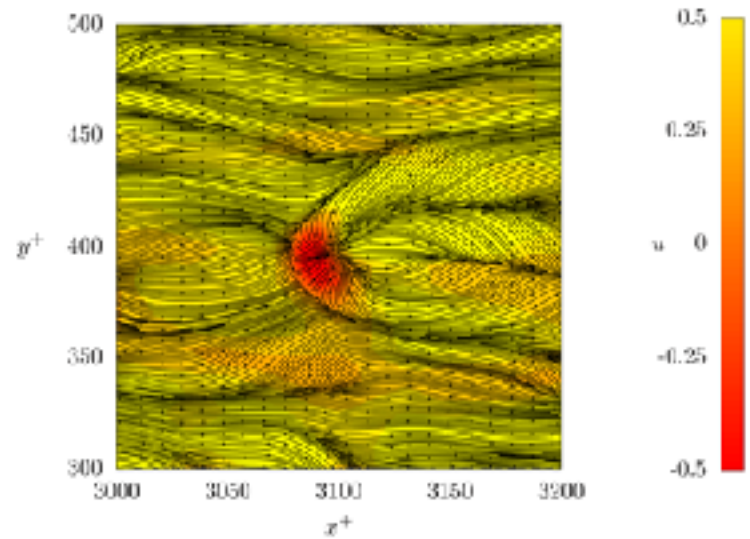


An important character: Wall-shear stress



Considering a single phase-flow, from literature:





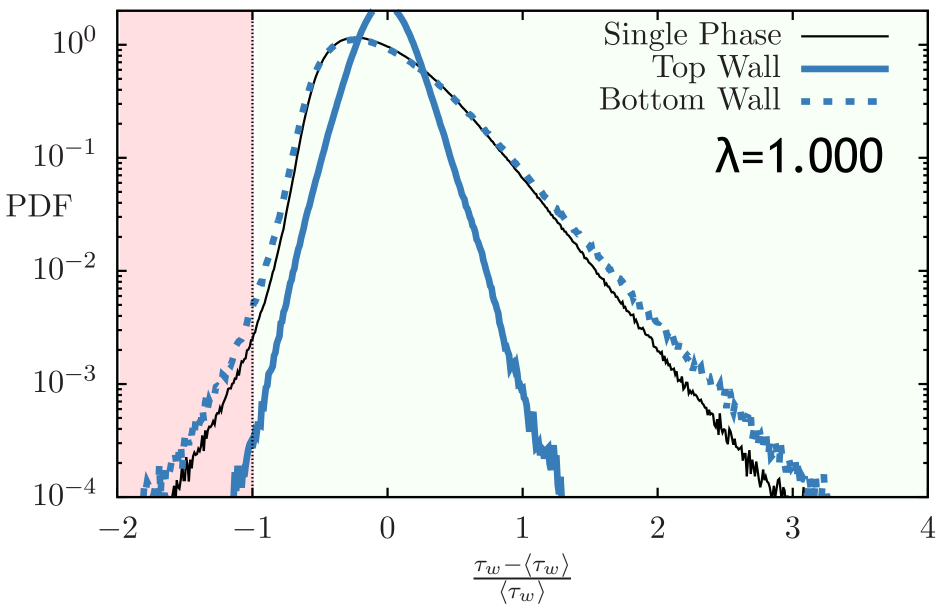
A. Wietrzak et al., Wall shear stress and velocity in a turbulent axisymmetric boundary layer, JFM (1994)
K.J. Colella et al., Measurements and scaling of wall shear stress fluctuations, EF (2003)
P. Leanars et al, Rare back-flow and extreme wall-normal velocity fluctuations in near-wall turbulence, PoF (2012)

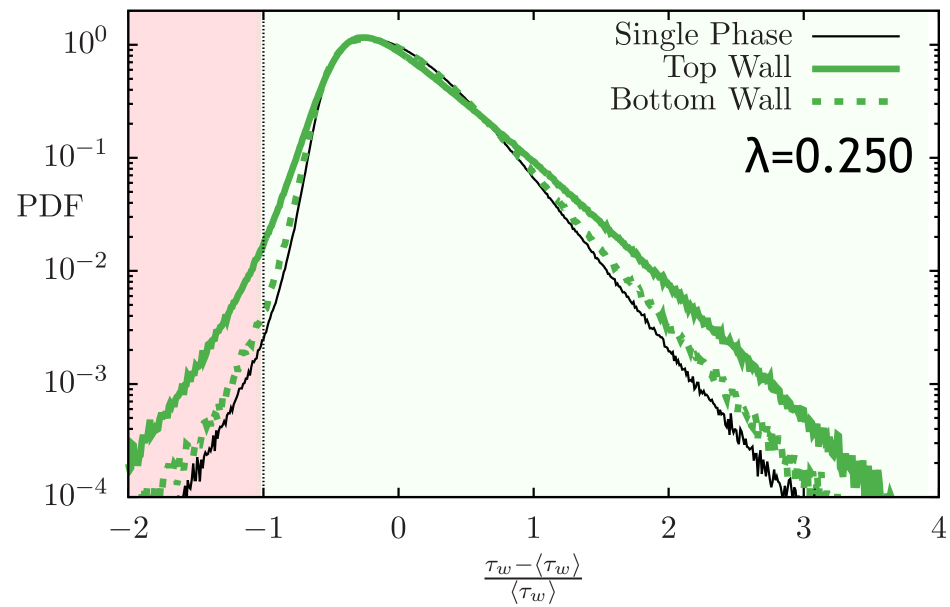
Wall-shear stress:stratified case

Consider the viscosity-stratified case and the wall shear stress fluctuations τ'_w :

$$\tau'_w = \frac{\tau_w - \langle \tau_w \rangle}{\langle \tau_w \rangle}$$

$\tau'_w < -1$ ⟶ Back-Flow Event





Top: Shape is modified, fluctuations reduced.
Bottom: Slight increase of the fluctuations.

Top: Increase of the fluctuations..
Bottom: Slight increase of the fluctuations.

S. Ahmadi et al, Turbulent drag reduction in channel flow with viscosity stratified fluids, C&F (2017)
S. Ahmadi et al, Turbulent drag reduction by a near wall surface tension active interface, FT&C (2018).
P. Leaners et al, Rare backflow and extreme wall-normal velocity fluctuations in near-wall turbulence, PoF (2017)

Simulations of turbulent channel flow

Common used approaches:

- Constant Flow Rate (CFR)
- Constant Pressure Gradient (CPG)

Study of DR with CFR and CPG might lead to some problems and influence the results:

- Different power injected
- Comparison is difficult.

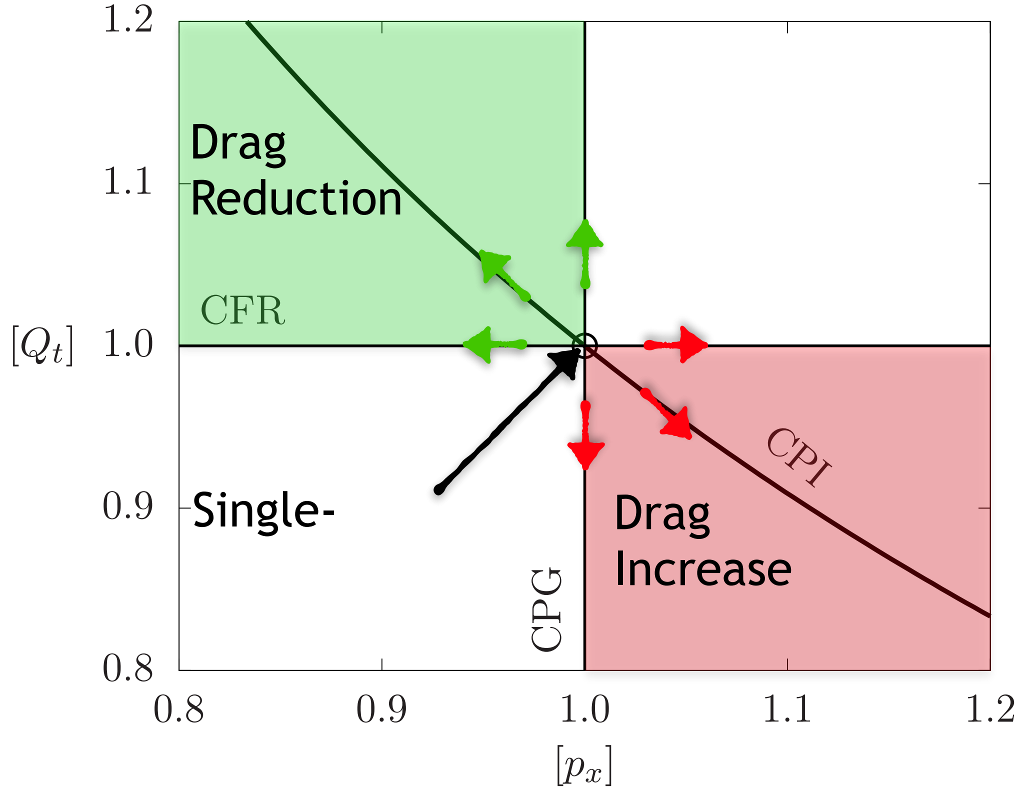
Third possible approach:

- Constant power input (CPI)

Power injected is kept constant adapting the mean pressure gradient to the flow-rate:

$$-p_x{}^{n+1} = \frac{3}{Re_\Pi u_b{}^n},$$

Mean pressure gradient   Bulk velocity (Flow-rate)



Roccon et al., Constant power input simulations of drag reduced viscosity stratified turbulent channel flow, FT&C (sub)
Roccon et al., Turbulent drag reduction by compliant lubricating layer, JFM-R (2019)
Ahmadi et al., Turbulent drag reduction in channel flow with viscosity stratified fluids, C&F (2018)
Ahmadi et al., Turbulent drag reduction by a near wall surface tension active interface, FT&C (2018)

Constant Power Input Simulations
Simulation setup

Characteristic velocity based on the power injected in the system:

$$u_\Pi = \sqrt{\frac{\Pi_m h}{3\mu_2}}$$

<u>Flow parameters:</u>

Reynolds number (inertia/viscous)

$$Re_\Pi = \frac{\rho u_\Pi h}{\mu_2} = 12220$$

Weber number (inertia/interfacial)

$$We_\Pi = \frac{\rho u_\Pi^2 h}{\sigma} = 830$$

<u>Phase field parameters:</u>

$$Pe_\Pi = \frac{u_\Pi h}{\mathcal{M}\beta} = 830 \qquad Ch = \frac{\xi}{h} = 0.01$$

*Roughly corresponding to a shear Re=300 (SP).

<u>We consider 5 different viscosity ratios λ :</u>

(ratio between the viscosity of the thin lubricating layer over the main layer)

$$\lambda = \frac{\mu_1}{\mu_2} = \frac{\text{Thin Layer}}{\text{Main layer}}$$

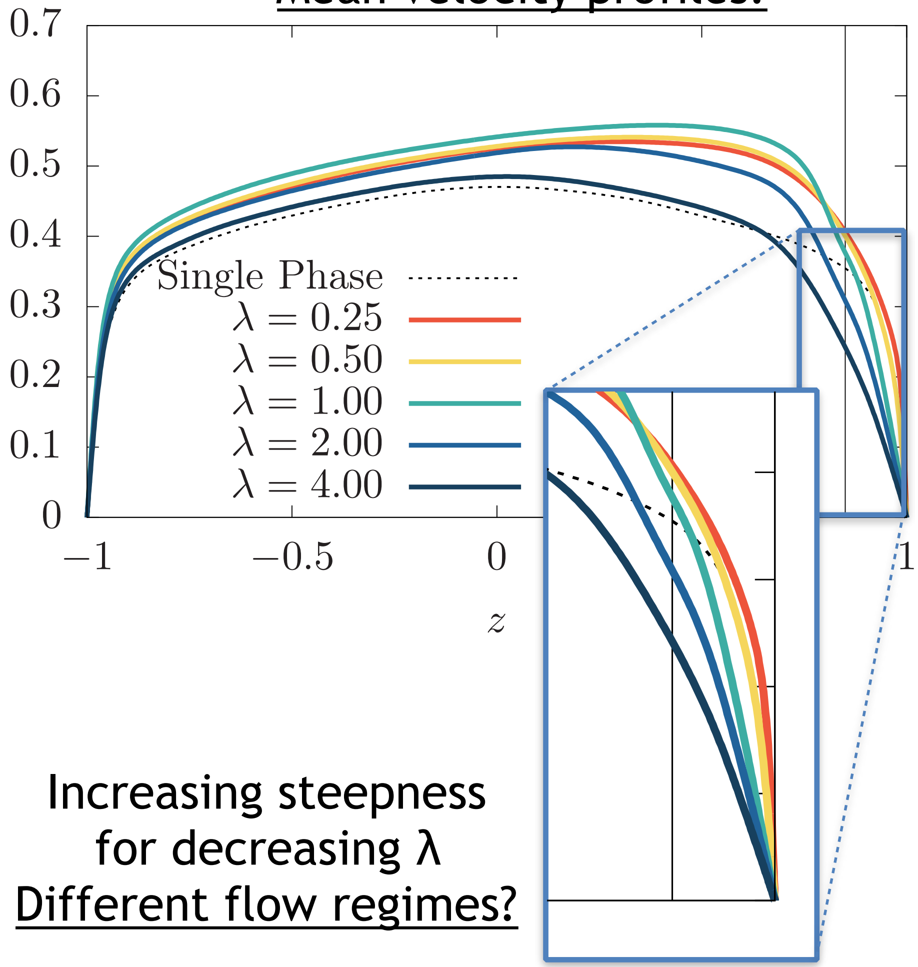
#	λ
SP	-
S1	0,25
S2	0,50
S3	1,00
S4	2,00
S5	4,00

Grid resolution:
512 x 256 x 257 (Single-phase)
1024 x 512 x513 (Stratified cases)

Roccon et al., Constant power input simulations of drag reduced viscosity stratified turbulent channel flow, FT&C (sub)
Roccon et al., Turbulent drag reduction by compliant lubricating layer, JFM-R (2019)
Ahmadi et al., Turbulent drag reduction in channel flow with viscosity stratified fluids, C&F (2018)
Ahmadi et al., Turbulent drag reduction by a near wall surface tension active interface, FT&C (2018)

Results
Macroscopic parameters (FR and PG)

Mean velocity profiles:

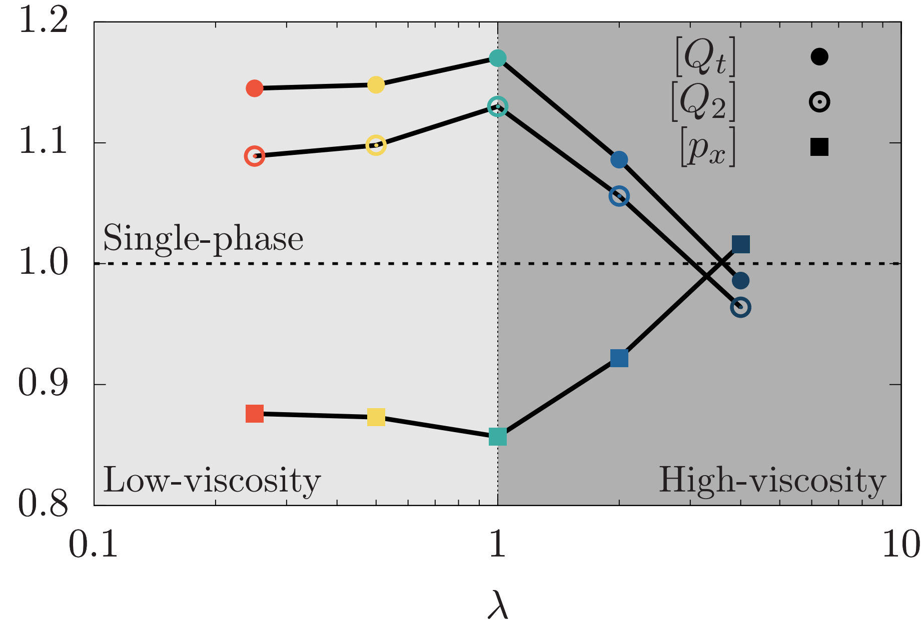


Increasing steepness for decreasing λ

<u>Different flow regimes?</u>

Drag reduction (CPI approach): Flow-rate increases and at the same time the mean pressure gradient decreases.

Flow-rates and pressure gradient:



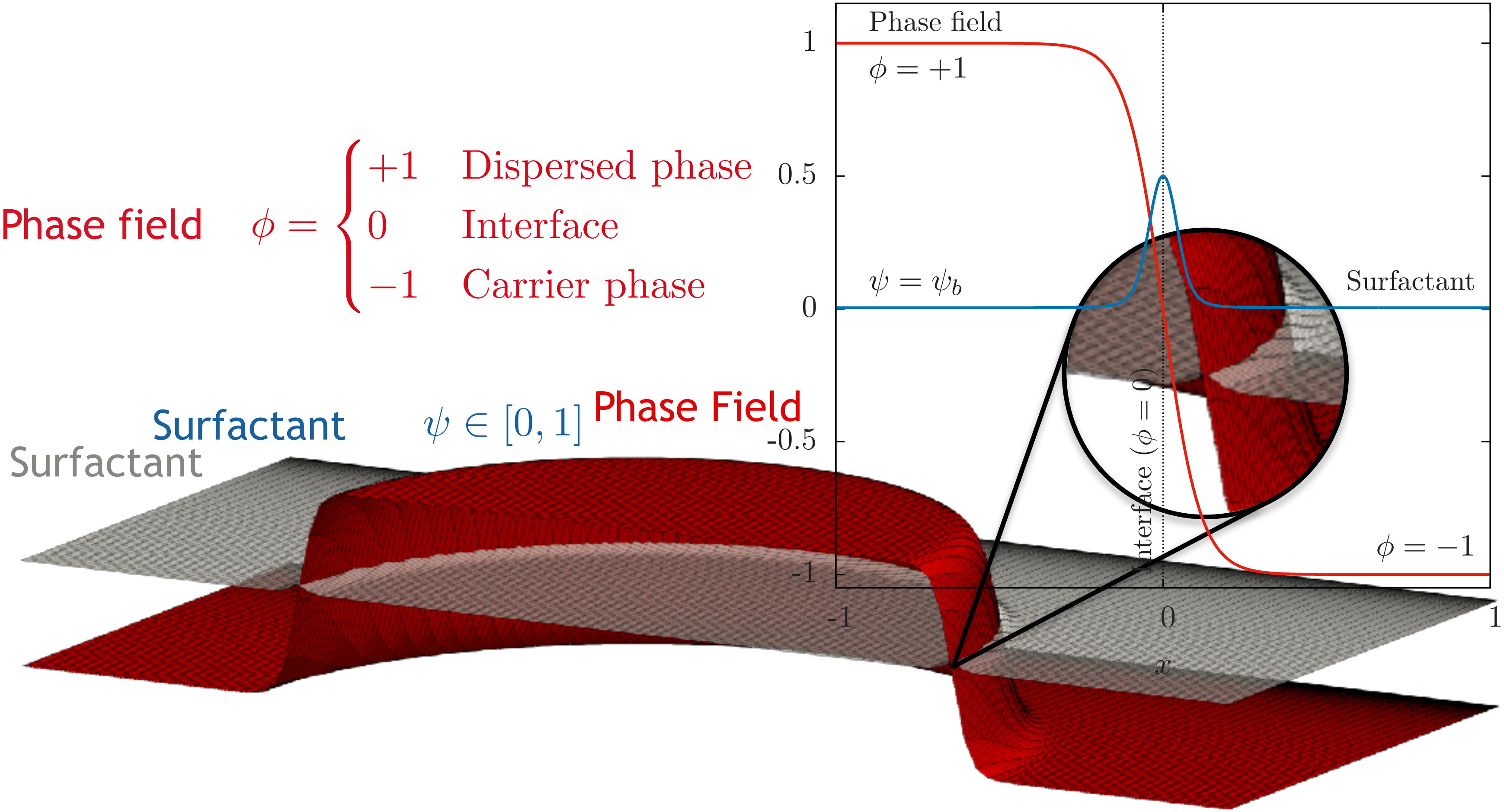
Roccon et al., Constant power input simulations of drag reduced viscosity stratified turbulent channel flow, FT&C (sub)

Fil Rouge

1. Historical Perspective, modelling and computational issues
2. A short story on droplets in turbulence (influence of viscosity/density contrast)
3. A short story on oil transport
4. A short story on drop coalescence/break-up (influence of surfactant)

Modelling the presence of surfactant with the Phase Field Method

Phase field $\phi = \begin{cases} +1 & \text{Dispersed phase} \\ 0 & \text{Interface} \\ -1 & \text{Carrier phase} \end{cases}$



Alfredo Soldati and Francesco Zonta

Modelling the presence of surfactant with the Phase Field Method

Taking the variation of the Ginzburg-Landau energy functional with respect to Φ and ψ we can compute the expression of the two chemical potentials:

$$\mu_\phi = \frac{\delta F(\phi, \nabla\phi, \psi)}{\delta\phi} = \phi^3 - \phi - Ch^2\nabla^2\phi$$

For Φ we neglect the coupling with ψ (Kim. 2012

$$\mu_\psi = \frac{\delta F(\phi, \nabla\phi, \psi)}{\delta\psi} = Pi \log\left(\frac{\psi}{1-\psi}\right) - \frac{1}{2}(1-\phi^2)^2 + \frac{1}{2Ex}\phi^2$$

… Final point is the two Advection Diffusion Equations for phase and surfactant!

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = \frac{1}{Pe_\phi}\nabla^2(\phi^3 - \phi - Ch^2\nabla^2\phi)$$

$$\frac{\partial\psi}{\partial t} + \mathbf{u}\cdot\nabla\psi = \frac{Pi}{Pe_\psi}\nabla^2\psi + \frac{1}{Pe_\psi}\nabla\cdot\psi(1-\psi)\nabla\left(-\frac{1}{2}(1-\phi^2)^2 + \frac{\phi^2}{2Ex}\right)$$

G.Toth & B.Kvamme, Analysis of Ginzburg-Landau-type models of surfactant-assisted liquid phase separation, PRE (2015)
S. Komure, H. Kodama, Two order parameter model for an oil-water-surfactant system, PRE (1996)
A. Yun, Y.Li & J.Kim, A new phase-field model for a water-oil-surfactant system, Appl. Math (2014)
S. Engblom et al. On diffuse interface modeling and simulation of surfactants in two-phase fluid flow, Comm. Comp. Phys (2012)

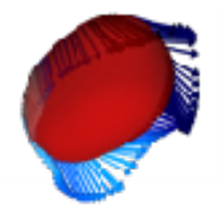
Phase Field Method
Coupling with Navier-Stokes

Assumptions:
- Matched density
- Matched viscosity
- Non-uniform surface tension

Equation of state for surface tension:

$$f_\sigma(\psi) = \frac{\sigma(\psi)}{\sigma_0} = 1 + \beta_s \log(1-\psi)$$

Flow:



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

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{Re_\tau}\nabla^2 \mathbf{u} + \frac{3}{\sqrt{8}}\frac{Ch}{We}\nabla \cdot [\tau_c f_\sigma(\psi)]$$

Interface:

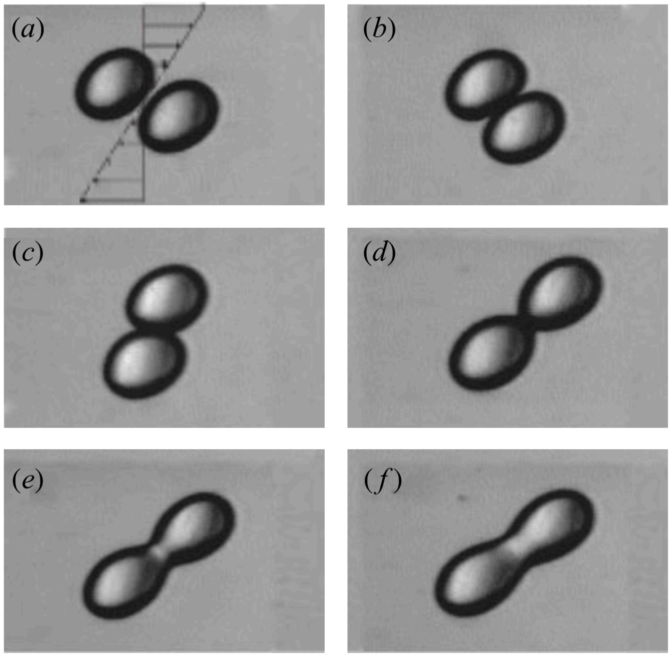
$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \frac{1}{Pe_\phi}\nabla^2 \mu_\phi \qquad \mu_\phi = \frac{\delta \mathcal{F}}{\delta \phi}$$

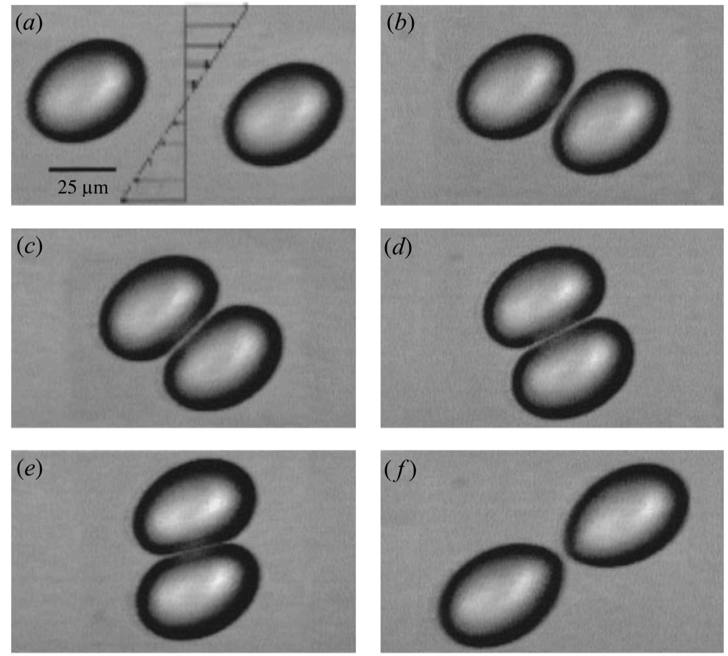
Surfactant:

$$\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi = \frac{1}{Pe_\psi}\nabla \cdot (\mathcal{M}_\psi(\psi)\nabla \mu_\psi) \qquad \mu_\psi = \frac{\delta \mathcal{F}}{\delta \psi}$$

S. Komura et al., Two-order-parameter model for an oil-water-surfactant system, PRE (1997)
G.I. Tòth et al., Analysis of Ginzburg-Landau-type models of surfactant-assisted liquid phase separation, PRE (2015)
G. Soligo et al., Coalescence of surfactant-laden drops by Phase Field Method, JCP, (2019)
S. Engblom et al., On diffuse interface modeling and simulation of surfactants in two-phase fluid flow, CCP (2013)

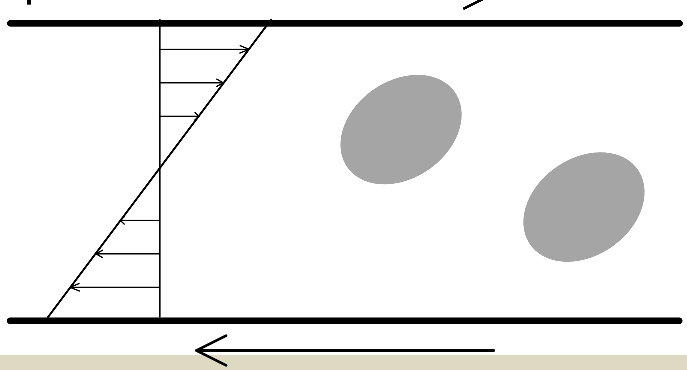
Droplets interactions





Coalescing droplets

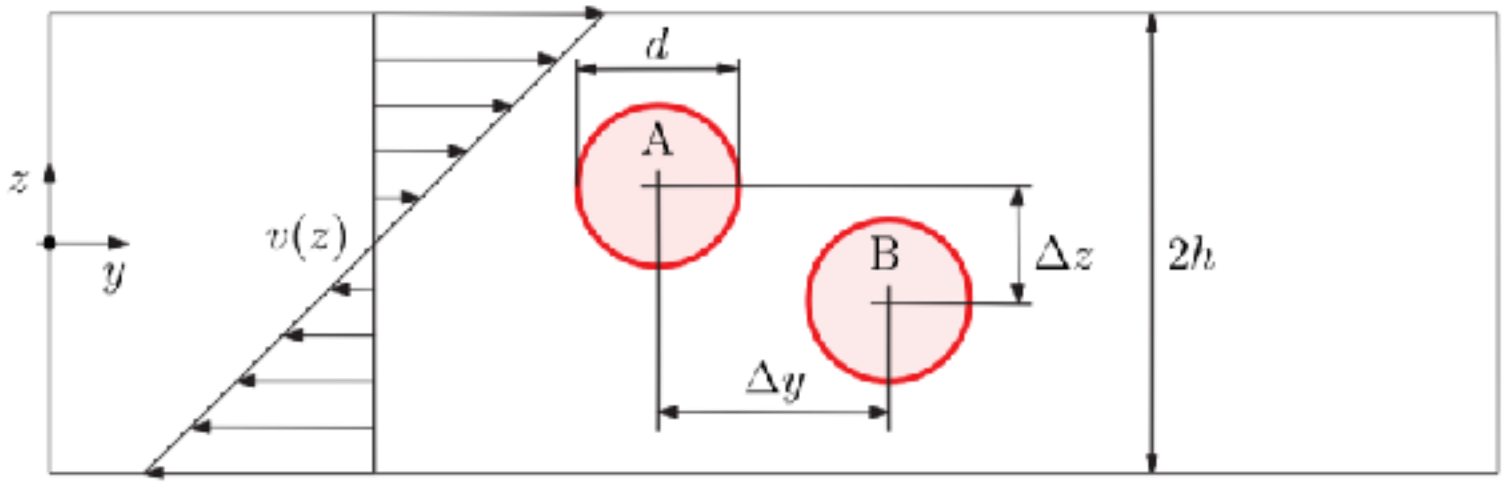
Non-coalescing droplets



[1] S. Guido and M. Simeone. Binary collision of drops in simple shear flow by computer-assisted video optical microscopy. J. Fluid Mech., 357: 1–20, 1998.

Simulation Setup
Replica of the Guido&Simeone experiment

Setup considered:



Two droplets with diameter:

$$d = 0.7h$$

Separated by a distance:

$$\Delta y = h$$

$$\Delta z = 0.5h$$

Laminar shear flow

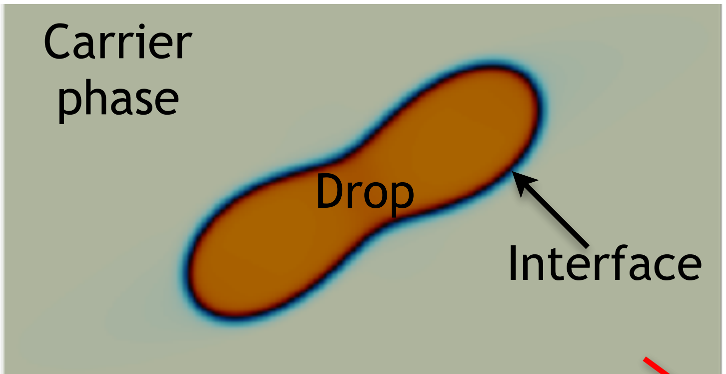
- Shear Reynolds number:

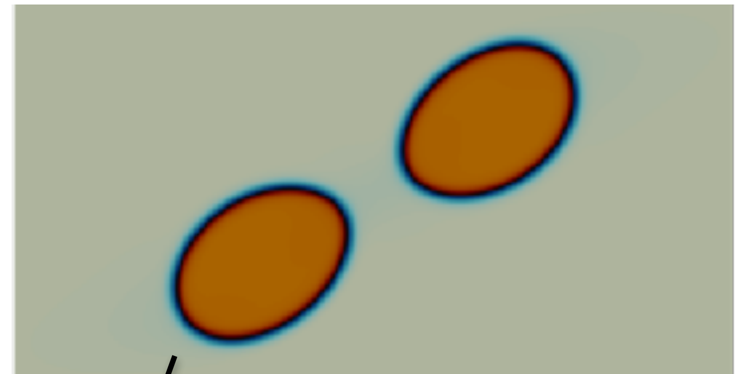
$$Re_\tau = \frac{\rho u_\tau h}{\eta} = 0.5$$

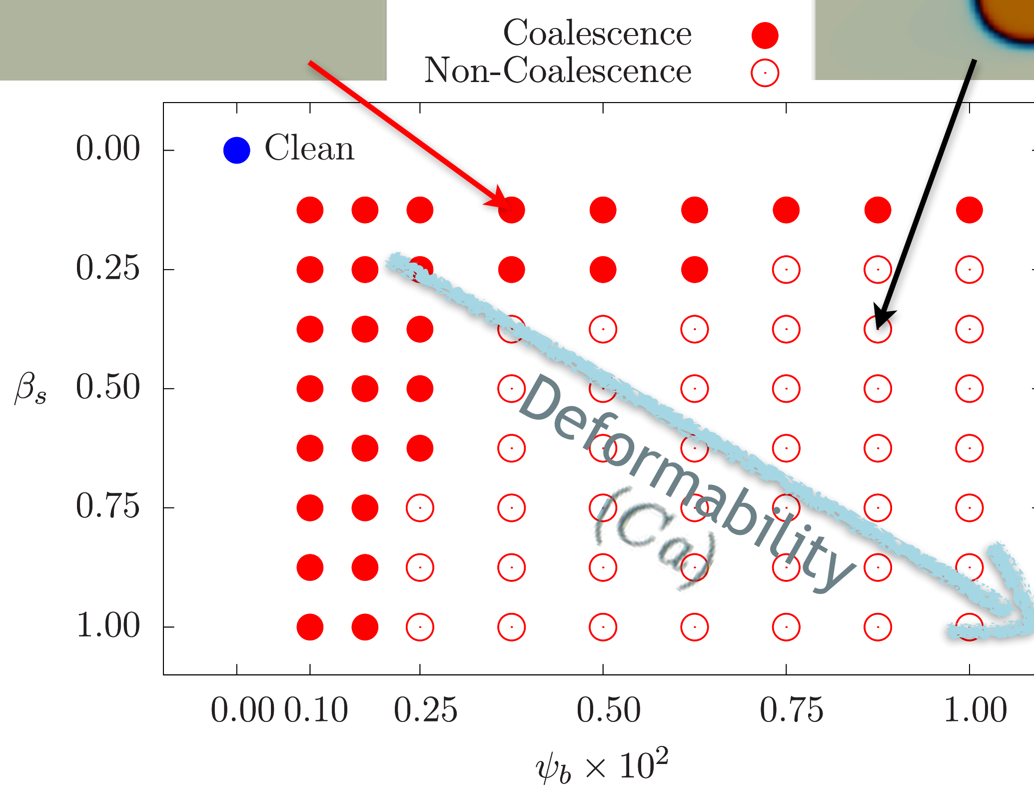
- Capillary number:

$$Ca = \frac{We}{Re}\frac{d}{2h} = \frac{\text{Viscous Forces}}{\text{Surface Tension Forces}} = 0.10$$

Coalescence *vs* non-coalescence: Explore the parameters range



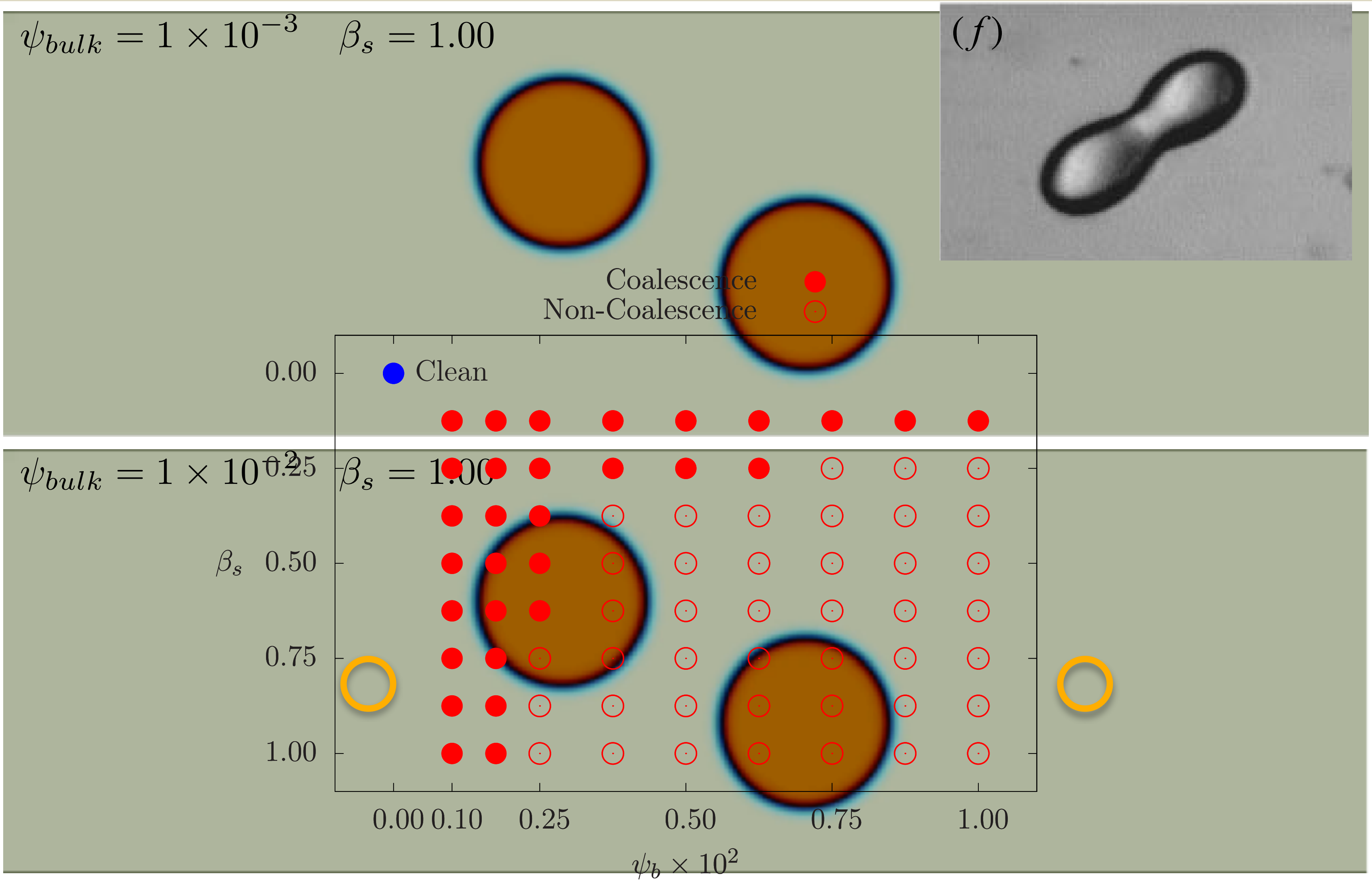




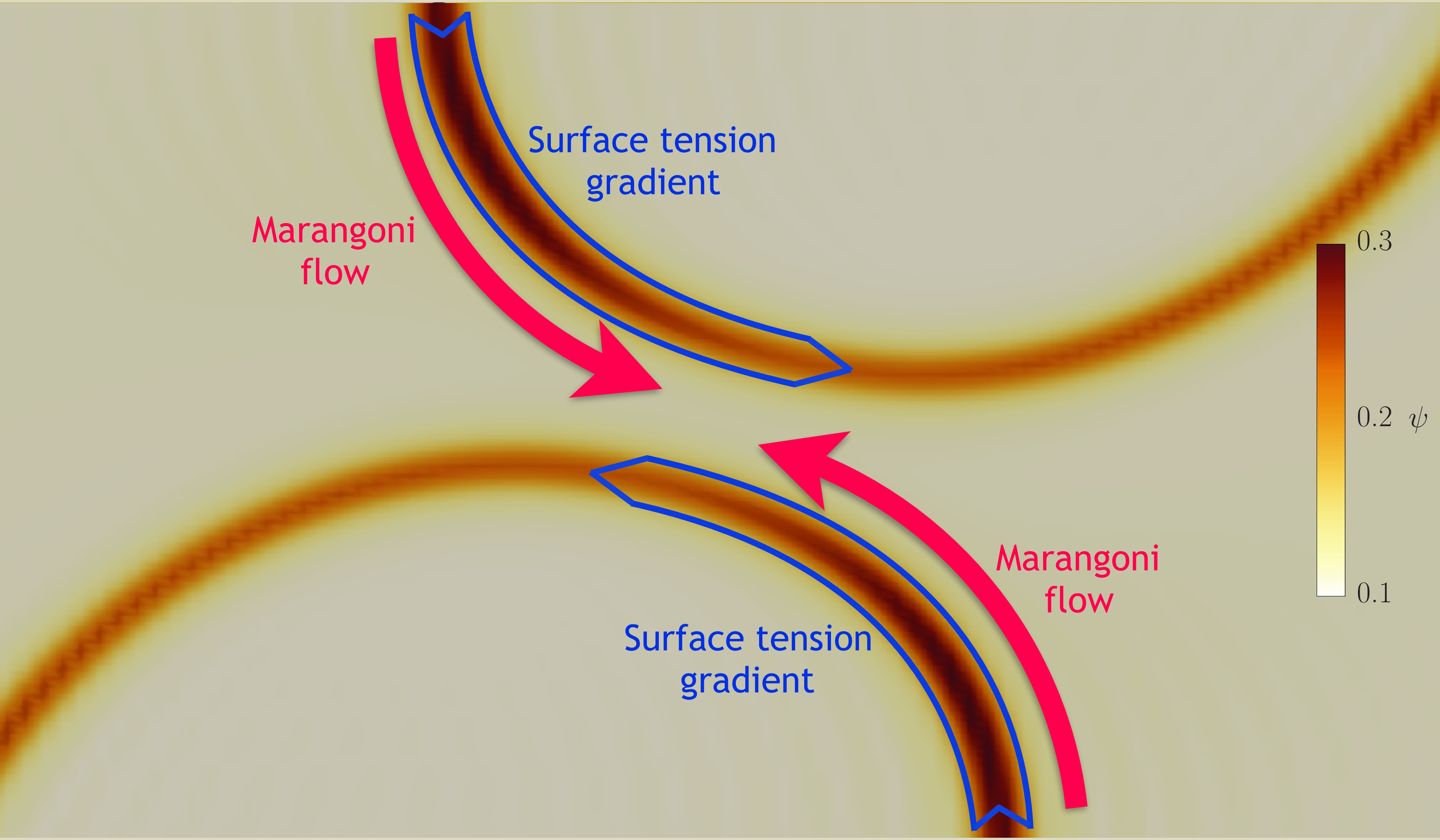
Capillary number

$$Ca = \frac{\eta u_w}{\overline{\sigma}}$$

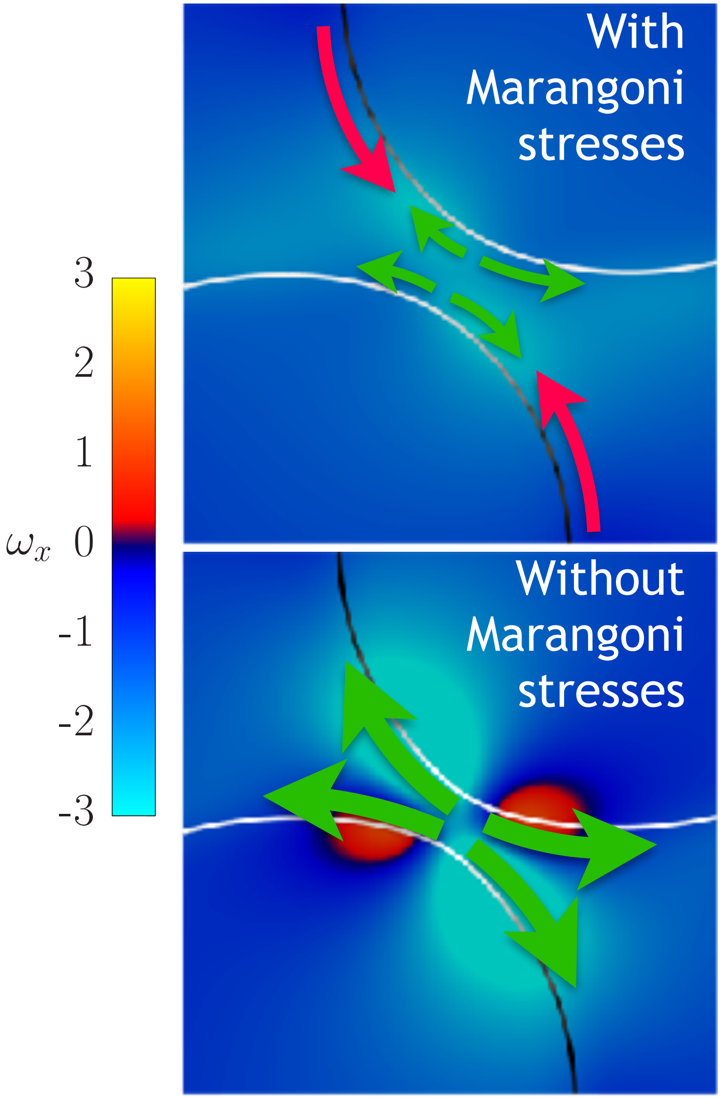
Coalescence *vs* non-coalescence
Explore the parameters range

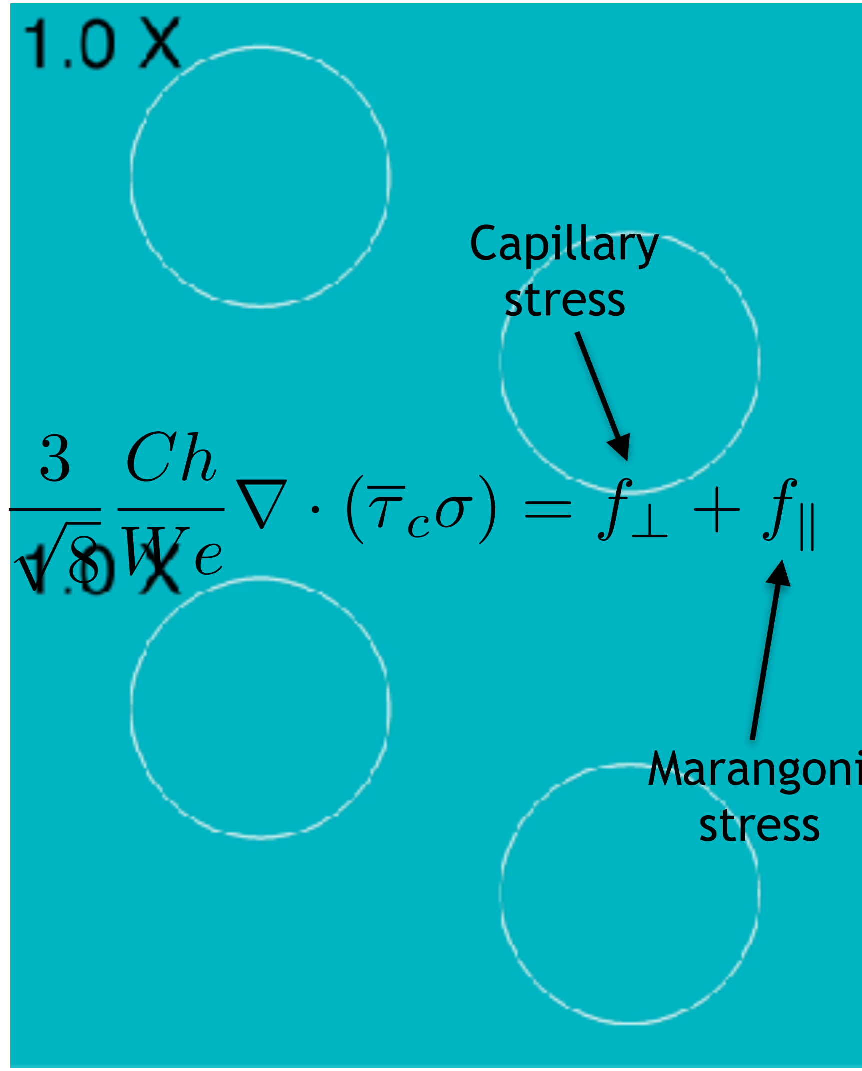


Role of Capillary and Marangoni stresses



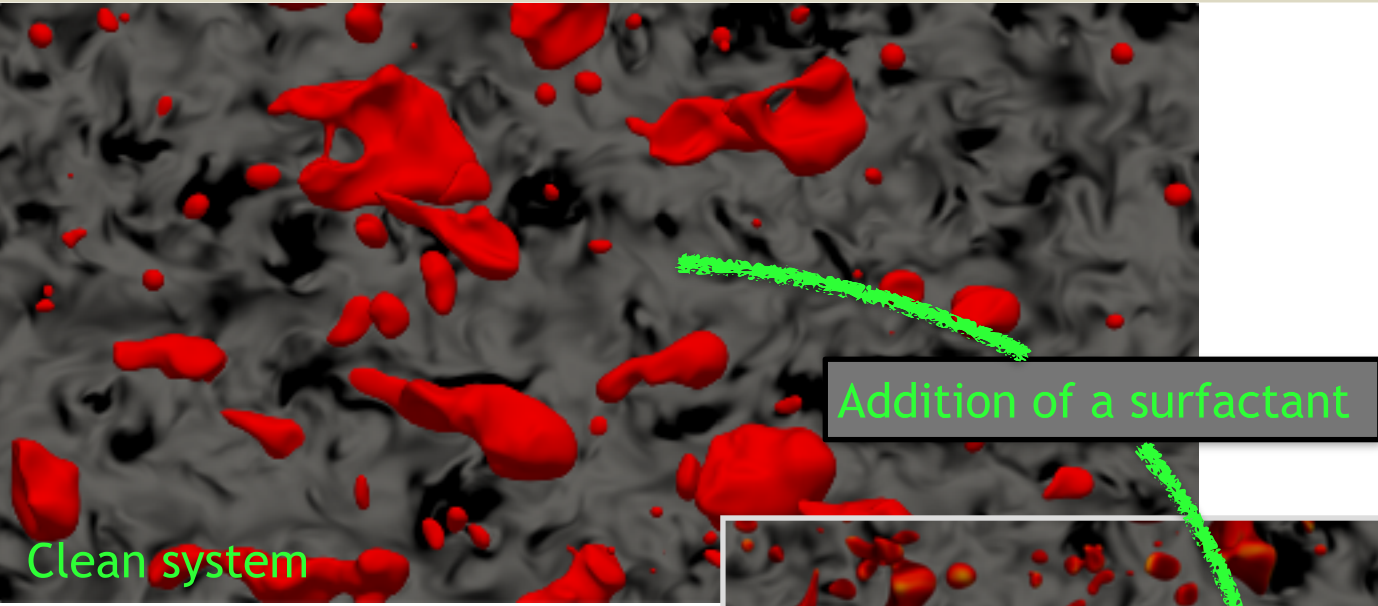
Role of Capillary and Marangoni stresses

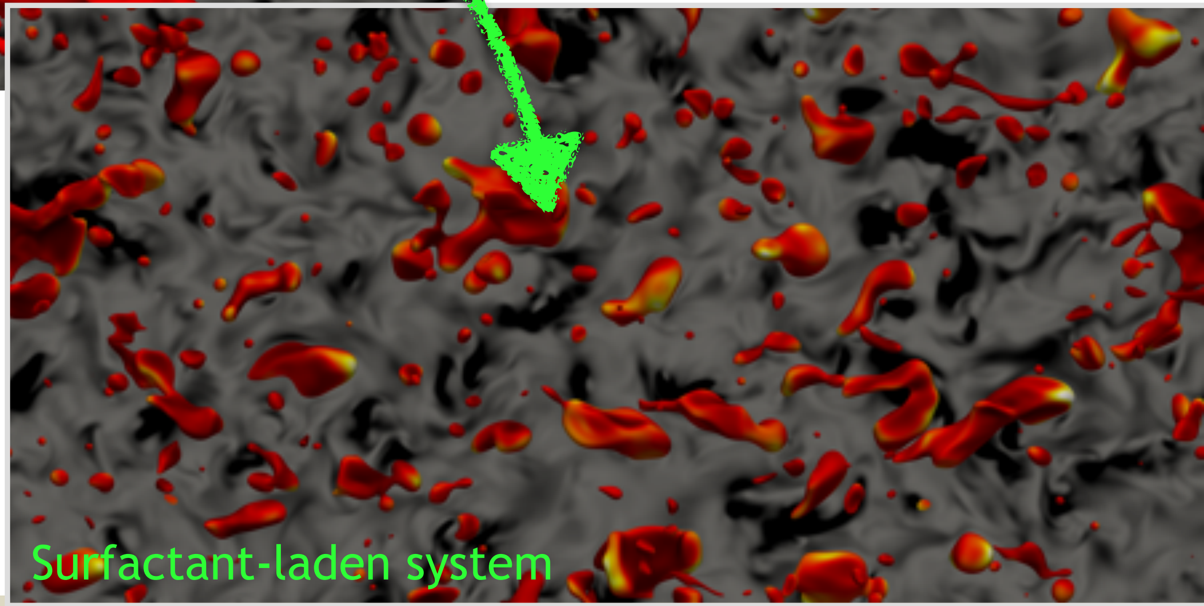




$$\frac{3}{\sqrt{8}}\frac{Ch}{We}\nabla\cdot(\overline{\tau}_c\sigma) = f_\perp + f_\parallel$$

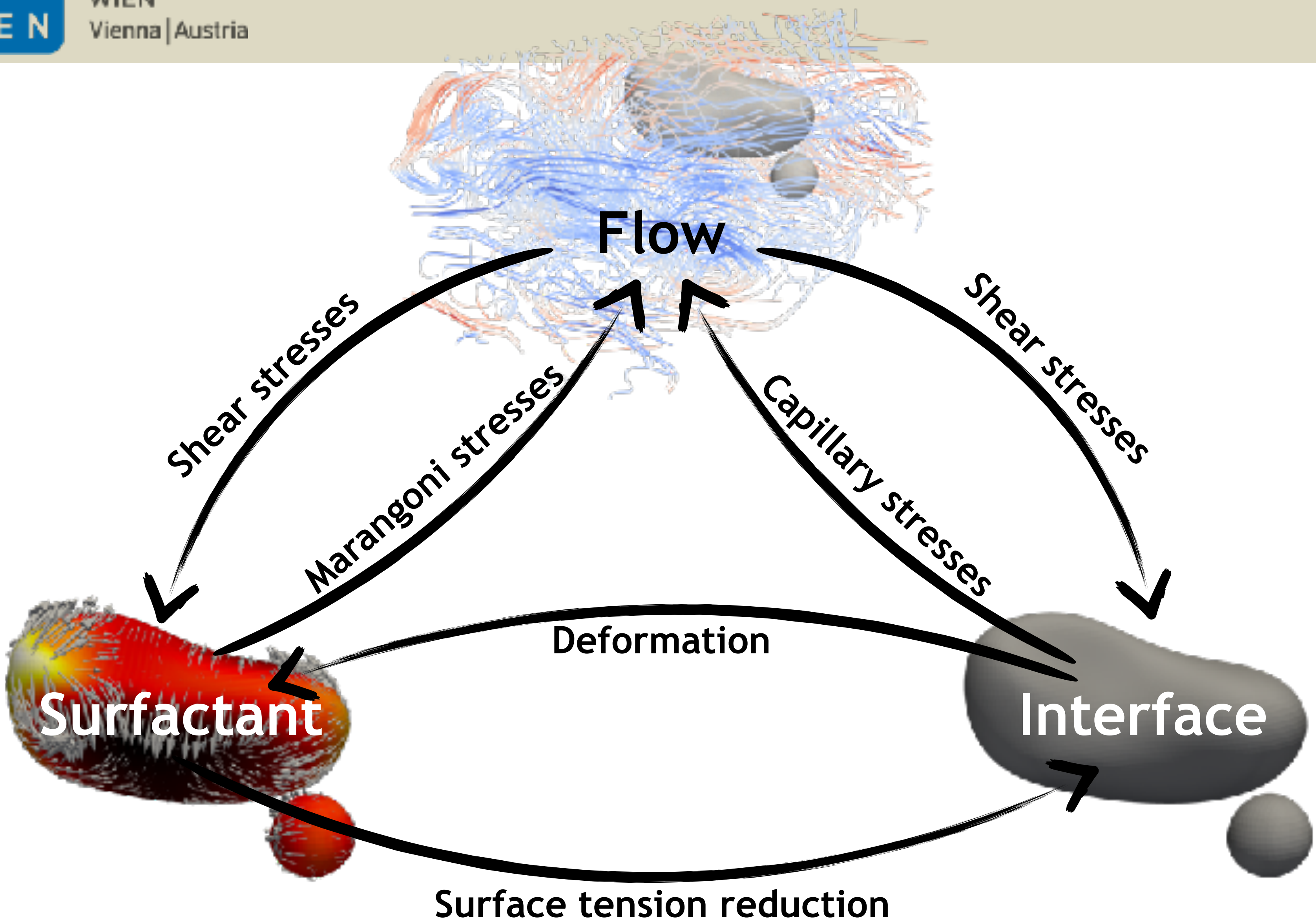
Surfactant-laden droplets in turbulent channel flow





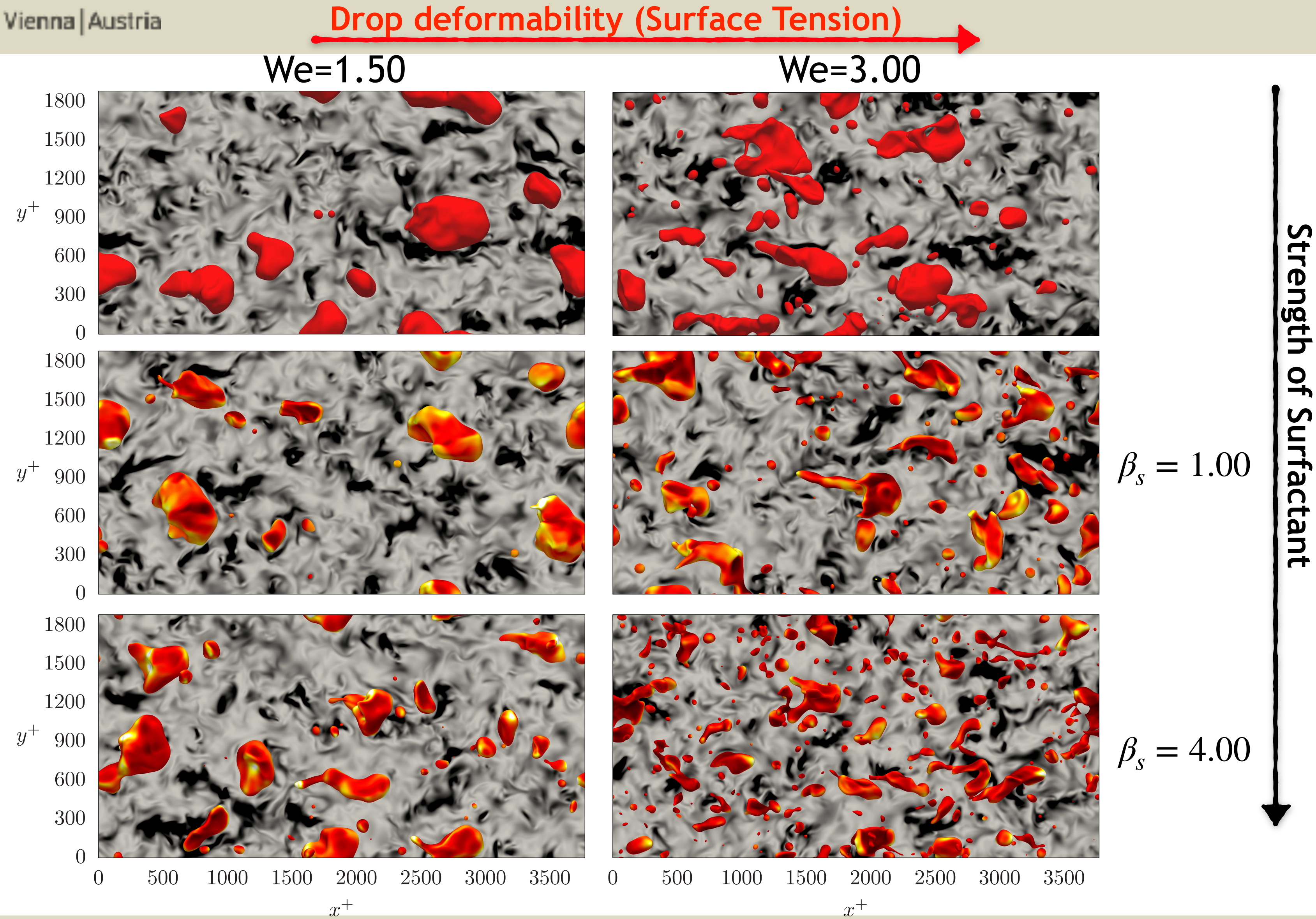
Effects of the surfactant:
- Dispersed phase morphology?
- Droplet size distribution?
- Surfactant distribution?
- Turbulence modifications?

Flow-Surfactant-Interface

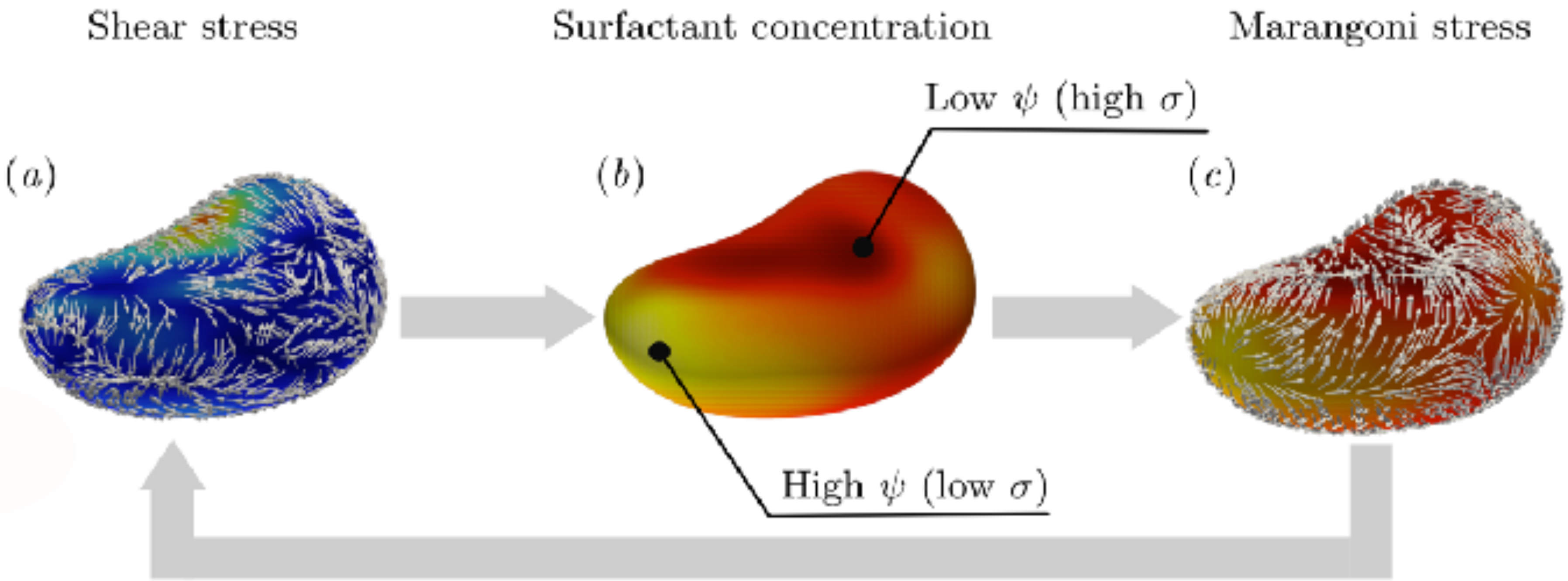


G. Soligo, A. Roccon, A. Soldati, Breakage, coalescence and size distribution of surfactant-laden droplets in turbulent flow, J. Fluid Mech. (2019)

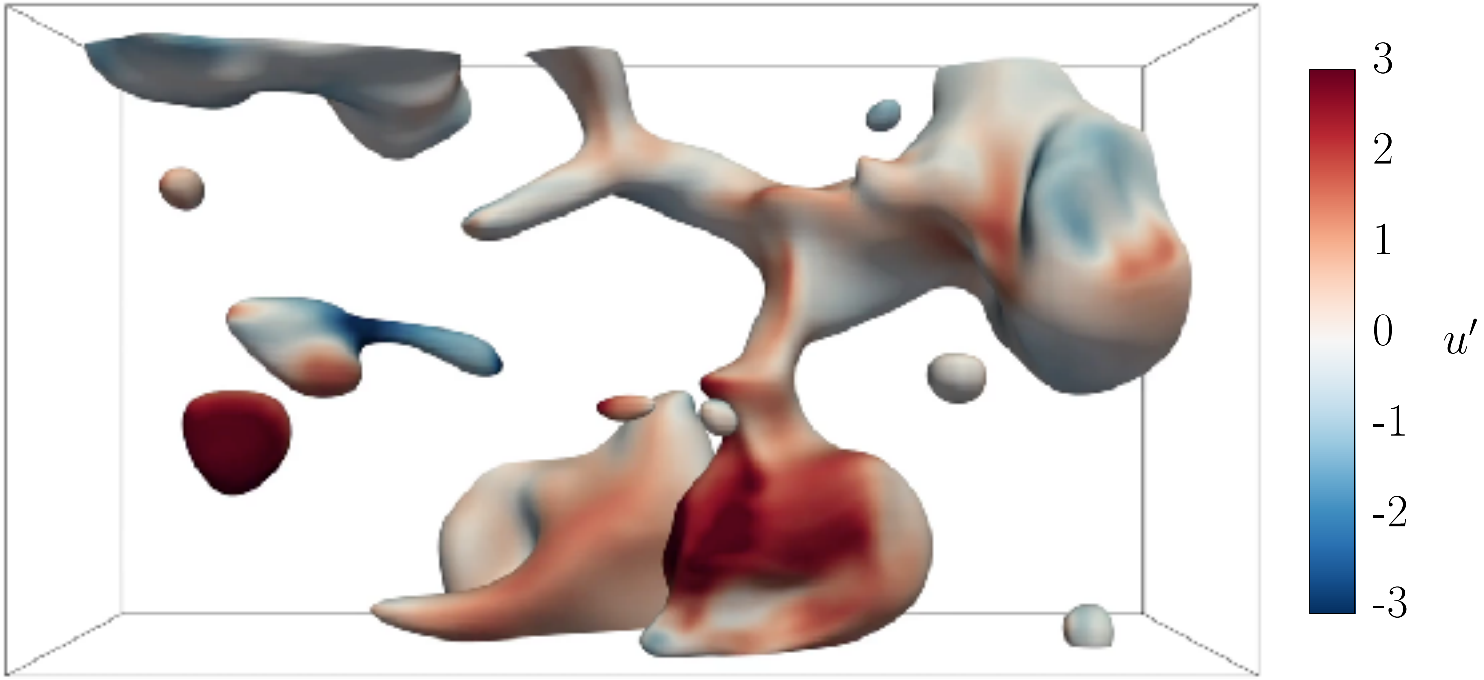
Qualitative view



Interface - Flow field Interactions



Coalescence and breakup rates



COALESCENCE

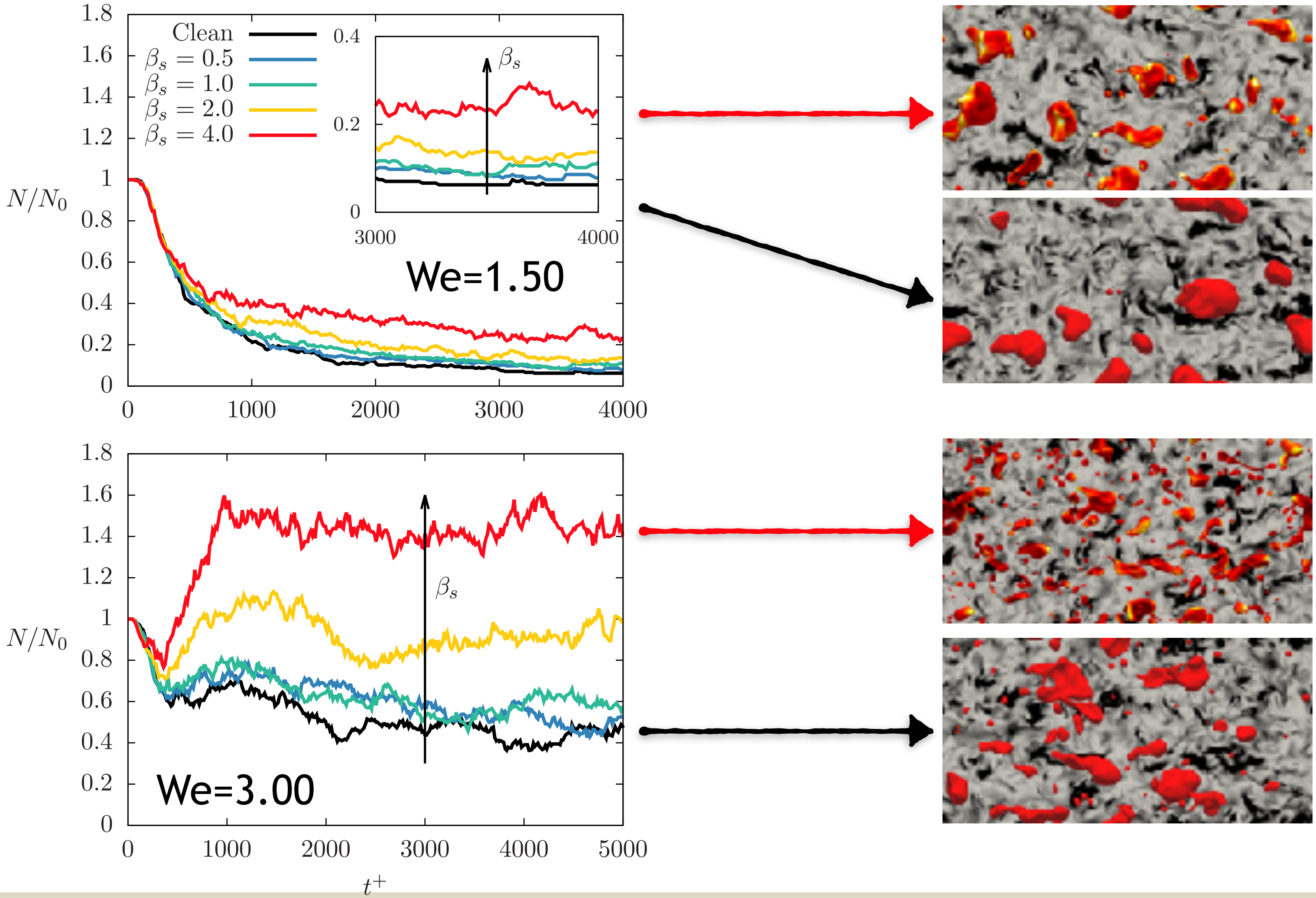
Turbulent fluctuations make two droplets collide. Upon collision, a small bridge can form between two droplets. Surface energy minimization tends to restore a spherical shape for the newly formed droplet.

BREAKUP

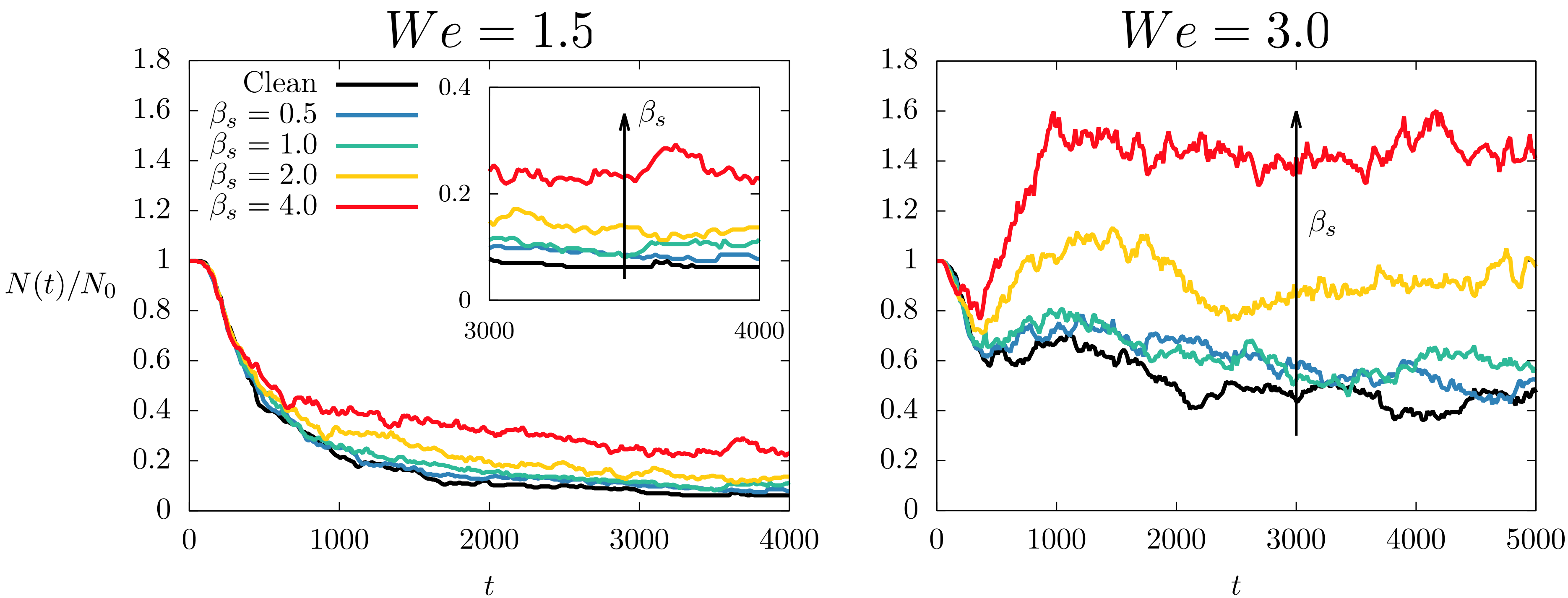
Shear stresses acting at the interface overcome surface tension force, leading to the formation and breakage of a thin liquid bridge. After the breakup surface tension restores the shape of the newly formed droplets.

Number of droplets

Number of droplets over time, initial number of droplets N_0=256



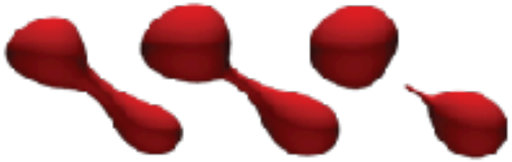
Number of droplets



	$We = 1.5$		$We = 3.0$	
$\beta_s = 0.0$	18.7		115.8	
$\beta_s = 1.0$	28.3	+51.1 %	147.8	+27.6 %
$\beta_s = 4.0$	63.3	+238.5 %	366.0	+216.1 %

Steady-state number of droplets

Coalescence/breakup rates



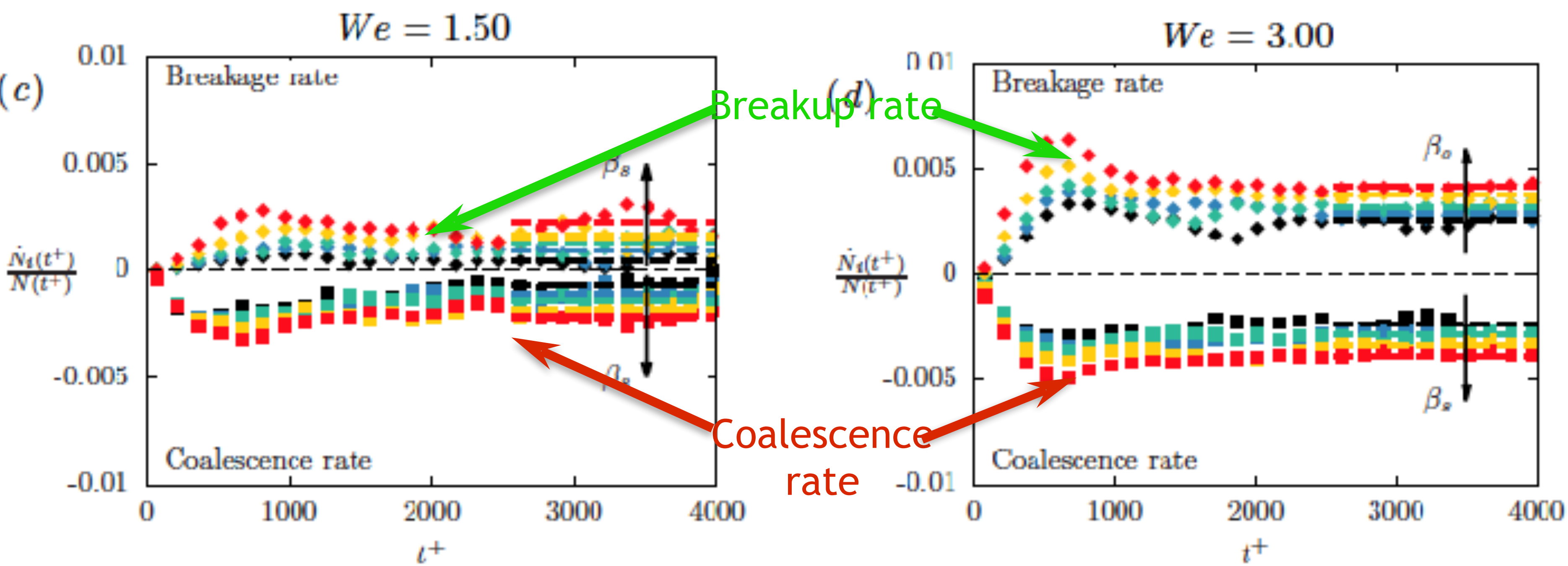
Breakup event

Breakup rate

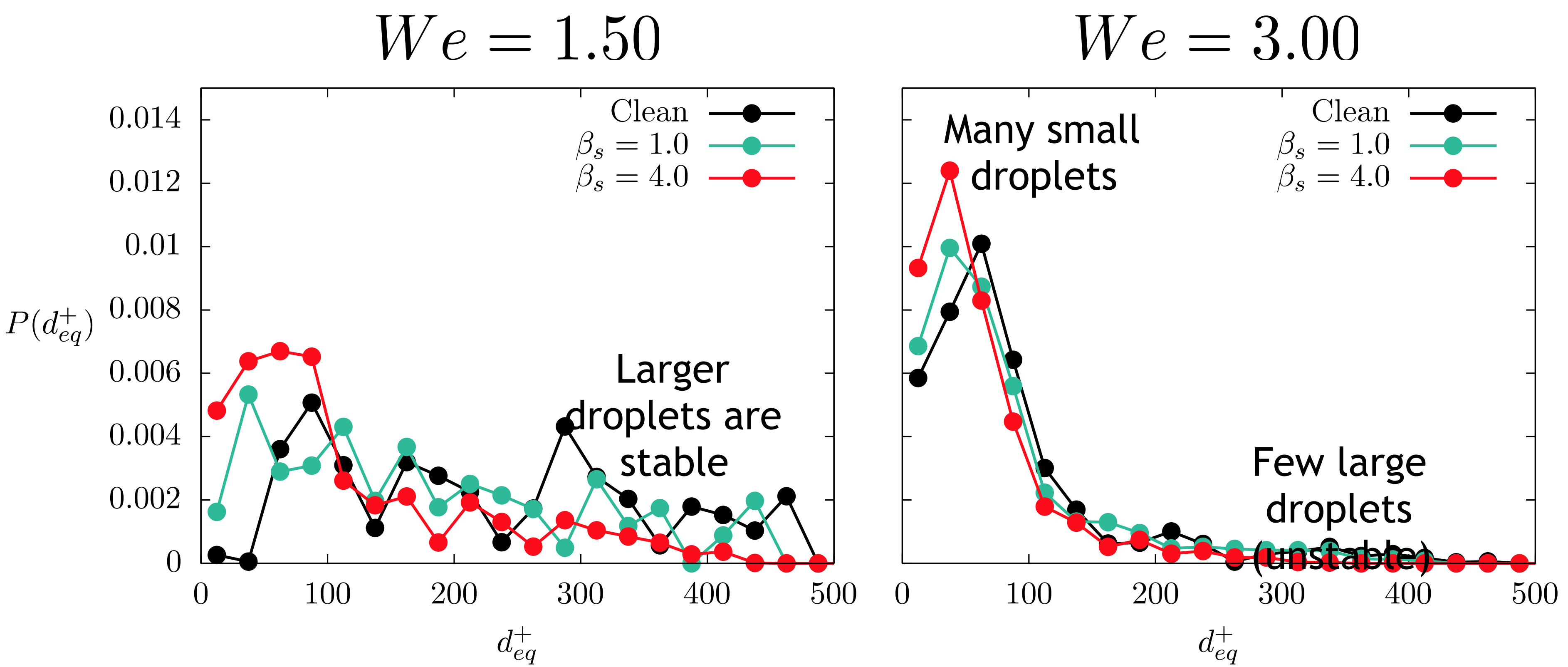
Coalescence rate

Coalescence event

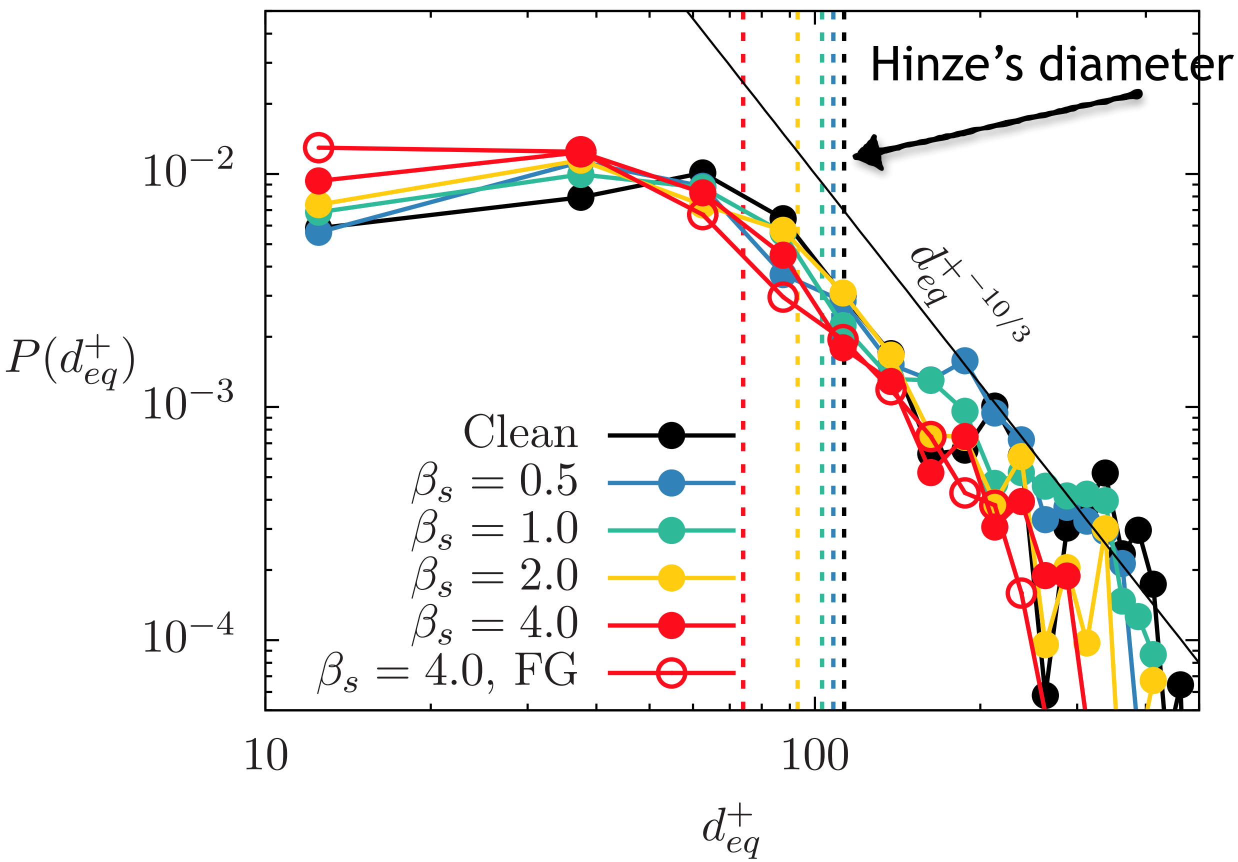
$$\frac{\partial N}{\partial t} = b(t) - c(t)$$



Droplet size distribution



Droplet size distribution
Comparison with literature



Garrett et al. (2000)

$$P(d^+_{eq}) \propto {d^+_{eq}}^{-10/3}$$

Experimental scaling valid for droplets larger than Hinze inviscid scale

Deike et al. (2016) report
A scaling of -1/3

$\beta_s = 4.0$, FG

$N_x \times N_y \times N_z = 2048 \times 1024 \times 1025$

[1] C. Garrett, M. Li & D. Farmer (2000) *J. Phys. Oceanogr.*

[1] Deike, Melville & S. Popinet (2016) *J. Fluid Mech.*

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