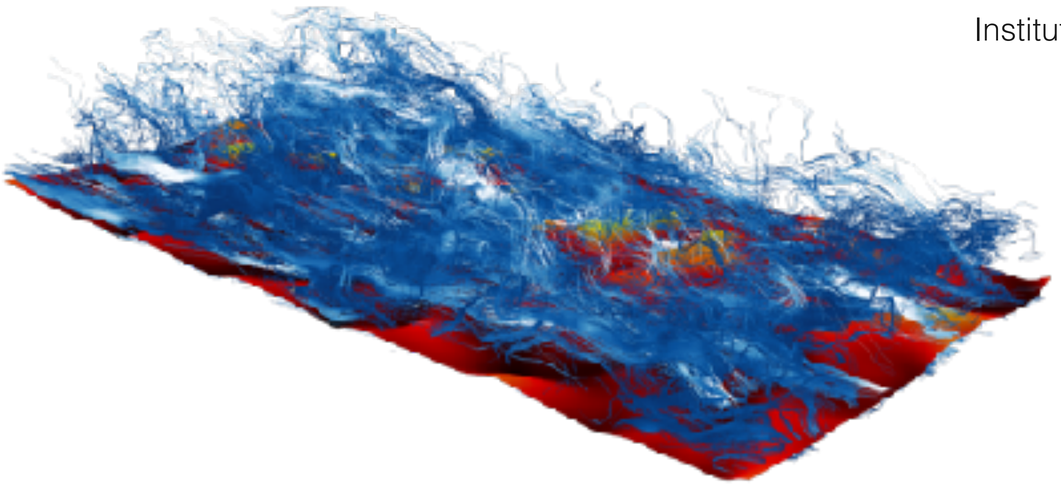
Modeling and Direct Numerical Simulation of Multiphase Flows

Francesco Zonta

Institute of Fluid Mechanics and Heat Transfer, TU Wien, Austria



XIV Workshop & Summer School "Multiphase Flows"

2-4.09.2021, Gdansk, Poland

Fil Rouge

1. Computational approaches to multiphase flows: a short introduction
2. The sharp interface approach: numerical modeling, boundary conditions, application (stratified air/water flow)
3. The Phase Field Method: recap on numerical modeling, application (oil transport in pipelines/channels)

Fil Rouge

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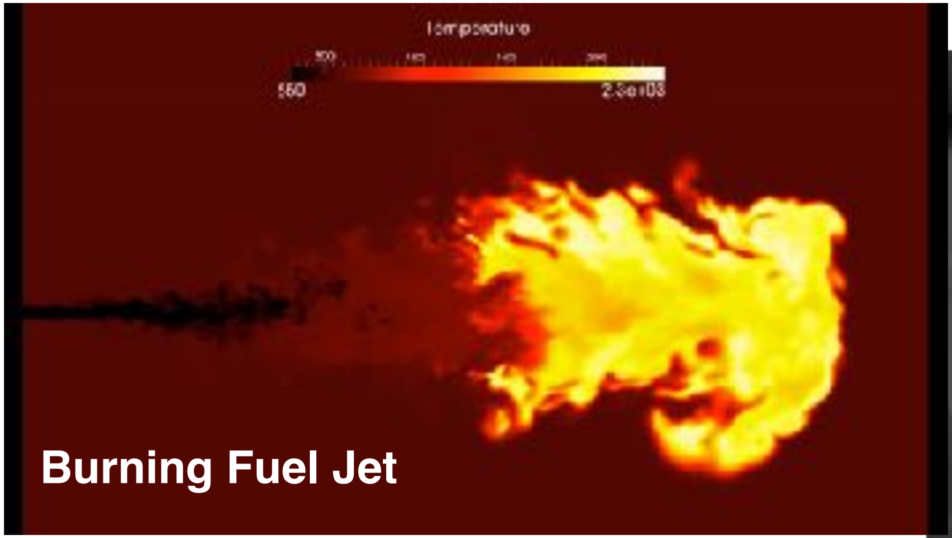
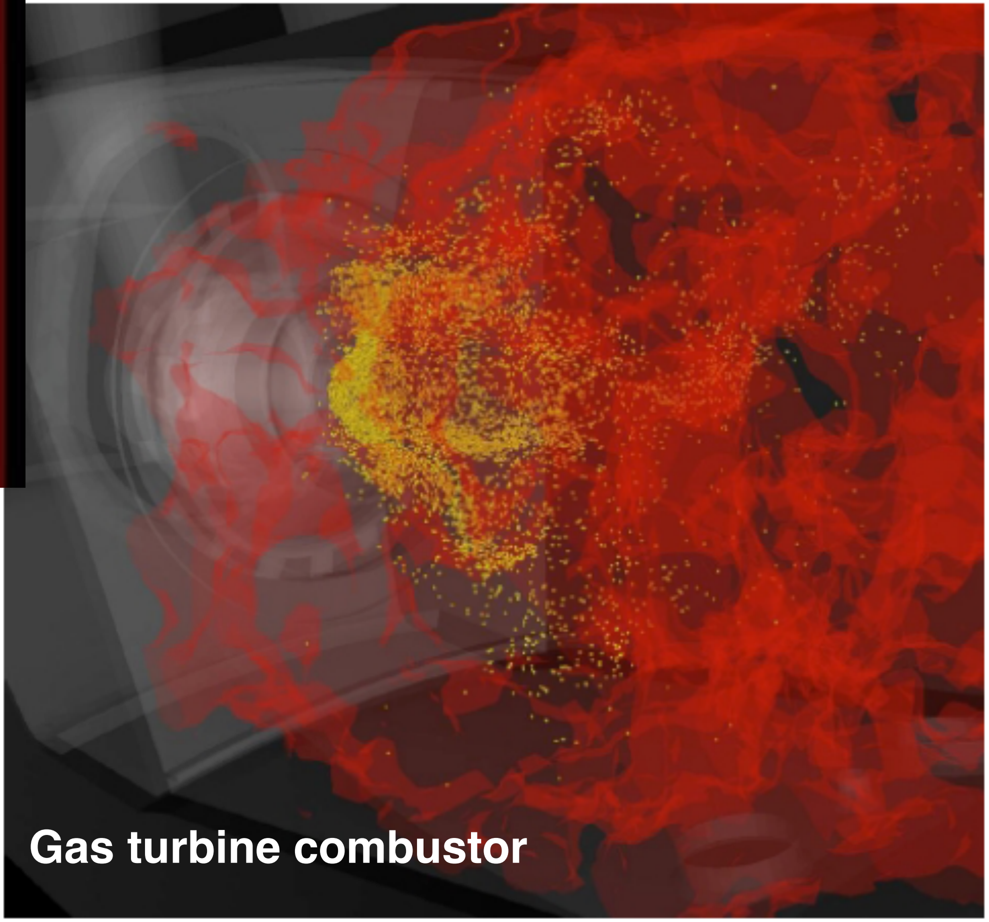
What is a multiphase flow? Just few examples…Industrial…





What is a multiphase flow? Just few examples…high seas…

But you might even have something smoother…

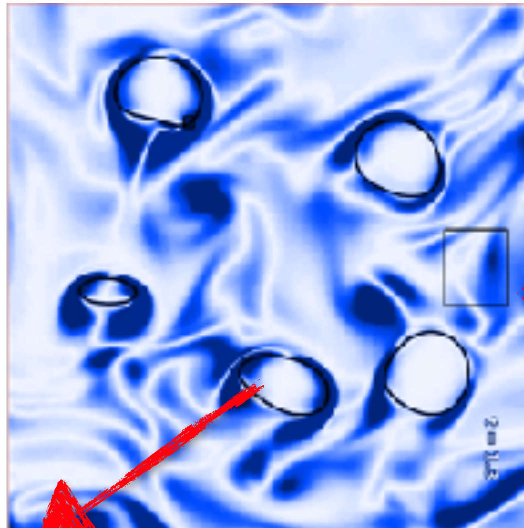
How to analyze such flows?

Interface ....?

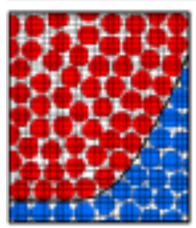
The idea of molecular orientation at an interface was conceived by Benjamin Franklin who, in 1765, spread olive oil on a water surface and estimated the thickness of the resulting film as one ten-millionth of an inch. Lord Rayleigh [8] in England and Miss Pockels [9] in Germany established that the film was only one molecule thick. Langmuir introduced novel experimental methods which resulted in new conceptions regarding these films.

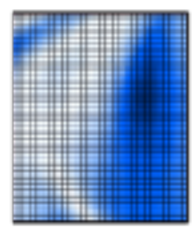
A. Pockels, *On the spreading of oil upon water*", Nature (1894)

The problem of computing interfaces: the grid resolution



Interface:
Scale ≃ 10^-9 m





Turbulence:
Largest Scale ≃ 1m
Smallest Scale ≃ 10^-3 m
<u>3 orders of magnitude.</u>
$N_P = 10^3 \times 10^3 \times 10^3 \simeq 10^9$
*for a 3D Cube ($Re_\lambda = 85$)

Interface $\mathcal{O}(10^{-9})$ — Kolmogorov scale $\mathcal{O}(10^{-3})$ — Large scales $\mathcal{O}(10^{0})$

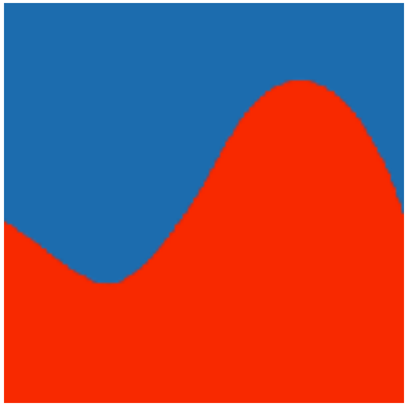
Length scale

Here? Here?

3-4 Orders of magnitude
In largest HPC centers!

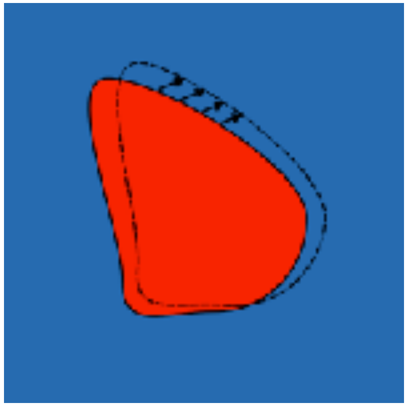
Flow Solution?

- Solving Navier-Stokes Eqs. in the whole domain?
- Solving Navier-Stokes Eqs. in separate domains?



Phase Tracking?

- Advection of a “color” function?
- Marker some points of the interface?

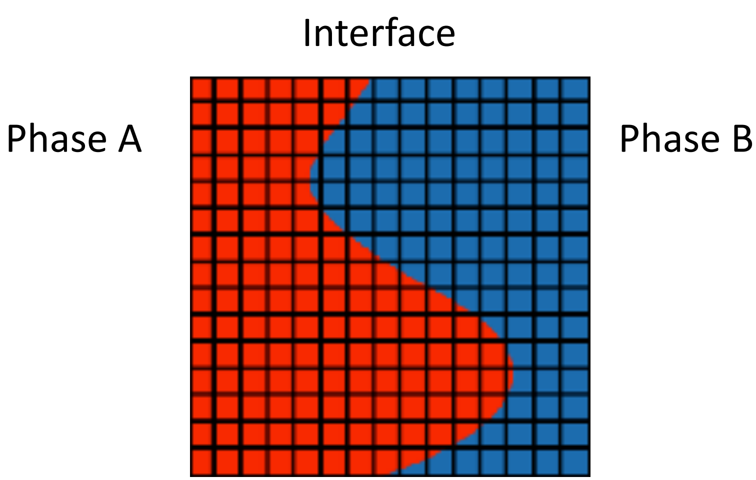


Flow Solution

Continuos approach

Solving NS equation in all the domain, interface is treated as the rest of the fluid domain.

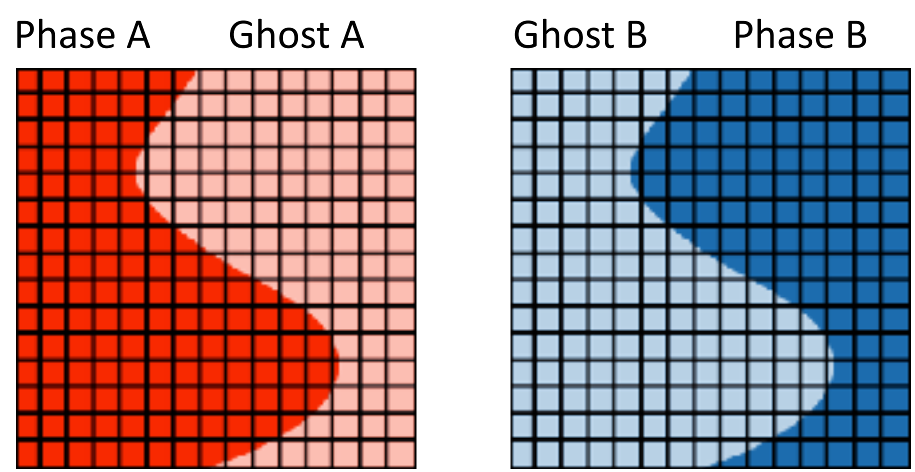
- Easy to implement, one-fluid approach.
- Surface tension forces undergo a "smoothing" operation.
- Velocity, density, viscosity profile are always smeared out.



Sharp approach

Treat the interface as a discontinuity.

- 1. Domain mapping.
- 2. *Ghost Fluid Method* (GFM), solving each phase in the whole domain (real and ghost) and accounts for interface jump conditions (velocity, pressure, density, viscosity). Not always a "real" sharp approach…
  Note: Sometimes, only few nodes of the ghost fluid required.



J. Brackbill et al, JCP, 1992
R. Scardovelli and S. Zaleski, ARFM, 1999
R. Fedwik, JSC, 1999
B. Lalanne et al, JCP, 2015

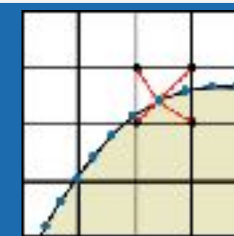
Phase Solution

Phase Tracking → Interface Tracking → Front Tracking (FT)

Phase Tracking → Interface capturing → Volume of Fluid (VOF), Level Set (LS), Phase Field Model (PFM)

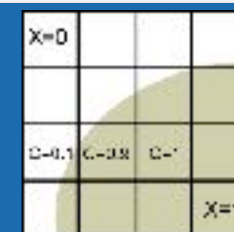
Front Tracking (FT)

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{u}_i$$



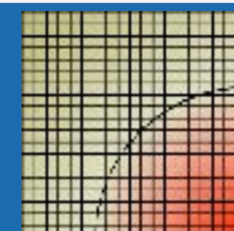
Volume of Fluid (VOF)

$$\frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C = 0$$



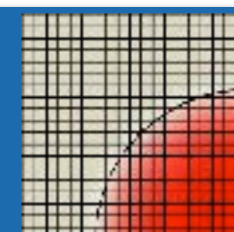
Level Set (LS)

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0$$



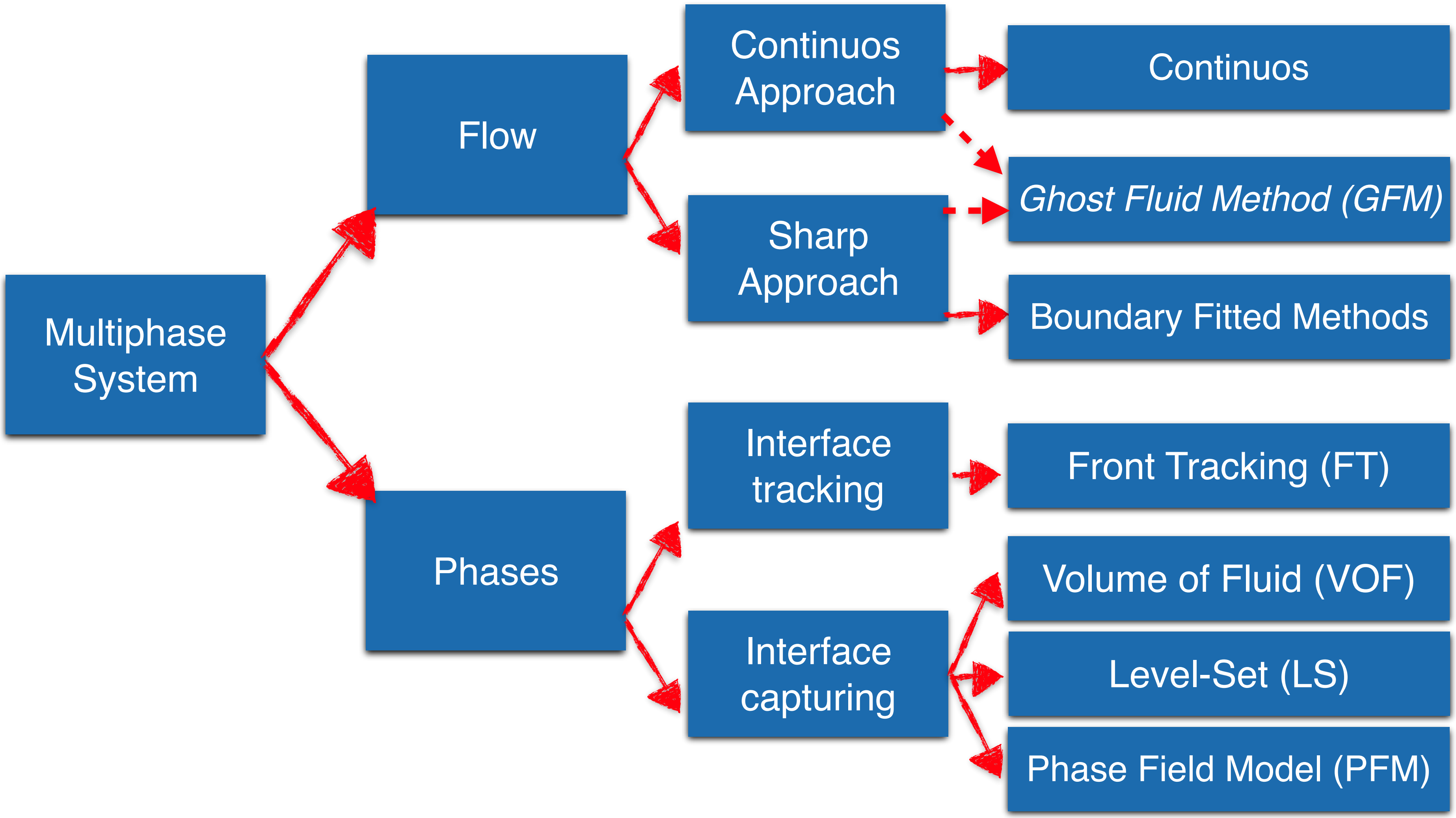
Phase Field Model (PFM)

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \nabla \cdot (M(\phi) \nabla \mu)$$



S.O. Unverdi and G. Tryggvason, *A Front-Tracking Method for Viscous, Incompressible, Multi-fluid Flows*, JCP, 1991
C.W. Hirt and B.D. Nichols, *Volume of fluid (VOF) method for the dynamics of free boundaries*, JCP, 1981
M. Sussmann et al, *A level set approach for computing solutions to incompressible 2 Phase flow*, JCP, 1994
D. Jaqmin, *Calculation of Two-Phase Navier–Stokes Flows Using Phase-Field Modeling*, JCP, 1999

Flow and Phase Solution (recap)



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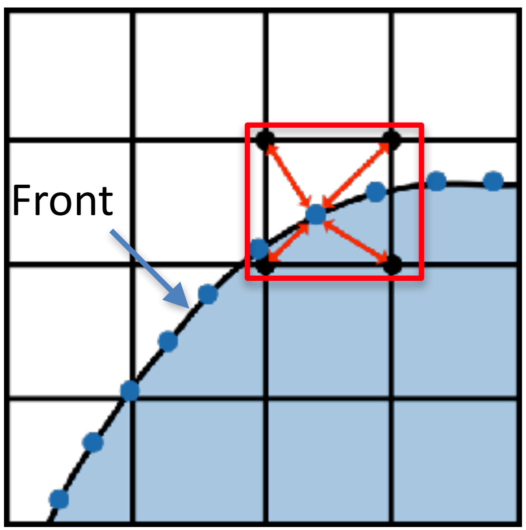
Front Tracking (FT)

Marker on the interface:

Tracking using a Lagrangian approach:

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{u}_i$$



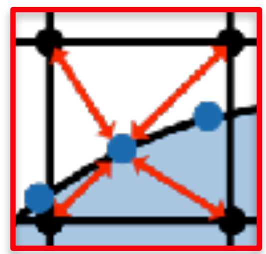
Interface is formed by segments (2D) or Elements (3D)

S.O. Unverdi and G. Tryggvason, *A Front-Tracking Method for Viscous, Incompressible, Multi-fluid Flows*, JCP, 1991; G. Trygvasson et al, *A Front-Tracking Method for the Computations of Multiphase Flow*, JCP 2001; A. Prosperetti and G.Tryggvason, *Computational Methods for Multiphase Flow*, Cambridge, 2009

Flow is solved on the Eulerian Grid.

↔ Communications Markers-Eulerian Grid

- Surface tension force:



Smoothing operation:
"Diffuse" the surface tension on the neighbor nodes of the eulerian grid.

- Velocity of the markers:

Interpolation from eulerian grid.

- Coalescence & Breakage of interface?

Interface reconnection needs some special model/treatment.

- Number of Markers:

Need to increase or decrease the number of markers if the interface stretches or compresses.

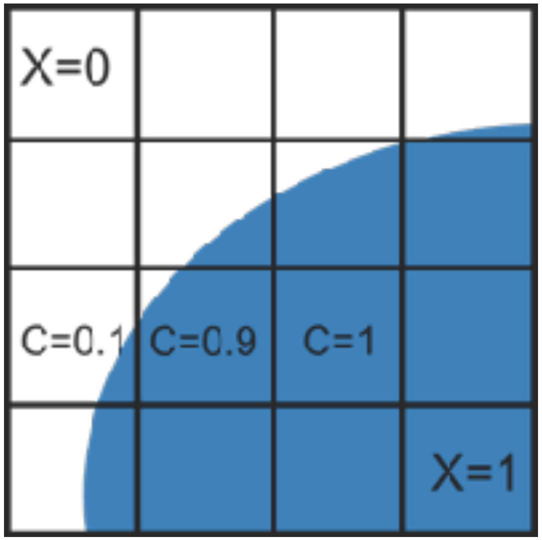
Volume of Fluid (VOF)

Definition of a Marker or Color function X:

- X=0 Phase A
- X=1 Phase B

Mean value on the cell volume

$$C = \frac{1}{V}\int_V \chi(x,y,z)dV$$



- C=0 Phase A
- 0<C<1 Interface
- C=1 Phase B

R. Scardovelli and S. Zaleski, *Direct numerical simulation of free surface and interfacial flow*, Ann. Rev. Fluid, 1999
A. Prosperetti and G. Tryggvason, *Computational Methods for Multiphase Flow*, Cambridge, 2009
C.W. Hirt and B.D. Nichols, *Volume of fluid (VOF) method for the dynamics of free boundaries*, JCP, 1981

Advection of the phase

$$\frac{\partial C}{\partial t} + \mathbf{u}\cdot\nabla C = 0$$

- Need of a specific advection scheme and to reconstruct the interface from a mean cell-value.

- Coalescence & Breakage of interface?

Automatically accounted

- Grid:

Use of Eulerian Grid for fluid and phase.

Level-set (LS)

Defining a marker function ϕ

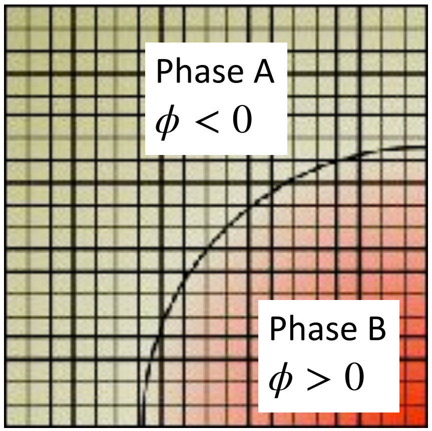
ϕ

$$\phi = -d \quad \text{Phase A}$$

$$\phi = 0 \quad \text{Interface}$$

$$\phi = +d \quad \text{Phase B}$$

(d, distance from the interface)



M. Sussmann et al, *A level set approach for computing solutions to incompressible two-phase flow*, JCP, 1994
S. Osher and A. Sethian, F. *propagating with curvature-dependent speed: Algorithms based on Hamilton-Jacobi formulations*, JCP, 1988
S. Osher and R. Fedwik, *Level Set Methods and Dynamic Implicit Surfaces*, Springer, 2003
J.A. Sethian, *Level Set Methods and fast marching methods*, Cambridge, 1996

Level-set function is advected by the equation:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0$$

Difficult to preserve as a distance function, need to reinizialitaze.

$$\frac{\partial \phi}{\partial \tau} = sign(\phi_0)(1 - |\nabla \phi|)$$

- Coalescence & Breakage of interface?

Topological change are automatically accounted, no closure models needed.

- Surface tension force?

Very accurate computation of curvature, force is "diffused" in 3 or more cells typically.

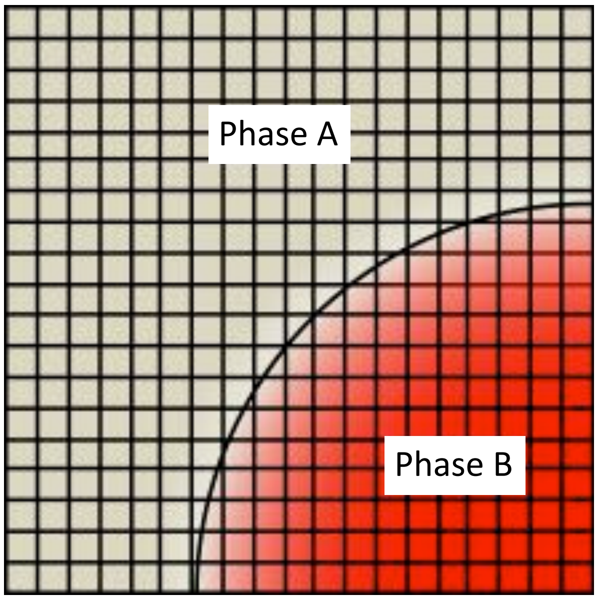
- Grid:

Use of Eulerian Grid for fluid and phase.

Phase Field Method (PFM)

Define a concentration ϕ :

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



Cahn-Hilliard equation (diffusion)

$$\frac{\partial \phi}{\partial t} = -\nabla \cdot J_\phi, \text{ with } J_\phi = -\mathscr{M}\nabla \mu_\phi \quad [\mathscr{M} \text{ mobility}]$$

(μ_ϕ is chemical potential)

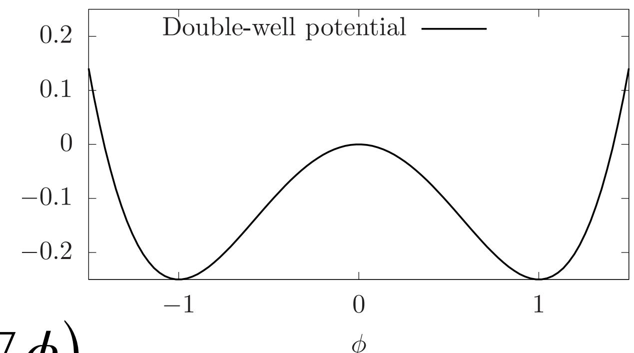
To find μ_ϕ, Ginzburg-Landau energy functional (immiscible fluids):

Double-well potential + controlled mixing (interface)

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

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

$$f_{int} = \frac{Ch^2}{2}|\nabla\phi|^2$$



Therefore: $\mu_\phi = \dfrac{\delta F\left(\phi, \nabla\phi\right)}{\delta\phi} = \phi^3 - \phi - Ch^2\nabla^2\phi$

(Ch = we will see it later...)

J.W. Cahn and J.E. Hilliard, *Free energy of a non-uniform system I, Interfacial free energy*, JCP, 1958

Phase Field Method (PFM)

Recalling the expression of the chemical potential: $\mu_\phi = \phi^3 - \phi - Ch^2 \nabla^2 \phi$

System at rest: $\mu_\phi = 0 \rightarrow \phi = \tanh\left(\frac{x}{\sqrt{2}Ch}\right)$

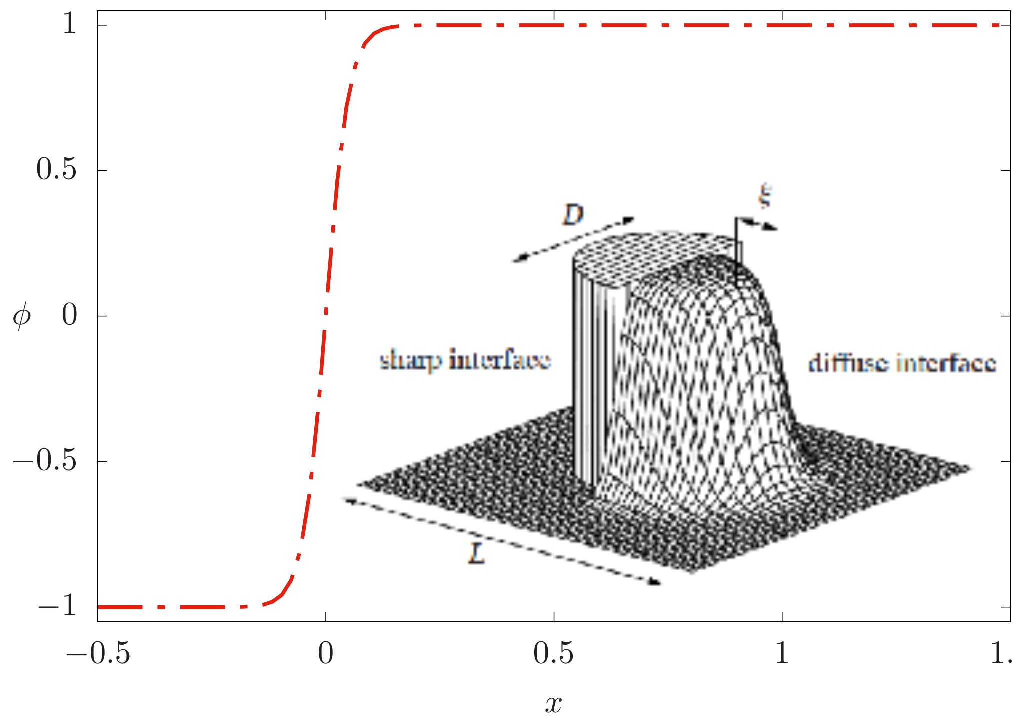
Ch = Dimensionless thickness of interface

For a real multiphase system, Cahn and Peclet are of the order of:

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

Impossible to perform simulations, we enlarge the interface so that simulations are possible:

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



D. Jaqmin, *Calculation of Two-Phase Navier–Stokes Flows Using Phase-Field Modeling*, JCP, 1999

Phase Field Method (PFM)

When convection is also present:

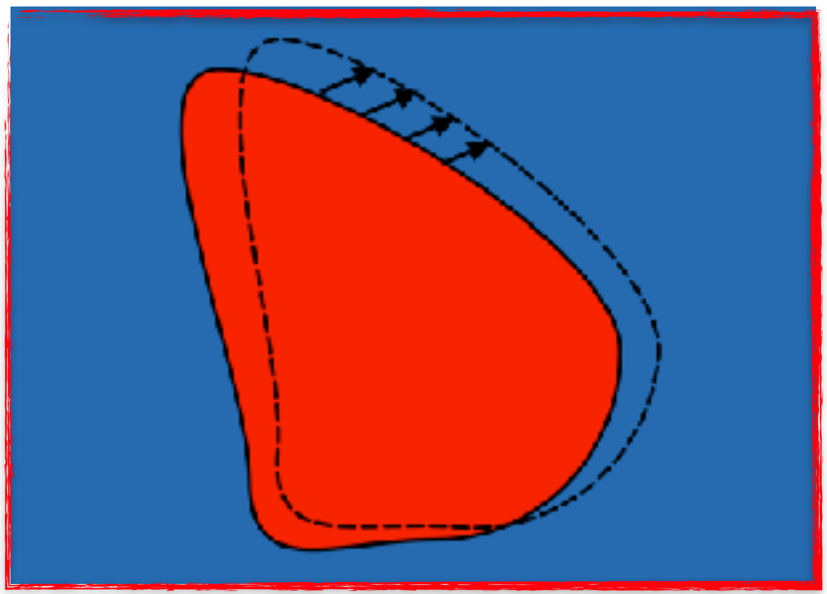
$$\frac{\partial \phi}{\partial t} + \underbrace{\mathbf{u} \cdot \nabla \phi}_{\text{Interface Advection}} = \underbrace{\frac{1}{Pe} \nabla^2 \mu}_{\text{Controlled Mixing}}$$

Note:

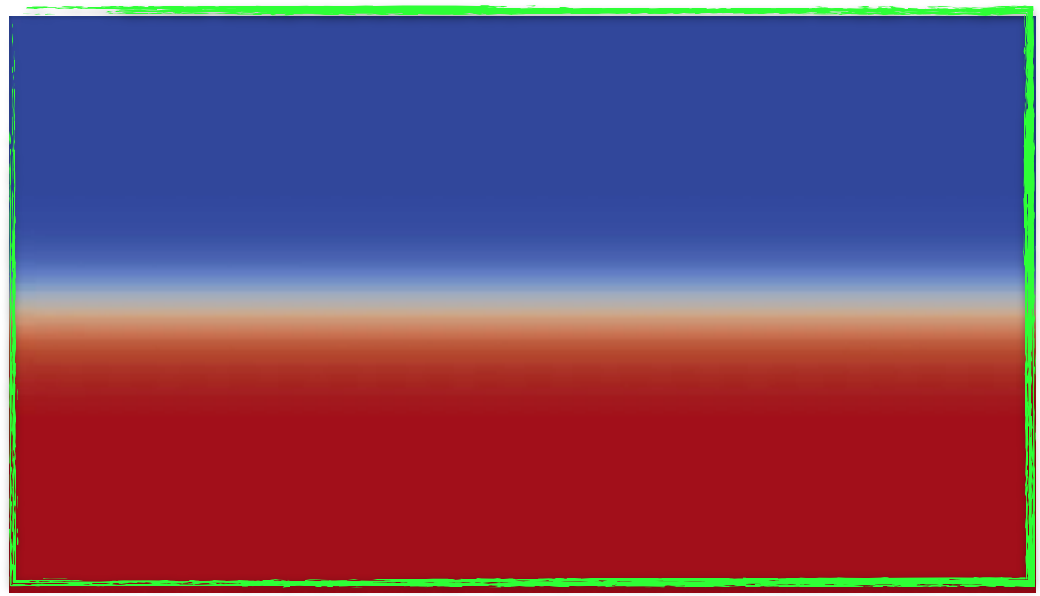
Level Set, advection modify the profile, profile must be reinitialise.

Phase Field Method, Chemical potential is able to restore and keep the profile during the computation.

Advection from the flow field **u**

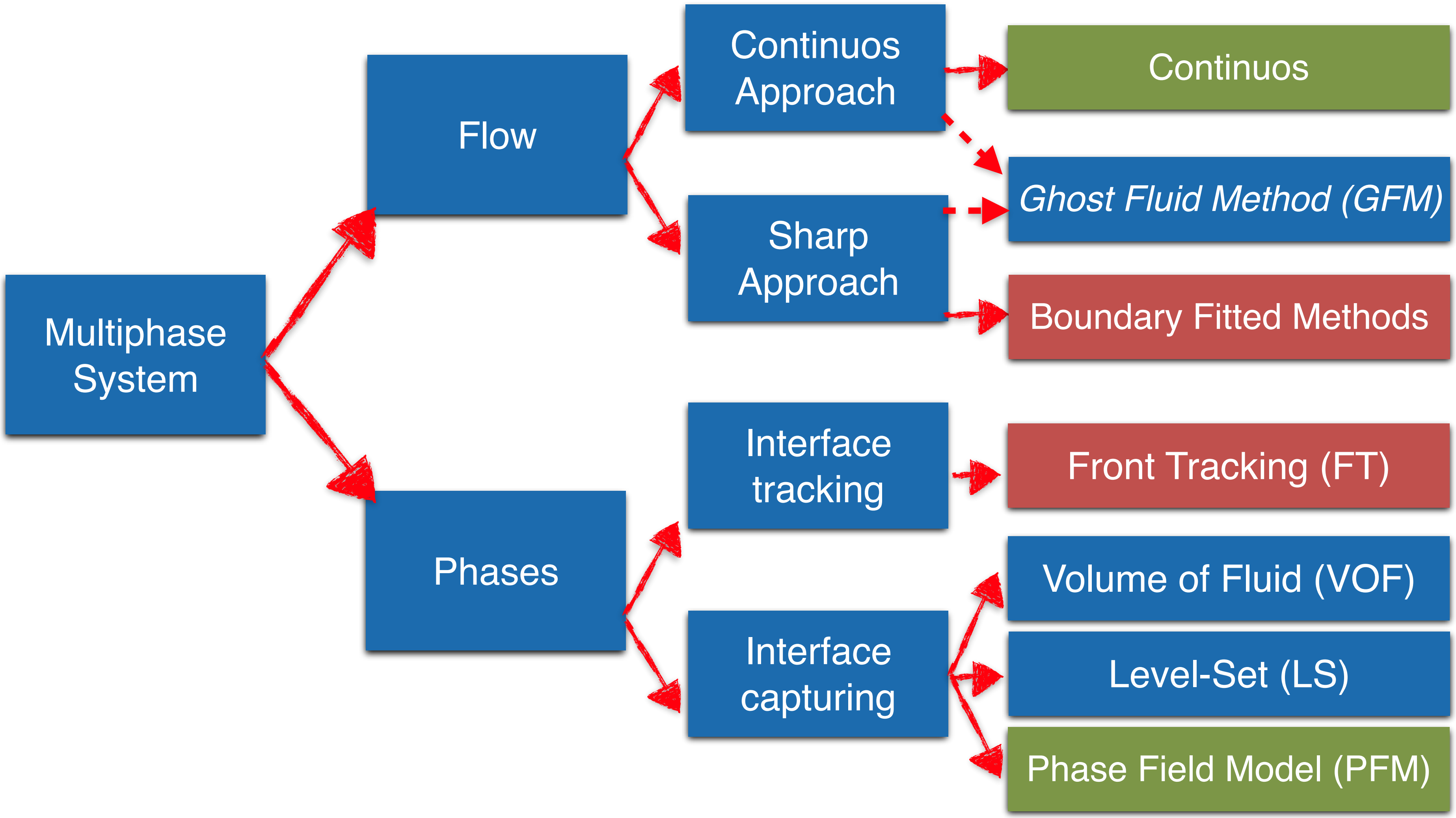


Restoring the interfacial equilibrium profile.



D. Jaqmin, *Calculation of Two-Phase Navier–Stokes Flows Using Phase-Field Modeling*, JCP, 1999

Focus of present lectures



Fil Rouge

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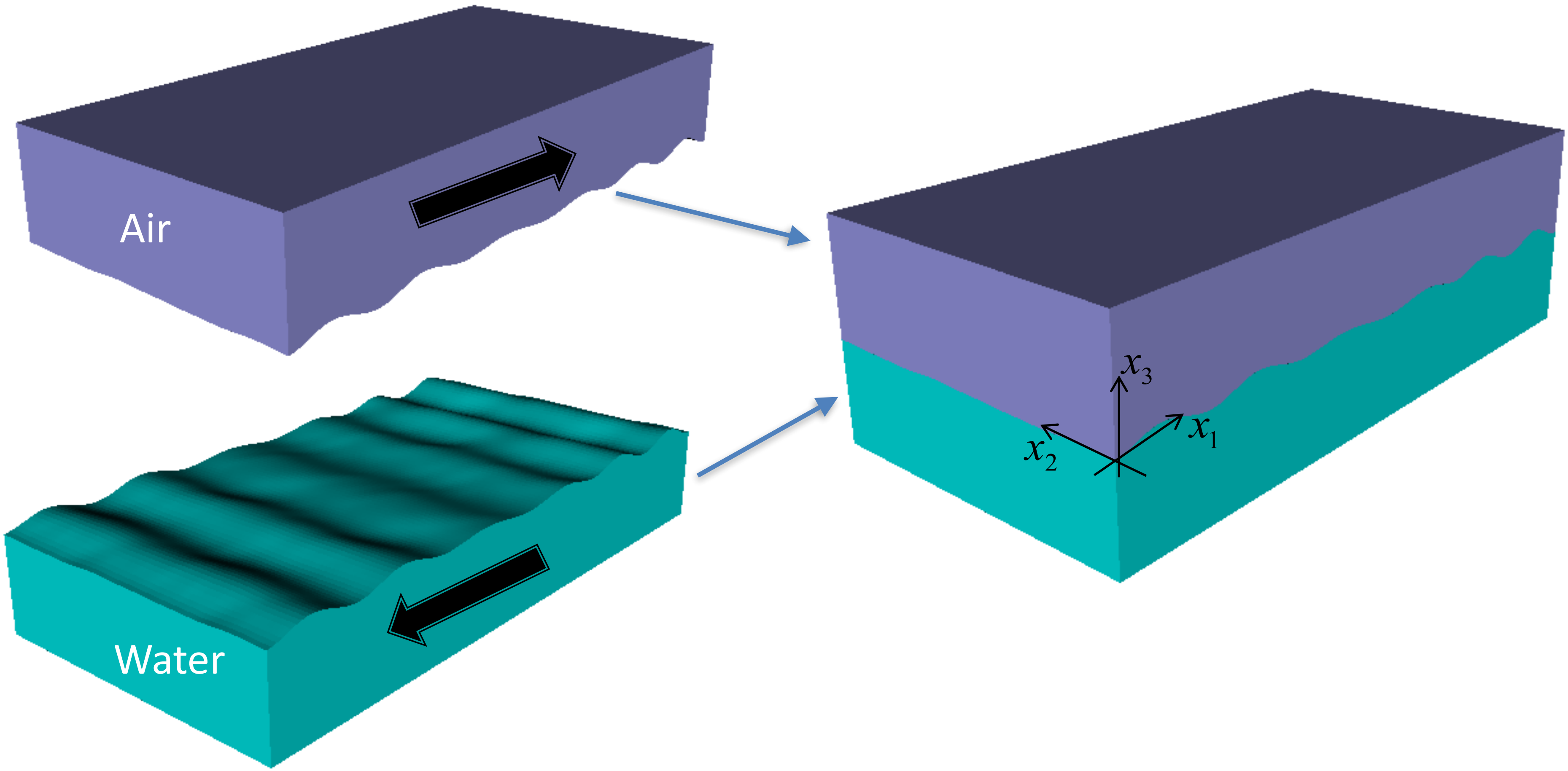
3. The Phase Field Method: recap on numerical modeling, application (oil transport in pipelines/channels)

Boundary fitted Method: Physical configuration

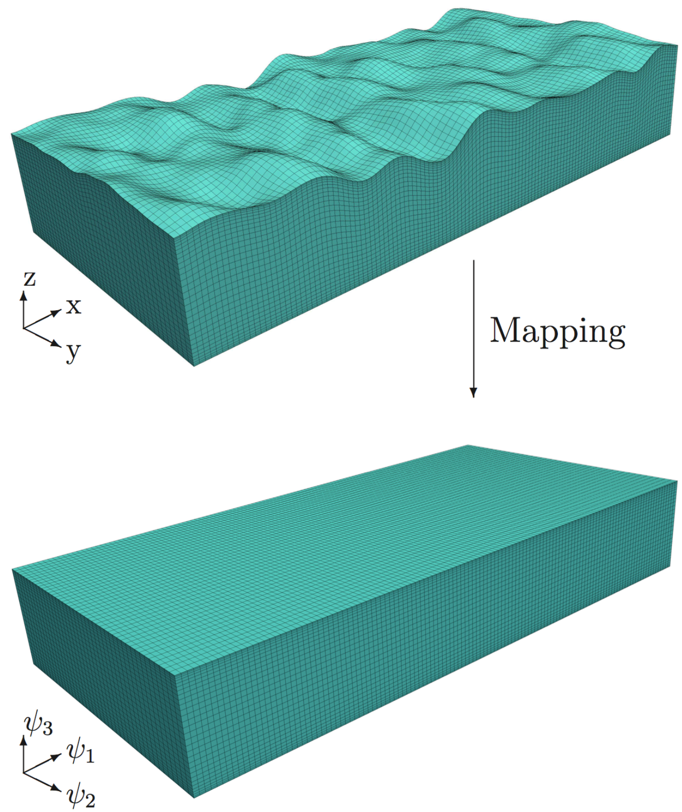


Boundary fitted Method: Equations and numerical modeling

Governing equations-Physical domain

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

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{Re} \nabla^2 \mathbf{u}$$



Algebraic mapping

$$\psi_1 = x \,, \quad \psi_2 = y \,, \quad \psi_3 = \frac{z}{h + \eta(x, y, t)} \,, \quad \tau = t$$

Interface “deformation”

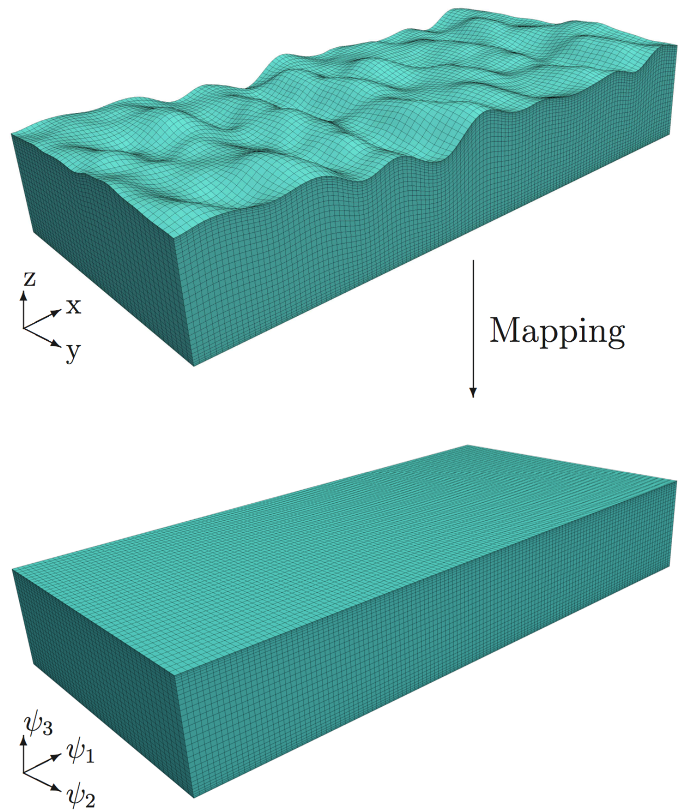
Reference height of the domain

Boundary fitted Method: Equations and numerical modeling

Governing equations-Physical domain

$$J = \frac{\partial \psi}{\partial X}$$

$$\partial_x = J \cdot \partial_\psi$$



$$\partial_X = \left(\partial/\partial x, \partial/\partial y, \partial/\partial z\right)^T$$

$$\partial_\psi = \left(\partial/\partial \psi_1, \partial/\partial \psi_2, \partial/\partial \psi_3\right)^T$$

Fractional step technique

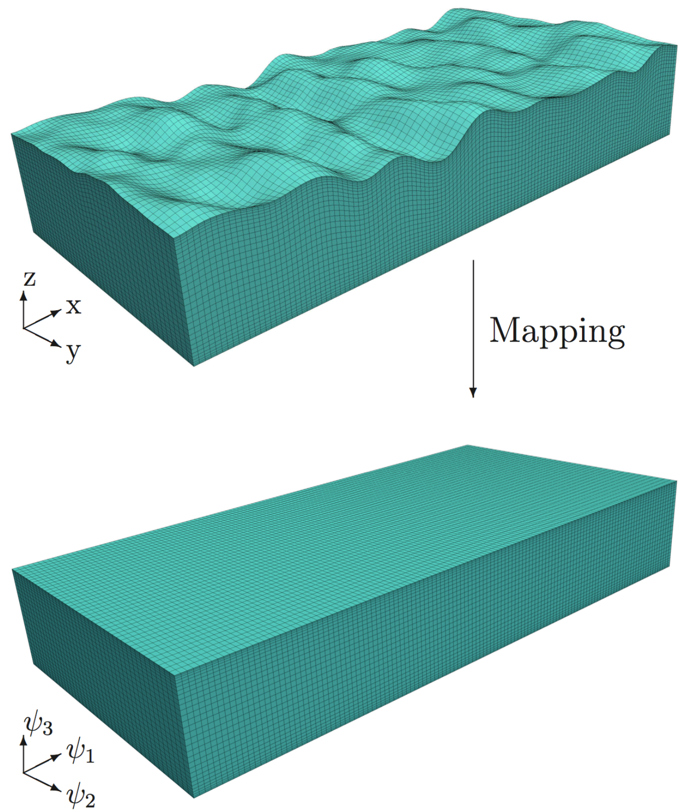
Momentum equation (no pressure)

Provisional time step

$$\frac{\tilde{\mathbf{u}} - \mathbf{u}^n}{\Delta t} + \sum_{q=0}^{M-1} \alpha_q \nabla \cdot (\mathbf{u}\mathbf{u})^{n-q} - \frac{1}{2Re_\tau} \nabla^2 \left(\tilde{\mathbf{u}} + \mathbf{u}^n\right) = 0,$$

Convective terms AB explicit: $M = 2, \alpha_0 = 3/2, \alpha_1 = -1/2;$

Diffusive terms CN implicit



Correction to obtain a divergence-free field

$$\frac{\mathbf{u}^{n+1} - \tilde{\mathbf{u}}}{\Delta t} + \nabla p^{n+1} = 0,$$

Taking divergence and assuming div-free field (@n+1)

$$\nabla^2 p^{n+1} = \frac{\nabla \cdot \tilde{u}}{\Delta t}$$

Obtain u^{n+1}, then p^{n+1}

Numerical Implementation: Spectral & pseudo-spectral methods

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

For spectral methods: global functions are defined in each node and are not zero

This brings some advantages for the representation of the derivatives

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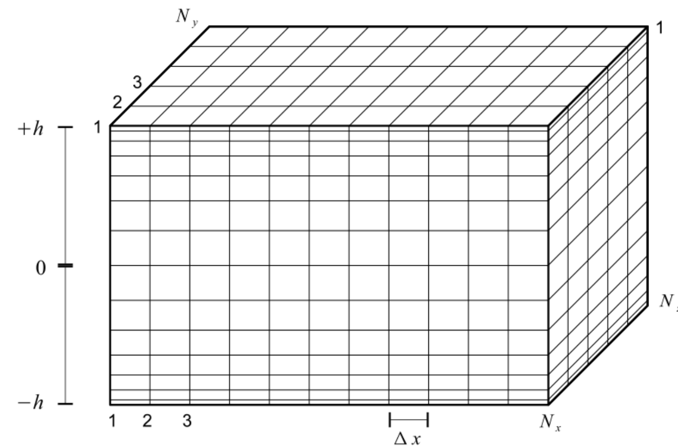
Numerical Implementation: Spectral & pseudo-spectral methods

Discrete geometry

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

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

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



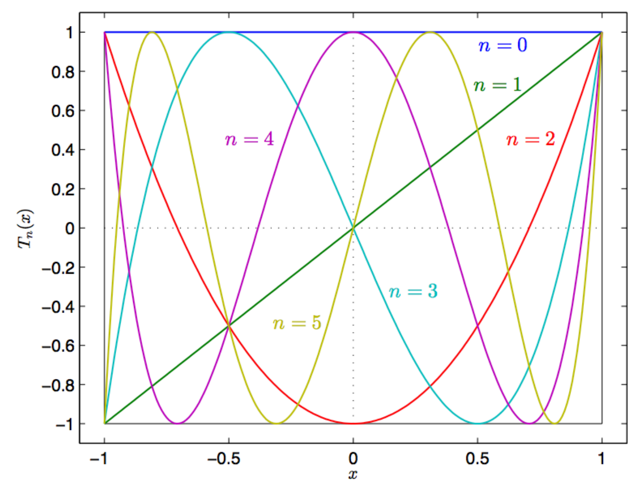
Spatial discretization of the solution (Fourier+Chebyshev)

Remember: approximate a function as the linear combination of test functions (which in this case are global)

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

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

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

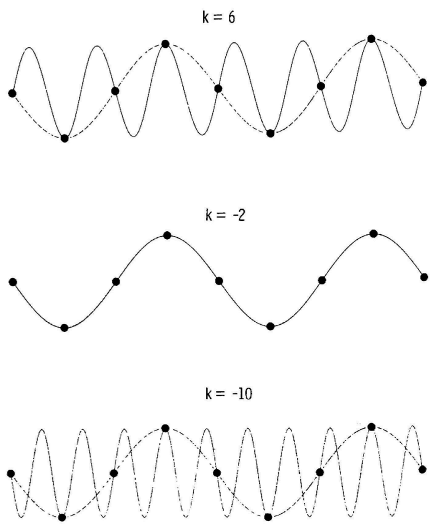


Numerical Implementation: Spectral & pseudo-spectral methods

Why pseudo-spectral?

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{Re} \nabla^2 \mathbf{u}$$

- Performing products in modal space, $\mathcal{O}\left(N^2\right)$
- Transform into physical, multiply, back to modal, $\mathcal{O}\left(N \log_2 N\right)$
- 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

Boundary conditions

Interface

Kinematic B.C.

$$\frac{\partial \eta}{\partial t} + u_x \frac{\partial \eta}{\partial x} + u_y \frac{\partial \eta}{\partial y} = u_z$$

Dynamic B.C. (B.C on stress and velocity)

$$@z = 0$$

$$\frac{1}{Re\tau}\left(\left(\tau_{\mathbf{L}} - \tau_{\mathbf{G}}\right) \cdot \mathbf{n}\right) \cdot \mathbf{n} + p_G - p_L + \frac{1}{We}\nabla \cdot \mathbf{n} - \frac{1}{Fr}\eta = 0$$

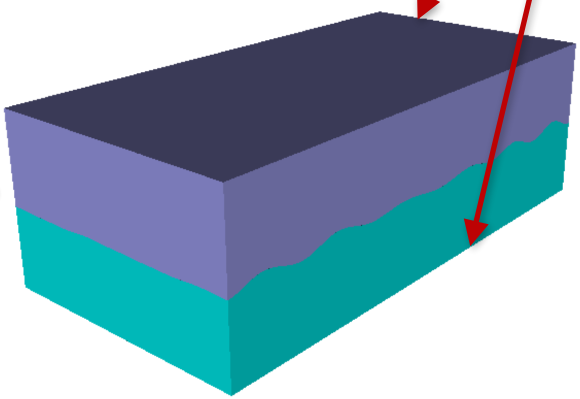
$$((\tau_L - \tau_G) \cdot \mathbf{n}) \cdot \mathbf{t}_i = 0 \ , \quad i = x, y$$

$$\mathbf{u}_G = \frac{1}{\mathscr{R}}\mathbf{u}_L; \ \mathscr{R} = \sqrt{\rho_L / \rho_G}$$

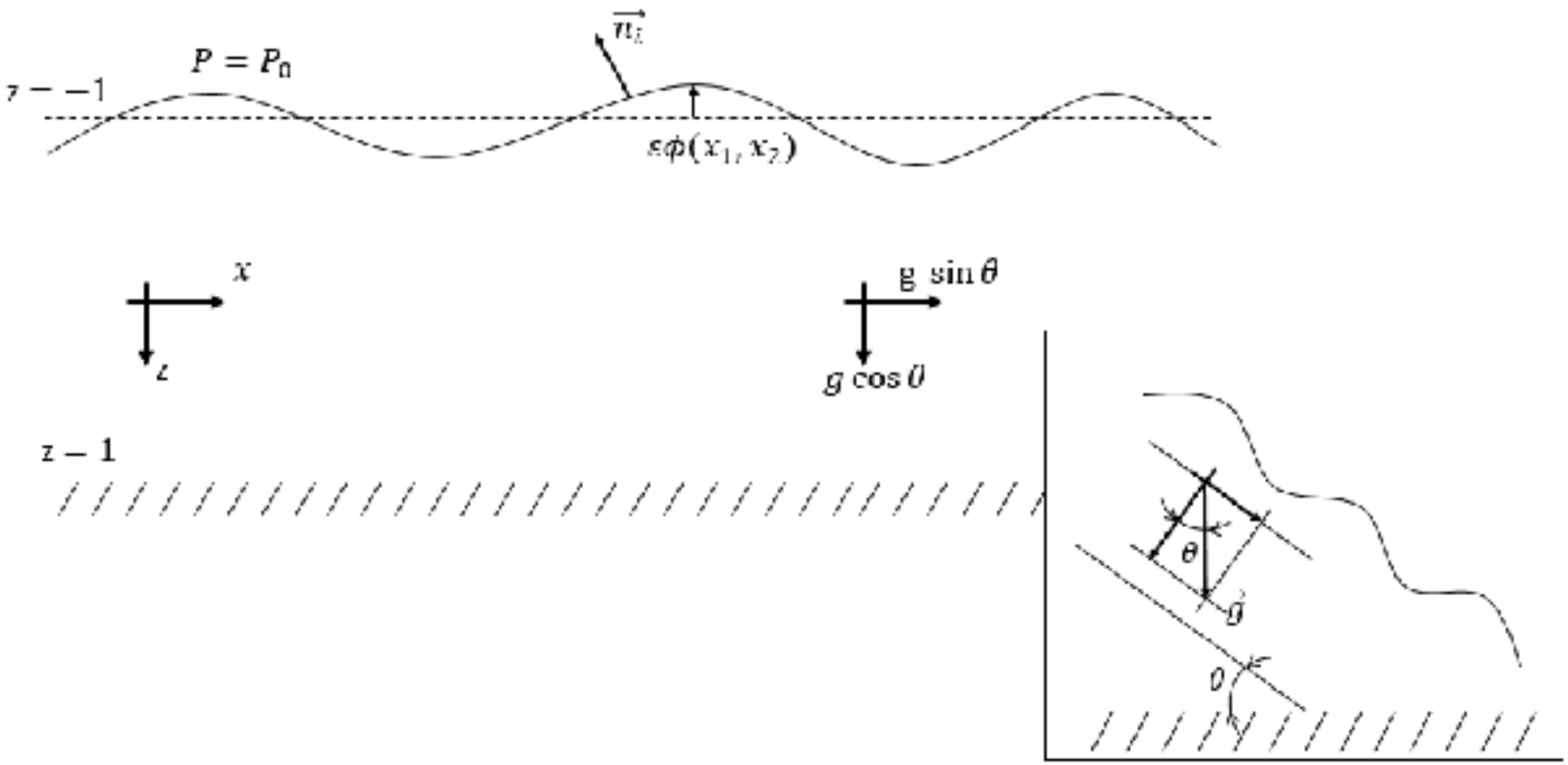
Outer boundaries (Free-slip B.C.)

$$@z = \pm h$$

$$\frac{\partial u_{x,y}}{\partial z} = \frac{\partial p}{\partial z} = u_z = 0$$



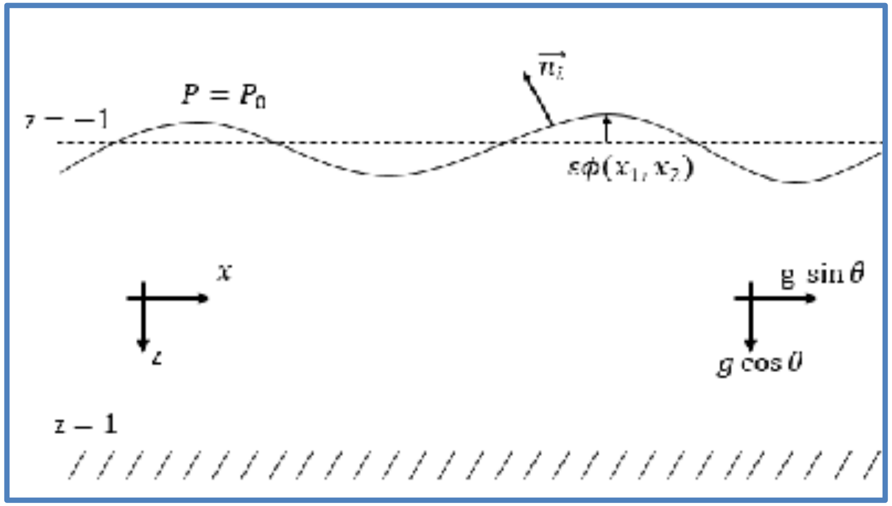
A note on the Boundary Conditions



Boundary fitted Method: Equations and numerical modeling

The stress balance at the free surface is

$$\tau_{ij} n_j = \sigma \frac{\partial n_j}{\partial x_j} n_i - P_0 n_i$$



For a Newtonian fluid:

$$\tau_{ij} = -P\delta_{ij} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

The interface can be described (implicit description) by:

Note: in the following (x_1, x_2, x_3) can be used instead of (x, y, z)

$$F(x_1, x_2, x_3) = x_3 + 1 + \epsilon\phi(x_1, x_2)$$

The surface unit normal n_i is:

$$n_i = \frac{\nabla F}{|\nabla F|}$$

Therefore, we get — using Taylor series exp. for $\sqrt{1+x^2} \simeq 1 + \frac{x}{2} - \frac{x^2}{8} + \frac{x^3}{16} - \dots$:

$$\begin{cases} n_1 = \frac{\partial F}{\partial x_1}\left(|\nabla F|\right)^{-1} = \epsilon \frac{\partial \phi}{\partial x_1} + o\left(\epsilon^3\right) \\ n_2 = \frac{\partial F}{\partial x_2}\left(|\nabla F|\right)^{-1} = \epsilon \frac{\partial \phi}{\partial x_2} + o\left(\epsilon^3\right) \\ n_3 = \frac{\partial F}{\partial x_3}\left(|\nabla F|\right)^{-1} = 1 + o\left(\epsilon^2\right) \end{cases}$$

The curvature can be computed as:

$$\nabla \cdot n = \epsilon \left(\frac{\partial^2 \phi}{\partial x_1^2} + \frac{\partial^2 \phi}{\partial x_2^2} \right)$$

Hence, the 3 components of the stress balance equations can be written as :

$$\mu\left[2\ \frac{\partial u_1}{\partial x_1}\ n_1 + \left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right)\ n_2 + \left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}\right)\ n_3\right] - (P - P_0)\ \ n_1 = \sigma\ \frac{\partial n_j}{\partial x_j}\ n_1$$

$$\mu\left[2\ \frac{\partial u_2}{\partial x_2}\ n_2 + \left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right)\ n_1 + \left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2}\right)\ n_3\right] - (P - P_0)\ n_2 = \sigma\ \frac{\partial n_j}{\partial x_j}\ n_2$$

$$\mu\left[2\ \frac{\partial u_3}{\partial x_3}\ n_3 + \left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}\right)\ n_1 + \left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2}\right)\ n_2\right] - (P - P_0)\ n_3 = \sigma\ \frac{\partial n_j}{\partial x_j}\ n_3$$

Previous equations, with u_i and P evaluated at the surface location x_3^S,

$$x_3^S = -1 - \epsilon\phi(x_1, x_2)$$

are exact equations.

Now we consider the free, wavy, surface as a perturbed surface about the mean position $x_3 = -1$. To do this, we approximate any fluctuation y at the surface by a first order Taylor series expansion at $x_3 = -1$

$$y\left(x_3^S\right) = y(-1) + (\underbrace{x_3^S}_{\Delta x_3 = x_3^S - (-1)} + 1)\,\frac{\partial y}{\partial x_3}(-1) + \cdots = y(-1) - \epsilon\phi\frac{\partial y}{\partial x_3}(-1) + o(\epsilon^2)$$

Therefore we have:

$$P(x_3^S) \simeq P(-1) - \epsilon\phi\frac{\partial P}{\partial x_3}(-1)$$

Boundary fitted Method: Equations and numerical modeling

Starting from the exact equations (evaluated at x_3^s):

$$\mu\left[2\ \frac{\partial u_1}{\partial x_1}\ n_1 + \left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right)\ n_2 + \left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}\right)\ n_3\right] - \left(P - P_0\right)\ n_1 = \sigma\ \frac{\partial n_j}{\partial x_j} n_1$$

$$\mu\left[2\ \frac{\partial u_2}{\partial x_2}\ n_2 + \left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right)\ n_1 + \left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2}\right)\ n_3\right] - (P - P_0)\ n_2 = \sigma\ \frac{\partial n_j}{\partial x_j} n_2$$

$$\mu\left[2\ \frac{\partial u_3}{\partial x_3}\ n_3 + \left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}\right)\ n_1 + \left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2}\right)\ n_2\right] - (P - P_0)\ n_3 = \sigma\ \frac{\partial n_j}{\partial x_j} n_3$$

And recalling that:

$$\begin{cases} n_1 = \epsilon \dfrac{\partial \phi}{\partial x_1}; \quad n_2 = \epsilon \dfrac{\partial \phi}{\partial x_2}; \quad n_3 = 1 \\ \dfrac{\partial n_j}{\partial x_j} = \epsilon \left(\dfrac{\partial^2 \phi}{\partial x_1^2} + \dfrac{\partial^2 \phi}{\partial x_2^2}\right) \end{cases}$$

…and that**(next slide):

$$P(x_3^S) \simeq P_0 + p(-1) - \epsilon\phi\left[\rho g \cos\theta + \frac{\partial P}{\partial x_3}(-1)\right]; \qquad \frac{\partial u_i}{\partial x_j}(x_3^S) \simeq \frac{\partial u_i}{\partial x_j}(-1) - \epsilon\phi \frac{\partial}{\partial x_3}\left[\frac{\partial u_i}{\partial x_j}(-1)\right]$$

Note that in general:

$$P(x_3) = P_0 + \rho g \cos\theta \left(1 + x_3\right) + p(x_3) \rightarrow \text{therefore } \; P(-1) = P_0 + p(-1);$$

$$\frac{\partial p}{\partial x_3}(-1) = \rho g \cos\theta + \frac{\partial p}{\partial x_3}(-1)$$

This gives:

$$P(x_3^s) \simeq P(-1) - \epsilon\phi \frac{\partial p}{\partial x_3}(-1) \simeq P_0 + p(-1) - \epsilon\phi \left[\rho g \cos\theta + \frac{\partial p}{\partial x_3}(-1)\right]$$

We get:

$$\mu\left[2\ \epsilon\frac{\partial\phi}{\partial x_1}\ \frac{\partial u_1}{\partial x_1}+\epsilon\frac{\partial\phi}{\partial x_2}\ \left(\frac{\partial u_1}{\partial x_2}+\frac{\partial u_2}{\partial x_1}\right)+\frac{\partial u_1}{\partial x_3}+\frac{\partial u_3}{\partial x_1}-\epsilon\phi\frac{\partial}{\partial x_3}\left(\frac{\partial u_1}{\partial x_3}+\frac{\partial u_3}{\partial x_1}\right)\right]-\epsilon p\frac{\partial\phi}{\partial x_1}=0$$

$$\mu\left[2\ \epsilon\frac{\partial\phi}{\partial x_2}\ \frac{\partial u_2}{\partial x_2}+\epsilon\frac{\partial\phi}{\partial x_1}\ \left(\frac{\partial u_1}{\partial x_2}+\frac{\partial u_2}{\partial x_1}\right)+\frac{\partial u_2}{\partial x_3}+\frac{\partial u_3}{\partial x_2}-\epsilon\phi\frac{\partial}{\partial x_3}\left(\frac{\partial u_2}{\partial x_3}-\frac{\partial u_3}{\partial x_2}\right)\right]-\epsilon p\frac{\partial\phi}{\partial x_2}=0$$

$$\mu\left[2\left(\frac{\partial u_3}{\partial x_3}-\epsilon\phi\frac{\partial}{\partial x_3}\frac{\partial u_3}{\partial x_3}\right)+\epsilon\frac{\partial\phi}{\partial x_1}\ \left(\frac{\partial u_1}{\partial x_3}+\frac{\partial u_3}{\partial x_1}\right)+\epsilon\frac{\partial\phi}{\partial x_2}\ \left(\frac{\partial u_2}{\partial x_3}+\frac{\partial u_3}{\partial x_2}\right)\right]$$
$$-p+\epsilon\phi\rho g\cos\theta+\epsilon\phi\frac{\partial p}{\partial x_3}=\sigma\epsilon\left(\frac{\partial^2\phi}{\partial x_1^2}+\frac{\partial^2\phi}{\partial x_2^2}\right)$$

Together with the dynamic BC, we also have the kinematic BC:

$$\begin{cases} \dfrac{\partial F}{\partial t} + u \cdot \nabla F = 0 \\ F(x_1, x_2, x_3) = 1 + x_3 + \epsilon\phi(x_1, x_2) \end{cases}$$

This gives:

$$\epsilon \frac{\partial \phi}{\partial t} + u_1 \frac{\partial F}{\partial x_1} + u_2 \frac{\partial F}{\partial x_2} + u_3 \frac{\partial F}{\partial x_3} = 0$$

$$\epsilon \frac{\partial \phi}{\partial t} + u_1 \epsilon \frac{\partial \phi}{\partial x_1} + u_2 \epsilon \frac{\partial \phi}{\partial x_2} + u_3 = 0$$

Therefore, $u_3 \sim o\,(\epsilon)$; we also expect $p \sim o\,(\epsilon)$; It can be also shown that $u_2 \sim o(\epsilon)$

From continuity,

$$\frac{\partial u_1}{\partial x_1} \sim o(\epsilon)$$

It can be also shown that, in the neighborhood of the interface

$$\frac{\partial u_1}{\partial x_3} \sim o(\epsilon); \frac{\partial u_1}{\partial x_2} \sim o(\epsilon)$$

Such approach tells us that, at first order — order ϵ — all terms in which ϵ is multiplied by $\frac{\partial u_1}{\partial x_j}$ or p will vanish

Boundary fitted Method: Equations and numerical modeling

Hence we have (1st order approximation of BC at the wavy surface, $x_3 = -1$)

$$\begin{cases} \dfrac{\partial u_1}{\partial x_3} + \dfrac{\partial u_3}{\partial x_1} = 0 \\ \dfrac{\partial u_2}{\partial x_3} + \dfrac{\partial u_3}{\partial x_2} = 0 \\ 2\mu \dfrac{\partial u_3}{\partial x_3} - p + \epsilon\phi\rho g \cos\theta = \sigma\epsilon\left(\dfrac{\partial^2\phi}{\partial x_1^2} + \dfrac{\partial^2\phi}{\partial x_2^2}\right) \end{cases}$$

To write them in dimensionless form:

$u \rightarrow u_\tau; \quad x \rightarrow h; \quad f \rightarrow \dfrac{\epsilon\phi}{h}$ with f surface fluctuation wrt $x_3 = -1$

After some algebra, and upon introduction of the following parameters:

$$Re_\tau = \frac{\rho u_\tau h}{\mu}; \quad Fr = \frac{u_\tau^2}{gh\cos\theta}; \quad We = \frac{\rho u_\tau^2 h}{\sigma}$$

Boundary fitted Method: Equations and numerical modeling

We get

$$\frac{2}{Re_\tau}\ \frac{\partial u_3}{\partial x_3} - p + \frac{1}{Fr}\ f = \frac{1}{We}\left(\frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2}\right)$$

We recall that f is the dimensionless deviation of the surface from $x_3 = -1$, which is computed from the kinematic condition:

$$\epsilon \frac{\partial \phi}{\partial t} + u_3 + \epsilon \frac{\partial \phi}{\partial x_1} u_1 + \epsilon \frac{\partial \phi}{\partial x_2} u_2 = 0$$

In dimensionless form:

$$\frac{\partial f}{\partial t} + u_3 + \frac{\partial f}{\partial x_1} u_1 + \frac{\partial f}{\partial x_2} u_2 = 0$$

Works fine for small wave steepness, $ak < 0.01$

Assume now that the interface deformation is negligible, $\epsilon = 0,\ f = 0$.

Hence we have (0th order approximation of BC at the free surface, $x_3 = -1$)

$$\begin{cases} u_3 = 0 \quad \text{(from kinematic cond.)} \\ \dfrac{\partial u_1}{\partial x_3} = 0 \\ \dfrac{\partial u_2}{\partial x_3} = 0 \end{cases}$$

Physical configuration (recall)

Boundary conditions

Interface

Kinematic B.C.

$$\frac{\partial \eta}{\partial t} + u_x \frac{\partial \eta}{\partial x} + u_y \frac{\partial \eta}{\partial y} = u_z$$

Dynamic B.C. (B.C on stress and velocity)

$$@z = 0$$

$$\frac{1}{Re\tau}\left((\tau_{\mathbf{L}} - \tau_{\mathbf{G}}) \cdot \mathbf{n}\right) \cdot \mathbf{n} + p_G - p_L + \frac{1}{We}\nabla \cdot \mathbf{n} - \frac{1}{Fr}\eta = 0$$

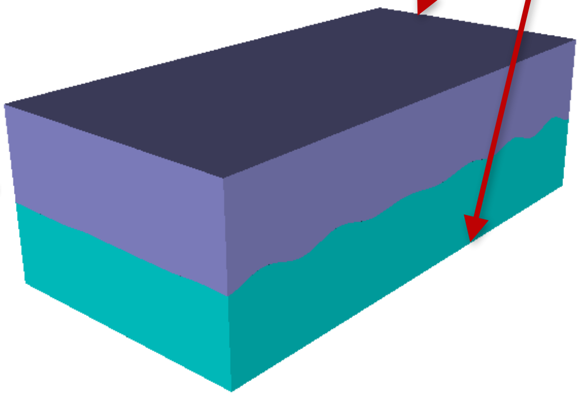
$$((\tau_L - \tau_G) \cdot \mathbf{n}) \cdot \mathbf{t}_i = 0 \;, \quad i = x, y$$

$$\mathbf{u}_G = \frac{1}{\mathscr{R}}\mathbf{u}_L; \;\; \mathscr{R} = \sqrt{\rho_L/\rho_G}$$

Outer boundaries (Free-slip B.C.)

$$@z = \pm h$$

$$\frac{\partial u_{x,y}}{\partial z} = \frac{\partial p}{\partial z} = u_z = 0$$



Simulations & Plan of experiments

Physical problem

Liquid (l) : Water

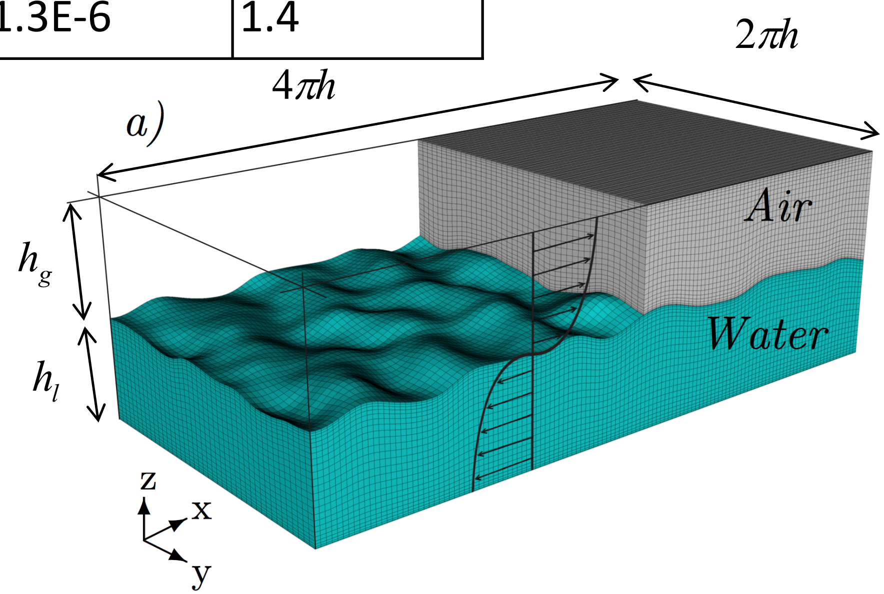
Gas (g) : Air

$$We = \frac{\rho_L h u_{\tau,L}^2}{\gamma}, \quad Fr = \frac{\rho_L u_{\tau,L}^2}{gh(\rho_L - \rho_G)}, \quad Re_\tau = \frac{u_{\tau,G} 2h}{\nu_G} = \frac{u_{\tau,L} 2h}{\nu_L}$$

Simulation	h[m]	Re_τ	We	Fr	$Fr^{1/2}/We$
S1	4.5E-02	170	8.5E-4	2.9E-6	2.03
S2	5E-02	170	7.6E-4	2.2E-6	1.93
S3	6E-02	170	6.3E-4	1.3E-6	1.4

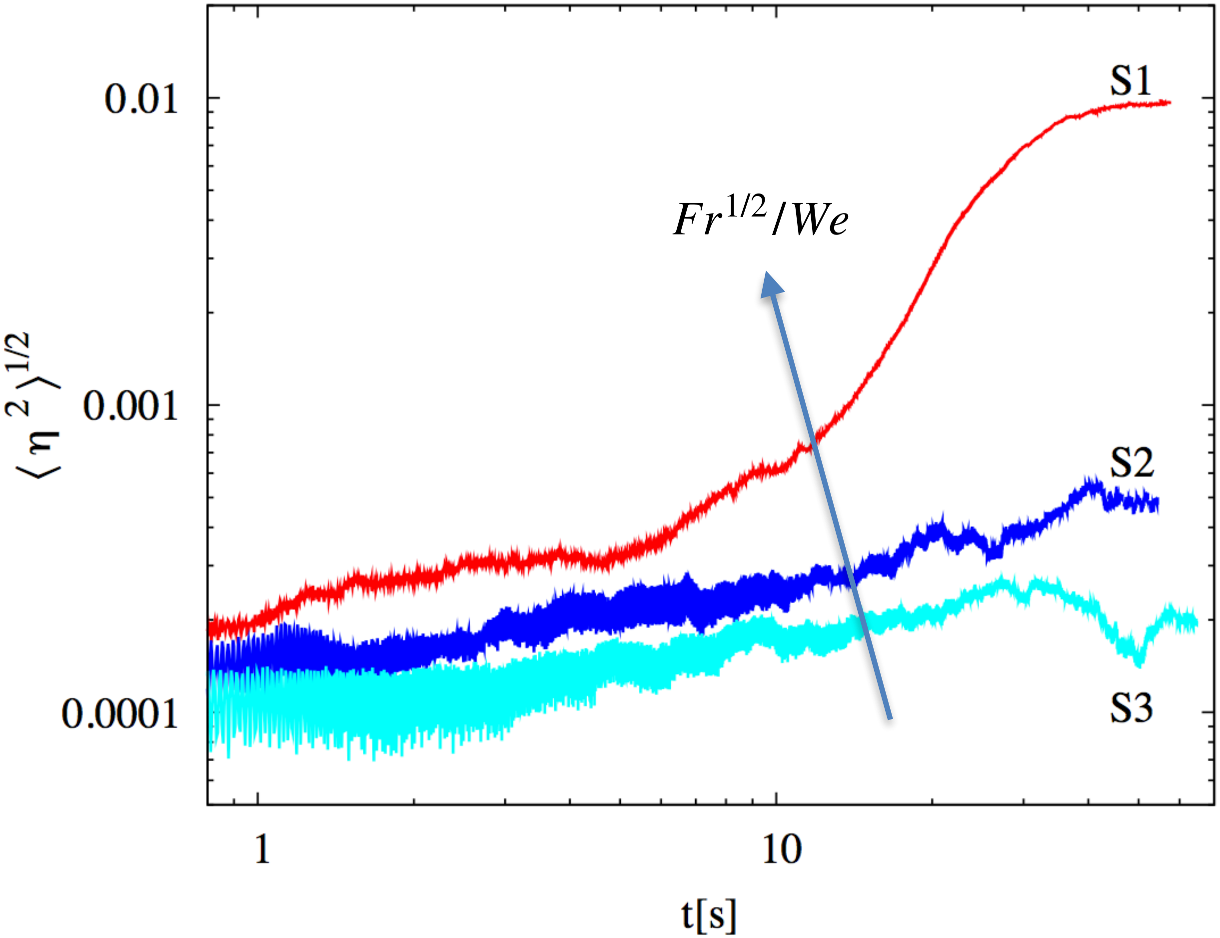
$Fr^{1/2}/We$ → Smaller (Surf. Tension dominates)

$Fr^{1/2}/We$ → Larger (Gravity important)



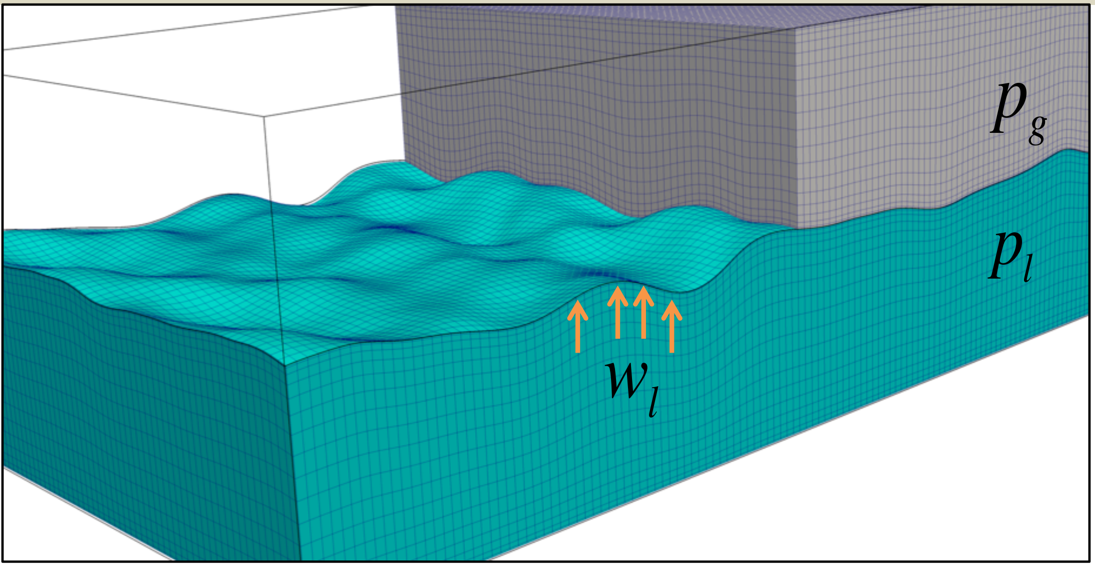
Transient growth of waves

Wave amplitude



How to explain this behavior?

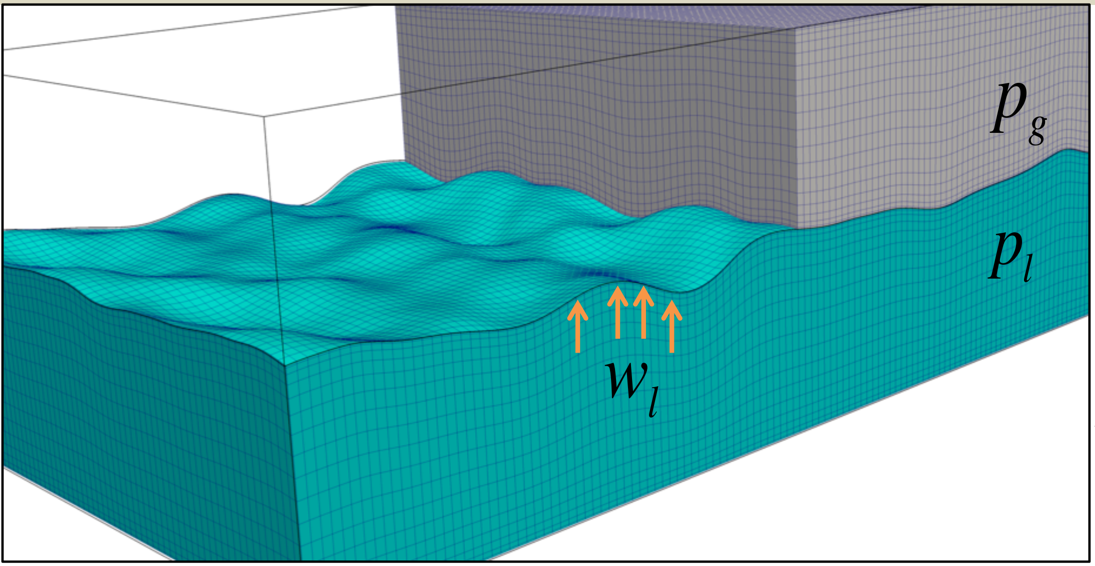
Consider the origin of a wave…



We express the variation of the interface area as (Hoepffner et al., PRL 2011):

$$\frac{dA}{dt} \propto h w_l$$

Consider the origin of a wave…

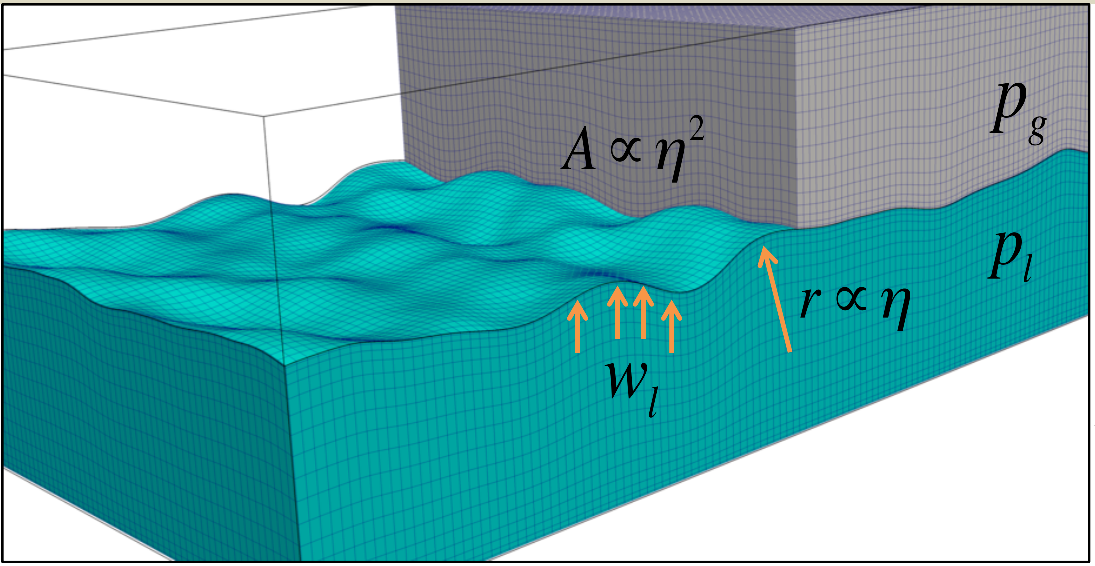


We express the variation of the interface area as (Hoepffner et al., PRL 2011):

$$\frac{dA}{dt} \propto h w_l$$

$$\begin{cases} \Delta p \propto \rho w_l^2 \\ \Delta p \propto \dfrac{\gamma}{r} \end{cases} \rightarrow \quad w_l \propto r^{-1/2}$$

Consider the origin of a wave…



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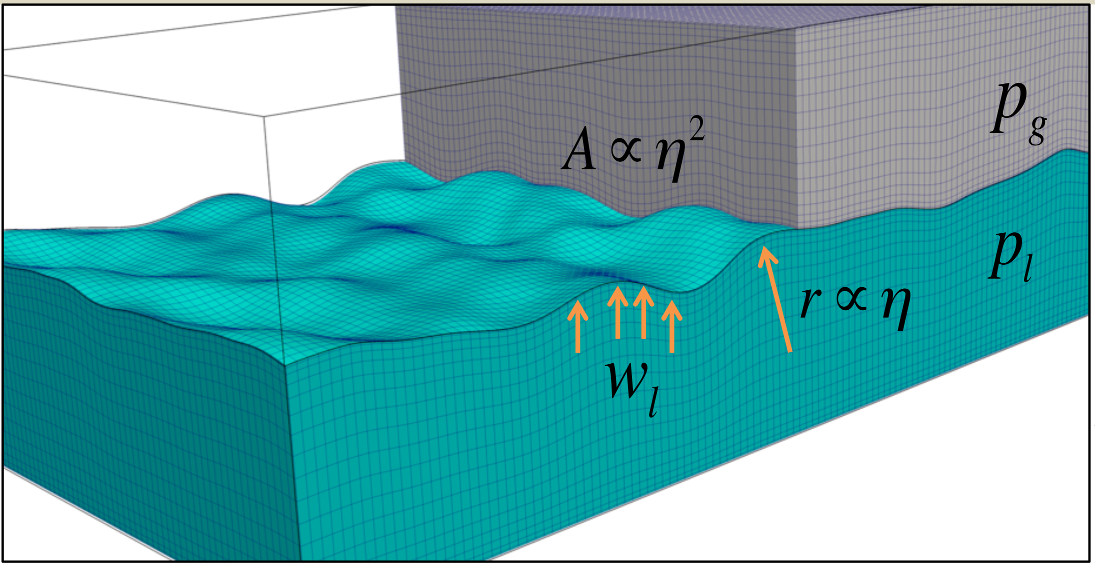

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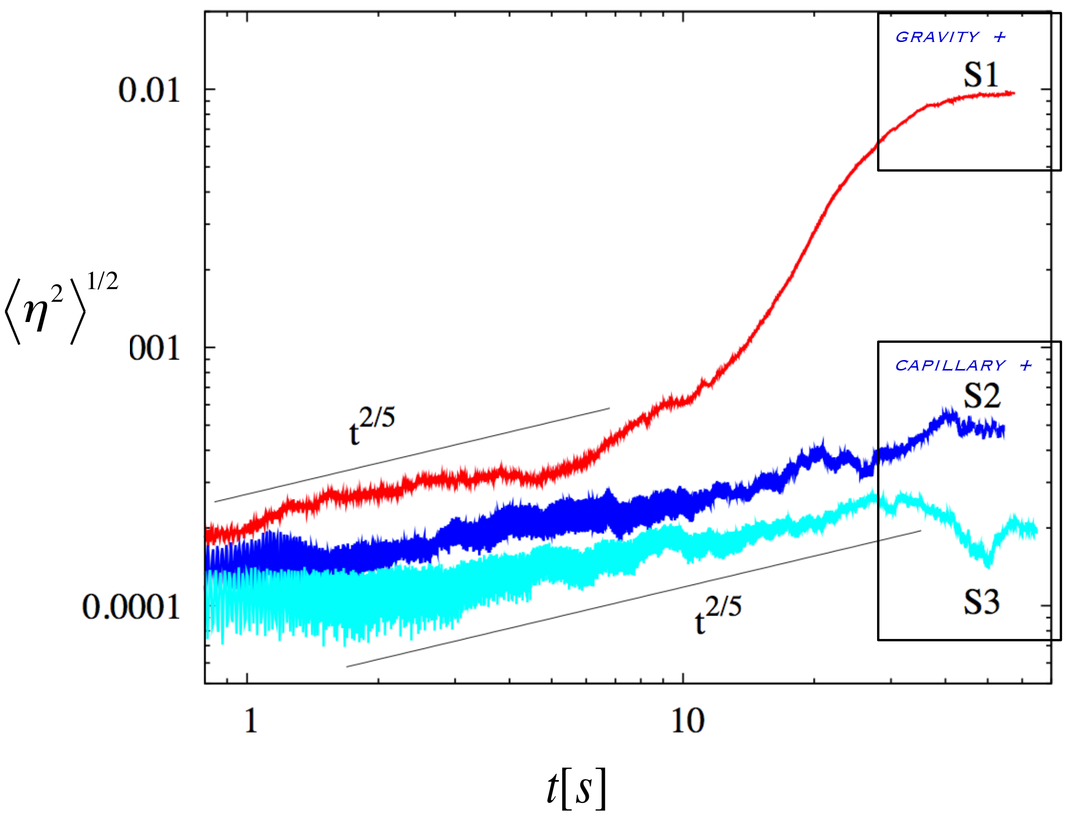
$$\begin{cases} \Delta p \propto \rho w_l^2 \\ \Delta p \propto \dfrac{\gamma}{r} \end{cases} \longrightarrow \quad w_l \propto r^{-1/2}$$

After some algebra:

$$\frac{d\eta^2}{dt} \propto \frac{1}{\eta^{1/2}} \longrightarrow \quad \eta \propto t^{2/5}$$

Transient growth of waves: DNS vs simplified model

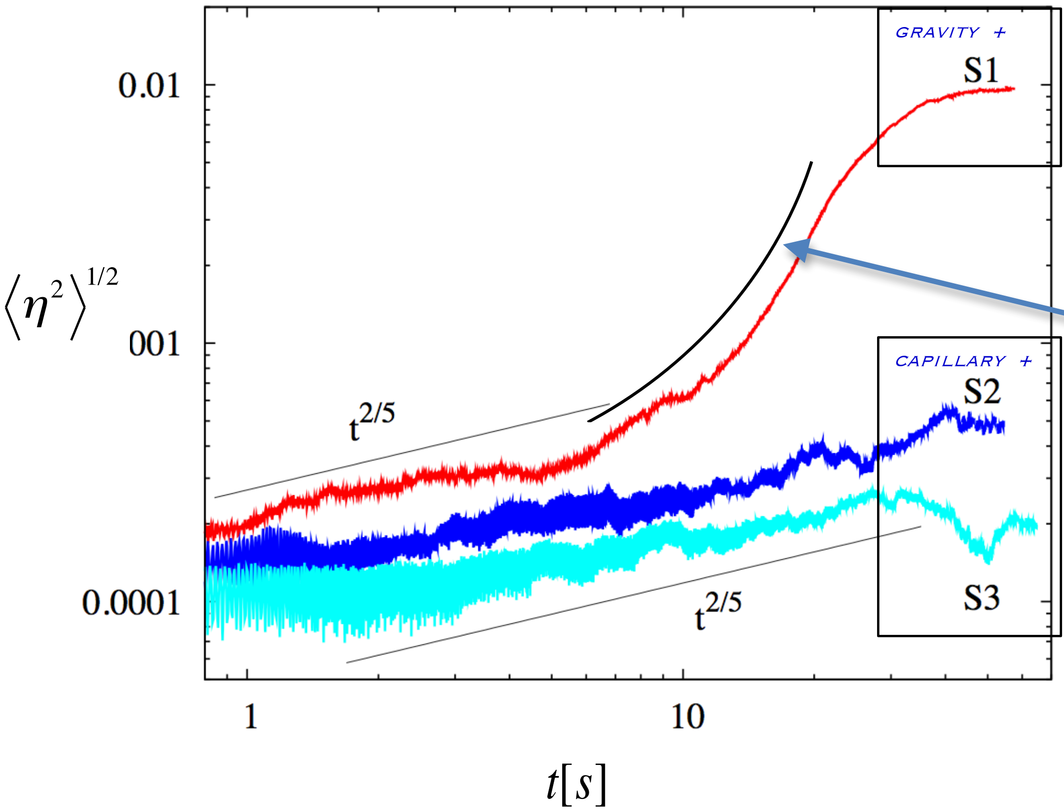


The proposed scaling is quite robust within the range of parameters investigated here

$$\eta \propto t^{2/5}$$

Whatever the value of the physical parameters, capillarity dominates at the beginning (Zonta et al. JFM 2015)

Transient growth of waves: DNS vs simplified model



For non-negligible gravity, i.e.

$$Fr^{1/2}/We \uparrow$$

after the initial scaling we observe

$$\eta \propto \exp(t)$$

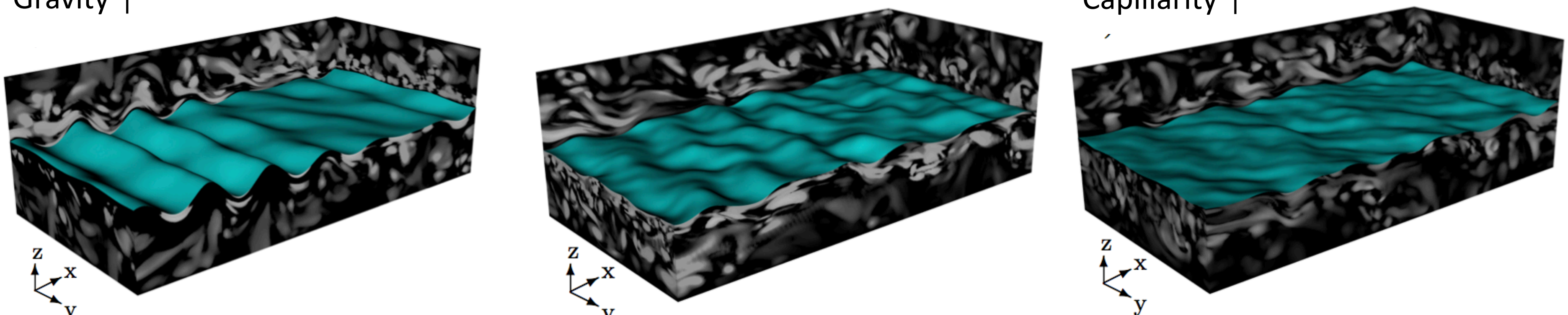
(resonance mechanism between waves and induced pressure/stress)

Lin et al. JFM 2008

Janssen, Cambridge press 2008

Structure of the interface deformation

Gravity ↑ Capillarity ↑

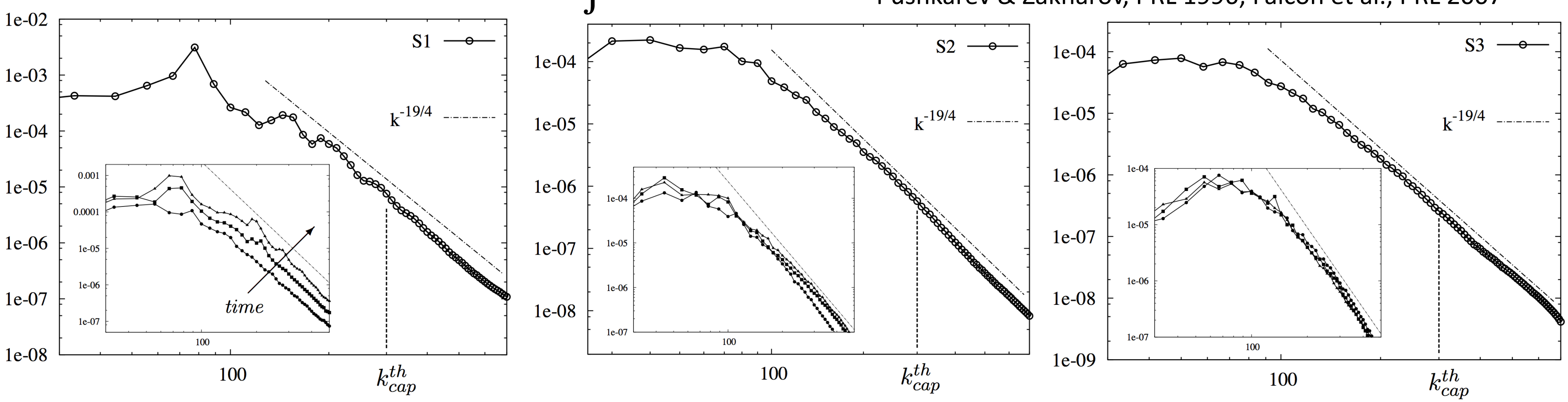


Quasy-sinusoidal wavy interface

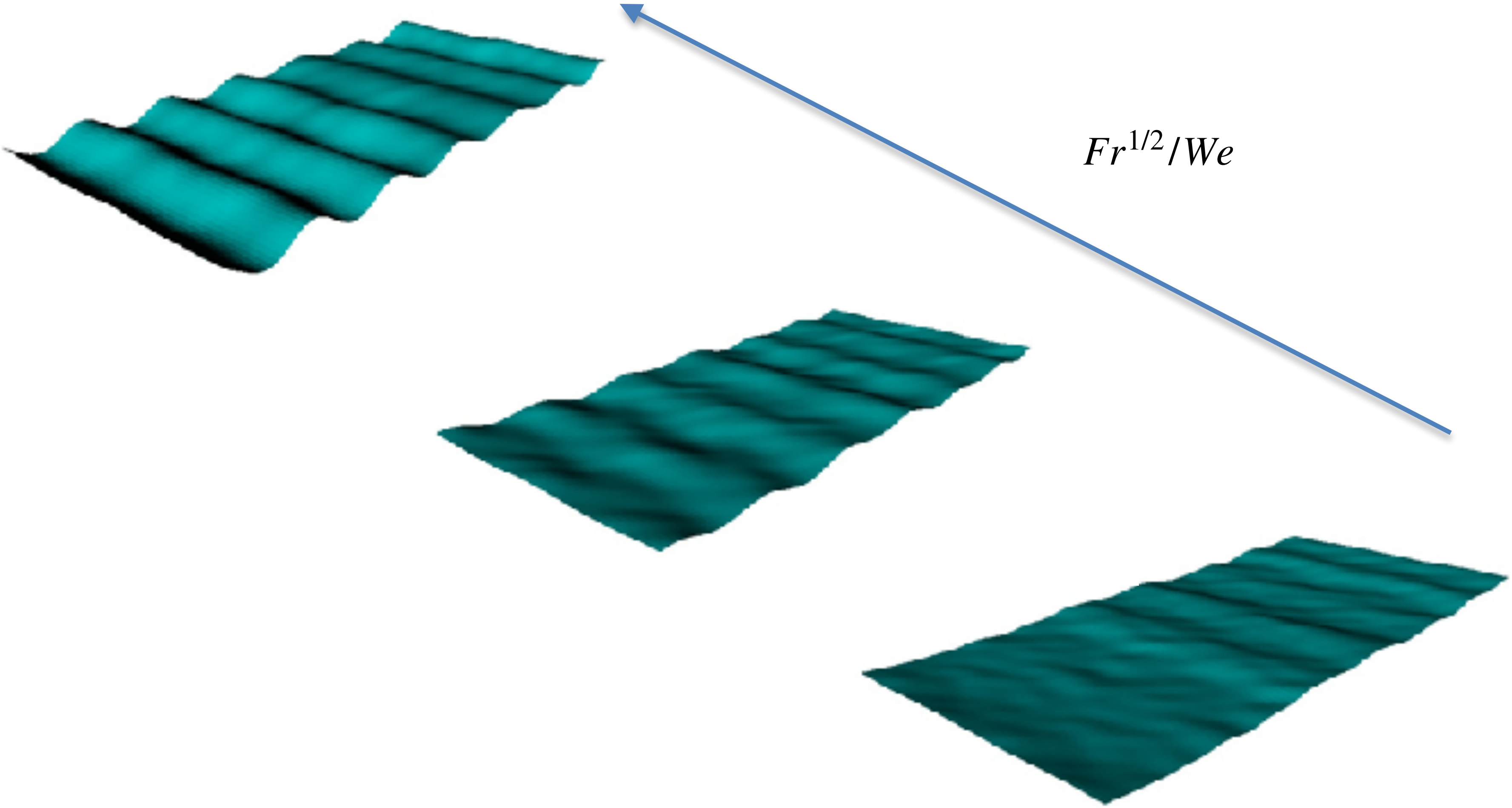
Surface roughness

Wavenumber spectrum $\hat{\eta}(k_x) = \int \hat{\eta}(k_x, k_y) dk_y$

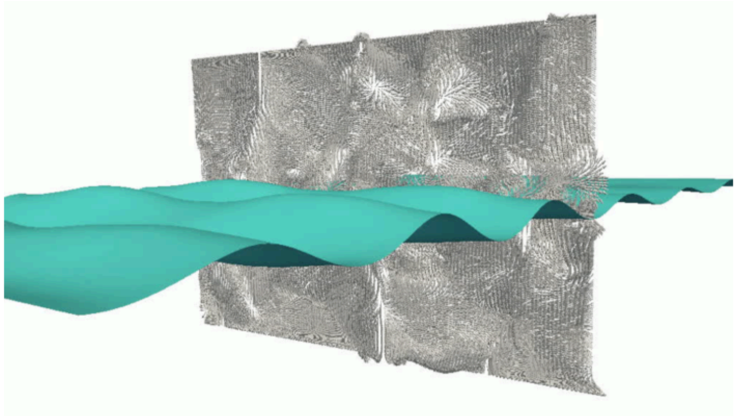
cfr wave turbulence theory
Pushkarev & Zakharov, PRL 1996; Falcon et al., PRL 2007

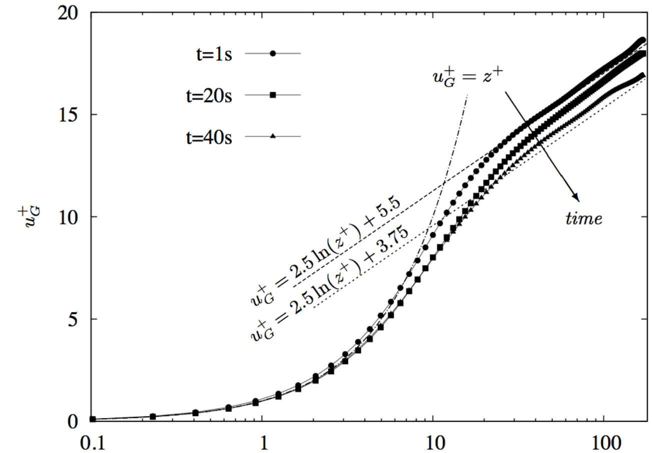


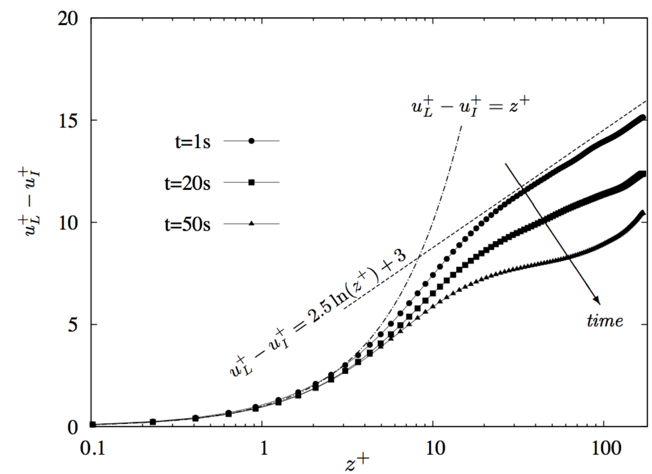
Structure of the interface deformation

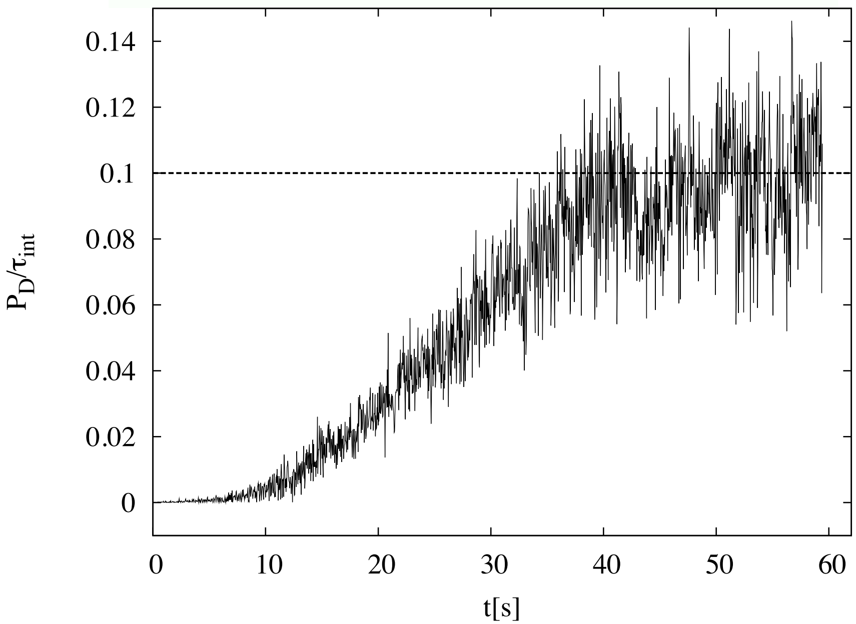


Structure of the interface deformation









As waves develop, we observe a drag increase (pressure drag+skin friction)

Fil Rouge

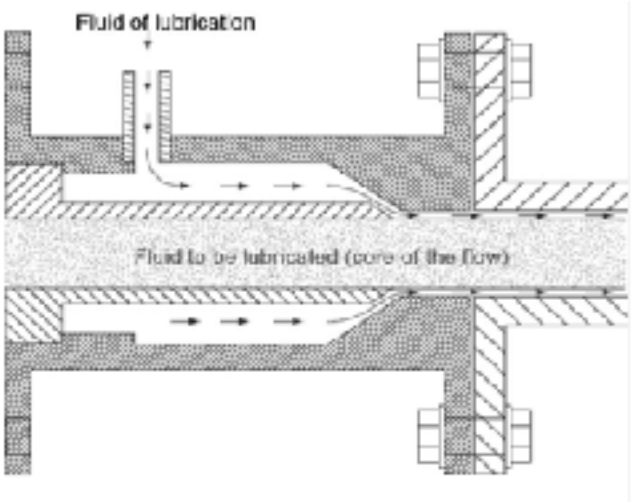
1. Computational approaches to multiphase flows: a short introduction

2. The sharp interface approach: numerical modeling, boundary conditions, application (stratified air/water flow)

3. The Phase Field Method: recap on numerical modeling, application (oil transport in pipelines/channels)

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 “

TECHNISCHE UNIVERSITÄT WIEN
Vienna | Austria

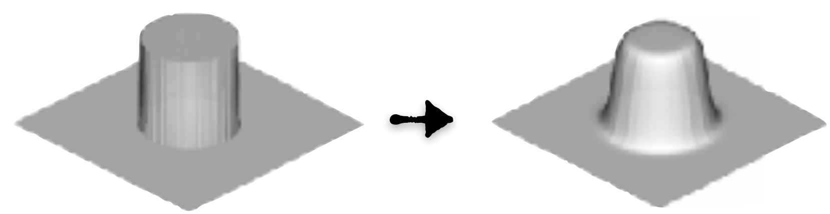
Numerical Implementation

Hypothesis:

-Matched density and incompressible flow.

-Different viscosity of the two phases.

Phase Field Method (PFM)



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

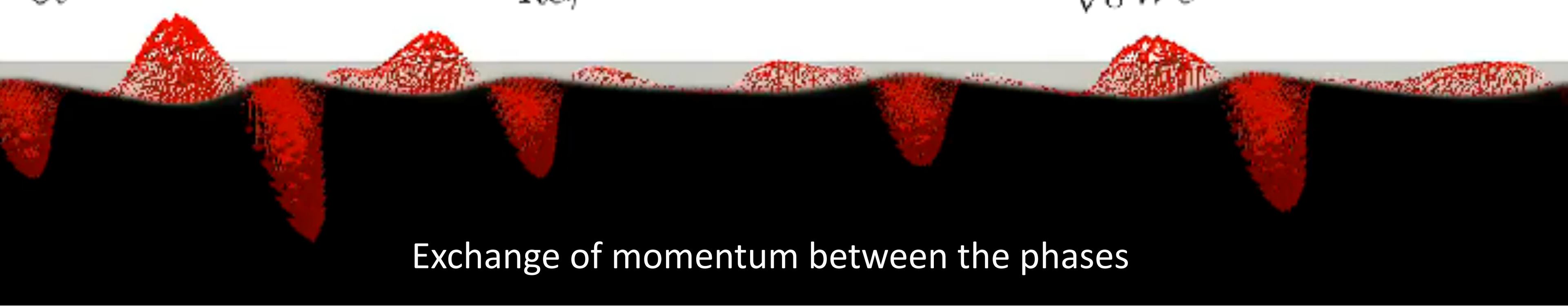
$$\nabla \cdot \mathbf{u} = 0$$

Flow driven by a constant mean pressure gradient (Π)

Viscosity Contrast: $(r(\phi, \lambda)(\nabla \mathbf{u} + \nabla \mathbf{u}^T))$

Surface tension forces: $\frac{3}{\sqrt{8}} \frac{Ch}{We}$

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



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)

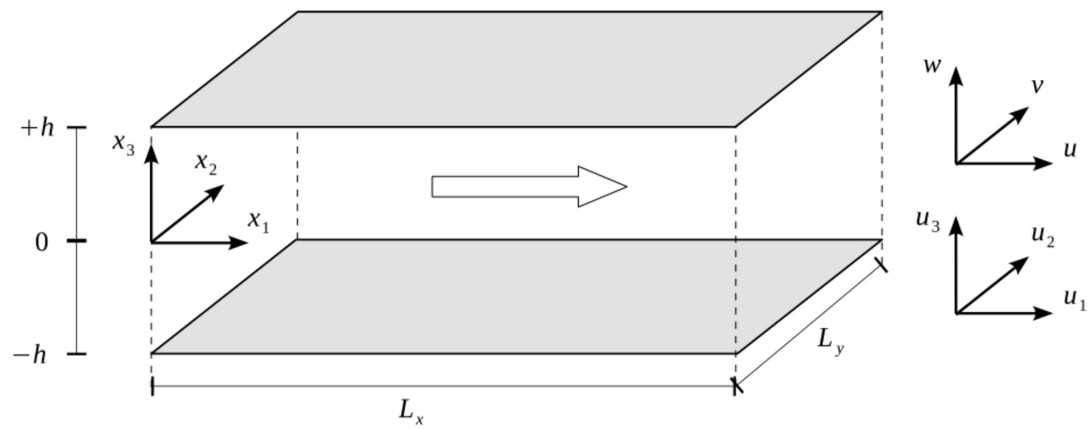
Numerical Implementation: Spectral & pseudo-spectral methods

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

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

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

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



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

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

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

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

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

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

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

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

Recall: 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

For spectral methods: global functions are defined in each node and are not zero

This brings some advantages for the representation of the derivatives

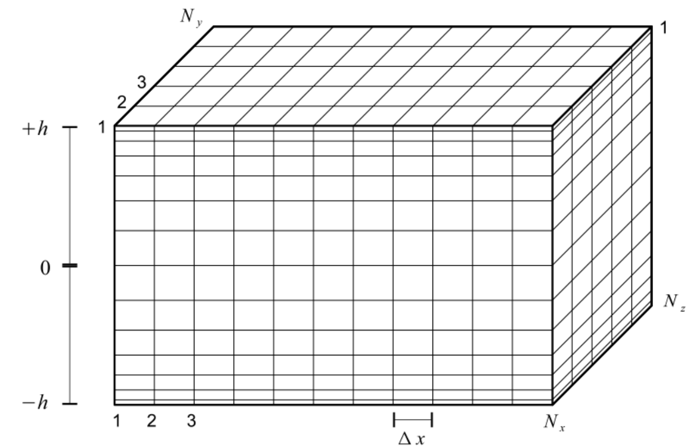
Numerical Implementation: Spectral & pseudo-spectral methods

Discrete geometry

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

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

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



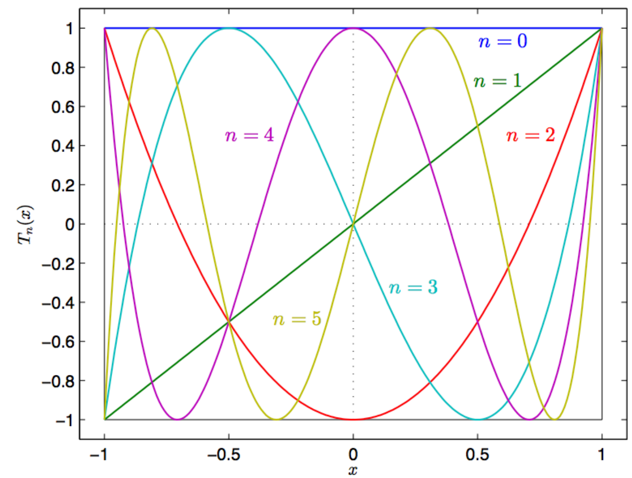
Spatial discretization of the solution (Fourier+Chebyshev)

Idea: approximate a function as the linear combination of test functions (which in this case are global)

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

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

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



Numerical Implementation: Spectral & pseudo-spectral methods

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

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

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

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

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

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

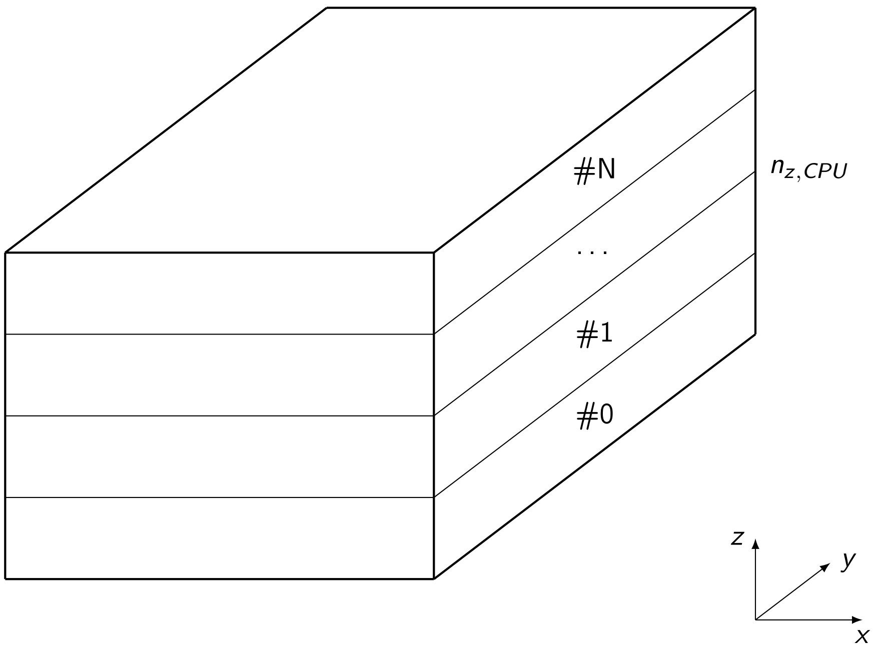
$$ik_1\hat{u}_1 + ik_2\hat{u}_2 + \frac{\partial \hat{u}_3}{\partial x_3} = 0$$

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

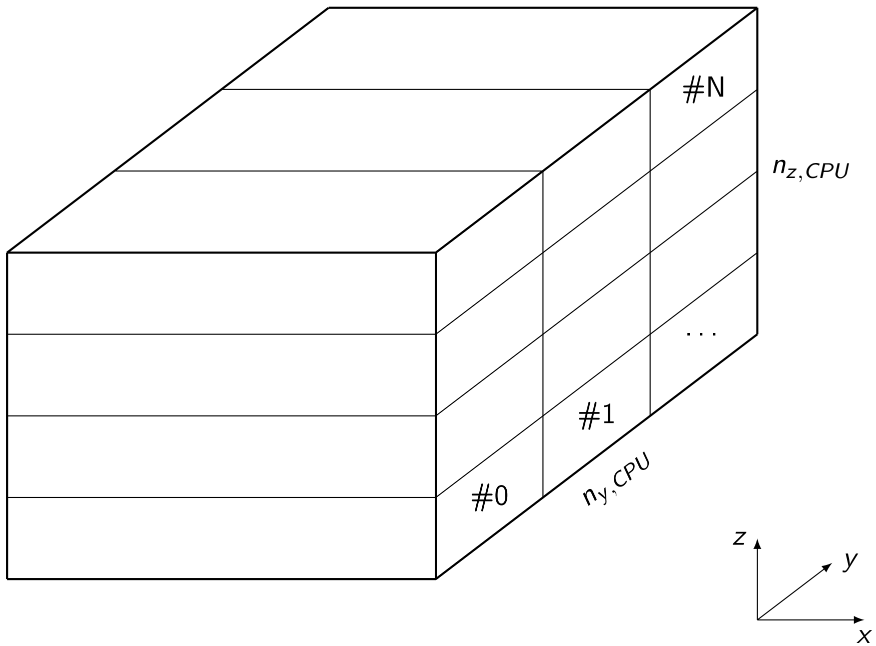
$$\left(\frac{\partial^2}{\partial x_3^2} - k^2 - \frac{s}{2Ch}\right)\left(\frac{\partial^2}{\partial x_3^2} - k^2 - \frac{s}{2Ch}\right)\hat{\phi}^{n+1} = \frac{\hat{H}_\phi^{\;n}}{\gamma}$$

Numerical Implementation: Spectral & pseudo-spectral methods

1D domain decomposition
"Slab"



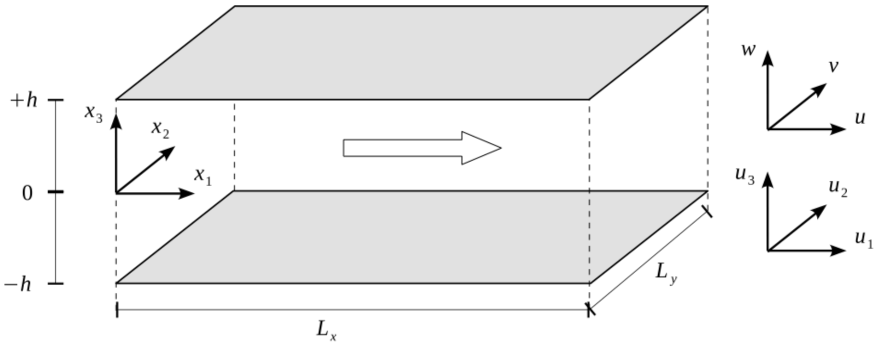
2D domain decomposition
"Pencil"



Numerical method (Recap)

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

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

<u>Solver NS (Vorticity-Velocity Formulation):</u>

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 Helmholtz 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 Helmholtz solver, Influence Matrix Method

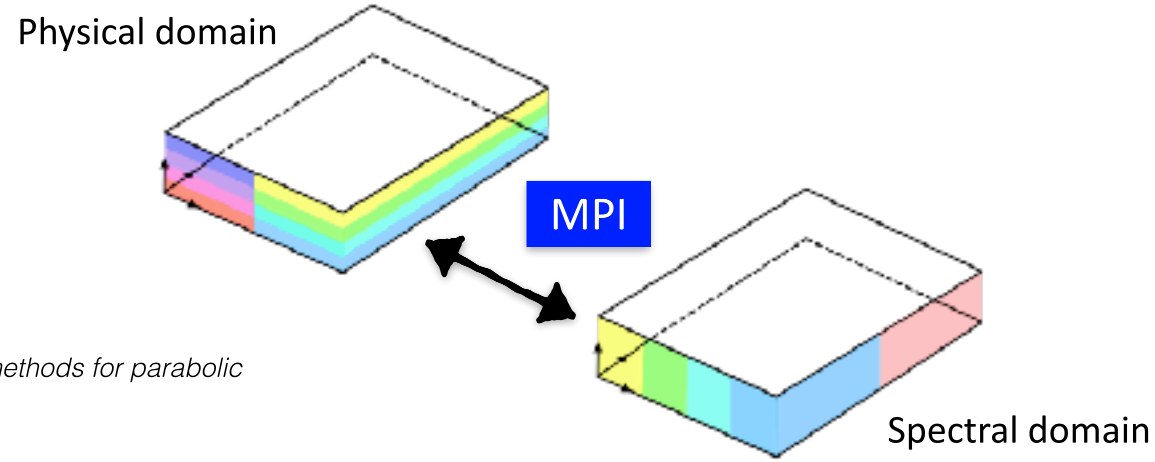
$$\frac{\partial \phi}{\partial t} = S_\phi + \frac{sCh^2}{Pe}\nabla^2 \phi - \frac{Ch^2}{Pe}\nabla^4 \phi$$

- Solve for phi
- 4th order PDE
- Double Helmholtz 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.*

Physical parameters

Weber Number (We):

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

Viscosity Ratio (λ):

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

Low We

Low λ
(Water+Hexane)

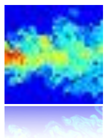
High We

High λ
(Water+Oil)

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

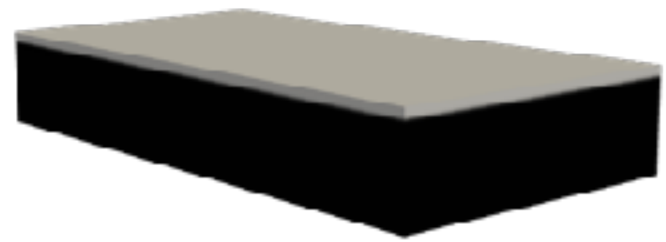
$$u_i(0) = u_i(L_x) \qquad \phi(0) = \phi(L_x)$$

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

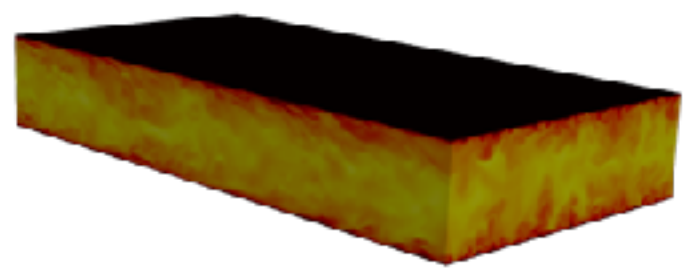
S. Ahmadi et al, *Turbulent Drag Reduction by a Near Wall Surface Tension Active Interface*, FTAC (2018)
S. Ahmadi et al, *Turbulent drag reduction in channel flow with viscosity stratified fluids*, CEF (2016)

Initial Conditions:

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



- Flow Field
  - Single Phase Flow $Re_\tau = 300.$



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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):

$$Ch = 0.02$$

F. Magaletti et al, *The sharp-interface limit of the Cahn–Hilliard/Navier–Stokes model for binary fluids*, JFM (2015)

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)

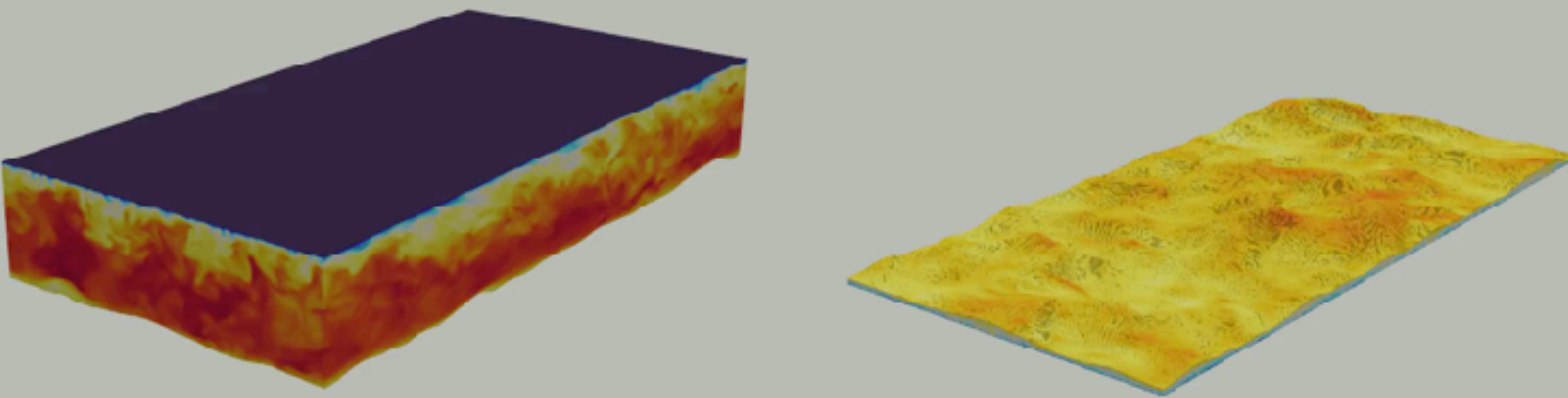
We consider 3 different viscosity ratio λ :

(ratio between the viscosity of the two phases)

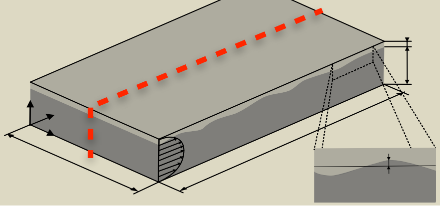
$$\lambda = \frac{\eta_w}{\eta_o} = \frac{\text{Water Viscosity}}{\text{Oil Viscosity}}$$

#	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

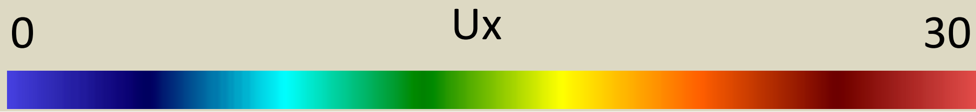
Visualization

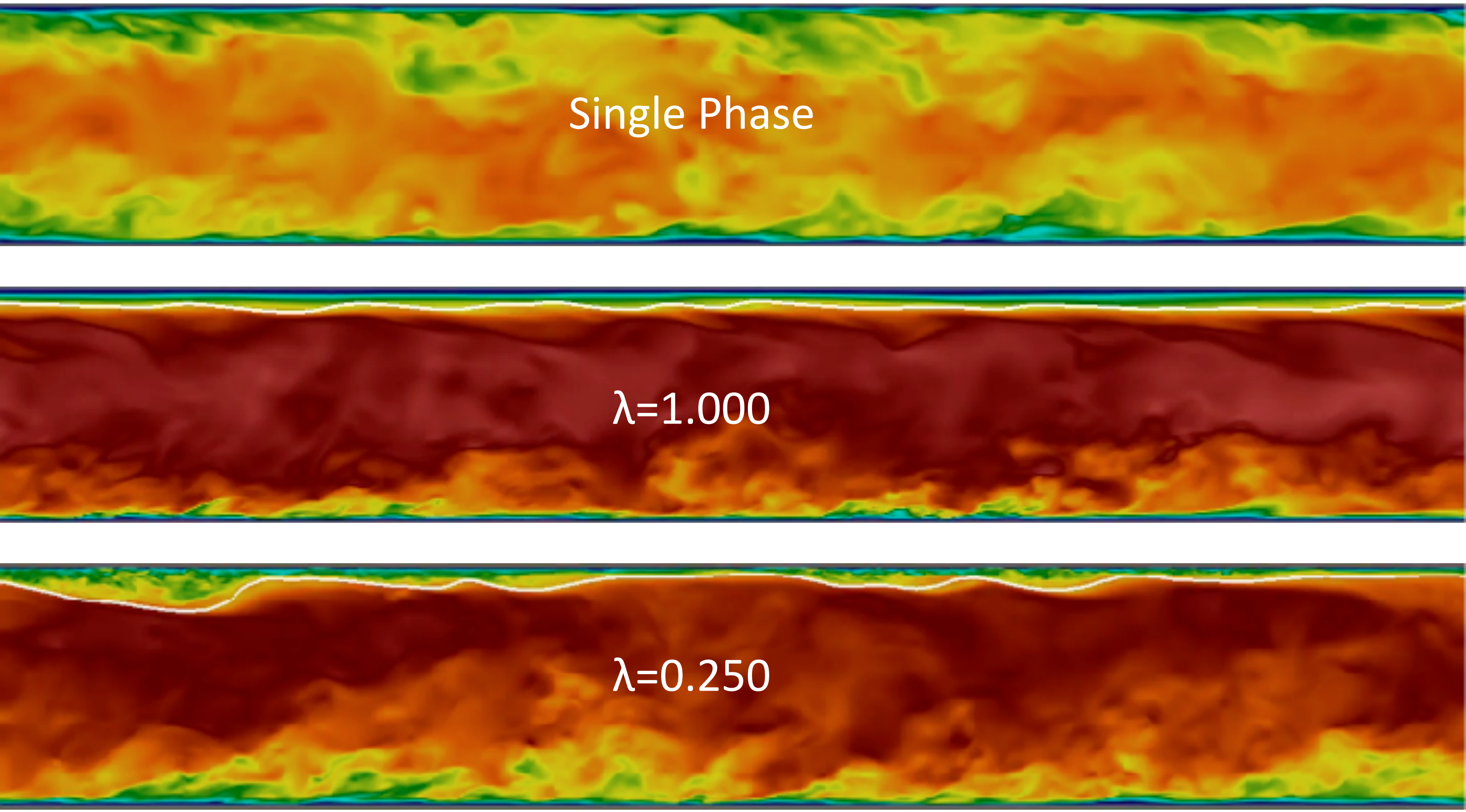


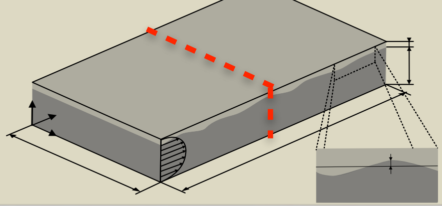
S. Ahmadi et al, Turbulent Drag Reduction by a Near Wall Surface Tension Active Interface, FTAC (2018)
S. Ahmadi et al, Turbulent drag reduction in channel flow with viscosity stratified fluids, CLF (2016)



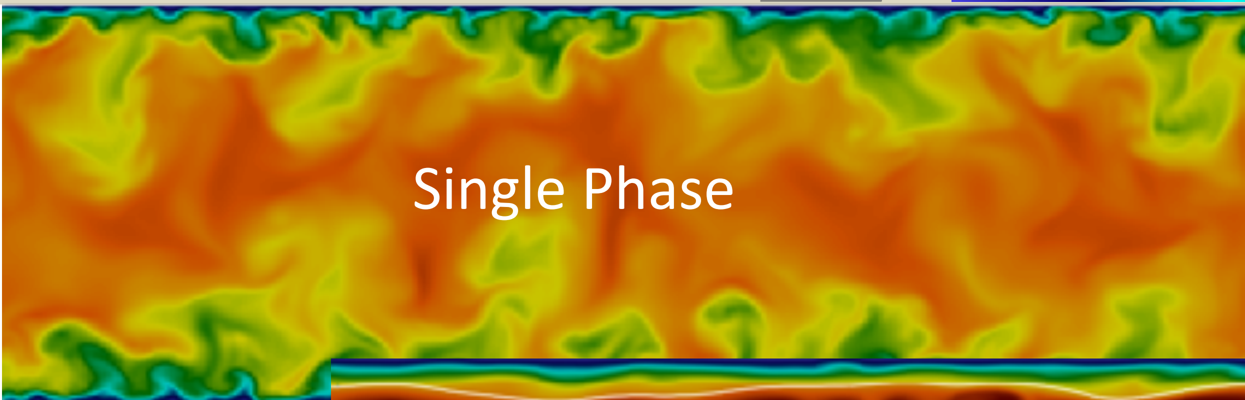
Visualization

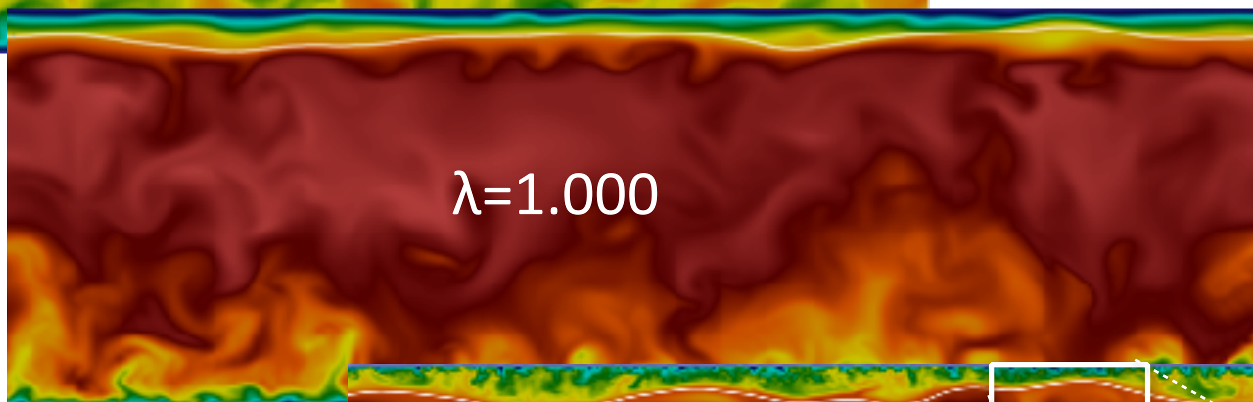






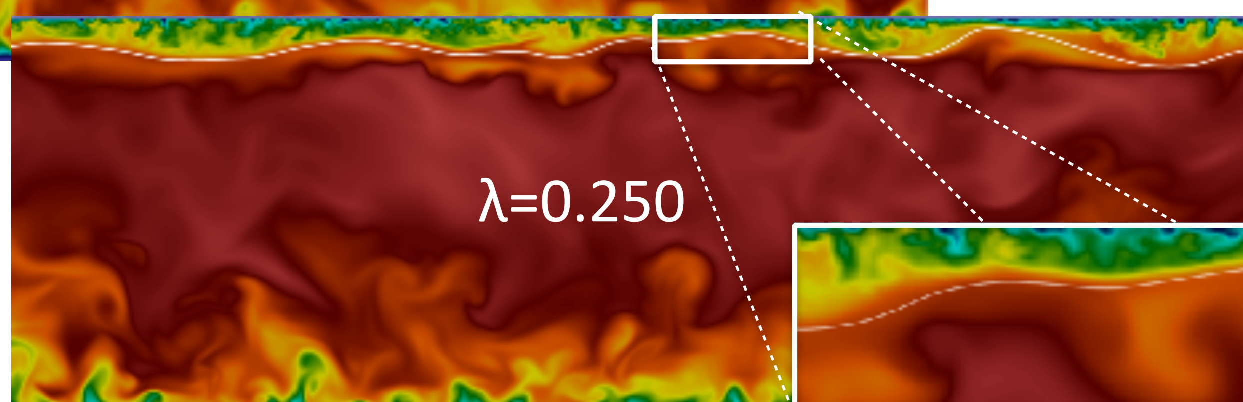
Visualization





$$Re_{local} \propto \frac{h}{\mu} \downarrow$$

DR driven by σ

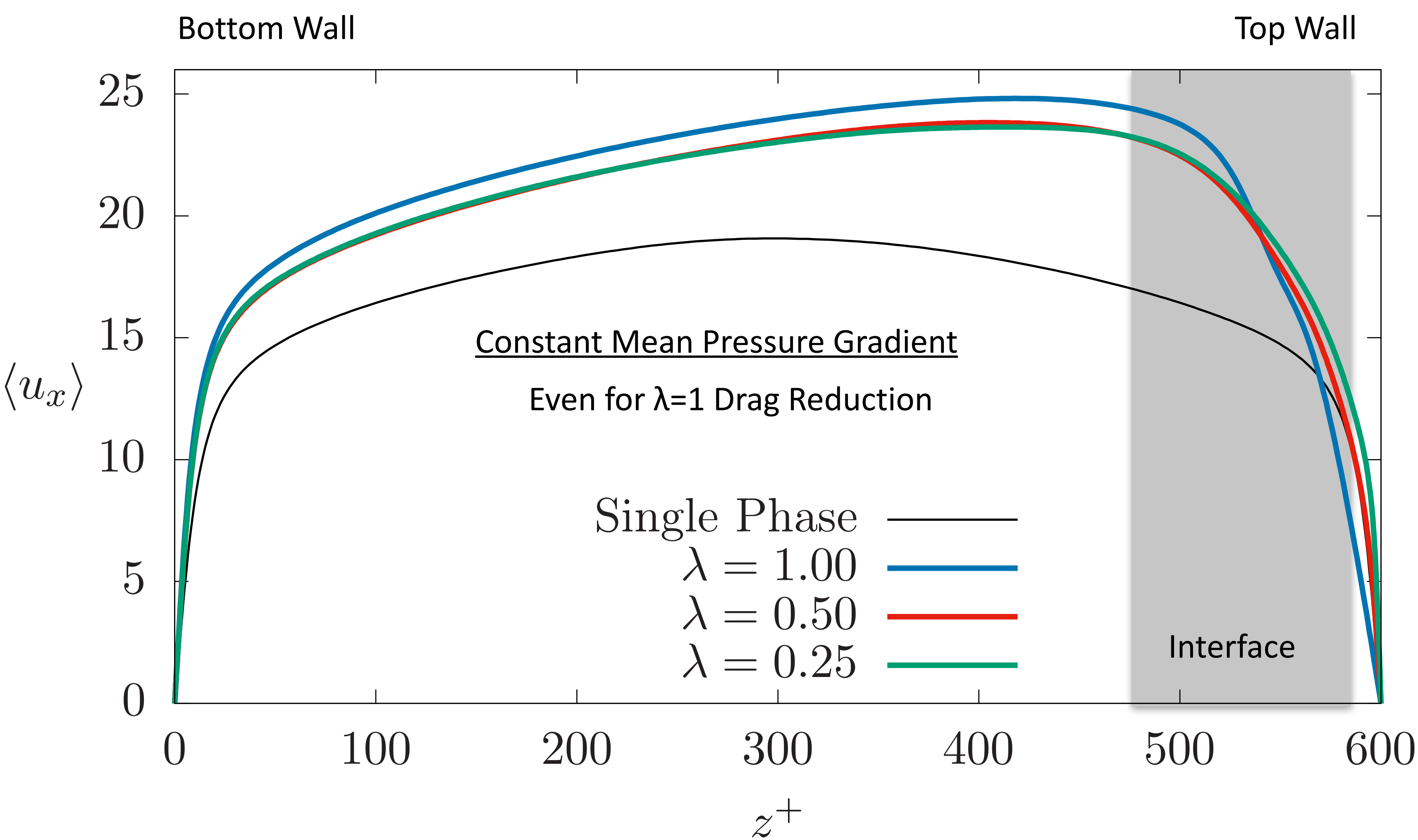


$$Re_{local} \propto \frac{h}{\mu} \uparrow$$

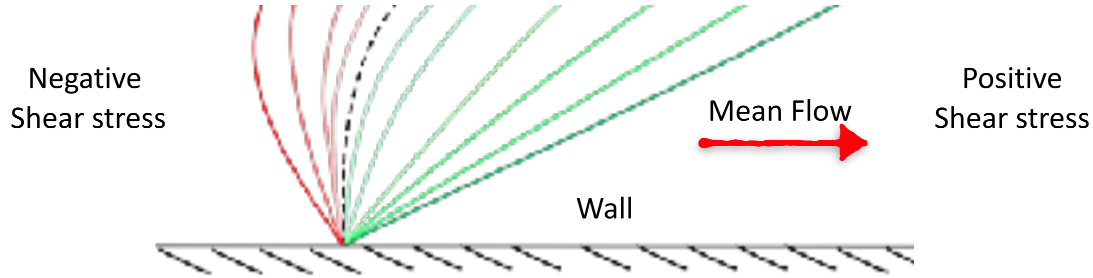
DR driven by λ

Roccon, Zonta, Soldati, *J. Fluid Mech.*, **70**, 040801 (2019)

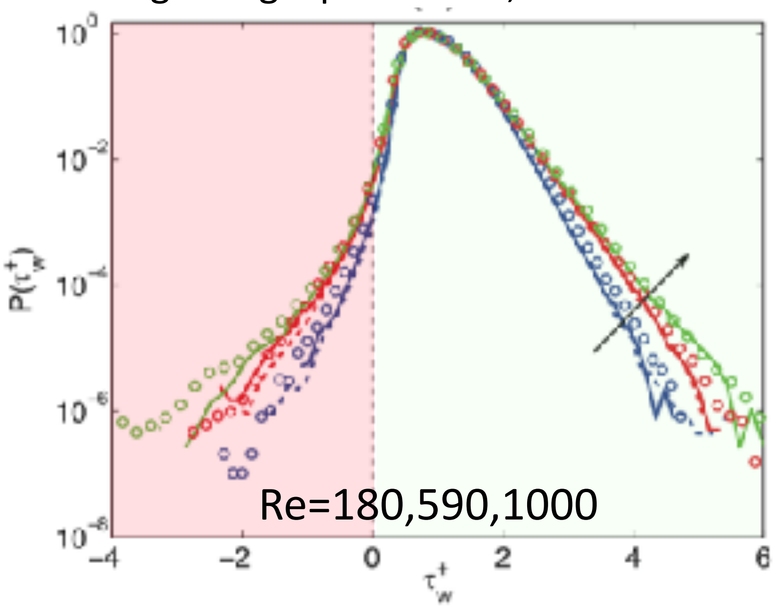
Mean Velocity Profile

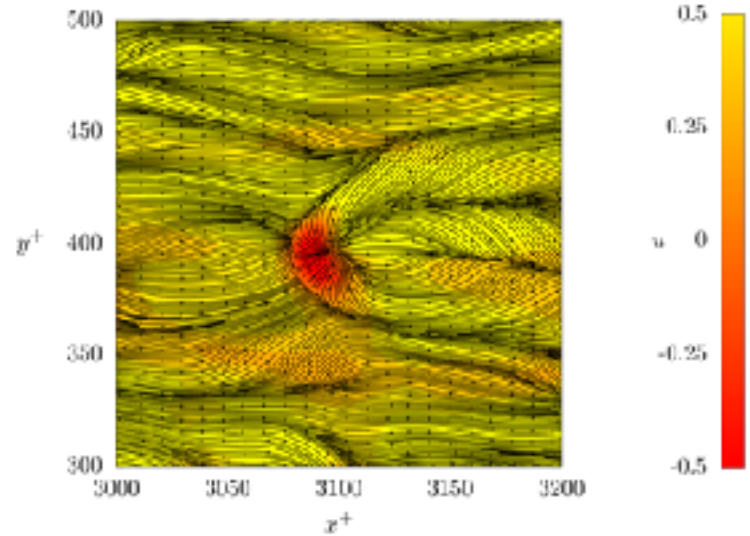


An important character: Wall-shear stress



Considering a single phase-flow, from literature:





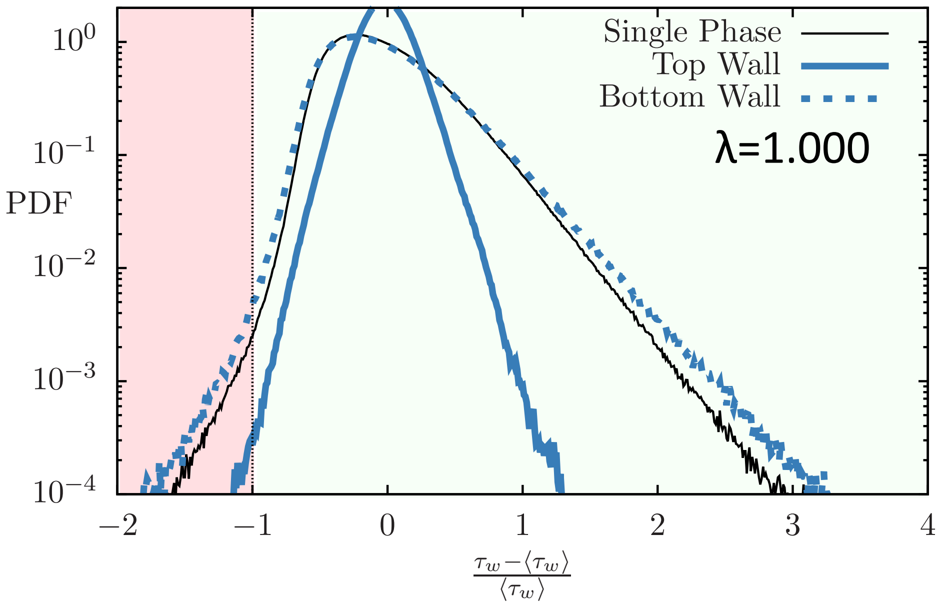
A. Wietrzak et al., *Wall shear stress and velocity in a turbulent axisymmetric boundary layer*, JFM (1994)
K.J. Colella et al., *Measurements and scaling of wall shear stress fluctuations*, EF (2003)
P. Leanars et al, *Rare back-flow and extreme wall-normal velocity fluctuations in near-wall turbulence*,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

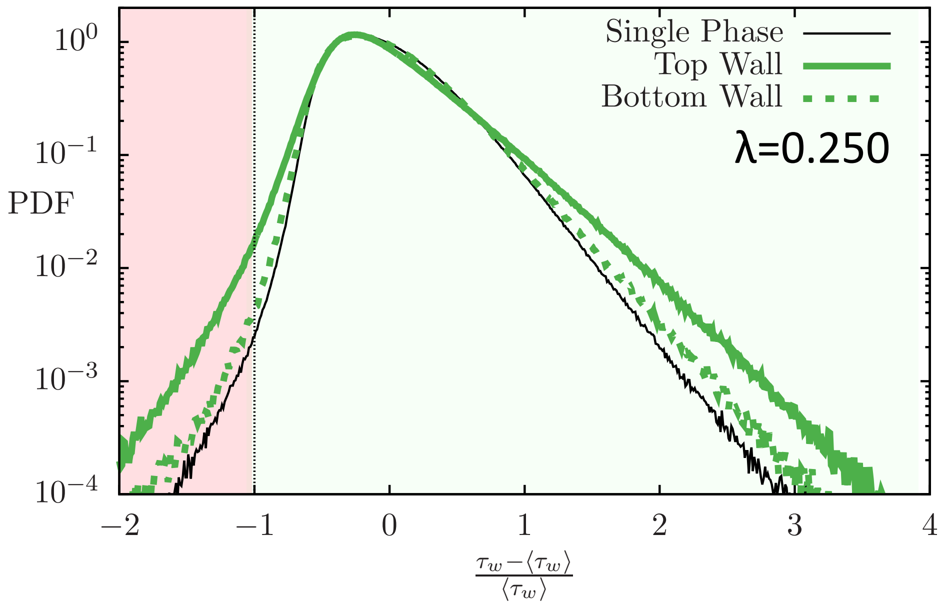
Wall-shear stress:stratified case

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





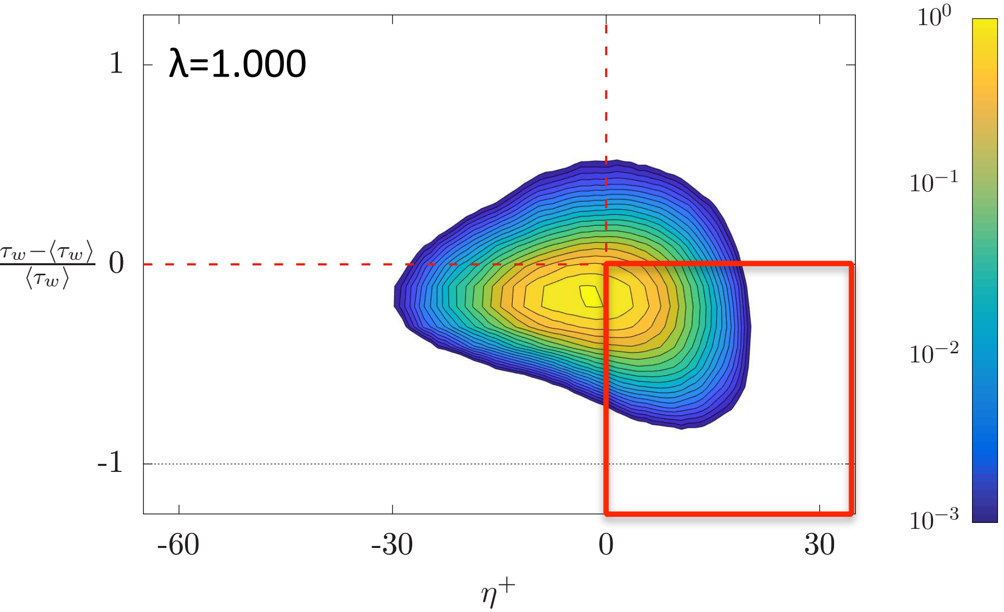
Top: Shape is modified, fluctuations reduced.
Bottom: Slight increase of the fluctuations.

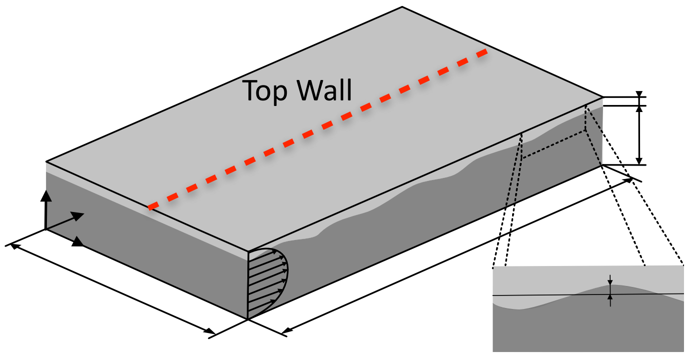
Top: Increase of the fluctuations..
Bottom: Slight increase of the fluctuations.

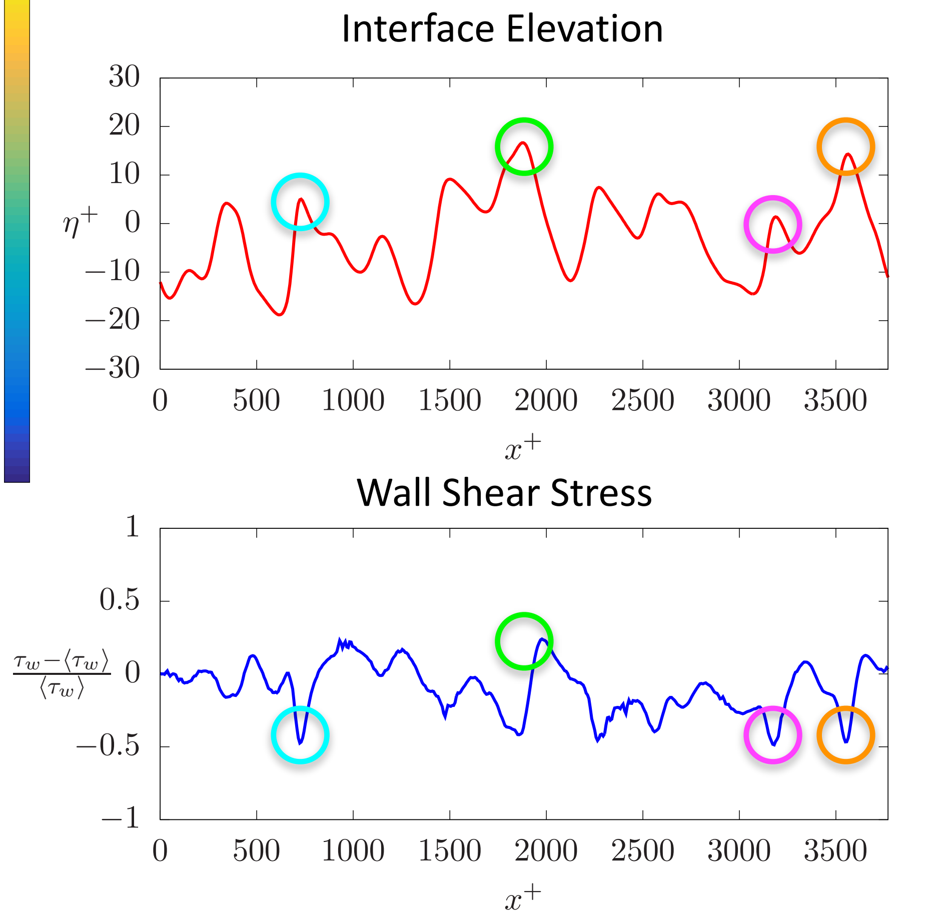
P. Leaners et al, *Rare backflow and extreme wall-normal velocity fluctuations in near-wall turbulence*, PoF (2017)
S. Ahmadi et al, *Turbulent drag reduction in channel flow with viscosity stratified fluids*, C&F (2017)
S. Ahmadi et al, *Turbulent drag reduction by a near wall surface tension active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

Interface-wall interaction

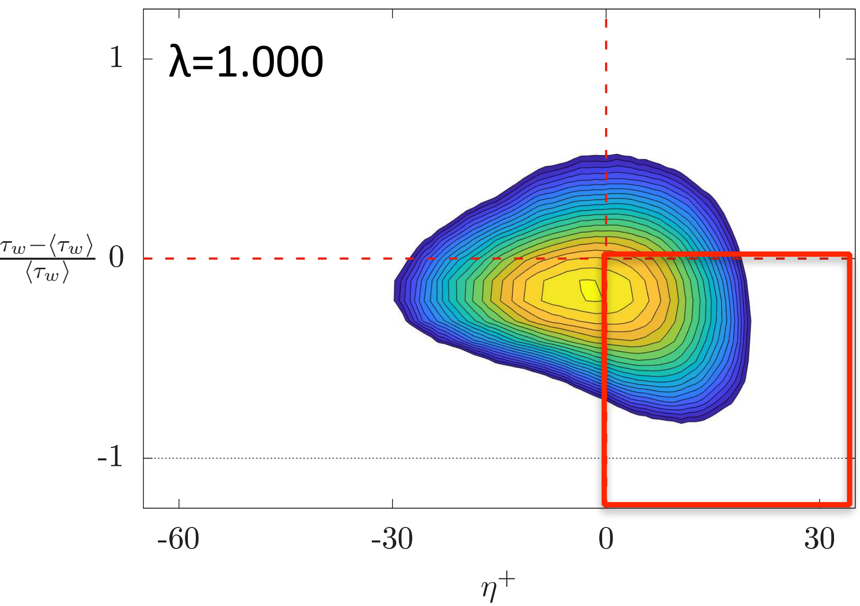
Joint-PDF between the wall shear stress and the interface elevation (Top Wall):

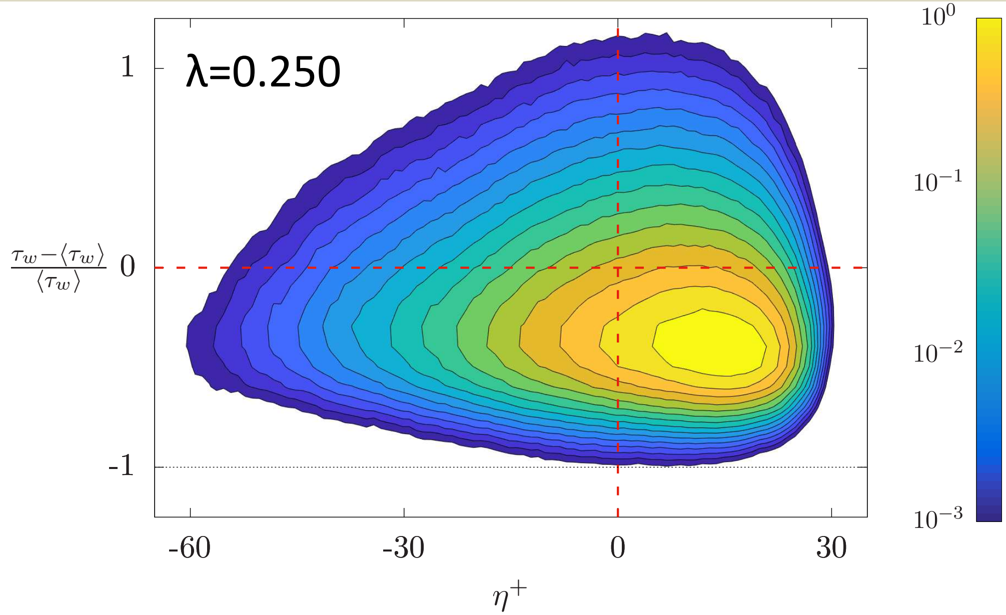






Interface-wall interaction



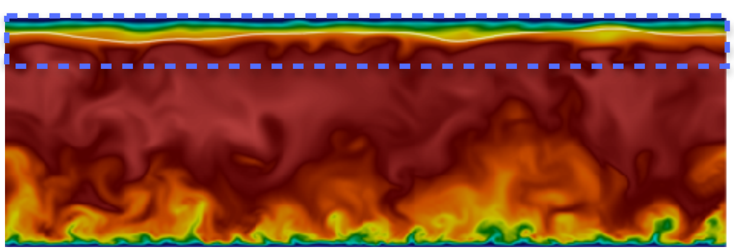


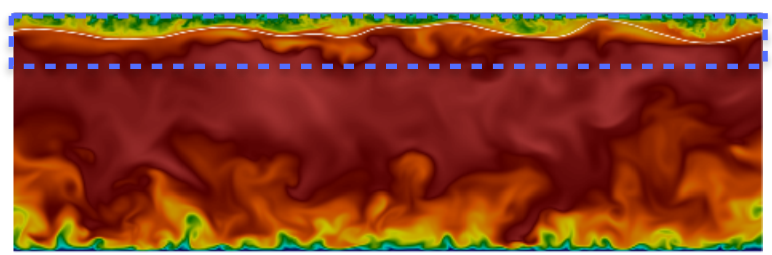
λ=1.000

Correlation between Wall Shear Stress And Interface Elevation

λ=0.250

Smaller Structures, interaction is weaker.





Constant Power Input (CPI) Simulations

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.

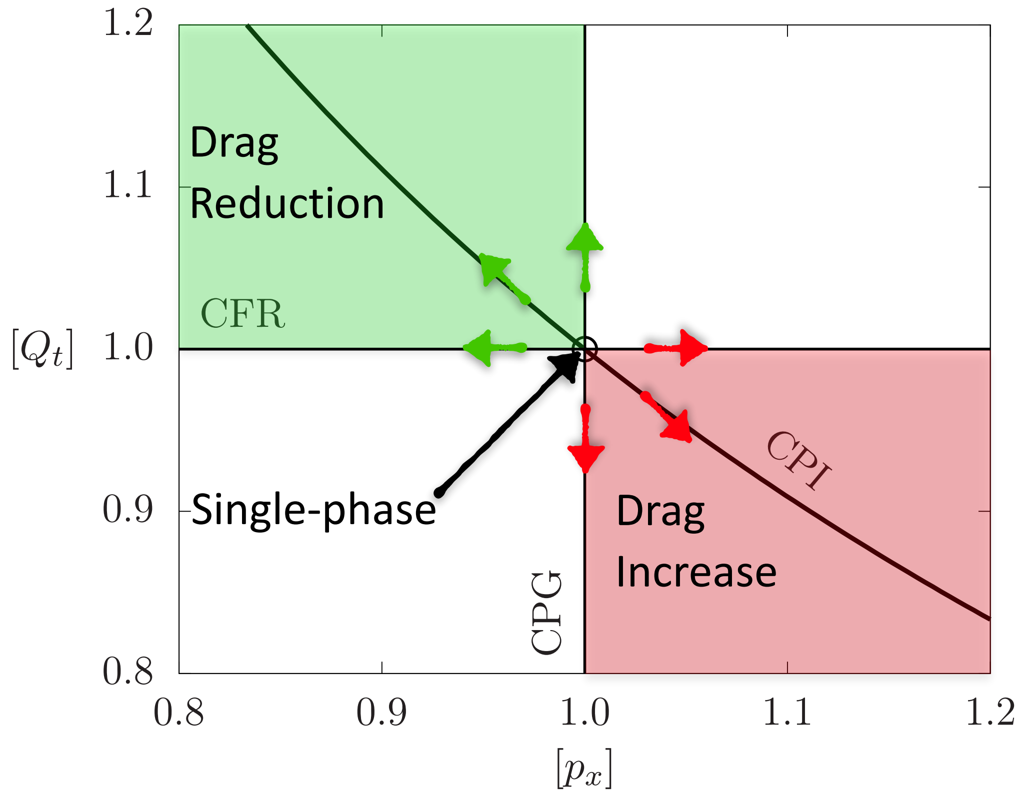
Third possible approach:

- 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., *Energy balance in lubricated drag-reduced turbulent channel flow* JFM (2021)
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)

CPI Simulations
Simulation setup

Characteristic velocity based on the power injected in the system:

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

Flow parameters:

Reynolds number (inertia/viscous)

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

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

Weber number (inertia/interfacial)

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

Phase field parameters:

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

We consider 5 different viscosity ratios λ :

(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

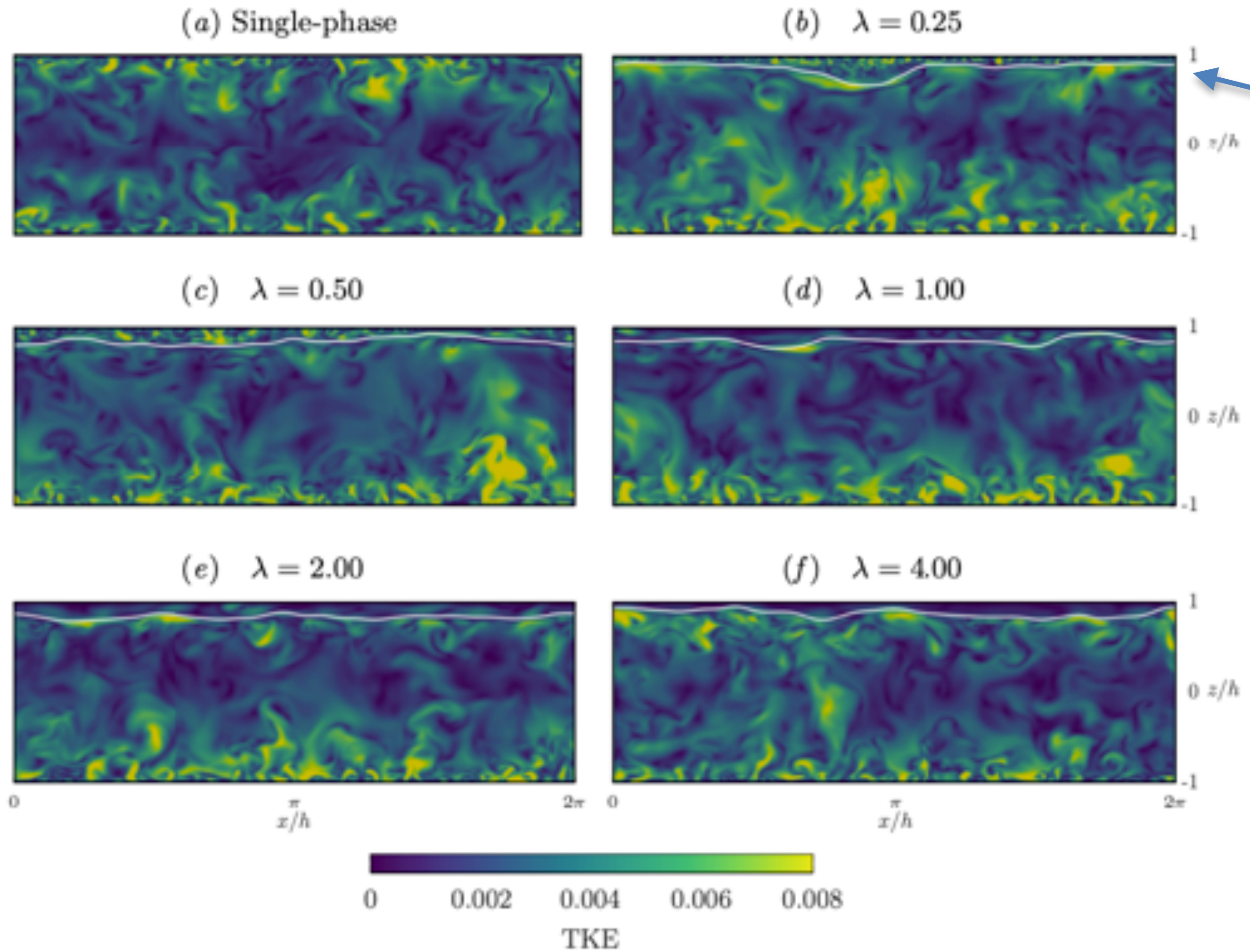
Grid resolution:

512 x 256 x 257 (Single-phase)

1024 x 512 x513 (Stratified cases)

Roccon et al., *Energy balance in lubricated drag-reduced turbulent channel flow*, JFM (2021)
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
Visualizations



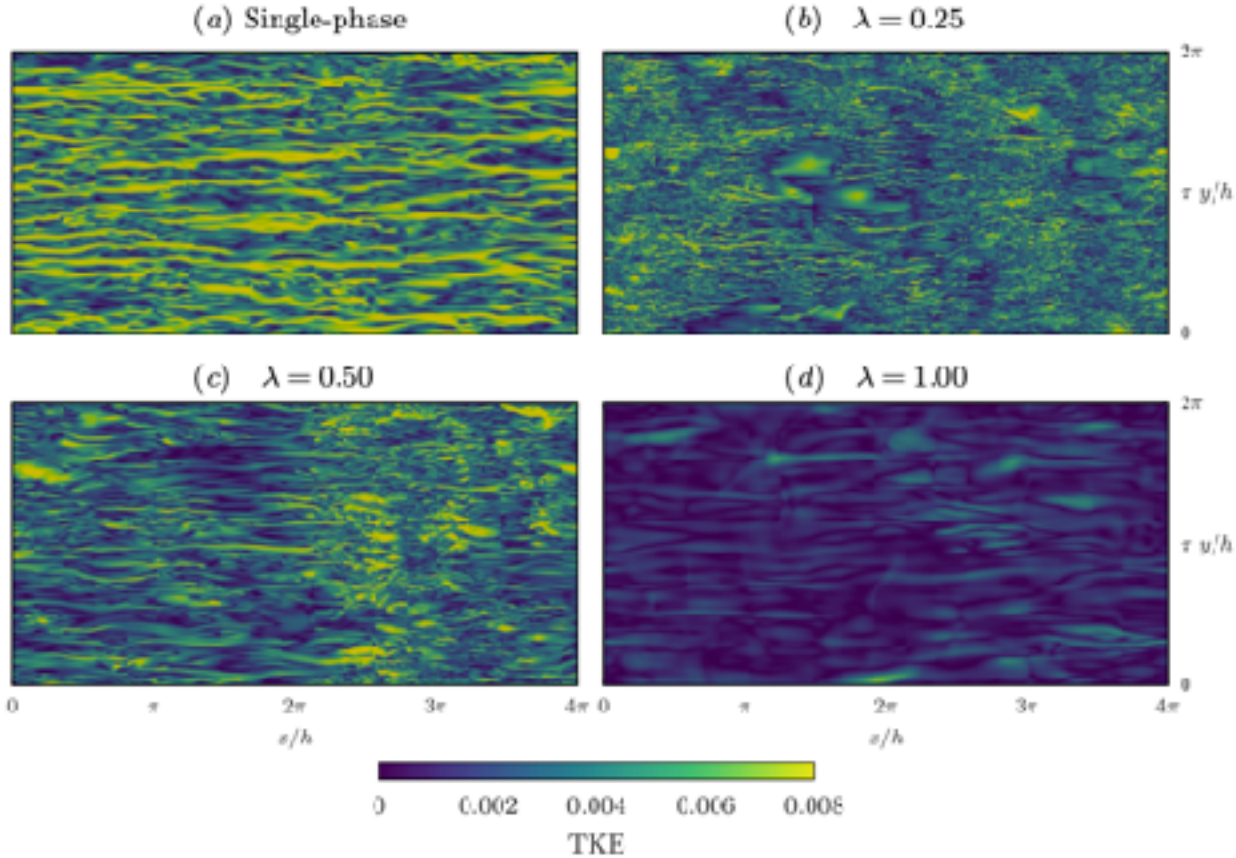
Interface: thin white line

Turbulence in the lubricating layer for $\lambda < 1$

Relaminarization in the lubricating layer for $\lambda > 1$

Roccon et al., Energy balance in lubricated drag-reduced turbulent channel flow JFM (2021)

Flow structures, focus on the lubricating layer (horizontal plane close to the top wall, $z/h = 0.97$)

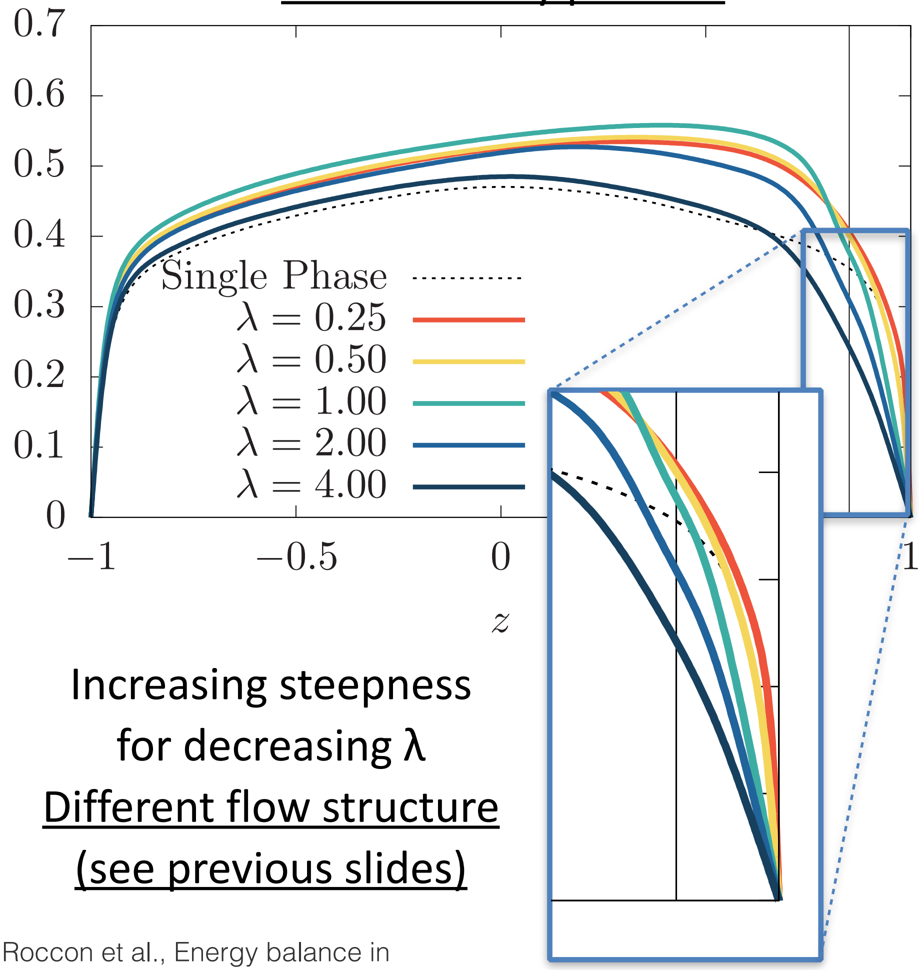


Laminar patches and turbulence, $\lambda < 1$

Relaminarization, $\lambda > 1$ (only $\lambda = 1$ is shown)

Roccon et al., Energy balance in lubricated drag-reduced turbulent channel flow JFM (2021)

Mean velocity profiles:



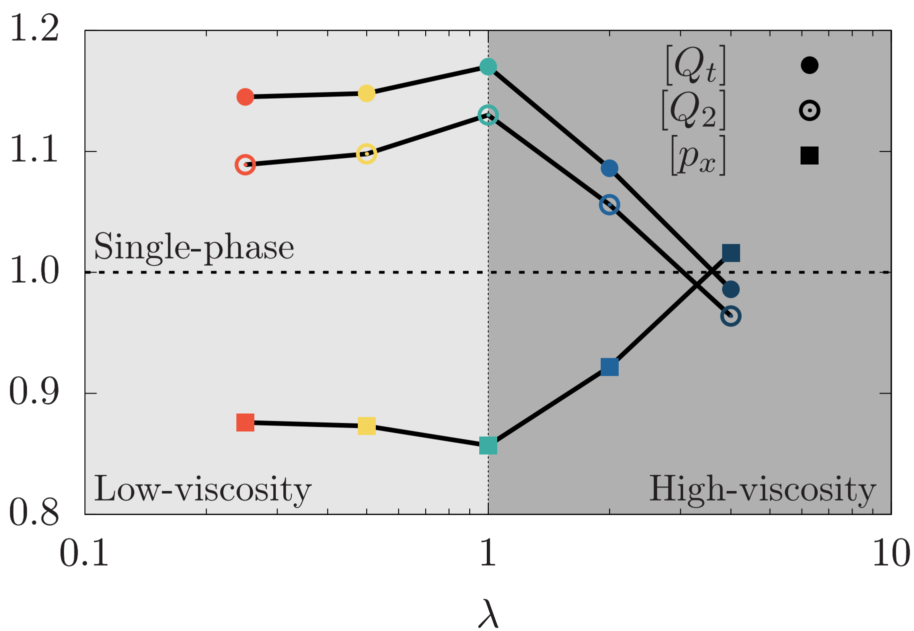
Increasing steepness for decreasing λ

Different flow structure (see previous slides)

Roccon et al., Energy balance in lubricated drag-reduced turbulent channel flow JFM (2021)

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

Flow-rates and pressure gradient:



Results
The energy box concept

Mean and Turbulent Kinetic energy budgets (single phase flow)

$$MKE = \frac{1}{2}\langle u_i\rangle\langle u_i\rangle; \quad TKE = \frac{1}{2}u_i'u_i'$$

$$\frac{D\,[\mathrm{MKE}]}{Dt} = \underbrace{-[\langle u_i\rangle\langle p_x\rangle]}_{\Pi_m} + \underbrace{\left[\langle u_i'u_j'\rangle\frac{\partial\langle u_i\rangle}{\partial x_j}\right]}_{P_k} - \underbrace{\left[\frac{\partial(\langle u_i'u_j'\rangle\langle u_i\rangle)}{\partial x_j}\right]}_{T_m} + \underbrace{\left[\frac{1}{2Re_\Pi}\frac{\partial^2\langle u_i\rangle^2}{\partial x_j^2}\right]}_{D_m} - \underbrace{\left[\frac{1}{Re_\Pi}\frac{\partial\langle u_i\rangle}{\partial x_j}\frac{\partial\langle u_i\rangle}{\partial x_j}\right]}_{\epsilon_m},$$

$$\frac{D\,[\mathrm{TKE}]}{Dt} = -\underbrace{\left[\frac{\partial\langle p'u_i'\rangle}{\partial x_i}\right]}_{\Pi_k} - \underbrace{\left[\langle u_i'u_j'\rangle\frac{\partial\langle u_i\rangle}{\partial x_j}\right]}_{P_k} - \underbrace{\left[\frac{1}{2}\frac{\partial\langle u_i'u_i'u_j'\rangle}{\partial x_j}\right]}_{T_k} + \underbrace{\left[\frac{1}{2Re_\Pi}\frac{\partial^2\langle u_i'u_i'\rangle}{\partial x_j^2}\right]}_{D_k} - \underbrace{\left[\frac{1}{Re_\Pi}\frac{\partial u_i'}{\partial x_j}\frac{\partial u_i'}{\partial x_j}\right]}_{\epsilon_k}.$$

Where:

Π_m = Power injected by mean pressure gradient
P_k = Production of TKE
T_m = Work done by Reynolds stresses
D_m = Viscous diffusion of MKE
ϵ_m = Mean flow viscous dissipation
Π_k = Pressure diffusion
T_k = Turbulent diffusion
D_k = Viscous diffusion of TKE
ϵ_k = Turbulent viscous dissipation

Integrating over the domain:

$$\overline{P_k} + \overline{\Pi_m} + \overline{\epsilon_m} = 0; \quad -\overline{P_k} + \overline{\epsilon_k} = 0;$$

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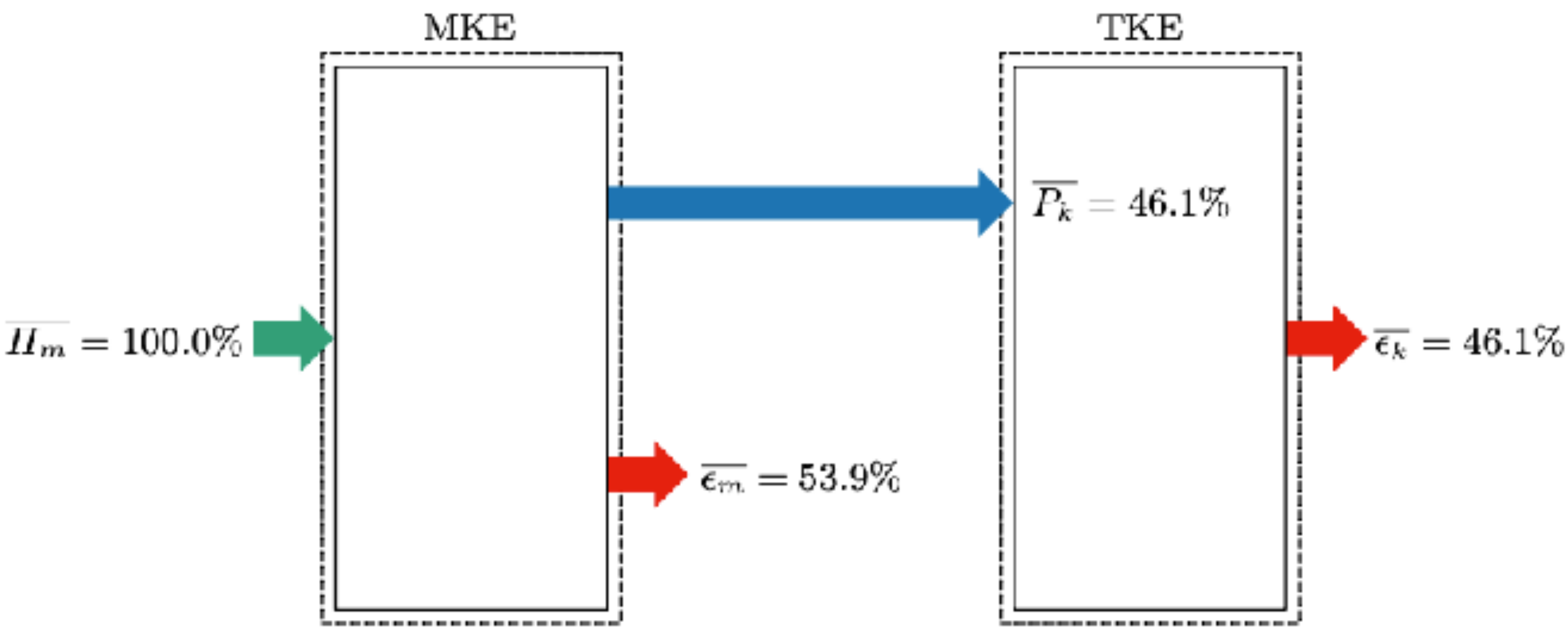
Results
The energy box concept

Energy Box representation



Integrating over the domain:

$$\overline{P_k} + \overline{\Pi_m} + \overline{\epsilon_m} = 0; \quad -\overline{P_k} + \overline{\epsilon_k} = 0;$$

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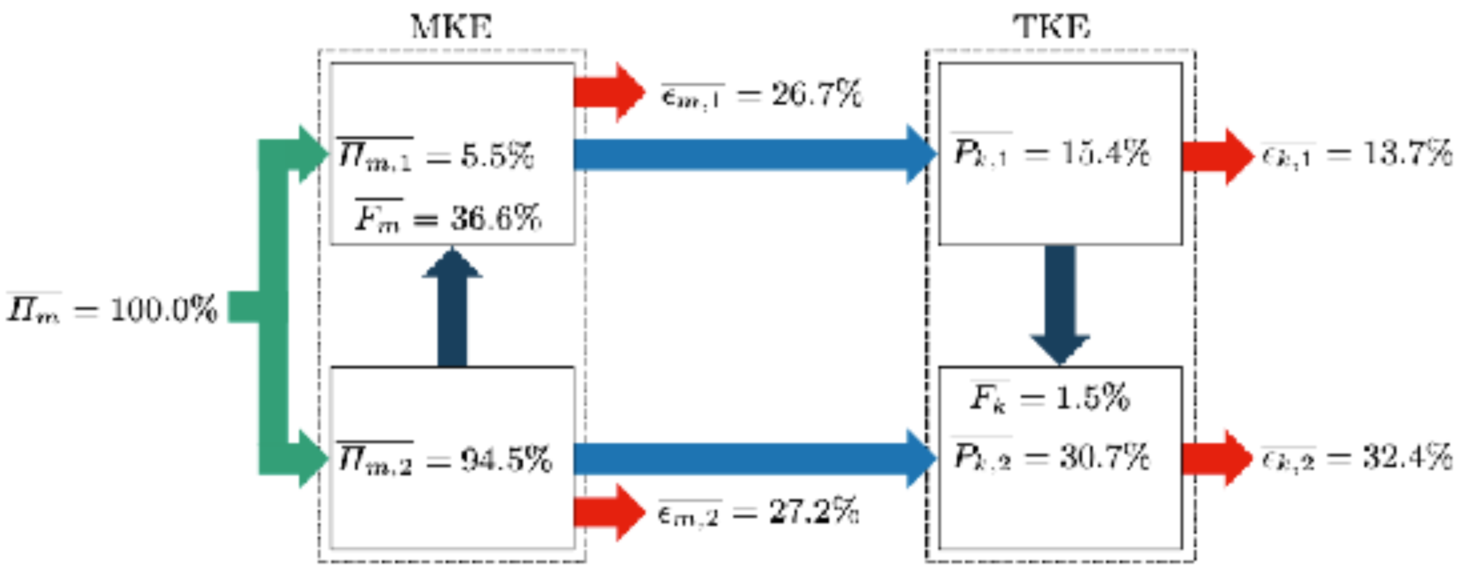
Results
The energy box concept

For the lubricated channel, we introduce the **phase-averaged energy box (**this grants us access to the exchange of energy between the two phases).

For example, take a **“virtually-lubricated” channel** (single phase channel, assuming a virtual separation interface —located where the real interface of the lubricate channel is)



We introduce an energy transfer efficiency:

$$\mathscr{H}_{sp} = \frac{\overline{\epsilon_{m,2}}}{\overline{\epsilon_{m,2}} + \overline{\epsilon_{k,2}}} = 0.456$$

i.e. energy dissipated by mean flow, compared to the maximum theoretical energy contained in the primary layer

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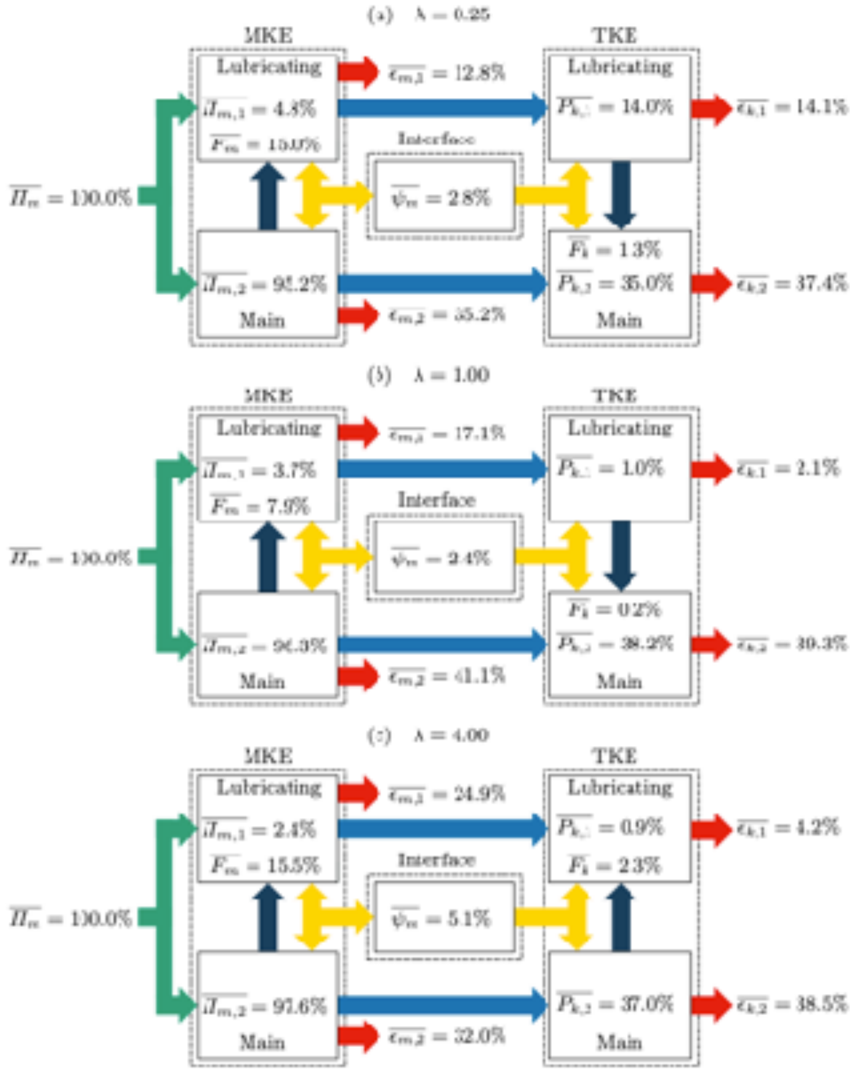
Results
The energy box concept

$\lambda = 0.25$:
$\mathscr{H}/\mathscr{H}_{sp} = 1.06$

$\lambda = 1$:
$\mathscr{H}/\mathscr{H}_{sp} = 1.11$

$\lambda = 4$:
$\mathscr{H}/\mathscr{H}_{sp} = 0.99$



Note: DR when ϵ_m increases and ϵ_k decreases

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