Physics and High Performance Computation of Turbulent Flows with Interfaces

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Outline of the seminar

- Part I   Introduction: Spectral and Pseudo-Spectral Methods
- Part II   thermally stratified fluids: internal waves and beyond
- Part III   Surface waves
- Part IV   Droplets in turbulence
- Part V   Carbon capture

Discussion on Numerics & Physics Involved

(always with **an eye on applications**)

Spectral and Pseudo-spectral

Methods to discretize the differential operators
Idea: approximate a function (unknown, which satisfies PDE+bc) using a linear combination of ''test'' functions that are <u>GLOBAL</u>

approximation

$$u(x) = \sum_{k=0}^{N} c_k \varphi_k(x)$$

Common also to finite difference and finite element methods

For spectral methods:
Global functions (defined in each node, and not equal to zero!)

Putting into the PDE equation+bc:

$$Lu(x) = s(x)$$ ← Domain

$$Bu(y) = 0$$ ← Boundary

Solution $\bar{u}$

$L\bar{u} - s$ Minimizes the residual

<u>We will obtain the solution (c_k)</u>

Spectral methods at a glance:

- Assume a basis (test functions; depend on the problem)

- Assume a number N of polynomials such that

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

- Substitute it into the pde+bc

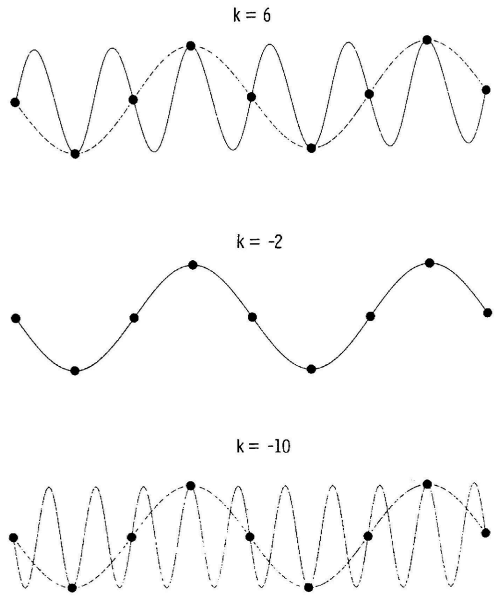
- Minimize the residual to find the coefficients of the spectral representation

Tau	Minimize the residual in each node
Galerkin	Minimize the integral of the residual (over the domain)

BC for tau methods: add BC to the system (extra equations)
BC Galerkin: combine the basic functions to form new functions fulfilling BC

WHY PSEUDO-SPECTRAL?

- Products in modal space: convolution $O(N^2)$
- Transform into physical space, multiply and back to modal $O(N \log_2 N)$
- Aliasing error (2/3 rules)



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

Aliasing of sin(-2x) wave by sin(10x) wave

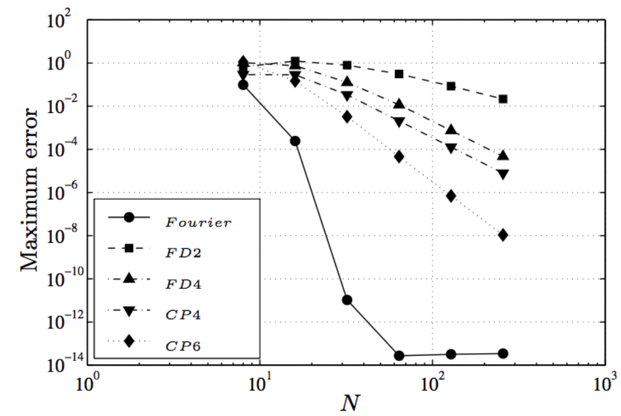
Canuto et al (1998)

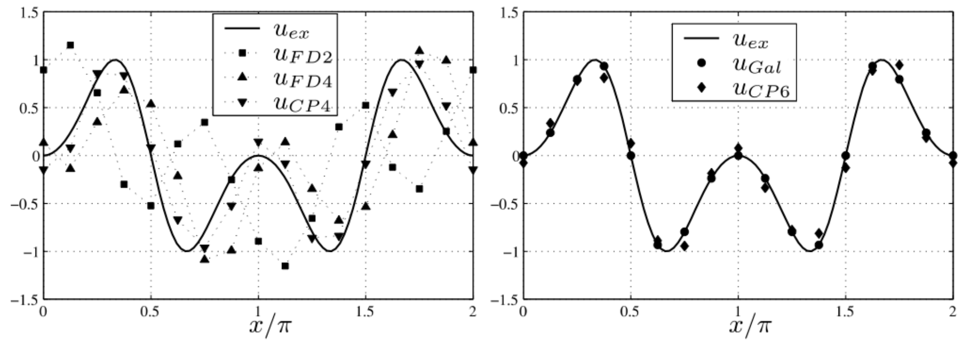
Spectral and Pseudo-spectral

Pro and Con

- In general, spectral accuracy and convergence

- With FFTW, good performances





- Aliasing

- Not easy to code

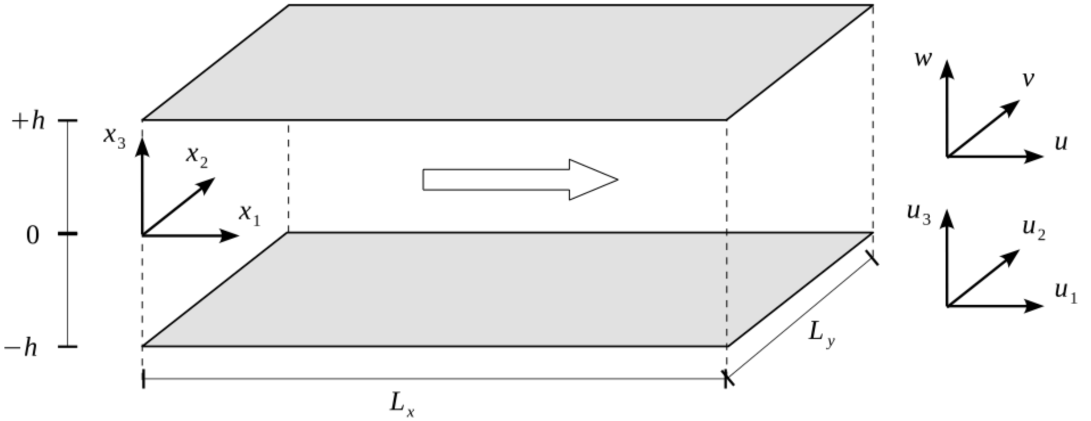
- Usually less flexible (simple geomtry). But…….

Canuto et al (2010)

$$\frac{\partial u_i}{\partial x_i} = 0$$

$$\frac{\partial u_i}{\partial t} = S_i + \frac{1}{\mathrm{Re}_\tau}\frac{\partial^2 u_i}{\partial x_j^2} - \frac{\partial p}{\partial x_i}$$

$$S_i = -\frac{\partial u_1 u_j}{\partial x_j} + \delta_{1,j}$$



Curl

$$\frac{\partial \omega}{\partial t} = \nabla \times S + \frac{1}{\mathrm{Re}_\tau}\nabla^2 \omega$$

2nd Curl+Continuity+Vectorial Identity

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

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

This leads to the following system:

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

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

$$\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} = -\frac{\partial u_3}{\partial x_3}$$

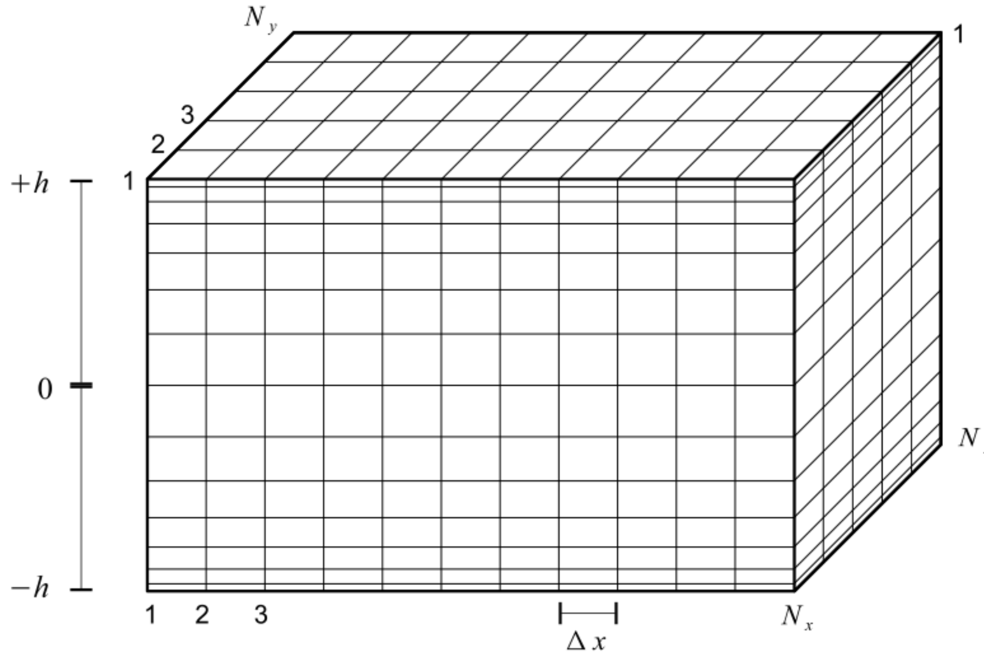
$$\frac{\partial u_2}{\partial x_1} - \frac{\partial u_1}{\partial x_2} = \omega_3$$

Discretization strategy

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

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

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



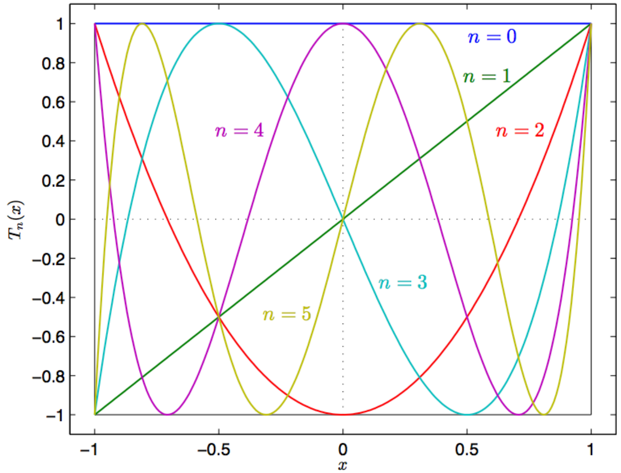
Spatial discretization: Fourier +

$$f\left(x_1,x_2,x_3\right)=\sum_{n_1}\sum_{n_2}\hat{f}\left(k_1,k_2,x_3\right)e^{i\left(k_1x_1+k_2x_2\right)}$$

$$k_1=\frac{2\pi n_1}{L_x};k_2=\frac{2\pi n_2}{L_y}$$

Chebyshev

$$f\left(x_1,x_2,x_3\right)=\sum_{n_1}\sum_{n_2}\sum_{n_3}\hat{f}\left(k_1,k_2,n_3\right)T_{n_3}(x_3)e^{i\left(k_1x_1+k_2x_2\right)}$$



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

We get the following discrete equations:

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

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

Continuity and vorticity

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

Vorticity transport

$$\frac{\partial \hat{\omega}_3}{\partial t} = \xi + \psi$$

Splitting of the operator

Convective terms: Adams Bashfort
Diffusive terms: cranck-Nicolson

$$\hat{\omega}_3^{n+1} = \hat{\omega}_3^n + \Delta t\left(\frac{3}{2}\xi^n - \frac{1}{2}\xi^{n-1}\right) + \frac{\Delta t}{2}\left(\psi^{n+1} + \psi^n\right)$$

After some algebra

$$\frac{\hat{\omega}_3^{n+1}-\hat{\omega}_3^{n}}{\Delta t}=ik_1\left[\left(\frac{3}{2}\hat{S}_2^{n}-\frac{1}{2}\hat{S}_2^{n-1}\right)+\frac{1}{2\,\mathrm{Re}_\tau}\left(\frac{\partial^2}{\partial x_3^2}-k^2\right)\hat{u}_2^{n}\right]$$

$$-ik_2\left[\left(\frac{3}{2}\hat{S}_1^{n}-\frac{1}{2}\hat{S}_1^{n-1}\right)+\frac{1}{2\,\mathrm{Re}_\tau}\left(\frac{\partial^2}{\partial x_3^2}-k^2\right)\hat{u}_1^{n}\right]+$$

$$+\frac{1}{2\,\mathrm{Re}_\tau}\left(\frac{\partial^2}{\partial x_3^2}-k^2\right)\omega_3^{n+1}$$

Finally

$$\left(\frac{\partial^2}{\partial x_3^2} - k^2\right)\omega_3^{n+1} = -\frac{1}{\gamma}\left(ik_1 H_2^n - ik_2 H_1^n\right)$$

$$H_i^n = \Delta t\left(\frac{3}{2}S_i^n - \frac{1}{2}S_i^{n-1}\right) + \left(\gamma\frac{\partial^2}{\partial x_3^2} + \left(1-\gamma k^2\right)\right)\hat{u}_i^n$$

Similarly for the vertical velocity

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

$$H^n = \frac{\partial}{\partial x_3}\left(ik_1 H_1^n + ik_2 H_2^n\right) + k^2 H_3^n$$

$$\gamma = \frac{\Delta t}{2\,\mathrm{Re}_\tau};\ \beta = \frac{1+\gamma k^2}{\gamma}$$

Dicrete ''version'' of the final system to be solved

$$\left(\frac{\partial^2}{\partial x_3^2} - k^2\right)\omega_3^{n+1} = -\frac{1}{\gamma}\left(ik_1 H_2^n - ik_2 H_1^n\right)$$

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

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

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

Helmholtz equations

CHEBYSHEV-TAU METHOD

$$\phi''(x) - \alpha^2\phi(x) = H(x)$$

General Helmholtz equation

$$p_1\phi(-1) + q_1\phi'(-1) = r_1$$
$$p_2\phi(+1) + q_2\phi'(+1) = r_2$$

Boundary conditions

Functions are represented through Chebyshev polynomials

$$\phi(x) = \sum_{n=0}^{N} a_n T_n(x) = a_0 T_0(x) + a_1 T_1(x) + \ldots$$

$$H(x) = \sum_{n=0}^{N} b_n T_n(x) = b_0 T_0(x) + b_1 T_1(x) + \ldots$$

$$\phi''(x) - \alpha^2 \phi(x) = H(x)$$

Integrated twice Helmholtz equation

$$\phi(x) - \alpha^2 \iint \phi(y)\, dy\, dy = \iint H(y)\, dy\, dy + Ax + B$$

Using the Chebyshev representation of the functions, we have

$$\sum_{n=0}^{N} a_n T_n(x) - \alpha^2 \iint \sum_{n=0}^{N} a_n T_n(y) dy dy = \iint \sum_{n=0}^{N} b_n T_n(y) dy dy + Ax + B$$

Integrals can be evaluated using some properties of Chebyshev series

$$\int \phi(y)\, dy = \int \sum_{n=0}^{N} a_n T_n(y) = \sum_{n=1}^{N+1} l_n T_n(x)$$

$$\iint \phi(y)\, dy = \int \sum_{n=1}^{N+1} l_n T_n(y) = \sum_{n=2}^{N+2} m_n T_n(x)$$

Where the coefficients l_n and m_n can be obtained from a_n using recursive rules of Chebyshev polynomials

We finally get

$$\sum_{n=0}^{N} a_n T_n(x) - \alpha^2 \sum_{n=2}^{N+2} m_n T_n(x) = \sum_{n=2}^{N+2} f_n T_n(x) + A T_1(x) + B T_0(x)$$

where

$$T_1(x) = x$$

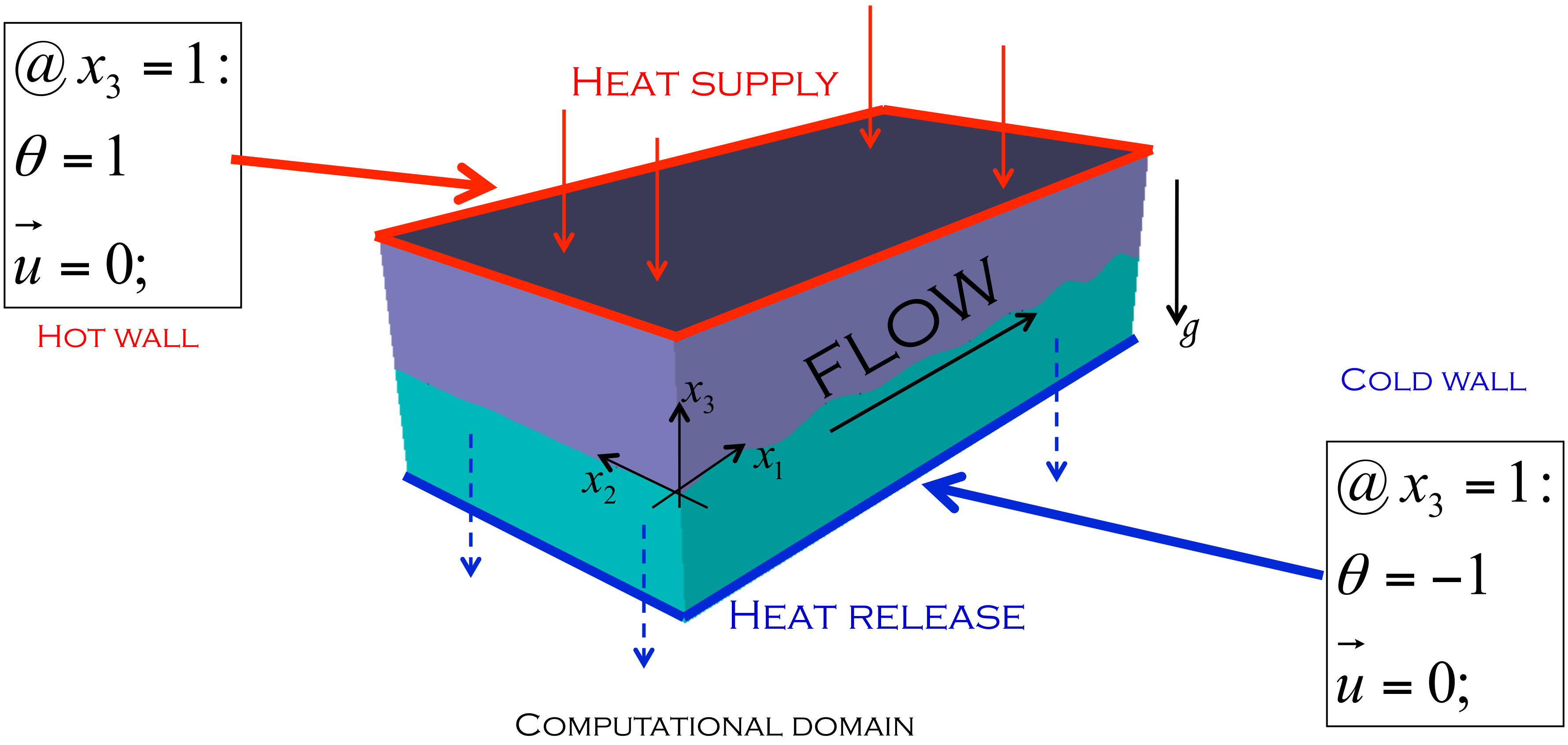
$$T_0(x) = 1$$

To solve this equation, we first define the residual:

$$R(x) = \left(a_0 - B\right) T_0(x) + \left(a_1 - A\right) T_1(x) + \sum_{n=2}^{N} s_n T_n(x)$$

Minimize R(x); solve a linear system (Gauss) to find the coefficients of the Chebyshev series a_n

$$s_n = a_n - \alpha^2 m_n - f_n$$


$@x_3 = 1:$
$\theta = 1$
$\vec{u} = 0;$
HOT WALL
HEAT SUPPLY
FLOW
g
x_3
x_1
x_2
COLD WALL
$@x_3 = 1:$
$\theta = -1$
$\vec{u} = 0;$
HEAT RELEASE
COMPUTATIONAL DOMAIN

Stably stratified turbulence: OB approx.

$$\frac{\partial u_i}{\partial x_i} = 0$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = \frac{1}{\mathrm{Re}_\tau}\frac{\partial^2 u_i}{\partial x_j^2} - \frac{\partial p}{\partial x_i} - \frac{1}{16}\frac{Gr}{\mathrm{Re}_\tau^2}\delta_{i,3}\theta$$

$$\frac{\partial \theta}{\partial t} + u_j \frac{\partial \theta}{\partial x_j} = \frac{1}{\mathrm{Re}_\tau \mathrm{Pr}}\frac{\partial^2 \theta}{\partial x_j^2}$$

$$Gr = \frac{g\beta\Delta\theta_{HC}(2h)^3}{\nu^2} \qquad \mathrm{Pr} = \frac{\mu c_p}{\lambda} = \frac{\nu}{k}$$

Physical parameters

$\Delta\theta_{HC} = 40°C$

$\theta_m = 50°C$

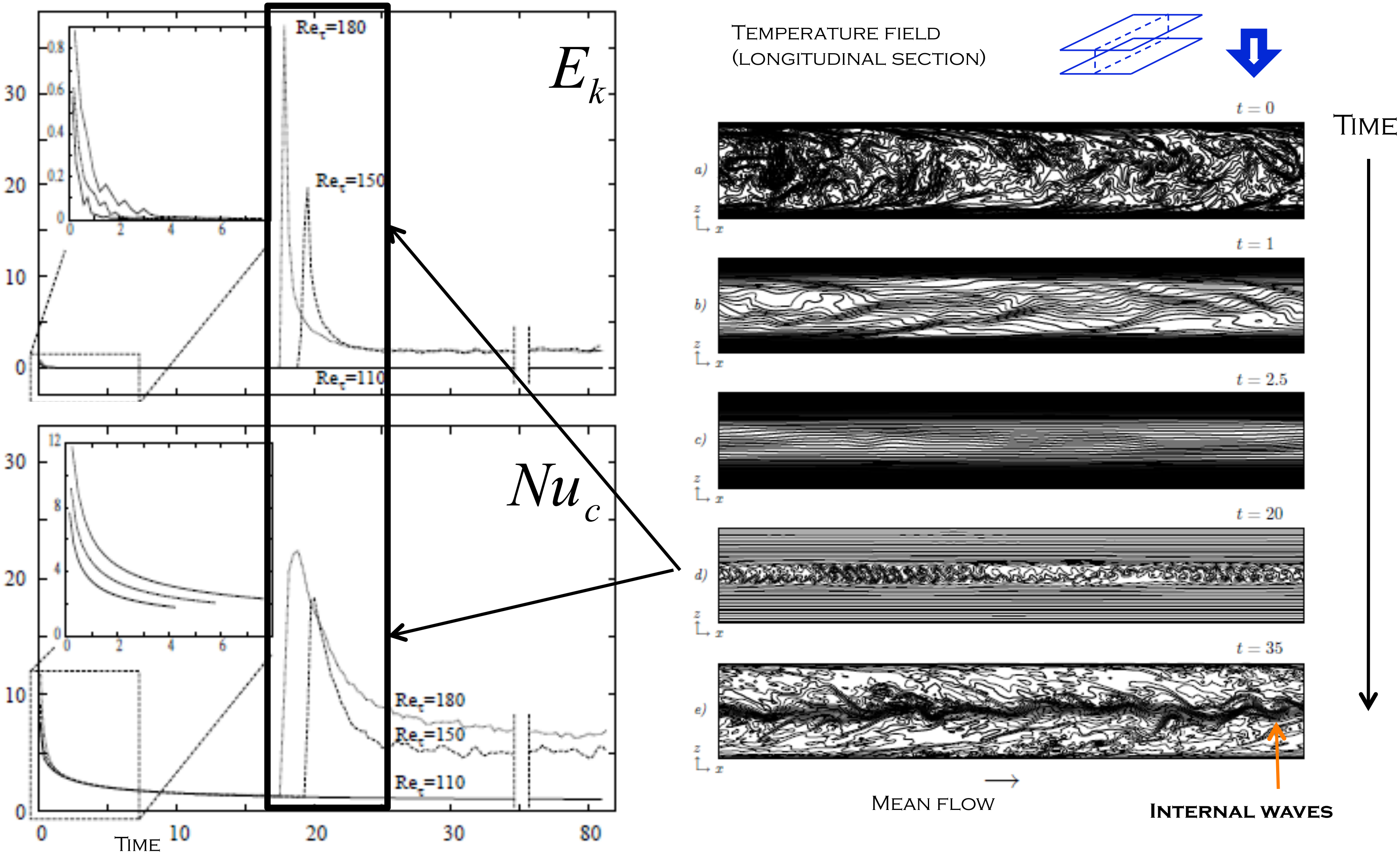
$\mathrm{Pr} = 3$

$\mathrm{Re}_\tau = 110 \div 180$

$Gr \approx 10^7$

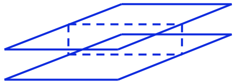
$Ri_\tau = \frac{Gr}{\mathrm{Re}_\tau^2}$

Stably stratified turbulence: Transient development of the flow

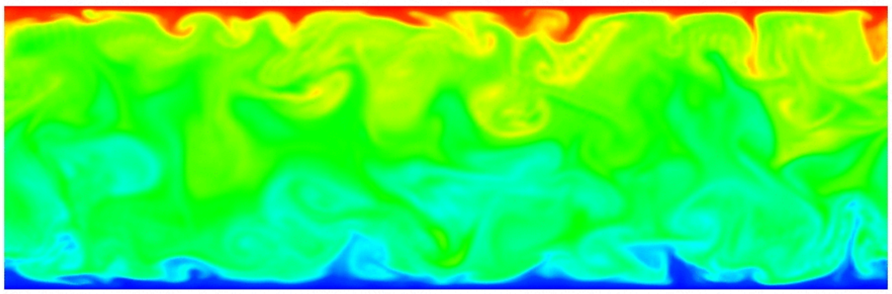


The role of buoyancy: Neutrally-buoyant vs stably stratified

Visualization on a cross section

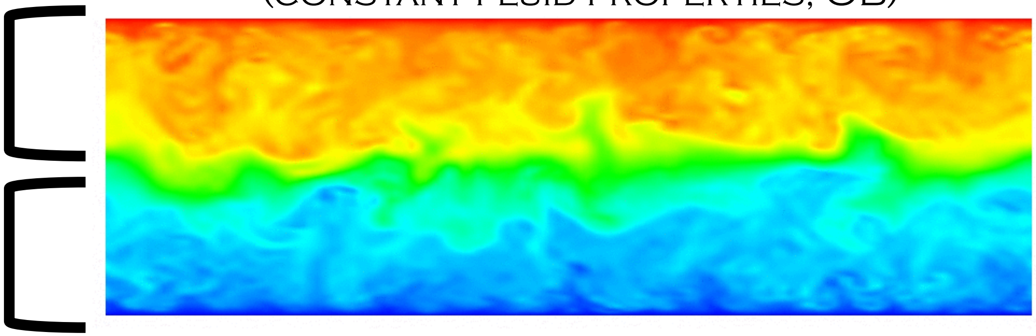


Neutrally buoyant



Mixing
(driven by turbulence structures)

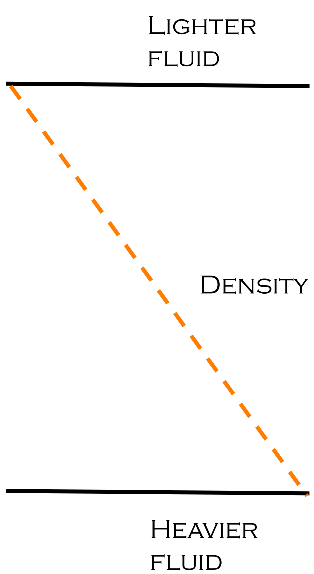
Stably-stratified
(constant fluid properties, OB)



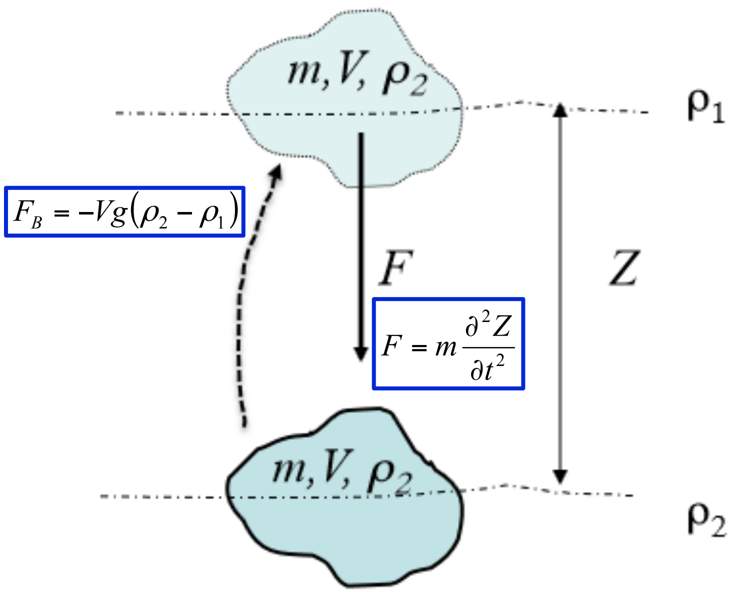
Internal waves=barrier
(two ''independent '' zones)

The oring of internal waves...next slide!

Stably stratified turbulence: The origin of Internal waves



Force balance on a fluid particle:



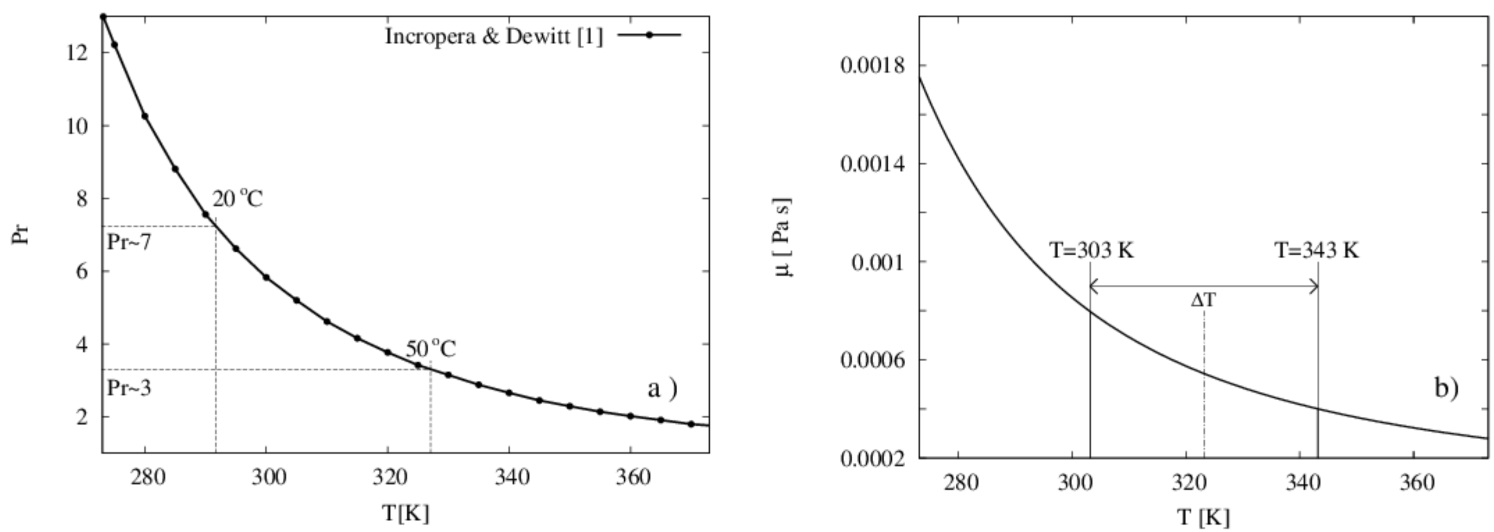
$$\begin{cases} \dfrac{\partial^2 Z}{\partial t^2} = \dfrac{g}{\rho}\dfrac{\partial \rho}{\partial z} Z = N^2 Z \\ N = \left(\dfrac{g}{\rho}\dfrac{\partial \rho}{\partial z}\right)^{1/2} \end{cases}$$

N: **Buoyancy frequency**
Or
Brunt-Vaisala frequency

Thermal-stratification in water beyond the Boussinesq assumption

So far we have considered uniform fluid properties

However…



μ, Pr

Stably stratified turbulence under NOB conditions: equations

$$\frac{\partial u_i}{\partial x_i} = 0$$

$$\frac{\partial u_i}{\partial t} = S_i + \frac{1}{\mathrm{Re}_\tau}\frac{\partial^2 u_i}{\partial x_j^2} - \frac{\partial p}{\partial x_i}$$

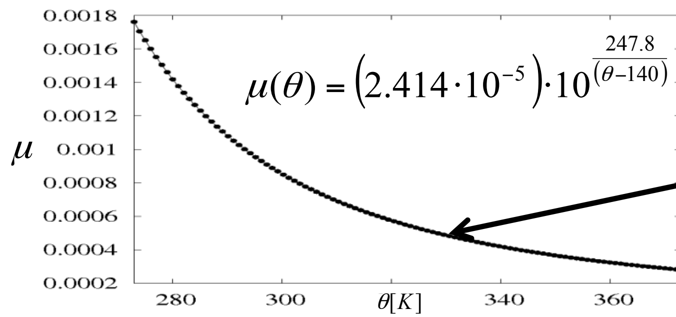
$$\frac{\partial \theta}{\partial t} + u_j \frac{\partial \theta}{\partial x_j} = \frac{1}{\mathrm{Re}_\tau \cdot \mathrm{Pr}}\frac{\partial^2 \theta}{\partial x_j^2}$$

$$S_i = -u_j \frac{\partial u_i}{\partial x_j} + \delta_{i,1} + \delta_{i,3}\frac{1}{16}\frac{Gr}{\mathrm{Re}_\tau^2}\theta$$

Uniform thermophysical properties (OB)

$$S_i = -u_j \frac{\partial u_i}{\partial x_j} + \frac{1}{\mathrm{Re}_\tau}\frac{\partial}{\partial x_j}\left(\mu_v \frac{\partial u_i}{\partial x_j}\right) + \delta_{i,1} + \delta_{i,3}\frac{1}{16}\frac{Gr}{\mathrm{Re}_\tau^2}\theta$$

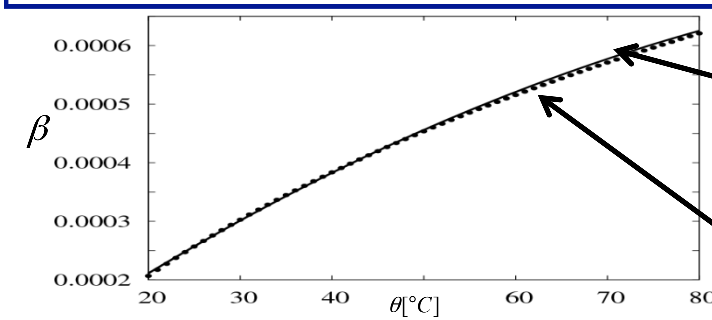
Temperature-dependent viscosity (NOB)



Symbols (Exp.): Incropera & Dewitt, (1985)

$$S_i = -u_j \frac{\partial u_i}{\partial x_j} + \delta_{i,1} + \delta_{i,3}\cdot g_i \cdot \rho_{ref}\left(\exp\left(-\int_{\theta_{ref}}^{\theta}\beta(\theta)d\theta\right) - 1\right)$$

Temperature-dependent thermal expansion coefficient (NOB)



Fitting (line)

$$\beta = 5.8\cdot 10^{-6} + 1.11\cdot 10^{-5}\theta - 4.196\cdot 10^{-8}\theta^2$$

Symbols (Exp.): Incropera & Dewitt, (1985)

$\Delta\theta = 40°C$

$\theta_m = 50°C$

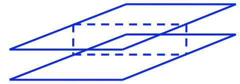
$\mathrm{Pr} = 3$

$Gr \approx 10^7$

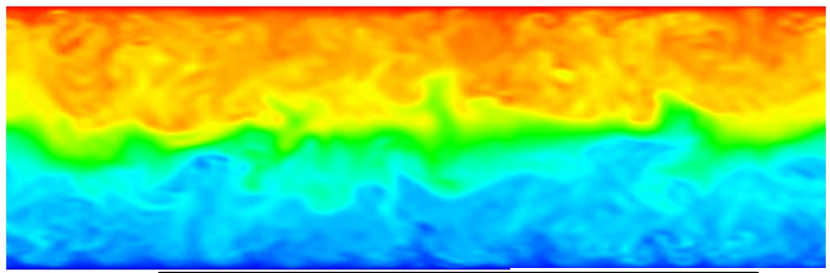
$Ri_\tau = \frac{Gr}{\mathrm{Re}_\tau^2}$

The role of Temperature dependent fluid properties

Visualization on a cross section

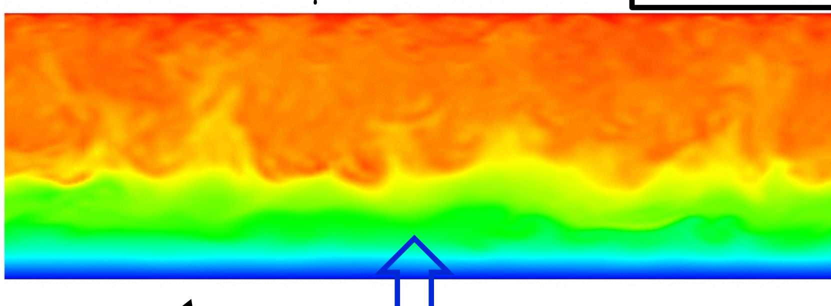


Stably-stratified
β,μ=constant - OB



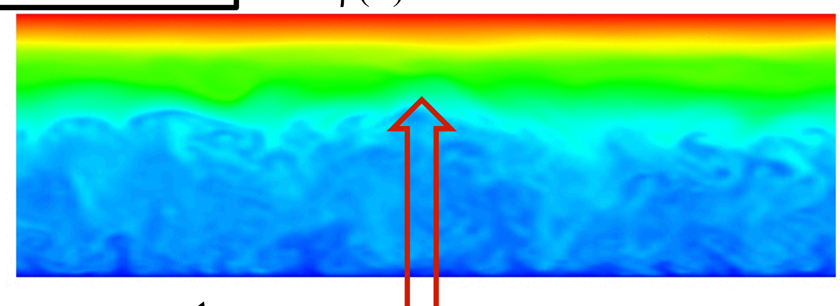
Local dynamics of the flow: VERY IMPORTANT (One-Sided Turbulence)

Stably-stratified
$\mu(T)$ - NOB



$\mu(T)\nearrow$ Laminar zone

Stably-stratified
$\beta(T)$ - NOB



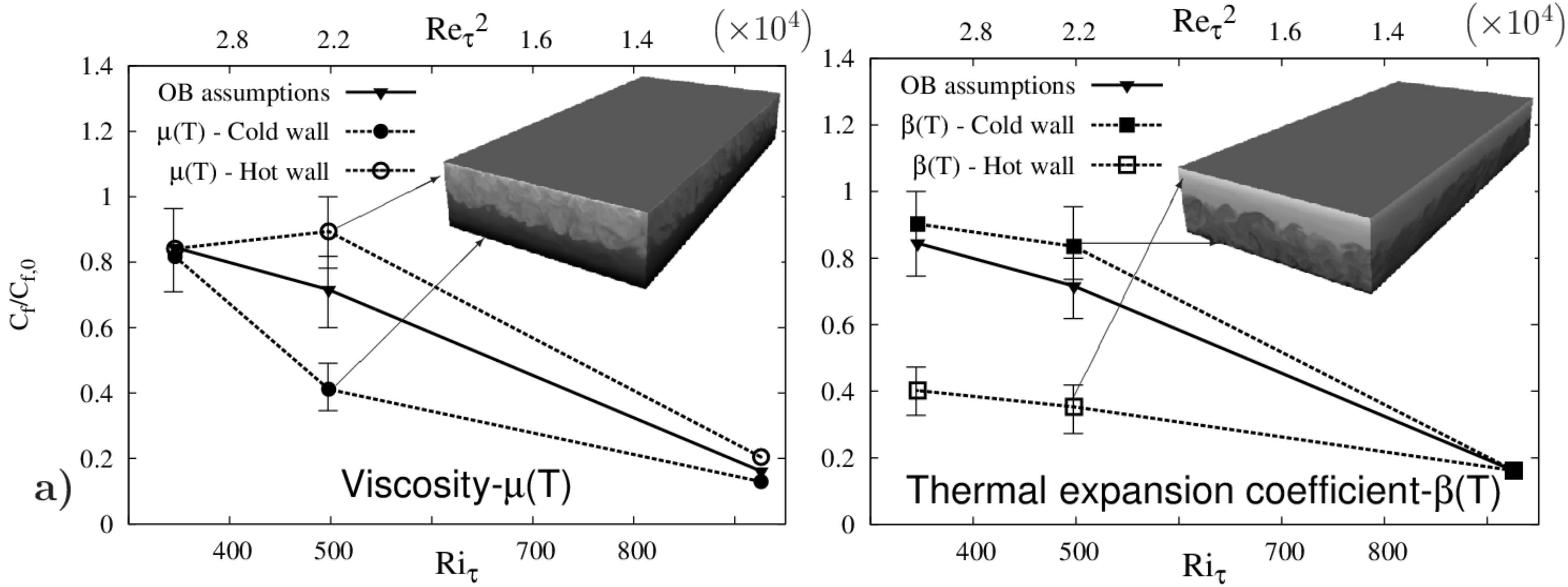
$\beta(T)\nearrow$ Laminar zone

Zonta et al., JFM, 697, 175-203 (2012)

Momentum and heat transfer coefficient-2

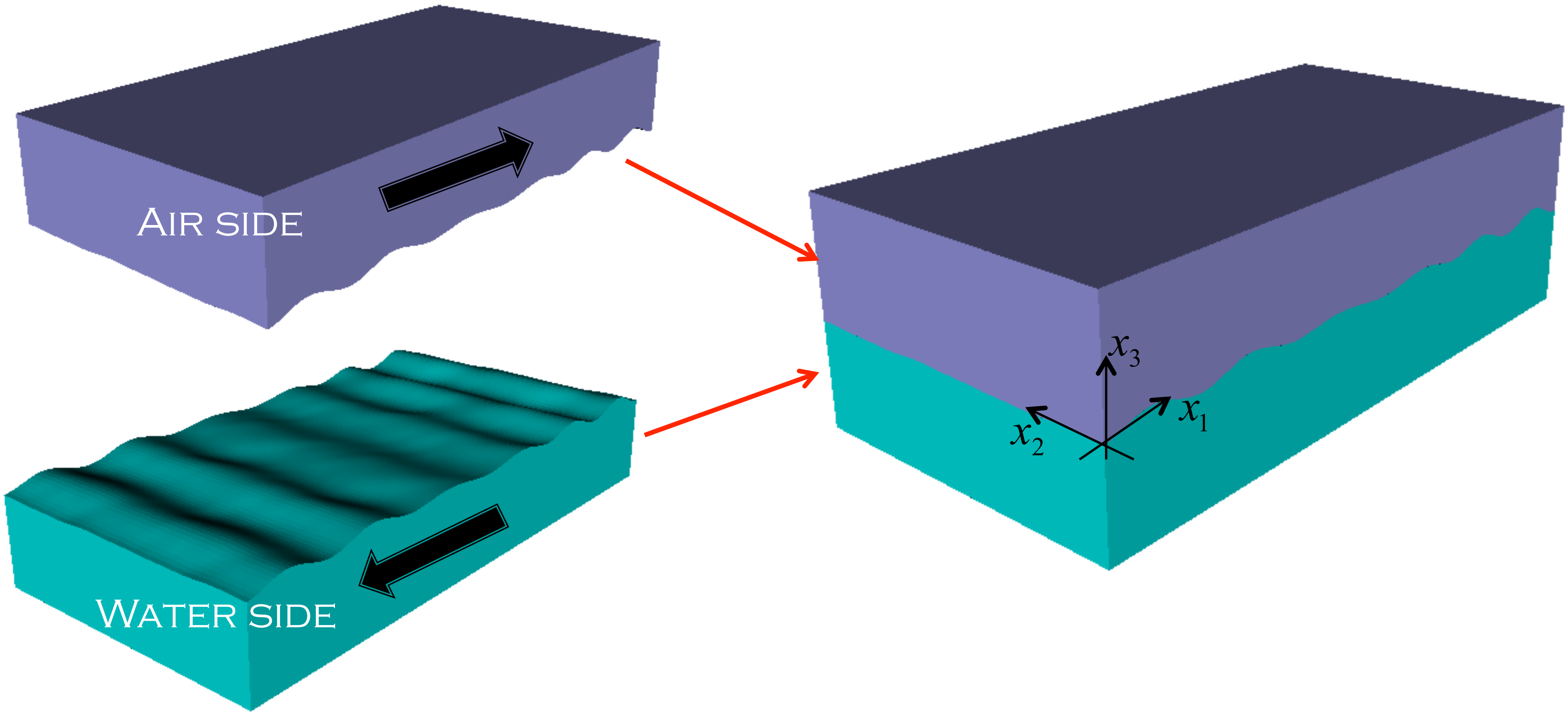
$$C_f = \frac{2\tau_w}{\rho u_b^2}$$

Local value of the shear stress



PART III: SURFACE WAVES

PHYSICAL CONFIGURATION

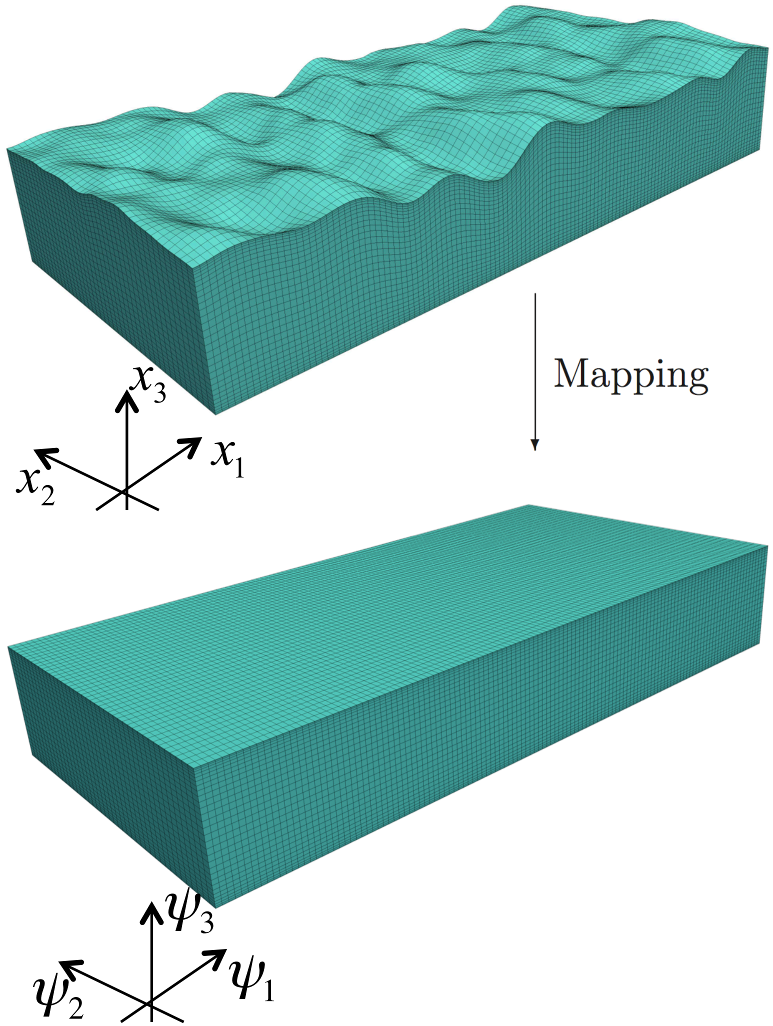


COUNTERCURRENT AIR-WATER FLOW
(DRIVEN BY PRESSURE GRADIENT)

GOVERNING EQUATIONS - PHYSICAL DOMAIN

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

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



ALGEBRAIC MAPPING

$$\psi_1 = x$$

$$\psi_2 = y$$

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

$$\tau = t$$

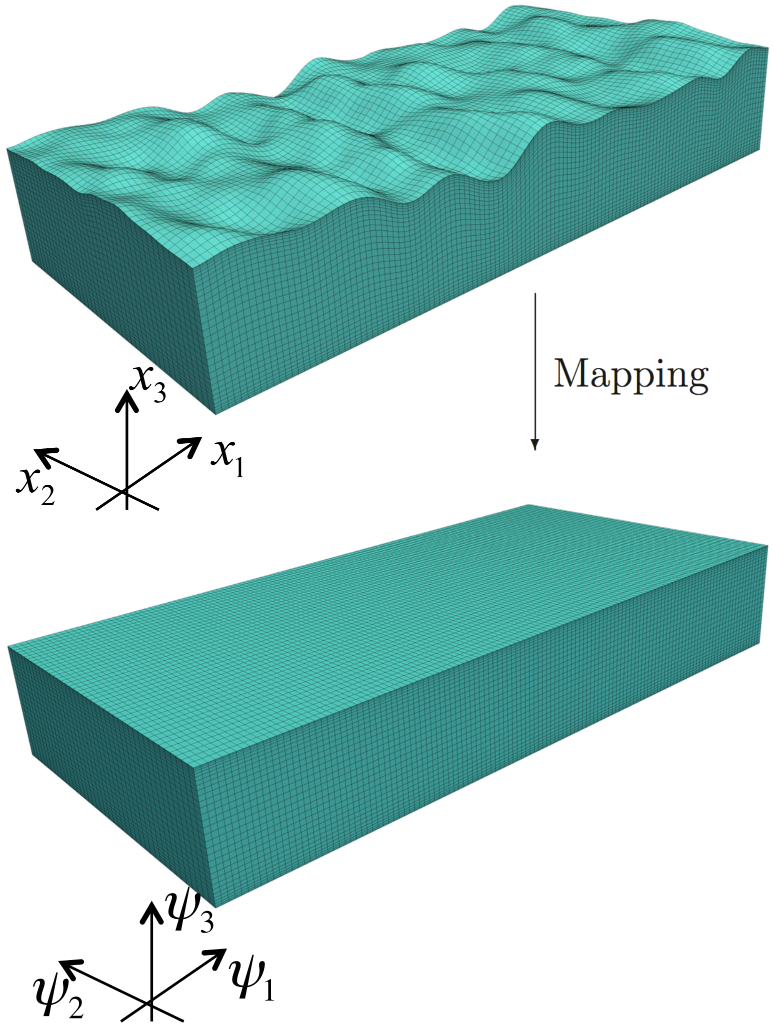
Jacobian & derivatives

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

$$\partial_X = J \cdot \partial_\psi$$

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

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



Equations & Numerical Methodology

Fractional-step technique

Provisional time step

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

Convective term: Adams-Bashfort explicit (M=2, α_0=3/2, α_1=-1/2)

Correction to obtain divergence-free field

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

Taking divergence & u^{n+1} div. free:

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

Solve to give p^{n+1} & u^{n+1}

Equations & Numerical Methodology

Spatial discretization

$$\Phi(\psi_i) = \sum_{k_1,k_2,k_3} \hat{\Phi}(k_1,k_2,n_3)\, e^{i(k_1\psi_1+k_2\psi_2)}\, T_{n_3}(\psi_3)$$

Spectral amplitude

Chebyshev polynomials

$$T_{n_3}(\psi_3) = \cos\left[n_3 \cos^{-1}(\psi_3 / h)\right]$$

Discretized governing eq.: Cheb-tau method With <u>proper b.c.</u>

$$\left(\frac{d^2}{d\psi_3^2} - \beta\right)\hat{\hat{u}}_i = \frac{\hat{H}_i}{\delta} - F\left(\nabla^2_{off} u_i^n\right)$$

$$\hat{H}_i = \Delta t\left(\frac{3}{2}\hat{S}_i^n - \frac{1}{2}\hat{S}_i^{n-1}\right) + F\left(\delta\nabla^2_{diag} u_i^n\right) + u_i^n$$

$$\beta = \frac{1+\delta k^2}{\delta}; \delta = \frac{\Delta t}{2\,\mathrm{Re}_\tau}$$

S_i^n (Convective terms)

<u>F (Four.-Cheb. Transform)</u>

Boundary conditions

Interface

Kinematic B.C.

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

Dynamic B.C.

$@\, x_3 = 0:$

$$p_g - p_l - g(\rho_l - \rho_g)\eta = \left(\left(\vec{\tau}_g - \vec{\tau}_l\right)\cdot \vec{n}\right)\cdot \vec{n} + \gamma\kappa;$$

$$\left(\left(\vec{\tau}_l - \vec{\tau}_g\right)\cdot \vec{n}\right)\cdot \vec{t}_{1,2} = 0;$$

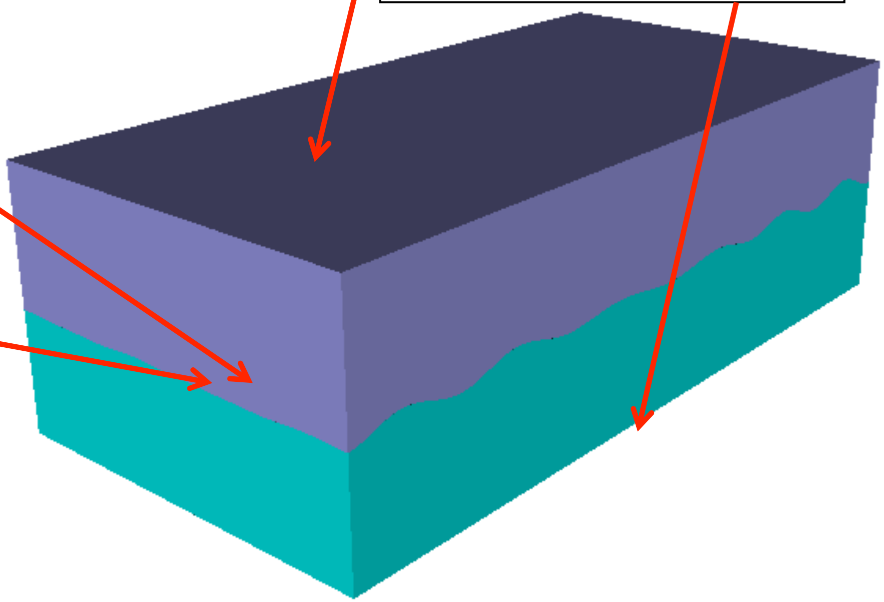
$$\vec{u}_g = \vec{u}_l;$$

(continuity of stress and velocity)

Free-Slip BC

$@\, x_3 = \pm h:$

$$\frac{\partial u_{1,2}}{\partial x_3} = \frac{\partial p}{\partial x_3} = 0; u_3 = 0;$$



Simulations: plan of experiments

Physical Problem
Liquid (l) : water
Gas (g): Air

Simulation	h	Re_τ	We	Fr	$Fr^{1/2}/We$
S1	0.045	170	8.5×10^{-4}	2.9×10^{-6}	2.03
S2	0.05	170	7.6×10^{-4}	2.2×10^{-6}	1.93
S3	0.06	170	6.3×10^{-4}	1.3×10^{-6}	1.4

Physical parameters

$$Re_{\tau,g} = \frac{\rho_g u_{\tau,g} h_g}{\mu_g}$$

$$Re_{\tau,l} = \frac{\rho_l u_{\tau,l} h_l}{\mu_l}$$

$$h_g = h_l$$

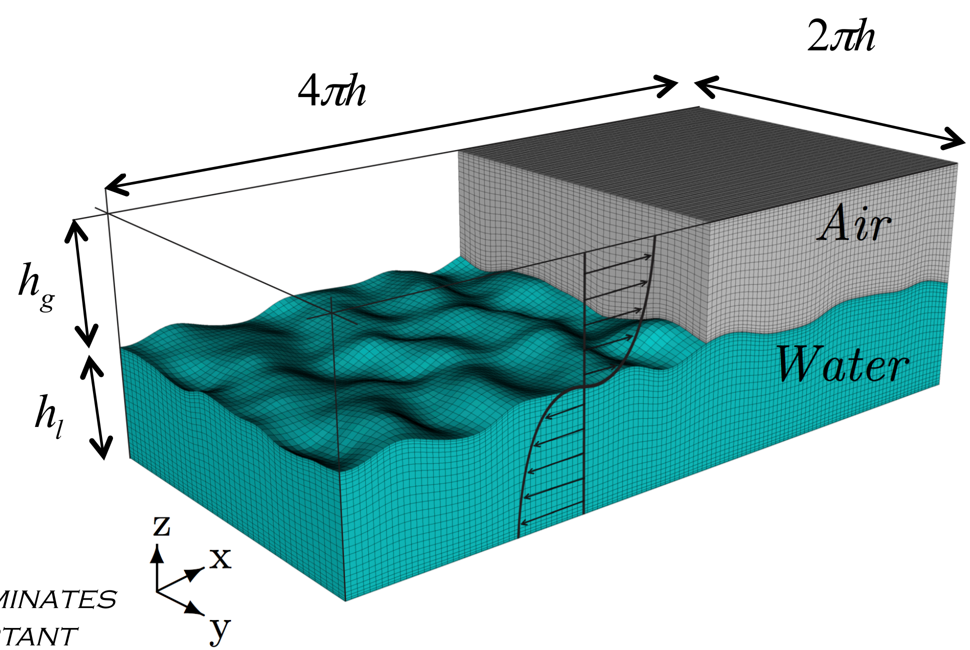
$$Re_{\tau,g} = Re_{\tau,l}$$

$$We = \frac{\rho_l h_l u_{\tau,l}^2}{\gamma}$$

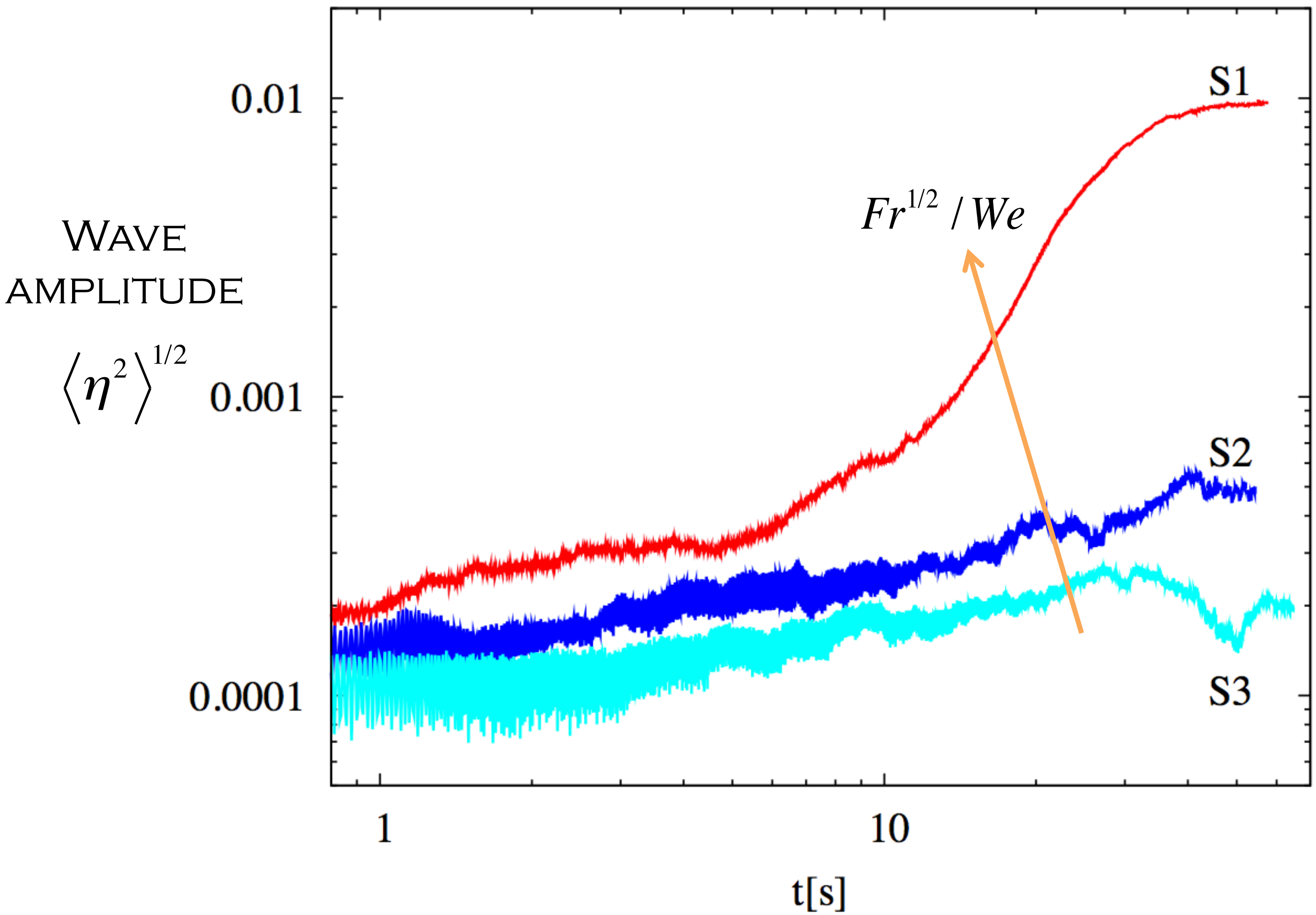
γ → *Surface tension*

$$Fr = \frac{\rho_l u_{\tau,l}^2}{g h_l (\rho_l - \rho_g)}$$

$Fr^{1/2} / We$ → *Smaller → surf. tension dominates*
Larger → gravity more important

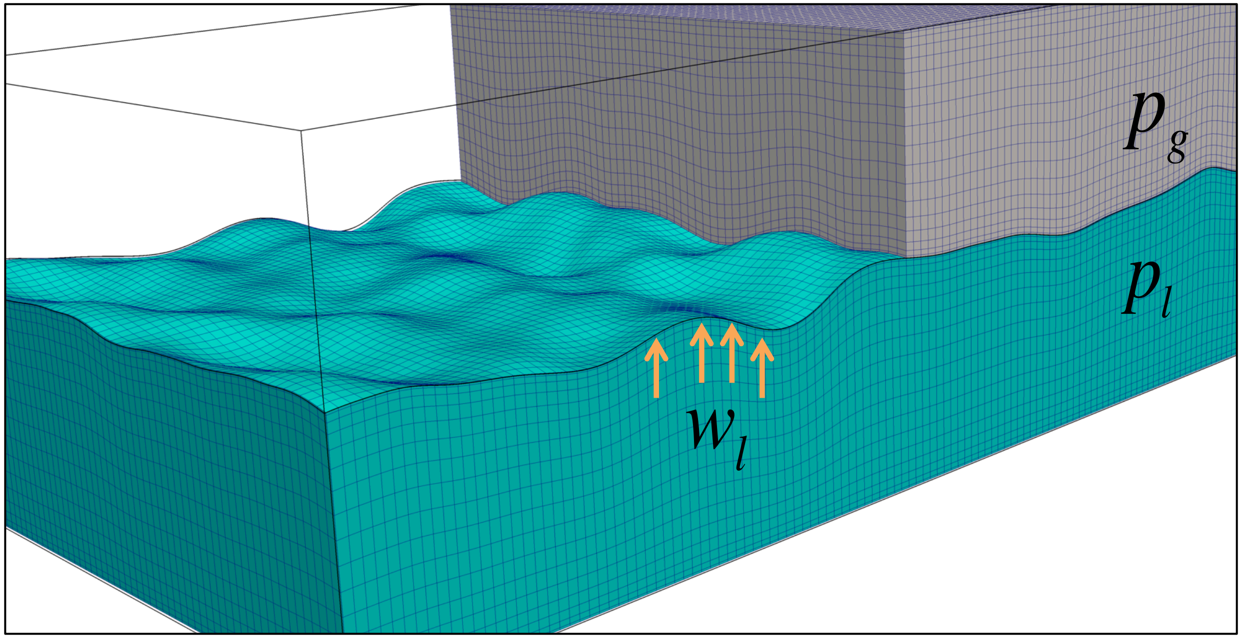


Transient growth of waves

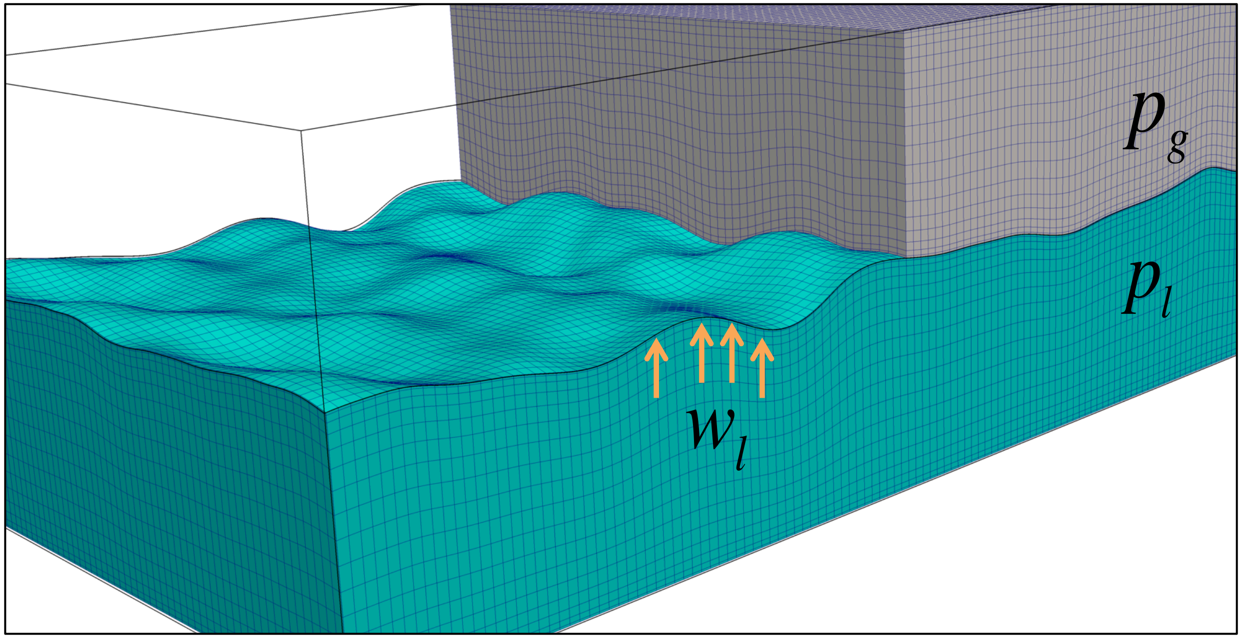


How to explain the time behavior of waves?

Consider the origin of a wave...



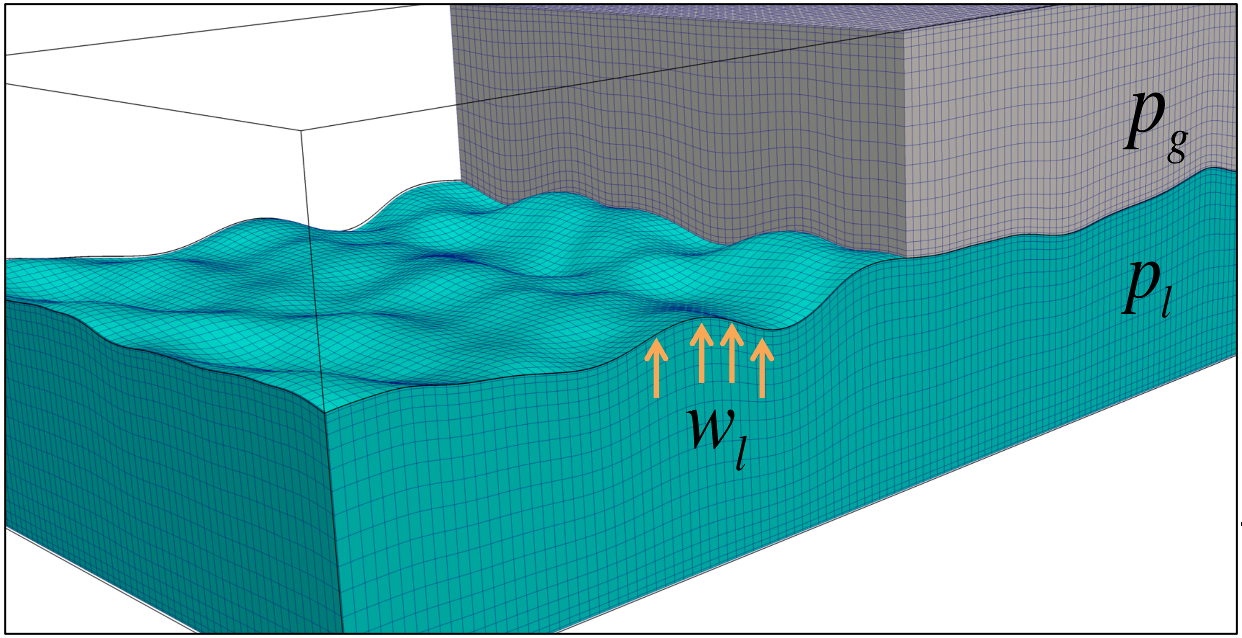
Consider the origin of a wave...



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

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

Consider the origin of a wave...



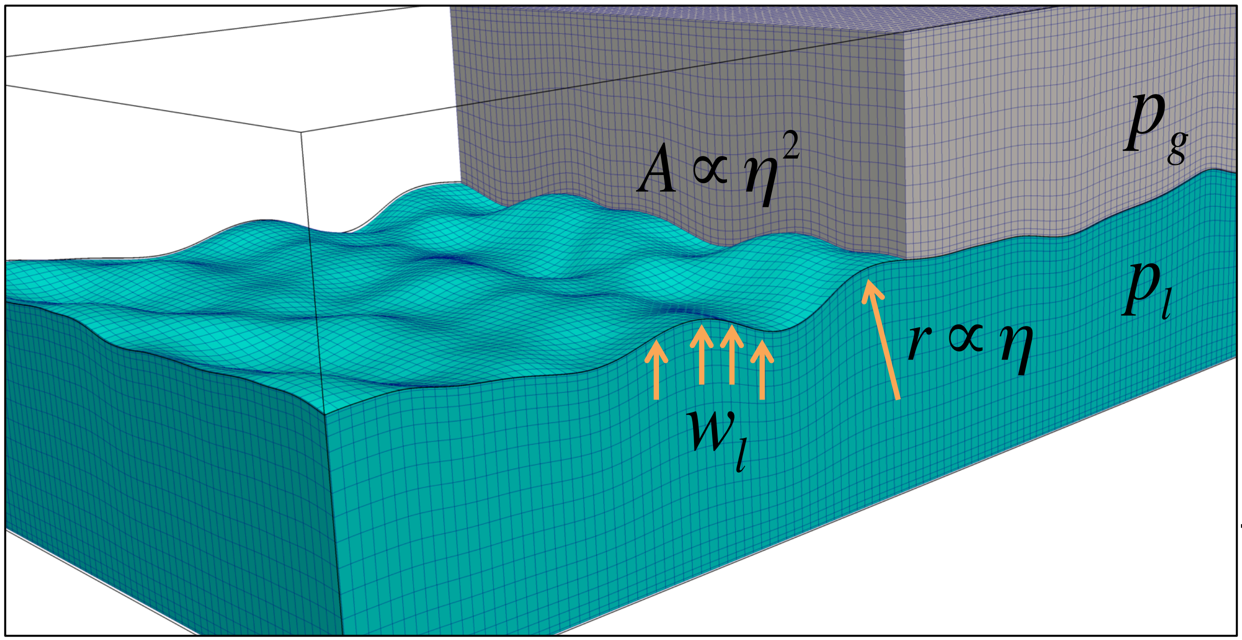
We express the variation of the interface area:
(Hoepffner et al., PRL 2011):

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

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

(Surface tension)

Consider the origin of a wave...



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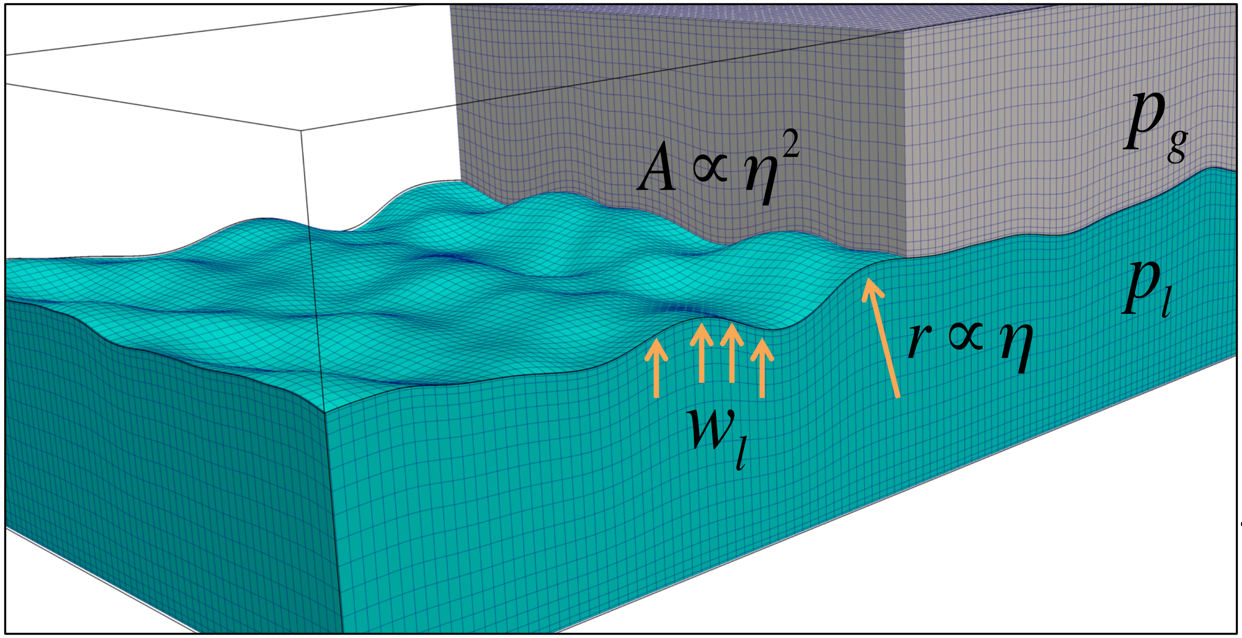
Consider the origin of a wave...



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

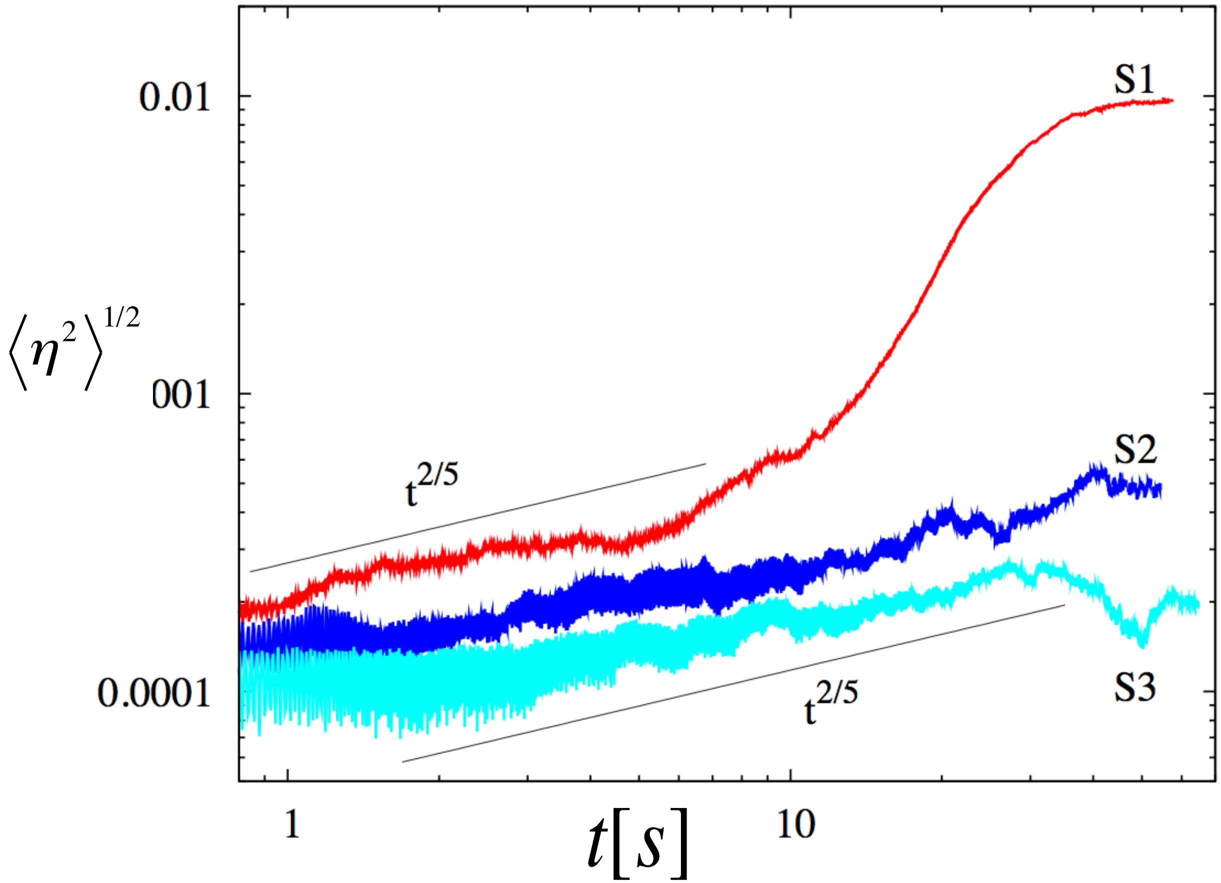
(Surface tension)

After some algebra:

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

Transient growth of waves: DNS vs simplified model

Wave amplitude over time



Initial scaling

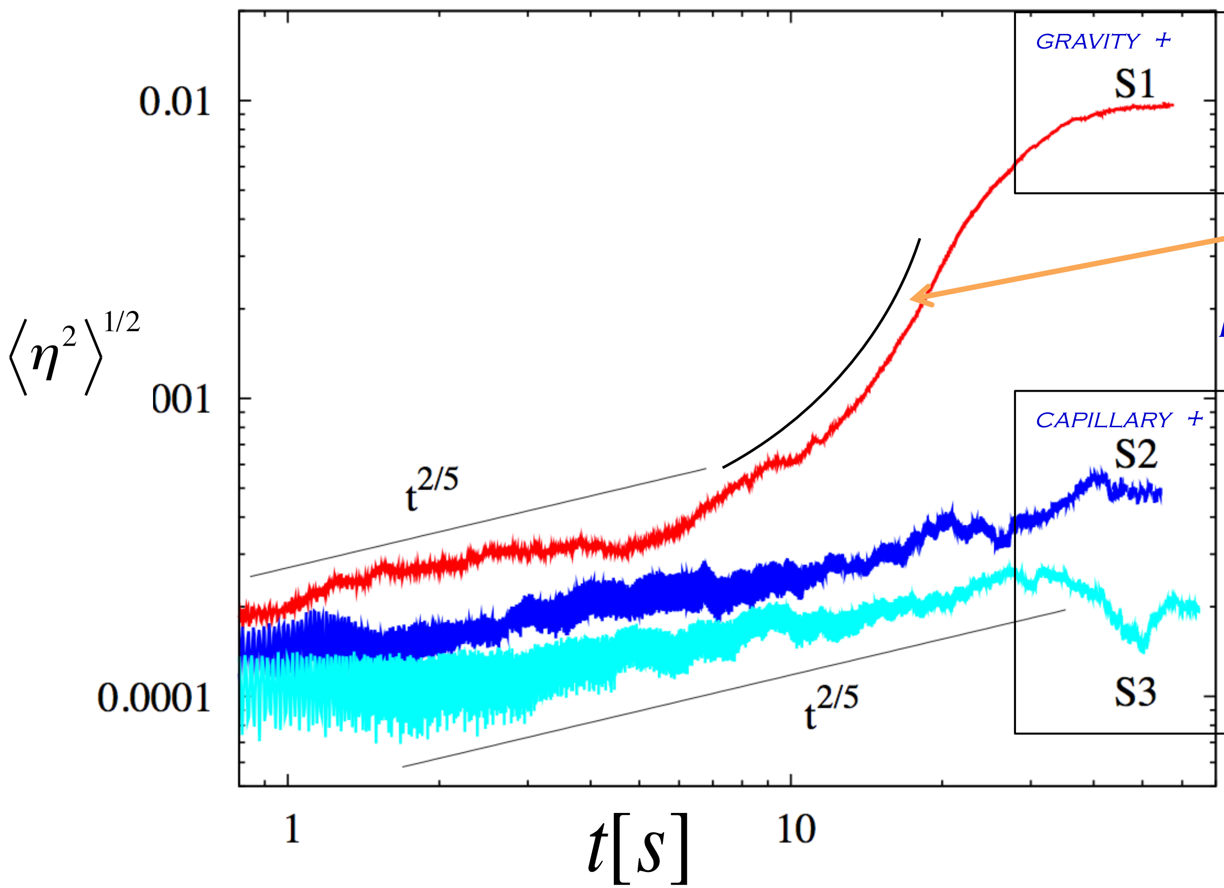
$$\eta \propto t^{2/5}$$

Quite ''robust'' within the range of parameters investigated

Whatever the physical parameters, capillarity dominates at the beginning

Zonta et al., JFM (2015)

Transient growth of waves: Small waves grow



After the initial scaling

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

For non-negligible gravity

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

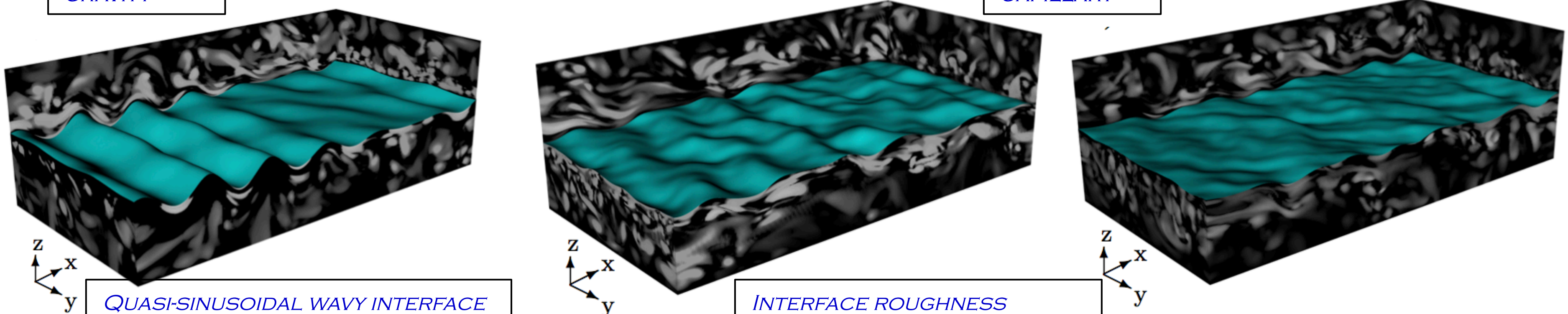
(resonance between waves-pressure/stress)

Lin et al., JFM (2008), Janssen, Cambridge Press (2004)

The structure of the interface deformation

GRAVITY +

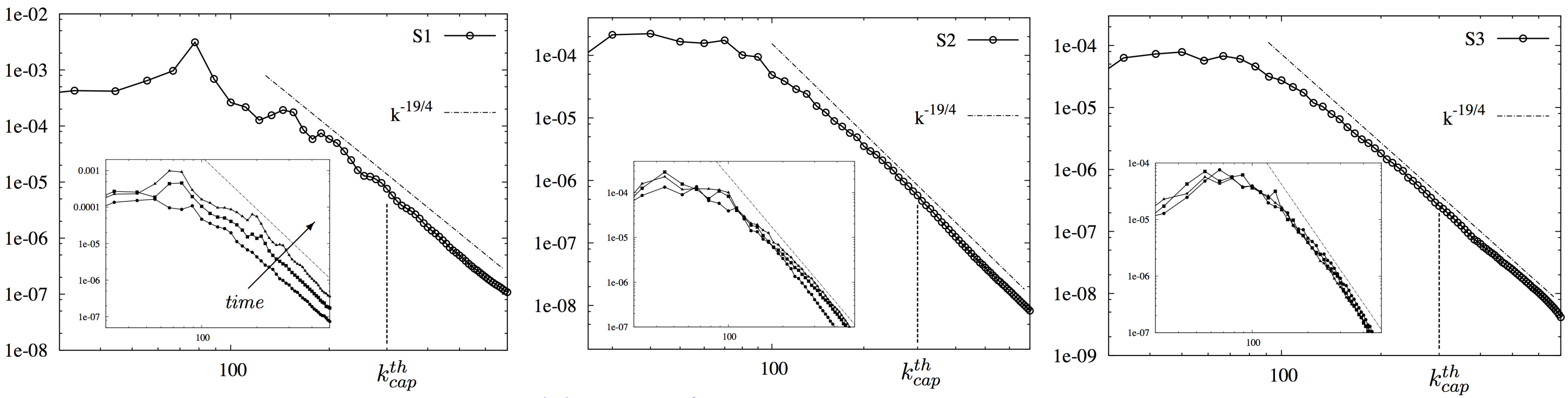
CAPILLARY +



QUASI-SINUSOIDAL WAVY INTERFACE

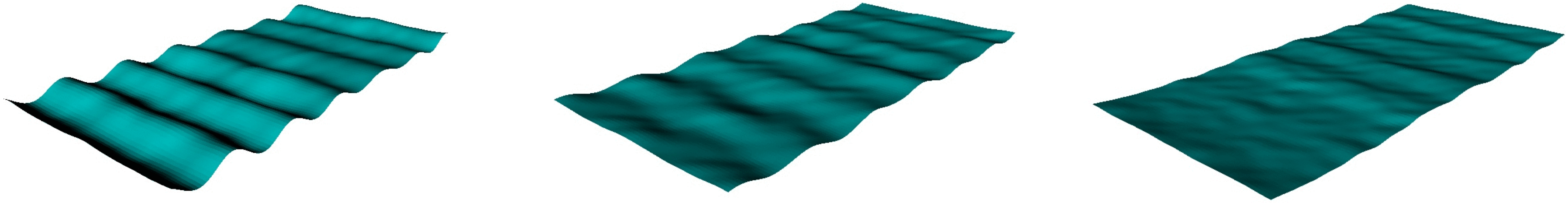
INTERFACE ROUGHNESS

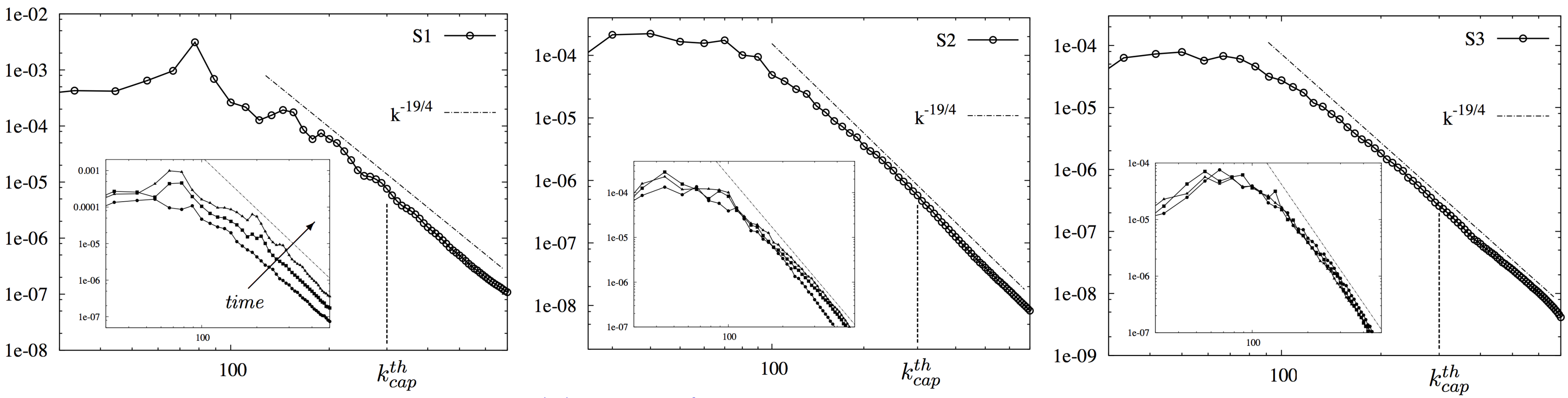
$$\hat{\eta}(k_x) = \int \hat{\eta}(k_x, k_y)\, dk_y$$



CFR. WITH WAVE TURBULENCE THEORY (Pushkarev & Zakharov, PRL 1996;Falcon et al., PRL 2007)

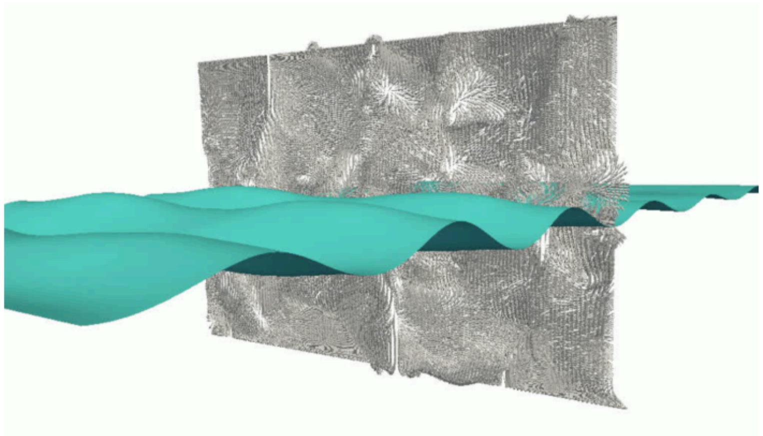
The structure of the interface deformation

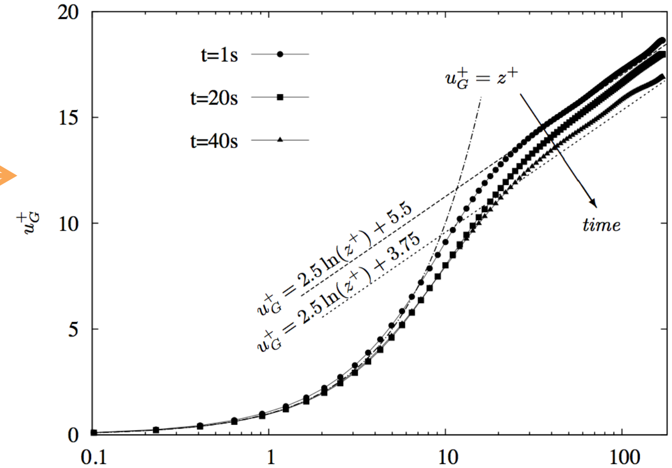


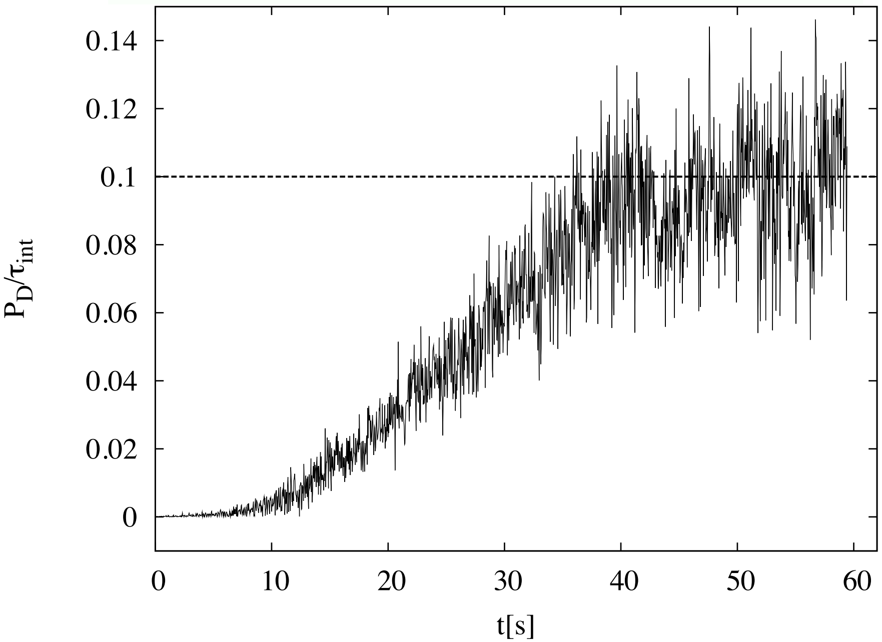


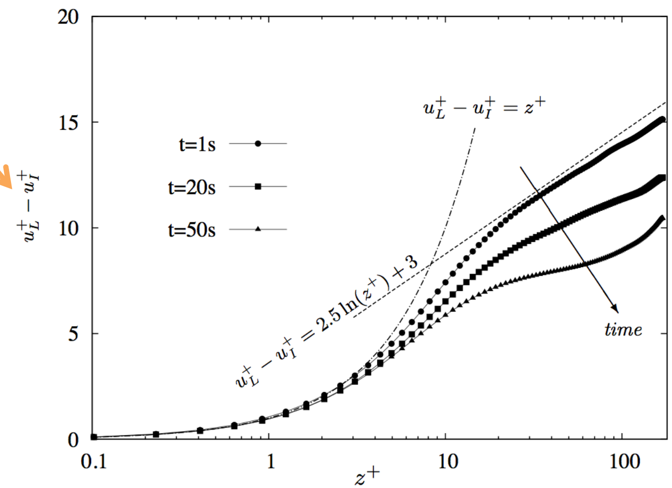
cfr. with Wave turbulence Theory (Pushkarev & Zakharov, PRL 1996;Falcon et al., PRL 2007)

TURBULENCE MODULATION BY INTERFACE DEFORMATION



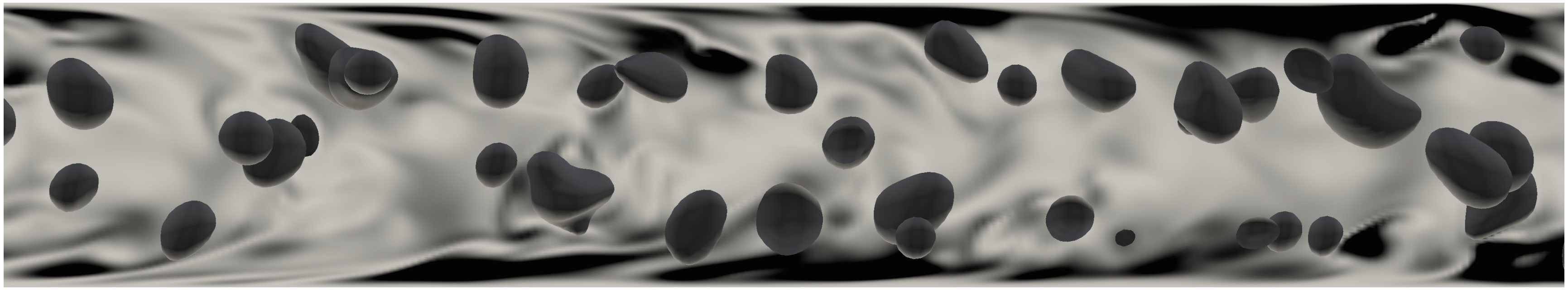






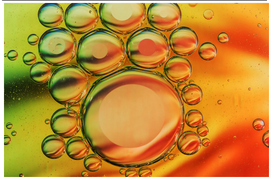
As waves develop, we observe a drag increase (pressure drag+skin friction)

PART IV:
DROPLETS IN TURBULENCE

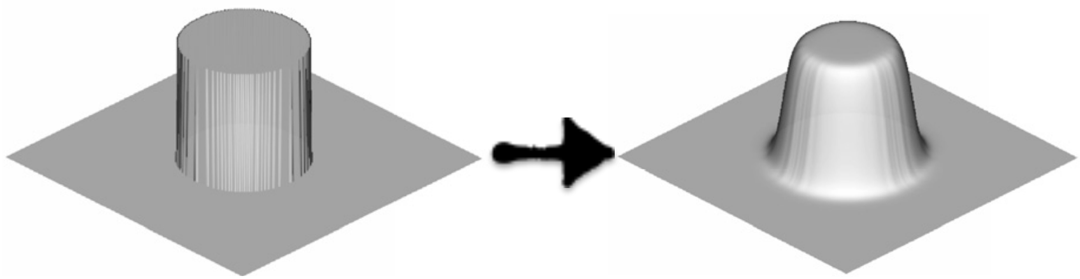


MULTIPHASE SYSTEM → TURBULENCE

MULTIPHASE SYSTEM → MULTIPHASE



Diffuse interface approach (PFM), the sharp interface is replace by a thin layer of transition:



The Phase Field is described by a transport scalar equation.

Hypothesis:
- Incompressible flow
- Matched Density multiphase system
- Different Viscosity of the two phases
- Constant Mobility

Mass Conservation:

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

Navier-Stokes equation:

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

Variable viscosity term (↑) *Capillary force term* (↑)

Cahn-Hilliard equation:

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

← *Chemical Potential*

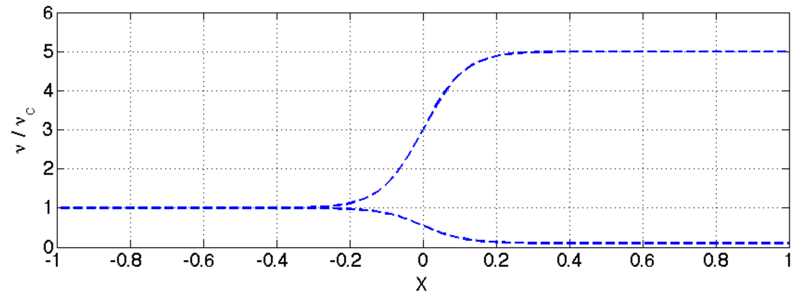
[1],[2],[3]

[1]Jacqmin,Calculation of Two-Phase Navier-Stokes Flows Using Phase-Field Modeling, JCP 1999;
[2]Badalassi et al. ,Computation of multiphase systems with phase field models, JCP 2003;
[3]Yue et al, A diffuse-interface method for simulating two-phase flwos of complex fluids, JFM 2004;

GOVERNING EQUATIONS

Viscosity can depends on Φ, using a linear interpolation of viscosity:

$$\nu(\phi) = \nu_c \frac{1-\phi}{2} + \nu_d \frac{1+\phi}{2}$$

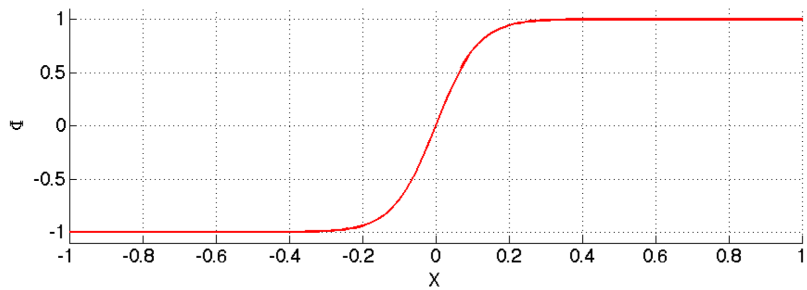


λ > 1

λ < 1

Defining λ as:

$$\lambda = \frac{\nu_d}{\nu_c} = \frac{\text{Drop Viscosity}}{\text{Continuos Viscosity}}$$



Φ profile

$$\phi = tanh \frac{x}{\sqrt{2}Ch}$$

Viscosity can be rewritten:

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

Inserting this expression in the NS equation, the diffusive term can be split as follows:

$$\nabla \cdot [\nu(\phi)(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathbf{T}})] = \nu_c \nabla^2 \mathbf{u} + \nu_c \nabla \cdot [(\lambda - 1)\frac{(\phi+1)}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathbf{T}})]$$

Linear Part

Non Linear Part

Weber Number (We):

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

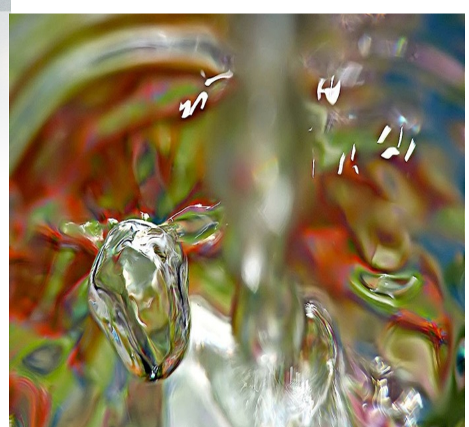
Viscosity Ratio (λ):

$$\lambda = \frac{\mu_d}{\mu_c} = \frac{\text{Droplet Viscosity}}{\text{Cont.Visocisty}}$$

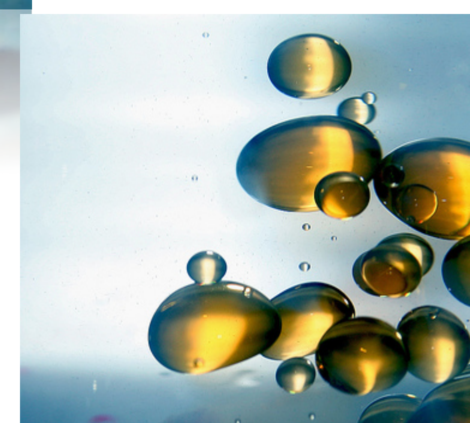
Low We

Low λ
(Water+Hexane)

High We



High λ
(Water+Oil)



PARAMETERS

μ_d μ_c $\lambda = \frac{\mu_d}{\mu_c}$

Fixed Parameters

Re$_\tau$*	***150.0***
Ch	***0.0185***
Pe**	***162.00***

Pe and Ch numerical parameters.

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

Grid: 512 x 256 x 257 (N_x-N_y-N_z)
Size: 4πH x 2πH x 2H (L_x-L_y-L_z)

$**Pe \sim 1/Ch$
* Based on the viscosity of the continuos phase (Φ=-1)

#	*We*	*λ*
S1		*0.01*
S2		*0.10*
S3	*0.75*	*1.00*
S4		*10.0*
S5		*100.*
S6		*0.01*
S7		*0.10*
S8	*1.50*	*1.00*
S9		*10.0*
S10		*100.*
S11		*0.01*
S12		*0.10*
S13	*3.00*	*1.00*
S14		*10.0*
S15		*100.*

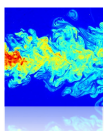
Numerical method

Method:

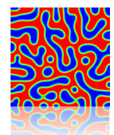
- Direct Numerical Solution (DNS);
- Pseudo-Spectral algorithm;
- N-S: Crank-Nicolson/Adams-Bashforth scheme
- C-H: Crank-Nicolson/Euler scheme

Boundary Conditions:

FLOW FIELD



PHASE FIELD



NO SLIP AT THE WALLS

$$\mathbf{u} = 0$$

90° CONTACT ANGLE

$$\frac{\partial \phi}{\partial z} = \frac{\partial^3 \phi}{\partial z^3} = 0$$

PERIODICITY ALONG X and Y

$$\mathbf{u}(0) = \mathbf{u}(L_y)$$

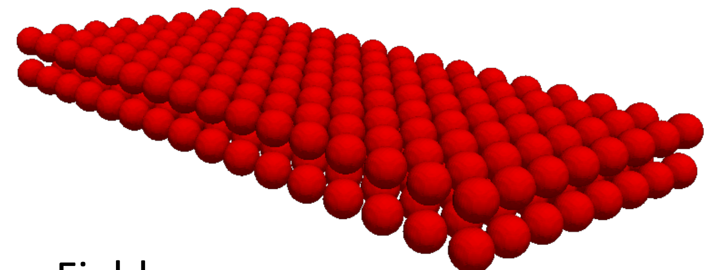
$$\mathbf{u}(0) = \mathbf{u}(L_x)$$

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

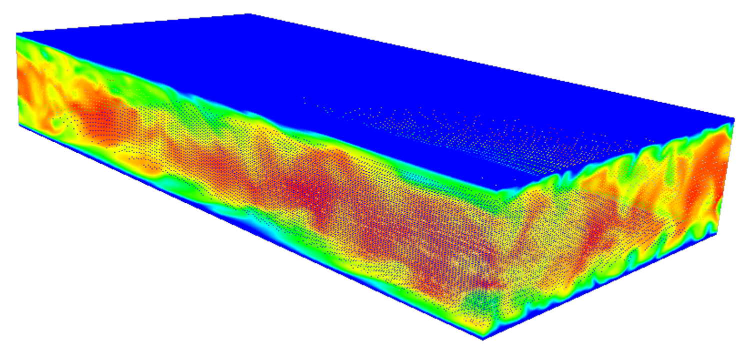
$$\phi(0) = \phi(L_y)$$

Initial Conditions:

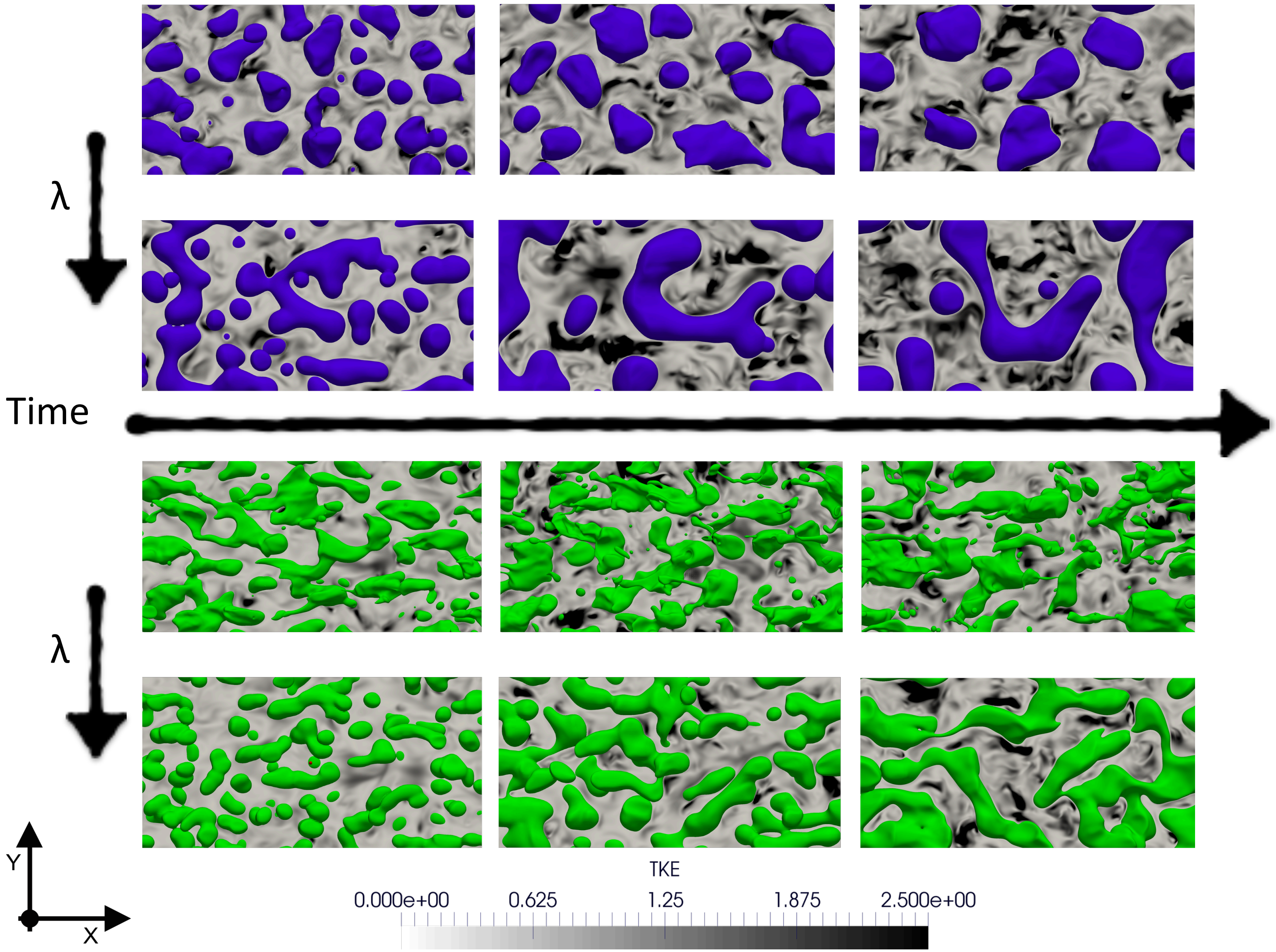
Phase Field
256 Droplets in two arrays
Vol=18.3% d^+=90 w.u.



Flow Field
-Fully Developed turbulent channel flow
DNS at Re_τ=150

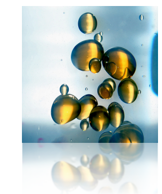


Results: collective dynamics



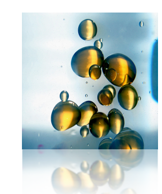
We=0.75
λ=0.01

We=0.75
λ=100.0



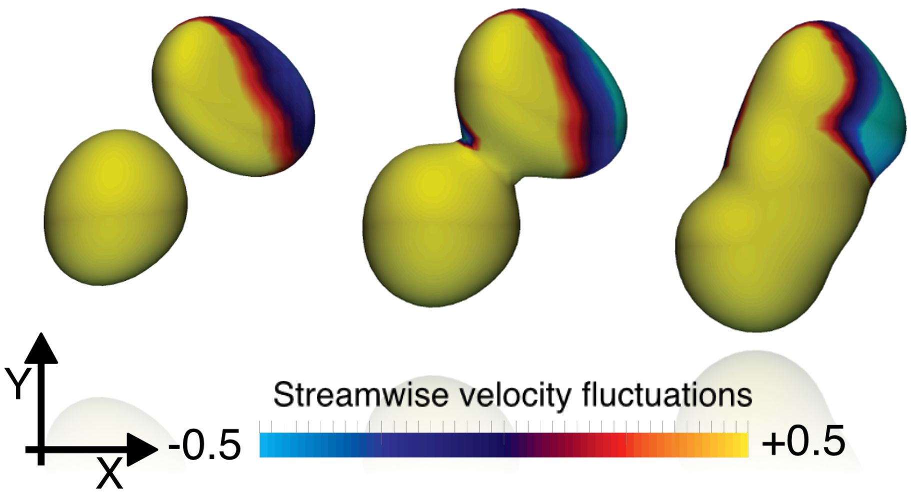
We=3.00
λ=0.01

We=3.00
λ=100.0



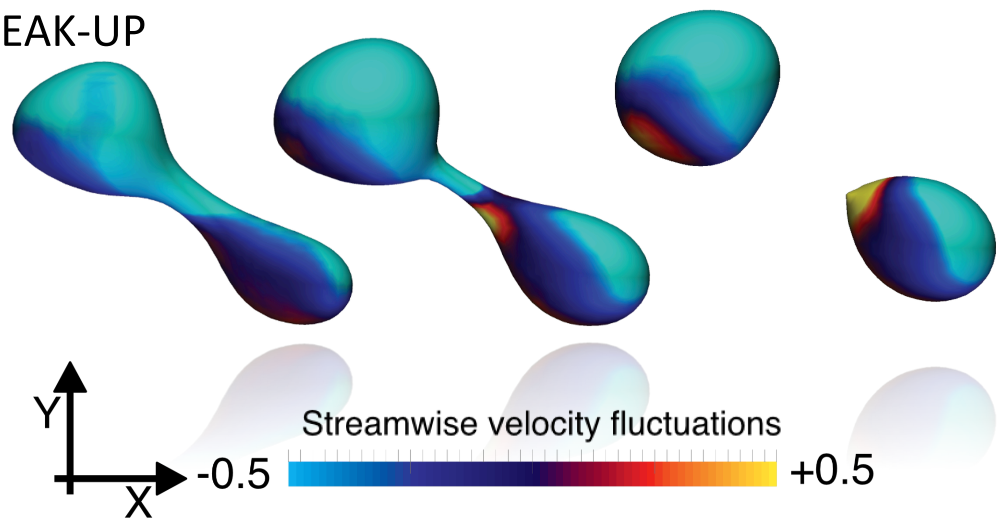
RESULTS: DROPLETS-DROPLETS INTERACTION

COALESCENCE



Turbulence fluctuations promote the coalescence phenomena. The new big droplet does not break only if the surface tension is strong enough.

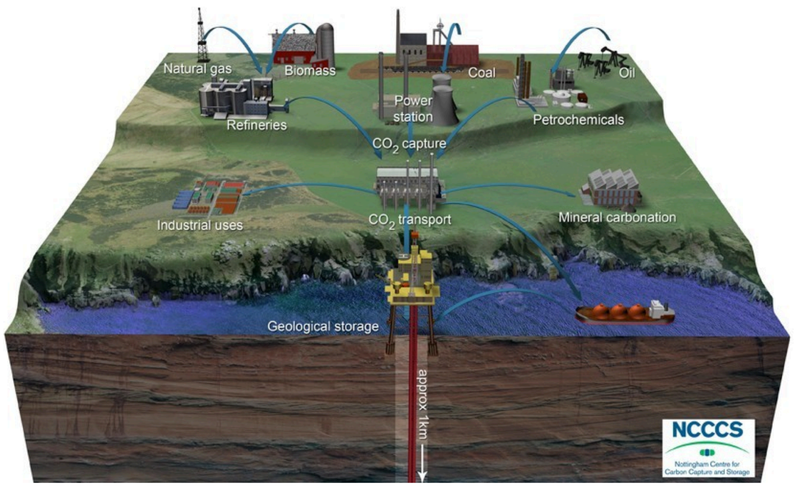
BREAK-UP



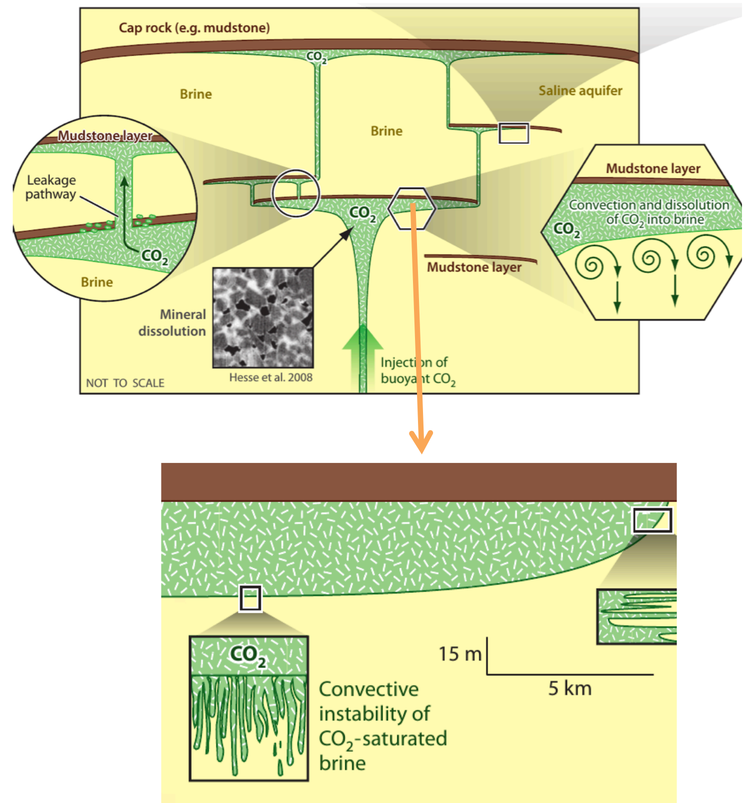
Turbulence fluctuations promote the brea-up phenomena; surface tension is not strong enough to keep the single droplet ''a single droplet''. A bridge is formed and the bridge breaks.

Results: Droplets dynamics

Part V: Geological CO_2 sequestration



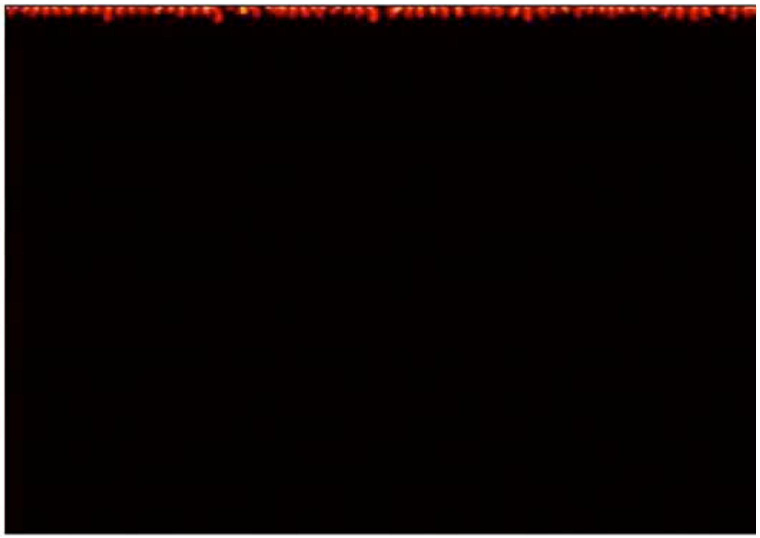
Liquid CO_2 is pumped beneath the earth surface



At the beginning, CO_2 moves upwards (lower density)
Later, it dissolves into brine and moves downwards

Huppert & Neufeld Annual Rev. Fluid. Mech. 2014

One-sided Config.
Prescribed Concentration
@ top wall.
Zero Flux @ bottom wall



Once this system starts
filling (i.e.the first finger
touches the bottom wall)
Its dynamics becomes
similar to the two-sided

Dimensionless equations

$$\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} = 0$$

$$\boldsymbol{u} = -\nabla p + \boldsymbol{k}\, C$$

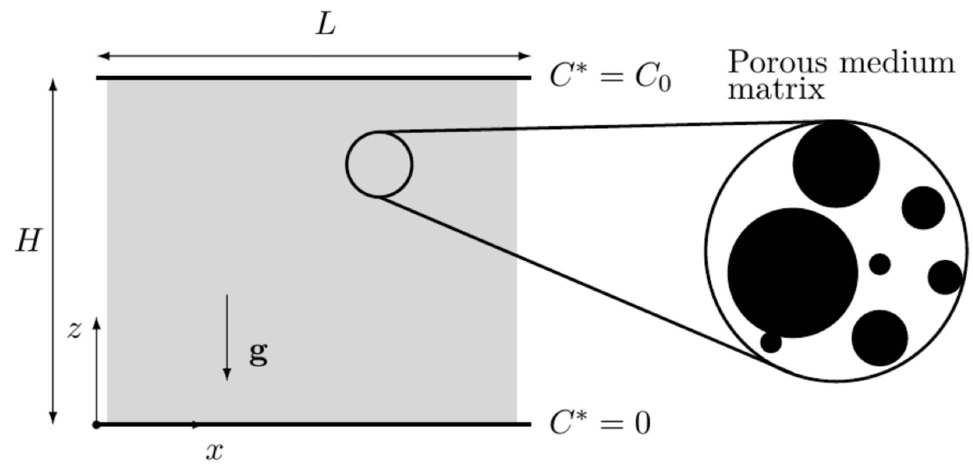
$$\frac{\partial C}{\partial t} + \boldsymbol{u} \cdot \nabla C = \frac{1}{Ra}\left(\gamma \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial z^2}\right)$$

where $\boldsymbol{u}, C$ are the fluid velocity and the CO_2 concentration, whereas

$$Ra = \frac{g\Delta\rho K_v H}{\mu\phi D} \text{ and } \gamma = \frac{K_v}{K_h}$$

contain information about fluid and porous medium properties

Numerical Simulations
We performed 2D Direct Numerical Simulations (DNS) using a pseudo-spectral method (Fourier + Chebyshev) up to **8192x1025** nodes.



Dimensionless boundary conditions

No-Penetration

$w = 0$ on $z = 0{,}1$

Fixed concentration

$C = 0$ on $z = 1$ — C fixed @ z=1

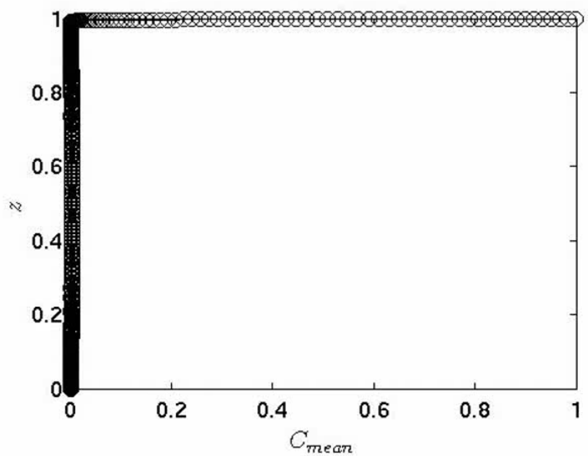
$C = -1$ on $z = 0$ — dC/dz fixed @ z=0

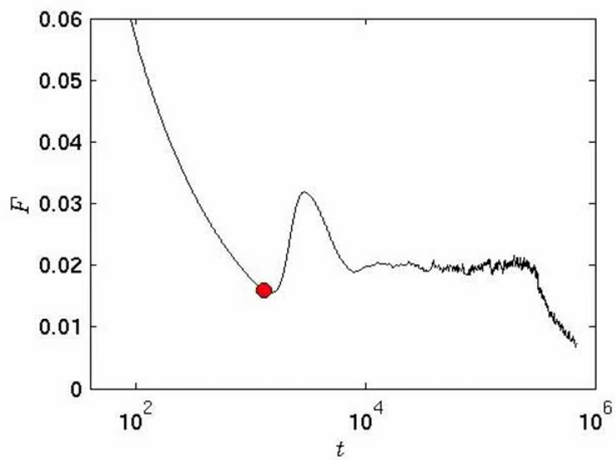
Periodic conditions

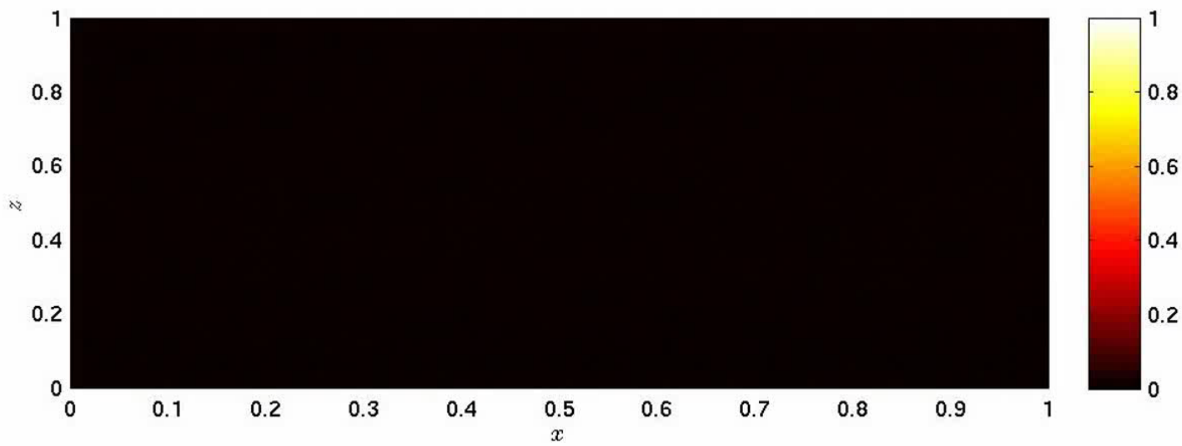
on $x = 0{,}1$

De Paoli et al., Phys. Fluids (2016)

Results: flux of CO_2







Thank you for your attention