MAE/NE-577
Multiscale Two-phase Flow Simulations

Instructor: Igor A. Bolotnov

About the instructor

- Igor Bolotnov, Professor, Nuclear Engineering
  - B.S. in Applied Mathematics & Informatics, Bashkir State University, Ufa, Russia (2002)
  - Ph.D. (2008) and M.S. (2003) in Engineering Physics, Rensselaer Polytechnic Institute, Troy, NY, U.S.A.
  - Professor since August 2021 (Ast. Prof. 2011 – 2017, Asc. Prof. 2017-2021).
- 15 years of research experience after Ph.D. degree:
  - Direct numerical / interface tracking simulations of complex flows
  - High-performance parallel computing applications
  - Multiscale analysis of Gen-IV reactor coolant flows
  - Development of models for two-phase turbulence
- 10 year collaboration with Oak Ridge National Laboratory (ORNL) as part of Consortium for Advanced Simulation of LWRs (CASL).
- Current research directions:
  - Interface tracking simulations: numerical tool development and analysis of bubbly turbulent flows
  - Advancing the boiling flows simulation capabilities in complex geometries
  - Development of single and two-phase turbulent models
- 240+ (140+ peer reviewed) conference papers, presentations and journal articles

Prominent publications

Igor Bolotnov

FOLLOWING

Professor of Nuclear Engineering, North Carolina State University
Verified email at ncsu.edu - Homepage

Multiphase flow · Nuclear Reactor Thermal H… · Two-phase flow · direct numerical simulation · Computational Fluid Dyna…

	All	Since 2018
Citations	1070	736
h-index	17	15
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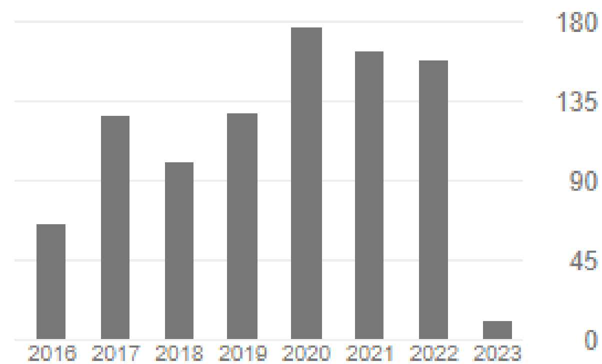

TITLE	CITED BY	YEAR
Detached direct numerical simulations of turbulent two-phase bubbly channel flow IA Bolotnov, KE Jansen, DA Drew, AA Oberai, RT Lahey Jr, MZ Podowski International Journal of Multiphase Flow 37 (6), 647-659	110	2011
Machine-learning based error prediction approach for coarse-grid Computational Fluid Dynamics (CG-CFD) BN Hanna, NT Dinh, RW Youngblood, IA Bolotnov Progress in Nuclear Energy 118, 103140	76 *	2020
Influence of Bubbles on the Turbulence Anisotropy IA Bolotnov Journal of Fluids Engineering 135 (1)	66	2013
Evaluation of bubble-induced turbulence using direct numerical simulation J Feng, IA Bolotnov International Journal of Multiphase Flow 93, 92-107	55	2017
Interface tracking simulations of bubbly flows in PWR relevant geometries J Fang, M Rasquin, IA Bolotnov Nuclear Engineering and Design 312, 205-213	55	2017
Estimation of shear-induced lift force in laminar and turbulent flows AM Thomas, J Fang, J Feng, IA Bolotnov Nuclear Technology 190 (3), 274-291	50	2015
Spectral analysis of turbulence based on the DNS of a channel flow IA Bolotnov, RT Lahey Jr, DA Drew, KE Jansen, AA Oberai Computers & fluids 39 (4), 640-655	46	2010
Direct numerical simulation of reactor two-phase flows enabled by high-performance computing J Fang, JJ Cambareri, CS Brown, J Feng, A Gouws, M Li, IA Bolotnov Nuclear Engineering and Design 330, 409-419	38	2018
Interfacial force study on a single bubble in laminar and turbulent flows J Feng, IA Bolotnov Nuclear Engineering and Design 313, 345-360	37	2017
Turbulent cascade modeling of single and bubbly two-phase turbulent flows IA Bolotnov, RT Lahey Jr, DA Drew, KE Jansen International journal of multiphase flow 34 (12), 1142-1151	31	2008
Slug-to-churn vertical two-phase flow regime transition study using an interface tracking approach MD Zimmer, IA Bolotnov International Journal of Multiphase Flow 115, 196-206	26	2019

Course web-site

https://moodle-courses2223.wolfware.ncsu.edu/course/view.php?id=5377

- Syllabus
- Selected notes
- Homework Assignments
- Announcements

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Schedule: MW 1:30pm - 2:45pm
327 111 Lampe Dr.

Office Hours: Wednesday 12:15pm-1:15pm (BU2153)

phone: (518)542-8939

You can always schedule an additional meeting by requesting it via e-mail (please allow at least a few hours between the request and the desired time/date)

Brief course outline

- **Introduction**
  - reactor systems applications
  - two-phase flow regimes
- **Direct numerical simulation (DNS)**
  - Navier-Stokes equations
  - Conservation of mass, momentum, energy
  - incompressible flows
  - Turbulence resolution requirements
- **Interface tracking methods (ITM)**
  - Overview of modeling approaches at various scales
  - One-fluid approach: incompressible N.S. incorporating interface treatment
  - Surface tension
  - Dimensionless groups
- **Numerical considerations:**
  - Overview of ITM methods
  - Time integration (explicit and implicit methods)
  - Spatial discretization
  - Boundary conditions
  - One-fluid approach:
    - Volume of Fluid method
    - Front-tracking method
    - Level-Set method
- **Computational Multiphase Fluid Dynamics (CMFD)**
  - Reynolds-averaged Navier-Stokes equations (RANS)
  - Turbulence modeling:
    - Gradient-diffusion and turbulent viscosity hypothesis
    - Shear stress and turbulent shear stress
    - law of the wall
    - turbulence models
  - two-phase modeling approach
  - interfacial forces
  - interfacial area density evolution
  - subcooled boiling modeling
  - critical heat flux

Introduction

1. **Introduction**
   - Multiphase flows definition and overview
   - two-phase flow regimes
   - reactor systems applications
2. **Direct numerical simulation (DNS)**
3. **Interface tracking methods (ITM)**
4. **Numerical considerations**
5. **Computational Multiphase Fluid Dynamics (CMFD)**.

Multiphase flow applications

Multiphase flows are everywhere:

- Rain, air/ocean interactions, combustion of liquid fuels, boiling in power plants, refrigeration, blood,

Research into multiphase flows usually driven by “big” needs

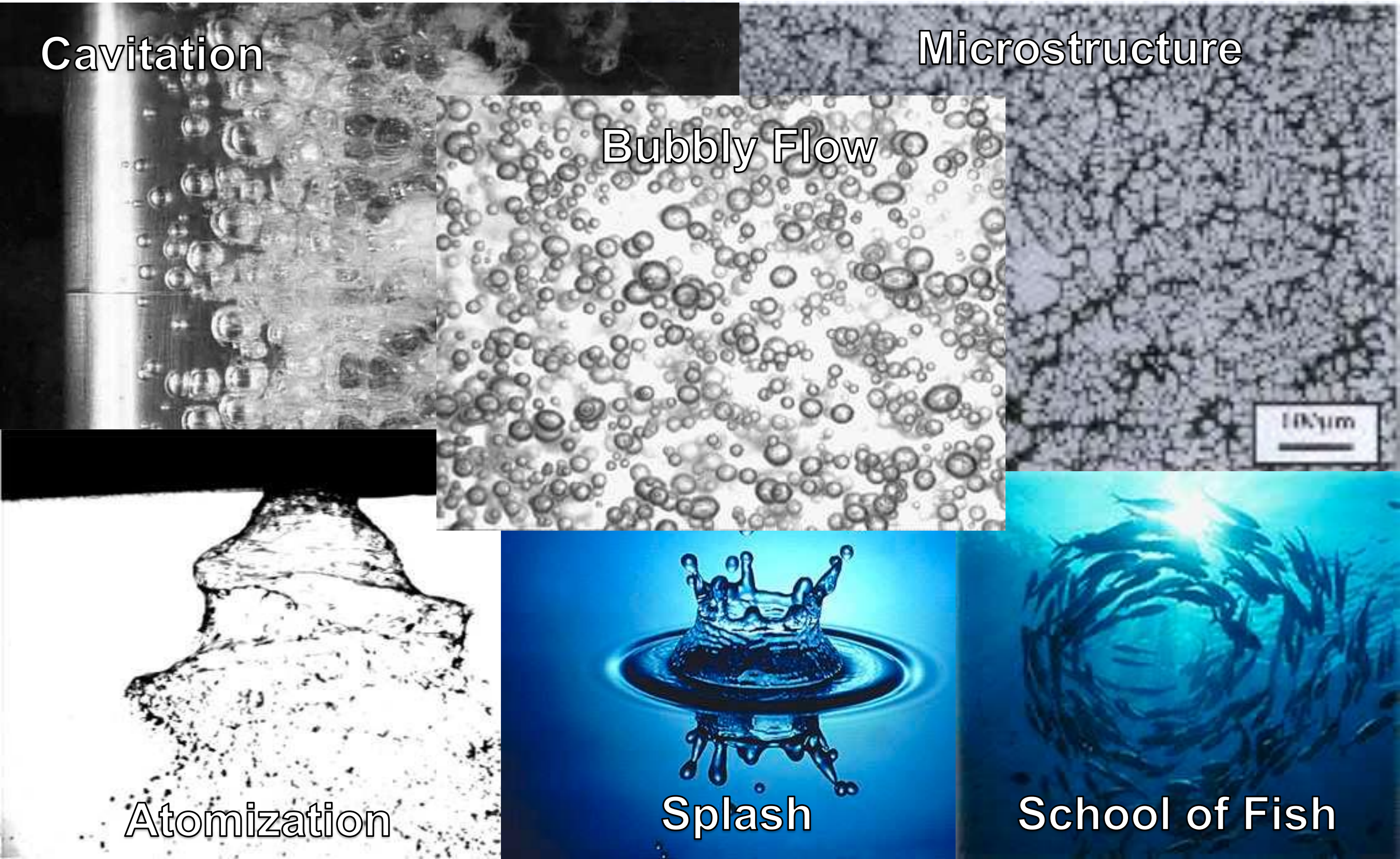
- Early Steam Generation
- Nuclear Power
- Space Exploration
- Oil Extraction
- Chemical Processes

Many new processes depend on multiphase flows

- Additive manufacturing, carbon sequestration

Multiphase flow applications

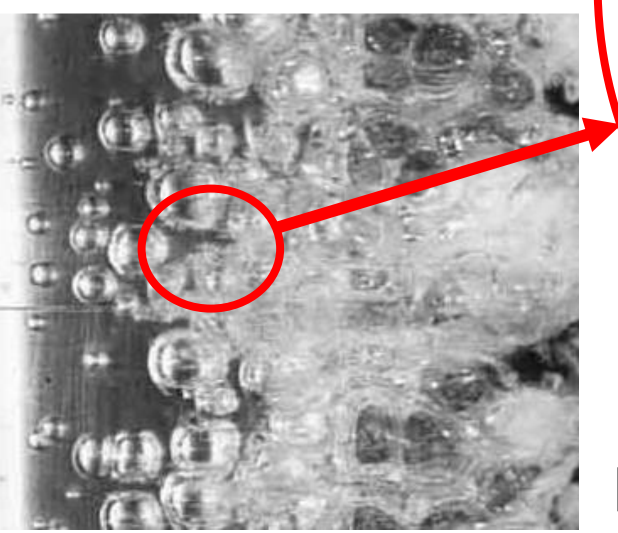
Examples

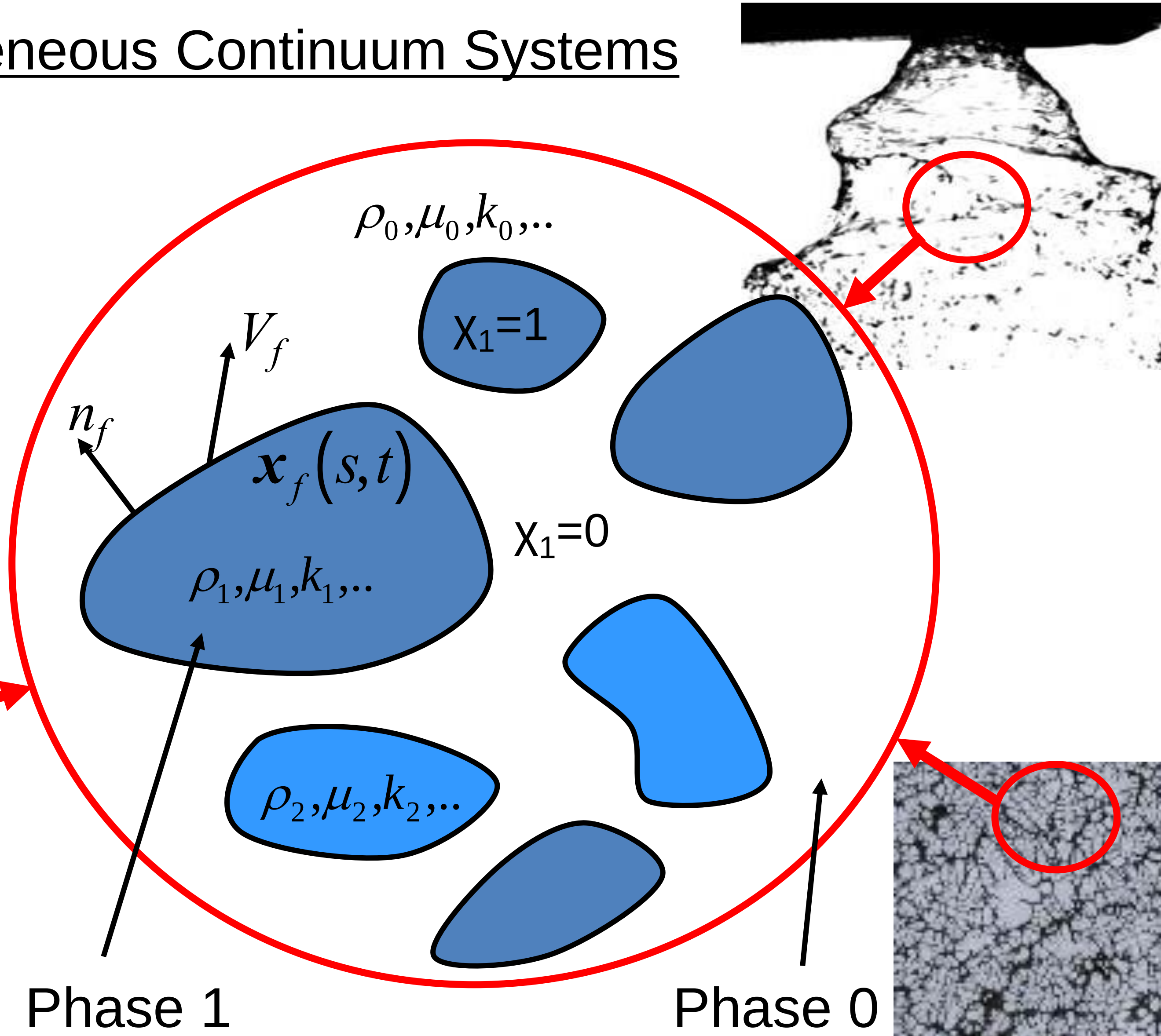


What is multiphase flow ?

Evolving Heterogeneous Continuum Systems

Systems composed of different phases and materials, separated by a ***sharp interface*** whose location changes with time





What is Multiphase flow ?

Multiphase flows are **characterized by**:

•Systems composed of different phases and materials, separated by a sharp interface whose location changes with time

•The physics is well described by continuum theories

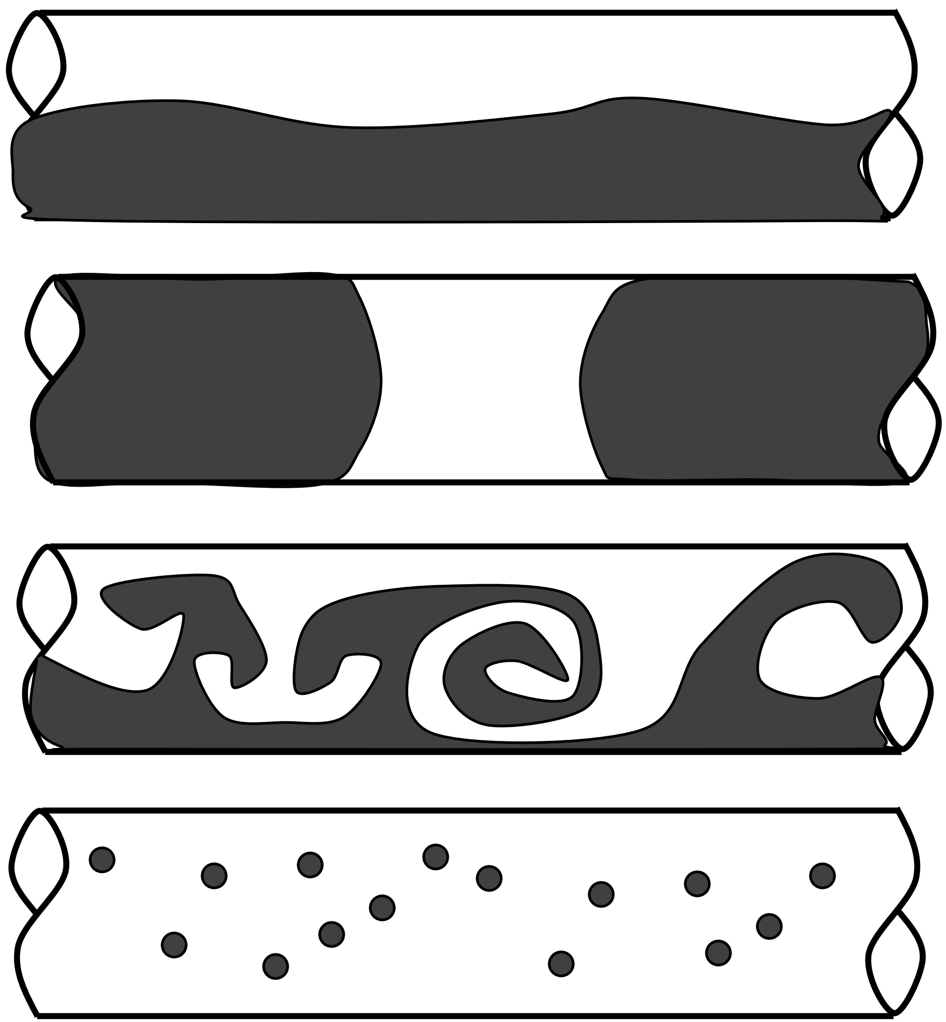
•The systems are sufficiently large so that simulations resolving the smallest and the largest scales are impractical

•There are good reasons to believe that the behavior of the smallest scales is—in some sense—universal

•The goal is to use **fully resolved** numerical simulations of the small scale behavior to help understand how the large and the small scale motion are coupled and to develop “closure” models

Flow Regimes

Flow in horizontal pipes



Stratified / Annular

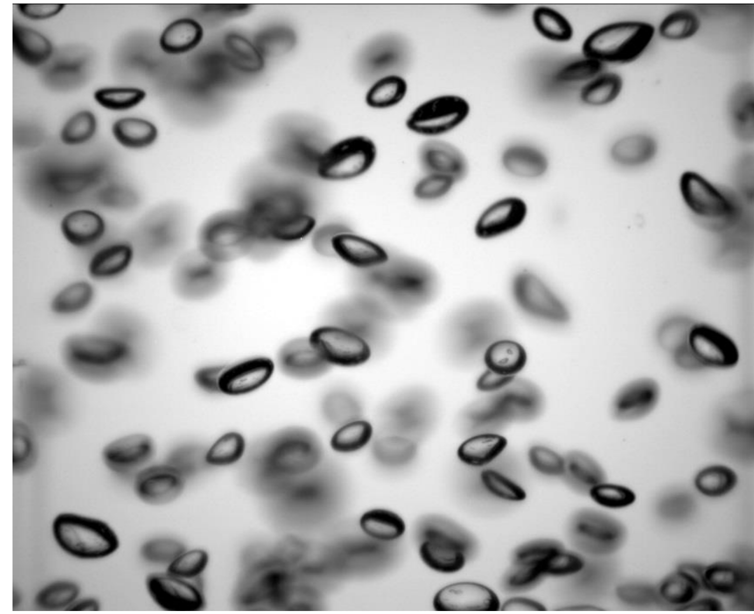
Slug / Taylor bubble

Churn-turbulent

Dispersed

Bubbly flows:

How does the void fraction and the bubble size and shape affect their **average rise velocity**



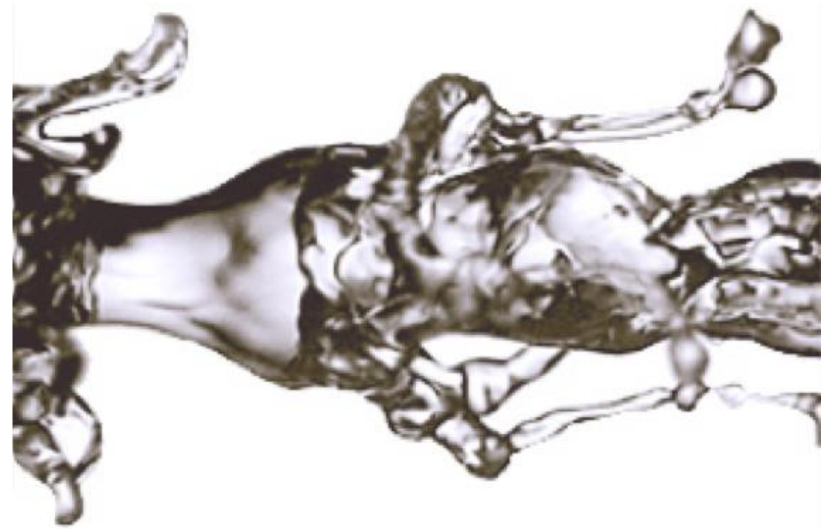
How do the bubbles **disperse** as they rise

Do the bubbles form **microstructures** as they rise and how do such structures affect rise velocity and dispersion

Does the bubbles **size distribution** change as the bubbles rise due to coalescence, breakup or size dependent migration

How do bubbles **interact with walls** and boundaries

Atomization of jets



What is the **drop size** and distribution, their velocities, and how does it depend on the initial nozzle shape and flow conditions ?

How long does it take for the jet to **break up** and how does it depend on the initial nozzle shape and flow conditions ?

What are the basic mechanisms that control the initial breakup and the **drop formation** and how do they depend on ***turbulence*** in the jet and the air flow ?

Can we develop models and reduced order descriptions ?

Finest scale simulations

Why Direct Numerical Simulations?

DNS provide us with **full details** of the flow in both space and time and allow us to compute any derived quantity

DNS allow us to turn the various physical processes **on and off** at will to determine their effect

DNS allow us to precisely define the **initial conditions** for each case and determine their effects

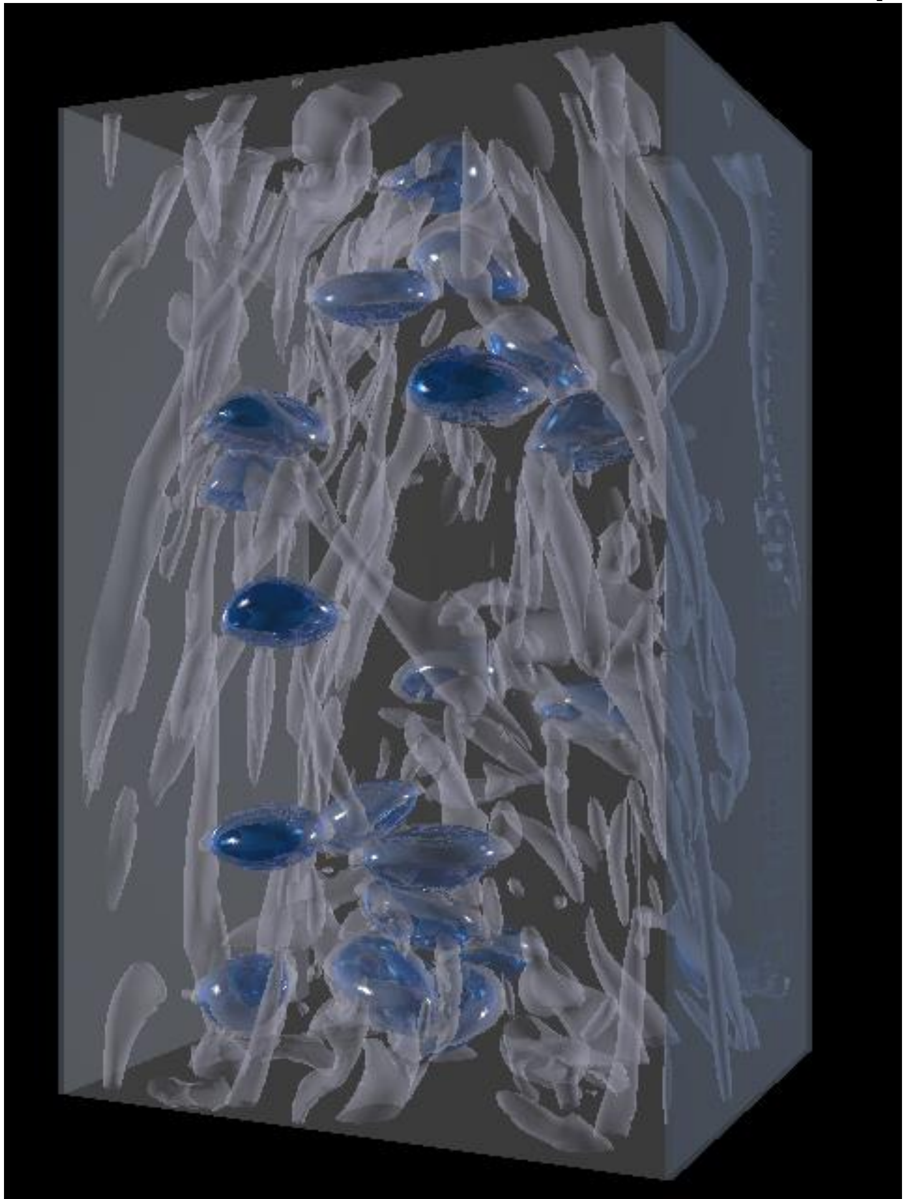
The purpose of DNS is not just to reproduce experiments!

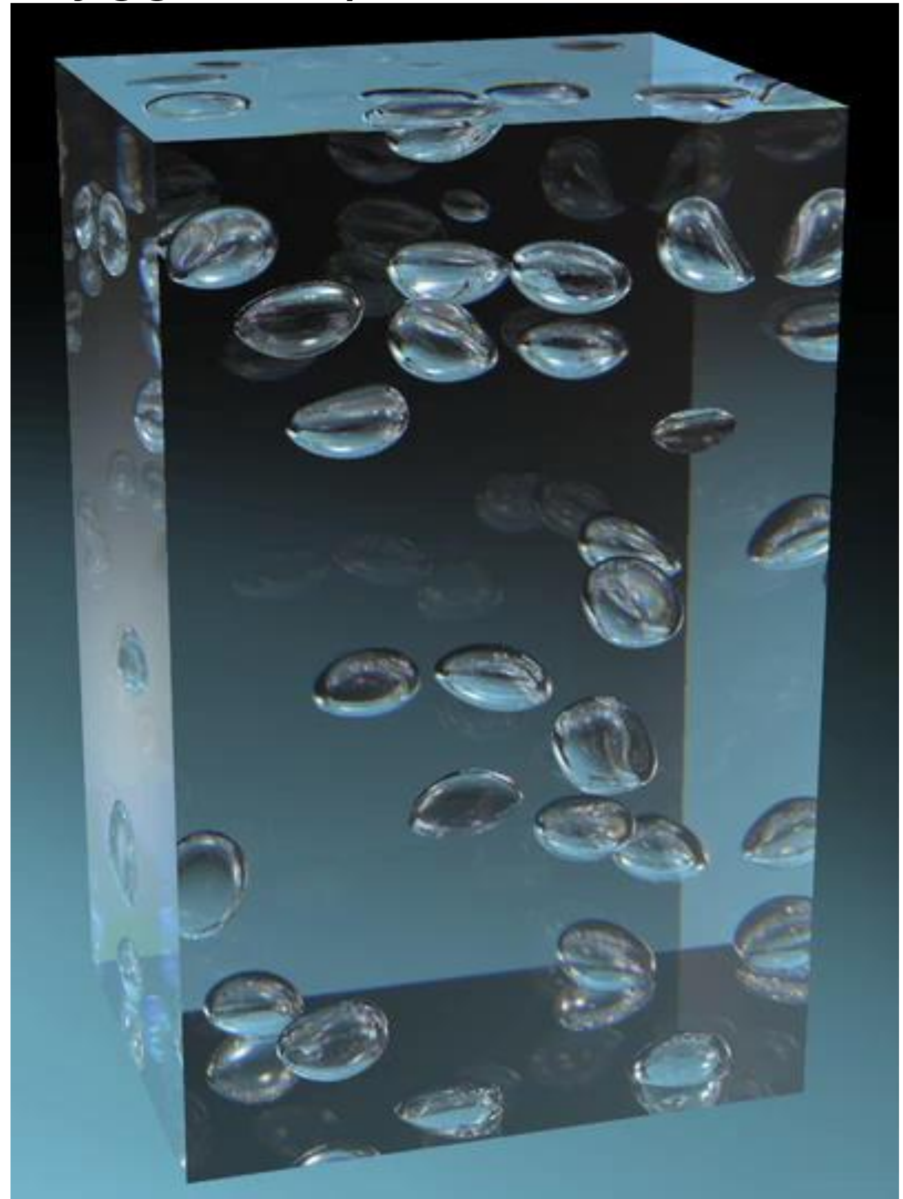
Direct Numerical Simulations:

Fully resolved and verified simulation of a validated system of equations that include non-trivial length and time scales

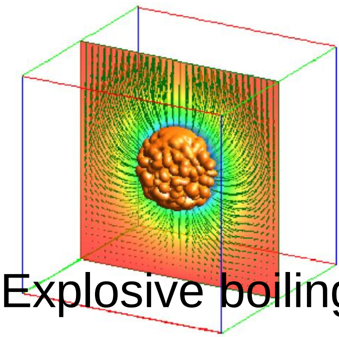
Bubbly flows

Bubbles in Vertical Channels (G. Tryggvason)

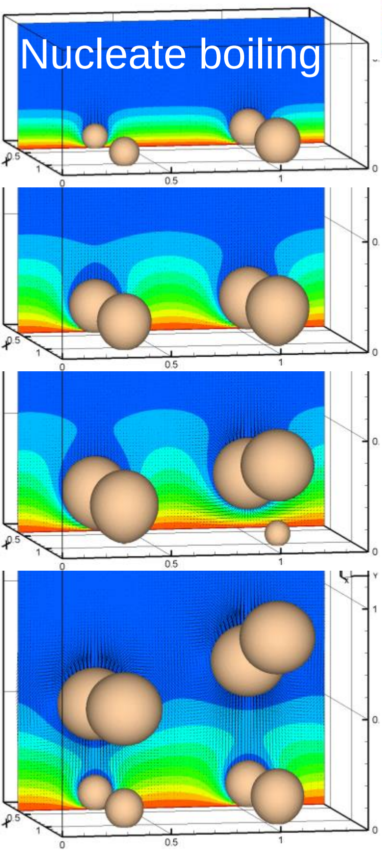




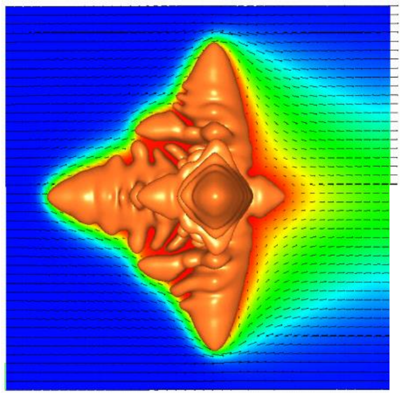
Multiphase flow simulations



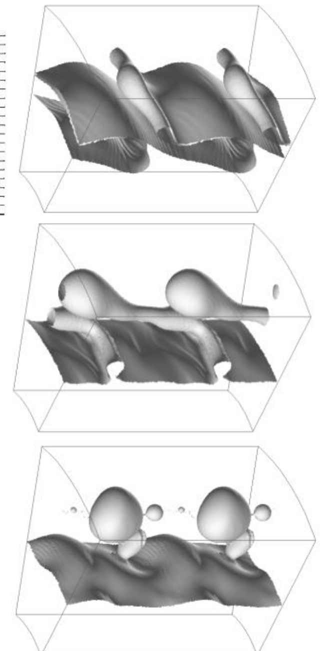
Explosive boiling



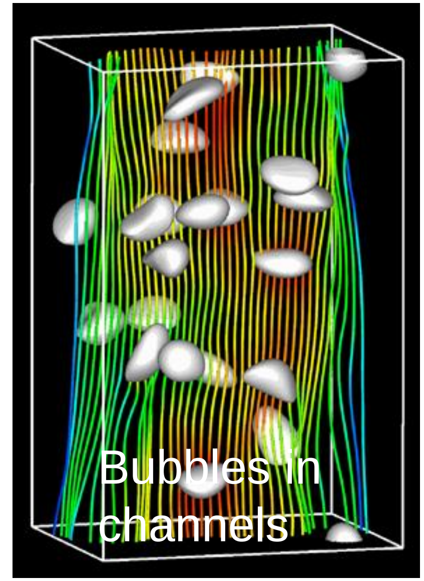
Nucleate boiling



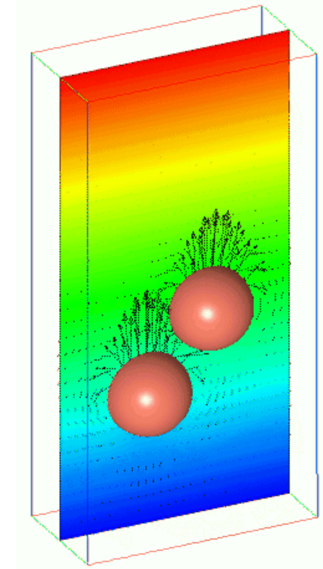
Solidification



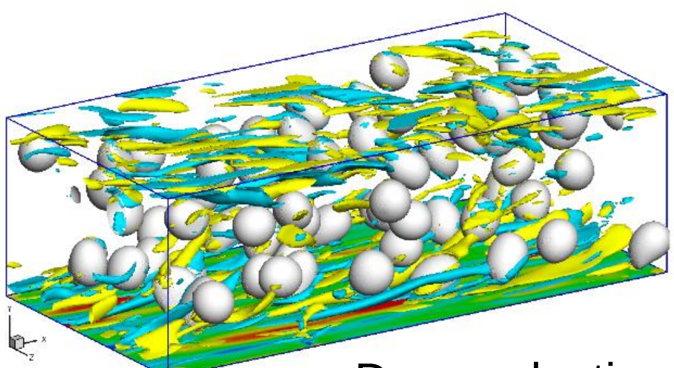
Atomization



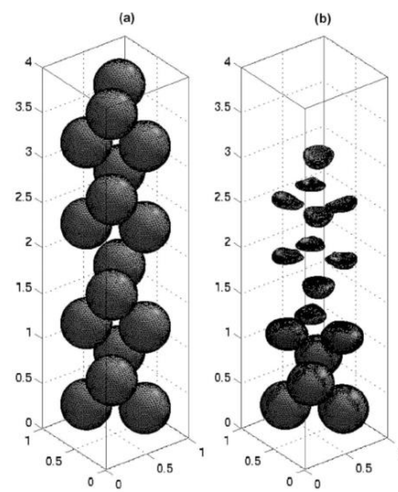
Bubbles in channels



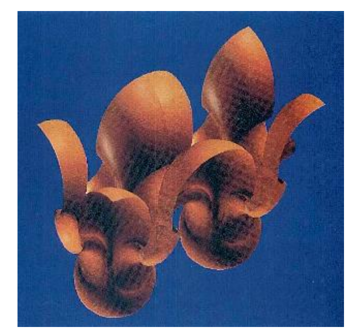
Thermo-capillary migration



Drag reduction



Cavitating bubbles



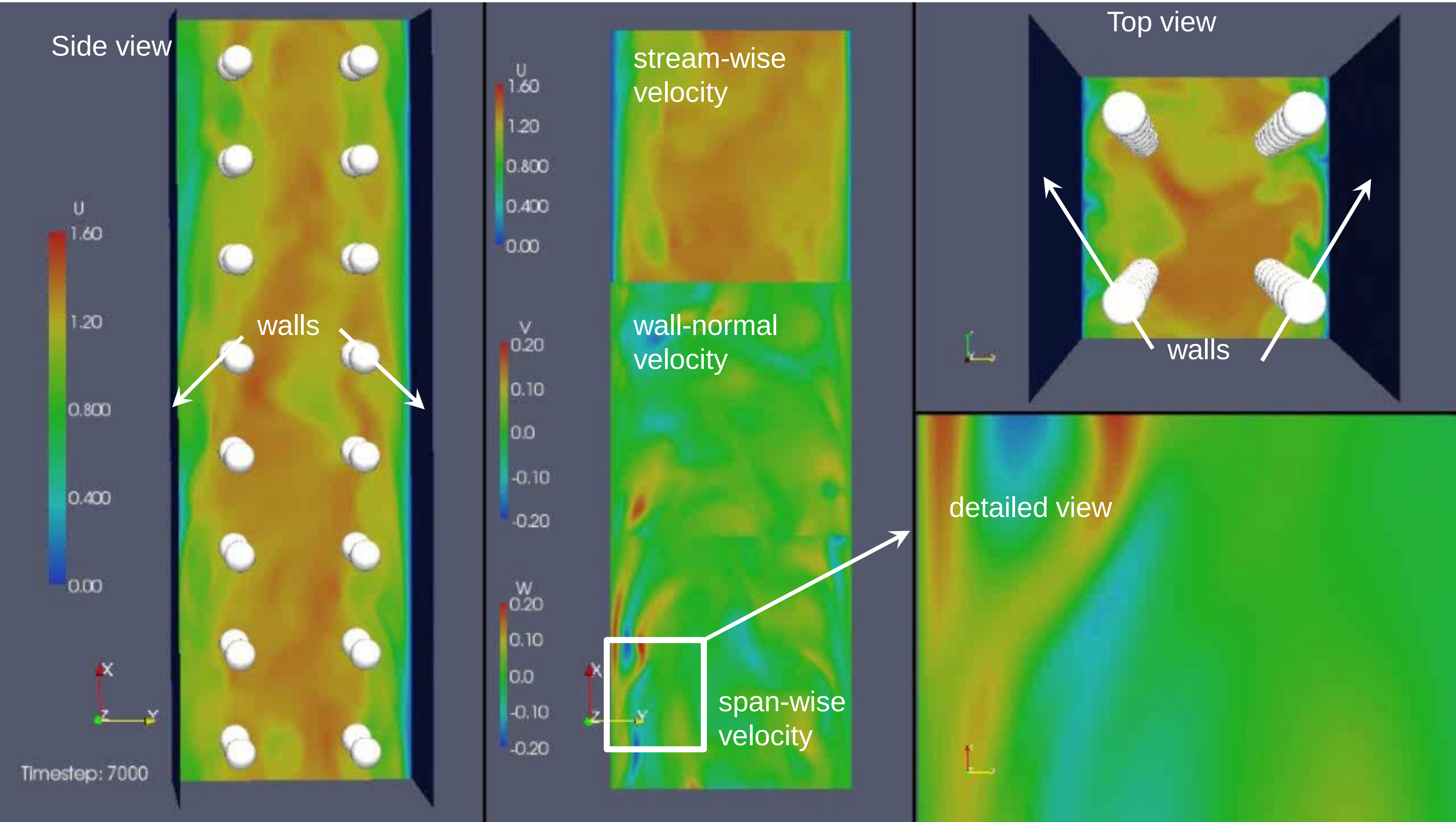
Rayleigh-Taylor Instability

Channel flow simulation

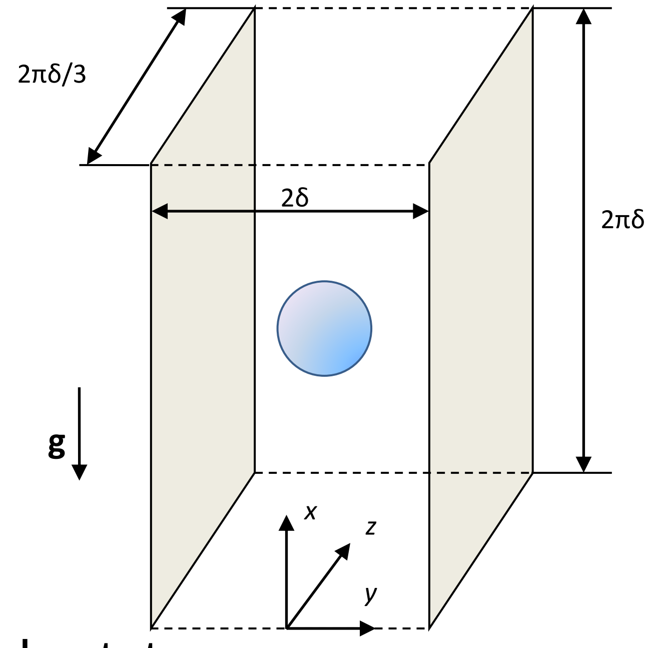
Domain size: ~9.8M elements
Liquid flow Re_{τ} = 180

Average Gas Volume Fraction: 1%
Initial number of bubbles: 32

ρ_l/ρ_g ~ 860



Lift force: introduction



Physics

- Four fundamental factors govern lift force (Hibiki & Ishii, 2007)
  - Relative velocity
  - Shear rate
  - Bubble rotational speed
  - Bubble surface boundary condition

Control Solution

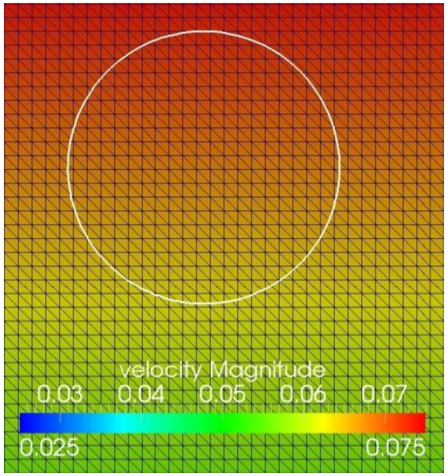
- PID-based controller
  - Control bubble's location at (quasi) steady state
  - Control forces balance lift and drag forces

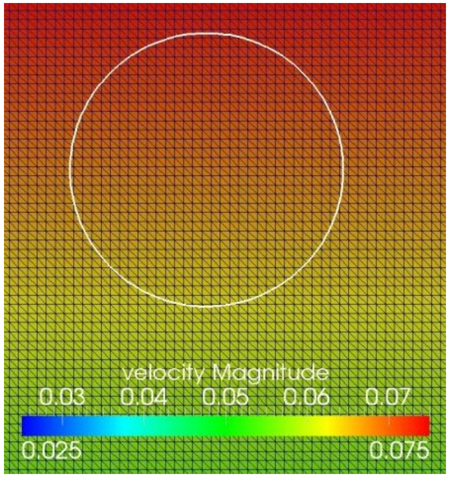
Force Balance:

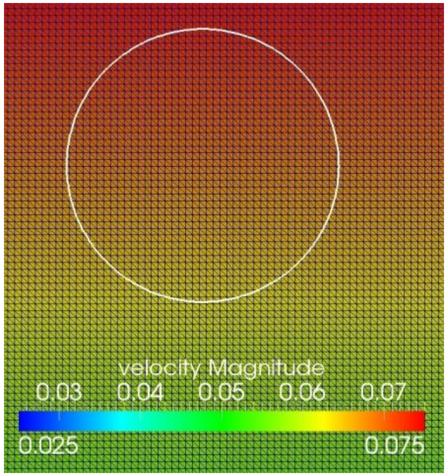
$$F_D = F_B + F_{xc} = (\rho_l - \rho_g)V_b g + F_{xc} = \frac{1}{2} C_D \rho_l v_r^2 A$$

$$F_L = F_{yc} = -C_L \rho_l V_b \vec{v}_r \times curl(\vec{v}_l)$$

Lift force: Mesh study







Resolution (elements across diameter)	C_d	C_l
20	0.16774	0.9628
30	0.1616	1.0282
40	0.1587	0.9964

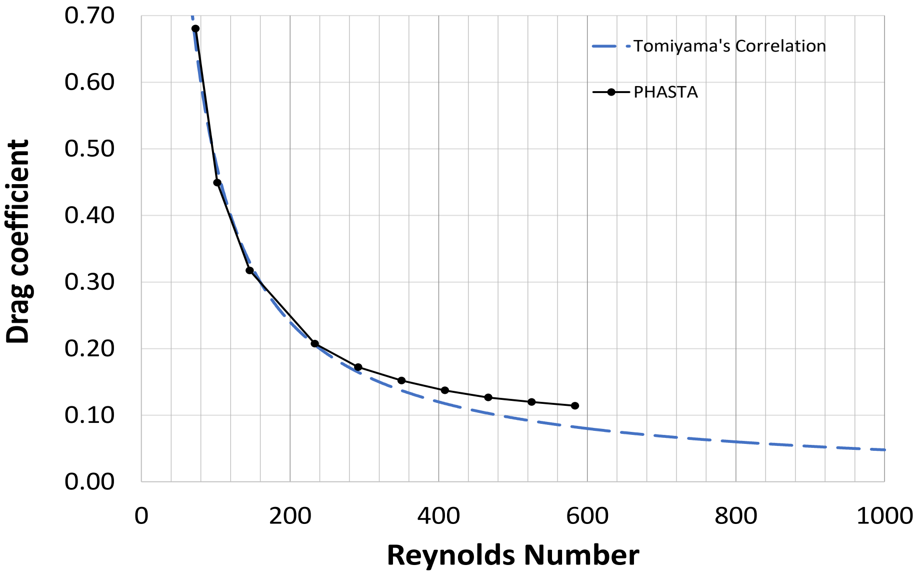
Drag force validation

Tomiyama A, Kataoka I, Zun I, Sakaguchi T. Drag coefficients of single bubbles under normal and micro gravity conditions. *JSME international journal.Series B, fluids and thermal engineering*. 1998;41(2):472-479

$$C_D = \min\left[\frac{16}{Re}\left(1 + 0.15Re^{0.687}\right), \frac{48}{Re}\right]$$

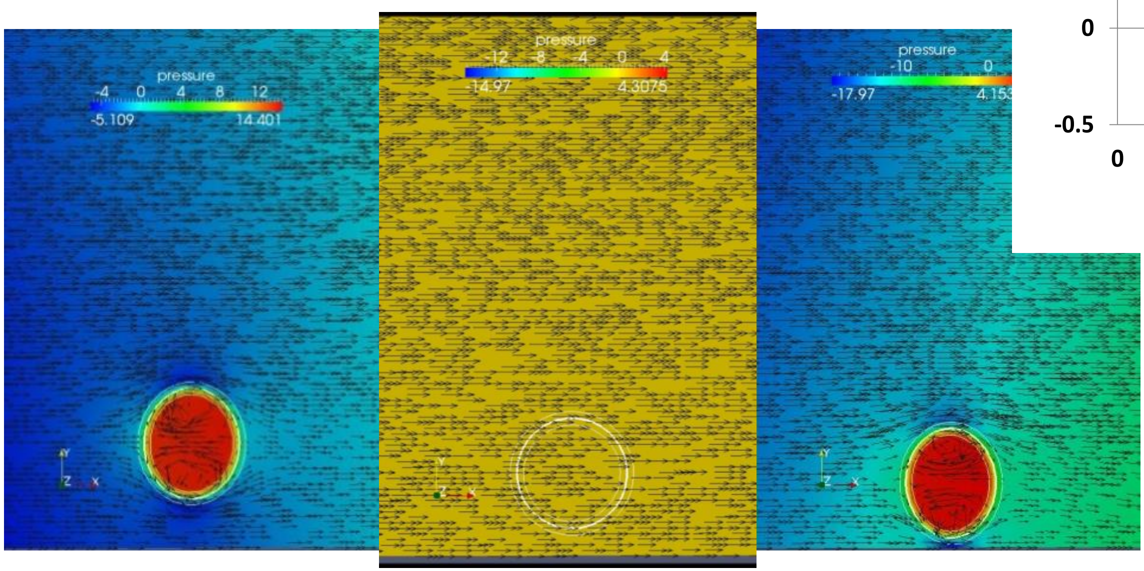
$$Re = \frac{\rho_L V_T d}{\mu_L}$$

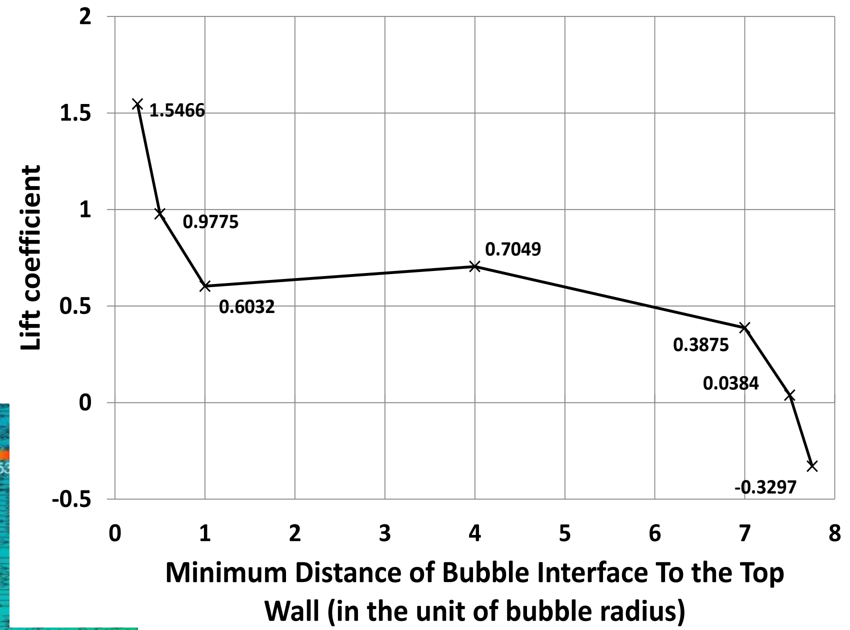
Case studies		Results	
		C_L	C_D
Relative velocity studies ($\frac{dv}{dy} = 1.0$)	R12.5:	0.3596	0.6805
	R17.5:	0.3775	0.4493
	R25:	0.3807	0.3172
	R40:	0.4086	0.2075
	R50:	0.4264	0.1722
	R60:	0.4223	0.1520
	R70:	0.4142	0.1372
	R80:	0.4177	0.1266
	R90:	0.3970	0.1198
	R100:	0.3925	0.1139



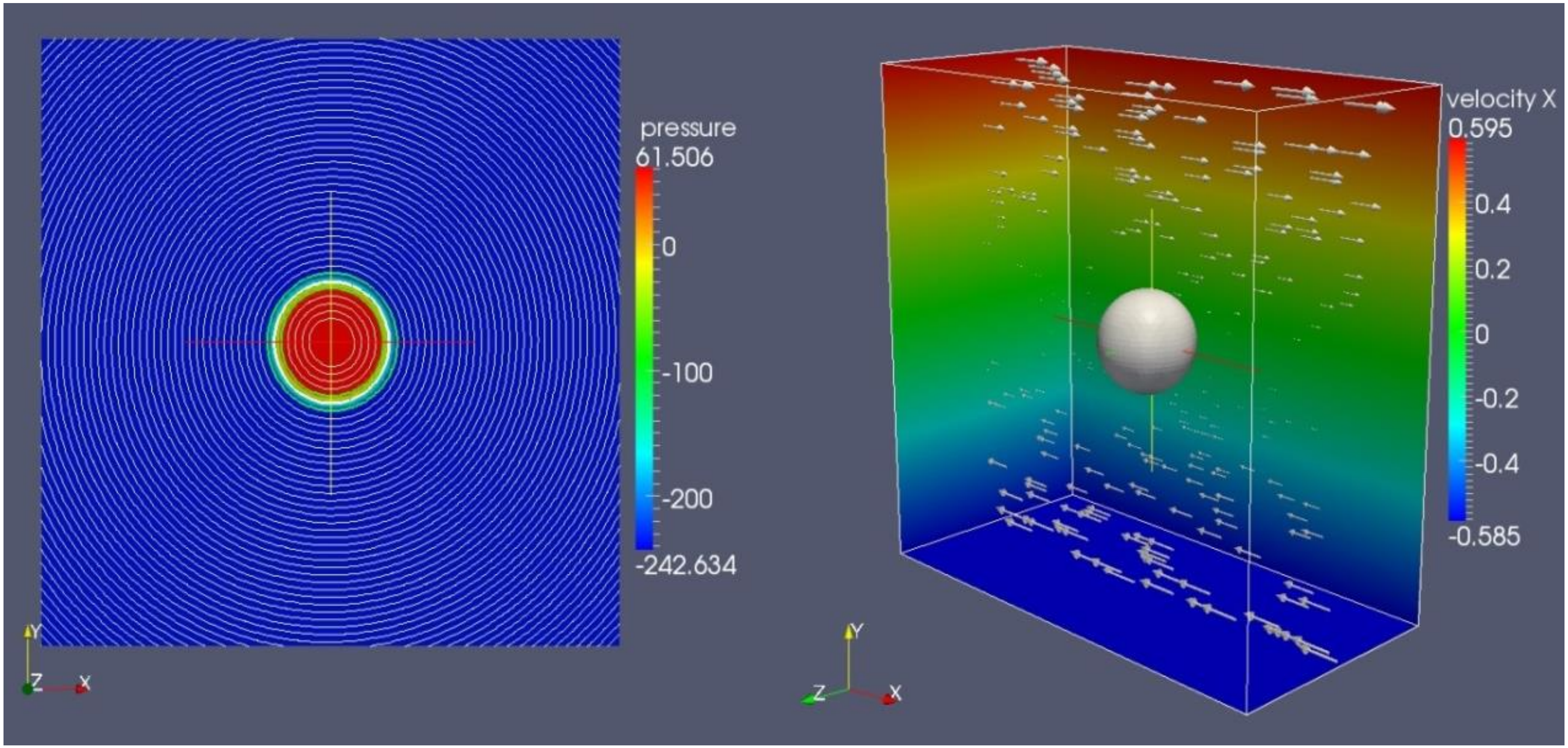
Wall effect study

Wall has the effect on the bubble behavior: emerging concept is to have variable lift force instead of counteracting "wall" force in multiphase CFD approach



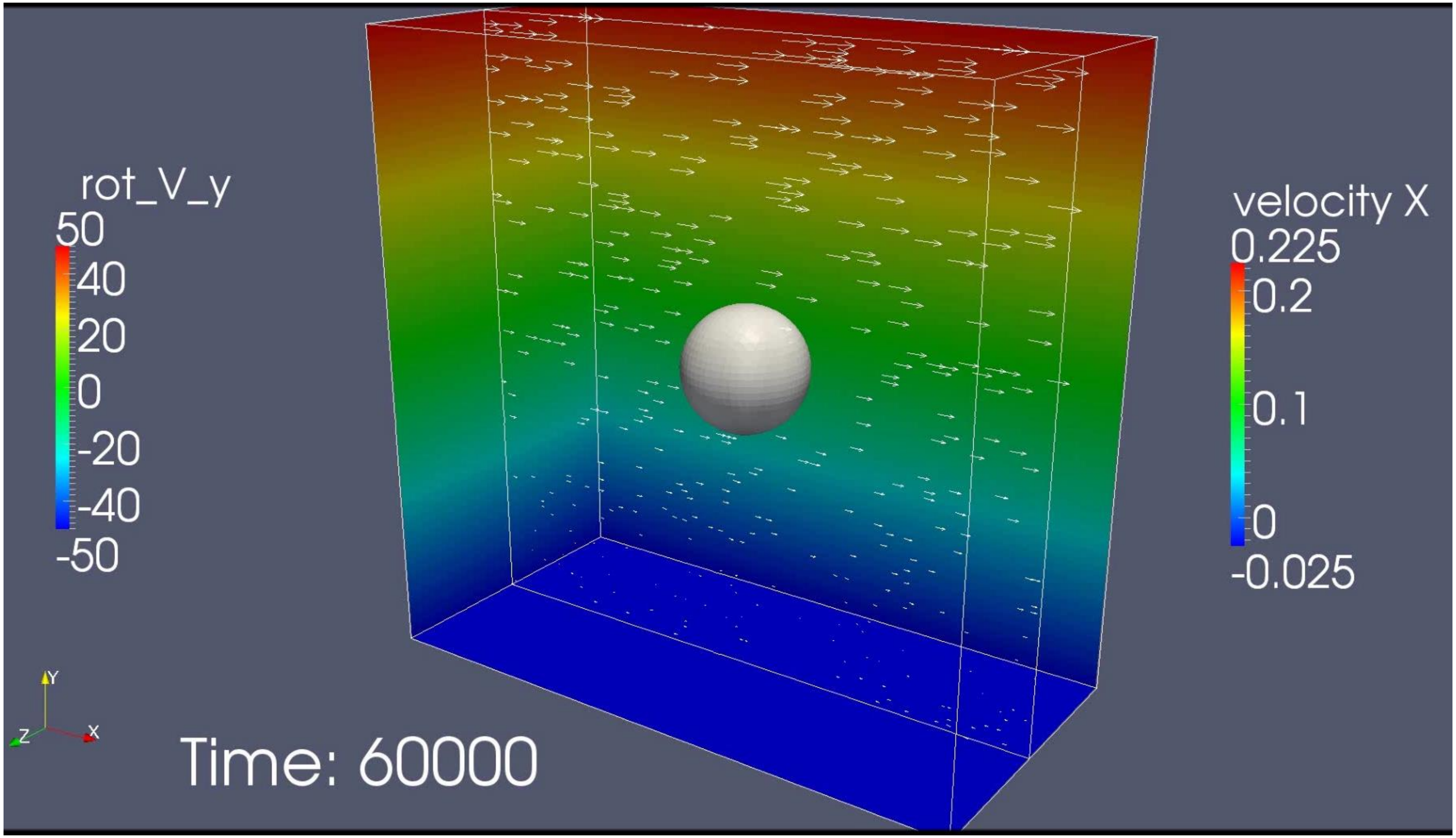


High shear rate simulations

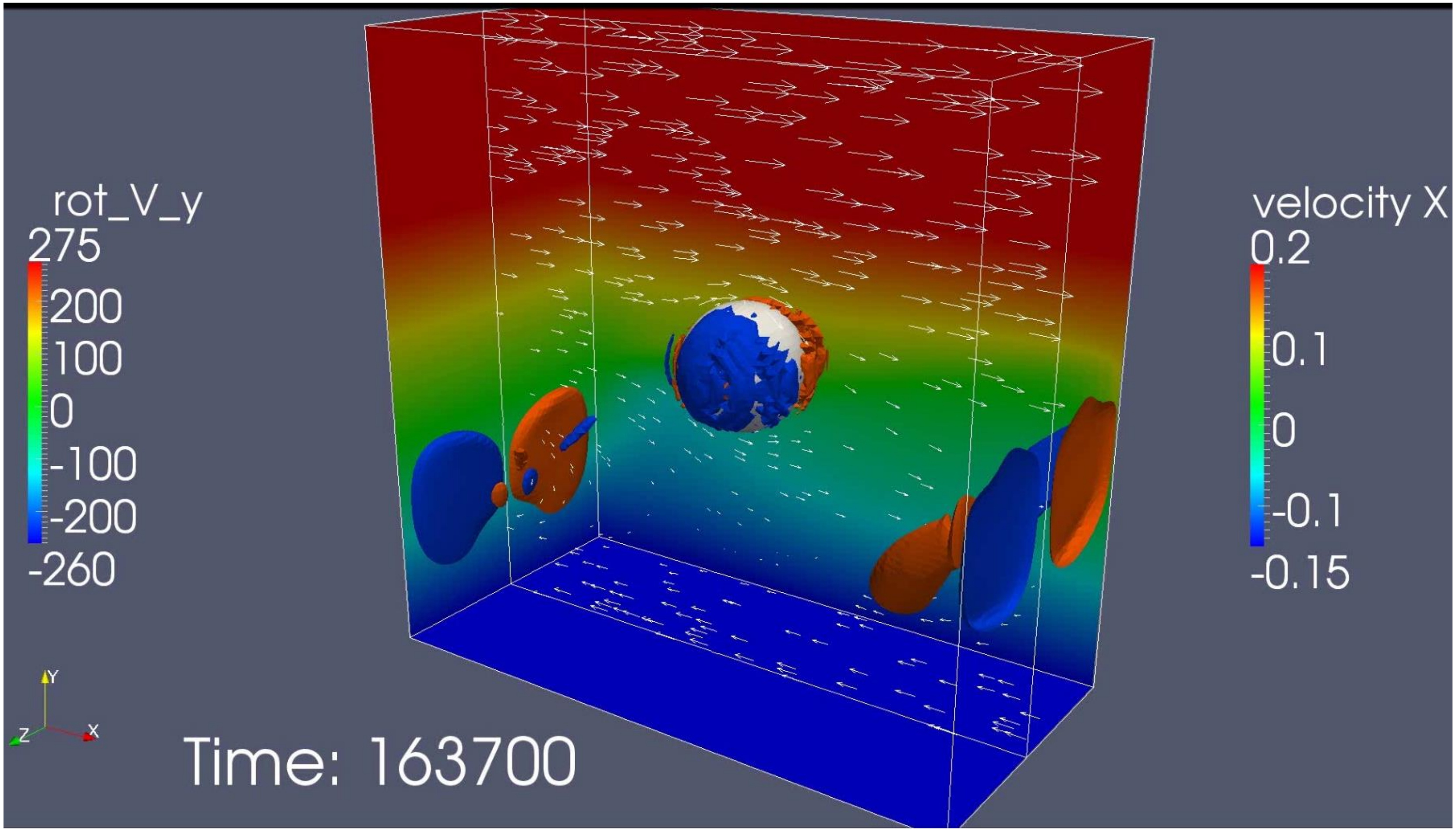


Typical case setup for a single bubble in high shear laminar flow

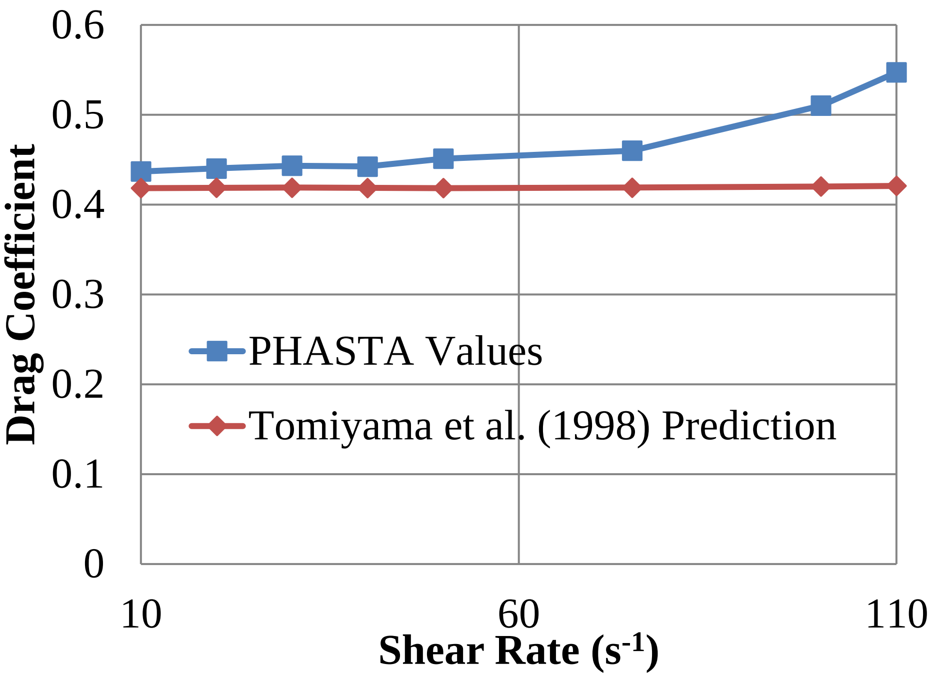
Medium Shear Laminar Flow (50 s^{-1})

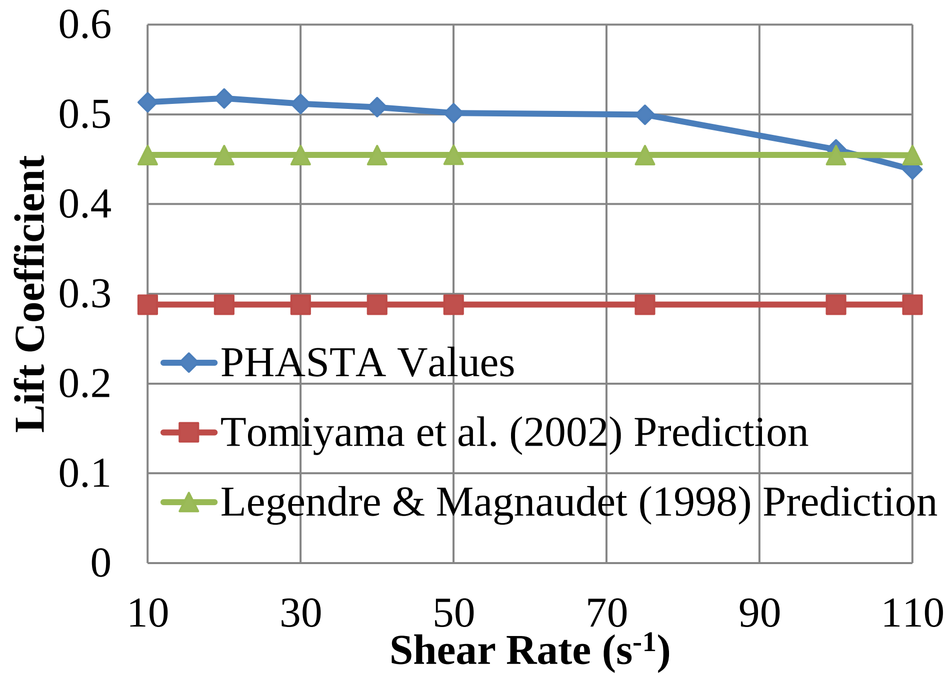


High Shear Laminar Flow (110 s^{-1})



Lift and drag coefficient vs. shear rate



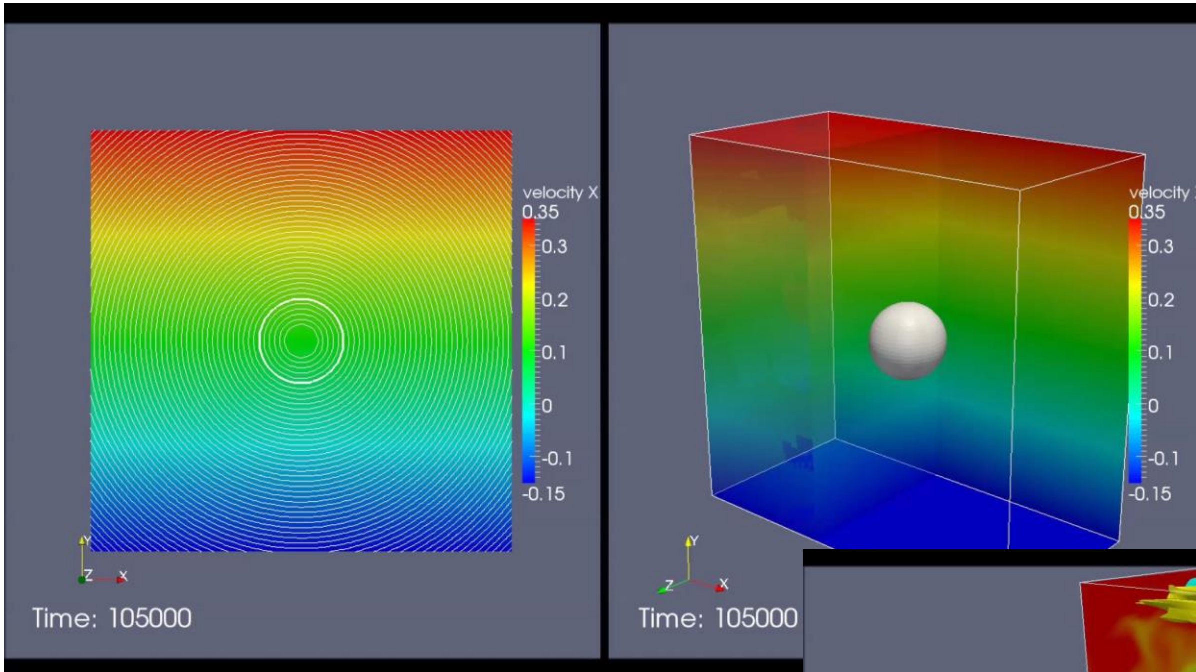


$$C_L = \sqrt{\left(\frac{6}{\pi^2}\frac{2.255}{(ReSr)^{0.5}(1+0.2Re/Sr)^{1.5}}\right)^2 + \left(\frac{1}{2}\frac{1+16/Re}{1+29/Re}\right)^2} \qquad Sr = \frac{\omega d}{v_r}$$

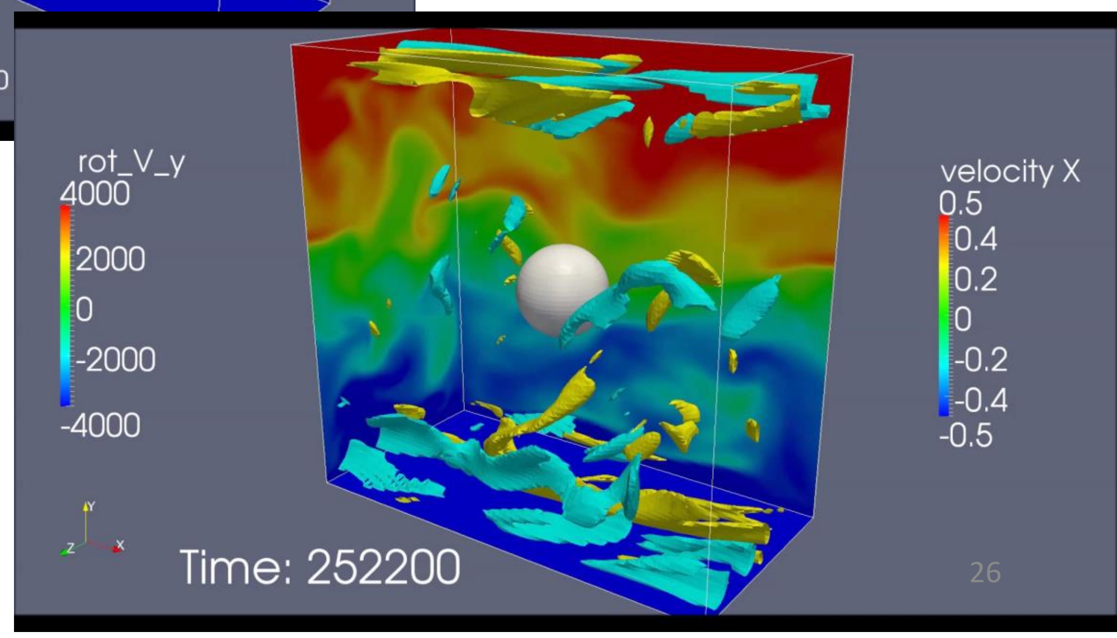
- Trends agree with Legendre & Magnaudet (1998) observation
- Correlations are independent of shear rate except Legendre & Magnaudet (1998)

Lift force: laminar and turbulent

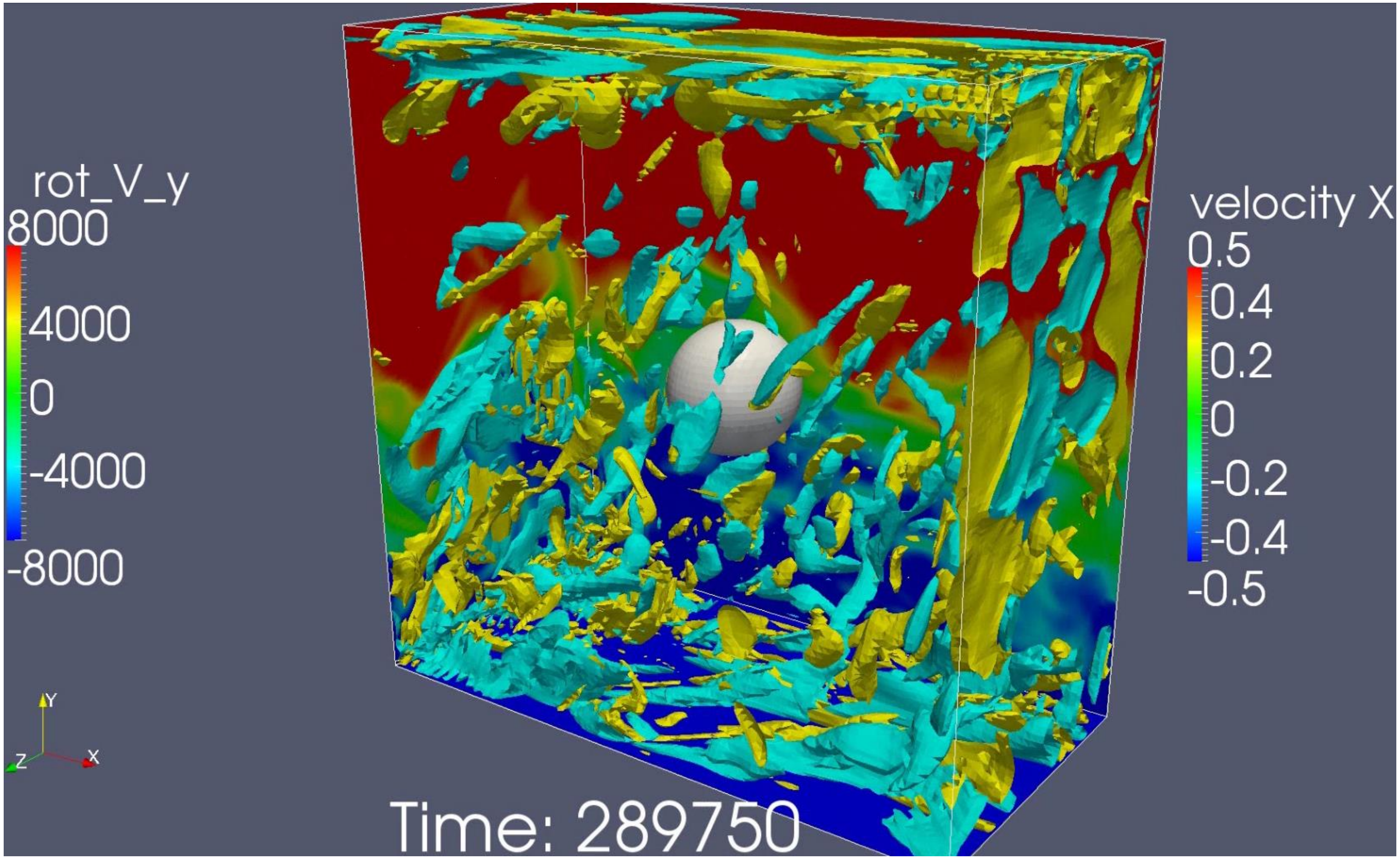
Laminar, shear rate: 100.0 s^{-1}



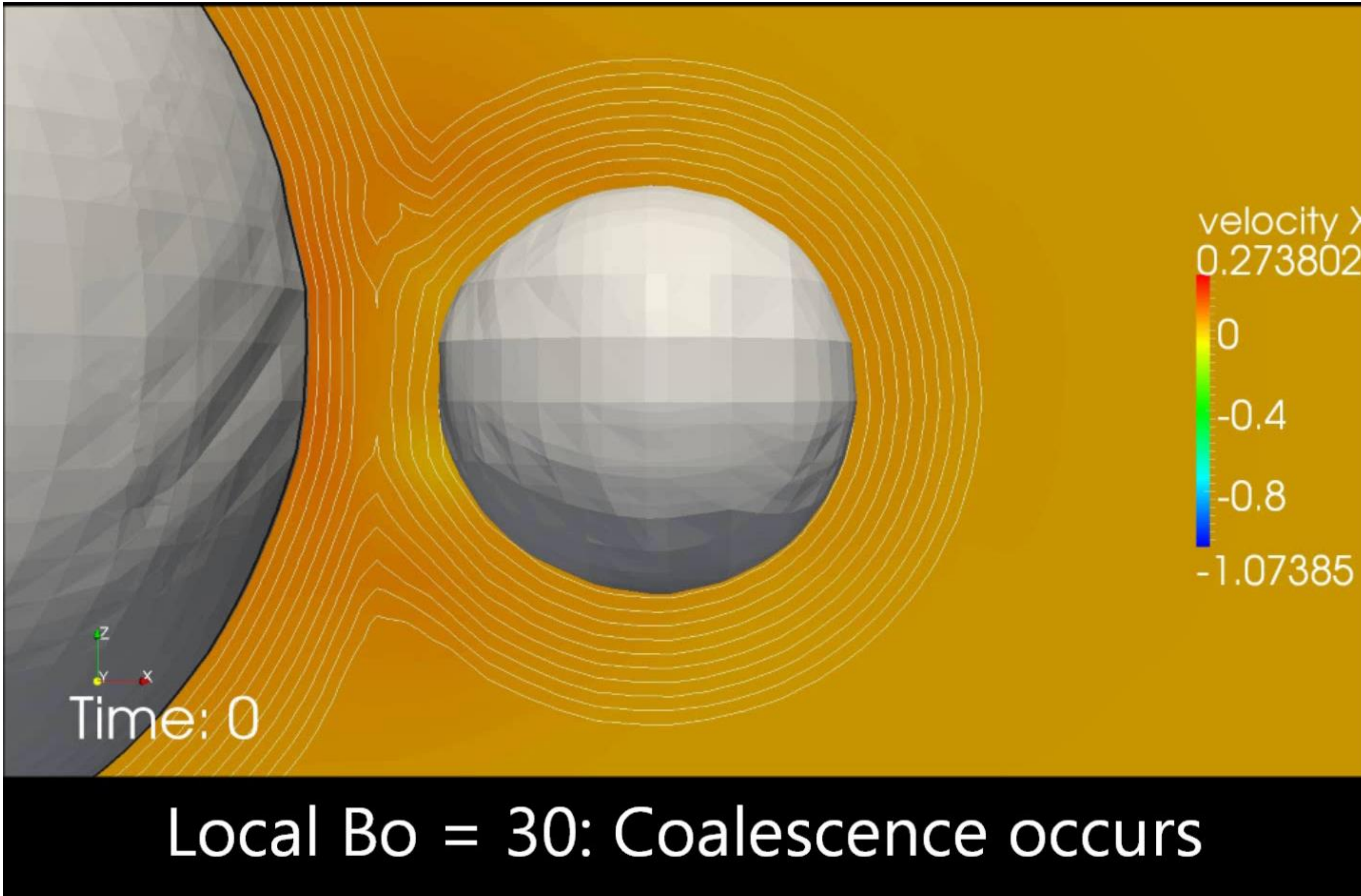
Turbulent, shear rate: 580.0 s^{-1}
(effective: 110.0 s^{-1})



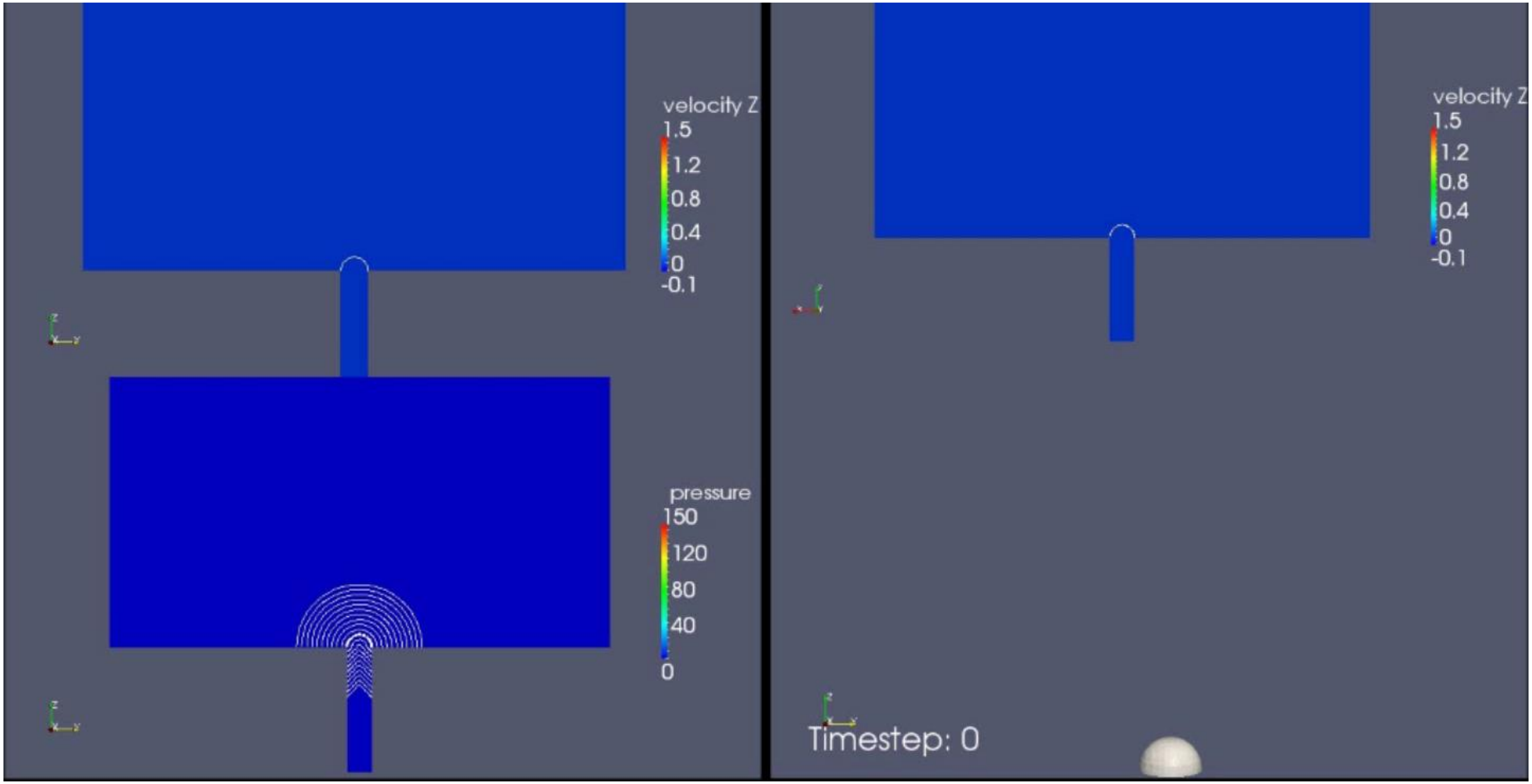
High shear turbulent (470 s^{-1})



Bubble Coalescence Control

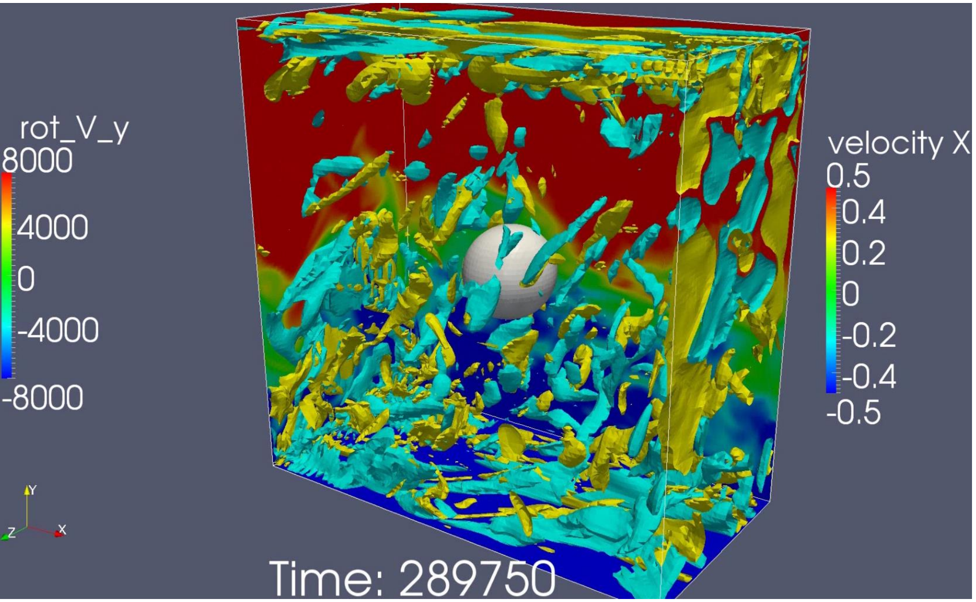


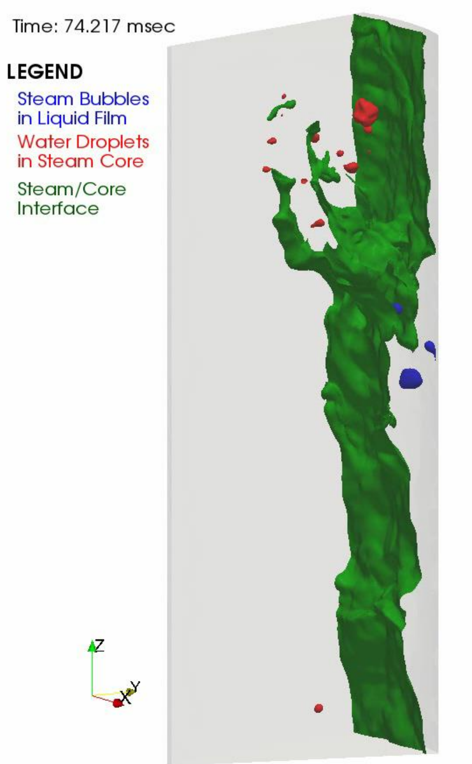
Bubble detachment

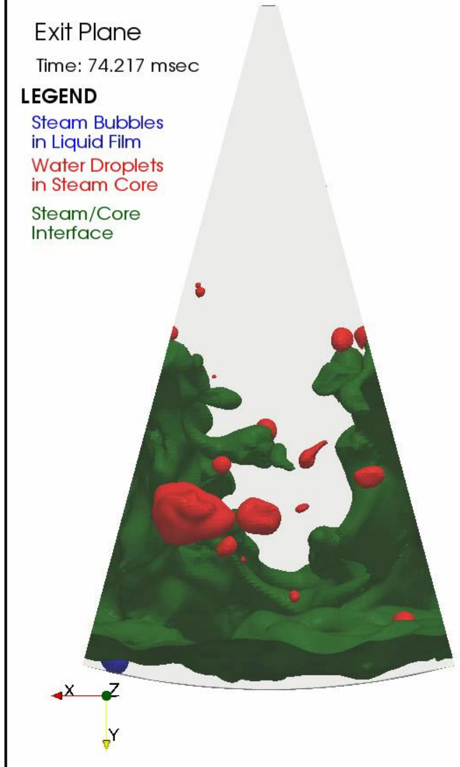


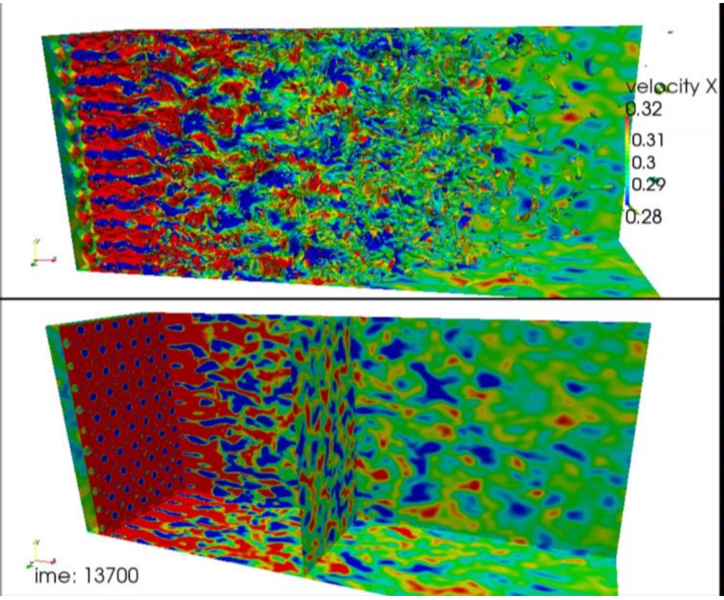
*Steve Palzewicz MNE project work

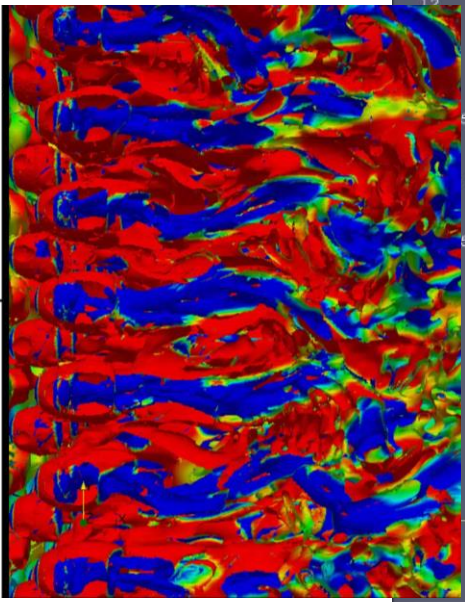
Simulations Examples

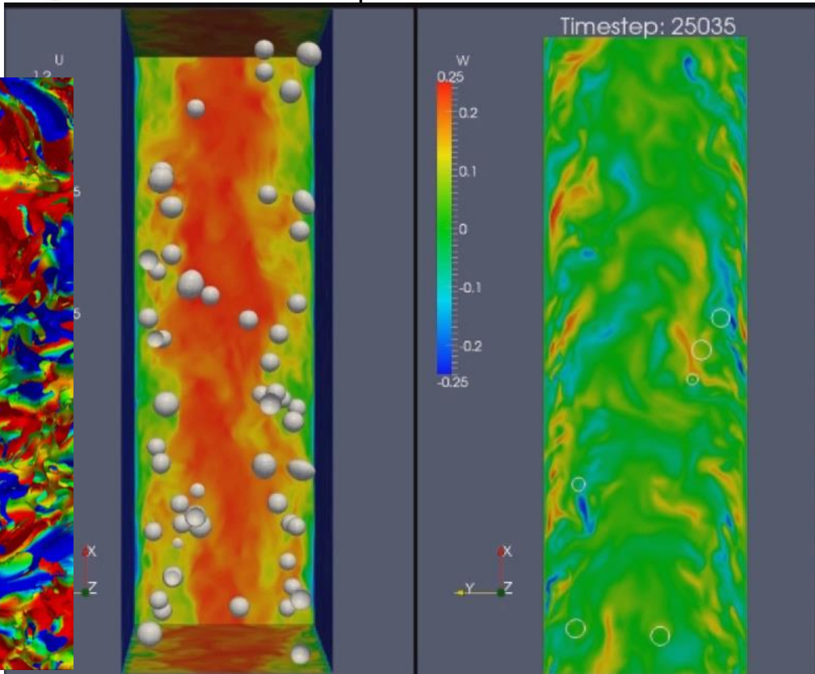












Multiple bubble simulations / Roughness study

Part 1: Turbulent bubbly flow in a channel

Overview:

Mesh resolution: 21 million elements

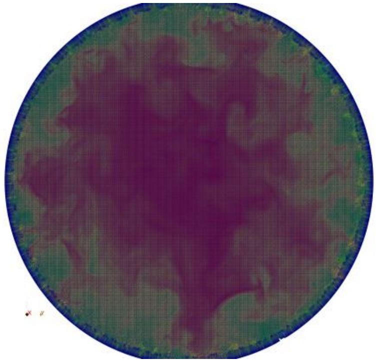
Computing resource: Jaguar supercomputer at ORNL; 11,200 cores used

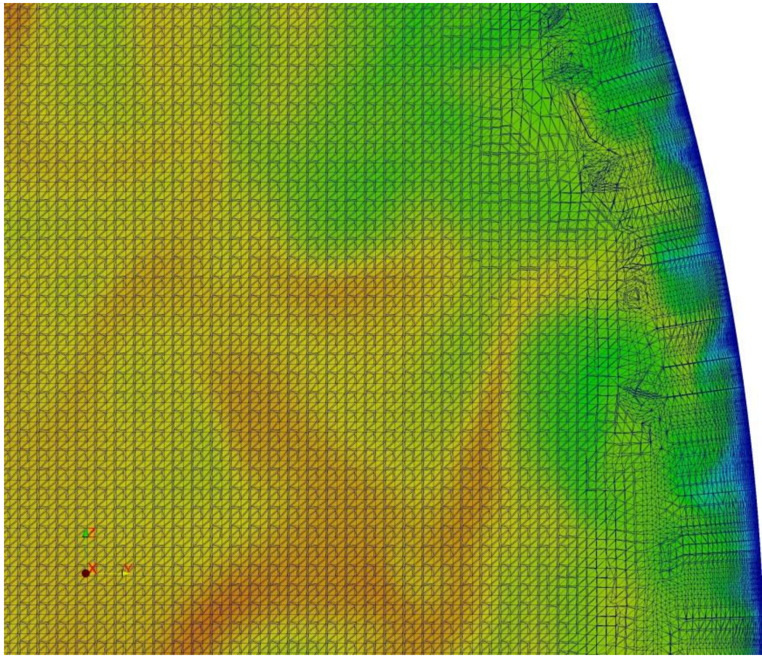
Turbulent Bubbly Pipe Flow Simulation

- 2014 **ASCR Leadership Computing Challenge (ALCC)** award from the U.S. Department of Energy Advanced Scientific Computing Research (ASCR) of 76.8 million CPU-hours at Argonne Leadership Computing Facility (ALCF) – IBM BG/Q based supercomputer with 768,000 cores.
- This allocation allows for direct overlap between experimental data and DNS capabilities
- We picked pipe flow experiments performed by M.E. Shawkat, C.Y. Ching, M. Shoukri "Bubble and liquid turbulence characteristics of bubbly flow in a large diameter vertical pipe" (IJMF **34**, 2008):
  - Pipe size: 200 mm ID
  - Liquid superficial velocities: 0.2 – 0.68 m/s
  - Gas superficial velocities: 0.005 – 0.18 m/s
  - Void fractions: 1.2 – 15.4 %
  - Average bubble diameter: 3 – 6 mm
- Selected DNS parameters:
  - Same pipe diameter, domain length is 628 mm with periodic boundary conditions
  - Liquid velocity: 0.35 m/s; Reynolds of 77,000 (Re based on friction velocity 1920)
  - Void fraction: 1% (3% and 5% are planned)
  - Bubble diameter: 7.5 mm
  - Gravity is reduced to keep the Eo number consistent with experiment

Turbulent Bubbly Pipe Flow Simulation

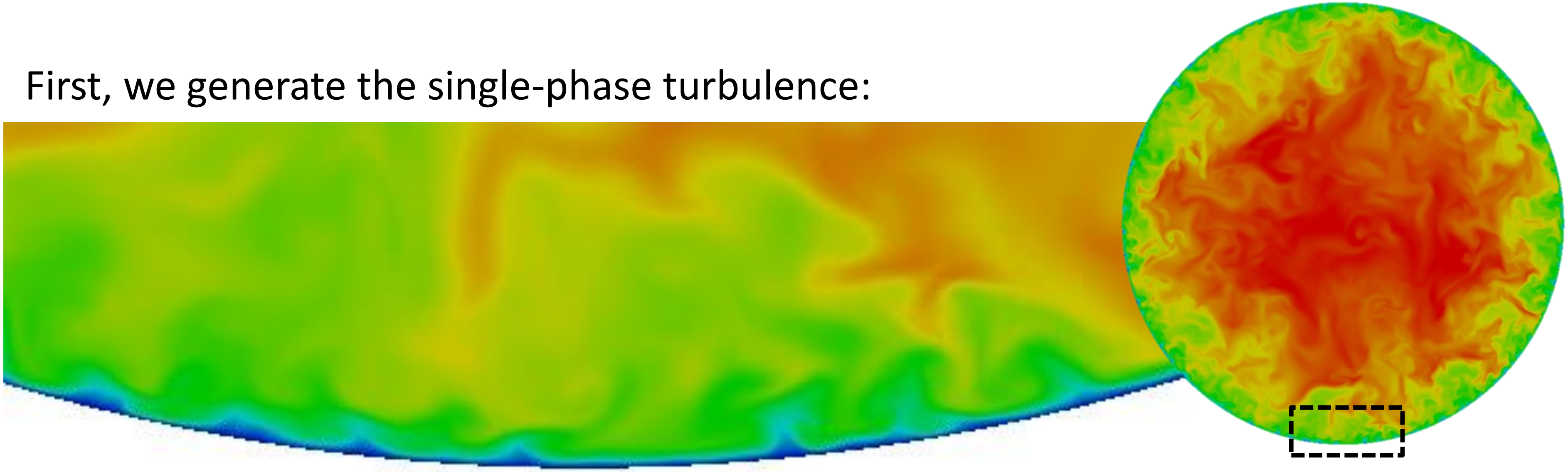
- Selected DNS parameters:
    - Same pipe diameter, domain length is 628 mm with periodic boundary conditions
    - Liquid velocity: 0.35 m/s; Reynolds of 77,000 (Re based on friction velocity 1920)
    - Void fraction: 1% (3% and 10% are planned)
    - Bubble diameter: 7.5 mm
    - Gravity is reduced to keep the Eo number consistent
- This results in the following requirements for DNS:
    - Mesh size:
        - Number of tetrahedral elements: 1,919,762,176 (1.9 billion)
        - Number of nodes: 321,798,909 (321 million)
    - Number of cores: 128x1024 (1/6 of the 5th largest world supercomputer)
    - Number of fully resolved bubbles (20 points across the diameter / fully deformable): 895 (1%), 2685 (3%) and 8950 (10%)





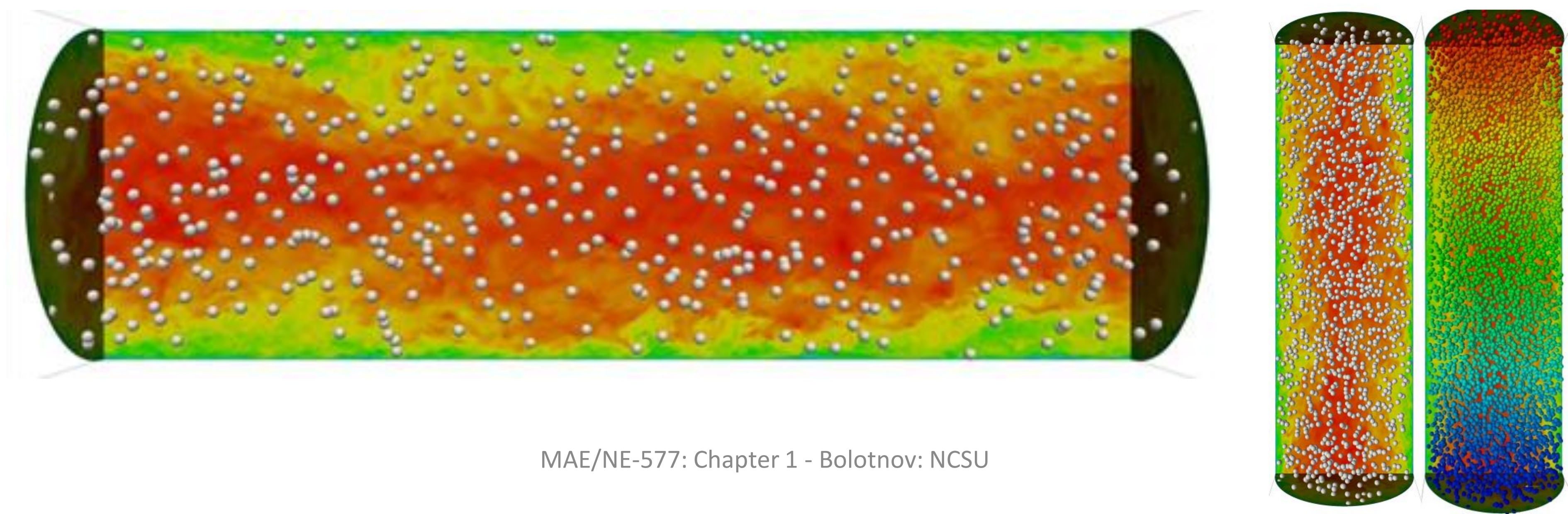
Turbulent Bubbly Pipe Flow Simulation

First, we generate the single-phase turbulence:



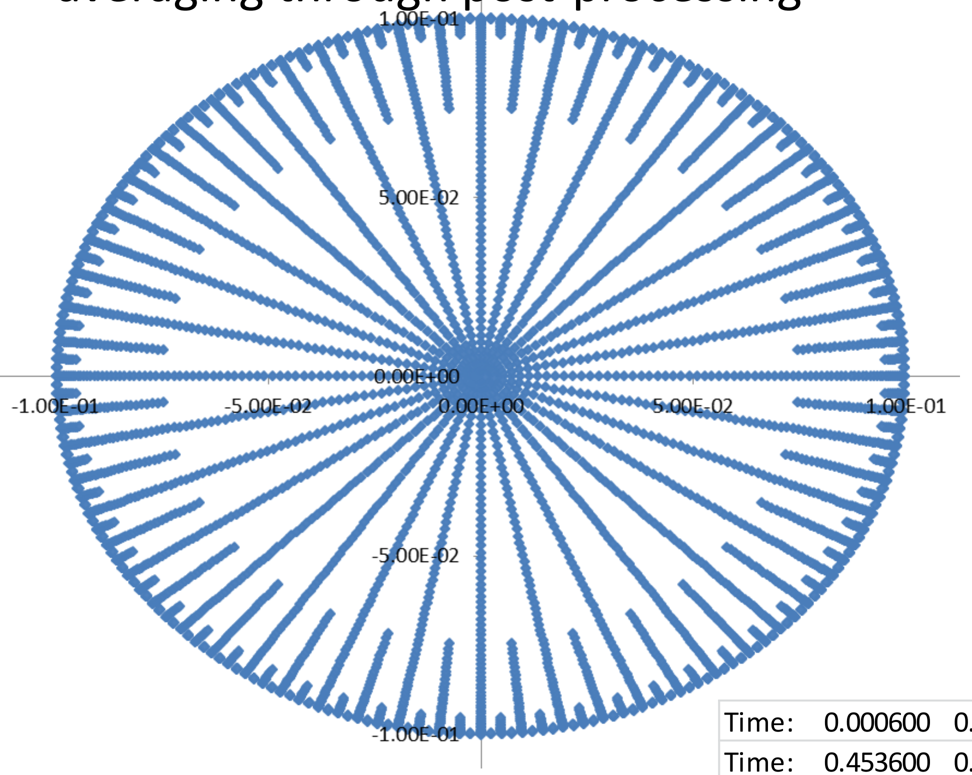
Then we place the bubbles (1% void fraction / random distribution):

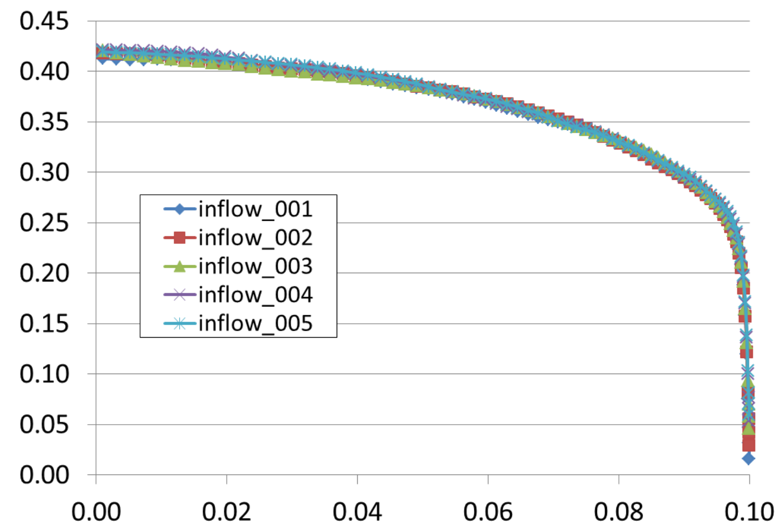
3% 10%

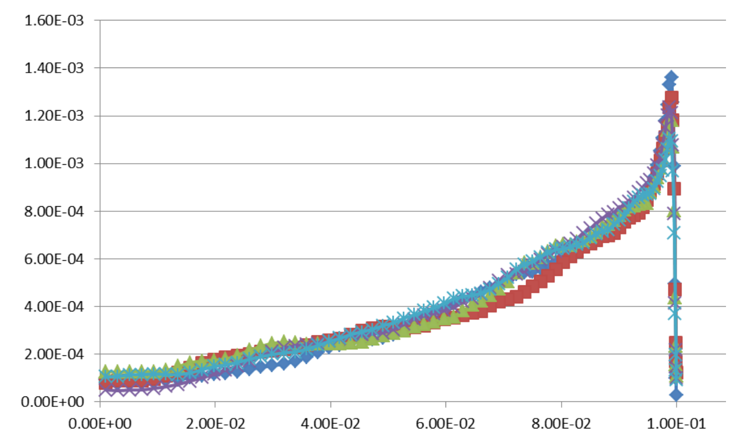


Turbulent Bubbly Pipe Flow Simulation

Basic analysis: place the virtual probes and record the time history of instantaneous velocities / pressures / phase indicator function for the averaging through post-processing



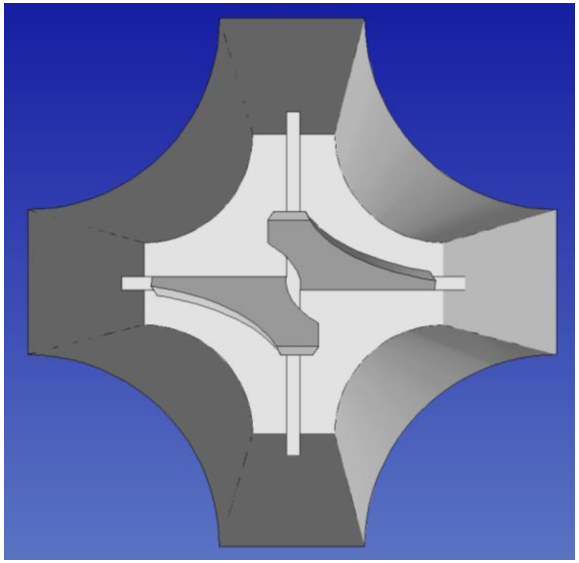


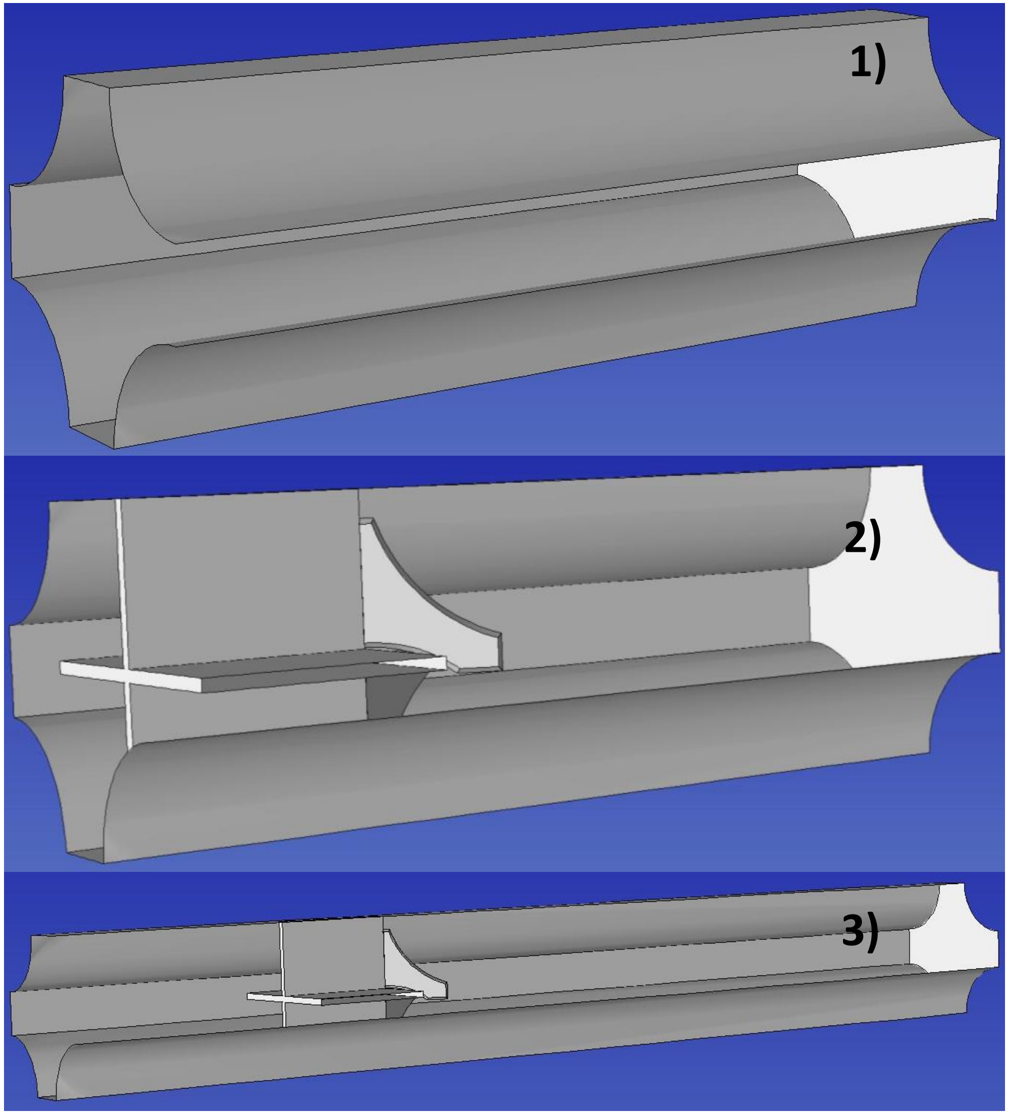


Time:	0.000600	0.227100	0.453600	0.453000	Steps:	15602	16254	16891	1289
Time:	0.453600	0.680100	0.906600	0.453000	Steps:	16891	17798	18930	2039
Time:	0.906600	1.133100	1.359600	0.453000	Steps:	18930	20063	21195	2265
Time:	1.359600	1.586100	1.812600	0.453000	Steps:	21195	22328	23460	2265
Time:	1.812600	2.041625	2.270650	0.458050	Steps:	23460	24605	25750	2290

Subchannel applications

1) Subchannel without internal structures
2) Subchannel with spacer grid and mixing vanes
3) Long subchannel with spacer grid and mixing vanes



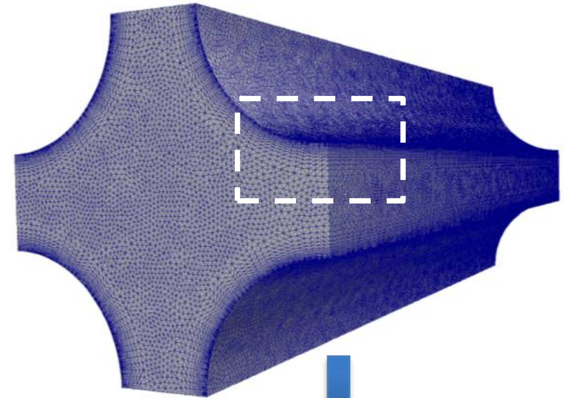


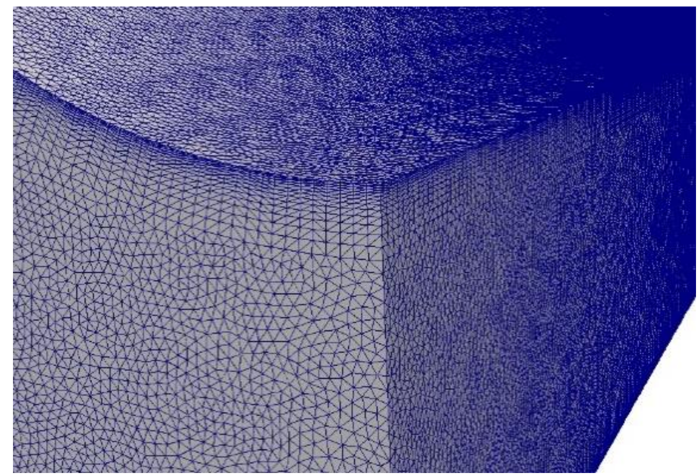
Subchannel applications

The computational mesh is created using an advanced unstructured meshing tool "Chef" allowing for outstanding performance in:

- Adaptive meshing
- Uniform mesh refinement
- Solution migration
- Dynamic load balancing

Large turbulent eddies are first developed on a coarse mesh, and then the solution can be migrated onto a finer mesh to allow smaller turbulent eddies/scales to develop, till a full DNS representation of the turbulent flow.





preUR
Coarse mesh
Mesh size: 17.36 M

→ 8x →

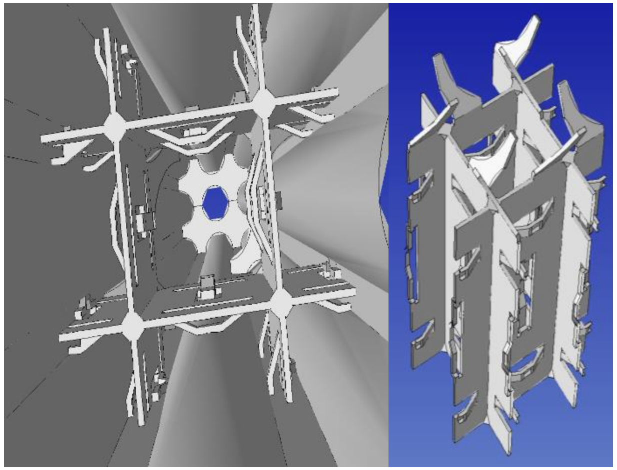
UR1
Intermediate mesh
Mesh size: 138.90 M

→ 8x →

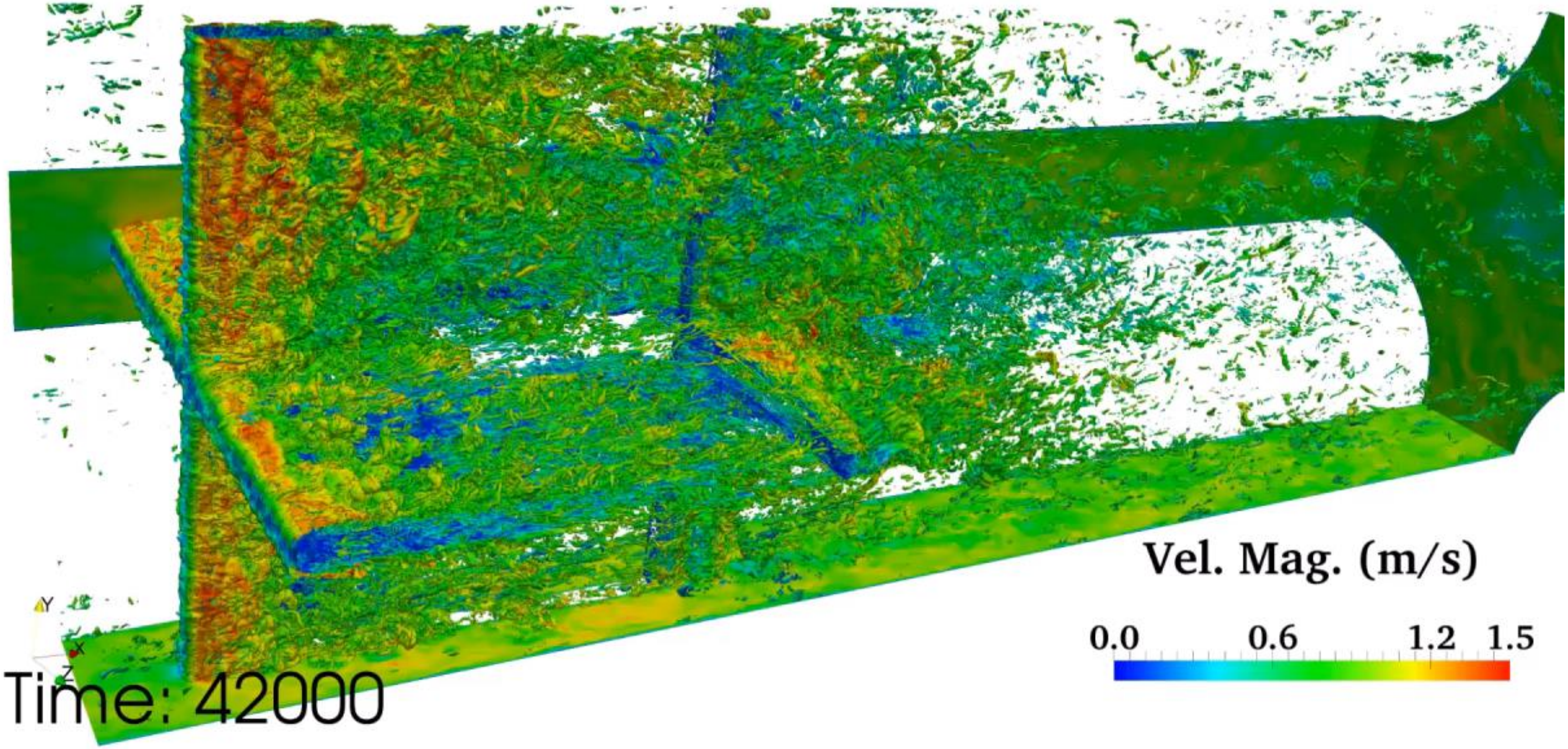
UR2
Fine mesh
Mesh size: 1.11 B

Subchannel applications

Realistic reactor spacer grids and mixing vanes used for turbulent flow simulations.



$Re_h \approx 80{,}000$; # of CPU cores used = 32,768;



Subchannel applications

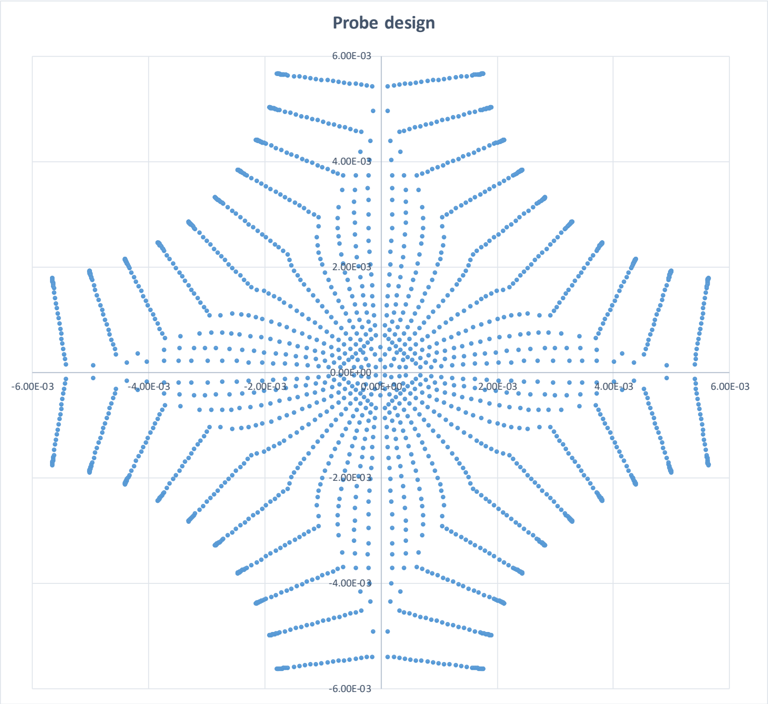
Conventional analysis can provide important time-averaged information, but a lot of details is **missing!**

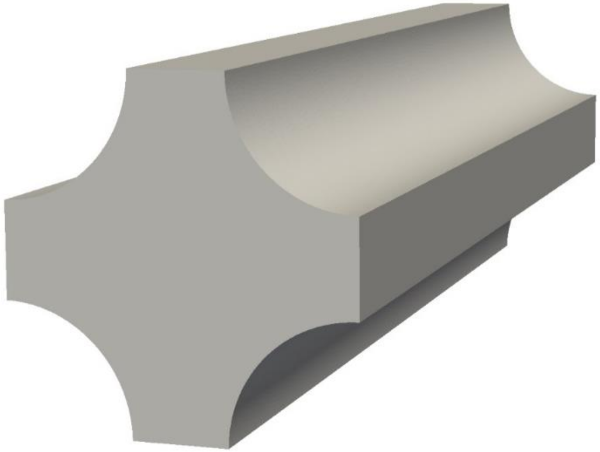
We need direct data about <u>bubble movements</u> to understand the bubble behavior patterns.

$$U_i(t) = \frac{1}{N_e}\sum_{m=1}^{N_e}\left(\frac{1}{N_w}\sum_{j=1}^{N_w} u_m^i(t+t_j)\right)$$

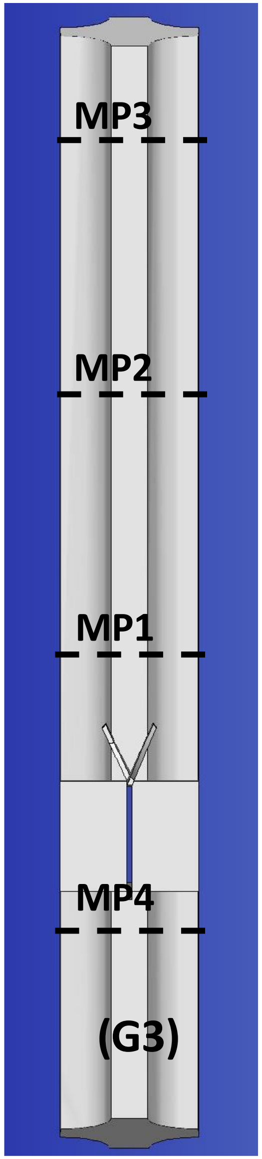
$$k(t) = \frac{1}{N_e}\sum_{m=1}^{N_e}\left(\frac{1}{N_w}\sum_{j=1}^{N_w}\sum_{i=1}^{3}\frac{1}{2}\left(u_m'^i(t+t_j)^2\right)\right)$$

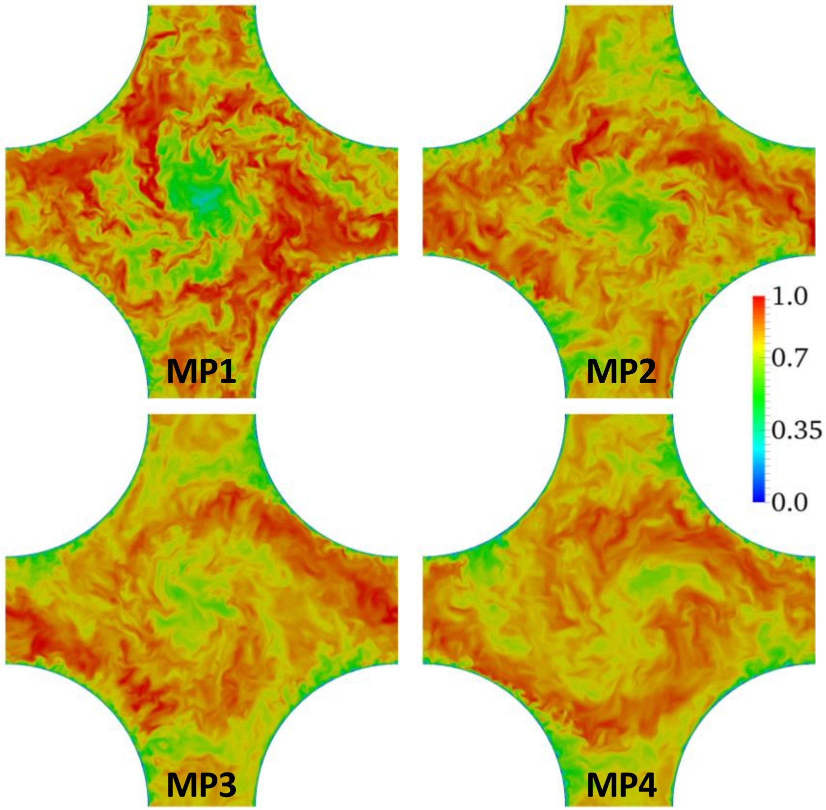
$$\alpha_k(t) = \frac{1}{N_e}\sum_{m=1}^{N_e}\left(\frac{1}{N_w}\sum_{j=1}^{N_w} X_k(t+t_j)\right)$$

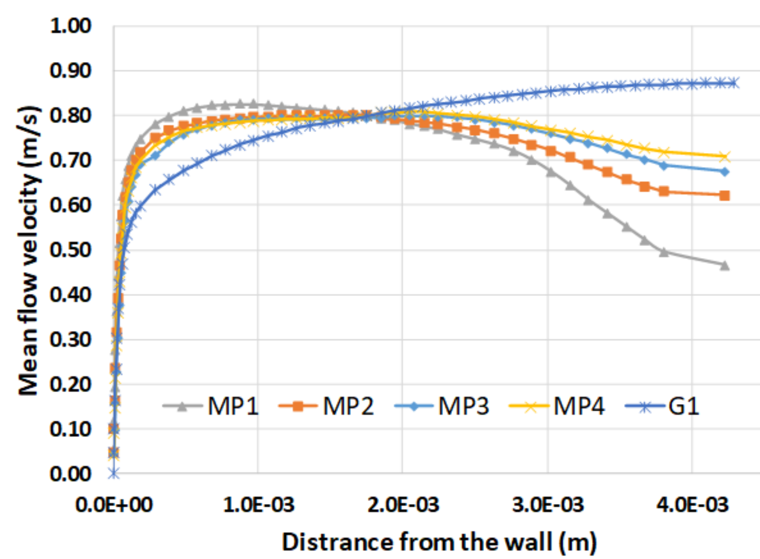


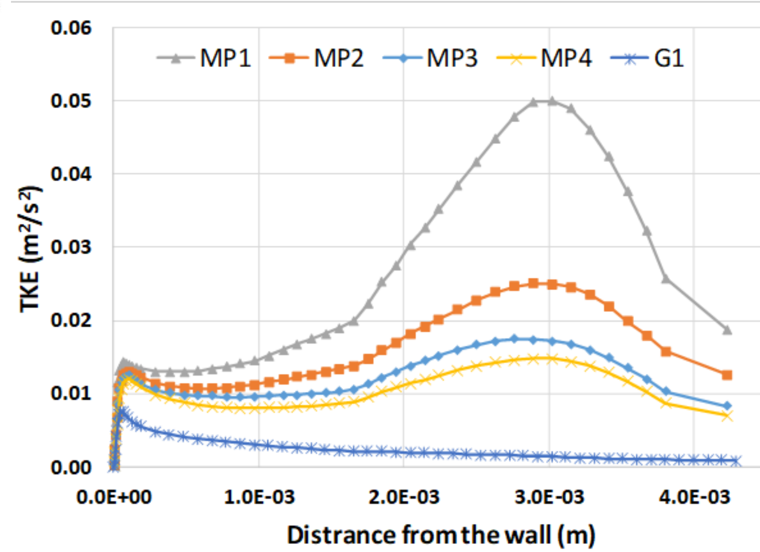


Subchannel applications







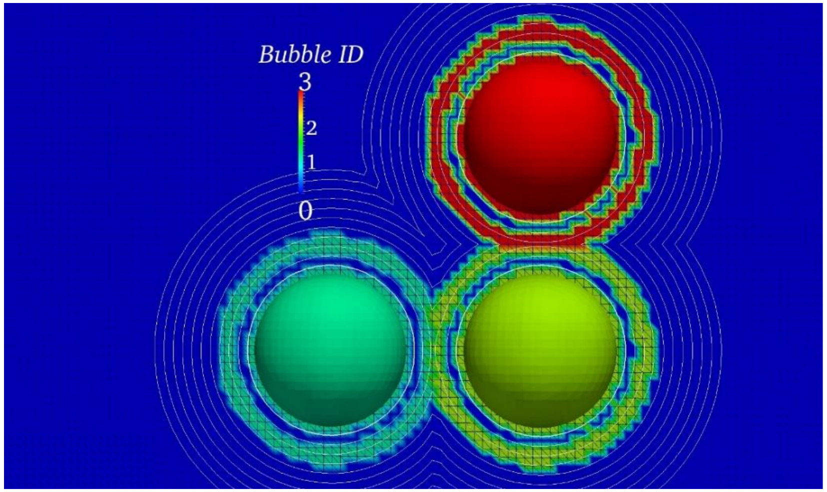


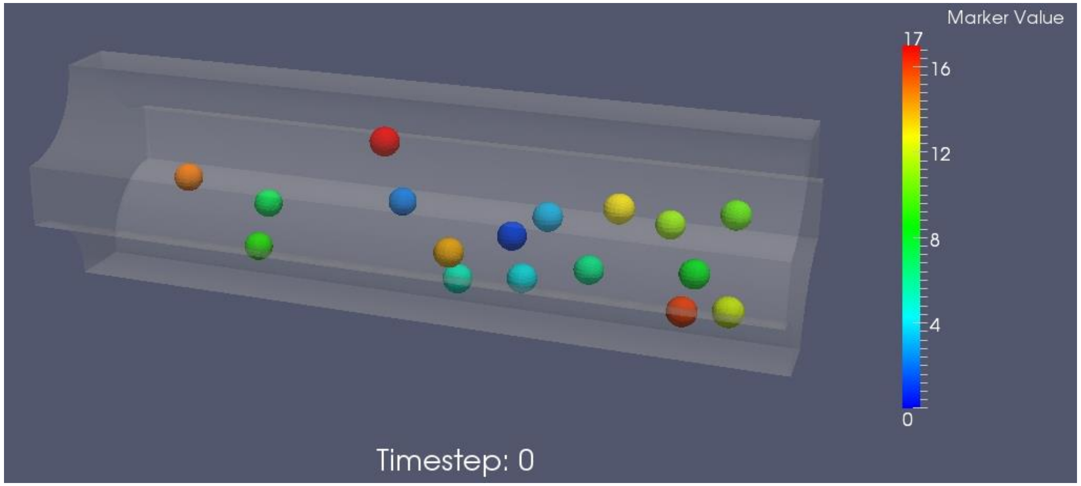
Bubble tracking

An ID/marker field is created along with level-set distance field.

Each bubble in the simulated domain gets assigned a unique ID.

Region of interest (ROI) usually consists of a bubble region and the local liquid shell.



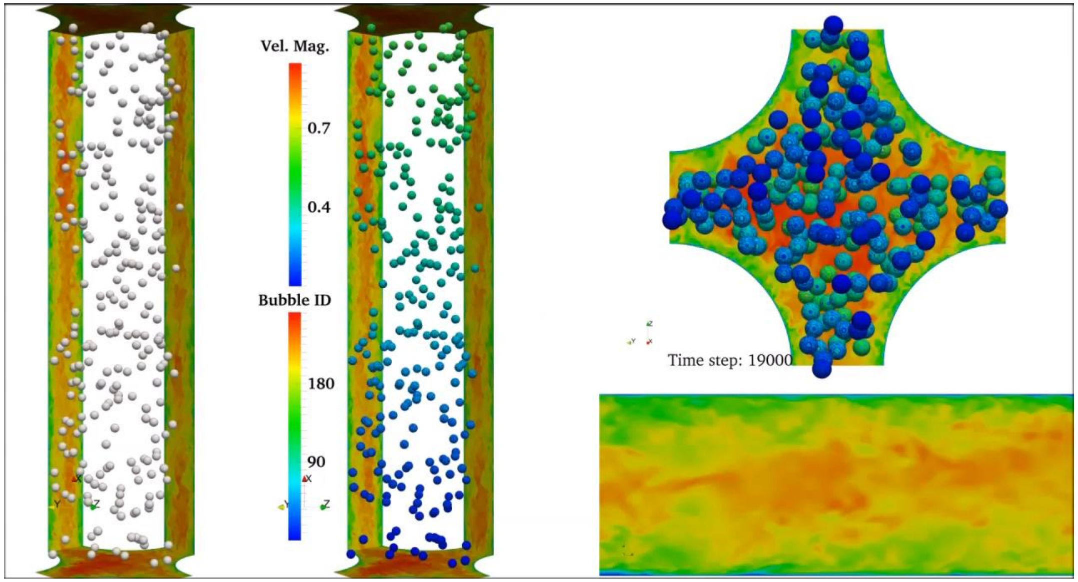


Bubble tracking data:

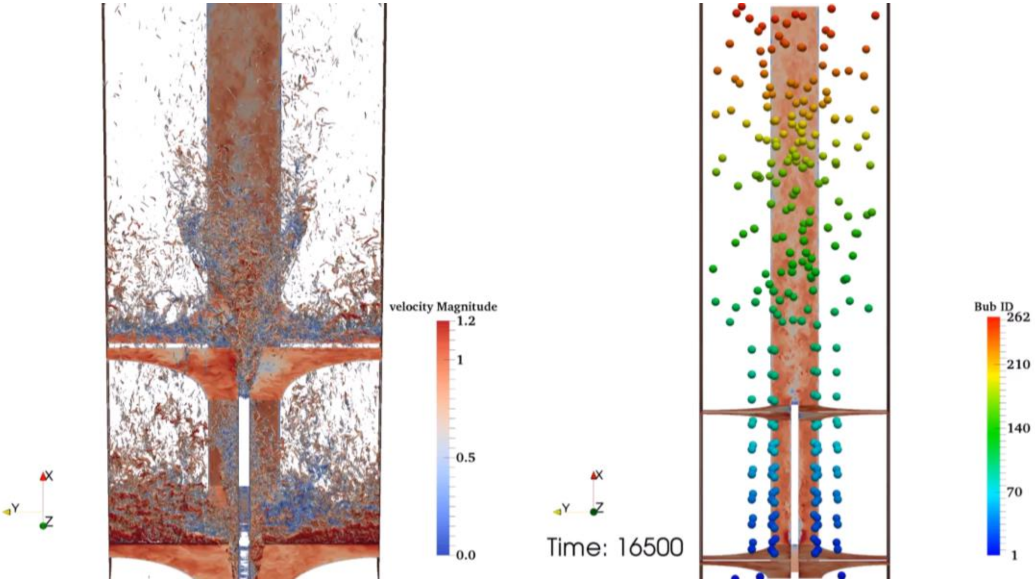
- Bubble volume & mass
- Average bubble position and velocity
- Bubble deformation level
- Local liquid velocity & shear rate

Two-phase flow through PWR geometry

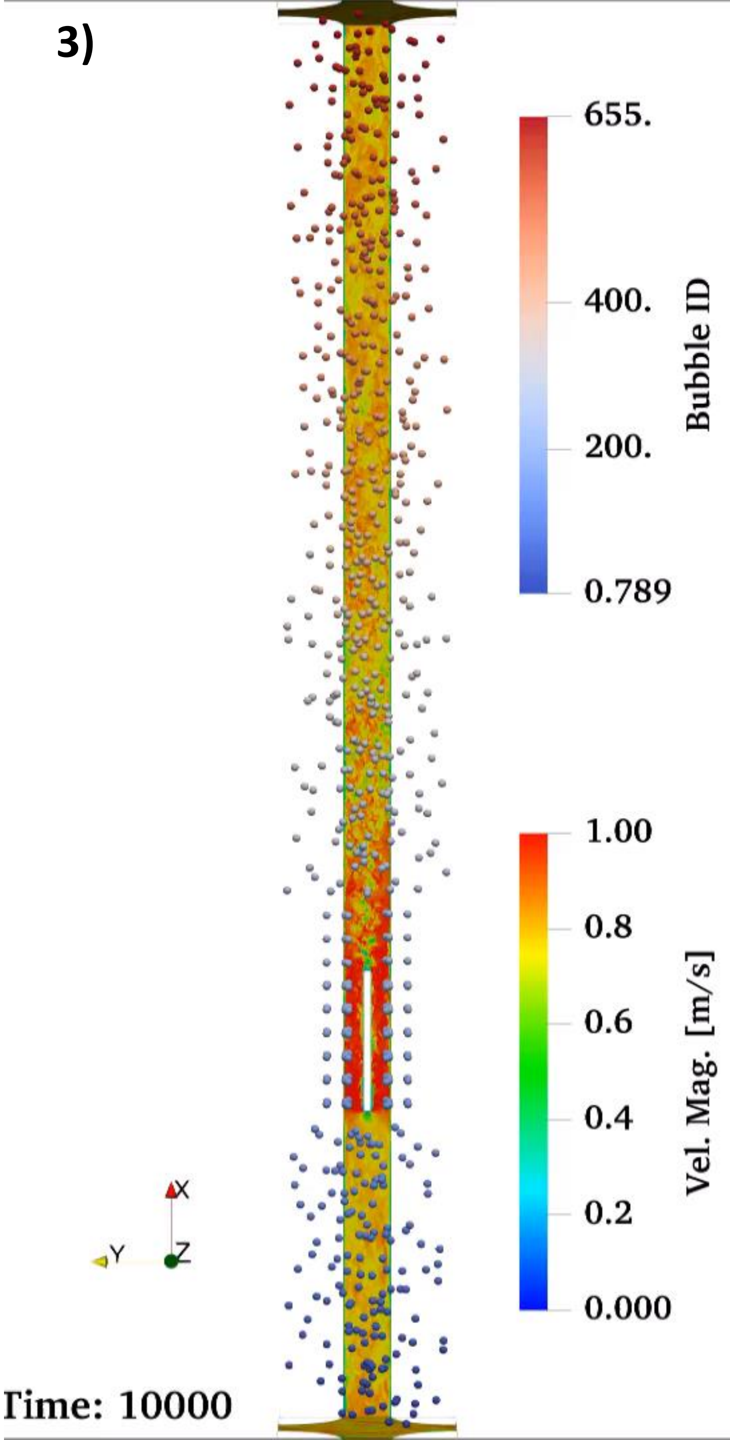
1)



2)

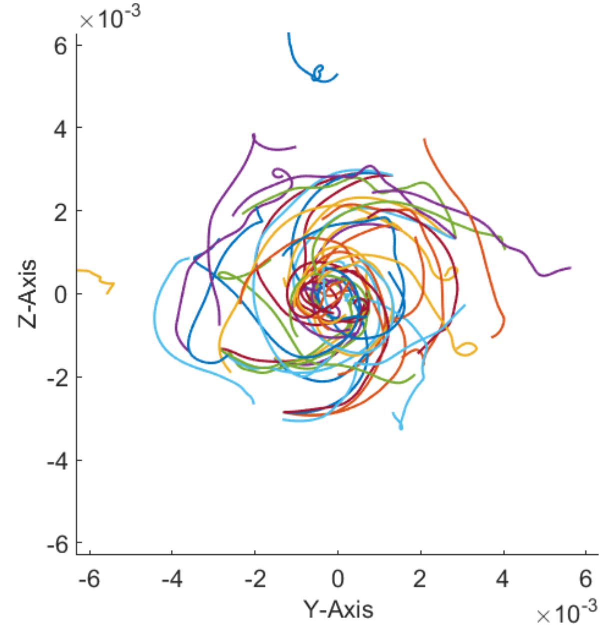


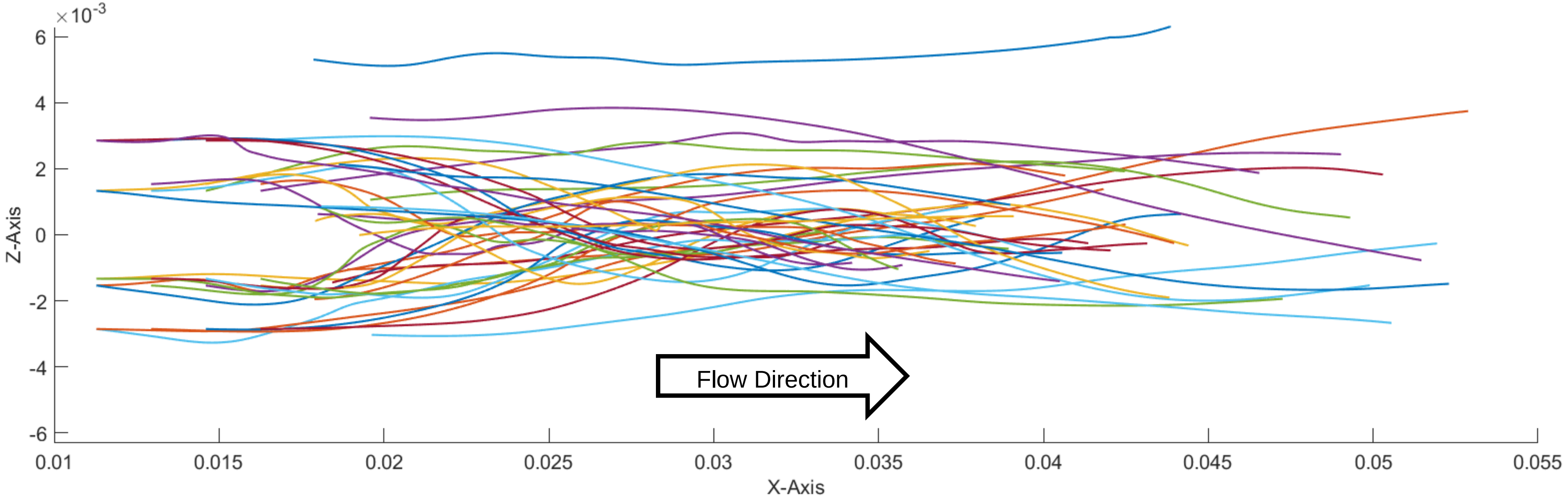
3)



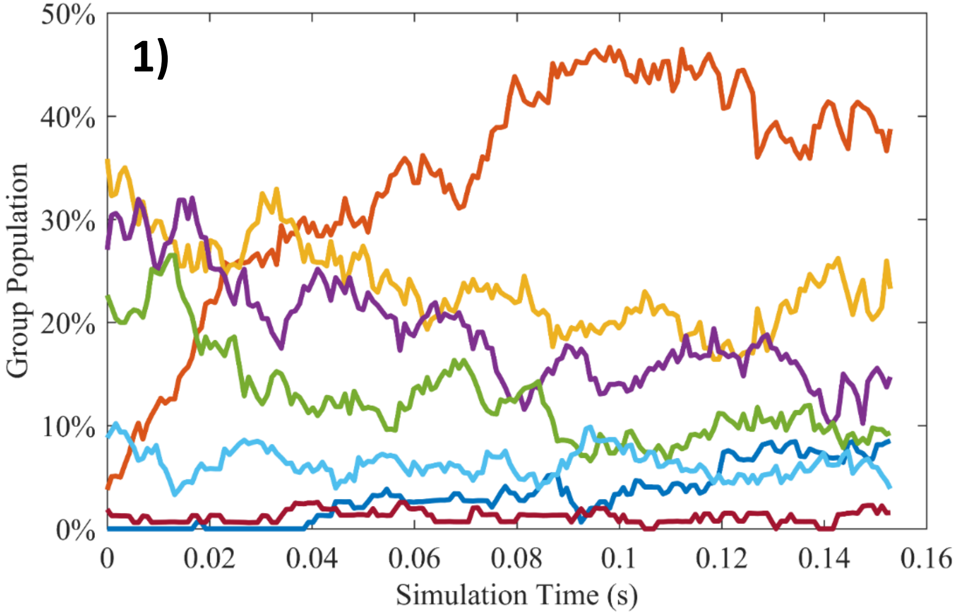
Two-phase flow through PWR geometry

- Bubble tracking allows for the novel visualization of each individual bubble within the flow
- Plotting the path of each bubble reveals the intense swirling and mixing produced by the mixing vane geometry



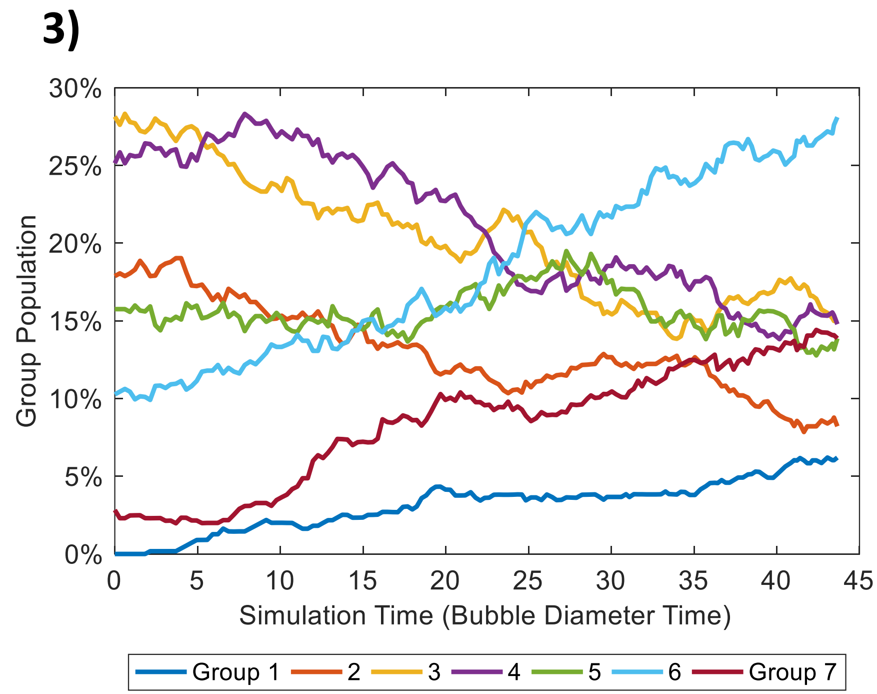


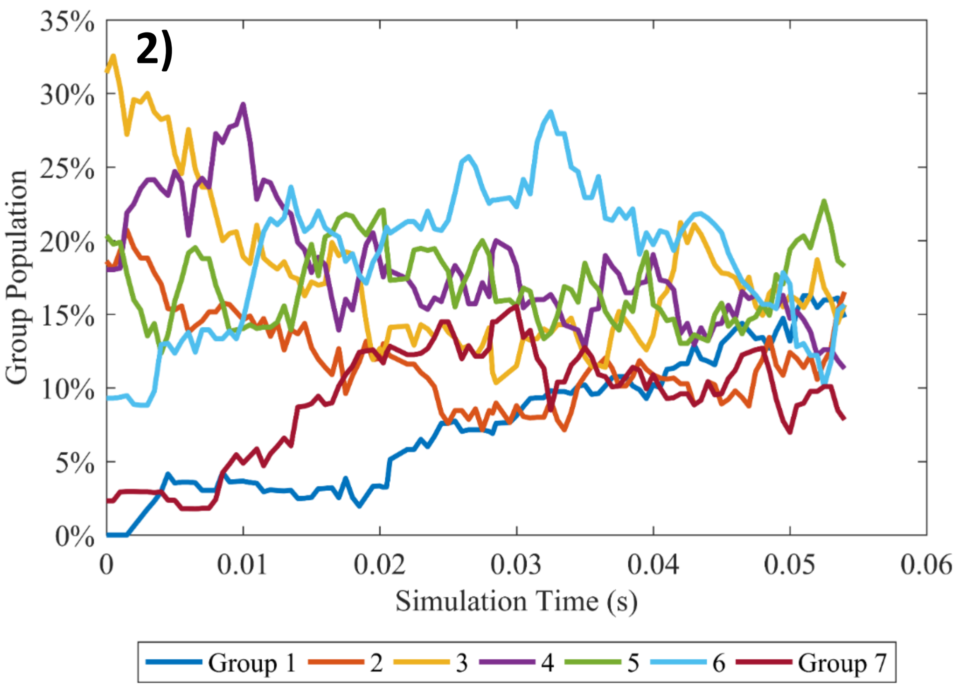
Two-phase flow through PWR geometry



Bubbles tend to migrate towards the walls in two-phase flows (lift force effects)

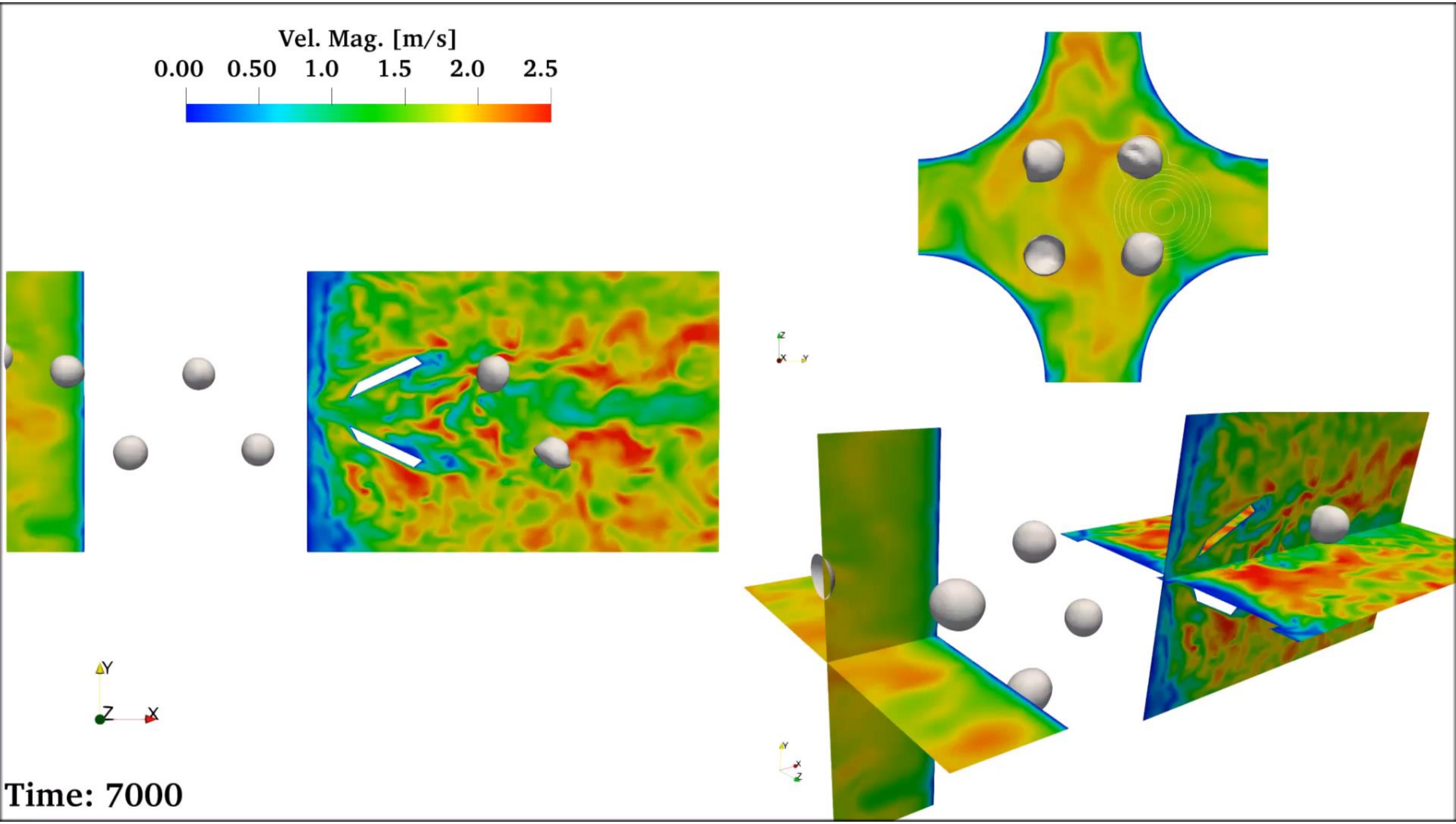
The mixing vane balances out the bubble population, cancelling the migration effect





Droplet flow

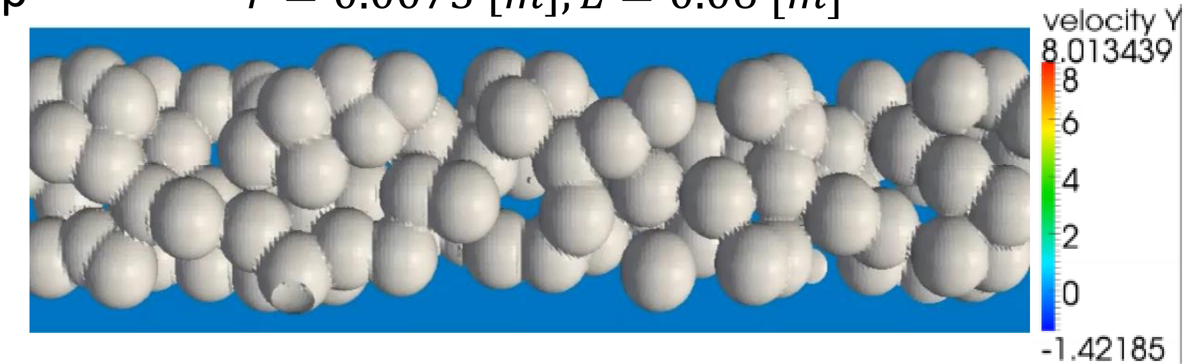
Dispersed flow film boiling (mist flow) regime exists under hypothetical loss-of-coolant accident (LOCA) conditions in PWRs



Simulating Flow Regime Transition

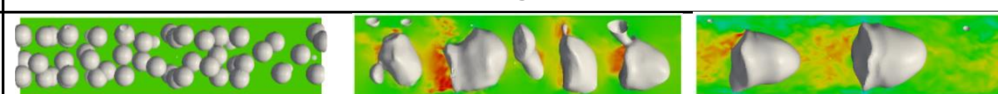
- α=0.4
- pressure gradient is step increased twice

$r = 0.0075\ [m], L = 0.06\ [m]$



Number of Elements [million]	5
y^+_{wall}	7.5
Wall Element Size [mm]	0.0385
y^+_{bulk}	46
Bulk Element Size [mm]	0.236

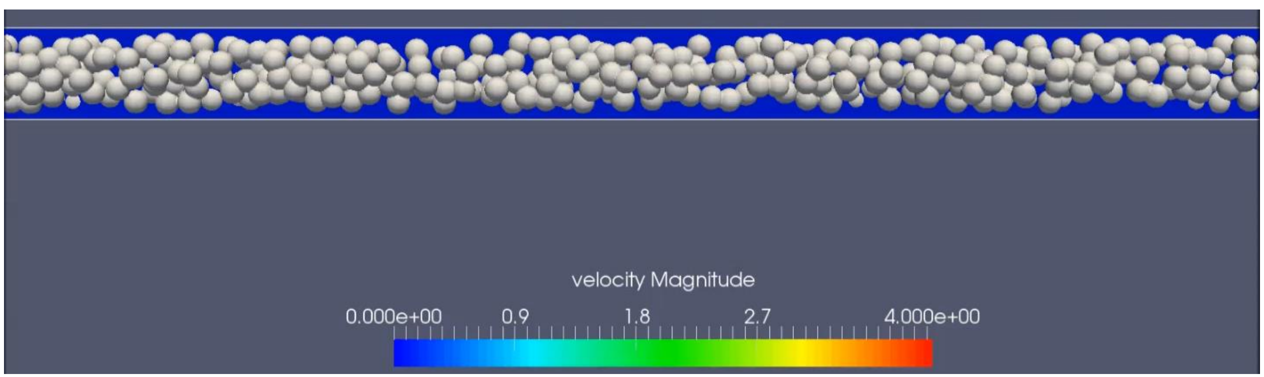
- Series of different void fractions/pressure gradients on the same mesh

Case	Void Fraction	Pressure Gradient [Pa/m]	Images
1	α=0.2	0.6	
2	α=0.3	3.0	
3	α=0.4	6.5	
4	α=0.4	1017	
5	α=0.4	15047	

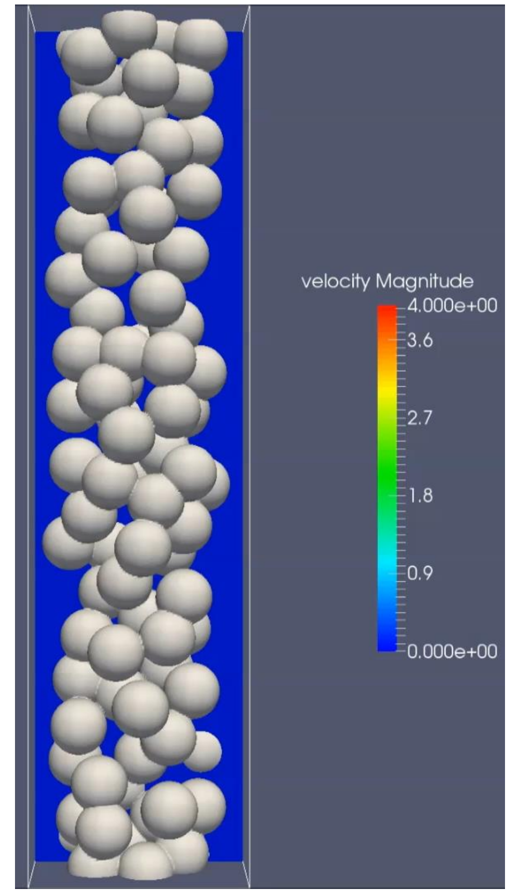
Simulating Flow Regime Transition

- Preliminary results for
  - First mesh refinement
  - 4x longer domain

	L/D=16 Domain	Refined Mesh
Number of Elements [million]	5	40
y^+_{wall}	7.5	3
Wall Element Size [mm]	0.0385	0.0154
y^+_{bulk}	46	24
Bulk Element Size [mm]	0.236	0.123
CPU Hours per Flow Through	10,000	12,600



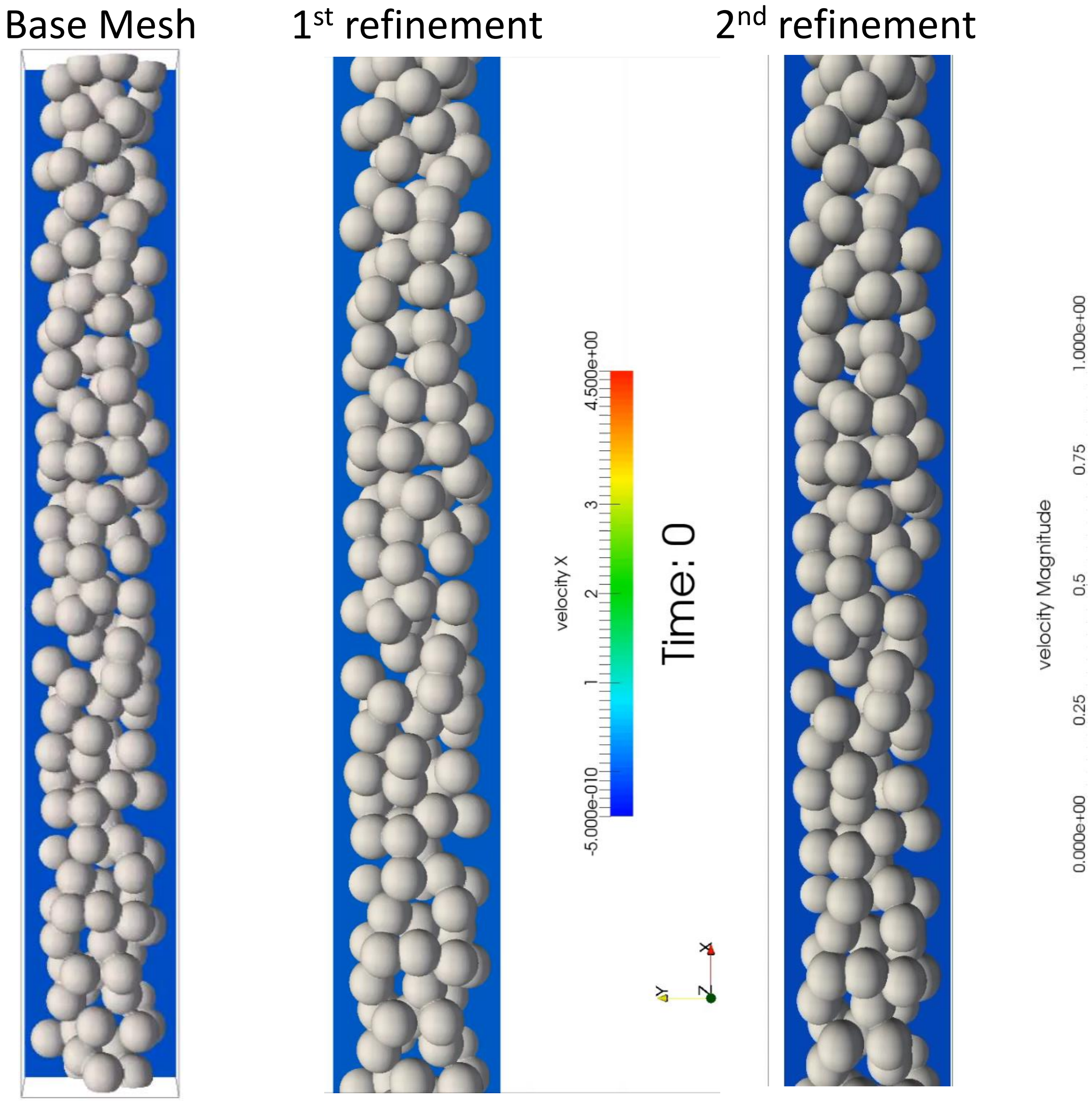
$r = 7.5\ [cm], L/D$=16



$r = 7.5\ [cm], L/D$ =4

Simulating Flow Regime Transition

- Simulation time to form a Taylor bubble
  - Base mesh: 0.433 [sec]
  - 1st refinement: 0.515 [sec]
  - 2nd refinement: 0.649 [sec]
- Bubble interface becomes smoother as mesh is resolved
- Liquid film “jets” are barely visible in base mesh
- Taylor bubble breakup
  - Base mesh: tail shearing
  - 1st refinement: nose elongation



Nuclear Reactor applications

- Predicting the two-phase flow behavior in reactor core, heat exchangers
- Determining the Departure from Nucleate Boiling / Dryout conditions
- Two-phase heat transfer prediction for various flow regimes
- Influence of the void fraction distribution on the neutron moderation in BWRs