

Multiphase flow modeling and simulation: HPC-enabled capabilities today and tomorrow

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**54th HPC User Forum
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Outline

- NC State:
 - College of Engineering
 - Department of Nuclear Engineering
- Massively parallel CFD-DNS code PHASTA:
 - Application examples
 - Scaling performance
- Interface tracking simulation examples:
 - Lift force evaluation
 - Bubble influence on the turbulence
 - Subchannel simulation of single/two-phase turbulent flows
 - Reactor subchannel geometry with spacer grids / mixing vanes
- Future applications:
 - Useful/usable virtual experiments for nuclear industry
 - Computing requirement / estimates / possible timeframe

NC State College of Engineering

- Fall 2013: Total enrollments 9,114
 - Undergraduate: 6,186
 - Masters: 1,803
 - PhD: 1,125
 - Size & quality indicators on the rise
- FY 13 Research expenditures > \$160M
- Among all U.S. engineering colleges:
 - 10th largest undergraduate enrollment
 - 9th largest graduate enrollment
 - 8th in number of BS degrees awarded
 - 14th in number of MS degrees awarded
 - 16th in number of PhD degrees awarded
- 281 tenured & tenure-track faculty members
 - 13 members of the National Academy of Engineering



Nuclear Engineering Department Brief History

- 1950 Established as graduate program in Physics Dept
- 1953 First non-governmental university-based research reactor
- 1954 Two PhDs awarded
- 1961 Department of Nuclear Engineering established
- 1965 Rapid growth from 4 to 9 faculty; thrust areas: (1) Fission power reactors; (2) Radiation applications
- 1973 1MW PULSTAR operational (4th on-campus reactor)
- 1983 Added Plasma/fusion graduate track
- 1994 Combined five-year BS/MNE degree established
- 2008 Master of Nuclear Engineering degree via Distance Ed
- 2014 PULSTAR is being licensed by NRC for 2MW operation

NCSU's Nuclear Engineering Today

- Our Faculty:
 - 8 active faculty in October 2007 ⇔ 14 today
 - 2 open positions currently in search
 - 2 endowed chairs: *Progress Energy* (in search) & *Duke Energy*
 - Multiple Joint Faculty Appointments with ORNL & INL
 - Lead in \$25M Consortium for Nonproliferation Enabling Capabilities
 - Pivotal role in CASL: Turinsky Chief Scientist, Doster Ed Programs
 - Gilligan: Director of NEUP (~\$60M annually in DOE research)
- Our Students:
 - Growing enrolments: ~100 Grads, ~150 UGs (sophomore – senior)
 - Won Mark Mills Award (best PhD) 10 times in Award's 55 years
 - ~10% win one or more award, scholarship, or fellowship annually
- Space:
 - Increased by more than 50% since 2008
 - Future move to new building on Centennial Campus

CFD-DNS code overview

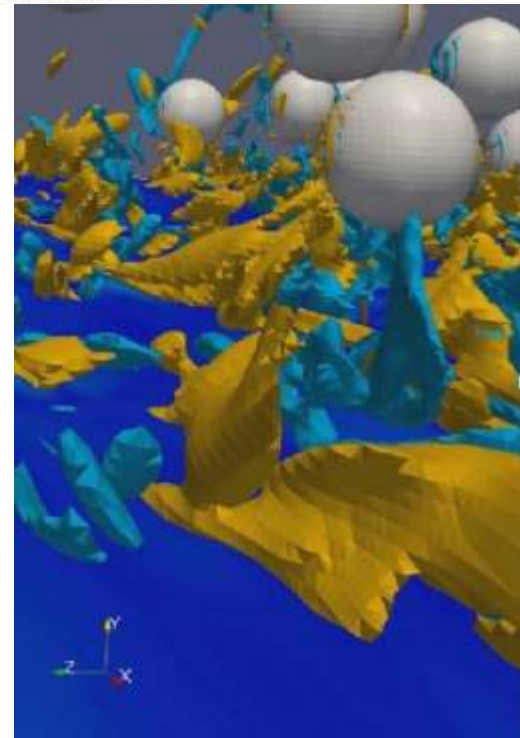
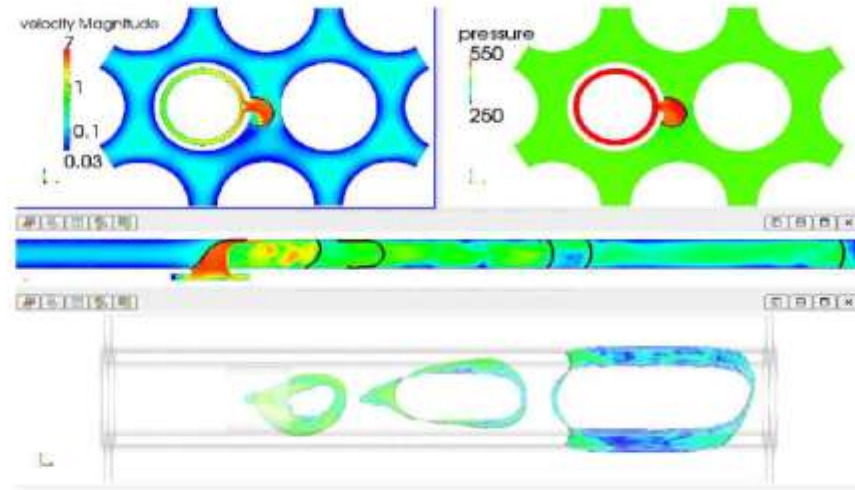
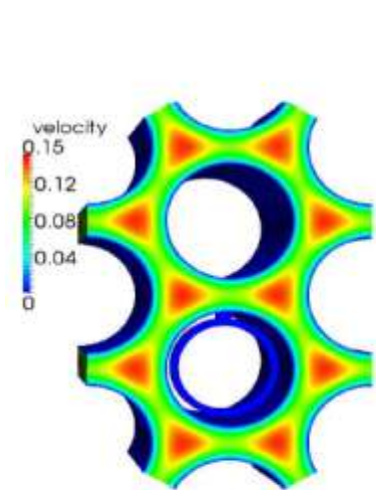
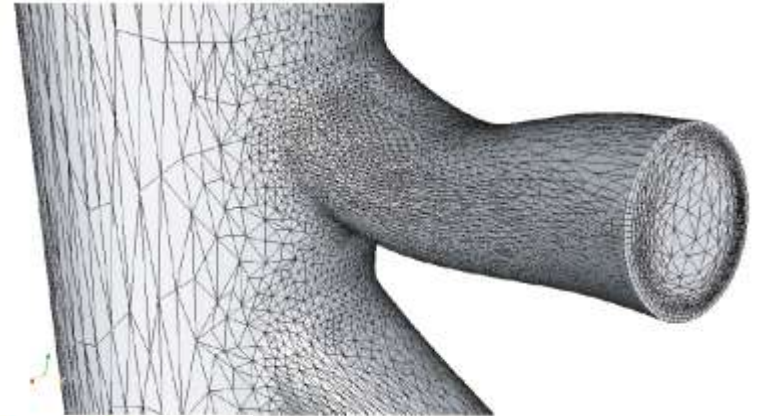
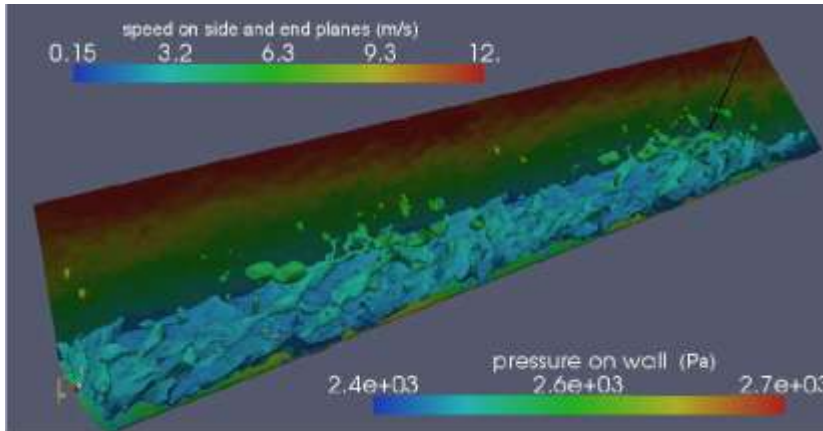
PHASTA is a **P**arallel, **H**ierarchic, higher-order accurate, **A**daptive, **S**tabilized, finite element method (FEM) **T**ransient **A**nalysis flow solver for both incompressible and compressible flows (Jansen, 1993).

Governing equations:

- Mass Conservation: $u_{i,j} = 0$
- Momentum Conservation: $\rho(\phi)u_{i,t} + \rho(\phi)u_j u_{i,j} = -p_{,i} + \tau_{ij,j} + f_i$
- Incompressible Newtonian Fluid: $\tau_{ij,j} = 2\mu(\phi)S_{i,j} = \mu(\phi)(u_{i,j} + u_{j,i})$
- Continuum Surface Tension (CST) model of Brackbill et al. (1992)

The Level-set Tracking method is implemented in PHASTA, which allows it simulate the two-phase phenomena.

PHASTA application examples

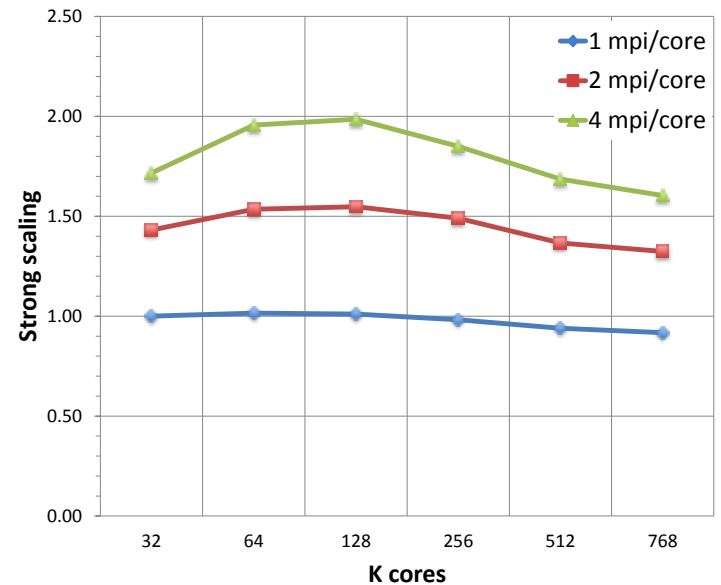


(a) Geometry of fuel bundle and initial velocity field $\| \mathbf{u} \|$.

(b) Top view cross sections of p and $\| \mathbf{u} \|$ (top), side view cross section of the velocity field (middle) and 3D shape of the interface (bottom).

Scaling performance

- Most recent: ANL's BG/Q "Mira":
 - Complex wing design on 11B elements
 - on up to 3M parts
- Strong scaling results with 5.07B elements up to 294,912 cores on JUGENE and up to 98,304 cores on Kraken



5.07B element mesh	eqn. form.		eqn. soln.		total	
	time	s_factor	time	s_factor	time	s_factor
JUGENE (IBM BlueGene/P) at JSC						
16,384 (base)	481.39	1	528.54	1	1009.94	1
32,768	240.78	1.00	301.47	0.88	542.25	0.93
65,536	119.64	1.01	162.59	0.81	282.23	0.89
131,072	59.69	1.01	84.09	0.79	143.78	0.88
262,144	30.02	1.00	43.24	0.76	73.26	0.86
294,912	26.71	1.00	39.15	0.75	65.86	0.85
294,912 (no LMod)	26.28	1.02	44.23	0.66	70.51	0.79
Kraken (Cray XT5) at NICS						
16,384 (base)	87.9	1	313.7	1	401.6	1
32,768	44.4	0.99	149.5	1.05	193.9	1.04
65,536	20.6	1.07	75.1	1.05	95.6	1.05
98,304	13.8	1.06	57.2	0.92	71.0	0.94



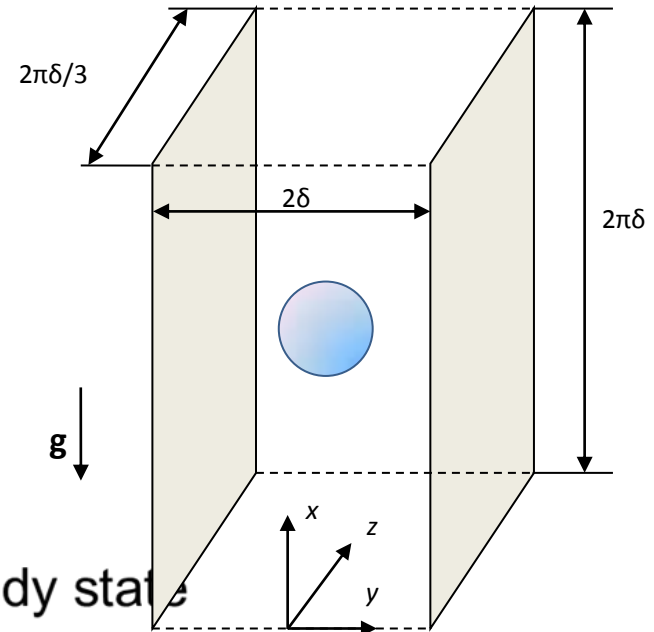
Lift force: introduction

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:

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

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

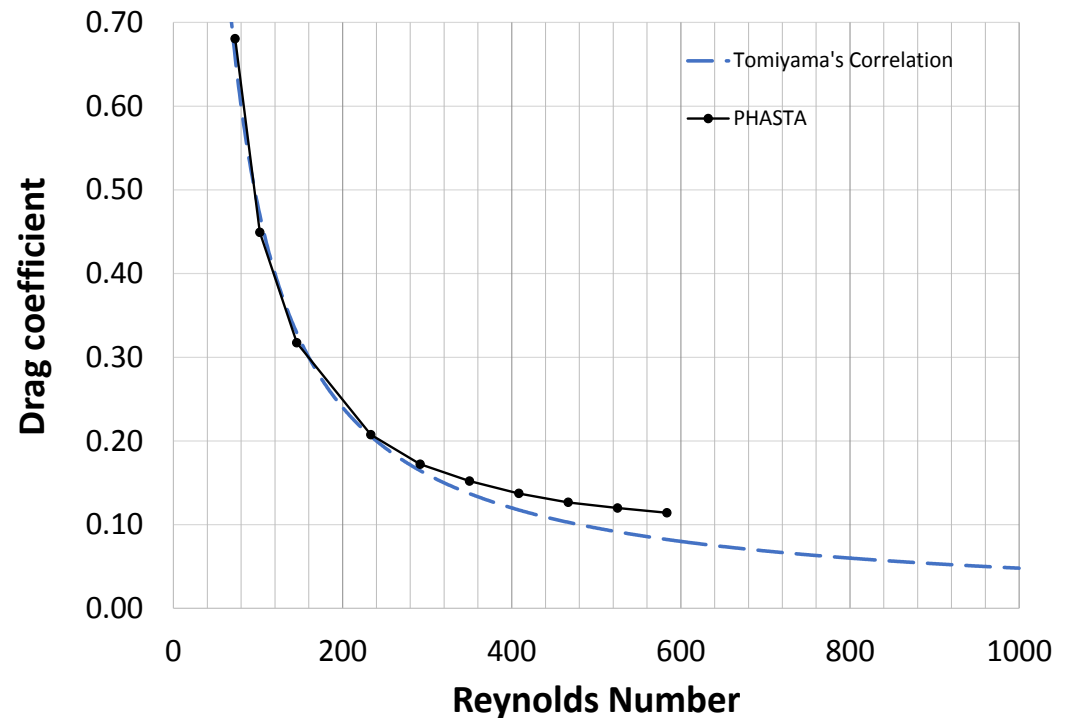
Drag force validation

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

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

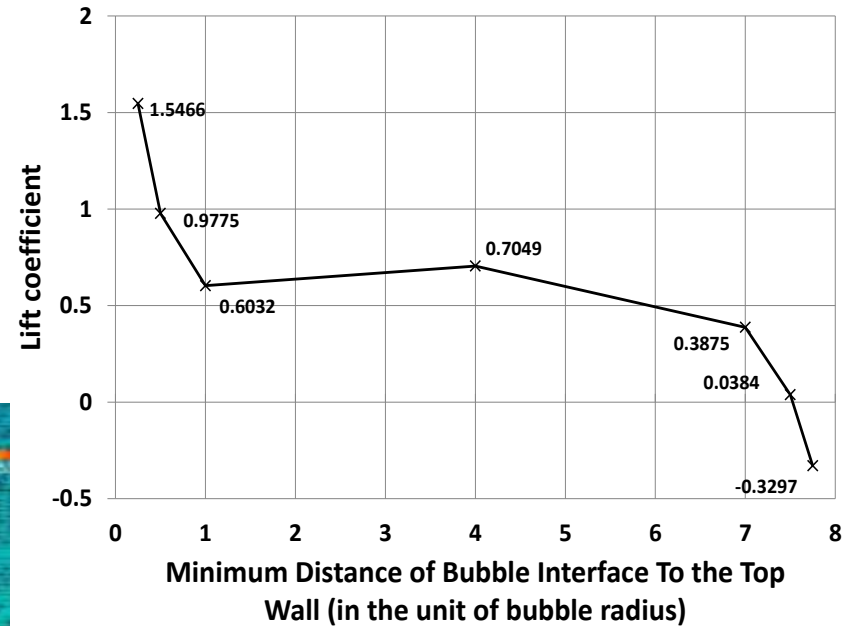
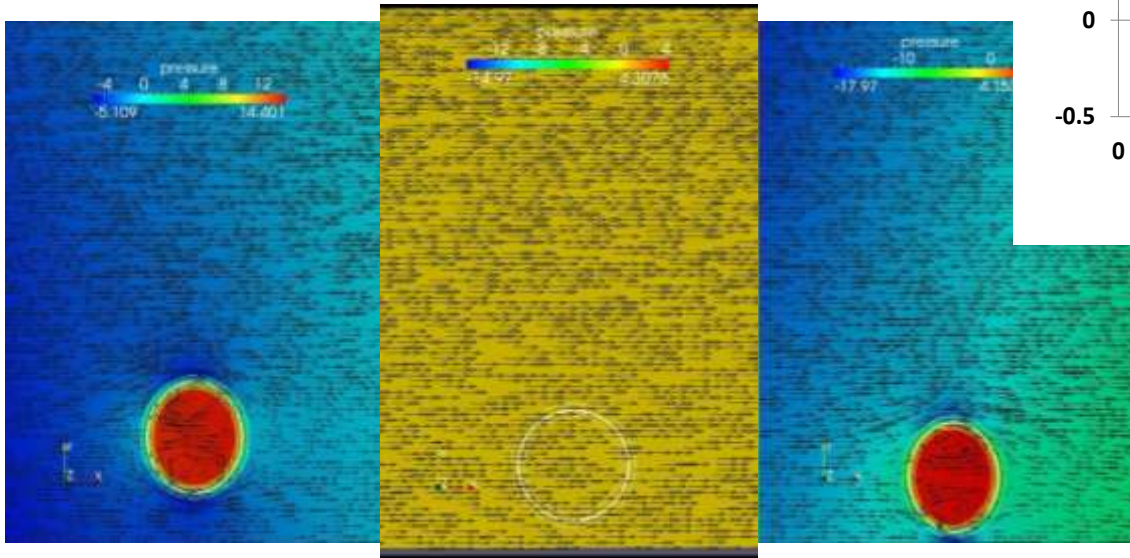
$$Re = \frac{\rho_L V_T d}{\mu_L}$$

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



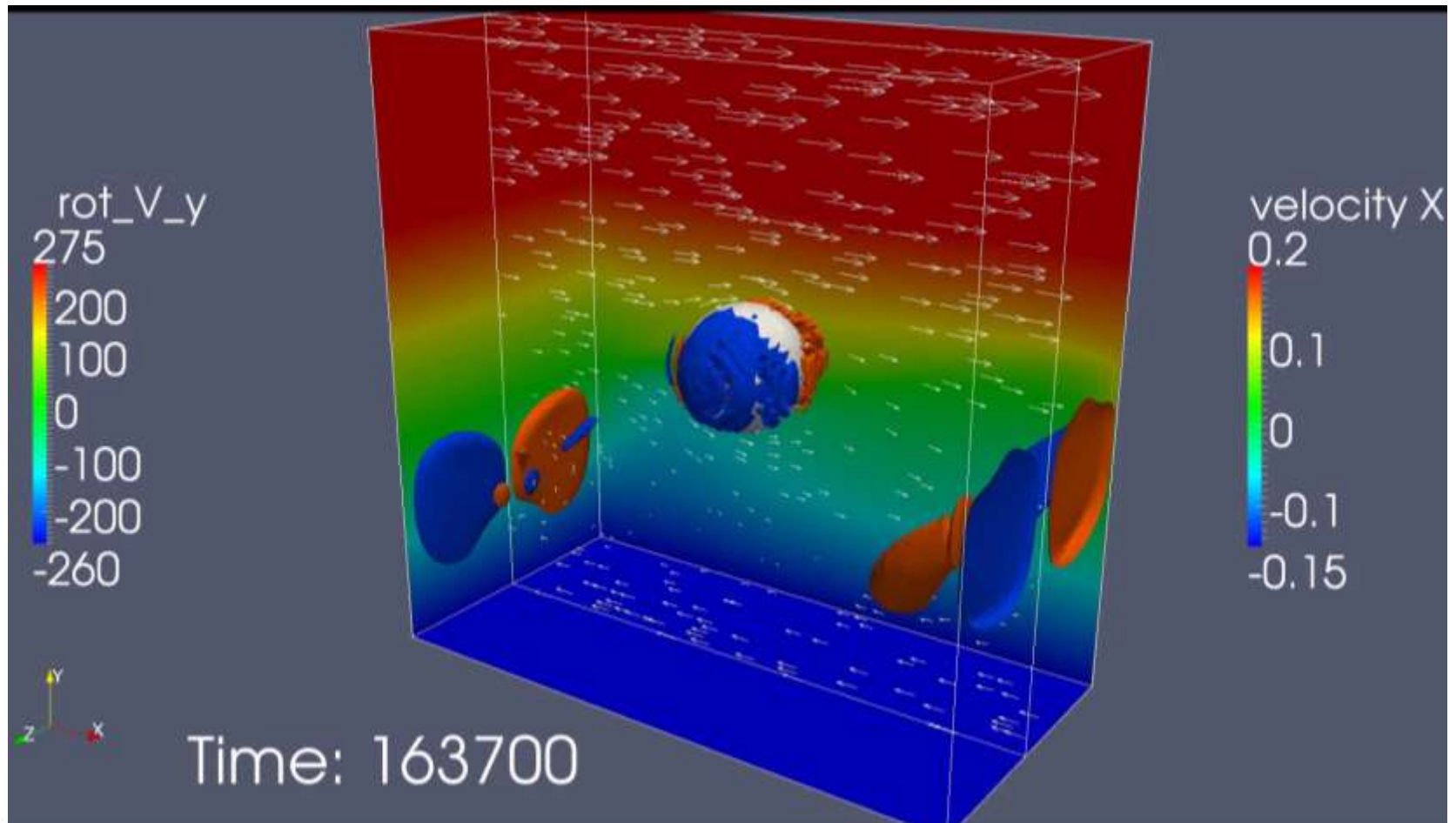
Wall effect study

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

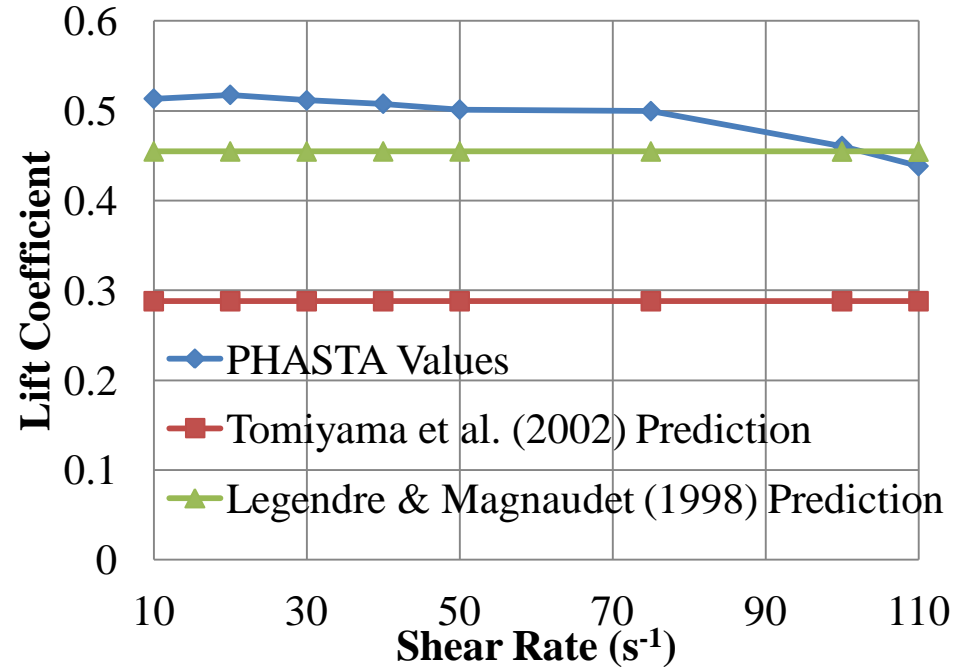
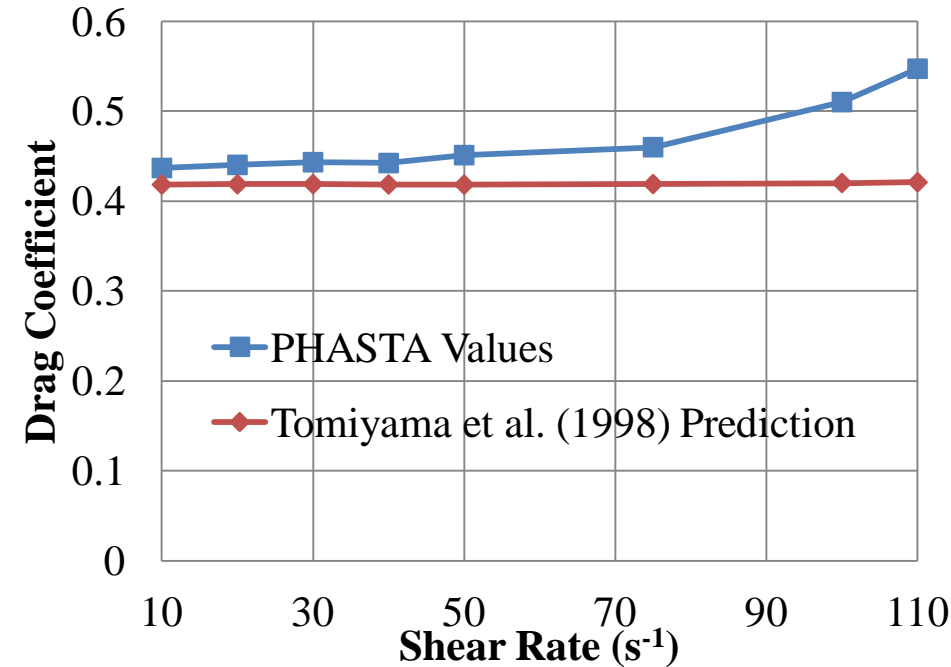


High Shear Laminar Flow (110 s^{-1})

About 1M cells, 64-core node runs for ~24 hours



Lift and drag coefficient vs. shear rate

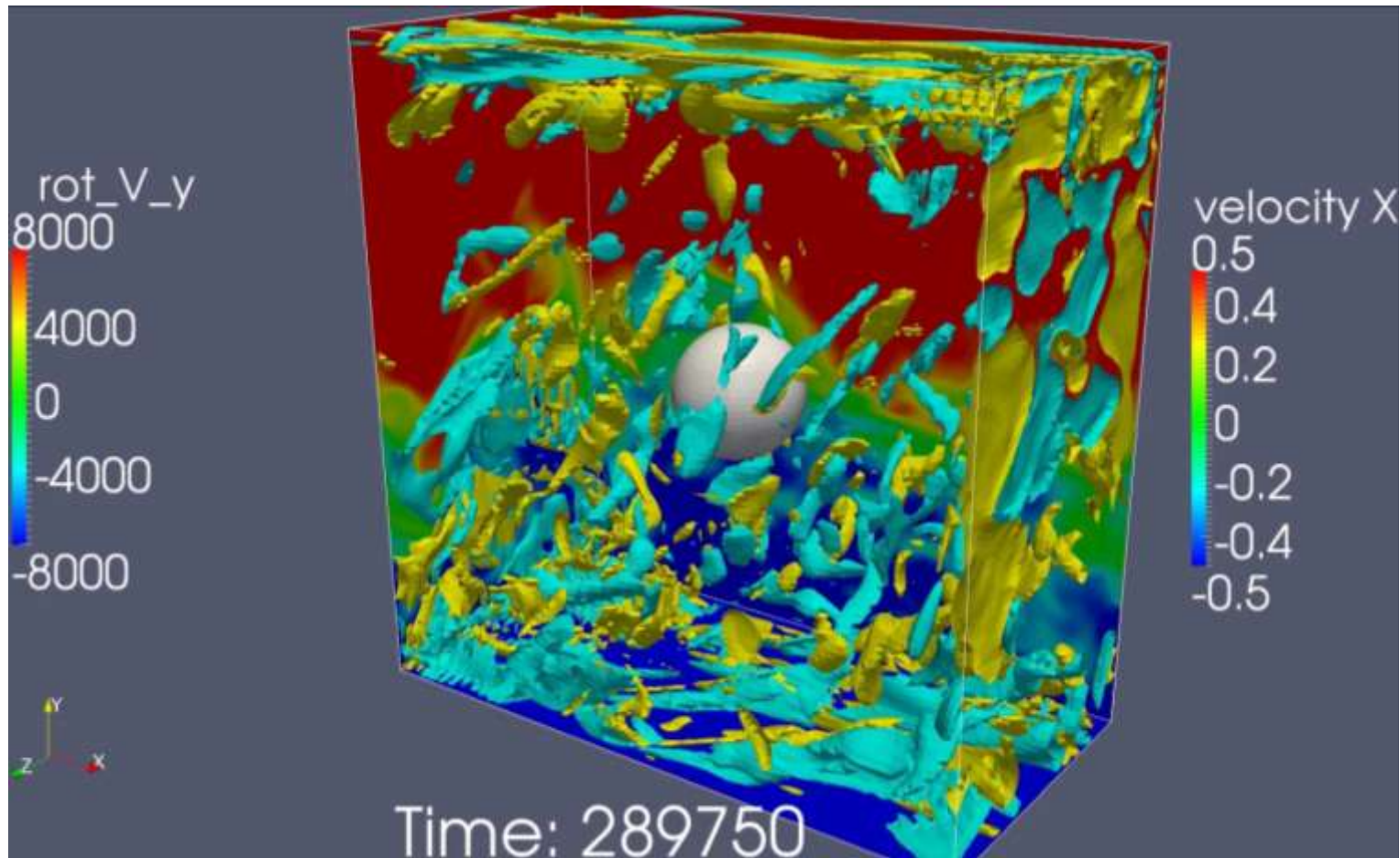


$$C_L = \sqrt{\left(\frac{6}{\pi^2} \frac{2.255}{(ReSr)^{0.5}(1 + 0.2Re/Sr)^{1.5}}\right)^2 + \left(\frac{11 + 16/Re}{21 + 29/Re}\right)^2}$$

$$Sr = \frac{\omega d}{v_r}$$

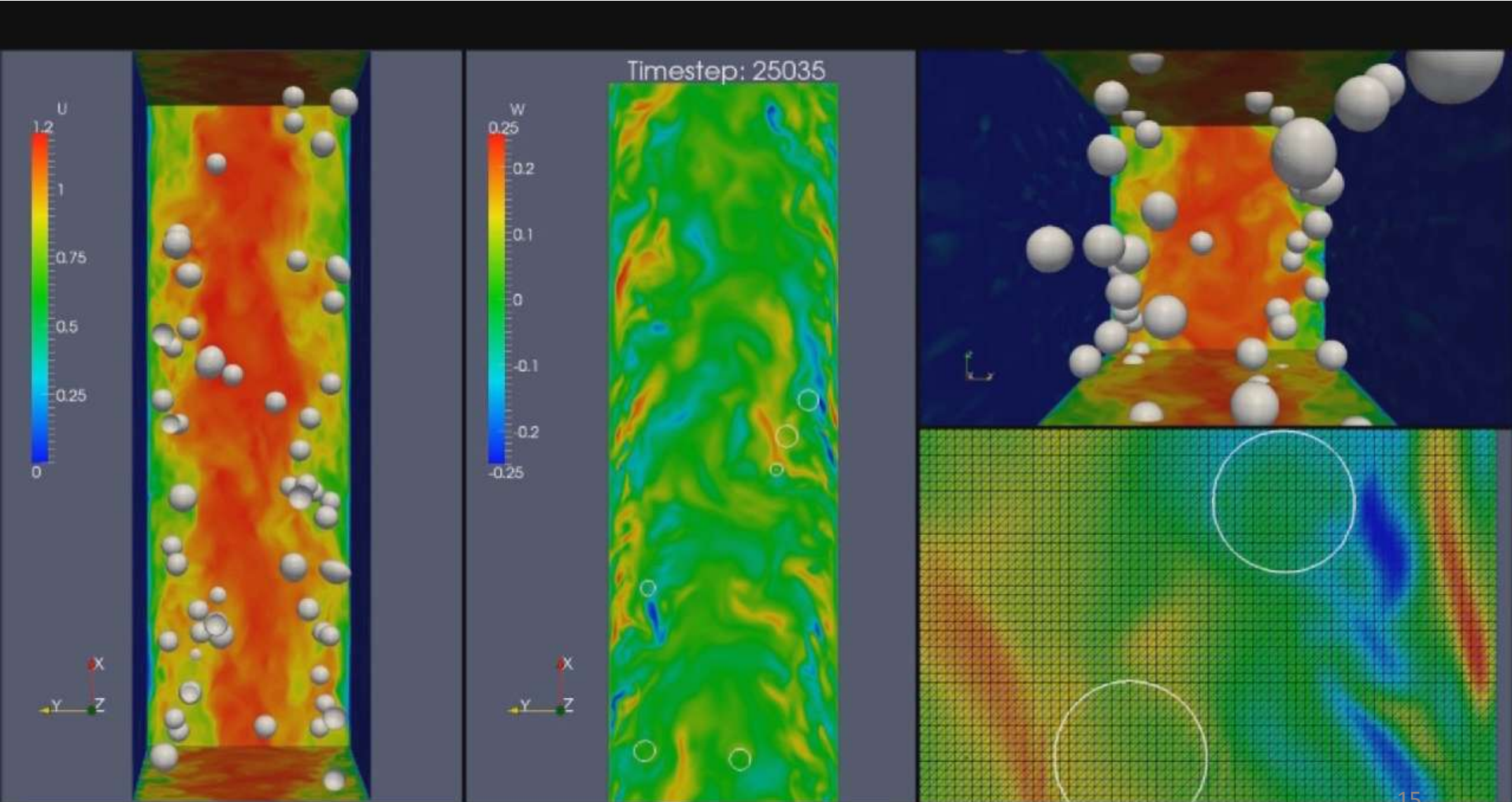
- Trends agree with Legendre & Magnaudet (1998) observation
- Correlations are independent of shear rate except Legendre & Magnaudet (1998)

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

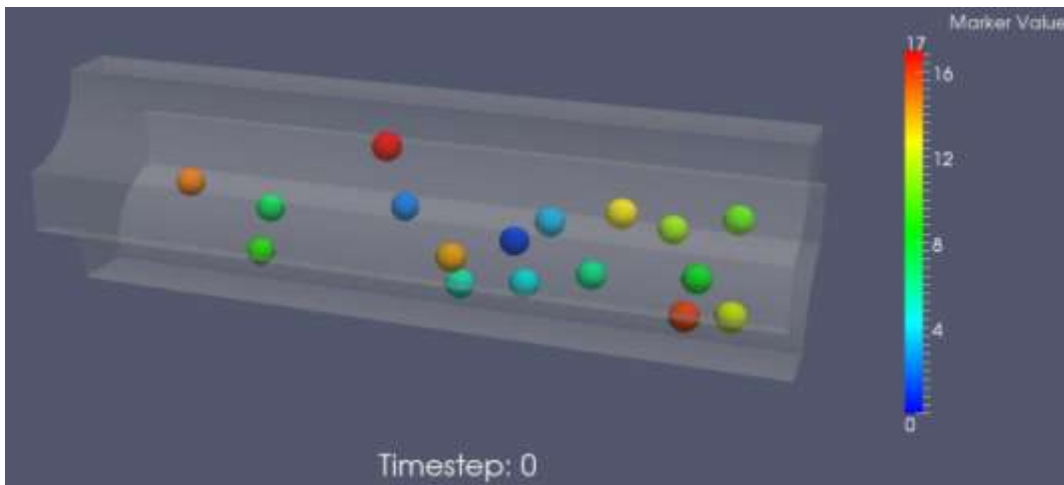
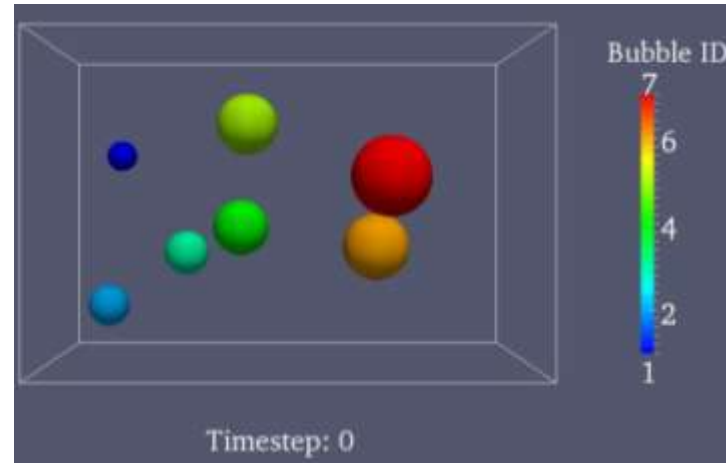
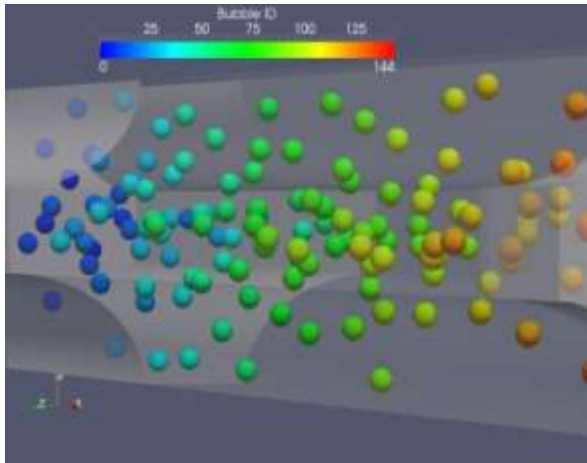


Multiple bubble simulations

60 bubbles; 20M hex cell mesh; ~4,096 core runs; ~5M CPU-hours for *good* statistics



Bubble tracking / advanced analysis



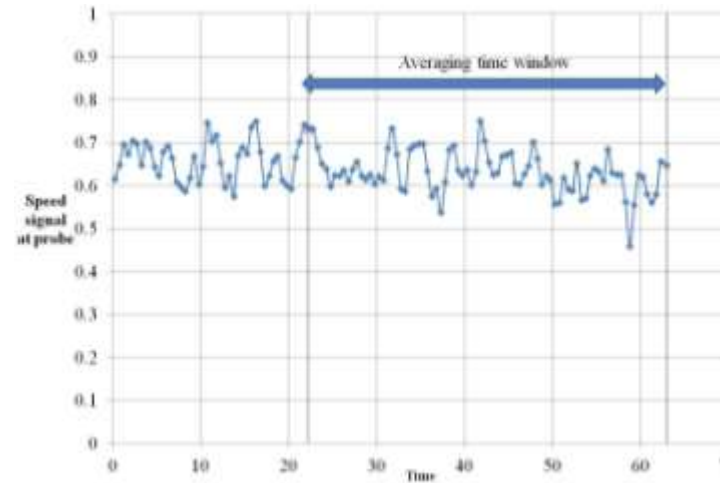
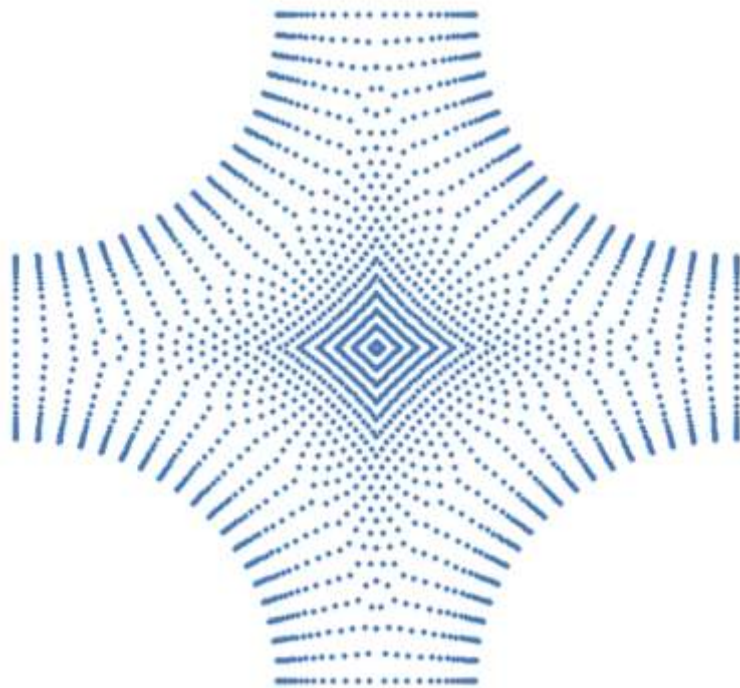
The bubbles can be marked by its unique ID and tracked during the simulations.

Data collection / analysis

Probes are created and placed in the domain in a flat plane arrangement as shown in the figure below.

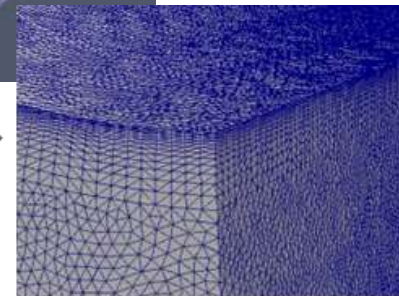
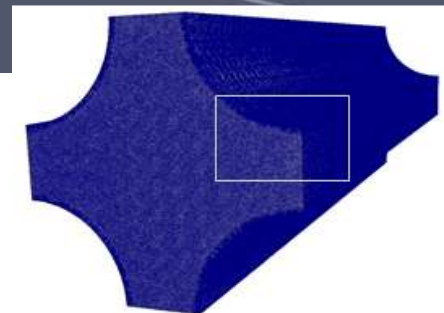
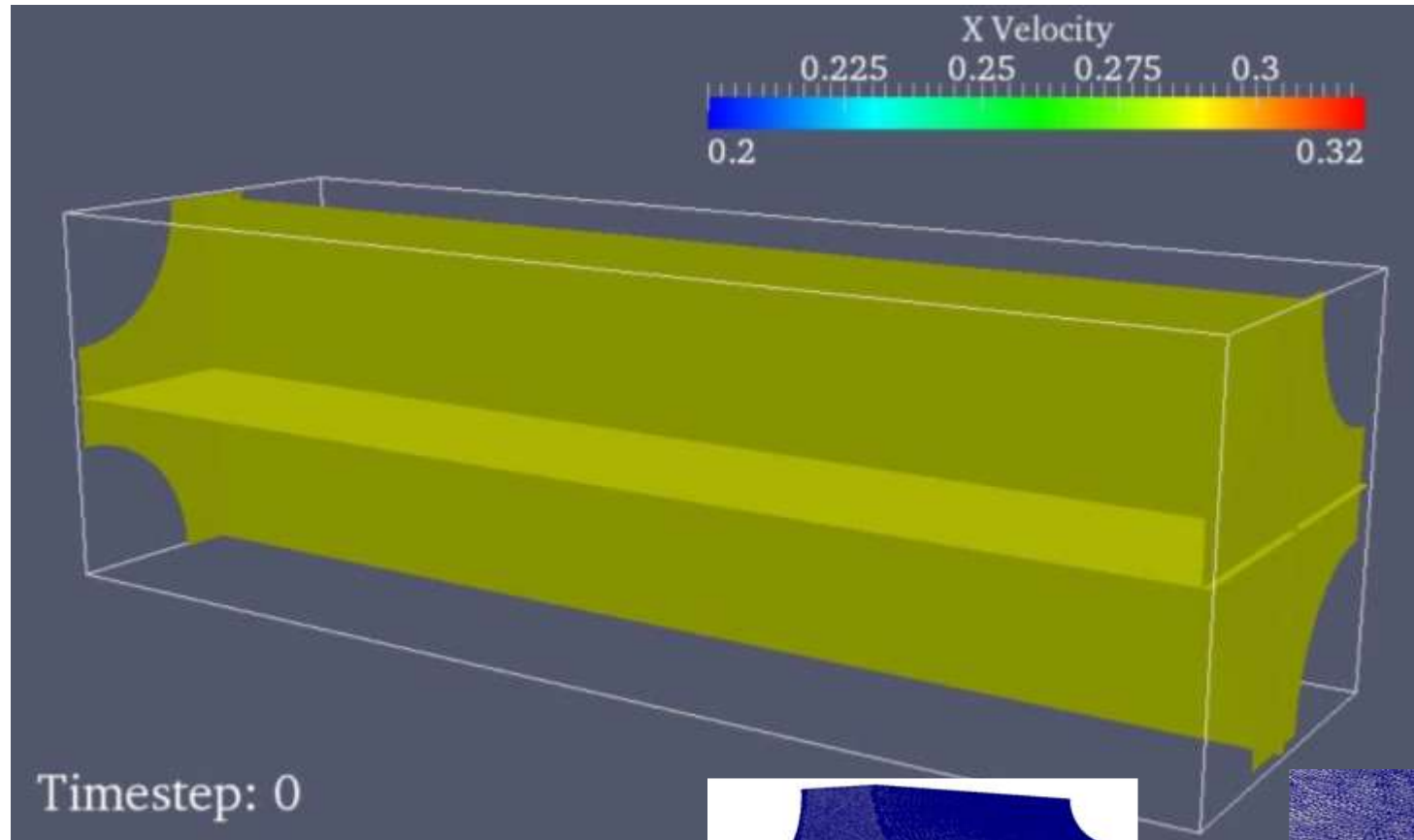
$$U_i(t) = \frac{1}{N_e} \sum_{m=1}^{N_e} \left(\frac{1}{N_w} \sum_{j=1}^{N_w} u_m^i(t + t_j) \right)$$

$$k(t) = \frac{1}{N_e} \sum_{m=1}^{N_e} \left(\frac{1}{N_w} \sum_{j=1}^{N_w} \sum_{i=1}^3 \frac{1}{2} (u_m^i(t + t_j))^2 \right)$$

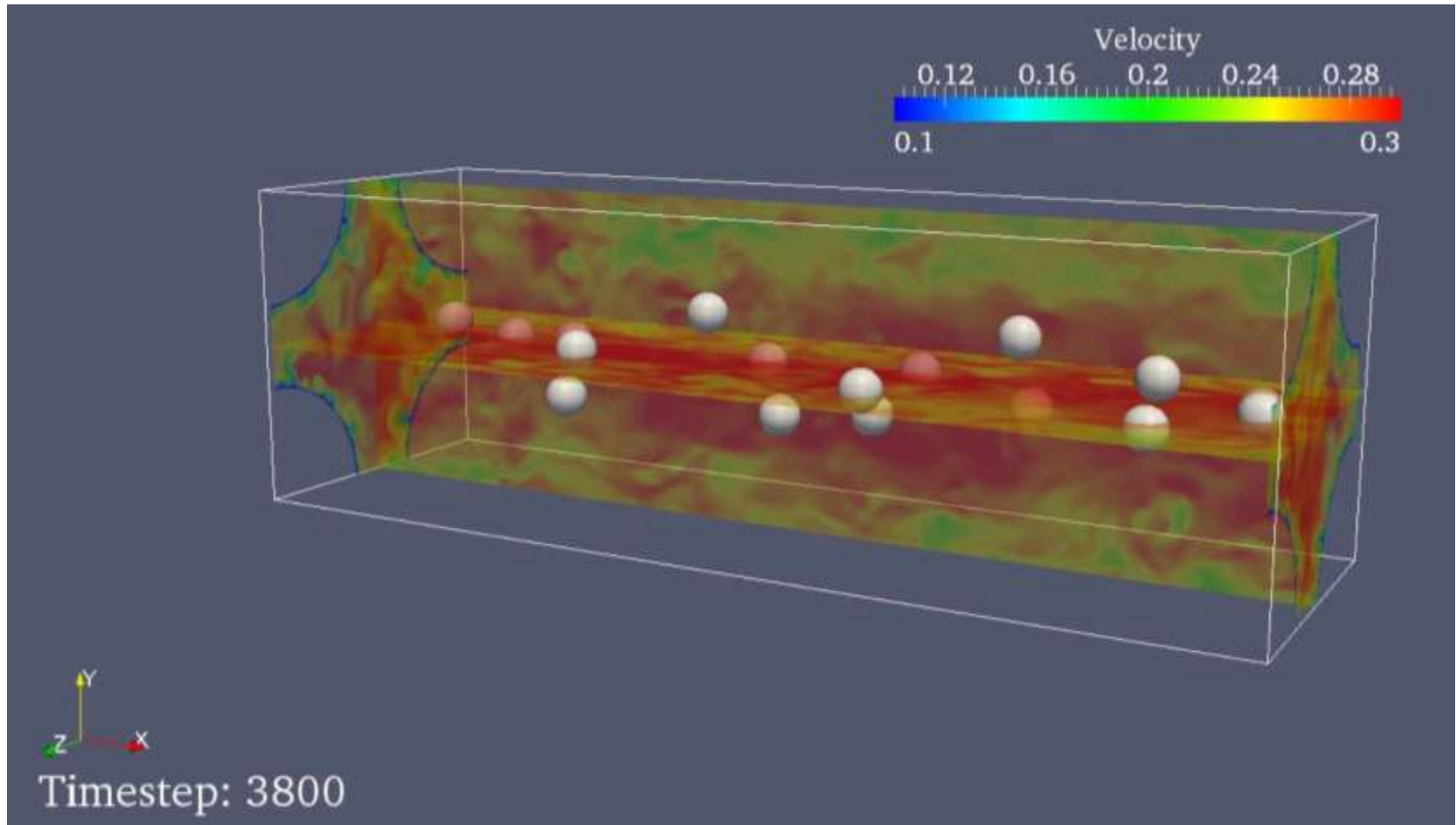


Subchannel flow - initialization

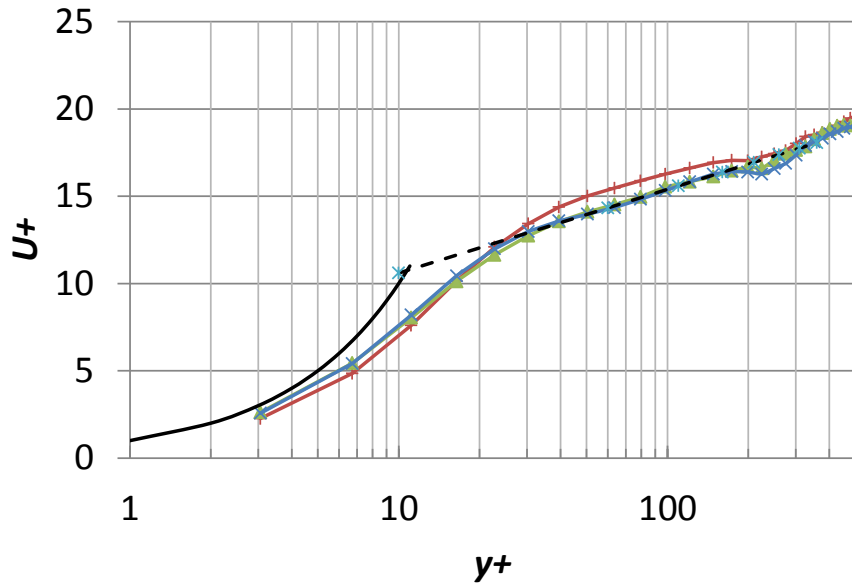
54 M tetrahedral unstructured mesh



Subchannel: two-phase flow



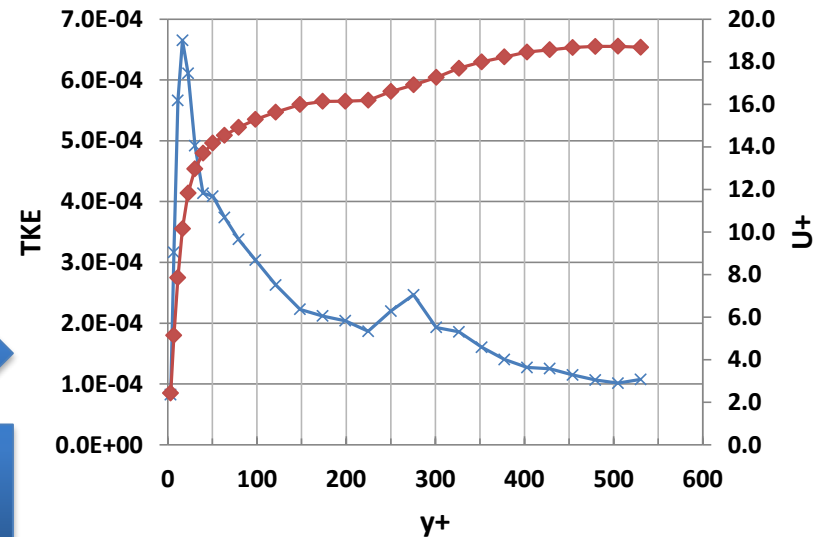
Averaged data



$$U^+ = \frac{1}{\kappa} \log y^+ + B$$

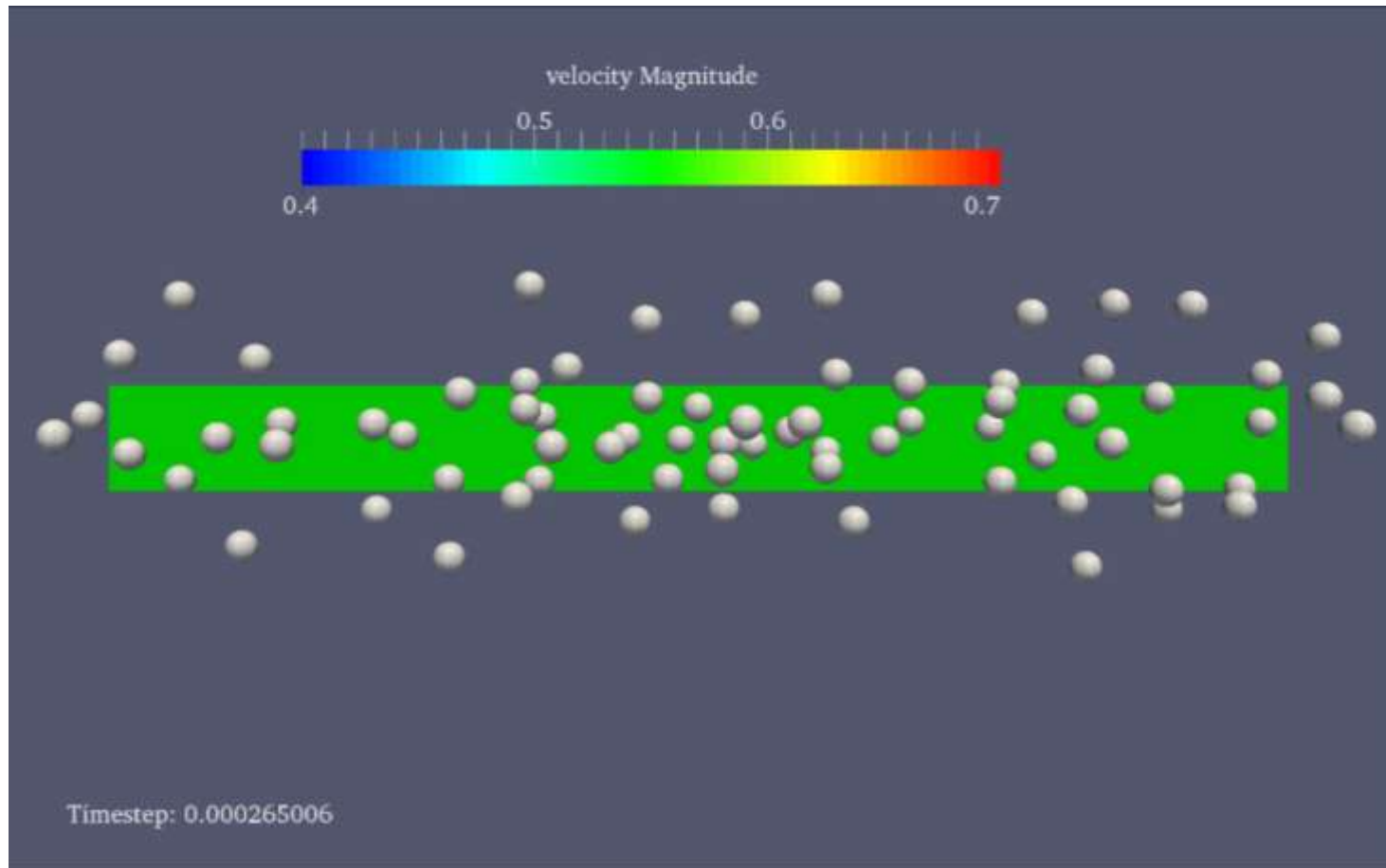
Law of the wall analysis shown in figure with dashed line results in the coefficients of $B = 5.8$ and $\kappa = 0.48$ observed in the subchannel simulation

Law of the wall profile for single phase simulation of a subchannel. Three time-averaged windows are shown in red, green and blue. Viscous sublayer (solid black) and log layer (dashed black) are shown.



Turbulent kinetic energy (TKE, blue) profile and dimensionless velocity (U^+ , red).

Multi-bubble single subchannel flow



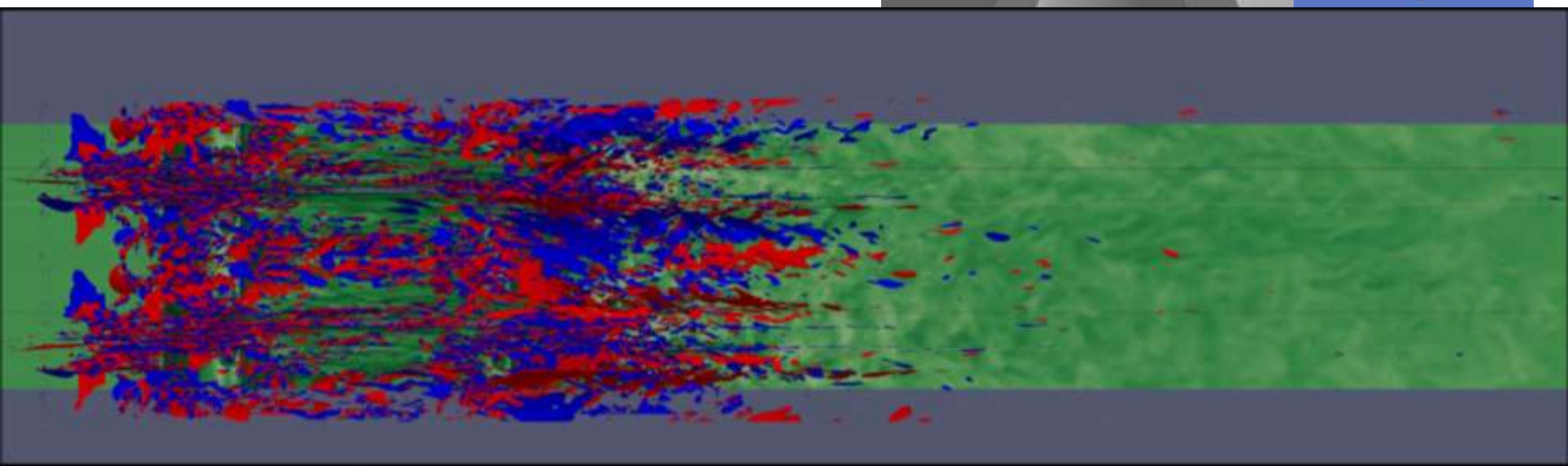
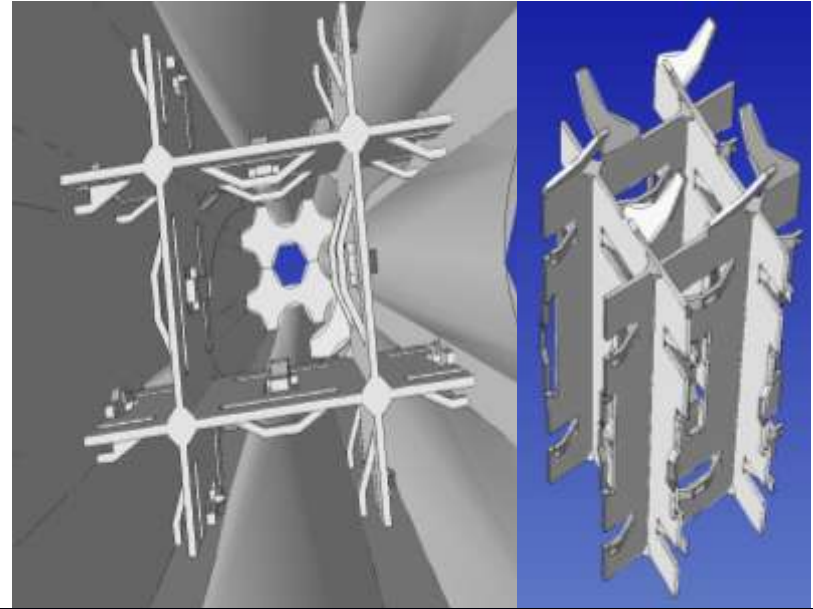
320 M elements; 72 bubbles at 1% void fraction; $Re = 60,000$

Simulated Mixing Vanes Design

Realistic reactor spacer grids (modified – not EC) and mixing vanes used for turbulent flow simulations.

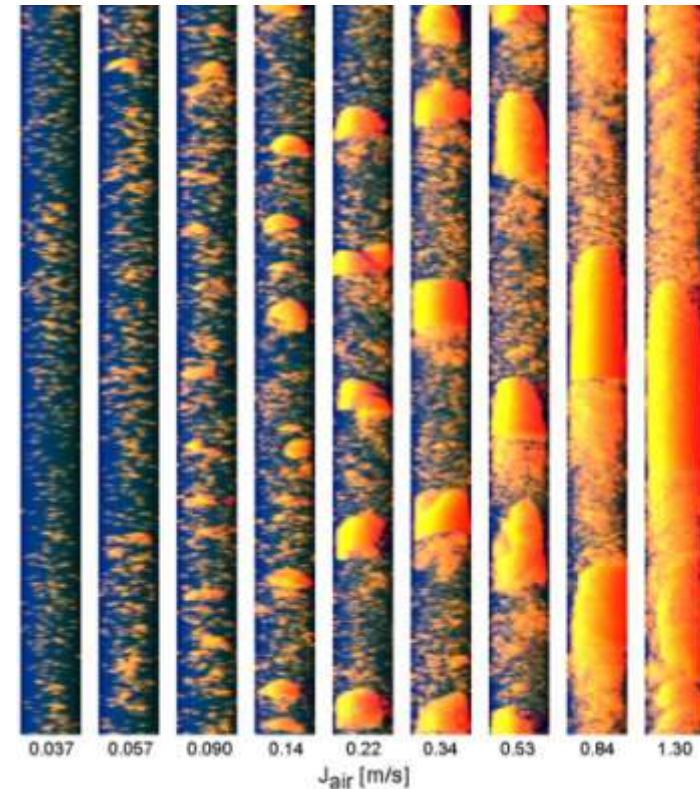
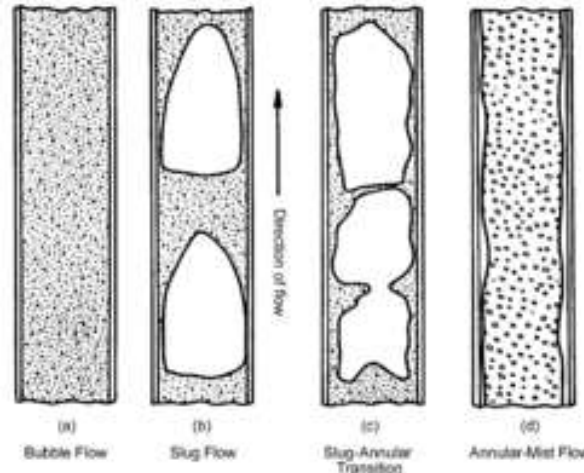
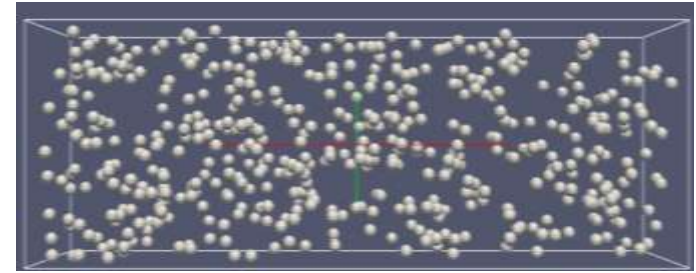
Movie produced by in-situ !

190M mesh:



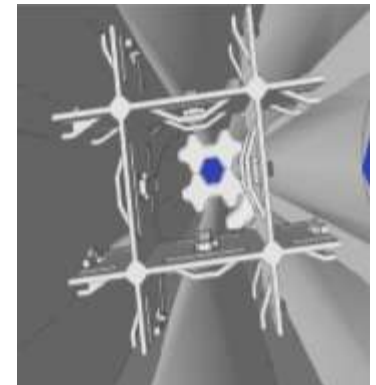
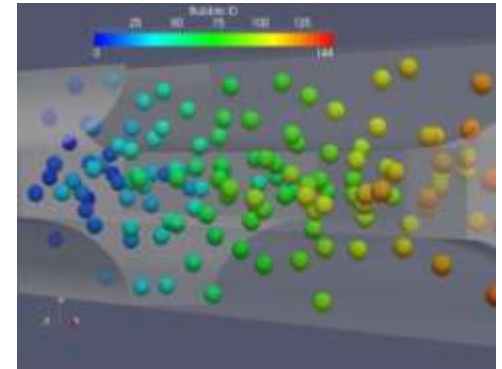
Some future virtual experiments

- Increasing fidelity of bubbly flow simulations
- Incorporate complex geometry analysis for nuclear applications
- Phase-change simulations
- Boiling flows at challenging conditions, including flow regime transition



PWR-relevant problem sizes

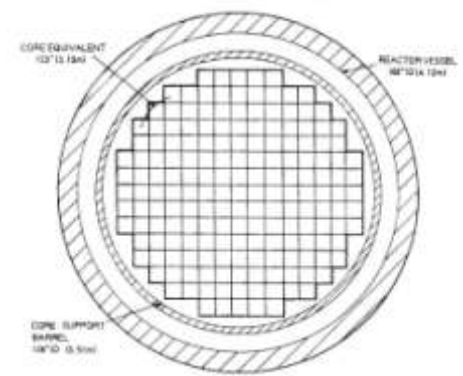
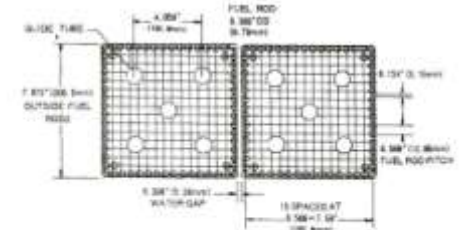
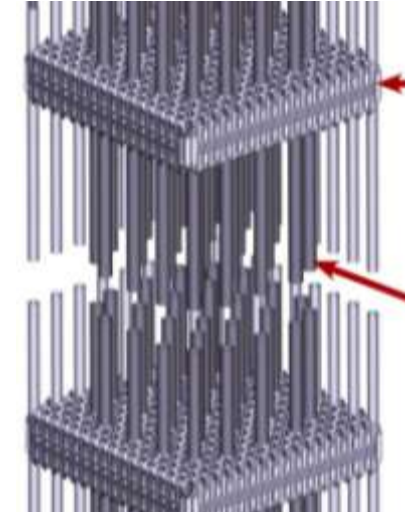
- Current runs (2013):
 - **2x2 subchannel, 40cm long**
 - Reynolds number of 180 (3.6% of typical normal operating conditions).
 - Mesh size: 190M elements
- Short term (2015):
 - Reynolds number of 500 (10% of PWR conditions)
 - Mesh size: 2B elements
 - Feasible on 512K BG cores at 4K elements per core
 - Would resolve 600 bubbles at 1% void fraction
- Mid term (2020):
 - Reynolds number of 5000 (typical PWR conditions)
 - Mesh size: 355B elements
 - Could run on up to 90M(!) cores at 4K elements per core
 - Would resolve 118,000 bubbles at 1% void fraction



Larger domain problem sizes



- Long term capabilities (2030 ?):
 - 17x17 subchannel, 4.0 m long
 - Reynolds number of 5000 (typical PWR conditions)
 - Mesh size: 256T elements
 - Could run on up to 16B cores at 16K elements per core
 - Would resolve 85M bubbles at 1% void fraction
- Direct simulation of *whole* reactor core (2060 ?):
 - About 160 fuel assemblies, 17x17 each
 - Reynolds number of 5000 (typical PWR conditions)
 - Mesh size: 40,000T elements
 - Could run on up to 320B cores at 128K elements per core
 - Would resolve 13.6B bubbles at average 1% void fraction
- Time domain – larger meshes require smaller timesteps to maintain fidelity in two-phase flow simulations
- Computing cost ? Advanced results must justify it!



Conclusions

- The ongoing effort will allow to equip the massively parallel ITM code, PHASTA, with validated capabilities for high fidelity simulation of multiphase flows.
- Advanced analysis tools is an integral component of large simulations which must be developed to take advantage of the vast amount of information provided by DNS/ITM approach.
- HPC development certainly allows to make high fidelity modeling and simulation applied to a much wider set of problems. High fidelity thermal hydraulic analysis will allow to support design and licensing of reactor core components in the new future.

Back-up: Resources / Capabilities

Local computing:

- Large memory (1,024 G RAM) rack-mounted workstation for mesh generation
- 6-node computing cluster with 64 cores per node, Infiniband interconnect (384 compute cores = about 3.3M CPU-hours annually)

Meshing:

- Simmetrix serial and parallel meshing tools for complex geometries (tested up to 92B elements)
- Pointwise license for CMFD meshing

Remote computing:

- 2014 ALCC award for 76.8M processor-hours at Mira (Argonne National Lab, #5 supercomputer, 768,000 computing cores on BG/Q)
- Access to Titan at ORNL (through CASL, about 5-20M processor-hours yearly), #2 supercomputer
- 2012 INCITE award for 14M processor hours on Titan