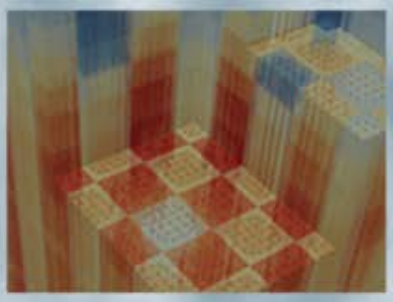
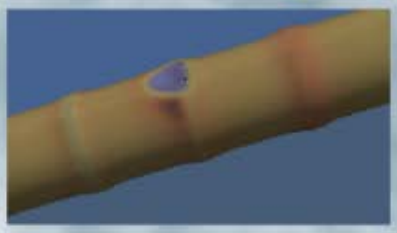
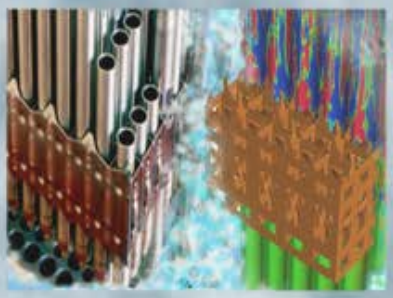
CASL-U-2015-0252-000

Development of Advanced Analysis Tools for Interface Tracking Simulations







Jun Fang, Igor A Bolotnov
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July 7, 2015

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

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Development of Advanced Analysis Tools for Interface Tracking Simulations

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A DOE Energy Innovation Hub

Introduction

The understanding of turbulent two-phase flows is very important due to the widespread occurrence of this phenomenon in natural and engineering systems. The development of high-performance computing (HPC) allows for increasingly large scale simulations to be conducted. Direct numerical simulation (DNS) coupled with interface tracking methods (ITM) stands out as a valuable tool to compliment and expand our ability to understand two-phase flow phenomenon.

Advanced data analysis techniques are highly desired for efficiently processing large-scale two-phase simulations in different geometries. The present work includes:

- A new capability developed which can estimate the drag and lift coefficients of the single bubble in uniform shear flows;
- Development of the **bubble tracking** capability for interface tracking simulations;
- **Advanced extraction algorithms** to collect detailed information regarding the individual bubble behaviors, such as location, velocity, local liquid flow field, and even bubble deformability;
- Some results from current simulations for pressurized water reactor (PWR) **subchannel** and progress in new computational tools development as well.

Numerical Methods

For our simulations we utilize **PHASTA** code, which is a parallel, hierarchic, higher-order accurate (from the 2nd to the 5th order accuracy, depending on function choice), adaptive, stabilized (finite element) transient analysis flow solver (both incompressible and compressible).

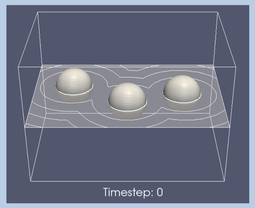
Governing equations:

- 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)

Level-Set approachis implemented for the two-phase simulations in PHASTA, which is actually the signed distance field described by:

- $\phi_i = \sqrt{(x-x_i)^2 + (y-y_i)^2 + (z-z_i)^2} - R_i$
- $\phi = \min\{\phi_i\}$

where x_i, y_i, and z_i, are the coordinates of the bubble center and R_i is the radius; **the interface is where $\phi = 0$**



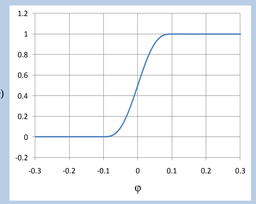
Properties dependent on distance from interface, e.g.

- density: $\rho(\phi) = \rho_l H_\varepsilon(\phi) + \rho_g(1 - H_\varepsilon(\phi))$
- viscosity: $\mu(\phi) = \mu_l H_\varepsilon(\phi) + \mu_g(1 - H_\varepsilon(\phi))$

Smoothed Heaviside function is used to describe the transient properties of bubble interface

$$H_\varepsilon(\phi) = \begin{cases} 0, & \phi < -\varepsilon \\ \frac{1}{2}\left[1 + \frac{\phi}{\varepsilon} + \frac{1}{\pi}\sin\left(\frac{\pi\phi}{\varepsilon}\right)\right], & |\phi| < \varepsilon \\ 1, & \phi > \varepsilon \end{cases}$$

where ε is the half thickness of interface

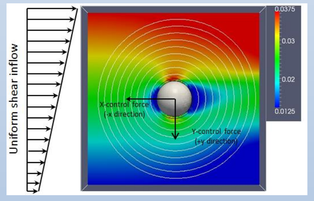


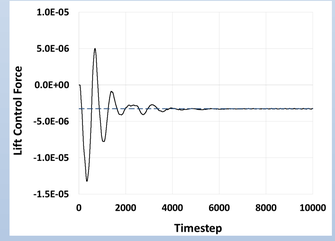
Measurement of Lift and Drag Forces

In order to evaluate the lift and drag forces, external control forces are applied in both lateral direction and stream-wise direction to balance them. Control forces can update themselves based on a simple modified **proportional-integral-derivative** (**PID**) controller:

$$CF_i^{(n+1)} = c_1\overline{CF_i} + c_2[CF_i^{(n)} + c_3(x_i - x_{i0}) + c_4 v_i + c_5\left(v_i^{(n)} - v_i^{(n-1)}\right)]$$

where CF stands for control force and the $\overline{CF_i}$ is the historical average of the force. The constants used for lift and drag control forces' expressions are listed in following table.

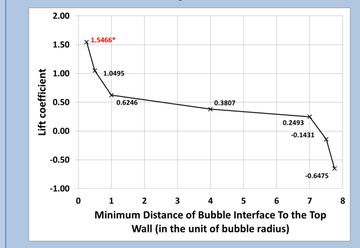


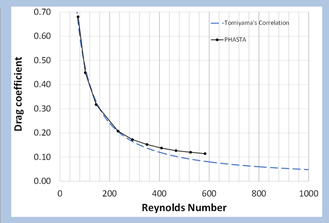


The Lift control force applied evolves during the simulation

$$F_L = -C_L\rho_L\frac{\pi d^3}{6}(V_b - V_L) \times \left(\frac{\Delta V}{L}\right)$$

$$F_D = C_D\frac{\pi d^2}{8}\rho V_b^2$$





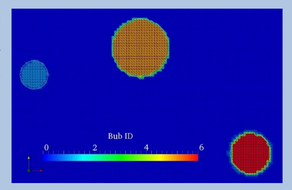
The drag coefficient measured under different bubble Reynolds number with Tomiyama's correlation

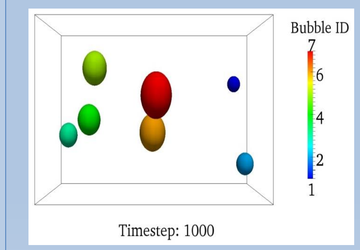
Thomas, A. M., Fang, J., Feng, J., & Bolotnov, I. A. (2015). Estimation of shear-induced lift force in laminar and turbulent flows. *Nuclear Technology, 109*, 1-18.

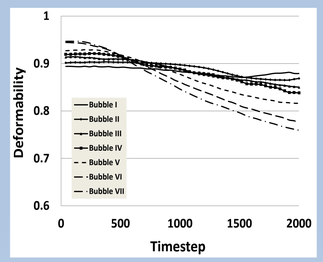
Bubble Tracking Capability and Information Extraction

Significant effort has been dedicated in developing the new capability of PHASTA to distinguish and track individual bubbles, and this new function is very crucial in the multi-bubble simulations.

$$D = \frac{|\phi_{\min}|}{R_{eq}}$$

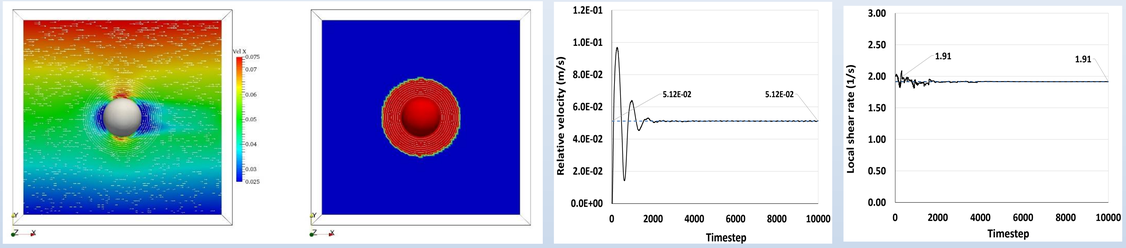






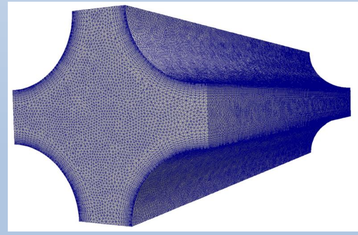
Left: The bubble with different deforming levels; Right: The deformability factors extracted for all the bubbles

Fang, J., & Bolotnov, I. A. (2014). Development of bubble tracking capability for level-set interface tracking method. *Transactions of the 2014 ANS Winter Meeting,* Anaheim, CA. , *111* 1658-1658.
Fang, J., Thomas, A. M., & Bolotnov, I. A. (2013). Development of advanced analysis tools for interface tracking simulations. *Transactions of the 2013 ANS Winter Meeting,* Washington D.C. , *109* 1613-1615.

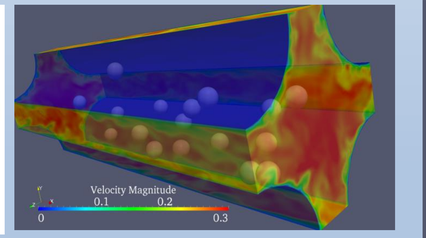


The bubble relative velocity and local shear rate measured in the flow with prescribed shear rate of 2.0 s^{-1} (left).

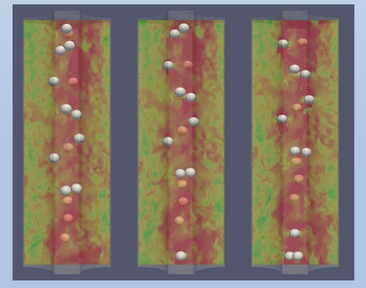
Subchannel Simulations and Computational Tools Development



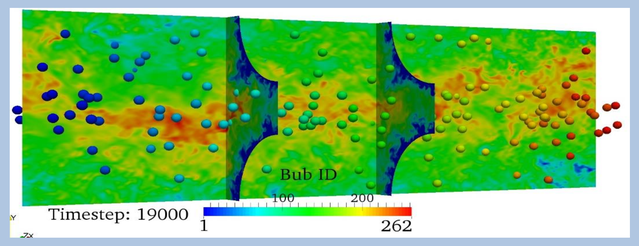
The unstructured mesh for a reactor subchannel



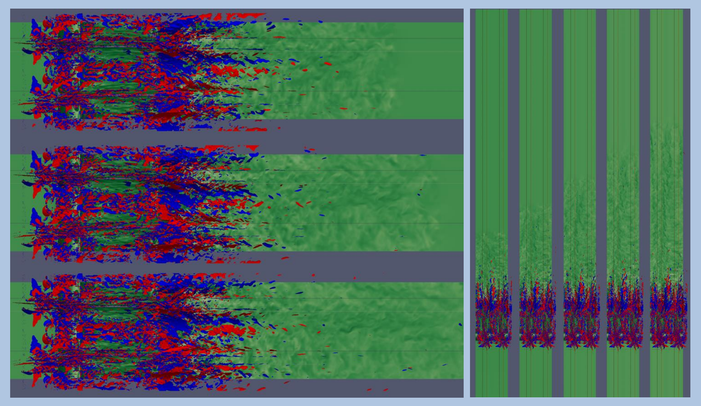
Several bubbles are placed in the domain based on the void fraction required.

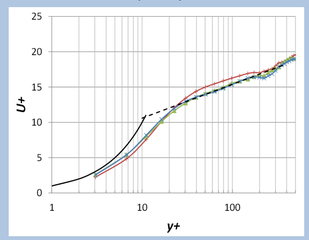


A set of screenshots showing the detailed process of bubbles moving through the single subchannel due to advection by the mean flow and buoyancy force.



The initial profile of a 262-bubble subchannel case with bubble ID's

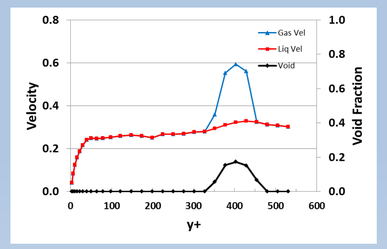




$$U^+ = \frac{1}{\kappa}\log y^+ + B$$

Three time averaged windows are shown in red, green and blue. Viscous sub-layer (solid black) and log layer (dashed black) are also shown above. **Law of the wall** analysis shown in the figure with dashed line results in the coefficients of B=5.8 and κ=0.48 observed in the subchannel simulation

For large scale DNS, there is a remaining challenge about how to efficiently process vast amount of raw simulation data. The conventional approach that record these data to disk storage for further post-processing and visualization is no longer a viable way due to prohibitive cost of disk access. To take full advantage of those high fidelity simulations, we have to develop and utilize the **in-situ visualization** and **simulation steering** tools. (The development is a cooperation with Dr. Hong Yi and Dr. Michel Rasquin)



The distribution for time-averaged gas velocity (in blue), liquid velocity (in blue) and void fraction (in black) at the subchannel inlet plane

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