

FLOW-3D Solver: Developments and Improvements

John Ditter
VP of Software Engineering

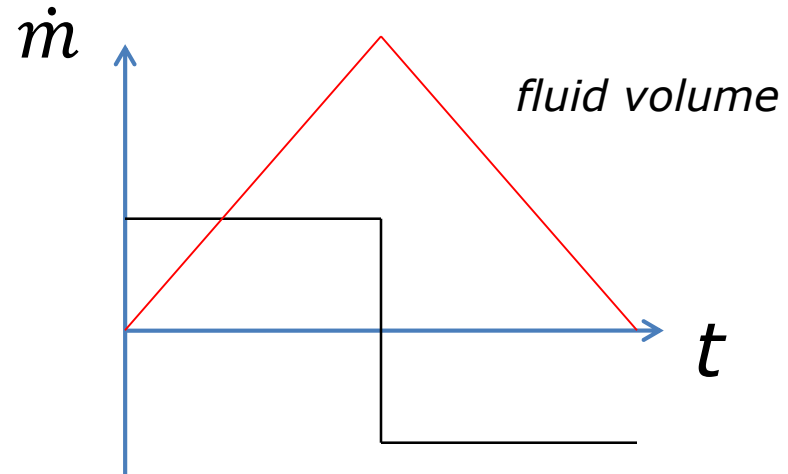
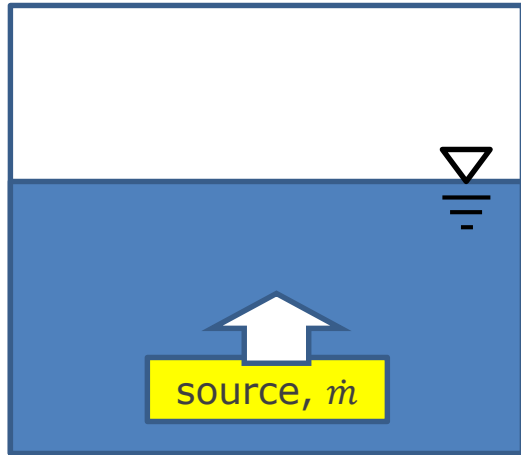
Improvements

- Automatic convergence of GMRES pressure solver
- FSI/TSE solver performance
- SMP parallel performance

GMRES pressure solver convergence

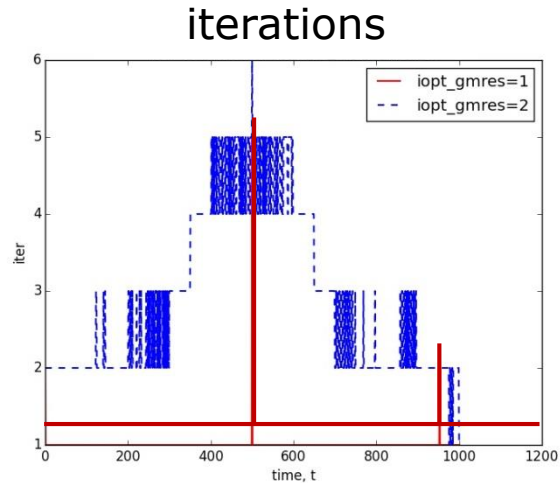
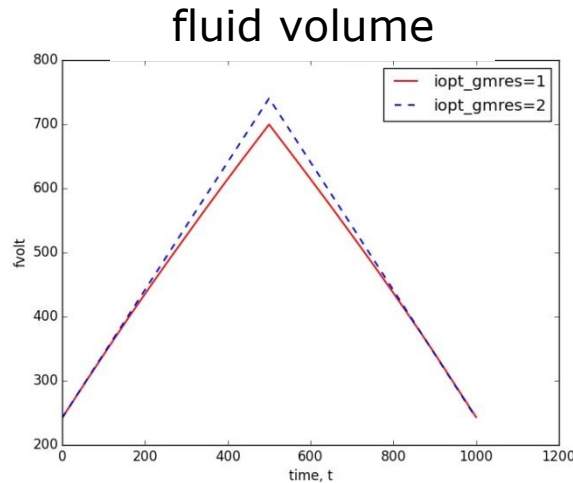
- The GMRES solver uses the same convergence criterion as the SOR and ADI solvers
 - May be insufficient for accurate and efficient solution
 - Often requires adjusting EPSADJ and ITMIN
- An additional criterion has been added, and *both* conditions must be satisfied for convergence

Example: Mass source/sink



Example: Mass source/sink

Convergence errors accumulate with time



- - - new, 0.5% error
— old, 7% error

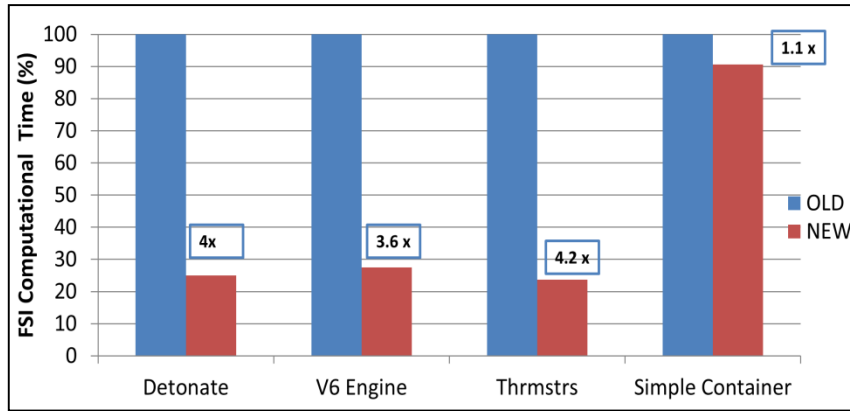
GMRES pressure solver: What to expect?

- More iterations for cases where solution was poorly converged
- Similar number of iterations for well behaved solutions
- More consistent results for different number of cores as well as between Linux and Windows OS
- No need to adjust EPSADJ and ITMIN

FSI/TSE solver performance

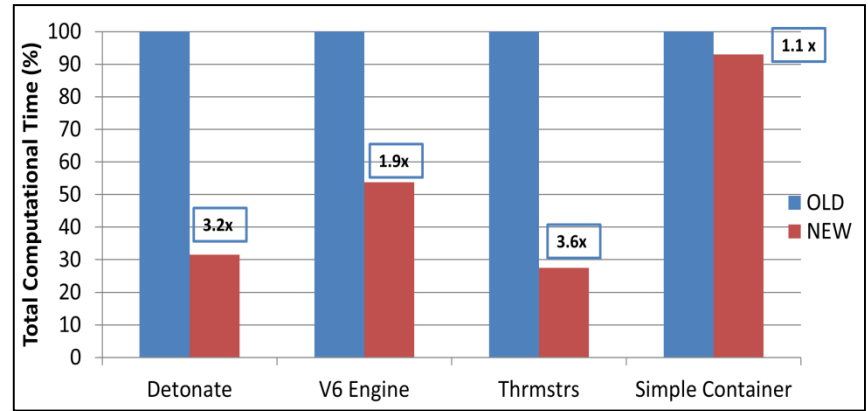
Optimized vector-matrix operations

FSI/TSE solver timing



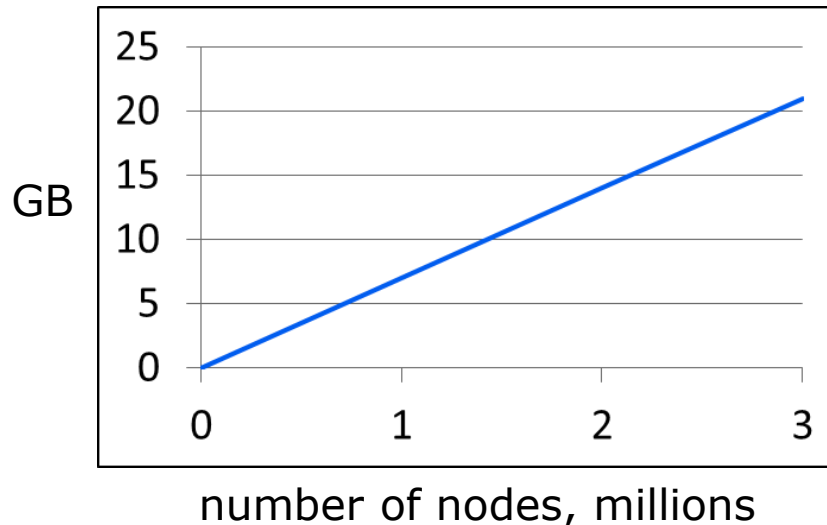
of nodes: 200K 480k 17k 26k

Total solver timing



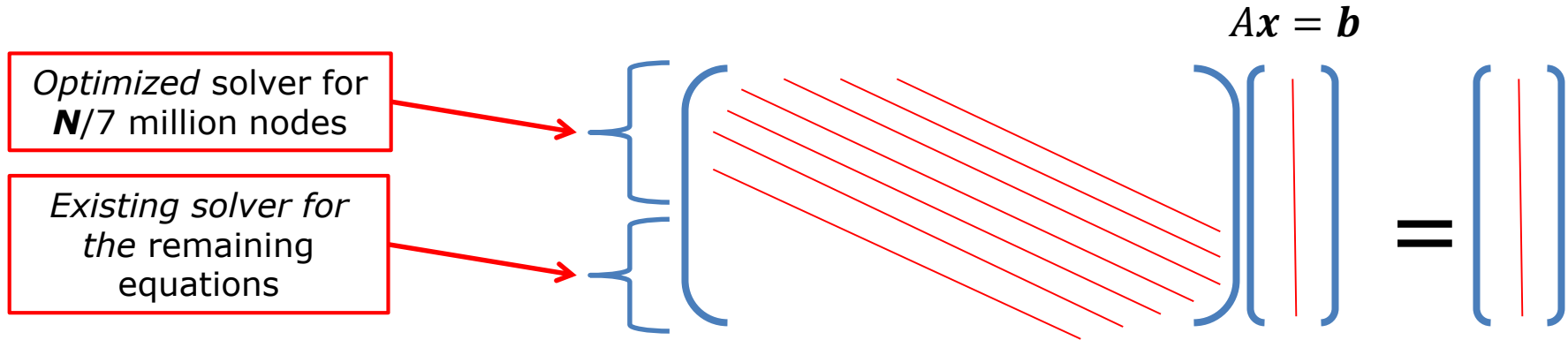
FSI/TSE solver performance: Memory penalty

Additional **7 GB** per **1 million** FE nodes (**14 GB** for tetrahedral mesh)



FSI/TSE solver performance: Hybrid approach

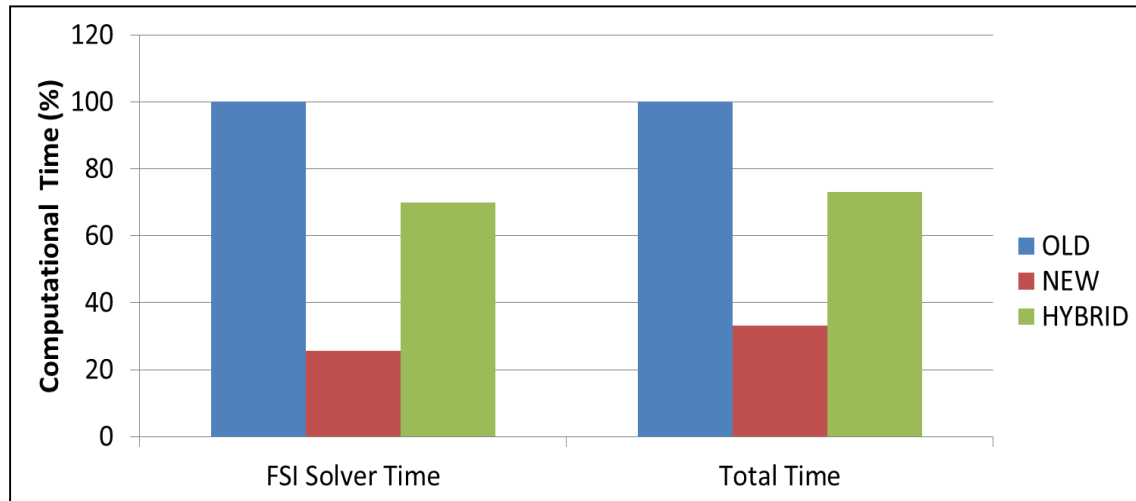
- Set a limit for the extra memory at N GB



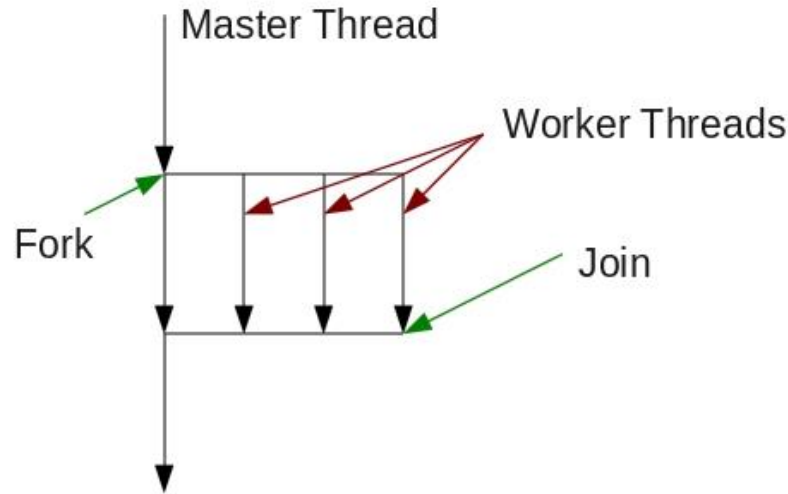
- Allow user to set N (default is 7 GB)

FSI/TSE solver performance: Hybrid approach

Hybrid performance from the hybrid solver



OpenMP overhead: Fork-Join



Number of fork-joins in GMRES solver: For MRSTRT=15, ITER=5, N=1500 per time step!

Reduced OpenMP overhead

| Examples | Pressure solver speed-up | Overall speed-up |
|-----------------------------|--------------------------|------------------|
| Continuous casting | 52% | 12% |
| Multi-block gravity filling | 27% | 27% |
| Marangoni | 48% | 32% |
| Mems | 47% | 23% |
| Slurry | 43% | 15% |
| Steam-air | 50% | 38% |
| Nirffluid | 56% | 43% |
| Pindrop | 42% | 23% |

Preliminary tests using 12 cores on Intel Xeon E5-2695 v2 @ 2.40GHz

New features

- Particle model
- Extensions to conforming mesh blocks
- Mooring line breaking
- Automatic wave-absorbing layer
- Dynamic droplet size for two-phase drift-flux model

Particle model

- Multiple species with different density and size
 - solid, fluid and gas particles
- Coulomb and dielectrophoresis forces
- Heat transfer with fluid and void:
 - evaporation/condensation
 - solidification
- Collisions with geometry components
 - sticking to stationary and moving components

Particle model physics

- Molecular and turbulent particle diffusion
- Two-way momentum coupling with fluid
- Host fluid:
 - fluid #1, fluid #2 or void.
- Macro-particles for better performance:
 - a numerical particle representing a small cloud of physical particles with identical properties

Particle classes

- Marker particles for tracers that move with fluid
- Mass particles for small solid objects
- Fluid particles are small droplets of fluid #1
- Gas particles for modeling small bubbles
- Void particles for tracking collapsed voids
- Probe particles represent probes, moving and stationary
- Source particles represent mass/momentum sources
- User-defined particles for customizations

Mass p

- Particle class properties are defined in *Physics*
- ≤ 10 species in each class
- Moving or stationary

Particles

Marker Mass Fluid Gas Add Class

Enable

Title:

Maximum allowed number of mass particles:

Species

Number of Species: 4

| | Title | Diameter | Density |
|---|-----------------|----------|-------------|
| 1 | sand grains | 0.001 | 2500 |
| 2 | Ti oxide powder | 0.004 | 2500 |
| 3 | Plastic pellets | 0.05 | 400 |
| 4 | Golf balls | 0.04267 | 1129.093467 |

Particle class properties

Host fluid

Fluid #1 and #2 (or void)

Fluid #1

Fluid #2 (or void)

Coefficients

Diffusion coefficient:

Drag coefficient:

Inverse Schmidt number:

Macro-particle coefficient:

Restitution coefficient:

Particle/fluid interaction

Implicit coupling with fluid

Ignore particle data in restart source file

Thermal properties

Specific heat:

Thermal conductivity:

Heat transfer coefficient to fluid:

Electrical properties

Dielectric constant:

AC coefficient:

Motion properties

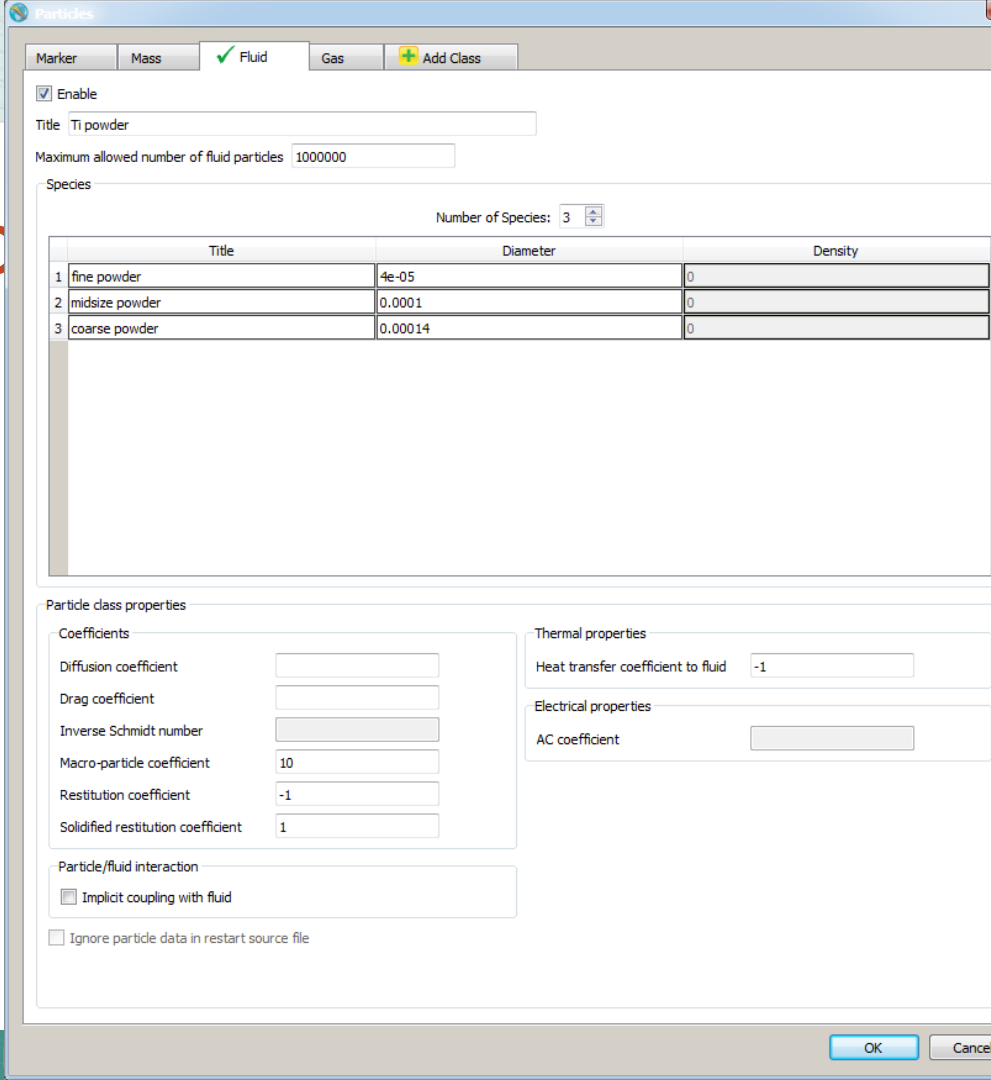
Stationary

Moving

OK Cancel

Fluid p

- Made of fluid #1
- Evaporation/condensation
- Solidification



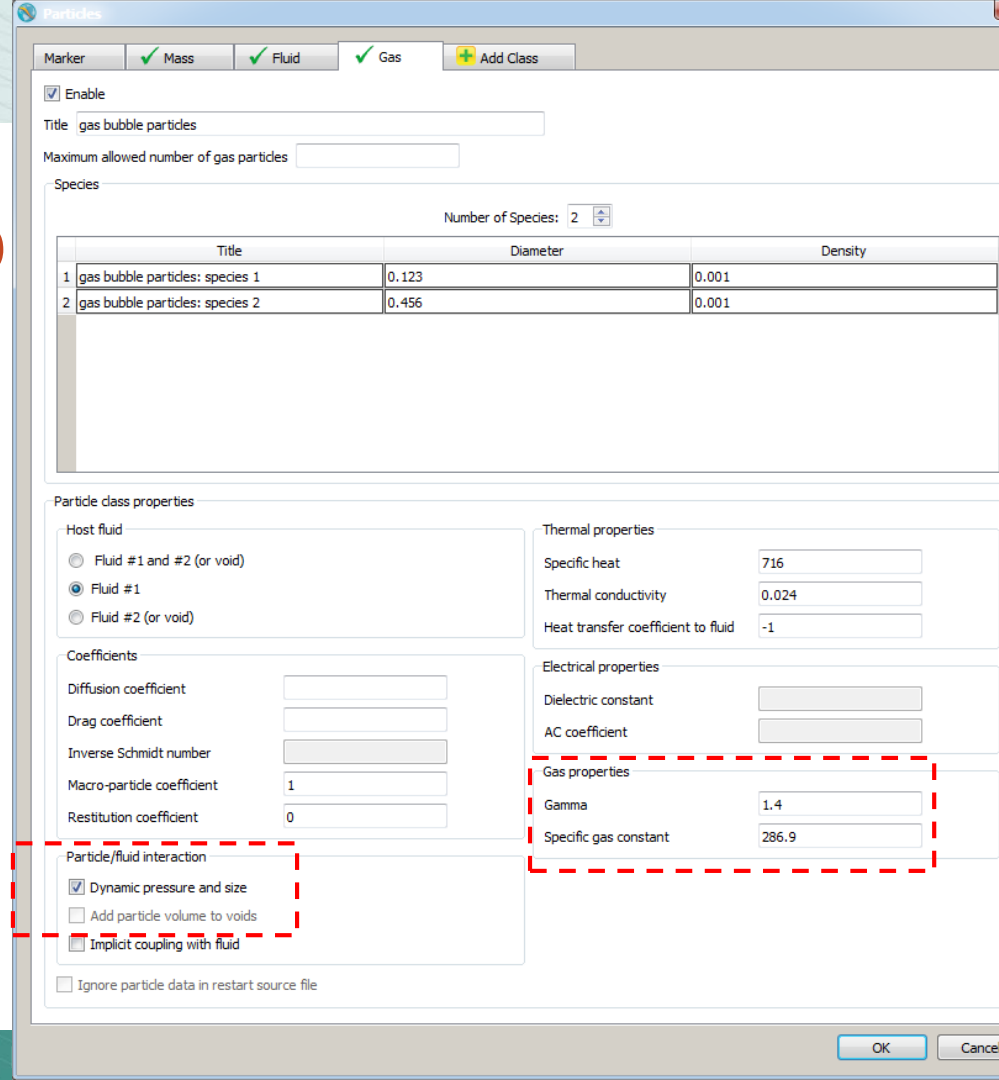
Gas p

- Dynamic pressure and size:

$$p_{particle} = p_{fluid} + \frac{4\sigma}{d}$$

- Equation-of-State

$$p = \rho RT$$



Generating particles

- Particles sources and blocks generate particles of specific class and species distribution
- A probe particle represents any existing species

User pa

- Material or marker
- Moving or stationary
- 3 extra attributes
- Customizable in source
 - particle_usr_force
 - particle_usr_vel
 - particle_usr_source
 - qsadd

Particles

Marker Mass Fluid Gas User Class 1 Add Class

Title: Birds flying from Australia to Iceland

Maximum allowed number of user class 1 particles: 532467

Species

Number of Species: 1

| | Title | Diameter | Density |
|---|---|----------|---------|
| 1 | Birds flying from Australia to Iceland: species 1 | 0.5 | 0.95 |

Particle class properties

Particle type

Marker particles

Material particles

Host fluid

Fluid #1 and #2 (or void)

Fluid #1

Fluid #2 (or void)

Coefficients

Diffusion coefficient

Drag coefficient

Inverse Schmidt number

Macro-particle coefficient

Restitution coefficient

Thermal properties

Specific heat

Thermal conductivity

Heat transfer coefficient to fluid

Temperature

Electrical properties

Dielectric constant

AC coefficient

Electric charge

Motion properties

Stationary

Moving

User class properties

Number of User Attributes: 0

Diameter

Density

Ignore particle data in restart source file

Note:

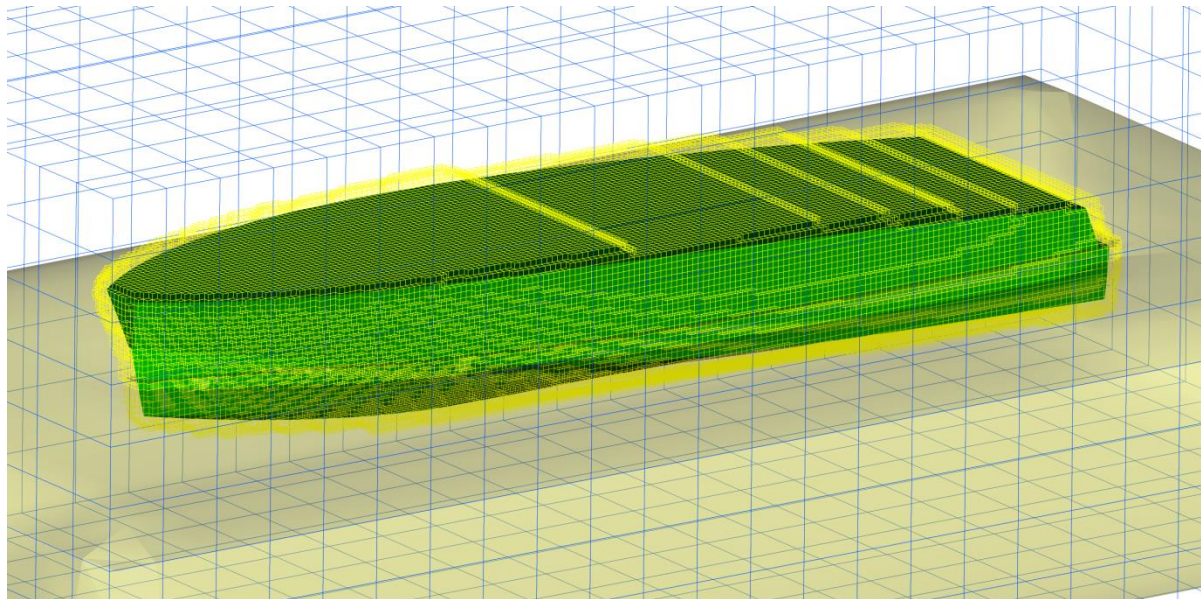
User customizable particle classes are based on the mass particle class and can be given custom attributes by modifying the supplied FORTRAN routines. For more information see the [Customization](#) chapter of the user manual.

Particle model summary

- Expanded modeling capabilities
- Improved accuracy:
 - particle-wall collision
 - 2nd order 3D trajectory integration
- User-customizable
- SMP/MPI parallelized

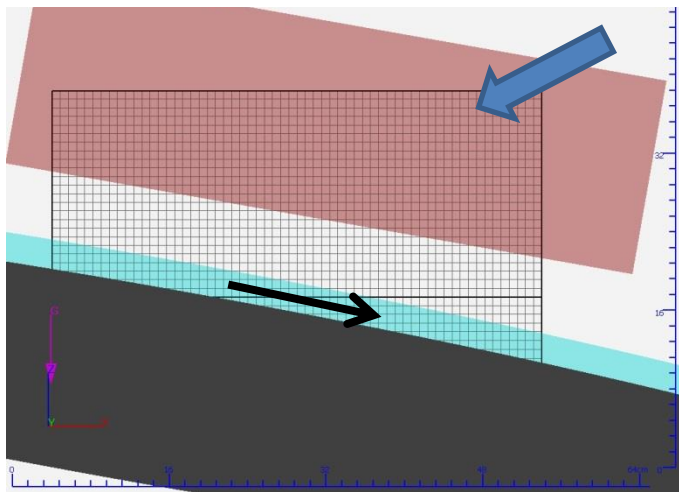
Extensions to conforming meshes

Concentrate fine mesh around an object

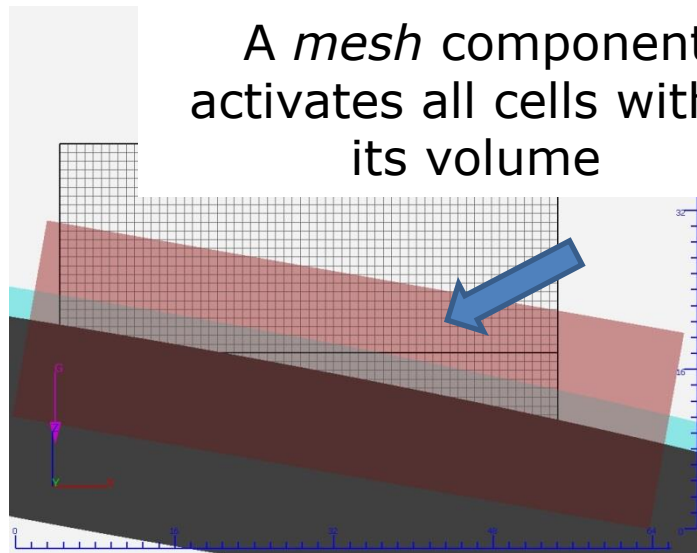


Mesh components

Domain removing components deactivate all cells within its volume

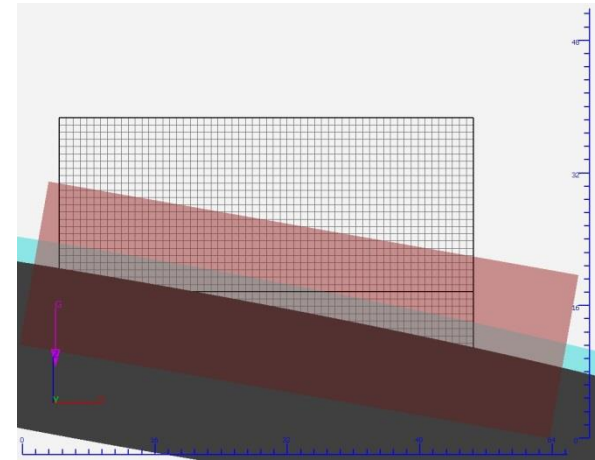


A *mesh* component activates all cells within its volume



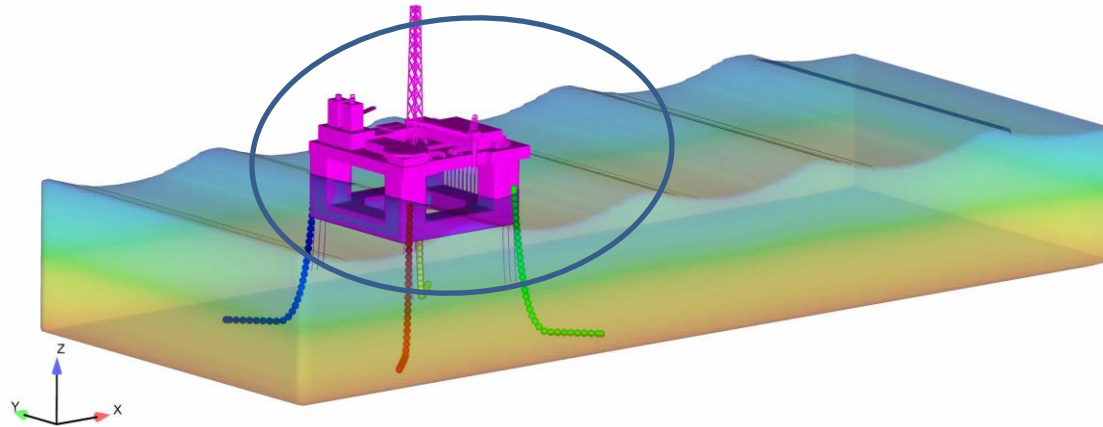
Mesh components

- Marks an arbitrary region in the domain
 - spanning open and solid volumes
- Mesh cells are active inside the region
 - with an optional overlap
- Multiple *mesh* components, STL & primitives.
- Complements Domain Removing Components



Refine the mesh in the path of a GMO

Time = 0.000

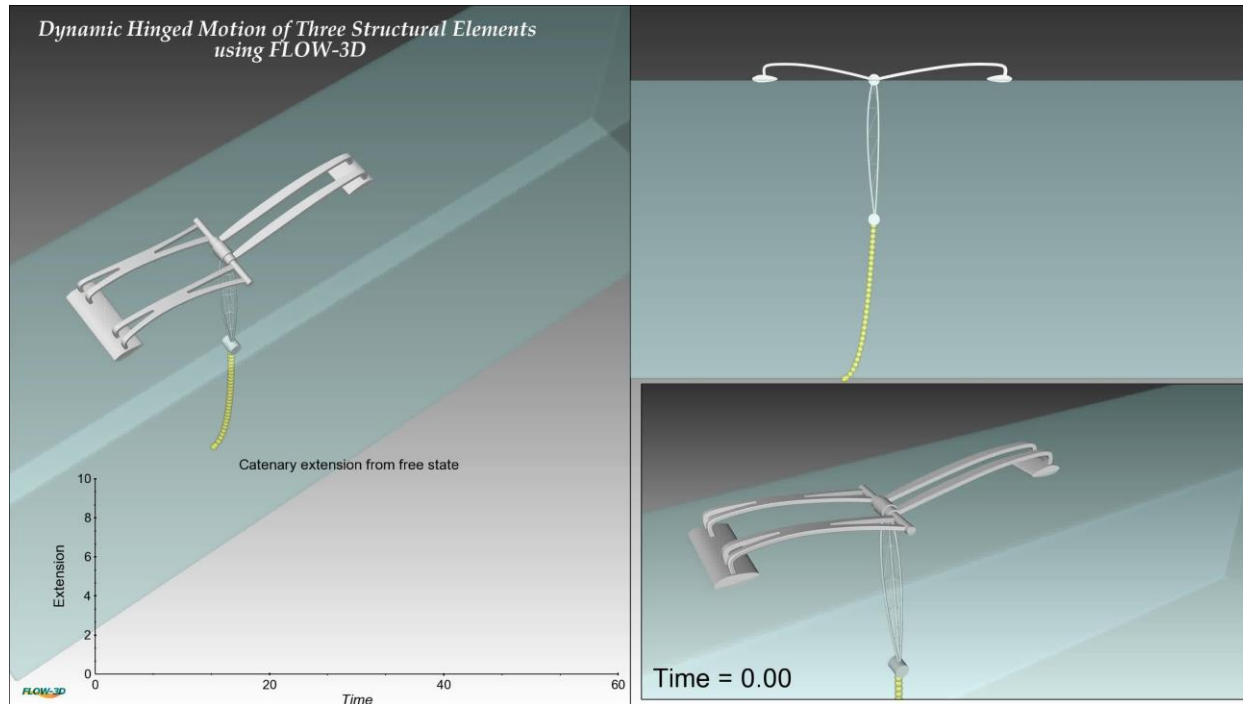


FLOW-3D

Conforming meshes summary

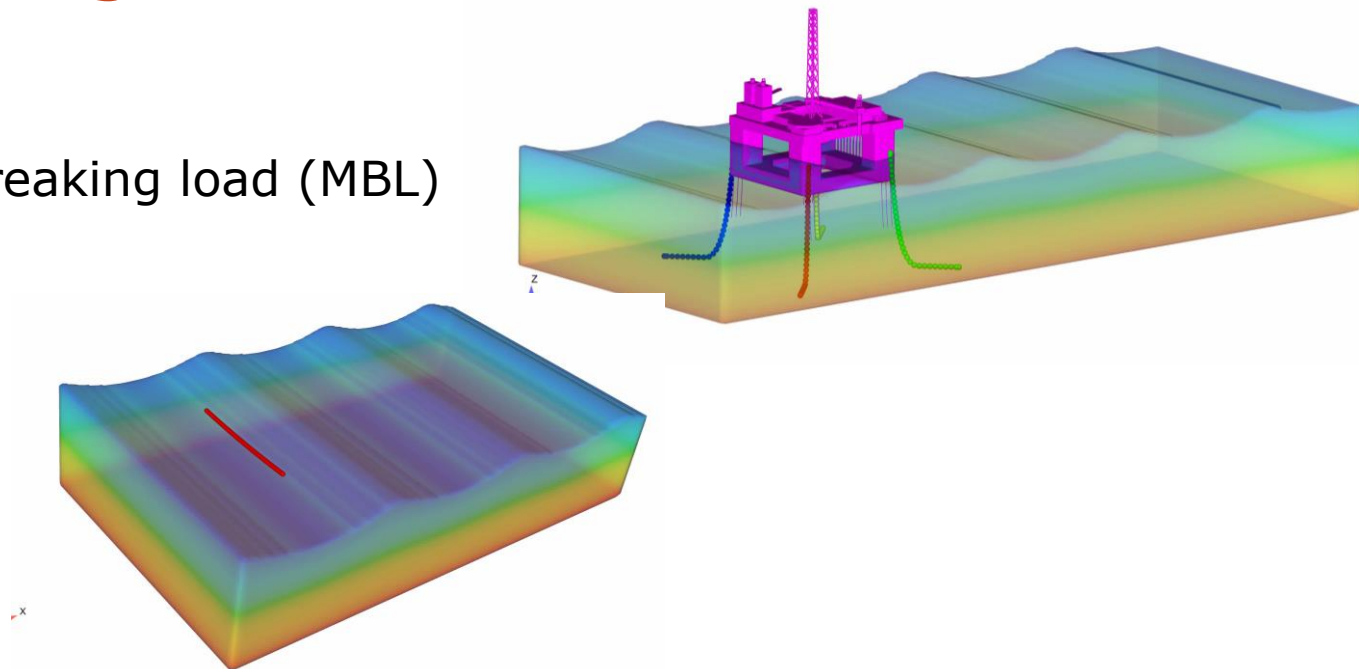
- Conforming to solid volume
 - selected components
- Conforming to *any* part of the domain
- Conforming to open volume
 - metal casting application only

Mooring line model



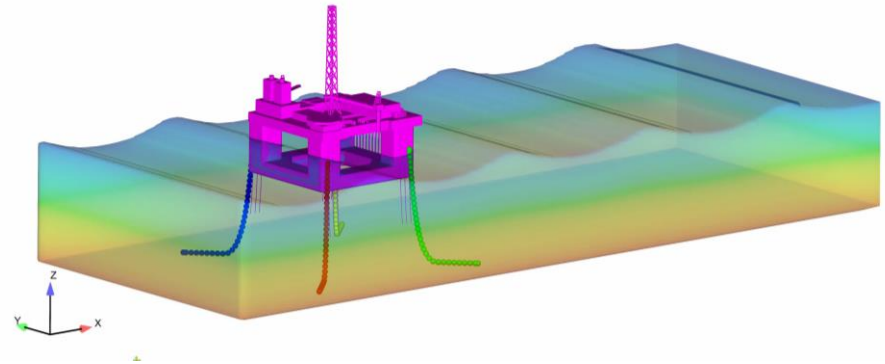
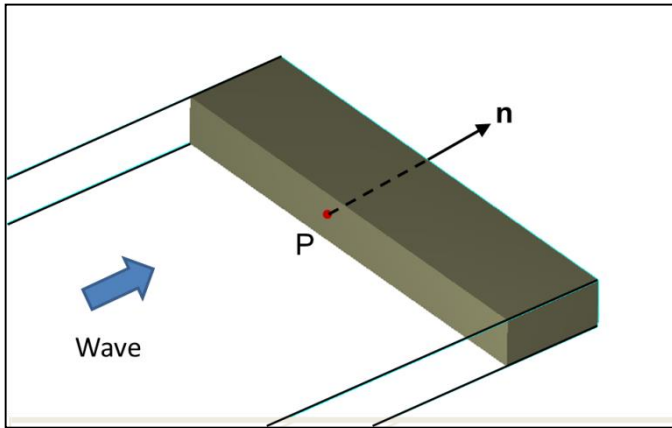
Mooring line model extensions

- Line failure
 - minimum breaking load (MBL)
- Free ends
- Fixed ends



Wave absorbing regions

Wave absorbing components are an effective way of preventing wave reflection at outflow boundaries.



Wave absorbing components

- Place non-turbulent
- Typical region boundary

Component Properties

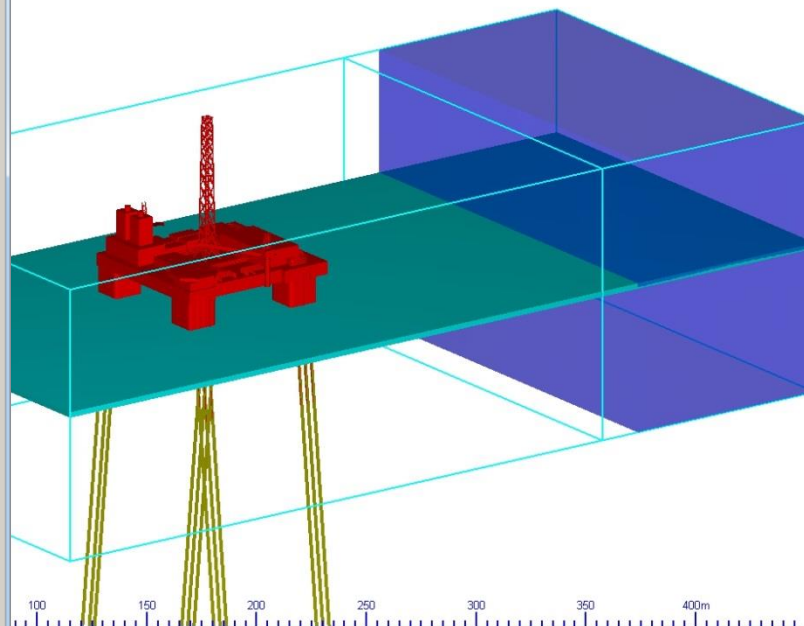
Surface Properties
 Thermal Die Cycling Properties
 Thermal Stress Properties
 Wave Absorbing Properties

Search for: Find

Wave Absorbing Properties

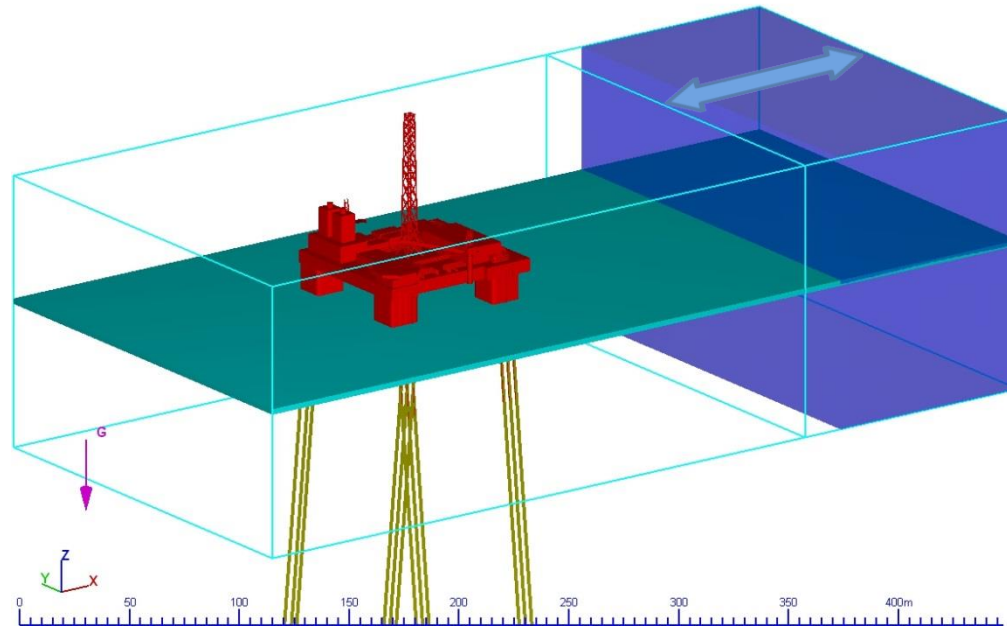
- Starting Point
 - X: 170
 - Y: 0
 - Z: 0
- Downstream direction
 - X: 1
 - Y: 0
 - Z: 0
- Background Stream Velocity
 - Prescribed
 - X: 0
 - Y: 0
 - Z: 0
- Damping coefficient of beginning: 0
- Damping coefficient of end: 1

Component 1: platform Component 2: wave absorber



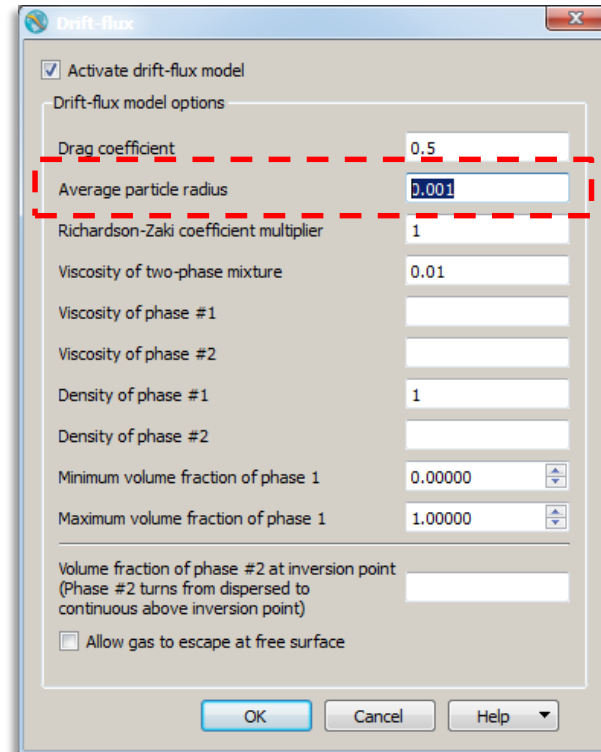
Wave absorbing boundaries

- New: a property of *Outflow* and *Continuative* mesh boundaries
- Only the thickness of the layer is required as input
- Placed inside the computational domain, upstream of the boundary
- Retain *Wave Absorbing* components



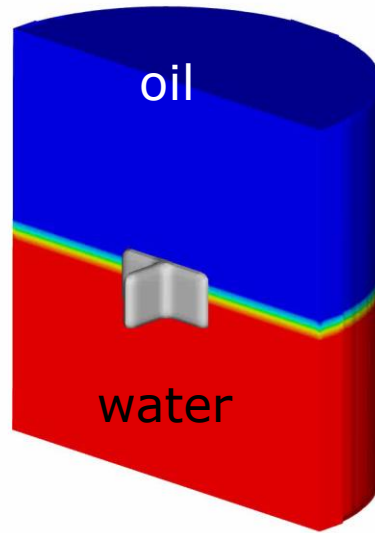
Dynamic droplet size in drift-flux model

- Using a fixed average droplet size is a major limitation of the two-phase model
- Dynamic size calculation for liquid droplets or gas bubbles, based on the critical Weber and Capillary numbers, $We = \frac{\rho u^2 l}{\sigma}$, $Ca = \frac{\mu u}{\sigma}$, $u \equiv \text{drift velocity}$
 - shear forces cause particles to break up
 - turbulence results in particle coalescence

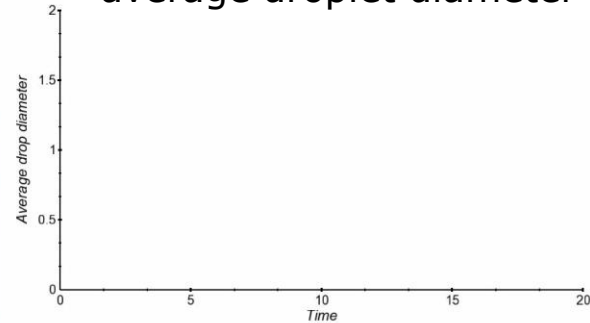


Dynamic droplet size in a mixing tank

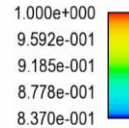
Time = 0.00



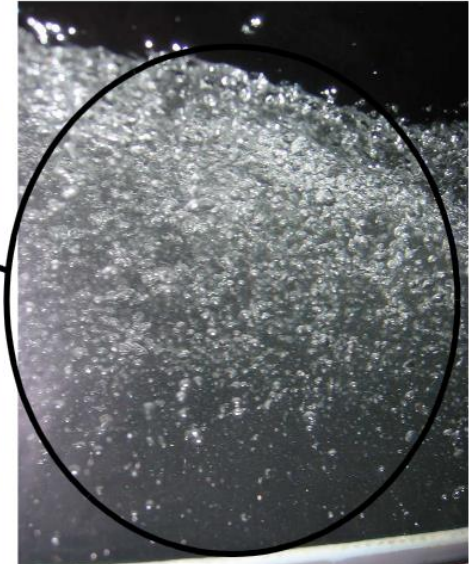
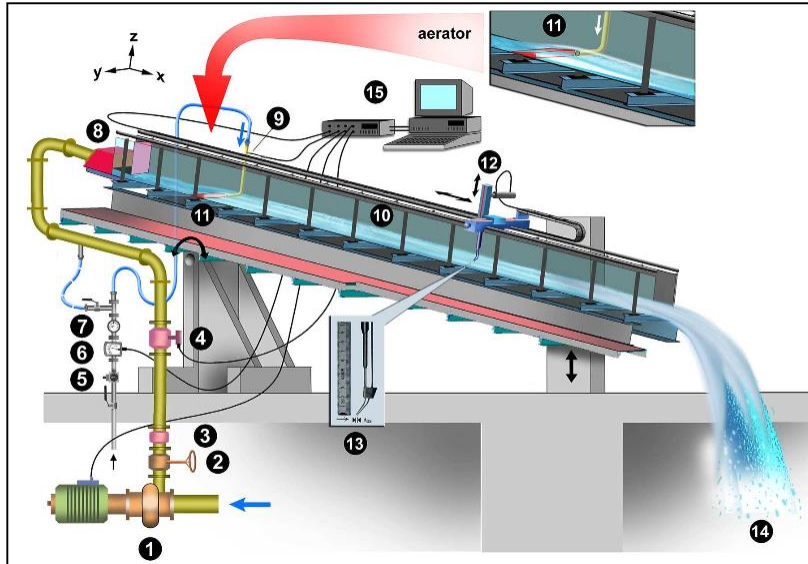
average droplet diameter



Macroscopic Density Selected

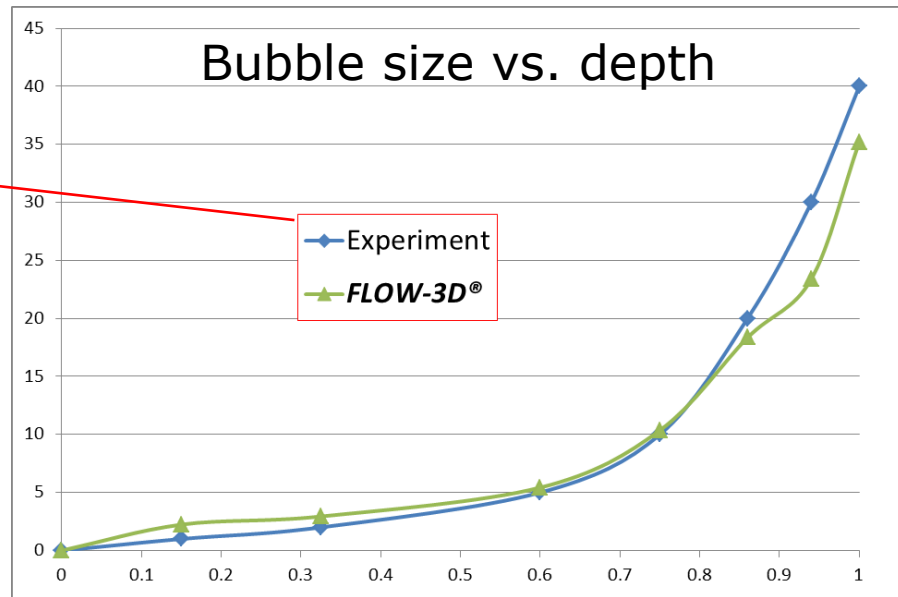
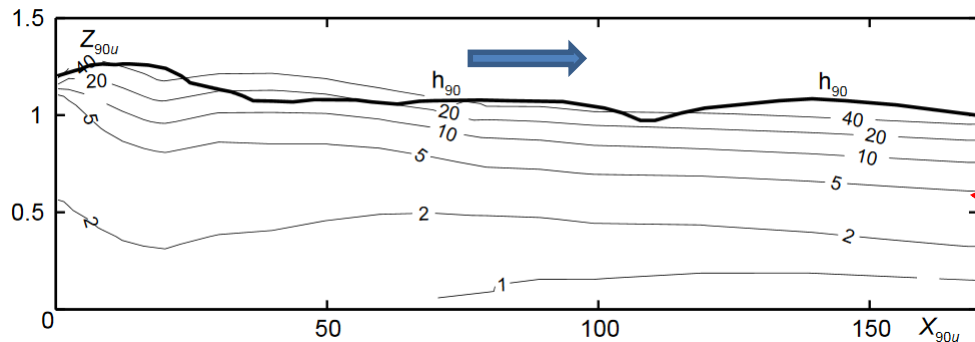


Air bubbles in an aerated chute



Kristian Kramer, ETH Zürich, 2004

Air bubbles in an aerated chute



Kristian Kramer, ETH Zürich, 2004

Thank you!