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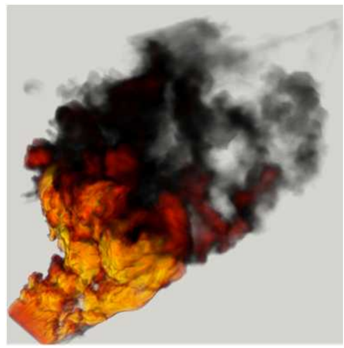

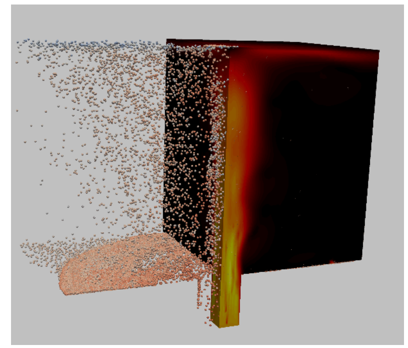

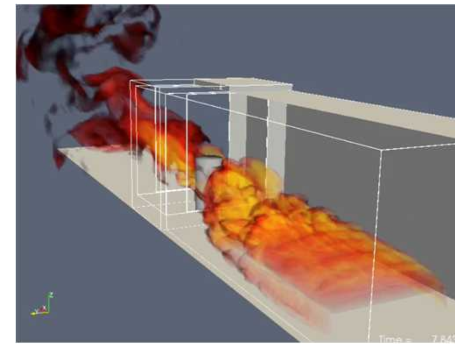

Particle Resuspension Simulation Capability to Substantiate DOE-HDBK-3010 Data

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U.S. DEPARTMENT OF ENERGY

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Outline

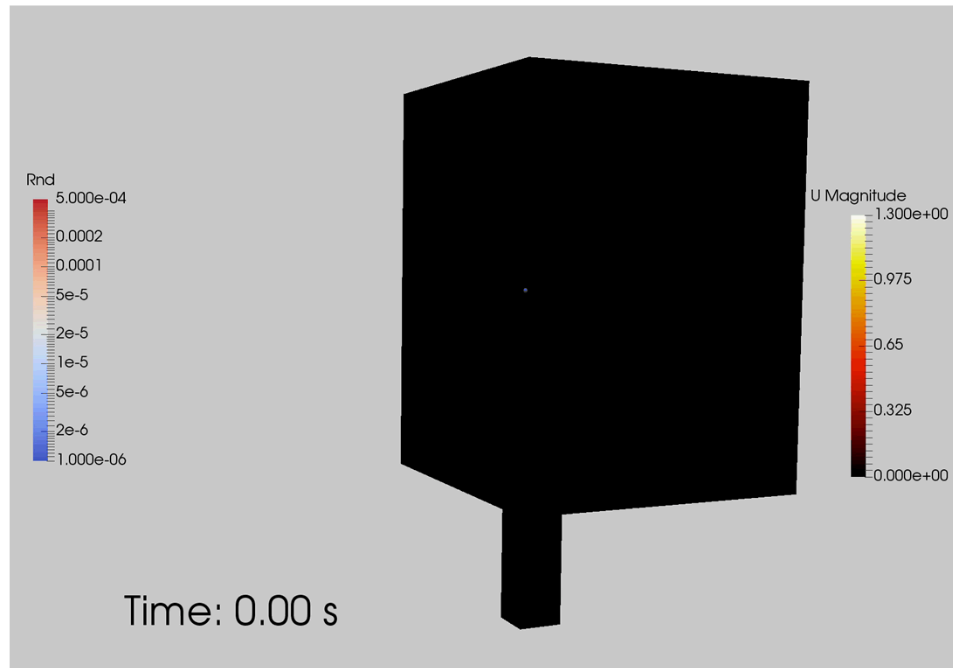
- Sierra/Fuego overview
- Particle transport algorithms
- Resuspension model overview
- Demonstration simulations
- Summary

Capability Overview

Sierra/Fuego[1]

Low-Mach fire simulation

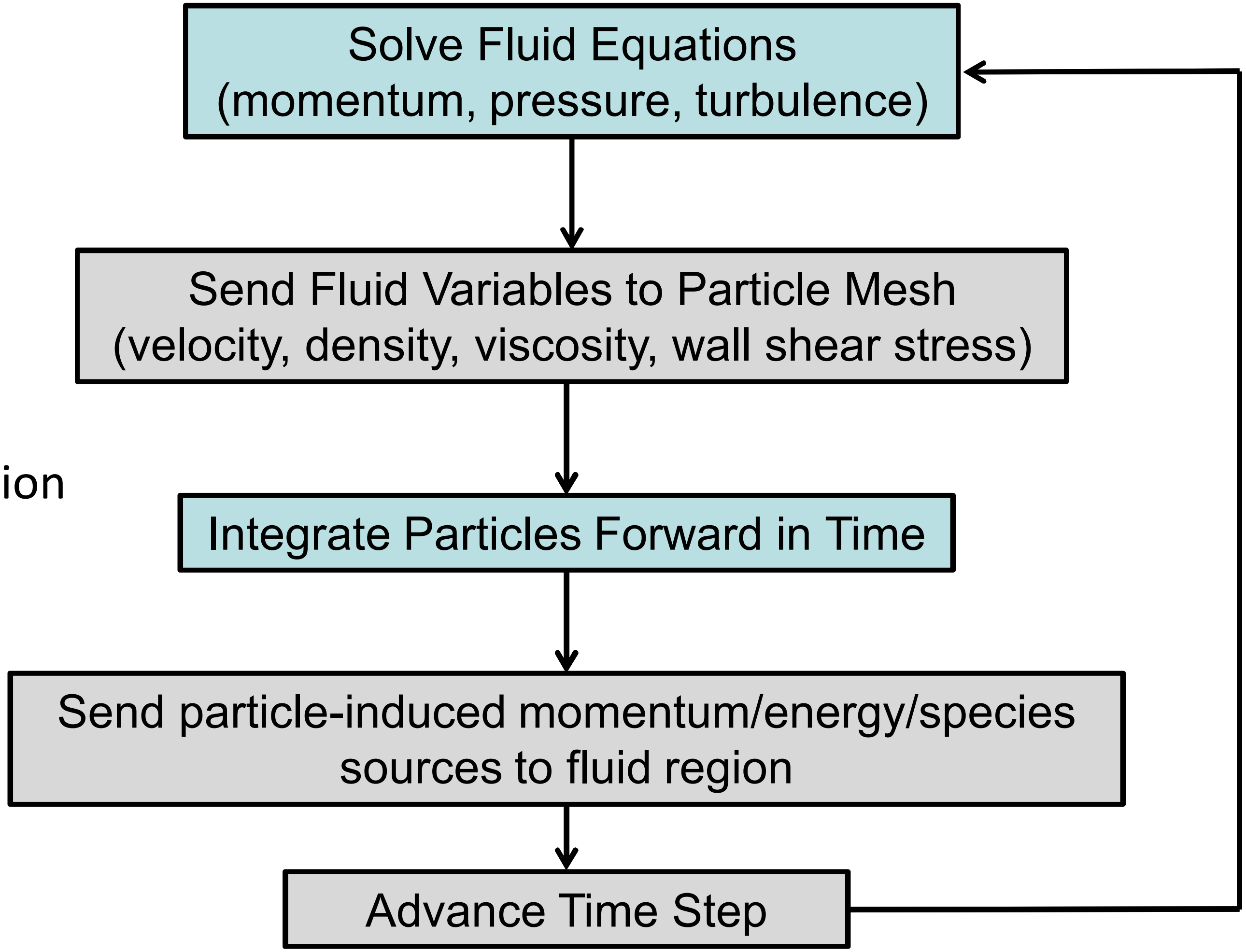
Demonstration simulation of particle-laden turbulent jet



1. Sierra Thermal/Fluid Development Team, SIERRA Low Mach Module: Fuego User Manual – Version 4.40, SAND2016-4157

Particle Transport

- Fluid/particle coupling algorithm
- 2-way coupling
- 1st order in time
- Particle mesh can have different parallel decomposition than fluid mesh



Particle Transport

- For this work, we consider only isothermal, inertial spherical particles

$$\begin{bmatrix}\dot{x}\\ \dot{v}\end{bmatrix} = \begin{bmatrix} v_p \\ \frac{1}{m_p}\left(F_{drag} + F_{buoy}\right)\end{bmatrix}$$

$$F_{buoy} = \frac{4}{3}\pi r^3\left(\rho_p - \rho_f\right)g$$

$$F_{drag} = 6\pi\mu_f r f_D(Re)\left(v_p - \left(v_f + v_f{}'\right)\right)$$

- The turbulent contribution to the velocity ($v_f{}'$) is a function of the turbulent kinetic energy ($\sqrt{\frac{2}{3}k}$) with a random orientation

- Wall shear stress is either calculated using an appropriate wall model (turbulent flow) or the local viscosity and velocity gradient (laminar flow)

- Turbulent variation in wall shear stress fit to experimental data by Keirsbulck et al.[2]

$$\frac{\tau_{w'}}{\overline{\tau_w}} = 0.0375\ln(u_\tau) + 0.482.$$

2. L. Keirsbulck, L. Labraga, M. Gad-el-Hak, Statistical properties of wall shear stress fluctuations in turbulent channel flows, International Journal of Heat and Fluid Flow 37 (2012) 1-8

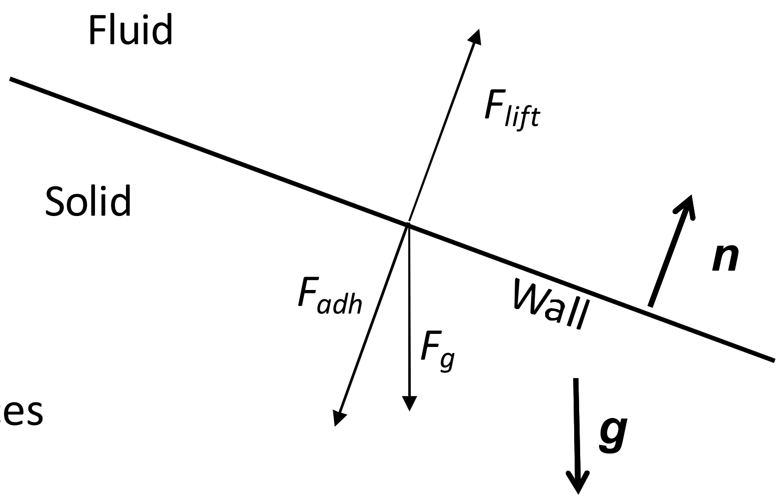
Particle-Wall Interactions

- Integration of the inertial particle ODE (previous slide) can result in the particle hitting a domain boundary

- Once it hits a boundary (wall) it can do several things:
  - Be deleted from the simulation
  - Rebound off the wall immediately
  - Permanently stick to the wall
  - Stick on the wall until its resuspension criteria is met and it is re-introduced back into the flow

Resuspension Force Balance

- Initial model is based on a force balance approach
  - Resuspends if $\boldsymbol{n} \cdot \left(\sum \boldsymbol{F}\right) > \boldsymbol{0}$
- Several models summarized by Young[3]
  - These typically do not include the buoyant force (gravity)
  - Most of the models can be cast in terms of different lift and adhesion forces



- Focused here on the Wichner model

$$\boldsymbol{F_{lift}} = \alpha \pi r^2 \tau_w \boldsymbol{n} \qquad \boldsymbol{F_{adh}} = -10^{-9}\frac{r}{\varepsilon}\boldsymbol{n} \qquad \boldsymbol{F_g} = \frac{4}{3}\pi r^3 (\rho_p - \rho_f)\boldsymbol{g}$$

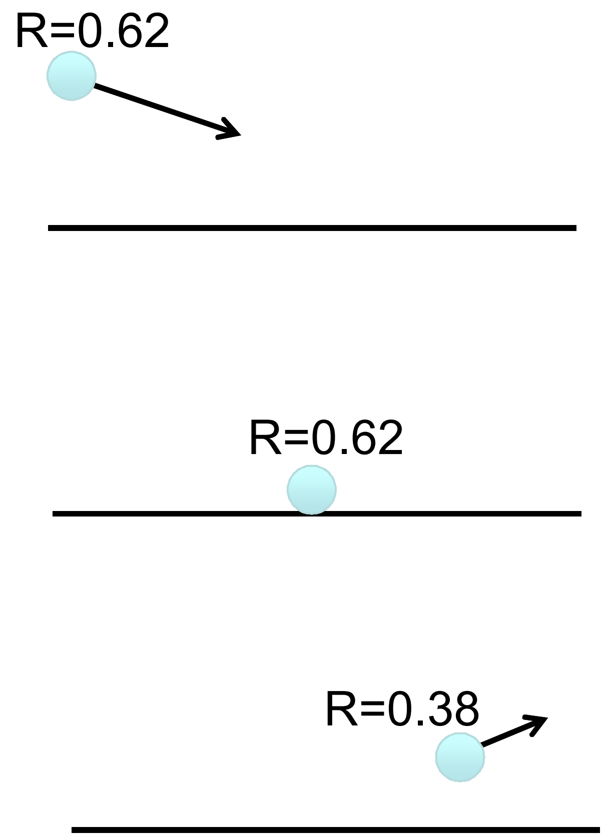
- Limitations of Wichner model:
  - Only applicable for small, solid particles (dust)
  - Requires knowledge of free parameter, α, and surface roughness, ε
  - Doesn't differentiate between liftoff resistance and rolling resistance

3. Michael F. Young, Liftoff Model for MELCOR, 2015, SAND2015-6119

Probabilistic Approach

- Want to account for randomness in the surface, and in the particle-surface interaction

1. Define a probability function (P)
2. Assign each particle a random number (R) at creation
3. For a stuck particle, the particle resuspends if F.n > 0 and P > R
4. Once the particle resuspends, it gets a new value for R



- For example, you could increase resuspension probability with higher lift forces using

$$P = 1 - \exp\left(-\frac{F_{lift}}{F_{adh}}\right)$$

Demonstration Cases

Wall Impact Test

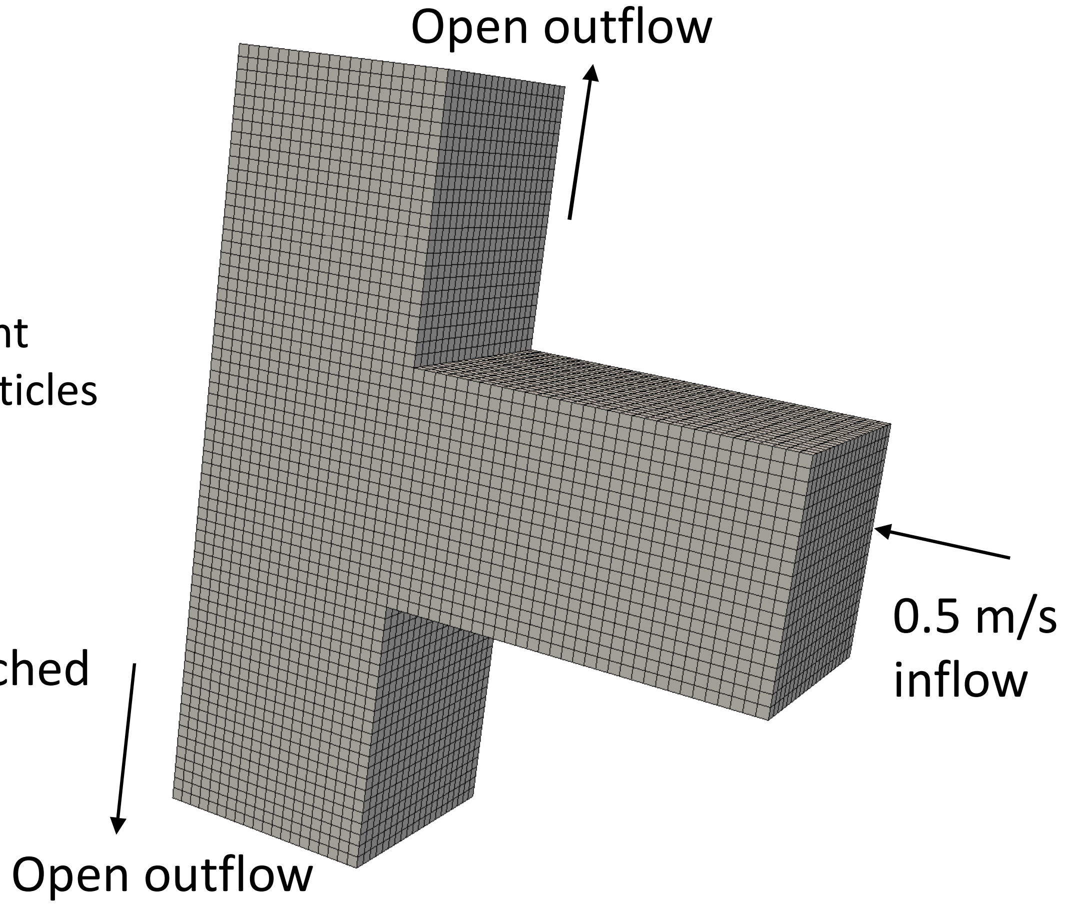
- Laminar gas flow impacting wall perpendicularly (Re = 950)
- No gravity forces
  - Only forces on particles are inertia and fluid drag
- Tests stokes number dependence of wall collision calculations
  - Laminar fluid drag alone should **never** cause particles to impact walls (streamlines do not cross though walls)
  - When inertial forces are high enough or flow is turbulent, particles can impact walls

Resuspension Model Tests

- Turbulent gas flow across a surface pre-loaded with particles (Re ~ 25,000)
- Gravity force active
  - Forces on particles are buoyancy, inertia, and fluid drag
- Particle size distribution is log-normal
- Compares constant and fluctuating wall shear stress models

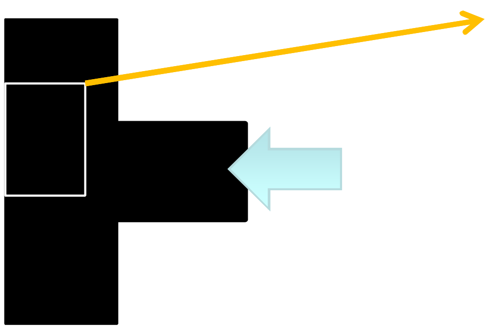
Wall Impact Test

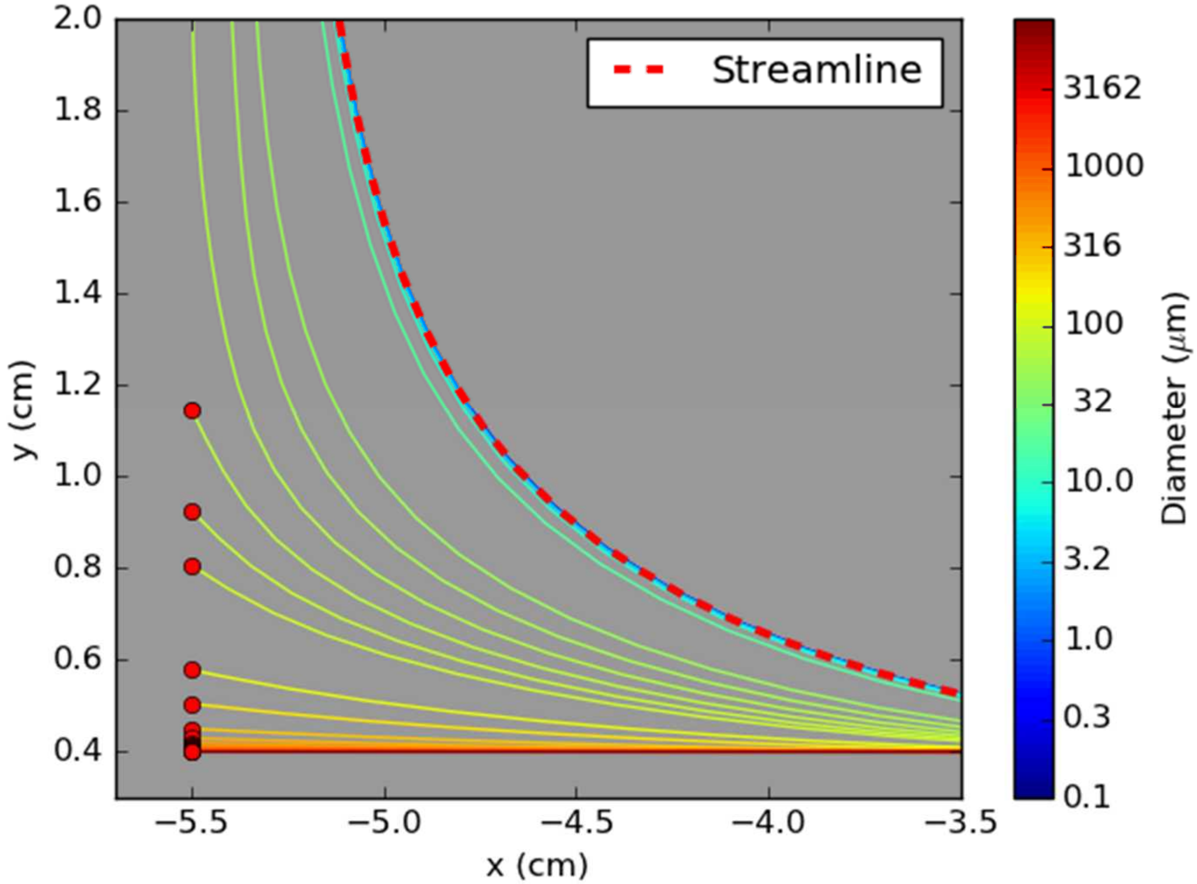
- Channels are 3 cm square
- Mesh is 1.5 mm
- Particle→Fluid coupling disabled
  - Each particle path is independent of the number/size of other particles
- Particles from 100 nm to 1 cm diameter inserted off-center in inflow branch after flow has reached steady state



Wall Impact Test

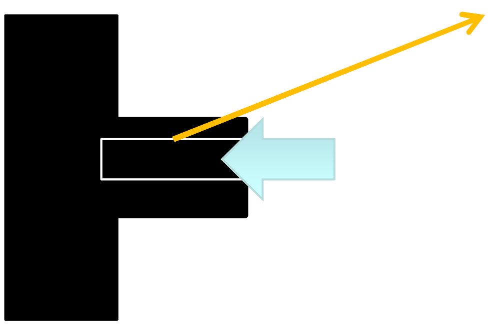
- Near-impact results show particles smaller than 80 μm diameter did not hit the wall
- Additional forces (electrostatic, Van der Waals) may be important for very small particles
- Small particles followed streamline
- Large particles had minimal deflection from initial trajectory

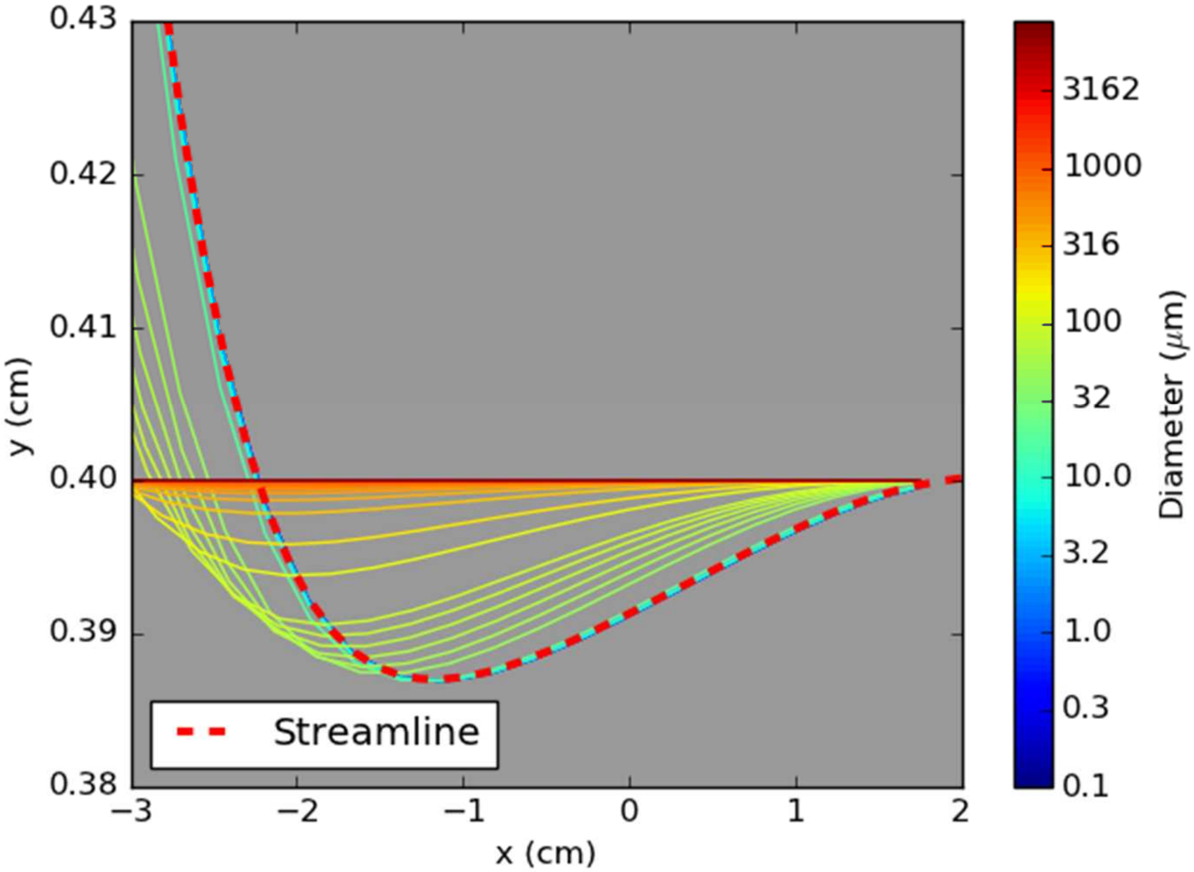




Wall Impact Test

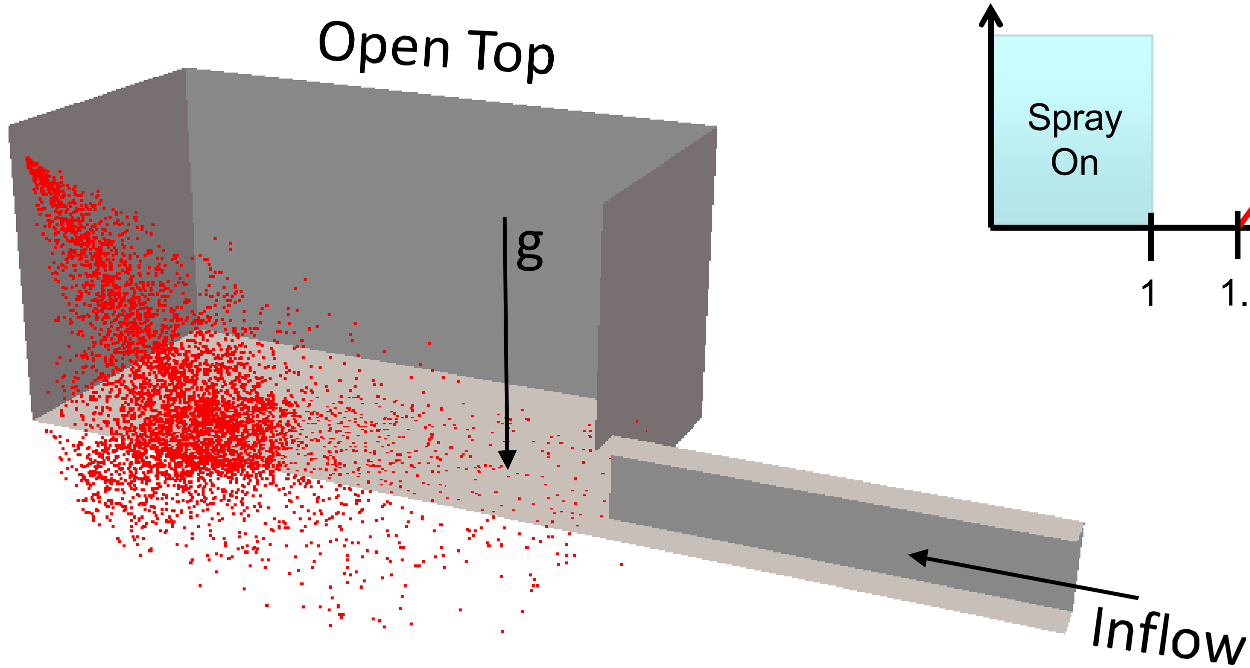
- Focusing on inflow region shows similar behavior
- Minimal deflection for large particles and small particles follow streamline
- 10 to 300 μm diameter particles partially deflected

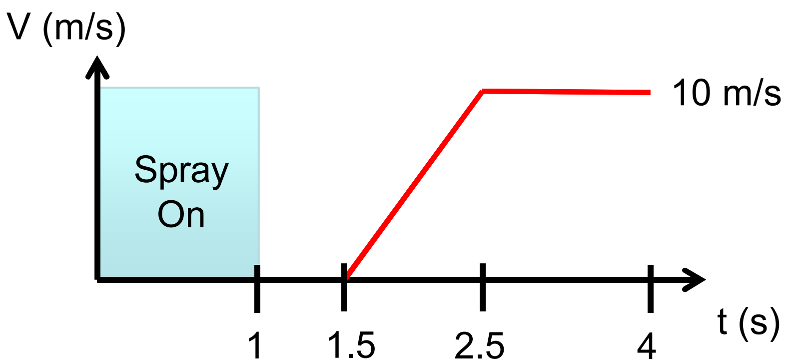




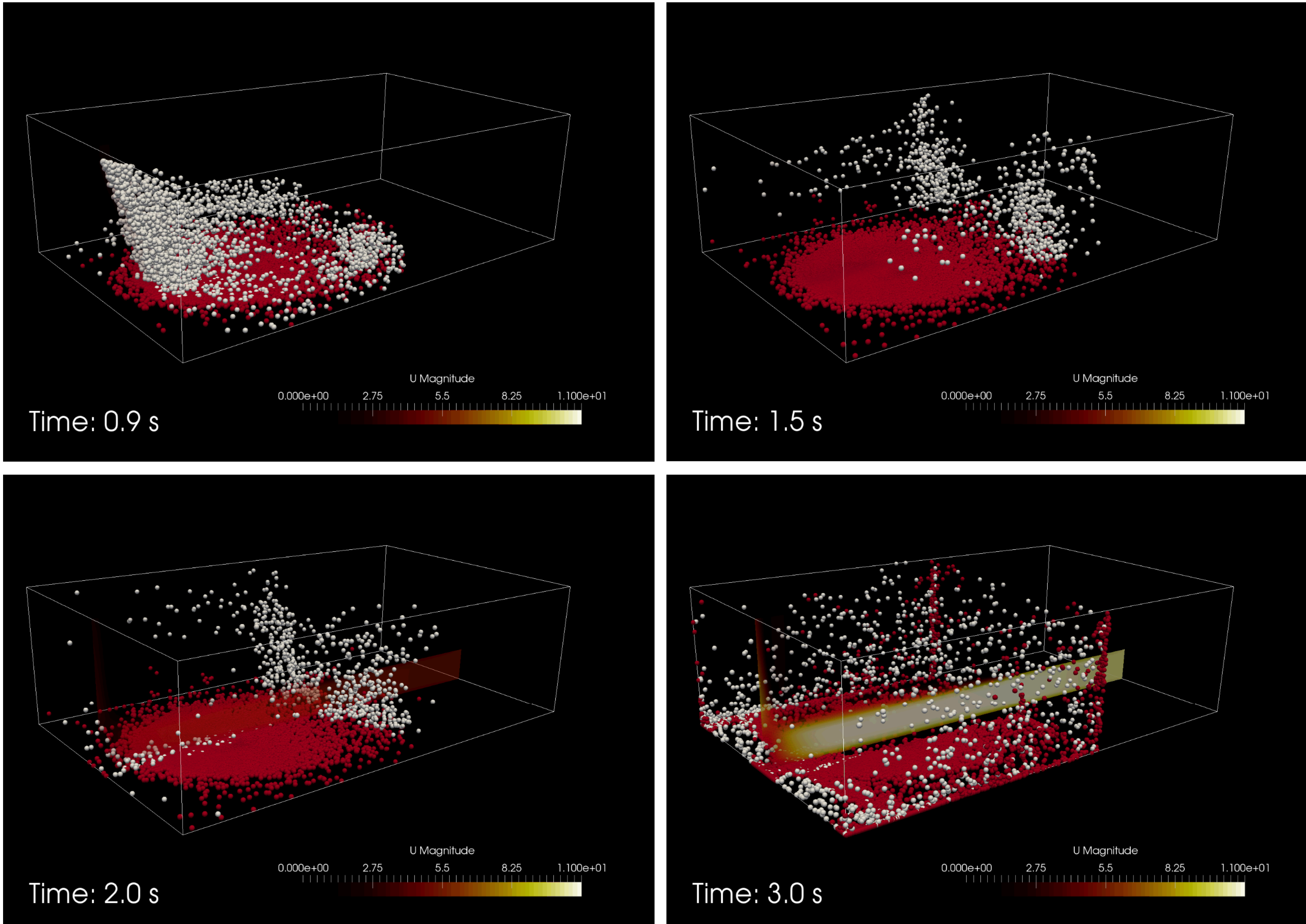
Resuspension Tests

- Notional scenario of a particle spray in an open box
- Box is 30 x 30 x 15 cm, inflow channel is 4 x 4 x 20 cm
- Particle spray active for 1 second, inflow jet starts at 1.5 seconds and ramps up to 10 m/s in 1 second, the holds constant for another 1.5 seconds
- Compare constant and variable wall shear stress models

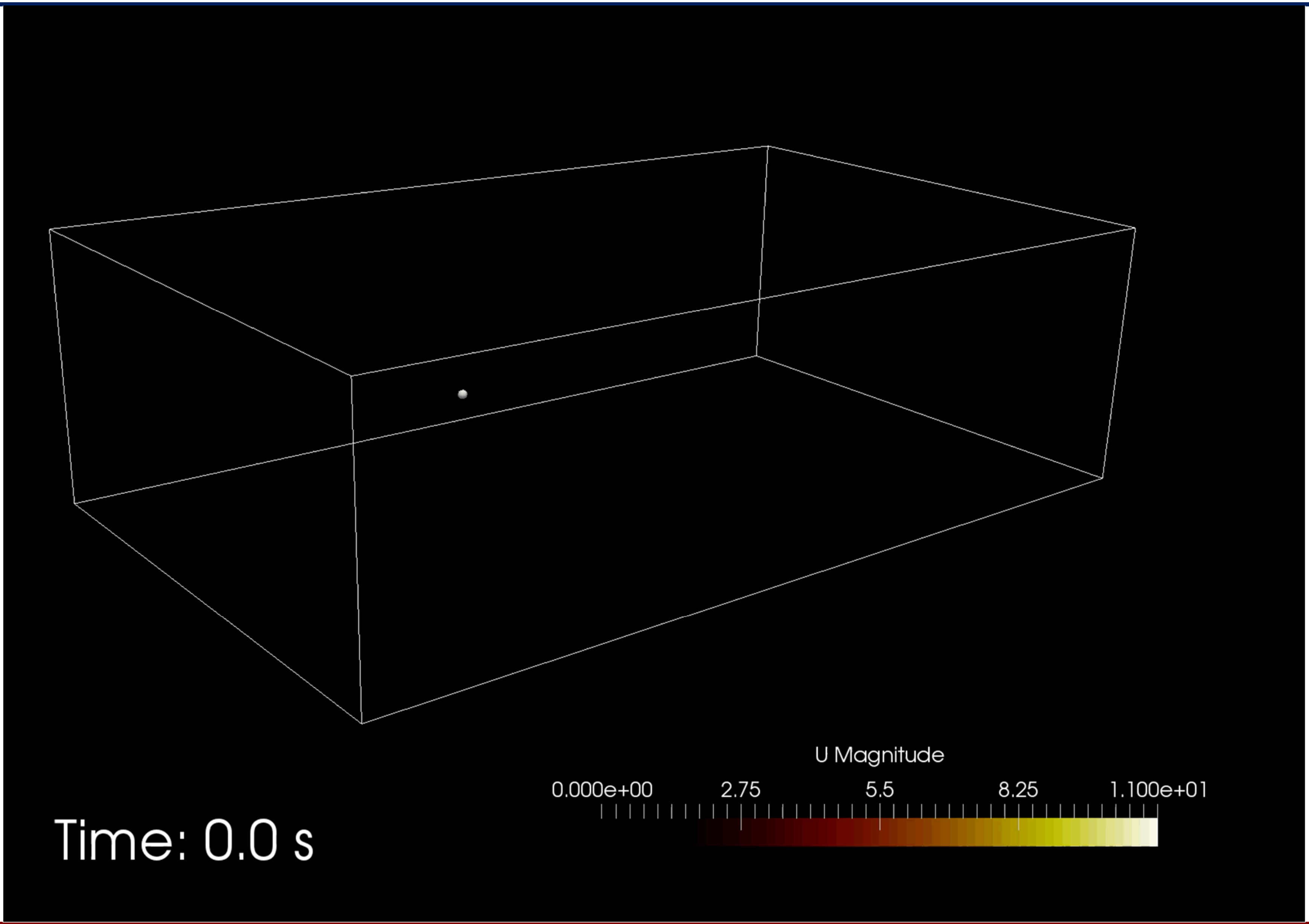




Resuspension Tests

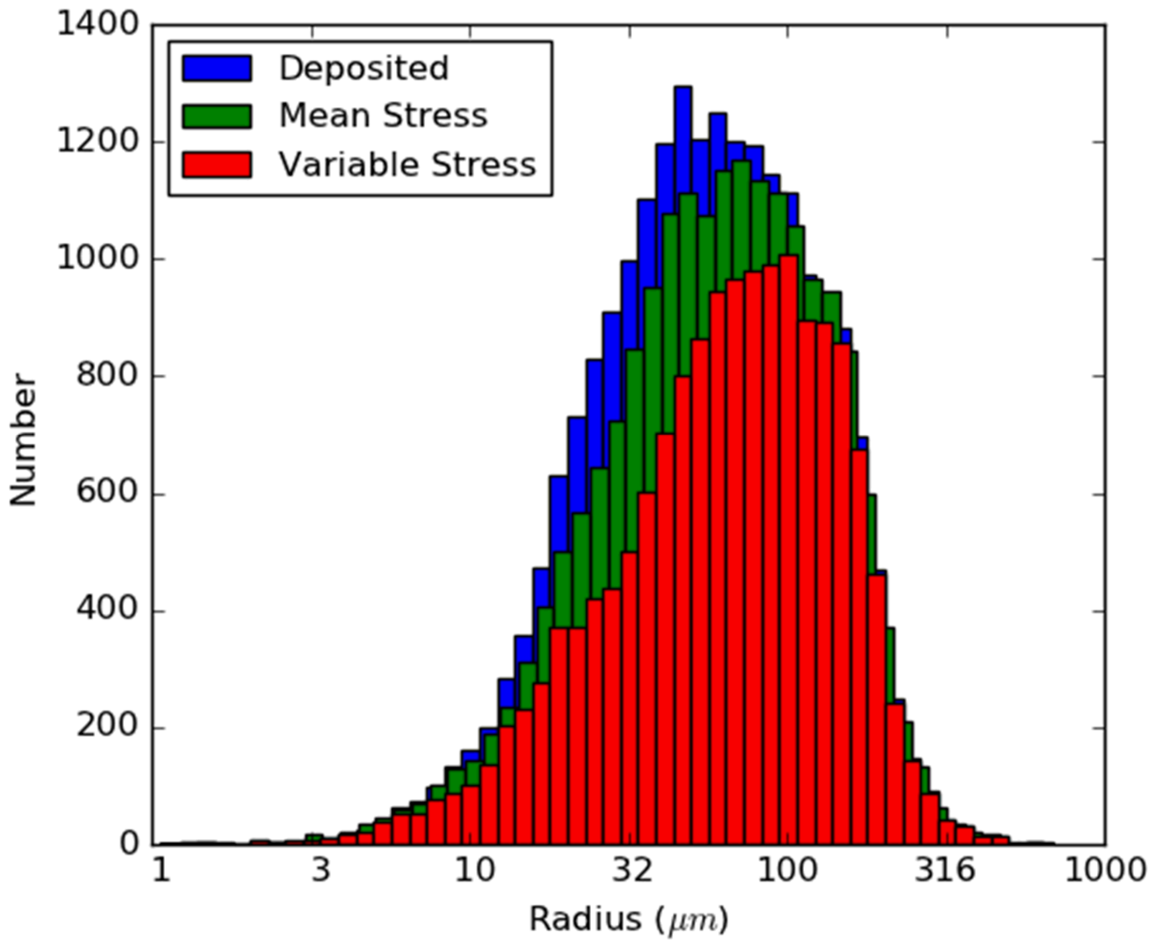


Resuspension Tests

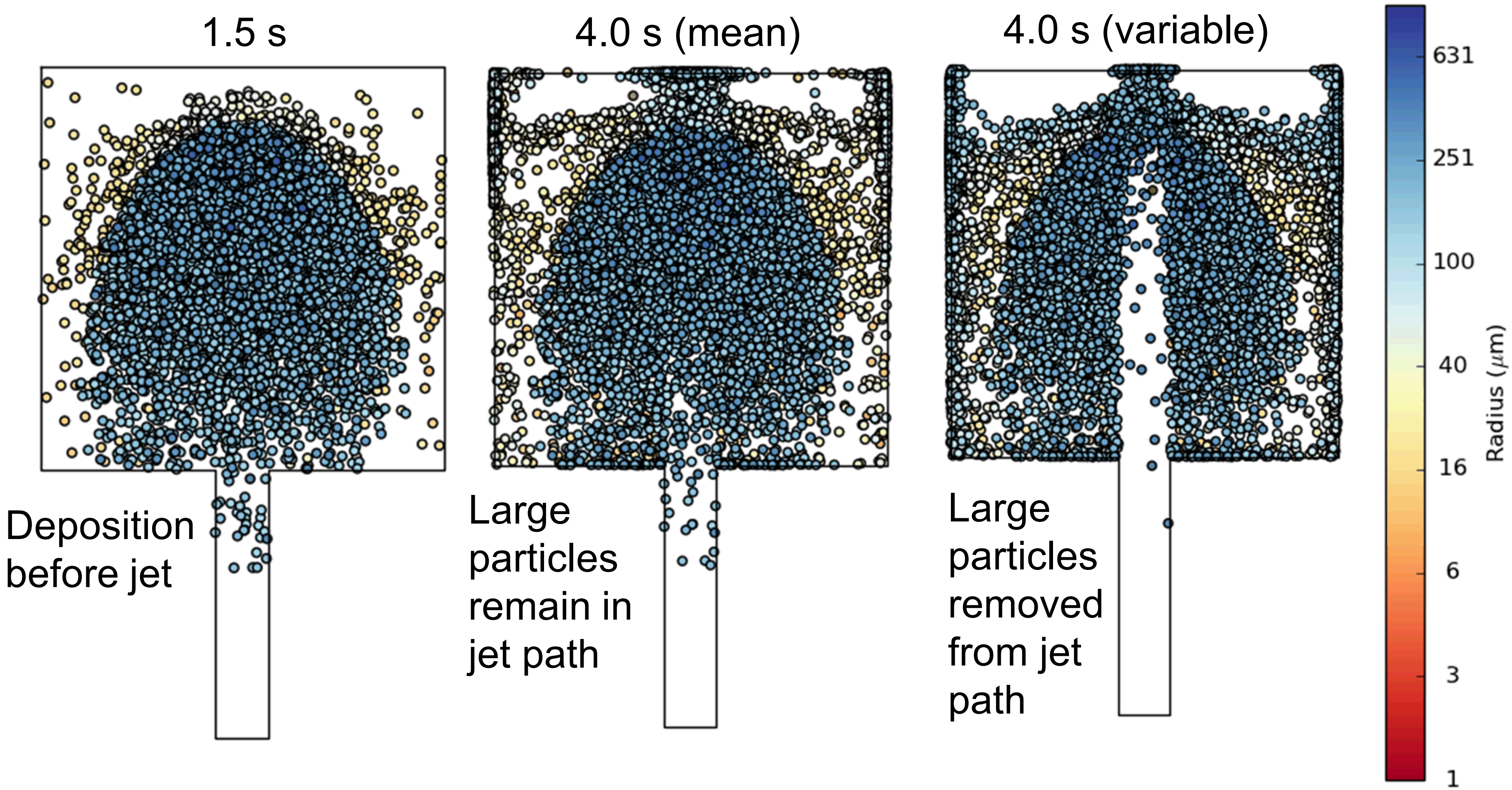


Stuck Particle Sizes

- Initial distribution of particles is log-normal
- Most resuspended particles between 10 and 100 μm
- Variable shear stress model removes more particles across the size spectrum



Spatial Distribution



Summary

- Sierra/Fuego particle transport simulations can include various force and probability based particle-wall interaction models

- Particle transport influenced by only buoyant, inertial, and drag forces may miss some relevant near-wall behavior for small particles

- Turbulent fluctuations in velocity and wall shear stress can significantly effect resuspended fraction

- Capability demonstrated for certain physically relevant use cases

Acknowledgements

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