Mars 2020 Launch, ULA Atlas V
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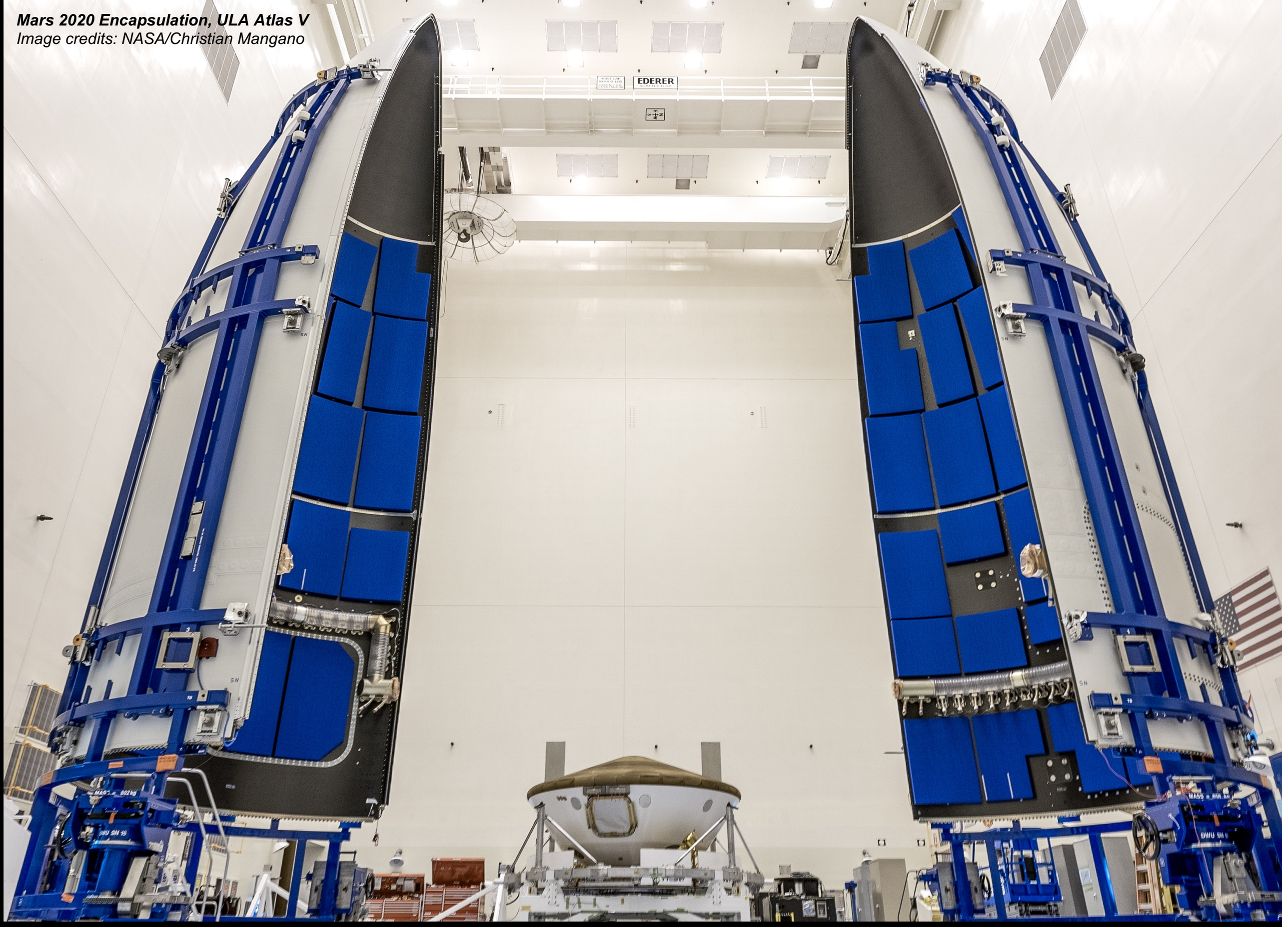

Mars 2020 Encapsulation, ULA Atlas V
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Modeling Particle and Spore Adhesion for Contamination Control and Planetary Protection Spacecraft Engineering Applications

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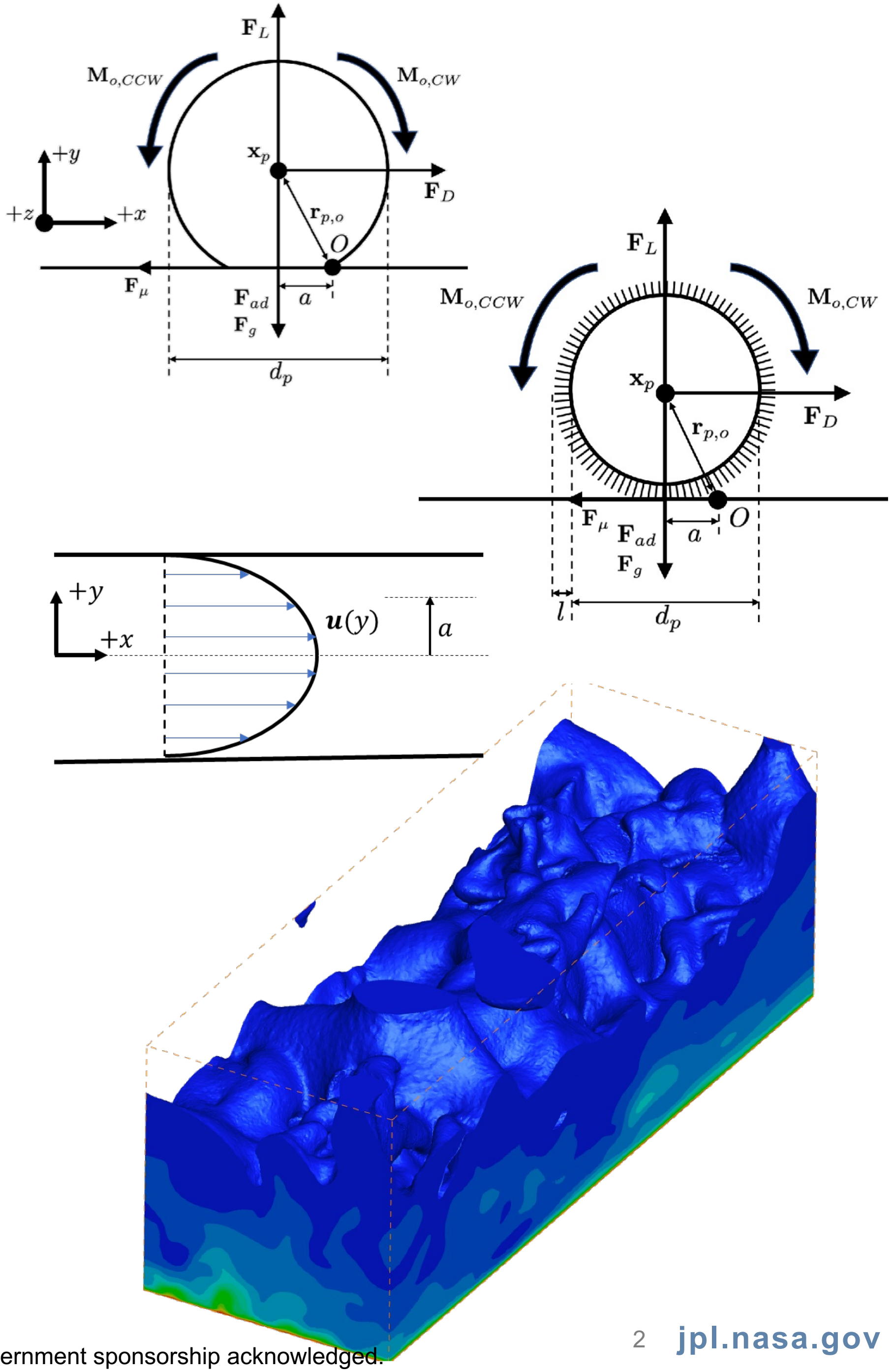
Outline:

- **Introduction**
    - Applications of particle redistribution
    - Existing methodologies – current assumptions for particle redistribution
- **Force modeling**
    - Relevant contribution typically modeled
    - Mechanisms for particle/spore removal
- **Validation work:**
    - Poiseuille Flow
    - Turbulent Boundary Layer
    - Spore Adhesion
- **Ongoing work**
    - Additional particle forces
    - Modeling improvements
    - Additional validation



Applications of particle redistribution

- **Rocket fairings quickly depressurize during launch ascent**: This generates a transient flows around the payload.

- Fairing and payload surfaces carry particulate and biological material. Depressurization-induced flows can:
  - ***Detach*** from fairing and payload surfaces,
  - ***Transport*** throughout the fairing environment, and
  - ***Redeposit*** onto other surfaces.

- Space exploration missions often have stringent Contamination Control (CC) and Planetary Protection (PP) requirements related to particulate deposition.
  - Contamination Control: Instrumentation and spacecraft hardware may be sensitive to the presence of particulate for proper operation (i.e. optical, thermal, and mechanical systems).
  - Planetary Protection: Biologics can redistribute onto the payload, which may risk forward contamination of the destination of interest impacting mission science objectives (i.e. biosignatures).

Applications of particle redistribution

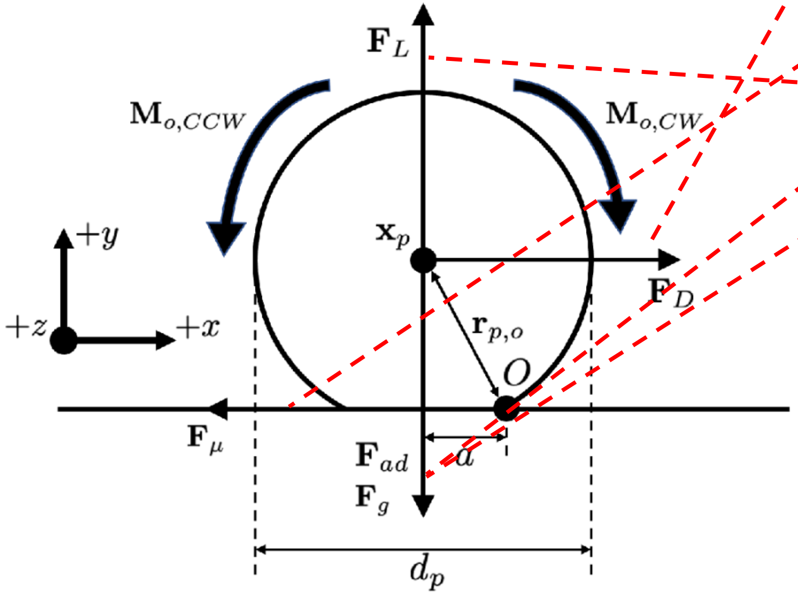
- **Rocket fairings quickly depressurize during launch ascent**: This generates a transient flows around the payload.
- Fairing and payload surfaces carry particulate and biological

- Existing methodologies assume particulate and/or biologic loading on all surfaces and stochastically redistribute them throughout the fairing.

- **<u>Physics based</u>** approaches are required to make predictions of particle and spore redistribution.

  to the presence of particulate for proper operation.
  - <u>Planetary Protection</u>: Biologics can redistribute onto the payload, which may risk forward contamination of the destination of interest, and may impact the ability to unambiguously detect biosignatures.

Traditional force modeling: Adhesion modeling



Experiments from Mikellides et al., 2020(a) (9) and simulations from from Mikellides et al., 2020(b) (10)

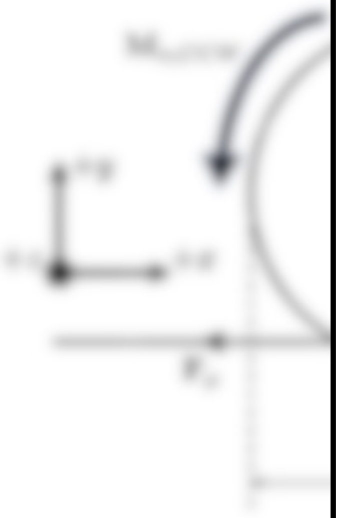
- Forces typically modeled (7-10)
  - Drag force: Variety of models exist to account for different regimes of flow (Stokes (3,11), Schiller-Naumann (11), Clift (11), White (12), Loth (13), etc.)
  - Friction force
  - Lift force
  - Gravitational force
  - Adhesion models (smooth surfaces) –
    - JKR Model (Johnson, Kendall, & Roberts; 1971) (14) – Larger particle adhesion
    - DMT Model (Derjaguin, Muller, Toporov; 1975) (15) – Smaller particle adhesion
    - Maugis Model (Maugis; 1992) (16) – Between small and large particulate, no closed form model.

Surface roughness can also have a significant effect on particle adhesion and resulting forces:

- ① Cheng et al.; 2002 (17)
- ② You & Wan; 2013 & 2014 (18,19) – Adhesion and capillary forces
- Rabinovitch; 2000 & 2002 (20,21) – Focus on capillary forces

Traditional force modeling: Adhesion modeling

- Forces typically modeled (7-10)
  - Drag force: Variety of models exist to account for different regimes of flow (Stokes (8,11), Schiller-Naumann (11), Clift (11), White (12), Loth (13), etc.)

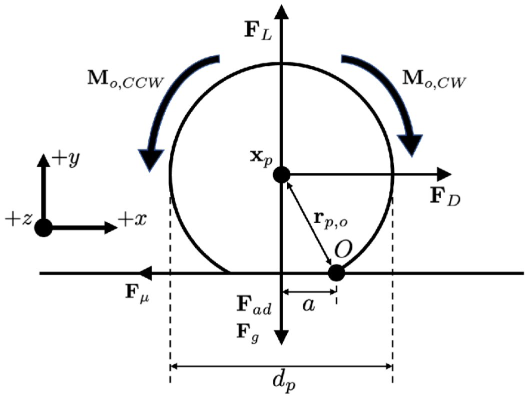


- Cheng-Ibrahim Model[8,17] →
  - Based on surface roughness theory, where one approximates the “fraction” of overlapping asperities through prior fits from Cheng (2002)[17].
- You and Wan Model[18,19] →
  - Directly model the variation in surface asperities as a convolution between two probability distributions, one for the particle surface and the other for the substrate.
- **Note**: Asperity being a rough element or protrusion on a surface and or particle.

  - Rabinovitch; 2000 & 2002 (20,21) – Focus on capillary forces

Traditional force modeling: Adhesion modeling

- Particles experience a wide range of forces from a surrounding flow (i.e. drag, unsteady effects, resolved pressure gradients, etc.) (5,6)
- Looking at literature we can simplify the forces being evaluated for a particle deposited on a surface. This results in a series of removal mechanisms. From Ibrahim et al.; 2003 & 2008 and Mikellides et al.; 2020: (7,8,10)



Experiments from Mikellides et al., 2020(a) (9) and simulations from from Mikellides et al., 2020(b) (10)

Forces of interest –

- F_D : Drag
- F_L : Lift
- F_F : Friction
- F_A : Adhesion
- F_G : Gravity

Removal Mechanisms –

- Aerodynamic Effects (Overcoming forces in y):

  ~~$F_L > F_A + F_G$~~

- Sliding (Overcoming friction):

  ~~$F_D \geq \mu_s(F_A + F_G - F_L)$~~

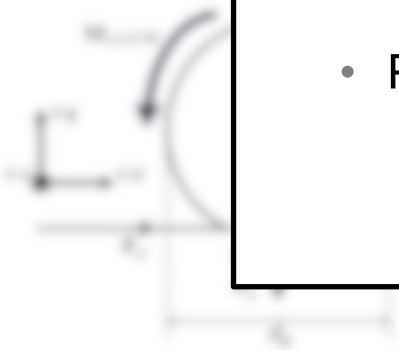
- Rolling (Moments about point 'o'):

  $M_o(F_D) \cancel{+ M_o(F_L}) > M_o(F_A) + M_o(F_G)$

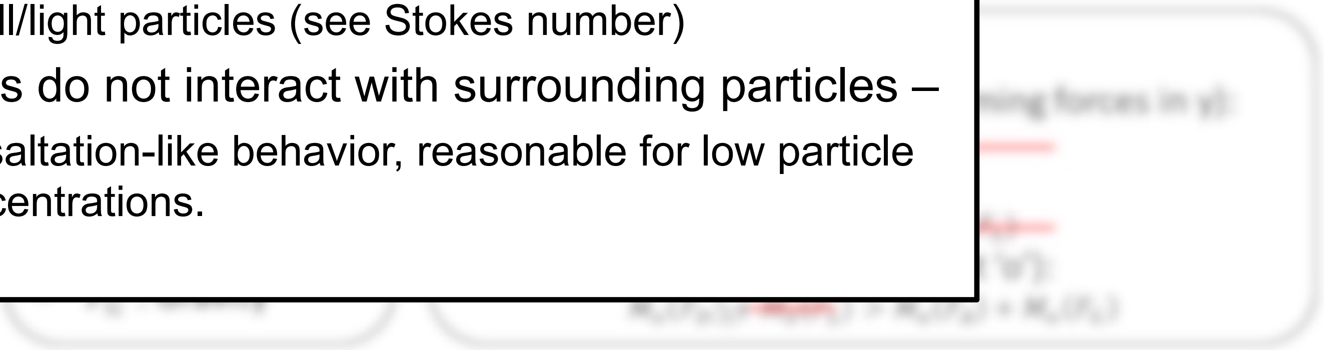
Traditional force modeling: Adhesion modeling

- Particles experience a wide range of forces from a surrounding flow (i.e. drag, unsteady effects, resolved pressure gradients, etc.) (5,6)

- **Assumptions** →
  - Spherical particles – Forcing models more mature
  - One-way coupling between particle and flow –
    - Flow only impacts particle, particle doesn't affect the surrounding flow
    - More reasonable for low particle concentrations and small/light particles (see Stokes number)
  - Particles do not interact with surrounding particles –
    - No saltation-like behavior, reasonable for low particle concentrations.



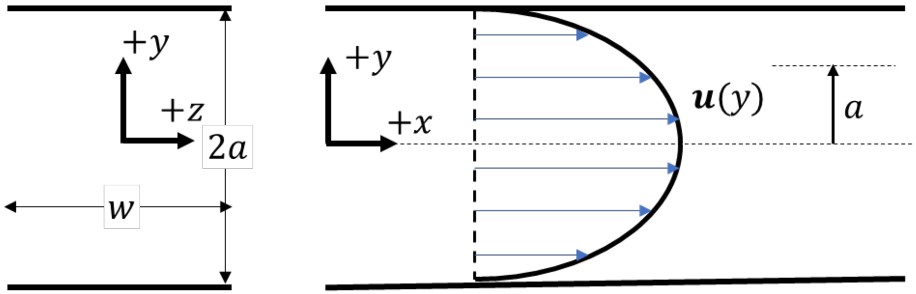
Experiments from Mikellides et al., 2020(a) (9) and simulations from from Mikellides et al., 2020(b) (10)

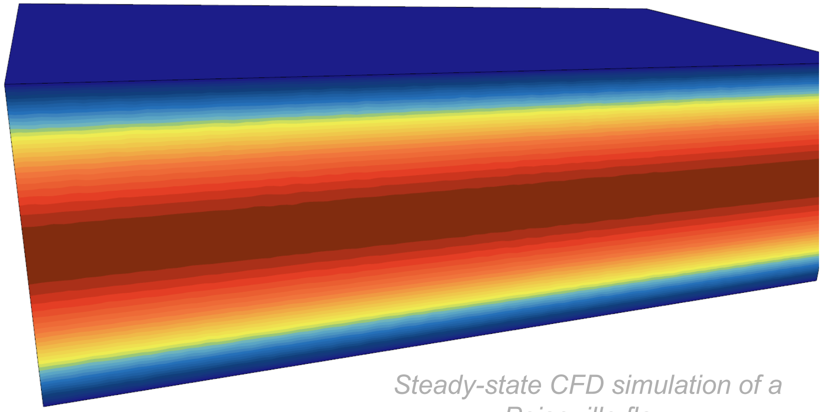


Model evaluation: Poiseuille flow

- Mikellides et al.; 2020(a) (9) describes experiments performed with a laminar flow device that evaluated the conditions by which particles were removed from a substrate of interest.

- The flow configuration described is known as a *Poiseuille flow,* which has a known flow solution for Navier-Stokes!

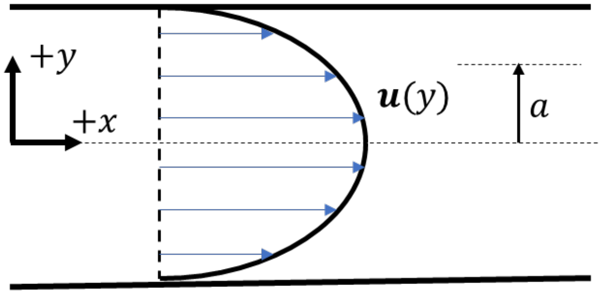




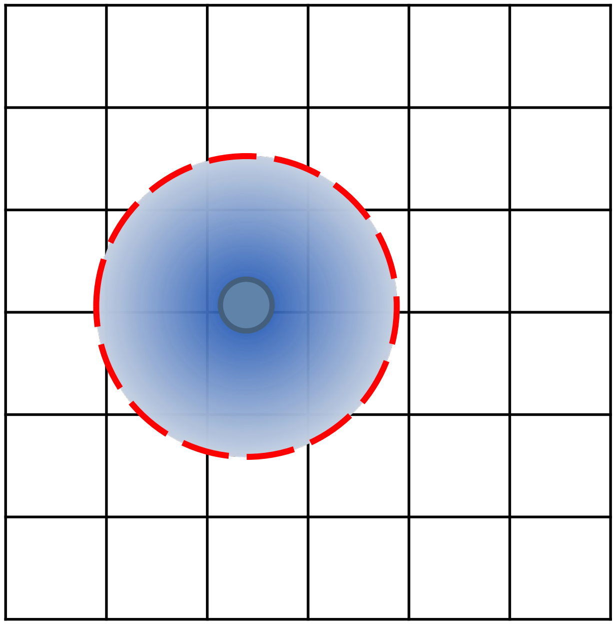
Steady-state CFD simulation of a Poiseuille flow

See fluid dynamics textbooks, such as Pozrikidis (2016) (22) for details on derivation and similar flow descriptions.

Model evaluation: Poiseuille flow

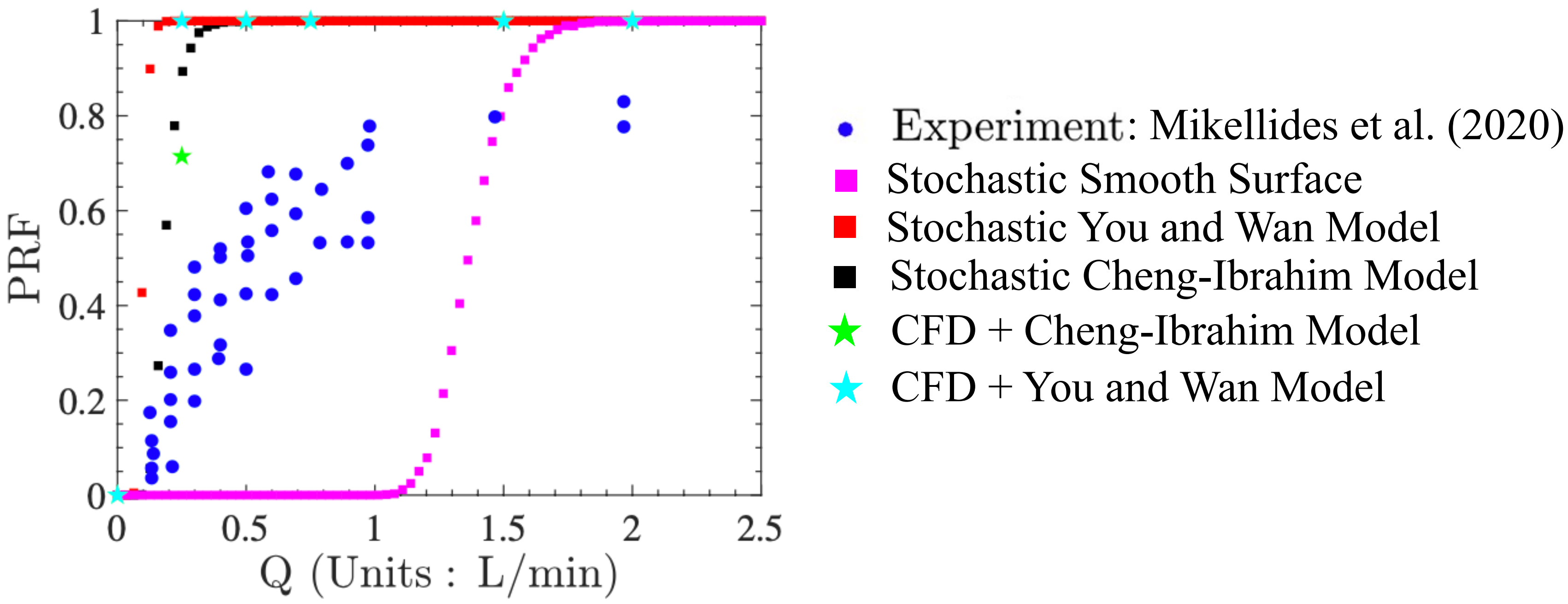


- Stochastic analysis (7,8,10)
  - Given flow/particulate parameters, stochastically sample particles to determine removal of particulate, given set of models.
- CFD based analysis (4,10)
  - Interpolation of information to particle is based on local sampling.
  - This evaluates the performance of the code when particles will have lots of information to sample from.



Experimental comparison: $\overline{d_p} = 70 \pm 5\ \mu m$

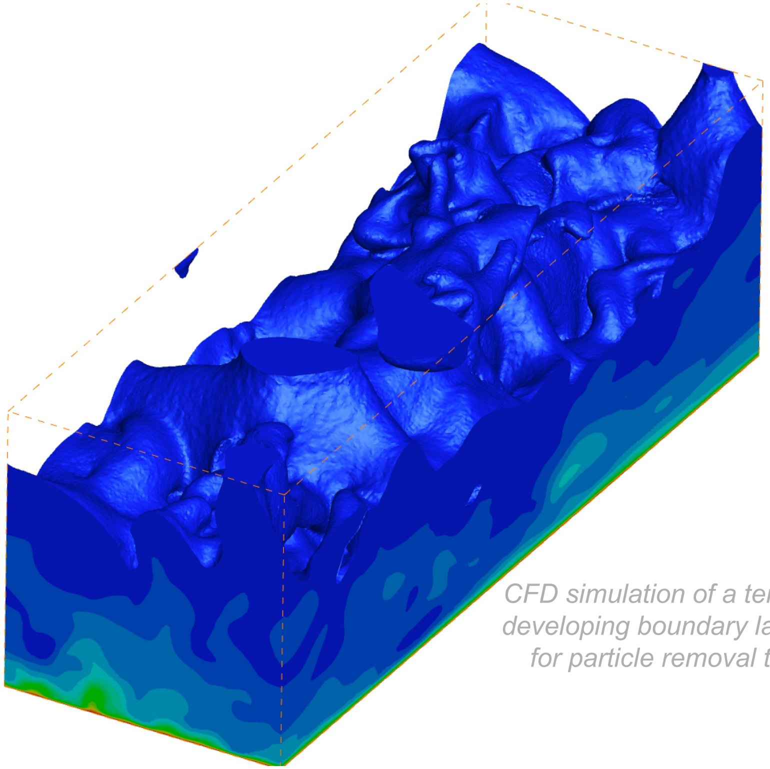
- Particles (with $\overline{d_p} = 70\mu m$ & $\sigma = 5\mu m$) are randomly sampled. Experimental data is from Mikellides et al.; 2020(a) (9).
- CFD performed with near wall grid refinement (prism layers) The following models are used for forcing:
  - Drag: Clift (11)
  - Adhesion: JKR (14)
  - Material properties: Glass spheres on glass substrate
- The particle removal fraction (PRF) is then evaluated for N_p = 5000 particles that are deposited onto the theoretical surface of interest:



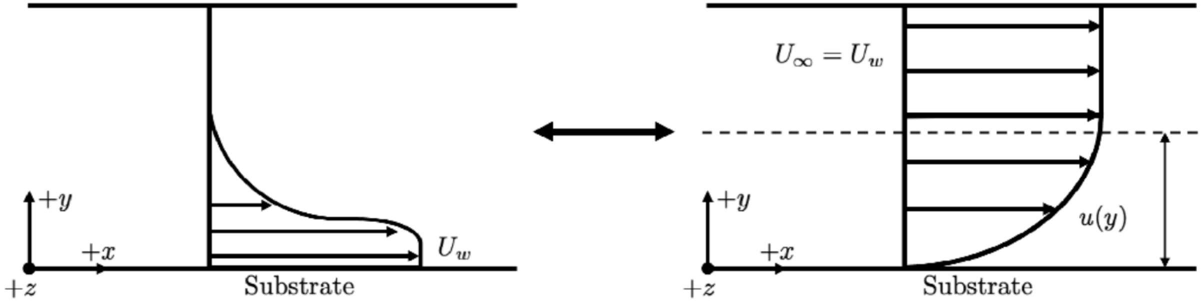
Model evaluation: Turbulent boundary layer

- Comparisons to experiments from Ibrahim et al. (2008)[8] where particles are removed from a substrate through a turbulent flow channel.

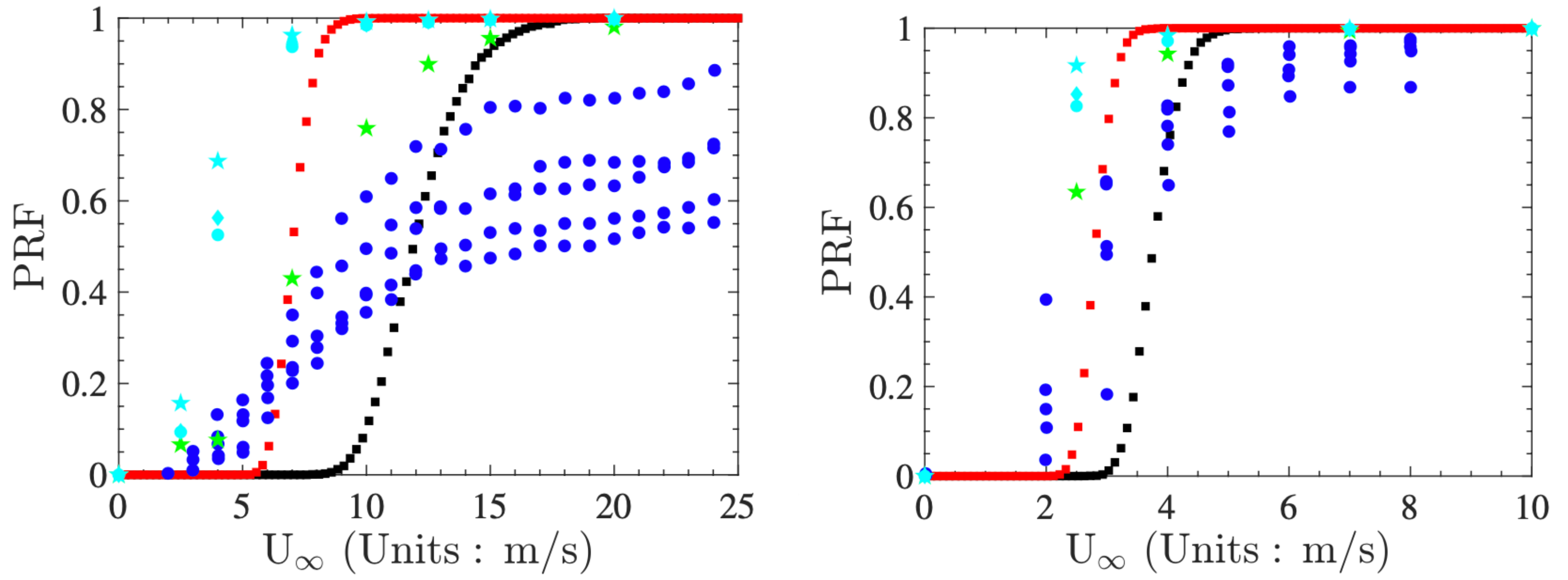
- Two comparisons →
  - Approximations of flow conditions from turbulent boundary layer theory.
  - CFD based on temporally developing boundary layer.



CFD simulation of a temporally-developing boundary layer used for particle removal testing.



Model evaluation: Turbulent boundary layer



$\overline{d}_p = 52.6\,\mu\text{m}$

$\overline{d}_p = 90.3\,\mu\text{m}$

- ● Experiment: Ibrahim et al. (2008)[8]
- ■ Stochastic You and Wan Model
- ■ Stochastic Cheng-Ibrahim Model
- ★ CFD + Cheng-Ibrahim Model
- ★ CFD + You and Wan Model

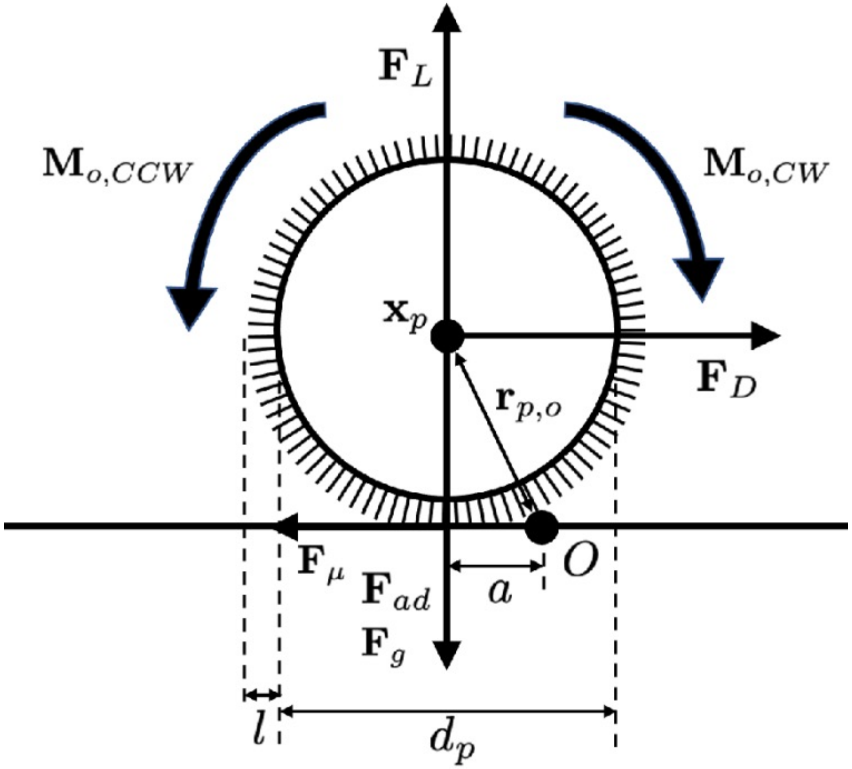
Sampling frequency variation of datasets:

- ★ $\Delta t = 0.1\ s$
- ◆ $\Delta t = 0.5\ s$
- ● $\Delta t = 1.0\ s$

Model evaluation: Spore adhesion

- Comparisons to experiments from Mercier-Bonin et al. (2011)[23] where spores are removed from a water driven shear flow (Poiseuille flow)

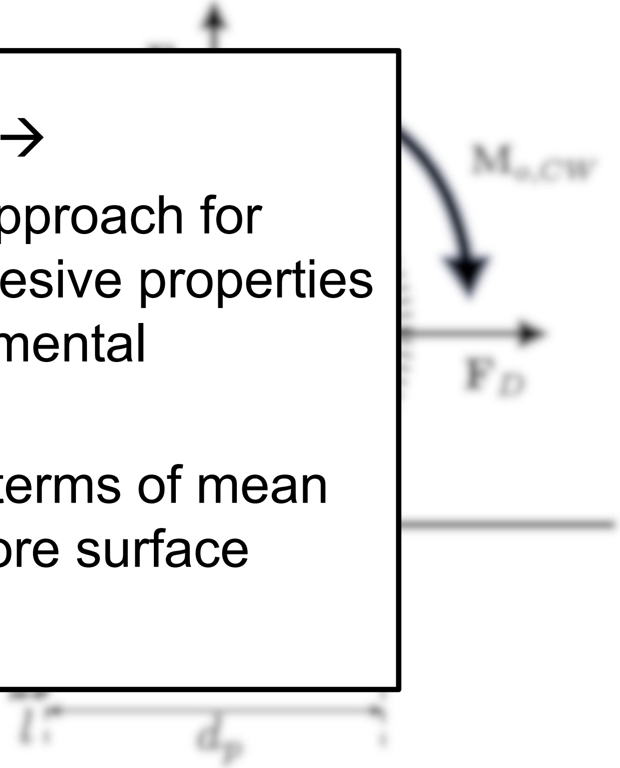
- Two spores for comparisons (against experiment and proposed model) →
  - *Bacillus cereus*
  - *Bacillus pumilus*



Note: Spore species impacts adhesion (shape, size, hair-like structures, behavior in different environments, etc.)

Model evaluation: Spore adhesion

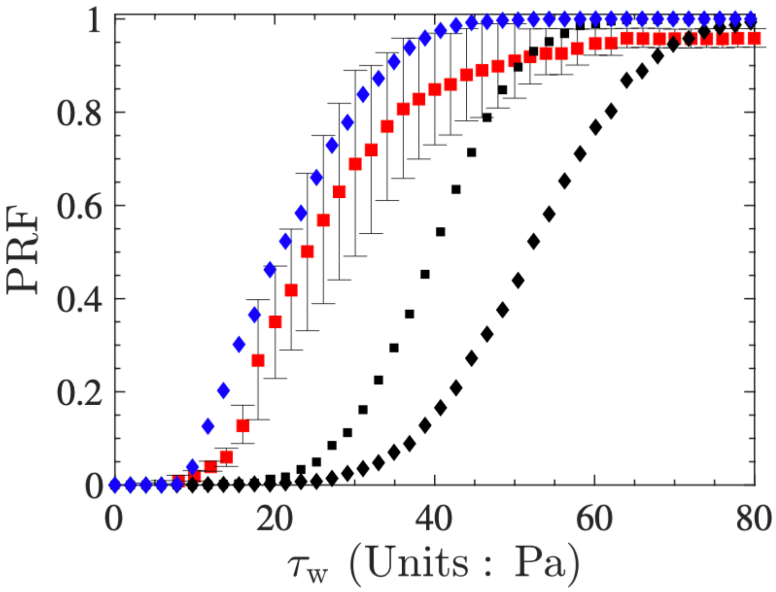
- Comparisons to experiments from Mercier-Bonin et al. (2011)[23] where spores are removed shear flo
- Two spo (against propose
  - *Bacil*
  - *Bacil*



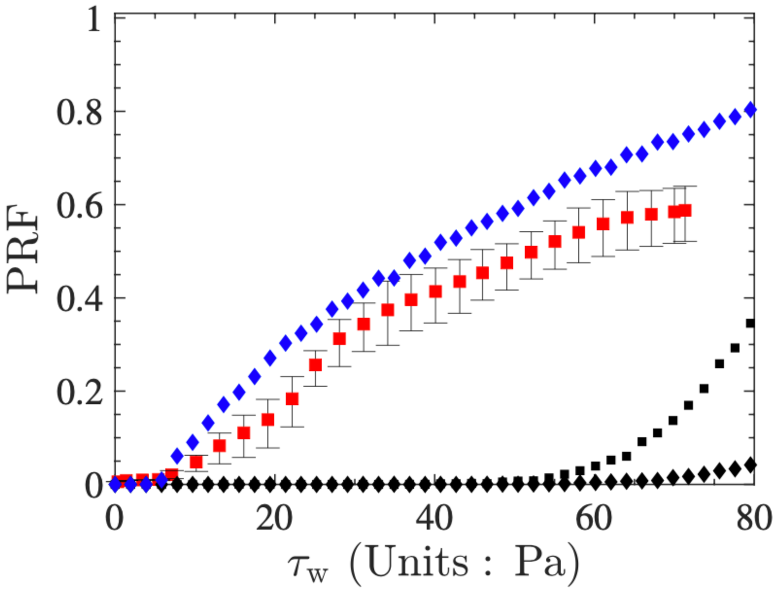
- **<u>Proposed modeling approach</u>** →
  - Apply a contact mechanics approach for adhesion → biochemical adhesive properties are highly spore and environmental dependent
  - Fit the contact mechanics in terms of mean and standard deviation of spore surface energy

<u>Note</u>: Spore species impacts adhesion (shape, size, hair-like structures, behavior in different environments, etc.)

Model evaluation: Spore adhesion



Bacillus cereus



Bacillus pumilus

- 🟥 Experiment: Mercier-Bonin et al. (2011)[23]
- 🔷 Stochastic: Surface energy fit, You and Wan Model
- ■ Stochastic: Mercier-Bonin slip model
- ◆ Stochastic: Mercier-Bonin rolling model

Conclusions

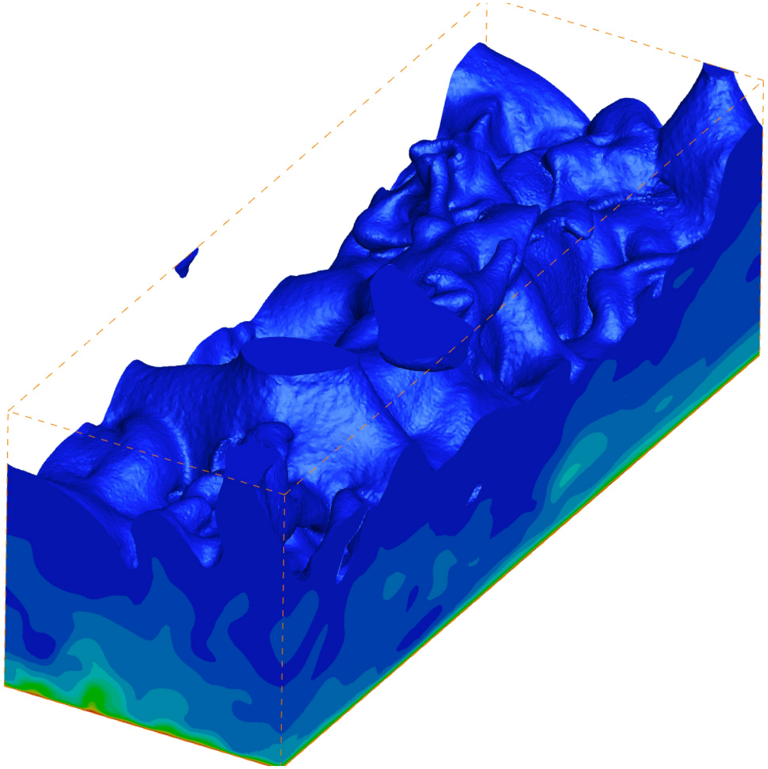
- **General overview; importance of particle adhesion and removal modeling:**
  - Applicable to Planetary Protection and Contamination Control
  - Provided brief overview of general force decompositions for Lagrangian particle tracking and adhesion/removal modeling
  - Discussion on model selection for adhesion and removal analysis

- **Models are highly sensitive to material property variation (i.e. surface roughness, Young's modulus, Poisson's ratio, surface energy)**

- **Showed the ability to simulate particle removal with surface adhesion:**
  - Demonstrated for different flow conditions
  - Demonstrated the ability to capture particle removal with adhesion modeling routines
  - Potential modeling procedure to capture arbitrary spore species adhesion forces

Future work

- **Additional validation:**
  - Other characteristic/canonical flows
  - Expand evaluation of spore removal from surface
- **Force modeling:**
  - Vibrational motion of particulate on surfaces
  - Additional models to improve transport estimations
  - Probabilistic particle removal – The surface energy of particles and substrates isn't always constant
- **Improvements to modeling can be made:**
  - More spore data for shear-based removal
  - Data for particle removal with atomic force microscopy (AFM) does exist; however, should be expanded to improve modeling capabilities
  - Temperature dependence
  - Material property information
    - Density, Young's modulus, modulus of elasticity, etc.



CFD simulation of a temporally-developing boundary layer used for particle removal testing.

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Traditional force modeling: Lagrangian representation

- The force on a Lagrangian particle is characterized by the integration of resolved stresses along the surface of a particle:

$$F = \int_S (-p\mathrm{I} \ + \sigma) dS$$

- Traditional definitions, such as the BBO and Maxey-Riley equations, were derived from phenomenological and disturbed versus undisturbed flow arguments respectively.

- These forcing definitions typically assume low Reynolds number creeping flow; however, provide insight into the forces that arise when considering flow over a particle.

- Transport equations for the i-th Lagrangian particle (excluding heat exchange):

$$\frac{d\boldsymbol{x}_p^{(i)}}{dt} = \boldsymbol{v}_p^{(i)}$$

$$m_p^{(i)} \frac{d\boldsymbol{v}_p^{(i)}}{dt} = \mathbf{F}_{resolved}^{(i)} + \ \mathbf{F}_{drag}^{(i)} + \mathbf{F}_{vu}^{(i)} + \mathbf{F}_{iu}^{(i)} + \mathbf{F}_{body}^{(i)} + \mathbf{F}_{lift}^{(i)} + \ \mathbf{F}_{coll}^{(i)}$$

$$I_p \frac{d\omega_p^{(i)}}{dt} = \sum_j \frac{d_p}{2} \boldsymbol{n}_{ij} \times f_{t,j\to i}^{col}$$

  - $\boldsymbol{x}_p^{(i)}, \boldsymbol{v}_p^{(i)}$, and $\omega_p^{(i)}$ are the position velocity and angular velocity respectively
  - I_p is the moment of inertia for a sphere $I_p = m_p d_p^2$
  - $\boldsymbol{n}_{ij}$ is the outward facing normal between particle i to particle j (or in this case wall j)
  - $f_{t,j\to i}^{col}$ is the tangential component of collisions between particle i and object j

Traditional force modeling: Lagrangian representation

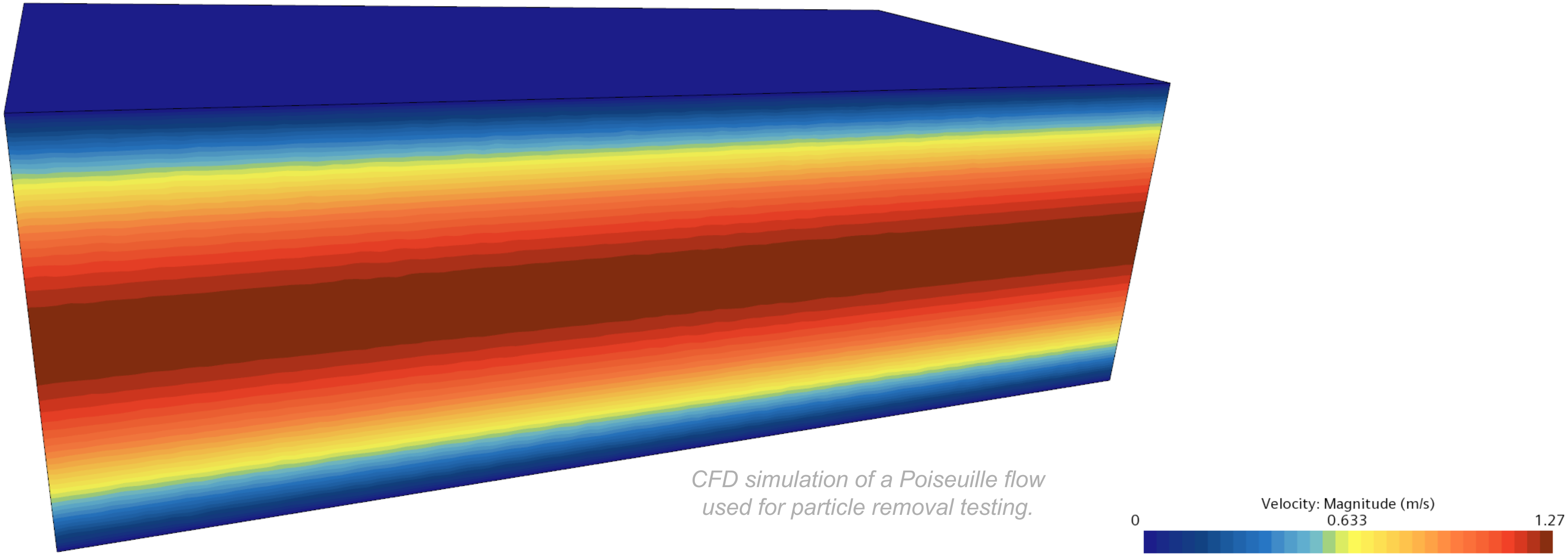
- The force on a Lagrangian particle is characterized by the integration of resolved stresses along the surface of a particle:

$$F = \int_S (-p\mathrm{I} \; + \sigma) dS$$

- Traditional definitions typically assume low Reynolds number creeping flow; however, provide insight into the forces that arise when considering flow over a particle: (2,3,5,6)
  - Resolved Forces – Viscous and pressure forces that arrive from the total stress tensor.
  - Aerodynamic Drag – Opposition of motion due to relative flow.
  - Viscous Unsteady – Basset history effect associated with boundary layer formation.
  - Inviscid Unsteady – Added mass due to displacement of “fluid.”
  - Lift - Shear or rotational induced.
  - Body Forces - External forces (i.e. gravity, electromagnetic, etc.)

Example: Poiseuille flow

- CFD simulations performed using commercial software (StarCCM+)
- Boundary conditions:
  - No-slip walls on top and bottom of domain
  - Periodic in streamwise direction
  - Cross stream boundaries are symmetry planes (no variation expected in cross-stream direction)
- Particle tracking is performed with an in-house one-way coupled Lagrangian particle tracking code (JPL SPLAT)



CFD simulation of a Poiseuille flow used for particle removal testing.

Existing methods predict particle redistribution

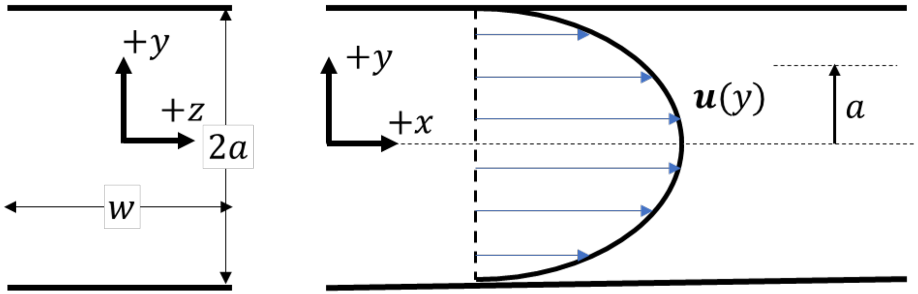
- Stochastic redistribution approach: Assume particulate and/or biologic loading on all surfaces and stochastically redistribute them throughout the fairing.(1)
  - Pros:
    - Well established
    - Easy to implement
    - Quick time to solution
  - Cons:
    - Errors for distribution of particulate
    - Does not represent reality
    - Cannot capture local concentrations of particles

- Physics approach: Calculate the force on every particle (2,3) and track trajectories during fairing redistribution process.(4)
  - Pros:
    - Removal is based on first principles (not all particles detach from surfaces)
    - Provides high fidelity data on classes of particles and their final locations
  - Cons:
    - Geometry dependent (no two missions are the same)
    - Can be computationally expensive

Model evaluation: Poiseuille flow

- Mikellides et al.; 2020(a) (9) describes experiments performed with a laminar flow device that evaluated the conditions by which particles were removed from a substrate of interest.

- The flow configuration described is known as a *Poiseuille flow,* which has an analytic flow solution! After manipulating the Navier—Stokes equations a bit, we get the following…



$$u(y) = \frac{(y^2 - a^2)}{2\,\mu}\frac{dP}{dx}$$

$$\tau = \mu\frac{du}{dy} = y\frac{dP}{dx}$$

$$\tau_{wall} = a\frac{dP}{dx}$$

$$Q = \frac{2wa}{3\mu}\frac{dP}{dx}$$

Variables -
- u: velocity
- μ: Dynamic viscosity
- P: Pressure
- Q: Volumetric flow rate
- τ: Shear stress

Assumptions –
- Flow is laminar (not turbulent)
- $\frac{dP}{dx}$ = Constant
- No-slip/no-penetration velocity condition at wall

See fluid dynamics textbooks, such as Pozrikidis (2016) (22) for details on derivation and similar flow descriptions.

Flow field comparison: Poiseuille flow (y vs. u)

- Flow field comparisons between analytic and CFD results (wall refinement)
- Low amount of error between the two plots