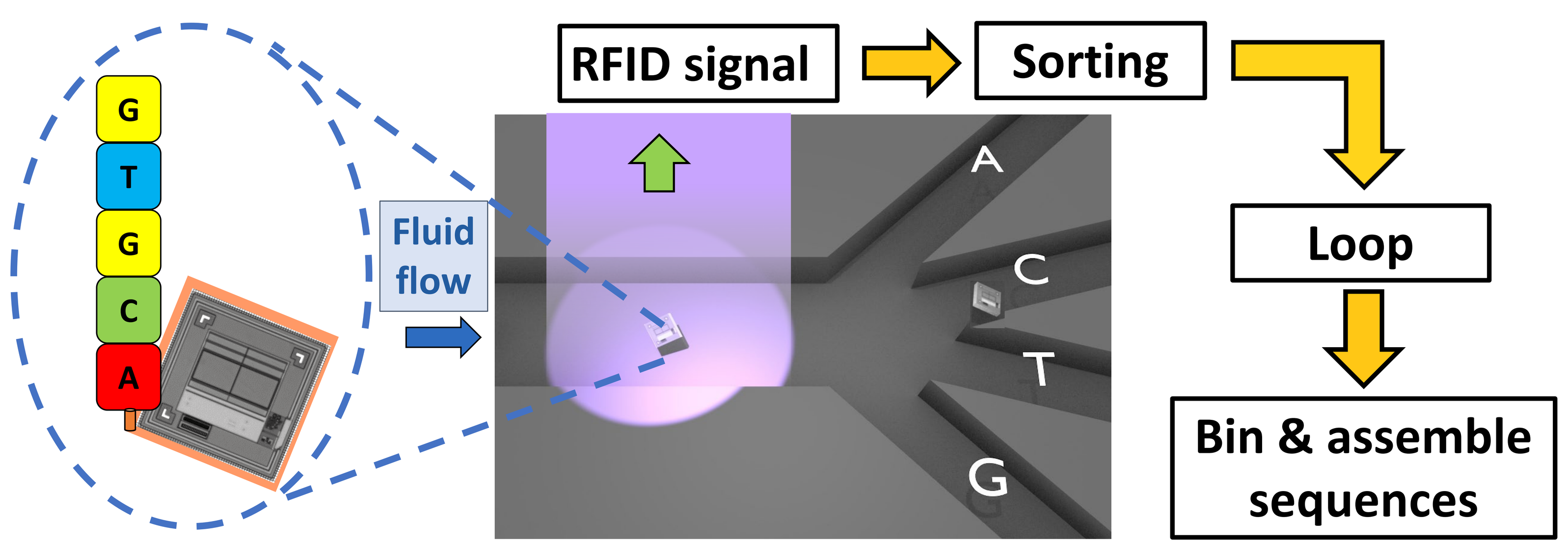
Development of a High-Throughput DNA Synthesizer: Predicting Motion of p-Chip Microtransponders in Fluid Flow

Raymond K. Yeung[1], Madeleine Chen[1], William Grover[1], Victor G. J. Rodgers[1], Philip Brisk[2]
[1]Department of Bioengineering, University of California, Riverside
[2]Department of Computer Science and Engineering, University of California, Riverside

Objective

- Towards the development of a high-throughput DNA synthesizer, we perform computational fluid dynamic (CFD) simulations to predict the trajectories of p-Chips in fluid flow and evaluate the interparticle spacings to achieve axially ordered trains of p-Chips.



- Point mass particle tracing methods disregard the particle orientation in calculating volume forces exerted on fluid elements and cannot accurately model particle-wall interactions [1-3].
- In this study, we investigate the transport of fluid-immersed, flat, rectangular solid particles in microchannels using a finite element CFD model of two-way coupled fluid-structure interaction that takes into account solid bodies using COMSOL.

COMSOL Fluid-Structure Interaction

- COMSOL Fluid-Structure Interaction (FSI) provides a direct numerical simulation that couples fluid flow and solid mechanics.

Laminar Fluid Flow

$$\rho_f \frac{\partial \overline{v_f}}{\partial t} + \rho_f \overline{v_f}\cdot\nabla\overline{v_f} = -\nabla p + \mu_f \nabla^2 \overline{v_f} \underbrace{-12\frac{\mu \overline{v_f}}{H^2}}_{\text{shallow channel approximation}} + \overline{F_f}$$

$$\nabla\cdot\overline{v_f} = 0 \qquad H: \text{channel height}$$

Solid Mechanics

$$\nabla\cdot\overline{\overline{\sigma_s}} + \overline{F_s} = \rho_s \frac{\partial^2 \overline{u_s}}{\partial^2 t}$$

$$\overline{\overline{\varepsilon_s}} = \frac{1}{2}\left[\left(\nabla\overline{u_s}\right)^T + \nabla\overline{u_s} + \left(\nabla\overline{u_s}\right)^T\left(\nabla\overline{u_s}\right)\right]$$

$$\overline{\overline{\sigma_s}} = C\overline{\overline{\varepsilon_s}}$$

$\overline{\overline{\sigma_s}}$: Cauchy stress tensor
$\overline{\overline{\varepsilon_s}}$: strain tensor
C: stiffness matrix

Fluid-Structure Interaction

$$\overline{f_s} = -\overline{n}\cdot\left[-p_f\overline{\overline{I}} + \mu_f\left(\nabla\overline{v_f} + \left(\nabla\overline{v_f}\right)^T\right)\right]$$

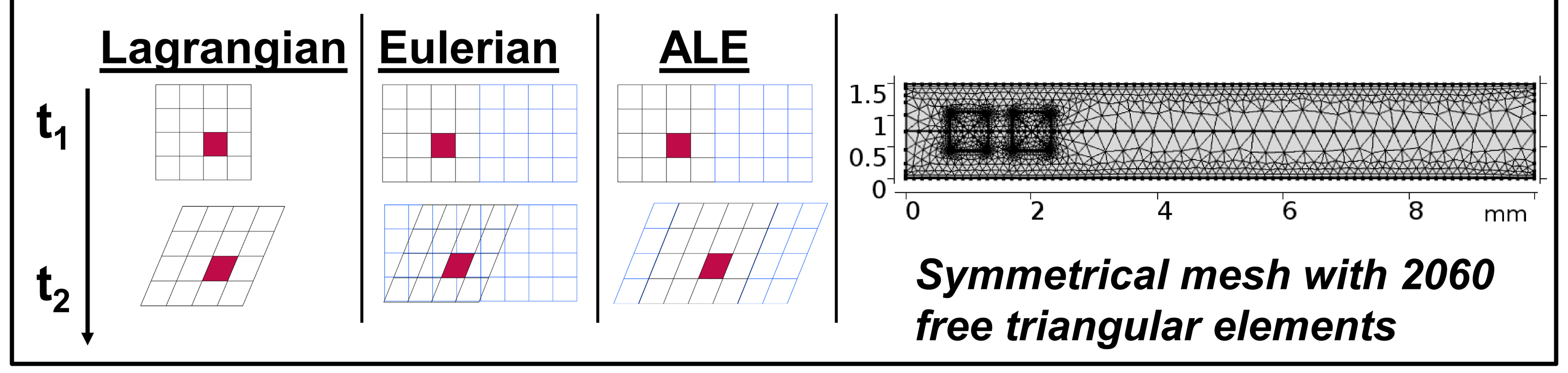
$$\overline{v_s} = \frac{\partial \overline{u_s}}{\partial t}, \quad \overline{v_f} = \overline{v_s}$$

$$\overline{F_s} = \overline{f_s}\frac{dv}{dV}$$

f_s = fluid load exerted on solid boundary
F_s = force on solid
dv = mesh element scale factor for spatial frame
dV = mesh element scale factor for material frame

Arbitrary Lagrangian Eulerian (ALE) Framework

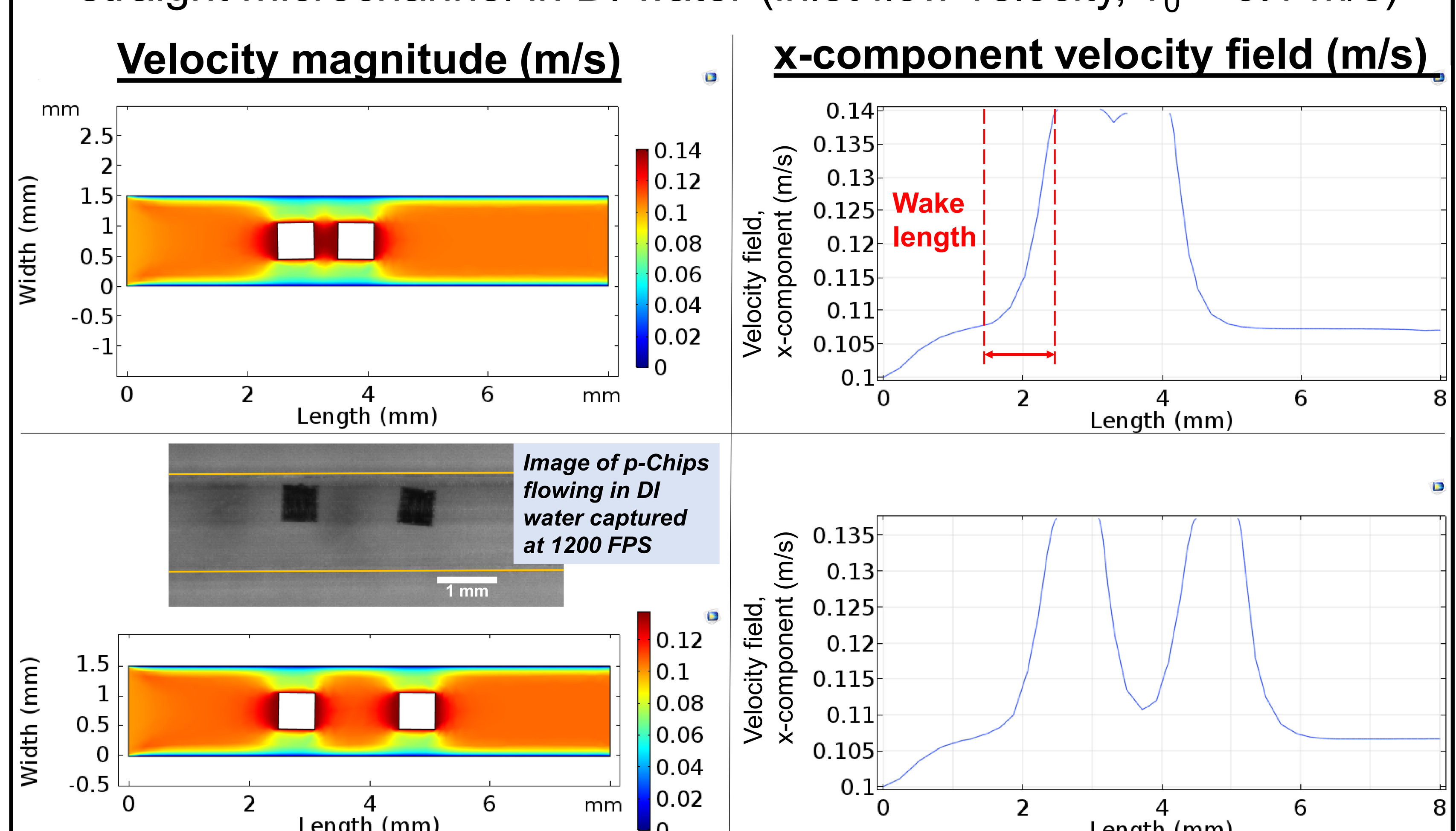
- ALE solves the set of Navier-Stokes and structural mechanics equations in a mesh frame with mathematical mapping to the spatial and material frames. The ALE mesh is automatically remeshed based on an established distortion expression.



Symmetrical mesh with 2060 free triangular elements

Effect of Particle Reynolds Number on Wake Length

- Channel dimensions: 1.5 mm width, 10 mm length, 0.2 mm height
- A 2-D FSI mesh independence study was performed for maximum mesh element sizes from 0.33 mm to 0.0525 mm. The evaluated numerical precision of the interparticle spacing and the rotation angle were 10^{-4} mm and 0.43 degrees, respectively.
- 2-D FSI studies were performed for square, micron-sized particles (diagonal length, D = 0.85 mm; sphericity: 0.55) flowing through a straight microchannel in DI water (inlet flow velocity, v_0 = 0.1 m/s)

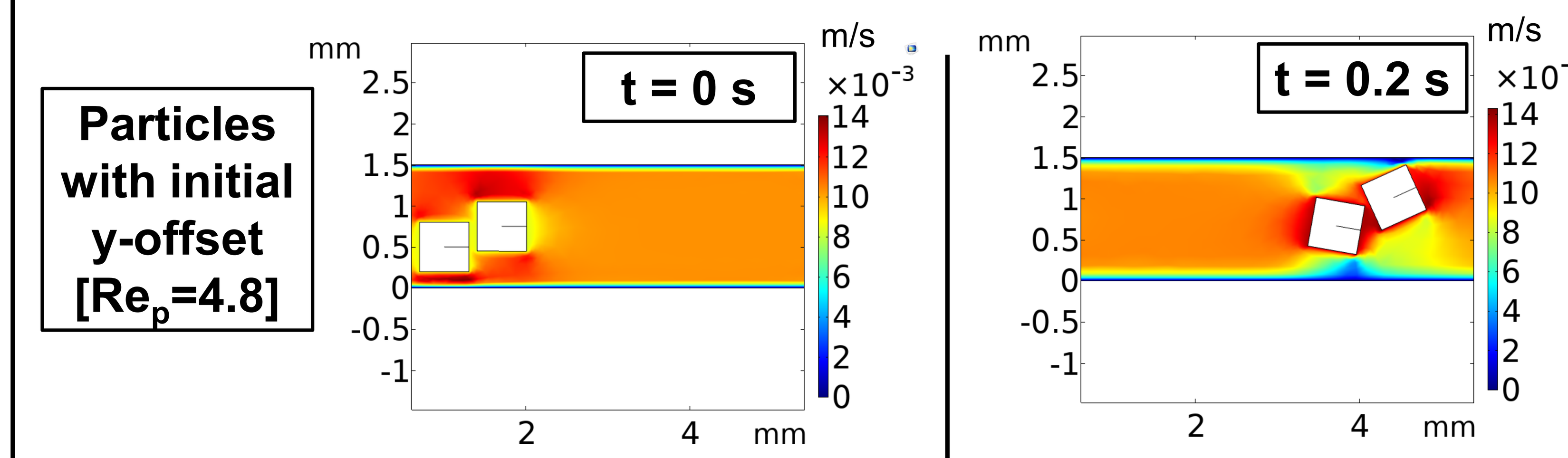


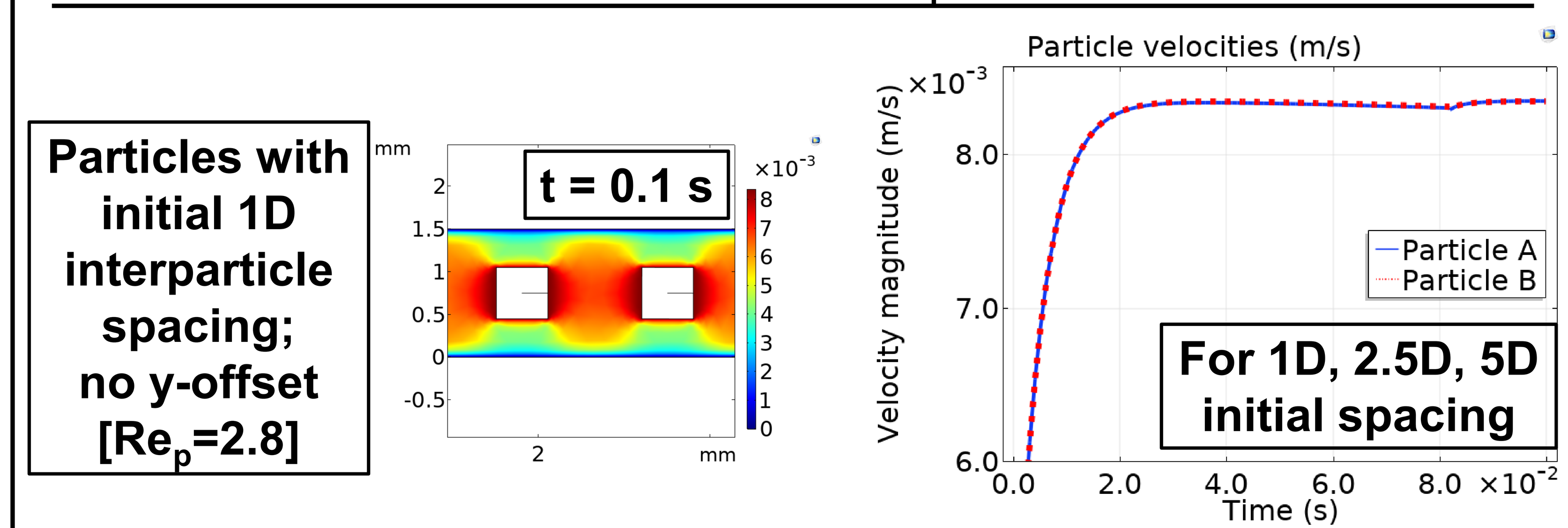
Effect of Particle Reynolds Number (Re_p) on Wake Length

Initial longitudinal interparticle spacing (mm)	Max. mesh element size (mm)	Inlet flow velocity (m/s)	Re_y	Re_c	Re_p	Wake Length (D)	Preferred axial spacing (D) of spherical particles at Re_p=5.6 [4]
2.0	0.33	0.01	15	3.5	4.8	1.8D	2.5D – 5D
		0.05	75	17.6	24	2.0D	
		0.10	150	35.2	48	2.5D	

Fluid-Particle, Particle-Particle Interactions

- Particle trajectories were evaluated for two square particles flowing through the microfluidic channel.





Discussion and Future Work

- The numerical simulations suggest the wake-influenced region of the trailing p-Chip is longer at higher Re_p.
- 2-D FSI studies at Re_p=2.8 indicate that changes in particle velocities are minimal at initial interparticle spacing values of 1D and greater. This suggests that for our application, highly ordered trains of rapidly flowing p-Chips may be achieved.
- The particle trajectories observed experimentally will be analyzed using a NI cRIO controller with LabVIEW and compared to predicted particle trajectories from numerical simulations.
- Two-way CFD-DEM coupling with COMSOL and LIGGGHTS as well as ANSYS Fluent and ROCKY DEM will be performed to evaluate contact forces during particle-particle and particle-wall interactions.

Acknowledgments

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References

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