Simulation and modeling of particle-laden compressible flows

Archana Sridhar*, Mehdi Khalloufi+ and Jesse Capecelatro+,*

*Department of Aerospace Engineering | +Department of Mechanical Engineering, The University of Michigan

Motivation

Disperse two-phase compressible flows are observed in many natural and engineering applications. Interactions between turbulence, shock waves, and particles present many challenges in understanding and modeling these systems.

Figure 1: Examples of particle-laden compressible flows. Top-left: Coal-dust explosions; Top-right: Shock-wave lithotripsy used for treating kidney stones; Bottom-left: Plume-surface interactions during planetary landing; Bottom-right: Detonation waves.

Key challenges

Significant progress has been made towards understanding and modeling turbulent particle-laden flows in the *incompressible* regime. Much less attention has been paid to particle-laden *compressible flows*. Key modeling challenges include:

- **Large number of interacting particles**
- **Wide range of length- and time-scales**
- **Strong two-way coupling**

Particle-resolved numerical simulations represent the most comprehensive approach to capture these interactions as all of the sub-grid scale dynamics are resolved, but are intractable due to the computational cost. Volume-filtering the governing equations enables simulations at larger scales but results in many unclosed terms, primarily drag and pseudo-turbulent kinetic energy (PTKE) [1]. We present a mathematical framework for compressible gas-particle flows and propose consistent closure models.

Numerics

Particle-resolved numerical simulations are used to guide the development of subgrid-scale models.

- Viscous compressible Navier–Stokes discretized using narrow-stencil finite difference that satisfy summation-by-parts (6^{th}-order interior, 3^{rd}-order at boundaries)
- Simultaneous approximation term (SAT) boundary treatment for energy stability
- Skew-symmetric-type splitting of convective fluxes for kinetic energy preservation
- Localized artificial diffusivity for shock capturing
- Ghost-point immersed boundary method to enforce boundary conditions at particle surface

Homogeneous suspension

Figure 2 shows a simulation of a homogeneous fully-developed flow past a suspension of particles with Reynolds number $\mathrm{Re} = 300$, volume fraction $\phi = 0.1$, and Mach number $\mathrm{Ma} = 0.8$. Particles create a nozzling effect that accelerates the gas to supersonic velocities resulting in multiple shocklets. These simulations are used to inform new drag models.

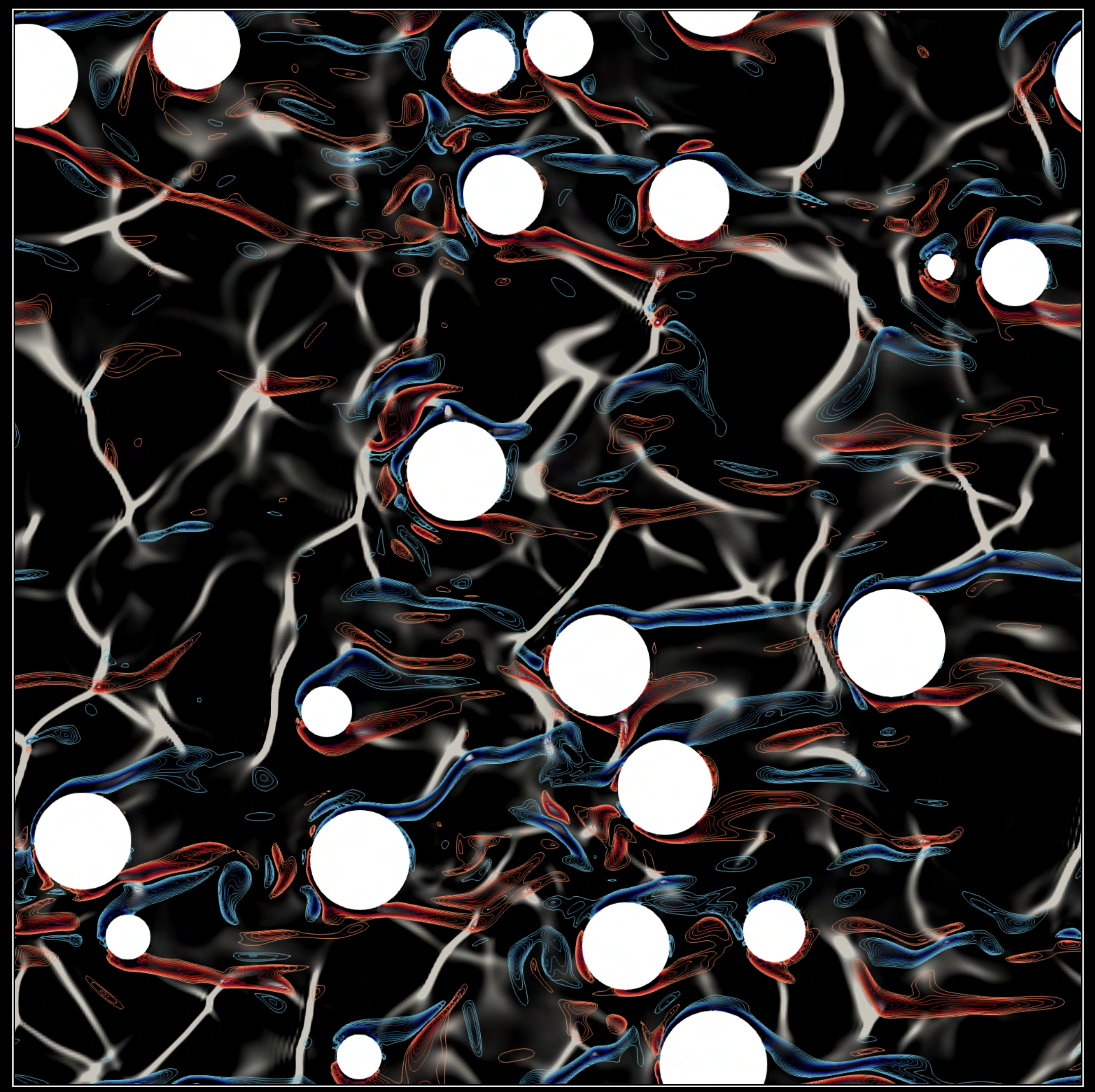
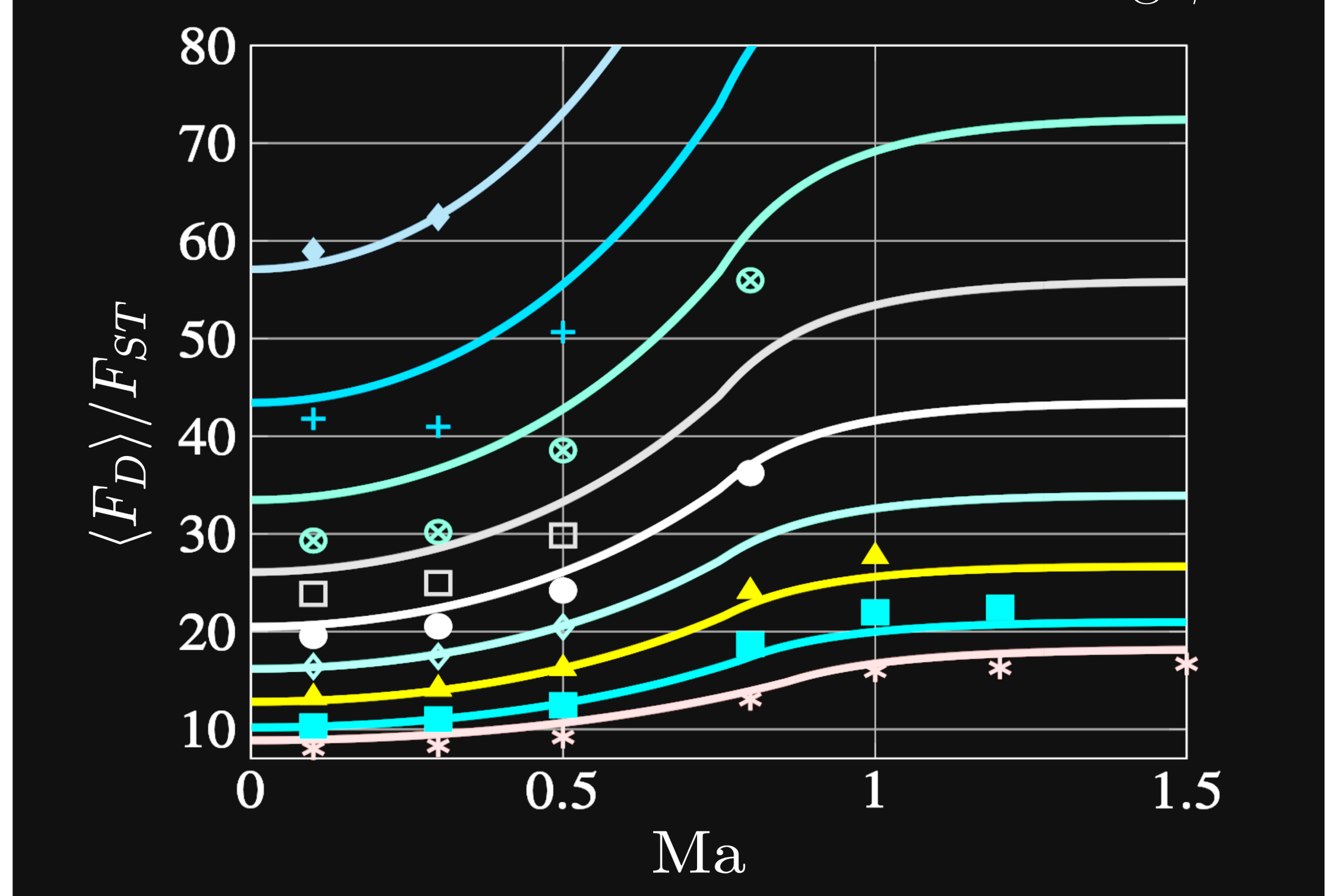


Figure 2: Compressible flow past a random assembly of fixed spheres showing a 2-D cross-section of the 3-D flow. Dilatation (black/white), vorticity (red: positive, blue: negative).

New drag correlation

The drag force in the suspension (normalized by Stokes drag) is shown in the figure below as a function of Ma and ϕ. Compressibility effects are observed to occur at lower Ma with increasing ϕ.

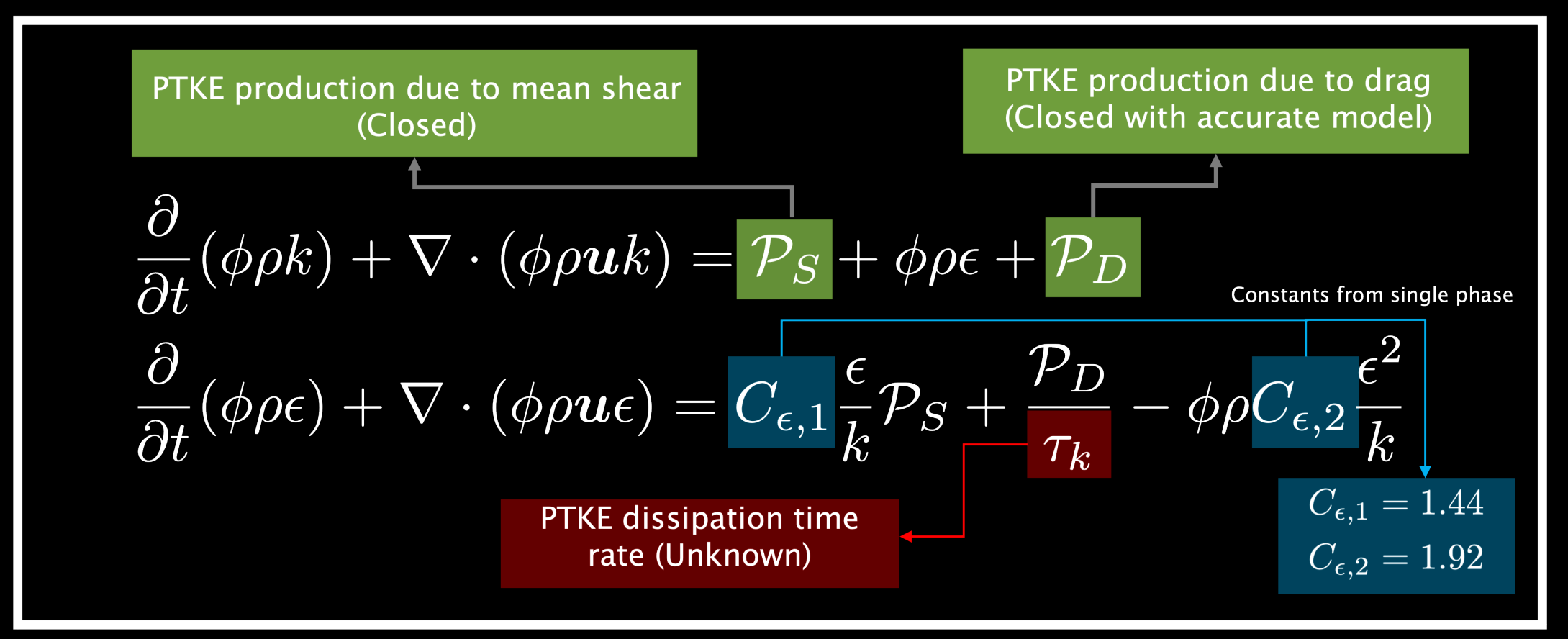


A new drag model was developed based on an effective Mach number (Ma^*) to capture these effects. The single particle drag correlation C_D^{iso} from [2] is augmented with the volume fraction correction $f(\phi)$ from [3] according to:

$$C_D(\mathrm{Re}, \mathrm{Ma}^*, \phi) = C_D^{iso}(\mathrm{Re}, \mathrm{Ma}^*) f(\phi)$$
$$\frac{\mathrm{Ma}^*}{\mathrm{Ma}} = 1 + \alpha(1 - e^{-\beta\phi}). \qquad (1)$$

Pseudo turbulence

Gas-phase velocity fluctuations induced by particles are termed PTKE. A two-equation model is proposed transporting $k = \widetilde{\boldsymbol{u}'' \cdot \boldsymbol{u}''}/2$ and its dissipation ϵ. Particle-resolved simulation are used to inform closure of the terms appearing below:



PTKE production due to mean shear (Closed)

PTKE production due to drag (Closed with accurate model)

$$\frac{\partial}{\partial t}(\phi\rho k) + \nabla\cdot(\phi\rho\boldsymbol{u}k) = \mathcal{P}_S + \phi\rho\epsilon + \mathcal{P}_D$$

Constants from single phase

$$\frac{\partial}{\partial t}(\phi\rho\epsilon) + \nabla\cdot(\phi\rho\boldsymbol{u}\epsilon) = C_{\epsilon,1}\frac{\epsilon}{k}\mathcal{P}_S + \frac{\mathcal{P}_D}{\tau_k} - \phi\rho C_{\epsilon,2}\frac{\epsilon^2}{k}$$

PTKE dissipation time rate (Unknown)

$C_{\epsilon,1} = 1.44$
$C_{\epsilon,2} = 1.92$

Figure 3 shows the flow physics associated with shock-particle interactions. Non-trivial hydrodynamic interactions result in size segregation with smaller particles moving further downstream.

References

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[2] N. Singh, M. Kroells, C. Li, E. Ching, M. Ihme, C. J. Hogan, and T. E. Schwartzentruber. General Drag Coefficient for Flow over Spherical Particles. *AIAA Journal*, 60(2):587–597, 2022.

[3] A. S. Sangani, D. Z. Zhang, and A. Prosperetti. The added mass, Basset, and viscous drag coefficients in nondilute bubbly liquids undergoing small-amplitude oscillatory motion, 1991.

Acknowledgements

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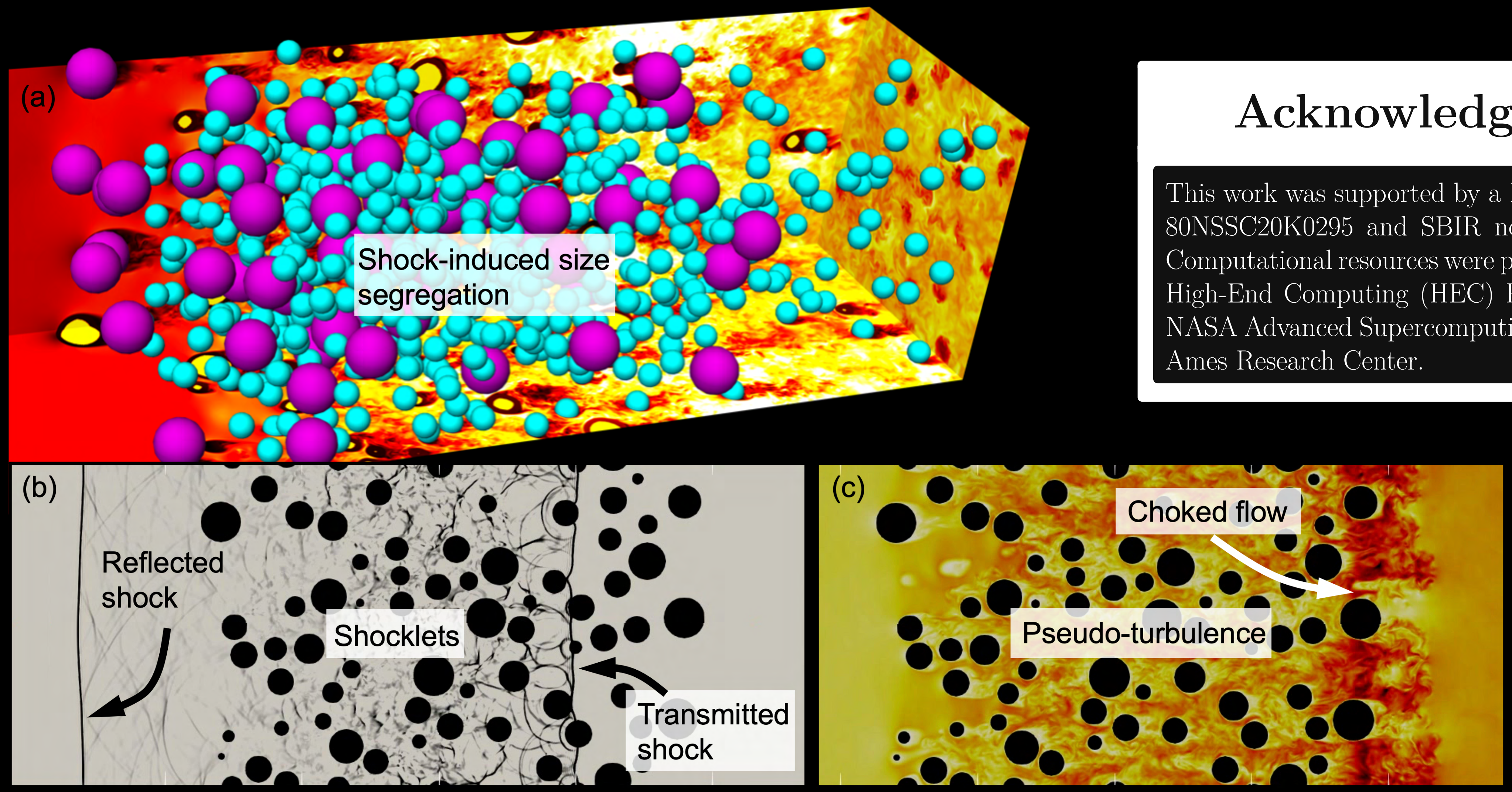

Figure 3: Particle-resolved simulations of a $\mathrm{Ma}_s = 1.66$ shock interacting with a particle curtain ($\phi = 0.21$.) (a) Shock-induced size segregation of a bidisperse suspension. (b) Numerical schlieren at an early time. (c) Local Mach number contour after the shock passes the curtain.