Bluebottle: A high-performance GPU-centric resolved-particle flow solver

Adam Sierakowski & Andrea Prosperetti

Motivation

Instances of systems of particles dispersed in fluid occur often in nature: dust storms, agricultural runoff, and beach erosion all exhibit particulate matter being moved by fluids. Additionally, we use particle-laden fluid flows in technological applications such as fluidized bed reactors which are used in producing oil products such as petroleum and plastics. In the future, we may take advantage of the energy-generation technology chemical looping combustion to reduce the release of carbon 14 products into the atmosphere.

Figure: Fluidized seed in the Mojave Desert (Wikipedia)

GPU-centric code design

We numerically solve the incompressible Navier-Stokes equations (1) and (2) to describe the motion of the fluid while the particles impose normal (friction) and no-penetration boundary conditions on the fluid.

\[ \rho u \cdot \nabla u = -\nabla p + \mu \nabla^2 u + g \] (1)

\[ \nabla \cdot u = 0 \] (2)

The Physalis method

The Physalis method takes advantage of the efficiency of a regular Cartesian finite-difference mesh while applying spectrally-accurate particle boundary conditions. In a particle reference frame in a region near the surface of a particle, due to the no-slip condition, (1) can be approximated as the Stokes equation.

\[ \nabla \cdot u = 0 \] (6)

Using \( P_h \phi_h \) and \( X_h \) total luminaries of order \( n \),

\[ \rho_h = \left( \frac{\delta}{2} \right) \sum_h \rho_h (\phi_h^2) \] (7)

Laudal provided the general solution of (6) in the presence of a spherical boundary with radius \( a \).

\[ u = \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^n}{2n+1} \left[ a^{n+3} \nabla \phi_n - \alpha a \phi_n \right] \] (8)

After finding the complex-valued dimensionless coefficients \( P_h \phi_h \) and \( X_h \) from the fluid field using scalar products (8), (9) determines particle boundary conditions (BC) at grid nodes near the particle surface. These boundary conditions are used to solve the fluid field, and the process is repeated until convergence. At convergence, the low-order \( P_h \phi_h \) and \( X_h \) give the hydrodynamic force (9) and moment (10) on the particle without any additional work.

\[ F_{1d} = x (y - y_0) (n - g) = \frac{1}{2} \left[ \frac{1}{2} \rho_0 u_0^2 \right] \int_{-a}^{a} \left[ (\nabla \phi_n)^2 \right] - N \left( \nabla \phi_n^2 \right) \] (9)

\[ \text{L} = \int \left[ \frac{1}{2} \rho_0 u_0^2 \right] \Omega \, d\omega = \frac{1}{2} \rho_0 u_0^2 \left( \int \nabla \phi_n^2 \right) \] (10)

State of the art

Utilizing experimental methods, it is very difficult to track the trajectories of individual particles, and it is nearly impossible to measure the forces on the particles and understand the fluid motion. We seek to learn about these fluid-particle systems using numerical simulations, but computers cannot accurately simulate an entire dust storm because of their wide range of length scales. To develop models of typical flow behavior, we use ensemble averaging to simulate many instances of the same particle configuration into a coarsened model that is more easily investigated.

The Physalis method

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\[ \rho u \cdot \nabla u = -\nabla p + \mu \nabla^2 u + g \] (1)

\[ \nabla \cdot u = 0 \] (2)

The flow solver

We numerically solve the incompressible Navier-Stokes equations (1) and (2) in the bulk flow on a staggered Cartesian grid using the projection method:

1. Calculate intermediate velocity \( \tilde{u} \) using the second-order Adams-Bashforth method for the convective term and an explicit forward-time central-space method for the diffusive term:

\[ \tilde{u} = u + \Delta t \left[ -\nabla u \nabla u \right] + \frac{3}{2} \Delta t \nabla^2 u + \frac{1}{2} \Delta t \nabla^2 u + g \] (3)

2. Solve for the pressure that will project \( \tilde{u} \) into a divergence-free space:

\[ \nabla \cdot \tilde{u} = 0 \] (4)

3. Step \( u \) forward to \( u^n+1 \) by projecting \( \tilde{u} \) into a divergence-free space to yield (5):

\[ u^{n+1} = u^n - \frac{3}{2} \Delta t \nabla^2 u^n + \frac{1}{2} \Delta t \nabla^2 u^n + g \] (5)

4. To incorporate the Physalis method into the projection method, we repeat the Physalis steps and the projection steps until solutions (4) and (5) converge proceeding to the next time step.

Open source code available

http://lucan.me.jhu.edu

Are you interested in learning more about Bluebottle or the Physalis method? Visit our website for more detailed development. Would you like to run some particle-laden flow simulations of your own? We have released Bluebottle under an open source license and we encourage you to download, share, and/or contribute to the source code.