Development of a Multiscale Eulerian-Lagrangian Method for High-Speed, Multimaterial Flows

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Outline

- Multi-Scale Modeling of High-Speed Flows with Particles and Droplets
- Macro-Models
  - SPARSE: Subscale Particle Averaged Reynolds Stress Equivalent
- Codes/Methods
  - Higher-Order Resolution Macro-Scale Particle-Source-In-Cell
  - SCMICTAR: High-Order Levelset Meso-Scale Code
- Meso-Scale Simulation of Shock-Cloud Interaction
  - Force Averaging
- Meta-Models: Dynamic Kriging
- Conclusions and Future Directions
High-Speed Multi-Material Flow
Explosion

Multi-Scale Physics in High-Speed, Multi-Material Environments
Multi-Scale Physics in High-Speed, Multi-Material Environments

Scramjet/Solid Rocket Propulsion

Macro-Scale

Micro-Scale

Droplet Dynamics

Meso-Scale

Liquid Fuel Injector/Atomization
Capturing Multiple Scales

- Existing methods cannot solve process-sized problems accurately and efficiently
  - Computational times for DNS solutions are prohibitively long
  - Current macro-scale models are limited in scope and accuracy
- The range of scales present in shocked particle-laden flows necessitate the use of advanced physical models and numerical schemes

Scramjet Engines
Multi-scale Approach

Mesoscale

Metamodle

Macroscale

0.8 < Ma < 1.2; Re < 10,000

NUMERICAL EXPERIMENTS

DRAG LAW

COMPUTATIONS


Modeling
Macro-Scale Point Particle

- Models a finite-sized particle as a volumeless, singular point
- Typical assumptions:
  - Spherical particle.
  - Modified Stokes drag forcing.
  - Particle scale is small as compared to smallest fluid scale.
- Enables computation with large number of particles.
- Omits finite-sized particles effects.

Should be considered statistical approach: model the averaged influence of many particles rather than the influence of individual particles

\[ F_{\text{Stokes}}^* = C_{D_\text{s}} 6\pi \rho^*_f d^* a^*_d (\overline{v}_{fd}^* - \overline{v}_{d}^*). \]

\[ C_{D_\text{s}} = 1 + \frac{Re_d^{2/3}}{6} \quad \text{Re}_d < 1000 \]
Computational vs. Physical Particle Phase

Each computational particle has an average velocity ($\bar{v}$)

$\bar{v}$ represents several physical particles with instant velocities ($\bar{v} + v'$) and drag profiles.

There are many other parameters (particle diameter for example) where this analysis is applicable as well.
Particle momentum equation,
\[ \frac{dv_p}{dt} = f(a) \cdot a \text{ where } a = u - v_p. \]

Decomposed, averaged computational particle cloud equation,
\[ \frac{d(\overline{v_p} + v'_p)}{dt} = f(\overline{a} + a') \cdot (\overline{a} + a'), \]
which, in typical Eulerian-Lagrangian methods, is truncated to
\[ \frac{dv_p}{dt} = f(\overline{a}) \cdot \overline{a}. \]

We Taylor expand the correction factor around \( \overline{a} \),
\[ f(\overline{a} + a') = f(\overline{a}) + \frac{df(\overline{a})}{da} \cdot a' + O(a'^2). \]

Using this expansion in the governing equation and simplifying,
\[ \frac{dv_p}{dt} = f(\overline{a}) \cdot \overline{a} + \frac{df(\overline{a})}{da} \cdot \overline{a}'a'. \]
SPARSE Model

Subgrid Particle Averaged Reynolds Stress Equivalent (SPARSE) model:

\[
\frac{d\bar{v}}{dt} = f(\bar{a})\bar{a} + f'(\bar{a})\bar{a}'\bar{a}'
\]

Looking closer at the averaged interphase velocity:

\[
\bar{a} = \bar{u} - \bar{v}
\]

Dispersion of the physical (“exact”) particle cloud influences the average fluid velocity:

\[
\overline{u_{fluid}(x_{exact})} \neq \overline{u_{fluid}(x_{exact})}
\]

Use an a priori closure model initially
“Exact” computation traces 10,000 particles

First Order and SPARSE models use a single computational particle

Background flow, $u_{\text{fluid}}$, is an analytical function

Randomized initial conditions with $-1 \leq \phi \leq 1$,

- $x_{p,\text{exact}} = 5 + \phi$
- $v_{p,\text{exact}} = 5 + 5\cdot\phi$

Error:

$$\varepsilon_{v_p} = \left| \frac{v_{p,\text{exact}} - v_{p,\text{model}}}{v_{p,\text{exact}}} \right|$$
Importance of RSE Term

- Constant background fluid velocity, $u_{\text{fluid}}(x, t) = 10$, enforces $u_{\text{fluid}}(x) = u_{\text{fluid}}(\bar{x})$.
- Only difference between First Order and SPARSE models is $f'(\bar{a})\alpha'\alpha'$
- Linear drag correction factor:

$$f(a) = \frac{0.1a}{St},$$

With a linear drag correction factor, the Taylor expansion is exact.
Importance of Average Fluid Velocity

- Constant drag correction factor: \( f(a) = \frac{24}{St} \)
- Only difference between **First Order** and **SPARSE** models is \( \overline{u} \)
- Spatially dependent background fluid velocity,
  \[
  u_{\text{fluid}} = \cos(\pi x) + x
  \]
3D Testing: Isotropic Turbulence

27,000 Particles

3\Delta x \approx 0.3

St = 0.01

Initial Particle Velocity

-2.5 < v_p < 2.5

\overline{x_p} and \overline{v_p} modeled using a single, initially stationary computational particle

\begin{equation}
 f(a) = \frac{3}{4} \left( 24 + 0.38 Re_p(a) + 4 \sqrt{Re_p(a)} \right) \left( 1 + \exp \left[ -\frac{0.43}{M_p(a)^{4.67}} \right] \right)
\end{equation}

Isotropic Turbulence

M_0 = 0.25

128^3 Nodes
3D Isotropic Turbulence

\[ |\mathbf{v}_p| = \sqrt{u_p^2 + v_p^2 + w_p^2}, \]

\[ \varepsilon_{|\mathbf{v}_p|} = |\mathbf{v}_{p,\text{exact}}| - |\mathbf{v}_{p,\text{model}}|, \]

Blue = First Order
Red = SPARSE
Green = Exact Spread
Codes
High-order resolution Eulerian Lagrangian method

Stable and high-resolution EL method for flows with discontinuities

Higher-Order TVD-RK time integration of particles

Use high-order ENO interpolation to determine field at particle position.

Solve Euler eq. with high-order WENO-Z

Weigh particle to grid through a smooth spline deposition function

[Jacobs and others, JCP, ’09, SIAM JSC ‘15, IJMF ’13, PoF ‘15]
SCIMITAR3D : High-Order Meso-Scale Simulation

Moving Shock in an Inviscid Ideal Gas

Cartesian Mesh

3rd Order in Time
TVD Runge-Kutta*

3rd Order in Space
Convex ENO**

Interface Tracked Sharply By Narrow Band Level Set Method***

Rigid, Fixed Particle

Interface Conditions Implemented By Ghost Fluid Method****

Test Problem: Cylinder in a Ma=1.3 Moving Shock
VERIFICATION
VERIFICATION AND CONVERGENCE

Meso-Scale Simulations and Meta-Modeling
Mesoscale Computations

- Shock, $Ma$
- Diameter, $d$

1 unit
Averaging of Representative Particles

\[ \overline{F_D} = \frac{1}{t^*} \int_{t=0}^{t^*} F_D^{avg} dt \]
Convergence of $F_D$

\[ y = 4.9825x^{-1.971} \]

Relative Error vs. $d/\Delta x$
Effect of Ma and Volume Fraction on $F_D$

Ma = 2.3; VF = 20.6%

Ma = 3.5; VF = 20.6%

Ma = 3.5; VF = 1.2%
Effect of Ma and Volume Fraction on $F_D$

NOT SELF SIMILAR

$F_D$ vs. $t$ for different $Ma$ and Vol. Frac.:
- $Ma = 3.5$
- $Ma = 2.3$
- $Ma = 1.1$
- Vol. Frac. = 20.6%
- Vol. Frac. = 11.6%
- Vol. Frac. = 1.3%
THE Metamodel: Dynamic Kriging (DKG)*

Sequential Sampling on a Sparse & Unstructured Grid in n dims

\[ f = ax + \theta \]

New Sample Location

Meta-Modeling: Kriging
Hypersurface of Averaged Drag
Convergence of Hypersurface

\[ y = 324.57x^{-2.684} \]

\[ \text{MSE} = \frac{\sum (F_{D}^{\text{avg}}|_{SC3D} - F_{D}^{\text{avg}}|_{DKG})^2}{\sum (F_{D}^{\text{avg}}|_{SC3D})^2} \]
Comparison with Experimental Model

Re = 5000; Kn = 10

Summary

- We have made great strides toward a multi-scale framework for simulation of high-speed, multi-physics flow:
  - Macro-scale: cloud modeling and coupling with meso-model
  - Meso-scale: simulations of particle-shock-cloud interaction and testing of representative particle
  - Meta-Modeling: Dynamic Kriging hypersurfaces in multi-dimensional space
  - Testing of shock-particle-cloud interaction (comparison with experiment) and isotropic turbulence
Next Project Period: UQ

DKG Equation

\[ y_i = a_{ij}x_j + \theta_j \]

Add a correction term to the diagonal

\[ y_i = (a_{ij} + \lambda \delta_{ij})x_j + \theta_j \]

Penalty Term: Comes from a Bayesian Probablity Model with a given mean and a variance