Algorithmic advances in droplet computations.
Computing fluid interactions in a turbulent background flow

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Cloud Physics Workshop Aug 2011
Outline

1. The cloud/droplet model
2. Krylov space methods
3. Droplet model investigations
4. Conclusions and future work
Stokes flow around spheres in a turbulent background flow.
Stokes flow around spheres in a turbulent background flow.

Features

- Spectrally resolved driven turbulent flow ($U$).
- Spheres are passive agents in the turbulent flow.
- Spheres induce a Stokes flow ($u$).
- Spheres interact with each other.
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Flow field induced by $k^{th}$ particle in isolation (free stream velocity $V_p$).

$$u_s(\vec{r}^{(k)}; a^{(k)}, V_p^{(k)}) = \frac{3}{4} \left[ \frac{a^{(k)}}{r^{(k)}} - \left( \frac{a^{(k)}}{r^{(k)}} \right)^3 \right] \frac{\vec{r}^{(k)}}{(r^{(k)})^2} (V_p^{(k)} \cdot \vec{r}^{(k)}) +$$

$$\left[ \frac{3 a^{(k)}}{4 r^{(k)}} + \frac{1}{4} \left( \frac{a^{(k)}}{r^{(k)}} \right)^3 \right] V_p^{(k)}$$
The mathematical model.

Interacting particles...

\[ u^{(k)} = \sum_{m=1, m\neq k}^{N_p} u_s \left( d^{(mk)}; a^{(m)}, V^{(m)} - U(Y^{(m)}, t) - u^{(m)} \right), \]

\[ k = 1 \ldots N_p \]
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\[ u(x, t) = \sum_{k=1}^{N_p} u_s(r^{(k)}; a^{(k)}, V^{(k)} - U(Y^{(k)}, t) - U^{(k)}) \]
The evolution of the algorithm

- Precomputation of A
- Analysis of methods
- Preconditioners...
  ...and more preconditioners...
- Cauchy integral equation
- GMRes with recycling

Simulation efficiency

Time

GMRes

Block Jacobi

<Improved droplet models>
Generalized Minimal Residual

Solving $Ax = b$ for our cloud system.

- Droplet interactions: $1/r$.
- Interactions are cut off when $r > 50a$. 
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Krylov space:

$$K_m(A, x_0) = \text{span} \left\{ x_0, Ax_0, A^2 x_0, \ldots, A^{m-1} x_0 \right\}$$

Big idea: We solve the system efficiently by finding solutions in $K_m$, $m < \text{dim}(A)$. 
Generalized Minimal Residual

General features of GMRes.

- GMRes constructs an orthonormal basis for \( K_m \) and \ldots
- GMRes minimizes \( \| b - Ax_m \|_2 = \| r \| \) over the space of all possible vectors \( x_m = x_0 + Vmy \).
- Like most good iterative methods, convergence is geometric under many circumstances.
- Unfortunately, our droplet system is not positive definite.
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\[
\|r_m\| \leq \left(1 - \frac{\lambda_{\min}(A + A^T)}{2\lambda_{\max}(A + A^T)}\right)^{m/2} \|r_0\|
\]

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Convergence of GMRes for non-PD matrices.

Sad truth: Our $A$ is not positive definite.
Convergence of GMRes for non-PD matrices.

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Happy result: We can still estimate a bound on the convergence rate.

$$\rho = \frac{M - m + 2\epsilon}{M + m + 2\sqrt{M m} + \epsilon^2}$$
Convergence of GMRes for non-PD matrices.

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Happy result: We can still estimate a bound on the convergence rate.

\[ \rho = \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} + \frac{2\varepsilon}{(\sqrt{M} + \sqrt{m})^2} + O(\varepsilon^2), \quad \kappa = \frac{M}{m} \]
Can we solve the droplet system under general circumstances?
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The cloud/droplet model
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Choose an appropriate $M$ to solve...

$$M^{-1}Ax = M^{-1}b$$

Ideal properties for $M$:

- $M^{-1}A$ has good convergence properties.
- $M^{-1}y = c$ can be solved quickly and accurately (unlike $Ax = b$).
Preconditioning

Choose an appropriate $M$ to solve...

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Schwarz Preconditioner

\[ Ax = (A_1 + A_2)x = b \]
\[ A_1 x^{m+1} = b - A_2 x^m \]
The current physical model

Droplets interact via Stokes flow.

\[ \psi = \frac{1}{4} \left( 2r^2 - 3r + \frac{1}{r} \right) \sin^2 \theta \]

- Valid for \( R = 0 \).
- Satisfies correct boundary conditions at sphere surface and in free stream.
- Stokes flow permits superposition.
- Problems: No \( R \) dependence. Slow decay. No wake. What is the convergent limit?
A proof-of-concept Oseen solution

\[ \psi = \frac{1}{2} r^2 \sin^2 \theta - \frac{3}{2R} (1 + \cos \theta) \left( 1 - e^{-\frac{1}{2} rR(1 - \cos \theta)} \right) \]

- Valid as an outer approximation for small \( R \) when \( r = O(1/R) \).
- Satisfies correct boundary conditions in free stream.
- Problems: Does not satisfy BC’s on the sphere. Does not permit superposition of solutions.
What is the residual, anyway?

\[ R = 10^{-2} \]
What is the residual, anyway?

\[ R = 10^{-1} \]
What is the residual, anyway?

\[ R = 10^0 \]
What is the residual, anyway?

\[ R = 5 \]
A new algorithm...

If the free stream were the same for all particles, we might use the Oseen solution.
A new algorithm...

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\[ \vec{V}_n = \vec{V}_i + \epsilon_{i,5} q_{i,5} \]

\[ \vec{V}_{n+3} = \vec{V}_i + \epsilon_{i,2} q_{i,2} \]

\[ \vec{V}_j = \vec{V}_i + \epsilon_{i,1} q_{i,2} \]

\[ \vec{V}_{n+1} = \vec{V}_i + \epsilon_{i,4} q_{i,4} \]

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Conclusions and future work

- GMRes has improved the efficiency of our simulation.
- Our analysis suggests that our solver is robust.
- We are expecting a factor of two improvement using precomputation.
- We will focus our efforts on improving the interacting droplet approximation to include $R$ dependence.

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