Toward faster and more accurate computation of hydrodynamic droplet-droplet interactions.

Computing fluid interactions in a turbulent background flow

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Peta-Apps Algorithms

Ax = b
Outline

1. The cloud/droplet model
2. Krylov space methods
3. Implications for our hydrodynamic interaction model
4. The algorithm warehouse
5. 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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Droplets are (were) a bottleneck
The mathematical model.

Flow field induced by $k^{\text{th}}$ particle in isolation (free stream velocity $V_p$).

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

$$\left[ \frac{3 a^{(k)}}{4 r^{(k)}} + \frac{1}{4} \left( \frac{a^{(k)}}{r^{(k)}} \right)^3 \right] V_p^{(k)}$$
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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\[ u(x, t) = \sum_{k=1}^{N_p} u_s(r^{(k)}; a^{(k)}, V^{(k)} - U(Y^{(k)}, t) - u^{(k)}) \]
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:

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

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 $x_m = x_0 + V_m y$.
- Like most good iterative methods, convergence is geometric under many circumstances.
- Unfortunately, our droplet system is not positive definite.
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\[
\| r_m \| \leq \left( 1 - \frac{\lambda_{\text{min}}(A + A^T)}{2\lambda_{\text{max}}(A + A^T)} \right)^{m/2} \kappa_2(V) \| r_0 \|
\]

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Sad truth: Our $A$ is not positive definite.
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Happy result: We can still estimate a bound on the convergence rate.

$$\rho = \frac{\lambda_M - \lambda_m + 2\delta}{\lambda_M + \lambda_m + 2\sqrt{\lambda_M\lambda_m + \delta^2}}$$
Sad truth: Our $A$ is not positive definite.

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

$$\rho = \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} + \frac{2\delta}{(\sqrt{\lambda_M} + \sqrt{\lambda_m})^2} + O(\delta^2), \quad \kappa = \frac{\lambda_M}{\lambda_m}$$
Simple analytic examples
Simple analytic examples

\[ a_1 / a_2 \]

\[ \lambda_1 \]

\[ \lambda_2 \]
Can we solve the droplet system under general circumstances?

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- Conclusions and future work
Preconditioning

There are two reasons to precondition our system.

1. Improve the quality of the solution.

\[ \frac{\| \vec{x} - \vec{x}_n \|}{\| \vec{b} \|} \leq \kappa(A) \frac{\| A\vec{x}_n - \vec{b} \|}{\| \vec{b} \|} \]

2. In our case, improve the distribution of eigenvalues of the system to be solved.
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1. Improve the quality of the solution.

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Preconditioning

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 $Ax = b$).
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Schwarz Preconditioner

$$M^{-1}\tilde{x} = \sum_l \hat{R}_l^T P_l \hat{A}_l^{-1} \hat{R}_l^T \tilde{x}$$
Normality

Asymmetric
Symmetric

\[ 10^4 \]
\[ 10^2 \]
\[ 10^0 \]
\[ 10^1 \]
\[ 10^2 \]
\[ 10^3 \]

\[ \kappa_2(V) \]

\[ N \]
## Performance summary

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<th>Solution Method</th>
<th>fixed cost</th>
<th>variable cost</th>
<th>$\epsilon = 10^{-6}$</th>
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<th>total time (sec)</th>
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</table>
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“We have top men working on it now...”

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2 Krylov space recycling...
3 Preconditioned preconditioning with the Cauchy Integral Equation...
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1. Fast multipole...
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3. Preconditioned preconditioning with the Cauchy Integral Equation...
Recall, Cauchy’s integral formula.

\[ f(z_0) = \frac{1}{2\pi i} \int_{\gamma} \frac{f(z)}{z - z_0} \, dz \]
A different way to solve preconditioned systems.

Recall, Cauchy’s integral formula.

\[ f(z_0) = \frac{1}{2\pi i} \int_C \frac{f(z)}{z - z_0} \, dz \]

It can also be used for matrix valued functions.

\[ f(M) b = \frac{1}{2\pi i} \int_C f(z)(zI - M)^{-1} b \, dz \]
Conclusions and future work

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