



ON THE SOLUTION OF A LARGE SPARSE LINEAR SYSTEM OF EQUATIONS ON A PARALLEL ARCHITECTURE

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A model flow for a droplet in a turbulent cloud

The continuous model:

$$u(x, t) = \sum_{k=1}^{N_p} u_s(r^{(k)}; a^{(k)}, V^{(k)} - U(Y^{(k)}, t) - u^{(k)}) \quad (1)$$

Definition of u_s :

$$u_s(r^{(k)}; a^{(k)}, V_p^{(k)}) = \frac{3}{4} \left[\frac{a^{(k)}}{r^{(k)}} - \left(\frac{a^{(k)}}{r^{(k)}} \right)^3 \right] \frac{\bar{r}^{(k)}}{(r^{(k)})^2} (V_p^{(k)} \cdot \bar{r}^{(k)}) + \left[\frac{3a^{(k)}}{4r^{(k)}} + \frac{1}{4} \left(\frac{a^{(k)}}{r^{(k)}} \right)^3 \right] V_p^{(k)} \quad (2)$$

The collocation points:

$$u^{(k)} = \sum_{m=1, m \neq k}^{N_p} u_s(a^{(mk)}; a^{(m)}, V^{(m)} - U(Y^{(m)}, t) - u^{(m)}), k = 1 : N_p \quad (3)$$

A complete study can be found in [1].

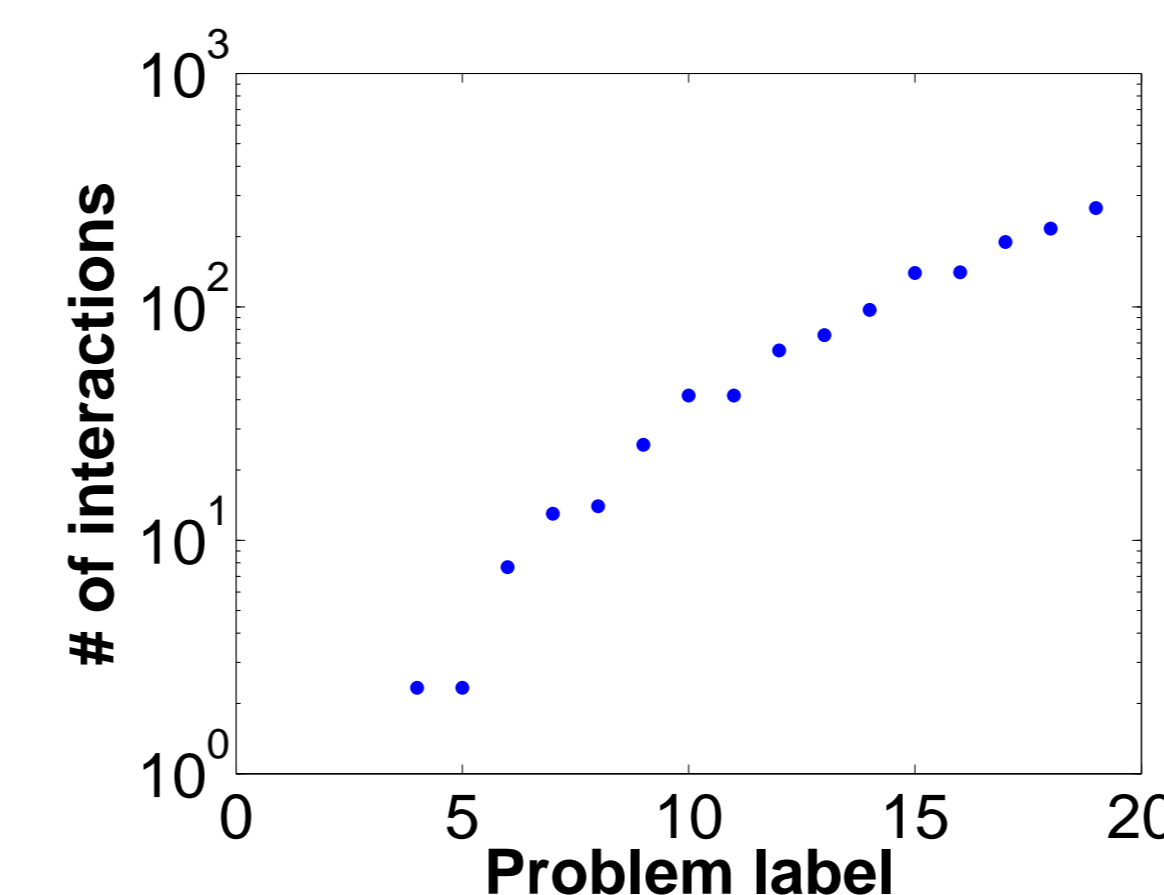
Current Approach

- Advantages
 - Easy implementation
 - Working and tested against Matlab
- Disadvantages
 - Starting to show slow convergence
- Mixture of Jacobi and Gauss-Seidel
 - Local Gauss-Seidel
 - Global Block-Jacobi

Discussion of J, GS, CGS, BiCG and GMRES

- Setup Experiments
 - Small experiments
 - Parameters initialized random
 - We add particles and kept radius fixed
- CGS and BiCG perform a little bit faster for smaller problems.
- GMRES [6] converges 50% faster for larger problems.

Tag	J	GS	CGS, BiCG, GMRES
4	C	C	C
5	C	C	C
6	C	C	C
→7	C	C	C
8	NC	C	C
9	NC	C	C
10	NC	C	C
11	NC	C	C
12	NC	C	C
13	NC	C	C
14	NC	C	C
15	NC	C	C
16	NC	C	C
17	NC	NC	C



Why GMRes?

- Advantages
 - Matrix-free approach
 - Only require Ax and not $A'x$
 - Performed better than CGS and BiCG in experiments with high # of interactions
 - Ax can be parallelized easily
- Disadvantages
 - Memory requirements increase quadratically with the number of iterations (but restart could be used)

Leveraging the dynamics

A and b vary slowly, which means we are solving a sequence of linear systems of the form $A^{(i)}x^{(i)} = b^{(i)}$, where $\|A^{(i)} - A^{(i+1)}\| \leq \epsilon$ and $\|b^{(i)} - b^{(i+1)}\| \leq \epsilon$, with $\epsilon \ll 1$. If so,

- Do we expect $\|x^{(i)} - x^{(i+1)}\| \leq \tilde{\epsilon}$?
- Can we take advantage of it?
- Has somebody tried to solve this before?
- Does it work for us?
- Since we want to use GMRes, are the Krylov sub-spaces $K_n(A^{(i)})$ and $K_m(A^{(i+1)})$ of linear systems (i) and $(i+1)$ respectively, close?

GMRes with Recycling

- Do we expect $\|x^{(i)} - x^{(i+1)}\| \leq \tilde{\epsilon}$?
 - Yes, in some sense.
- Can we take advantage of it?
 - See next question
- Has somebody tried to solve this before?
 - Yes, there is an algorithm called GCRO-DR that was built to solve problems of type $A^{(i)}x^{(i)} = b^{(i)}$, but in a finite elements context [5].
- Does it work for us?
 - No, it does not work as expected. The reason is not clear yet, but we think it is related to the eigenvalue distribution. The problems they work on lead to a very ill-conditioned matrix and our matrix is not ill-conditioned. We tested it with a code provided by them with our test problem. The improvement is minimal with our matrices but with their matrices the improvements are consistent.
- Since we want to use GMRes, are the Krylov sub-spaces $K_n(A^{(i)})$ and $K_m(A^{(i+1)})$ of linear systems (i) and $(i+1)$ respectively, close?
 - This is an open question. Based on the unsuccessful result from previous question we might be biased to say no. However, we still believe that we can recycle an older Krylov sub-space in the form of a preconditioner.

GMRes with Preconditioner

We could have left, right or both types of preconditioner, but what would be a good preconditioner?

- Use same kernel as (1) but increase order to $1/r^3$.
 - *Advantage:* Very fast convergence
 - *Disadvantage:* Does not speed up convergence of the original system
- Recycling and preconditioning can be used together. They complement each other.

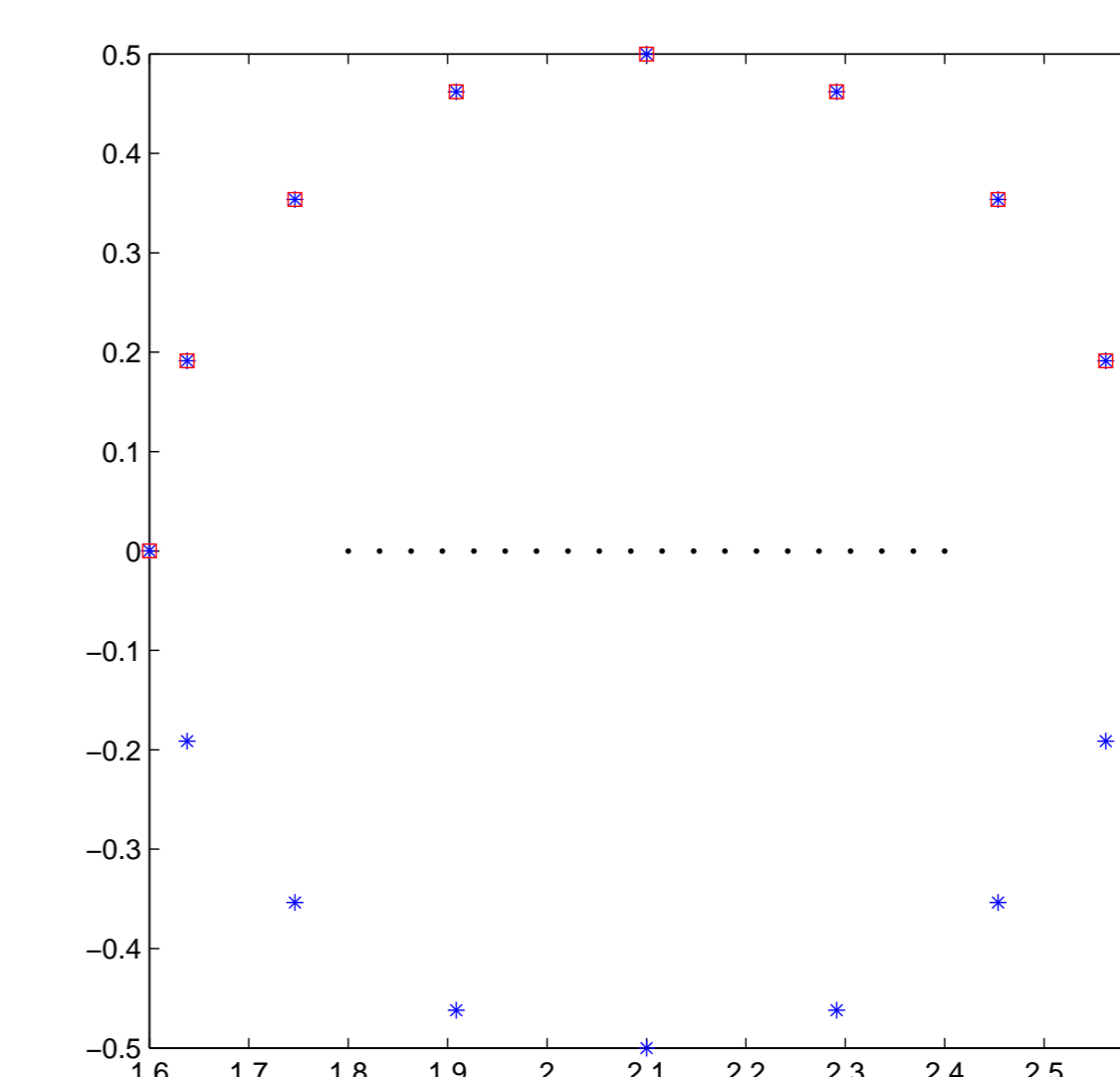
References

- [1] O. Ayala, W. Grabowski, and L. Wang. A hybrid approach for simulating turbulent collisions of hydrodynamically-interacting particles. *Journal of Computational Physics*, 225(1):51–73, July 2007.
- [2] P. Davies and N. Higham. Computing $f(A)$ for matrix functions f . *QCD and numerical analysis III*, 2005.
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- [5] M. L. Parks, E. de Sturler, G. Mackey, D. D. Johnson, and S. Maiti. Recycling Krylov Subspaces for Sequences of Linear Systems. *SIAM Journal on Scientific Computing*, 28(5):1651, 2006.
- [6] Y. Saad and M. H. Schultz. GMRES: A Generalized Minimal Residual Algorithm for Solving Nonsymmetric Linear Systems. *SIAM Journal on Scientific and Statistical Computing*, 7(3):856, 1986.

Cauchy contour approach with GMRes

- This idea has been around for long time [2, 3, 4]
- Strong requirements needed
- Idea: Instead of solving the system directly we solve several ‘easier’ linear system of equations.
- How:

$$A^{-1}b = \frac{1}{2\pi i} \int_{\gamma} \frac{1}{z} (zI - A)^{-1} b dz \quad (4)$$



Some simplification can be made after using trapezoidal rule since the eigenvalues are all real and positive (based on experiments) but not necessarily symmetric, i.e. only compute half of the contour and then take its real part since we will get complex conjugate values for the approximation.