HPC final project: Parallelized Ewald summation of stokes potential

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Periodic Stokes potentials

Consider a system of N point sources at location $\mathbf{x}_n$ with strength $\mathbf{f}_n$, in the periodic setting, the velocity field is

$$\mathbf{u}(\mathbf{x}) = \sum_{n=1}^{N} \sum_{\mathbf{p}} \mathbf{S}(\mathbf{x} - \mathbf{x_n} + \mathbf{p})\mathbf{f}_n, \tag{1}$$

with $\mathbf{S}$ the Oseen-Burgers tensor:

$$\mathbf{S}(\mathbf{x}) = \frac{\mathbf{1}}{|\mathbf{x}|} + \frac{\mathbf{xx}}{|\mathbf{x}|^3}. \tag{2}$$

where $\mathbf{p}$ form the discrete set $\{[iL_x \ jL_y \ kL_z] : (i, j, k) \in \mathbb{Z}^3\}$.
Warning: Eq.(1) **decays as** $1/|\mathbf{x}|$**!**
We need **Ewald summation** to compute this.

Ewald summation

$$\mathbf{u}(\mathbf{x}_m) = \sum_{n=1}^{N} \sum_{\mathbf{p}} \mathbf{A}(\xi, \mathbf{x_m} - \mathbf{x_n} + \mathbf{p})\mathbf{f}_n$$

$$+ \frac{1}{V} \sum_{\mathbf{k} \neq 0} \mathbf{B}(\xi, \mathbf{k}) e^{-k^2/4\xi^2} \sum_{n=1}^{N} \mathbf{f}_n e^{-i\mathbf{k}\cdot(\mathbf{x}_m - \mathbf{x}_n)}$$

$$- \mathbf{u}_{\mathrm{self}} \tag{3}$$

By the formulation by Hasimoto [2], we have

$$\mathbf{A}(\xi, \mathbf{x}) = 2\left(\frac{\xi e^{-\xi^2 r^2}}{\sqrt{\pi} r^2} + \frac{\mathrm{erfc}(\xi r)}{2r^3}\right)(r^2\mathbf{I} + \mathbf{xx}) - \frac{4\xi}{\sqrt{\pi}} e^{-\xi^2 r^2}\mathbf{I} \tag{4}$$

$$\mathbf{B}(\xi, \mathbf{k}) = 8\pi\left(1 + \frac{k^2}{4\xi^2}\right)\frac{1}{k^4}(k^2\mathbf{I} - \mathbf{kk}) \tag{5}$$

$$\mathbf{u}_{\mathrm{self}}(\mathbf{x}_m) = \frac{4\xi}{\sqrt{\pi}}\mathbf{f}_m \tag{6}$$

ξ is a positive constant known as the **Ewald parameter**.

Acceleration & parallelization

- Compute u^F (k-space) by FFT

$$\mathbf{u}^F(\mathbf{x}_m) = \frac{1}{V}\sum_{\mathbf{k}\neq 0} e^{-\eta k^2/8\xi^2} e^{-i\mathbf{k}\cdot\mathbf{x}_m} \cdot \mathbf{B}(\xi,\mathbf{k}) e^{-(1-\eta)k^2/4\xi^2} \left(\sum_{n=1}^{N} \mathbf{f}_n e^{-\eta k^2/8\xi^2} e^{i\mathbf{k}\cdot\mathbf{x}_n}\right) \tag{7}$$

Non-uniform FFT = Gaussian Gridding + FFT

  - **Gaussian Gridding**:
    Compute $\sum_{n=1}^{N} \mathbf{f}_n e^{-2\xi^2|\mathbf{x}-\mathbf{x}_n|_*^2/\eta}$
    Can be accelerated with Greengard's trick [1] and OpenMP[6]
  - **FFT**:
    Paralleled with CuFFT (GPU) [5] (v.s. FFTW (CPU serial)[4])

- Accelerate u^R (real space) by OpenMP [6]

Important Parameters & Error bound

Free parameters:

- ξ : Ewald parameter
- M: Number of layers of k-space
- p_∞: Number of layers of real-space
- P, m: Parameter of Gaussian gridding ($\eta = (PL\xi/Mm)^2$)

Error Bound: **Spectral accurate!**

$$E = E^F + E^Q + E^R \tag{8}$$

$$E^F \leq C_F e^{-\frac{M^2\pi^2}{4L\xi^2}} \quad \text{(truncation of k-space)} \tag{9}$$

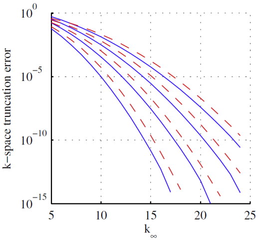
$$E^R \leq C_R\left(\frac{1}{\xi^2} + \frac{p_\infty}{\xi}\right)e^{-p_\infty^2\xi^2}. \quad \text{(truncation of real space)} \tag{10}$$

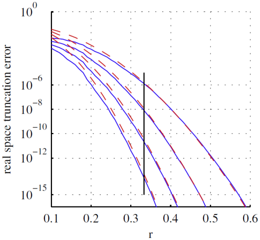
$$E^Q \leq 4e^{-\frac{\pi^2 P^2}{2m^2L^2}} + \operatorname{erfc}(m/\sqrt{2}) \quad \text{(quadrature)} \tag{11}$$

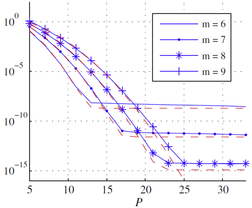
Ewald parameter ξ trades off between real space and k-space!

Spectral convergence

The three type of error versus the corresponding parameter, all has **spectral convergence**! (result from [3])







Time Complexity & Work load balance

The total computational cost of the method is

$$\underbrace{O(NP^3)}_{\text{Gaussian gridding}} + \underbrace{O(M^3\log(M^3))}_{\text{FFT + iFFT}} + \underbrace{O(M^3)}_{\text{Scaling on k-space}} + \underbrace{O(N^2p_\infty^3)}_{\text{Real space}} + \underbrace{O(N)}_{\textit{self}} \tag{12}$$

if no FFT acceleration, the cost is

$$\underbrace{O(N^2M^3)}_{k-space} + \underbrace{O(N^2p_\infty^3)}_{\text{Real space}} + \underbrace{O(N)}_{\textit{self}} \tag{13}$$

Ewald parameter ξ trades off between real space and k-space!

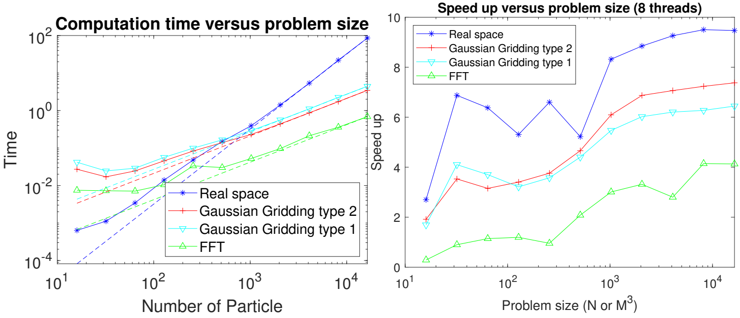
- Larger $\xi \to$ larger M, smaller p_∞.
- Smaller $\xi \to$ smaller M, larger p_∞.

How we choose the parameters:

- **Balance the error**
- **Balance the time**

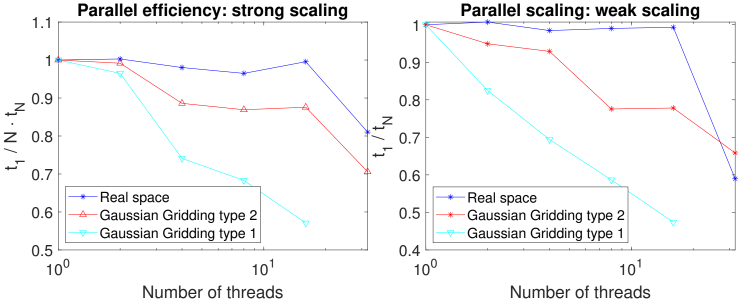
Time Complexity result & speed up

Prince sever, 8 CPU cores, 1 GPU, cuda-10.1 gcc-6.3 fftw-3.3.6 mpi/openmpi-x86_64 -O3 -march=native



Scaling result

Prince sever, 32 CPU cores, gcc-6.3 fftw-3.3.6
mpi/openmpi-x86_64 -O3 -march=native



References I

- Greengard, Leslie, and June-Yub Lee. "Accelerating the nonuniform fast Fourier transform." SIAM review 46.3 (2004): 443-454.
- Hasimoto, Hidenori. "On the periodic fundamental solutions of the Stokes equations and their application to viscous flow past a cubic array of spheres." Journal of Fluid Mechanics 5.2 (1959): 317-328.
- Lindbo, Dag, and Anna-Karin Tornberg. "Spectrally accurate fast summation for periodic Stokes potentials." Journal of Computational Physics 229.23 (2010): 8994-9010.
- Frigo, Matteo, and Steven G. Johnson. "The design and implementation of FFTW3." Proceedings of the IEEE 93.2 (2005): 216-231.

References II

- https://developer.nvidia.com/cufft
- Dagum, Leonardo, and Ramesh Menon. "OpenMP: An industry-standard API for shared-memory programming." Computing in Science Engineering 1 (1998): 46-55.

Link of the project:
`https://github.com/CecilMartin/Ewald_Summation`

Team work:

- Zhe Chen: Write codes, presentation
- Guanchun Li: Develop algorithm into pseudo-code, run codes, write slides
- Together: Literature research