Homework set 3 — MATH 393C — Spring 2019

Due on Thursday March 25. Please hand in solutions to problems 3.1 – 3.3.

Problem 3.1: The objective of this problem is to computationally investigate the error incurred by truncating multipole expansions. Consider the following geometry: Let Ω_τ and Ω_σ be two well-separated boxes with centers $\boldsymbol{c}_\tau$ and $\boldsymbol{c}_\sigma$. Let $\boldsymbol{y} \in \Omega_\sigma$ be a source point and let $\boldsymbol{x} \in \Omega_\tau$ be a target point. Consider the error function

$$e(P) = \sup\left\{\left|\log|\boldsymbol{x}-\boldsymbol{y}| - \mathsf{B}_P(\boldsymbol{y},\, \boldsymbol{c}_\tau)\,\mathsf{Z}_P(\boldsymbol{c}_\tau,\, \boldsymbol{c}_\sigma)\,\mathsf{C}_P(\boldsymbol{c}_\sigma,\, \boldsymbol{x})\right| \,:\, \boldsymbol{y} \in \Omega_\sigma\ \boldsymbol{x} \in \Omega_\tau\right\}$$

where P is the length of the multipole expansion, and where

$\mathsf{C}_P(\boldsymbol{c}_\sigma,\, \boldsymbol{y}) \in \mathbb{C}^{P\times 1}$	maps a source to an outgoing expansion
$\mathsf{Z}_P(\boldsymbol{c}_\tau,\, \boldsymbol{c}_\sigma) \in \mathbb{C}^{P\times P}$	maps an outgoing expansion to an incoming expansion
$\mathsf{B}_P(\boldsymbol{x},\, \boldsymbol{c}_\tau) \in \mathbb{C}^{1\times P}$	maps an incoming expansion to a target

(a) Estimate $e(P)$ experimentally for the geometry:

$$\Omega_\sigma = [-1,1]\times[-1,1], \qquad \Omega_\tau = [3,5]\times[-1,1].$$

(b) Fit the function you determined in (a) to a curve $e(P) \sim c\cdot\alpha^P$. What is α?

(c) Is the supremum for a given P attained for any specific pair $\{\boldsymbol{x},\, \boldsymbol{y}\}$?
If so, find (experimentally) the pair. Does the choice depend on P?

(d) Repeat questions (a), (b), (c) for a different geometry of your choice. (Provide a picture.)

Hint: The provided file `main_T_ops_are_fun.m` might be useful.

Problem 3.2: The objective of this exercise is to familiarize yourself with the provided prototype FMM. The questions below refer to the basic FMM provided in the file `main_fmm.m` when executed on a uniform particle distribution. For this case, precompute only the translation operators $\mathbf{T}^{(\text{ofo})}$, $\mathbf{T}^{(\text{ifo})}$, and $\mathbf{T}^{(\text{ifi})}$ (i.e. set `flag_precomp=0`).

(a) Estimate and plot the execution time of the FMM for the choices

$$N_{\text{tot}} = 1\,000,\ 2\,000,\ 4\,000,\ 8\,000,\ 16\,000,\ 32\,000,\ 64\,000.$$

Set `nmax=50`. Provide plots that track the following costs:

t_{tot}	total execution time, including initialization.
t_{init}	cost of initialization (computing the tree, the object `T_OPS`, etc.).
t_{ofs}	cost of applying $\mathbf{T}^{(\text{ofs})}$.
t_{ofo}	cost of applying $\mathbf{T}^{(\text{ofo})}$.
t_{ifo}	cost of applying $\mathbf{T}^{(\text{ifo})}$.
t_{ifi}	cost of applying $\mathbf{T}^{(\text{ifi})}$.
t_{tfi}	cost of applying $\mathbf{T}^{(\text{tfi})}$.
t_{close}	cost of directly evaluating close range interactions.

(b) Repeat exercise (a) but now for a few different choices of `nmax`. Which one is the best one? Provide a new plot of the times required for this optimal choice.

Problem 3.3: Repeat Problem 3.2 but now use a non-uniform point distribution of your choice.

Problem 3.4: *[Optional]* Can you think of a better way of computing the interaction lists? Here "better" could mean either a cleaner code that executes in more or less the same time, or a code that executes significantly faster than the provided one. If your code is ***both*** cleaner and faster then so much the better!

Problem 3.5: *[Optional]* Code up the single-level Barnes-Hut method and investigate computationally how many boxes you should use for optimal performance for any given precision and given total number N_{tot} of charges. Create a plot of the best possible time t_{optimal} for several N_{tot} and estimate the dependence of t_{optimal} on N_{tot}. To keep things simple, consider only uniform particle distributions. You need only consider a fixed precision (say $P = 10$) but an ambitious solution should compute the optimal time for several different choices (say $P = 5,\ 10,\ 15,\ 20$).