AM126 lec 16

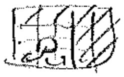
· ACMS 4pm
· X-hr: LaTeX for slides!

· projects — start putting slides together — can use LaTeX.
short write-up due Fri 9th, 5pm.

① 2/28/12

Last time: $O(N^{3/2})$ alg. for applying interaction matrix $a_{ij} = \ln\frac{1}{|y_i - y_j|}$ to vector x_j of charges, the (2d Laplace kernel) between N particles

Assuming? uniformly distributed in rectangle.

Trick: (M boxes)  nearby: sum directly. far boxes: eval multipole expansion.

Relies on A matrix coming from elliptic PDE.

Why is $\vec{x} \mapsto A\vec{x}$ important to apply fast?

- enables iterative soln. ("Krylov" methods: apply A repeatedly) of large Nyström lin. sys. for BVP.
- Other apps: compute forces in large gravitational, fluid (point vortices), molecular (electrostatic) simulation. Timestep to evolve.

note: methods are either iterative or direct

don't know how many iters needed... (ill-cond = bad!)

eg $\{$ $O(N^3)$ algs. for dense solves, Gaussian elim. / 'fast' direct solvers — Gillman colloq. this Th. $\}$ fixed effort, even for ill-cond.

Bottleneck: each target box has many $\left(\frac{N}{M}\right)$ targets at which many (M) m'pole exps have to be eval'ed.

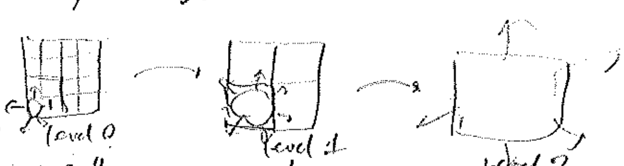
Better: combine to 'local expansion' before eval'ing at targets in box:

→ ③ 2/23/12 (see next page).

— break.

Hierarchical (multilevel) versions:

'Tree code': (small boxes w/ O(1) particles per box)

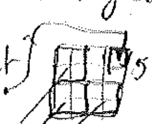


level 0 → level 1 → level 2

once got src box m'pole exps, gather in groups of 4 to give new m'pole exps (M2M) (all have same order p)

requires 'quad tree' structure: each box has a level, a list of children (unless level 0, a 'leaf' box), a parent.

↑ gathering up the tree

to eval. at targ. box:  near do directly O(1)

3 level-1 m'poles. (no local exps used).

get $O(N \ln N)$ effort ~ close to linear in N. (optimal, since must operate on each charge, & N of them).

Adaptivity:

what if not uniform? Subdivide to different levels until O(1) charges per box.

harder to code, but same scaling w/ N.

'Fast multipole method' (FMM): gather m'pole exps on way up the tree, translate (M2L) to local exps. on top-level boxes, separate local exps on way down tree. ◯ → 8 → ∞ etc.

Finally eval. local exps. on leaves at all targets; excluding O(1) nearby sources which are summed directly.

Bookkeeping tricky! at each level there are boxes not well-sep. for M2L; have to do using child boxes: interaction lists.

Effort: $O(N)$, Greengard-Rokhlin '87. Also adaptive version. 3d is much messier!

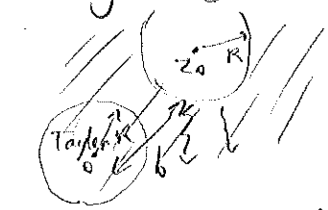
③ 2/28/12

Where's the bottleneck? If could make smaller box size L, less interactions could be done directly. But currently would have more boxes hence more effort evaluating all their m'pole exp's at the $O(N)$ distant pts!

$\Rightarrow$ Need a way to combine m'pole exp's so all target pts in a box can be eval'ed from single expansion... a 'local expansion' = Taylor expansion.

start

Say $z_0 \in \mathbb{C}$ is source box center, rep. by m'pole. @ z_0, $|z_0| \geq 2R$, then can be rep. by Taylor @ 0 in $|z|<R$.



Consider terms in m'pole,

e.g. monopole $\ln \frac{1}{z-z_0} = \ln \frac{1}{z_0} - \ln\left(\frac{z}{z_0} - 1\right)$ ↙ $\ln(x-1) = x - \frac{x^2}{2} + \frac{x^3}{3} - \dots$ for $|x|<1$.

$$= \ln \frac{1}{z_0} - \frac{1}{z_0} z + \frac{1}{2z_0^2} z^2 - \frac{1}{3z_0^3} z^3 + \dots$$

n^{th}-pole $(z-z_0)^{-n}$ has

0^{th} Taylor coeff $= (z-z_0)^{-n}\big/_{z=0} = (-z_0)^{-n} = (-1)^n z_0^{-n}$

1^{st} " " $\frac{d}{dz}\Big|_{z=0} (z-z_0)^{-n} = -n(z-z_0)^{-n-1}\Big|_{z=0} = -n(-z_0)^{-n-1} = (-1)^n z_0^{-n-1} n$

m^{th} " " $\frac{1}{m!}\frac{d^m}{dz^m}\Big|_{z=0}(z-z_0)^{-n} = \frac{1}{m!}(-1)^n n(n+1)\cdots(n+m-1) z_0^{-n-m}$

So,

$$= (-1)^n \binom{n+m-1}{n-1} z_0^{-n-m}$$

Thm (M2L, "multipole to local"): m'pole exp. $u(z) = c_0 \ln \frac{1}{z-z_0} + \sum_{n\geq 1}^{\infty} c_n (z-z_0)^{-n}$ can be written as Taylor expansion $\sum_{n=0}^{\infty} a_n z^n$, abs. convergent in $|z| < |z_0|$, with coeffs

$$\begin{cases} a_0 = c_0 \ln \frac{1}{z_0} + \sum_{n=1}^{\infty} (-1)^n z_0^{-n} c_n \\ a_m = c_0 \frac{(-1)^m}{m} z_0^{-m} + \sum_{n=1}^{\infty} (-1)^n \binom{n+m-1}{n-1} z_0^{-n-m} c_n, \quad m = 1, 2, \dots \end{cases}$$

Thm (error of M2L): if sources $\{y_j\}_{j=1}^N$ lie in $|z-z_0|<R$, $|z_0| > b+R$ for some $b>R$, then error of truncating above sums to p terms is, in $|z|<R$, bnded by $c\left(\sum_{j=1}^N |x_j|\right)\left(\frac{R}{b}\right)^p$

pf: Greengard-Rokhlin '87

Same exponential convergence rate as before; dep on $\frac{R}{b}$ tot. charge

'Far' eval. can now become:
- for each target box compute a_m coeffs due to each m'pole src box c_n's
- evaluate local (Taylor) exp at all targets in the target box.

Effort is $O(p^2 M^2)$ since p^2 to map c_n's to a_m's, & M^2 translations z_0 (many are actually same)
$+ O(pN)$ eval. p^{th}-order local exp. at all N target pts.

Total effort now $\underset{\substack{\text{S2M src-to}\\ \text{-m'pole}}}{pN} + \underbrace{\underset{\text{direct}}{9\frac{N^2}{M}} + \underset{\text{M2L}}{p^2M^2}} + \underset{\text{L2T}}{pN}$ → balance, $M = N^\gamma$

$2-\gamma = 2\gamma$, $\gamma = 2/3$

Overall scaling $O(p^2 N^{4/3})$
$= O(N^{4/3})$ if fixed p. Best yet.

Can do even better w/ heirarchical version: FMM.