Numerical Lab #2

- Eigenvalue Problems (ARPACK)
- N-Body Simulators (FMM)
- Multigrid

Overview: Lab #2

- Eigenvalue Problems
  - Algorithm Overview
  - ARPACK Introduction
- FMM in 3D
- "Hands-On" Experiments
  - Explore ARPACK
  - Multigrid Software
**ARPACK: Overview**

- **ARPACK = ARnoldi PACKage**
- ARPACK is freely available:
  - [http://www.caam.rice.edu/software/ARPACK/](http://www.caam.rice.edu/software/ARPACK/)
  - Fortran 77 code

- Solves large scale Hermitian, non-Hermitian, standard or generalized eigenvalue problems.

**ARPACK: Overview**

- Computes a few (k) eigenvalues with specified features:
  - eigenvalues of largest magnitude
  - eigenvalues of smallest magnitude
  - simultaneous computation of eigenvalues at both ends of the spectrum
- Eigenvectors also available upon request.
**ARPACK: Overview**

- Uses these driver routines:
  - dsaupd : Real double precision symmetric problems
  - dnaupd : Real double precision non-symmetric problems
  - znaupd : Complex double precision problems (Hermitian or non-Hermitian)
- For each of these, there are associated routines to compute eigenvectors.

**ARPACK: Overview**

- Uses a reverse communication interface:

```plaintext
10 continue
   call dnaupd(ido, n, which, wrk, ...)
   if (ido .eq. newprod) then
       call matvec('A',n,wrk(iptr(1)),wrk(iptr(2)))
   else
       return
   endif
   goto 10
```

- ARPACK doesn’t care how A is stored!
- Ideal when w←Av has O(n) cost.
**ARPACK: Overview**

- Requires a fixed, predetermined amount of storage.
- \( n \cdot O(k) + O(k^2) \), where
  - \( n \) = order of the matrix
  - \( k \) = number of requested eigenvalues

**ARPACK: Lab Exercises**

- Use the real non-symmetric driver to compute eigenvalues for matrices generated by MATPDE.
FMM : 3D

- See Leslie Greengard’s Ph.D. thesis:  
  *The Rapid Evaluation of Potential Fields in Particle Systems.*

FMM : 3D

- Obvious way of doing N-body simulation:
  - Compute forces on all N particles using Coulomb’s law.
  - Advance position of particles for some timestep Δt using Newton’s laws.
  - Repeat.

- Cost Per Timestep: $O(N^2)$
FMM : 3D

- FMM Goal: Do N-body simulation using only O(N) steps.
- Some N-body solvers compute forces directly - FMM computes the potential.
- Solution to Laplace's Equation:

\[
\varphi = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left( L_n^m r^n + \frac{M_n^m}{r^{n+1}} \right) Y_n^m (\theta, \phi)
\]

FMM : 3D

- Suppose that k charges of strengths \( \{q_i, i = 1...k\} \) are located at the points \( \{S_i = (\rho_i, \alpha_i, \beta_i), i = 1...k\} \), with \( |\rho_i| \leq a \), for some \( a \).
- The potential at \( \vec{r} = (\rho, \theta, \phi) \in \mathbb{R}^3 \) is

\[
\varphi(\vec{r}) = \sum_{i=1}^{k} \sum_{n=0}^{m} \frac{M_n^m}{r^{n+2}} Y_n^m (\theta, \phi)
\]

\[
M_n^m = \sum_{i=1}^{k} q_i \rho_i^n Y_n^m (\alpha_i, \beta_i)
\]
**FMM : 3D**

For some precision $\epsilon$, is we keep only $p$ terms in the expansion, we have

$$\left| \varphi(\mathbf{r}) - \sum_{n=0}^{p} \sum_{m=-n}^{n} \frac{M_n^m}{r^{n+1}} Y^m_n(\theta, \phi) \right| \leq \frac{Q}{r-a} \left( \frac{a}{r} \right)^{p+1}$$

where $Q = \sum_{i=1}^{k} |q_i|$ 

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**Basic Data Structure**

- In the 3D case, an octtree is used.
- Octree:
  - Root of tree is 3D cube containing entire system
  - Each child of a node is a subdivision of that node's region into eight equal parts
  - For a tree of depth $l$, there are $8^l$ leaves.
**Basic Data Structure (2D)**

- $l = 0$
- $l = 1$
- $l = 2$
- $l = 3$

**Basic Definitions**

- *nearest neighbor:* For box $i$ at level $l$ in the octtree, a nearest neighbor is a box at the same level of refinement which shares a boundary point with box $i$.

- *second nearest neighbor:* For box $i$ at level $l$ in the octtree, a second nearest neighbor is a box at the same level of refinement which shares a boundary point with a nearest neighbor of box $i$. 
Basic Definitions

- **Interaction list**: for box \(i\) at level \(l\), it is the set of boxes which are children of the nearest and second nearest neighbors of \(i\)'s *parent* box and the *parent* box's nearest and second nearest neighbors.

- \(\Phi_{i,l}\): the \(p\)th-order multipole expansion (about the box center) of the potential field created by the particles contained inside box \(i\) at level \(l\).

Basic Definitions

- \(\Psi_{i,l}\): the \(p\)th-order multipole expansion about the center of box \(i\) at level \(l\) describing the potential field due to all the particles outside the box and its nearest and second nearest neighbors.

- \(\Psi_{i,j}\): the \(p\)th-order multipole expansion about the center of box \(i\) at level \(l\) describing the potential field due to all the particles outside of its *parent* box and the *parent* box's nearest and second nearest neighbors.
Basic Assumptions

- All the particles are stored in an octree.

- The leaf nodes of the octree contain the particles.

- For a fixed precision $\epsilon$, we choose the number of terms in the multipole expansion to be $p$, where $p = \lceil -\log_2(\epsilon) \rceil$.

FMM Step #1 (Upward Pass)

- For all leaf nodes $i$ in the octree, form a $p^{th}$-degree multipole expansion $\Phi_{i,n,p}$, where $n$ is the depth of the octree.

- This expansion is the potential that all well-separated boxes at level $n$ will feel due to the particles in box $i$.

- Really, we just need to form the moments $M_\gamma^n$. This is the only data the other boxes would need.
FMM Step #2 (Upward Pass)

- For $l = n-1$ to 0 do
  - For all interior nodes $i$ in the octtree at level $l$, form a $p^{th}$-degree multipole expansion $\Phi_{i,l}$ by using a translation operator to shift the center of each child’s expansion to the current box center and add them together.
  - For each box, the expansion represents the potential field due to all particles contained in one box.

FMM Step #2 (Upward Pass)

- 2D Pictorial Representation:
**FMM Step #3a (Downward Pass)**

- Set $\tilde{\psi}_{1,1} = \tilde{\psi}_{1,2} = \tilde{\psi}_{1,3} = \tilde{\psi}_{1,4} = \tilde{\psi}_{1,5} = \tilde{\psi}_{1,6} = \tilde{\psi}_{1,7} = \tilde{\psi}_{1,8} = 0$

- There is no potential being felt from anything outside the octtree!

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**FMM Step #3b (Downward Pass)**

- For $l = 1$ to $n-1$ do
  - For all interior nodes $i$ in the octtree at level $l$, form $\psi_{ij}$ by translating each multipole expansion $\Phi_{ij}$ for each box $j$ in the interaction list of box $i$ to a local expansion about the center of box $i$, adding these expansions together, and adding the result to $\tilde{\psi}_{ij}$

- This accounts for all interactions that were not accounted for at the parent’s level.
FMM Step #3c (Downward Pass)

- For \( l = 1 \) to \( n-1 \) do
  - For all interior nodes \( i \) in the octtree at level \( l \), form \( \Psi_{n,i} \) for \( /s \) children by translating \( \Psi_{n,i} \) to each of the children's centers.

FMM Step #4 (Downward Pass)

- For all leaf nodes \( i \) in the octtree, form \( \Psi_{n,i} \) by translating each multipole expansion \( \Phi_{n,i} \) for each box \( j \) in the interaction list of box \( i \) to a local expansion about the center of box \( i \), adding these expansions together, and adding the result to \( \Psi_{n,i} \).

- This accounts for all interactions that were not accounted for at the parent's level, and which can be safely computed using a multipole expansion.
**FMM Step #5 (Downward Pass)**

- For all leaf nodes \( i \) in the octtree, and for each particle \( p_i \) at point \( P_i \) in the \( i^{th} \) box, evaluate \( \Psi_{n_i}(P) \).

- We have now computed the potential experienced by every particle due to those particles that are not in its nearest or second nearest neighbors.

- This is the potential which can be safely computed using a multipole expansion!

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**FMM Step #6 (Downward Pass)**

- For all leaf nodes \( i \) in the octtree, and for each particle \( p_j \) in the \( i^{th} \) box, compute interactions with all other particles within the box and its nearest and second nearest neighbors.

- These cannot be computed using a multipole expansion, and must be computed directly using the \( O(N^2) \) algorithm.
FMM Step #7 (Downward Pass)

- For all leaf nodes $i$ in the octtree, and for each particle $p_j$ in the $i^{th}$ box, add the direct terms (computed in step #6) and the far-field terms (computed in step #5) together.

Computing the Force:

- How can we compute $-\nabla \varphi$ without using finite differences?

- Recall that we have computed a complex-valued potential at each point.

- There exist formulas that allow us to compute the force directly from the complex potential.
Sample Images

- Two Point Charges in X-Y Plane:

Sample Images

- (Approximate) Ring of Charge:
Sample Images

- Two Half-Rings of Charge of Opposite Sign:

![Graph](image1.png)

Sample Images

- Sinusoidal Distribution:

![Graph](image2.png)
FMM: Parallel Implementation

- Assume distributed memory message passing environment (MPI)
- Assign each octtree node to an individual processor.
- Each processor processes the nodes it owns, blocking if information unavailable, and sending information it computes to other processors if necessary.

FMM: Parallel Implementation

![Graph: Speedup vs. Number of Processors]
ARPACK: Lab Exercises

1) Copy /scratch/tra1/ARPACK_work/* to your own workspace.
2) Type 'make all'.
3) Read (skim) dnsimp.f
4) Run dnsimp
5) Change parameters (nev, etc.) within dnsimp.f and explore.