Moore’s Law

• Every 18 months, the speed of your computer is doubled

• Every 18 months, the memory on your computer is doubled

• At the same time, the cost of your computer goes down - not quite exponentially, because the box does not become much cheaper!

• A good number to look at

\[ R_{1970} = \frac{\text{Cost of CPU time}}{\text{Cost of human time}} \]

• 1970 is the year

• Different CPUs, different humans, etc.
Observation

- \( R_{1945} \gg 1000 \)
- \( R_{1960} \gg 100 \)
- \( R_{1970} \gg 10 \)
- \( R_{1980} \sim 1 \)
- \( R_{2000} \ll 0.01 \)

- Unlike men, not all CPUs are created equal! But then, most CPUs do not vote...

- The thing is not slowing down, though eventually . . .

- What should we be doing as applied mathematicians, numerical analysts, etc.?
Consequences

- Ticket reservations
- Phone systems
- Tactical bombing
- Experimental science
- Manufacturing
- . . .
Missing from the list

- Philosophy
- Theater
- Politics
- Dealing with teen-age children
- Mathematics
- Numerical simulation of physical phenomena (????!!!)
Structure of the Talk

- Changing paradigm in the numerical use of computers
- Interaction of Moore’s law with numerical algorithms
- Characteristics of a modern numerical algorithm
- Example: rapid evaluation of radiation fields
- Pontification
Paradigm as of 1945

- Critical mission (Manhattan project, for example)
- Willingness to expend human time on programming (ouch!), debugging of the numerical scheme, interpretation
- Limited computer resources: only small-scale problems can be solved
- Extremely uncomfortable programming environment
- Air of heroism and desperation
- No difference between theoretical numerical analysts and practitioners
- Numerical approaches appropriate to small-scale problems
- Numerical algorithms usually written from scratch
Paradigm as of 1970

• Mission not necessarily critical (oil exploration, NACA airfoils, more involved aerodynamics, civil and mechanical engineering, rocket fuel stoichiometry, . . .)

• Willingness to expend human time on programming (still pretty uncomfortable), interpretation

• Improved computer capabilities; CPU time still quite expensive, but the flop rate is much higher; one can try running things at night

• The air much less heroic; most applications in non-desperate environments

• Numerical algorithms appropriate to small-scale problems

• Most numerical codes written from scratch
Paradigm as of 2000

- Mission usually not critical: computer games, medical imaging, design of fishing rods, Boeing-767’s . . .

- Limited willingness to expend human time on programming (could be fun, though!), interpretation. . . and most interpreters are not named Teller, Ulam, or Fermi. . .

- Very much improved computer capabilities; CPU time dirt cheap, and flop rate is about to become gigaflop rate

- Air not heroic at all; lots of applications, and most in non-desperate environments

- Numerical algorithms appropriate to small-scale problems

- Most numerical codes written from scratch
The Purpose of a Modern Numerical Algorithm

- Produce engineering (physical, biochemical, etc.) results with a minimum expenditure of *human* time

- CPU time is irrelevant *as long as it is affordable* (!!!)

- Note to the algorithm designer: torpedoes should not be aimed at the present location of the ship!
Illustration: Algorithms with CPU time estimates $O(n^3)$, $O(n \cdot \log(n))$

- To a large extent, the choice of the algorithm is determined by the power of one's computer (!!!)
What do We Want from a Numerical Algorithm?

- Speed, in the asymptotic sense
- Adaptivity
- Robustness
- Rapid convergence and controlled accuracy: fallacy of the “engineering accuracy” argument; high cost of low precision
- Surprise: adaptivity implies controlled condition numbers; integral vs. differential equations; fast algorithms
- Related surprise: in order to be efficient (or even simply useful), certain algorithms have to be fairly complicated (think about modern cars)
Subject of This Talk

- Talk is cheap - examples are needed
- FMMs for the Helmholtz (Maxwell’s) Equation in the “wideband” environment - explain
- Something of a misnomer - *mea culpa*
- Disclaimer: Boeing, HRL, Illinois, MadMax...
- A post-mortem for a project
- Connections with Moore’s law, etc.
FMM for the Helmholtz (Maxwell) Equation

- Function: evaluate potentials, fields, etc. of charge distributions. $N^2$ vs. $N$ or $N \cdot \log(N)$, or $N \cdot (\log(N))^2$. . .

- Does not provide discretizations, integral formulations, iterative solvers, etc. (left to the user as an exercise)

- Indifferent to all of these issues - explain

- In reality, consists of two procedures. One is used on the subwavelength scale (or in low-frequency environments), the other is used in the high-frequency environment; transition is seamless
Low-Frequency (Subwavelength) Environment

- Similar to Laplace - explain
- Very simple “bare-bones” scheme, more involved “modern” versions
- Fairly fast: (several times slower than the Laplace FMM) for groups up to 4 \( \lambda \) or so (define the groups)
- Break-even points
- Behavior as groups increase
- Serious deterioration for groups greater than 5 to 8 \( \lambda \)
- Fairly simple implementations produce acceptable results
High-Frequency Environment

- Not at all similar to the Laplace case: “oscillatory behavior”

- Example with the Moon

- “At a fixed number of points per $\lambda$, the rank of each submatrix is proportional to its size” - not quite true, Michielssen counterexample

- How bad is it?

- Let us see
At the Bottom of the Scheme

\[ V(Q_i) = \sum_{j=1}^{N} q_j \frac{e^{ik\|Q_i - P_j\|}}{\|Q_i - P_j\|} \]

Direct evaluation requires \( O(NM) \) work
At the Bottom of the Scheme II

\[ V(Q) = V(r, \theta, \phi) \approx \sum_{n=0}^{p} \sum_{m=-n}^{n} M_n^m Y_n^m(\theta, \phi) h_n(kr), \]

with multipole moments

\[ M_n^m = \sum_{j=1}^{N} q_j Y_n^{-m}(\theta_j, \phi_j) j_n(kr), \quad P_j = (r_j, \theta_j, \phi_j) \]

In the low frequency regime, the error in the multipole approximation decays like \((R/|Q|)^{p+1}\).

For our simple example, \( R/|Q| < 1/2 \), so that setting \( p = \log_2(\frac{1}{\varepsilon}) \) yields a precision of \( \varepsilon \).
At the Bottom III

- Evaluate multipole coefficients $M^m_n$ for $n = 0, \ldots, p$

- Evaluate expansion at target points $Q_j$, for $j = 1, \ldots, M$

- Total operation count: $p^2 \cdot (N + M) = (N + M) \cdot \log^2(\frac{1}{\epsilon})$

- The schemes depend critically on $p^2$ being much smaller than $N$
Hard Life at High Frequencies

\[ V(r, \theta, \phi) \approx \sum_{n=0}^{p} \sum_{m=-n}^{n} M_n^m Y_n^m(\theta, \phi) h_n(kr) \]

- Coefficients \( M_n^m \) do not start decaying until \( n > |k \cdot R| \), after which decay is extremely rapid.

- Condition \( p > |k \cdot R| + O(|k \cdot R|^{1/3}) \) is needed if we are to have any accuracy at all.
- $p$ is proportional to $\frac{R}{\lambda}$

- In BIE discretizations: fixed number of nodes per $\lambda^2$

- Thus, total number of elements in the expansion is of the same order as $N$

- None of the $O(N \cdot \log(N))$ schemes (Barnes-Hut, etc.) will work in this regime
- Another way to put it: the rank approach will not work because the ranks are high

- Cooked goose, vicious gloating

- The situation is a little better when volume distributions and volume integrals are considered, but not enough - and there is FFT-based competition

- What about order $N$ algorithms (FMMs)?
Translation Operators \((h \rightarrow h)\)

\[
\sum_{n=0}^{p} \sum_{m=-n}^{n} M_n^m Y_n^m(\theta, \phi) h_n(kr) \rightarrow \\
\rightarrow \sum_{n=0}^{p} \sum_{m=-n}^{n} N_n^m Y_n^m(\alpha, \beta) h_n(k\rho)
\]

- Cost: \(O(p^4)\)
- \(O(p^3)\) via “point and shoot” procedure
- Fatal in the BIE environment
Translation Operators \((h \rightarrow j)\)

\[
\sum_{n=0}^{p} \sum_{m=-n}^{n} M^m_n Y^m_n(\theta, \phi) h_n(kr) \rightarrow \\
\sum_{n=0}^{p} \sum_{m=-n}^{n} L^m_n Y^m_n(\alpha, \beta) j_n(k\rho)
\]

- No better than \(h \rightarrow h\)

- Dominant type of translation in an FMM
Translation Operators \((j \rightarrow j)\)

\[\sum_{n=0}^{p} \sum_{m=-n}^{n} L_n^m Y_n^m(\theta, \phi) j_n(kr) \rightarrow \]

\[\sum_{n=0}^{p} \sum_{m=-n}^{n} O_n^m Y_n^m(\alpha, \beta) j_n(k\rho)\]

- Same as \(h \rightarrow h\)
A Grim Observation

- Ranks of translation operators in the high-frequency Helmholtz (Maxwell’s, etc.) environment are proportional to the sizes of the groups in wavelengths (with subtle exceptions - Michielssen)

- For surface distributions of charges, any FMM that as much as creates translation operators will be of order at least $O(N^2)$ - horror!

- Translation operators in their “point and shoot” form reduce best possible order to $O(N^{3/2})$ - not nearly good enough

- Classical translation operators are of little use in the construction of Helmholtz FMMs, except at low frequencies
What Is Needed

- Bases in which translation operators are diagonal, or at least very sparse

- Transitions between such bases must be very sparse

- Transitions between the standard representations (partial wave expansions) and the new bases must be very sparse

- Alternatively, it should be possible to carry out the whole procedure in the “dual” bases

- Where does one find such paragons?
A Pleasant Observation

- All translation operators on a given level are diagonalized by the same unitary operator

- All diagonal forms are available analytically

- Transitions between bases (corresponding to different levels) can be done in a “fast” manner

- The whole procedure is quite simple, as long as it is understood in an appropriate weak sense
Radiation Potentials and $T_{hh}$

\[ P(r, \theta, \varphi) = \sum_{n=-\infty}^{+\infty} \sum_{m=-n}^{n} M_n^m Y_n^m(\theta, \phi) h_n(kr) \]

\[ P(\tilde{r}, \tilde{\theta}, \tilde{\varphi}) = \sum_{n=-\infty}^{\infty} \sum_{m=-n}^{n} \tilde{M}_n^m Y_n^m(\tilde{\theta}, \tilde{\phi}) h_n(k\tilde{r}) \]

Sommerfeld condition:

\[ \lim_{r \to \infty} P(r, \theta, \varphi) \cdot r \cdot e^{-i \cdot k \cdot r} = F(\theta, \phi) \]
Observation

The mapping

\[ U : \{M^m_n\} \rightarrow F(\theta, \phi) \]

diagonalizes the translation operator

\[ T_{hh} : \{M^m_n\} \rightarrow \{\tilde{M}^m_n\} \]

On the diagonal

\[ e^{i \cdot k \cdot a \cdot \cos(\psi)} \]

\((r, \theta, \varphi)\)

\((\tilde{r}, \tilde{\theta}, \tilde{\varphi})\)
Proof:

For large $r$,

$$(\bar{\theta}, \bar{\varphi}) \sim (\theta, \varphi),$$

which means that the mapping

$$U^{-1} \circ T_{hh} \circ U : F \rightarrow \bar{F}$$

is diagonal. For large $r$,

$$\bar{r} - r \sim a \cdot \cos(\psi),$$

and

$$(U^{-1} \circ T_{hh} \circ U)(\theta, \varphi) = e^{i \cdot k \cdot a \cdot \cos(\psi)}$$
What Is U?

For large $r$

$$h_m(kr) \sim \frac{e^{i \cdot k \cdot r}}{k \cdot r}$$

(up to some powers of $i$), and

$$\sum_{n=0}^{p} \sum_{m=-n}^{n} M_n^m Y_n^m(\theta, \varphi) h_n(kr) \sim \frac{e^{i \cdot k \cdot r}}{k \cdot r} \sum_{n=0}^{p} \sum_{m=-n}^{n} M_n^m Y_n^m(\theta, \varphi) = F(\theta, \varphi)$$

\[(r, \theta, \varphi)\]
\[\psi\]
\[a\]
\[(\tilde{r}, \tilde{\theta}, \tilde{\varphi})\]
What Have We Achieved?

- $T_{hh}$ is a spherical convolution; it is diagonalized by the spherical harmonic transform; its diagonal form is a function living on $S^2$.

- $T_{hh}$ is unitary; its diagonal is $e^{i \cdot k \cdot a \cdot \cos(\psi)}$

- Direct result of the Sommerfeld condition, and has been known for a long time

- And what about $T_{jj}$ and $T_{hj}$?
Diagonalizing $T_{jj}$

For large $r$

$$j_m(kr) \sim \frac{\cos(k \cdot r)}{k \cdot r}$$

(up to some phase corrections), and

$$\sum_{n=0}^{p} \sum_{m=-n}^{n} M_n^m Y_n^m(\theta, \varphi) j_n(kr) \sim$$

$$\sim \frac{\cos(k \cdot r)}{k \cdot r} \sum_{n=0}^{p} \sum_{m=-n}^{n} M_n^m Y_n^m(\theta, \varphi) = F(\theta, \varphi)$$

- A Sommerfeld condition of sorts
Diagonalizing $T_{jj}$ II

$$\sum_{n=0}^{p} \sum_{m=-n}^{n} M_n^m Y_n^m(\theta, \varphi) j_n(kr) \sim \cos(k \cdot r) \frac{1}{k \cdot r} \sum_{n=0}^{p} \sum_{m=-n}^{n} M_n^m Y_n^m(\theta, \varphi)$$

- Makes no physical sense whatsoever
- As $p \to \infty$, the limit usually does not even exist!
- First truncate, then take the limit; for this, we will pay later
- Diagonalized by the harmonic transform, same as $T_{hh}$; the same $e^{i \cdot k \cdot a \cdot \cos(\psi)}$ on the diagonal
- Purely formal expedient
Corollary

Far-field signature of a unit charge is given by the formula

\[ F(\theta, \varphi) = e^{i \cdot k \cdot a \cdot \cos(\psi)}; \]

The potential at the point \((a, \theta, \varphi)\) of the \(J\) – expansion with the far-field signature \(\sigma\) is given by the formula

\[ P(a, \theta, \varphi) = \int_{S^2} \sigma(\tilde{\theta}, \tilde{\varphi}) \cdot e^{-i \cdot k \cdot a \cdot \cos(\psi)} ds \]
What about $T_{hj}$?

- Operators $T_{hh}, T_{jj}$ are diagonal in the far-field representation, and $T_{hh} = T_{jj}$

- Furthermore,

$$T_{jj} \circ \tilde{T}_{hj} = \tilde{T}_{hj} \circ T_{hh}$$

- Inevitable consequences

- Commutative diagrams, morality, etc.
What Is On The Diagonal?

\[ \sum_{n=0}^{\infty} (2n + 1) h_n(k \rho) P_n(\cos(\psi)) \]

- “Addition theorem”

- Abramovitz and Stegun

- Series above is divergent; truncation, accuracy, dynamic range, etc.

- Usual situation with convolutions with divergent sequences

- Analysis is a little detailed; results are summarized below

- Variations: beam-like translation operators, etc.
Summary

- All translations within one level are diagonalized by the far-field signature

- Far-field signatures of charge (dipole, whatever) distributions are given by simple formulae, and fairly inexpensive to evaluate

- Far-field signatures are smooth functions on the sphere, and can be represented by tables of their values - elaborate

- Transitions between levels involve interpolation and filtering of functions on the sphere. Interpolation is easy; filtering has been taken care of (Alpert-Jacob-Chien Algorithm, Dembart and VR, etc.)
“Low-Frequency Break-Down”

- Outgoing $h$-expansion behaves as $j_n(kr)$

- Incoming $j$-expansion is a convolution of the outgoing $h$-expansion with the original (physical space) translation operator; the latter behaves as $h_n(k\rho)$

- The potential at a point within the target sphere (circle) is obtained as an inner product of the incoming $j$-expansion with a sequence behaving as $j_n(kr)$
“Low-Frequency Break-Down”

II

Behavior of Bessel Functions:

- When convolutions are done explicitly, the procedure is numerically stable as long as the spheres do not intersect (physics never lies, even if it takes a conspiracy)
“Low-Frequency Break-Down”

III

- When convolutions are done via Fourier Transforms (or via spherical transforms) the *dynamic range* of each sequence must not be large. In other words, $J_n(kr)$ must **implode** before $H_{2n}(kr)$ **explodes**

- For sufficiently large $kr$, the condition $\rho \geq 3r$ is sufficient. For smaller $r$, greater separation is needed

- Separation depends on the required accuracy, $kr$, and the machine $\varepsilon$ - explain

- In this case, a table is worth a thousand theories
“Low-Frequency Break-Down”:

Table

- Double precision calculations

  3 digits  0.25λ side of the cube
  6 digits  3.50λ side of the cube
  9 digits  12.0λ side of the cube

- Similarity with evaluation $\sin(a \cdot x)$
  via Taylor series - explain

- Marginal improvements are possible
“Low-Frequency Break-Down”: Remedy

- What does one do in the subwavelength regime?
- Use the low-frequency version of the FMM
- Transition to the high-frequency (diagonal) version at the appropriate point
- We have not tried to play with the size of the buffer
Numerical Examples
- 50 wavelengths in size
- Smallest triangle: 1.06E-6 \( \lambda \)
- Largest triangle: 2.86E-1 \( \lambda \)
- Number of triangles: 706,300
- Single node per triangle
### A-10 - Helmholtz

<table>
<thead>
<tr>
<th>$T$ (dir.)</th>
<th>Acc.</th>
<th>Error (pot.)</th>
<th>Error (grad.)</th>
<th>$T$ (sec.)</th>
<th>Mem. (Mb)</th>
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### A-10 - Laplace

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<th>Error (grad.)</th>
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</table>
Horse

- 50 wavelengths in size
- Smallest triangle: $9.34 \times 10^{-3} \lambda$
- Largest triangle: $3.27 \times 10^{-1} \lambda$
- Number of triangles: 872,694
- Single node per triangle
## Horse - Helmholtz

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<th>Error (pot.)</th>
<th>Error (grad.)</th>
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## Horse - Laplace

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</table>
Sphere

- 50 wavelengths in size
- Smallest triangle: 4.91E-2 \( \lambda \)
- Largest triangle: 6.27E-2 \( \lambda \)
- Number of triangles: 619,520
- Single node per triangle
### Sphere - Helmholtz

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<th>$T$ (dir.)</th>
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<th>Error (pot.)</th>
<th>Error (grad.)</th>
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### Sphere - Laplace

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</table>
Cube

- 50 wavelengths in size
- Smallest triangle: 9.12E-2 λ
- Largest triangle: 9.12E-2 λ
- Number of triangles: 668,352
- Single node per triangle
## Cube - Helmholtz

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<th>Error (pot.)</th>
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## Cube - Laplace

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</tr>
</tbody>
</table>
Observations

- A fairly mature technology

- Unlike the Laplace case, it is technical (as opposed to incantational), even on the most basic level - explain

- It is not enough to “invent” an order $n$ (or $n \cdot \log(n)$, or whatever) scheme any more - constants matter

- Robustness and ease of use, accuracy control, careful testing, implementation practices, etc.

- A little mathematics goes a long way - implications

- Algorithms are becoming technical and involved; have to be developed by competent groups

- An engineering discipline vs. black art
Conclusions

- Fast BIE solvers for Elliptic, parabolic, hyperbolic equations

- “Fast” algorithms for fast computers

- A different collection of collateral issues: surface descriptions, high-order discretizations, volume integrals, etc.

- Other environments involving “fastness” - Moore’s law and its consequences

- There are still some freebies left!

- What else?
Conclusions II

- Direct vs. iterative solvers

- BIEs in two dimensions

- Direct solvers for the Lippman-Schwinger equations, non-oscillatory and otherwise - scope and promise

- “Fast” SVDs and eigendecompositions

- DIRECT SOLVERS!!!

- Applications: Singular perturbation problems, problems in the vicinity of resonances, non-linear problems, inverse scattering

- INVERSE SCATTERING!!!