Fast Methods for Fast Computers

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Outline

- Introduction
  - Scaling Laws
  - Retrospective
- Economics of Computation
- The Modern Approach
  - High-Order Discretizations
  - Fast (Sparse) Decompositions
  - Well Conditioned Formulations
- Recent Work - Time Domain
- Wrapup

Introduction

- The best way to do computational physics changed when computers got big, because of scaling laws governing computational cost (FLOPs and memory) vs.
  - problem size
  - accuracy required

Thirty Years Ago

Theorists are not "practical", because they can only do simple problems.

Economics of Computation:

- Elasticity
  - A fundamental, but frequently misunderstood principle

Elasticity (1)

- Weak Form

$$\frac{d\,D}{d\,p} < 0 \qquad \frac{d\,S}{d\,p} > 0$$

- Strong Form

$$\frac{d\,(p\,D)}{d\,p} < 0 \qquad \frac{d\,(p\,S)}{d\,p} > 0$$

Elasticity (2)

If we interchange the role of currency and commodity,

$$S \longleftrightarrow p\,D$$
$$D \longleftrightarrow p\,S$$
$$p \longleftrightarrow \frac{1}{p}$$

Weak Elasticity ↔ Strong Elasticity!

Elasticity (3)

The fallacies ignore this law, for example:

- If people are taxed at a higher rate, they will work more (to reach their "target income").
- Demand for communication channels will be reduced by data compression technology.
- Computational science and engineering will replace theory and analysis.
- People will buy more computers if they have slow programs to run on them.

The New Math

- Dogma
- Analysis-Based Fast Methods
- High-Order Methods
- Well Conditioned Formulations

Dogma

- Is there a place for dogma in science or math?
- How about in art or music?

Stravinsky Dogma

I am fully aware that the words dogma and dogmatic, however sparingly one may apply them to aesthetic matters . . . , never fail to offend - even to shock - certain mentalities more rich in sincerity than strong in certitudes. For that very reason I insist all the more that you accept these terms to the full extent of their legitimate meaning, and I would advise you to recognize their validity and become familiar with them; and would hope that you will come to develop a taste for them. If I speak of the legitimate meaning of these terms, it is to emphasize the normal and natural use of the dogmatic element in any field of activity in which it becomes categorical and truly essential.

. . . Every formal process proceeds from a principle and the study of this principle requires precisely what we call dogma. . . . I use the words dogma and dogmatic, then, only insofar as they designate an element essential to safeguarding the integrity of art and mind, and I maintain that in this context they do not usurp their function.

Rokhlin Dogma

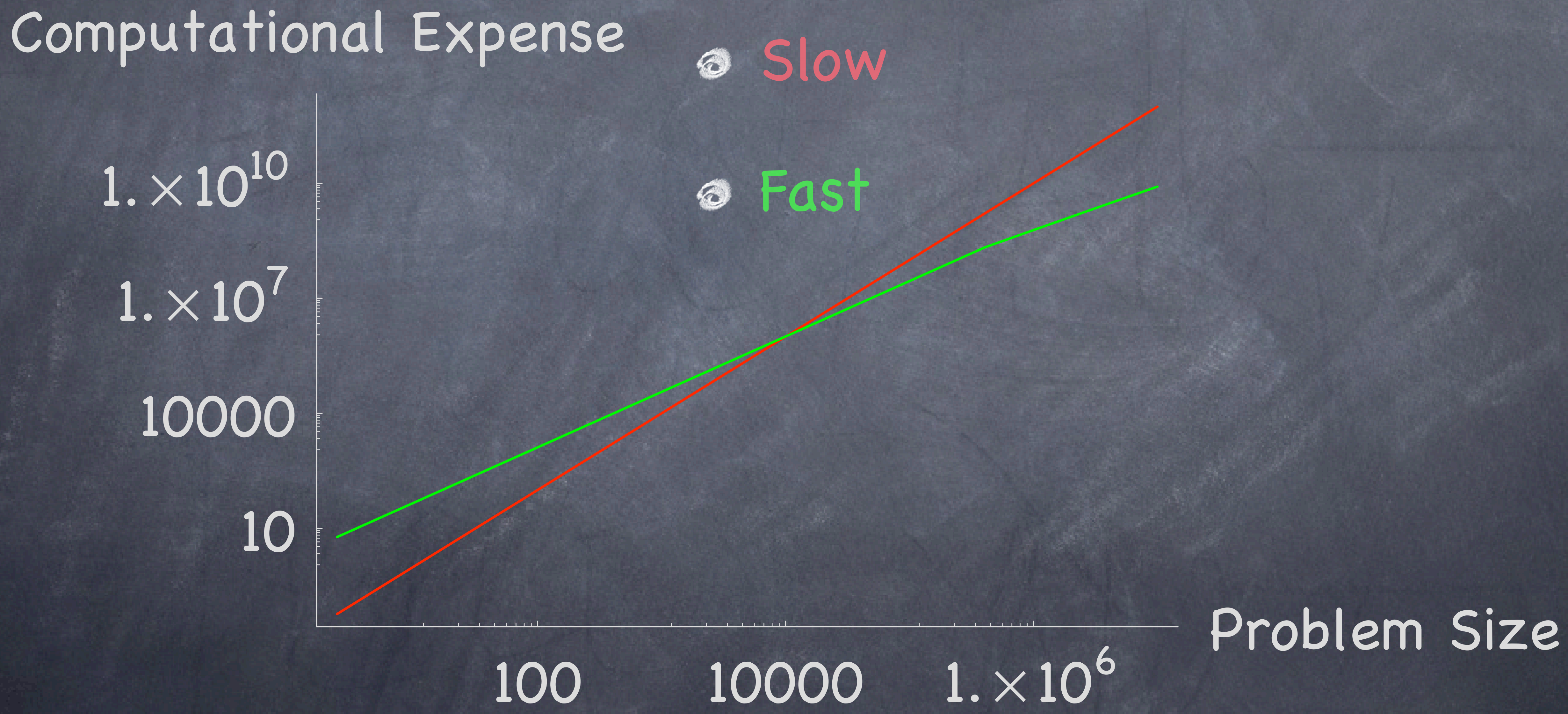
- METHODS MUST BE FAST
- ERRORS MUST BE CONTROLLED
- METHODS MUST BE HIGH ORDER
- DISCRETIZATIONS MUST BE POINT-BASED
- FORMULATIONS MUST BE WELL CONDITIONED
- GOD DID NOT INVENT POLYNOMIALS, HE INVENTED EXPONENTIALS

Any deviation will be regarded as an escape attempt.
Guards will shoot without warning.

Analysis Based Fast Methods

- FMM, Multigrid, Particle in Cell, . . .
- All amount to smart SVDs (often aided with FFTs).

The Time for Slow Methods Has Passed



Examples from Frequency Domain Computational Electromagnetics

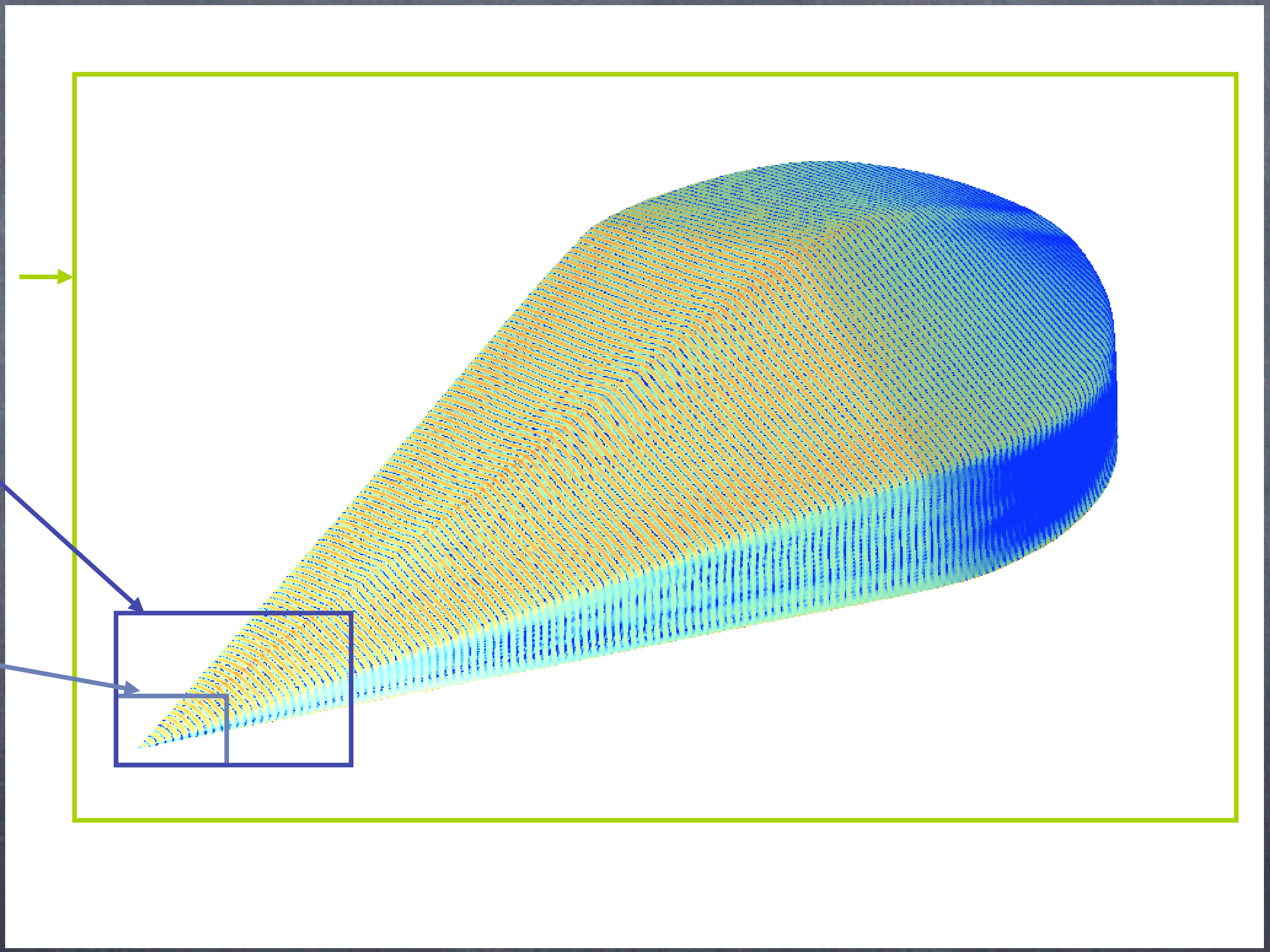
- Dart
- Sphere

Dart at 18 Ghz
State of the Art Scattering Calculations: 92 vs. 99

1999: Small supercomputer, fast methods

1999: Largest supercomputer, slow methods

1992: Largest supercomputer, slow methods



- 1999 fast methods result 10 times more accurate as well
- Could do an even bigger problem with bigger computer

State of the Art, Spheres:

1992 vs. 1999

Compare the state of the art: 1992 vs. 1999 for large spheres (courtesy of Mark Stalzer):

Year	1992	1999
Code	Patch	FastScat
Computer	Touchstone Delta	SGI O2k
# Processors	512	64
Radius / λ	5.31	60
Area / λ^2	354	45239
Accuracy (db RMS)	~ 2	0.12
# Unknowns	48672	2160000
Memory	38 GB	45.5 GB
Time	19.6 hr	27.9 hr
Cost / λ^2	~$10000	$50

- FastScat: At least 10x greater accuracy on much larger target
- For Patch to improve accuracy 10x and do R=60 sphere:
  - Roughly 1300x increase in unknowns
  - 2,200,000x increase in time
- Nine orders of magnitude improvement in seven years

The High Order Imperative

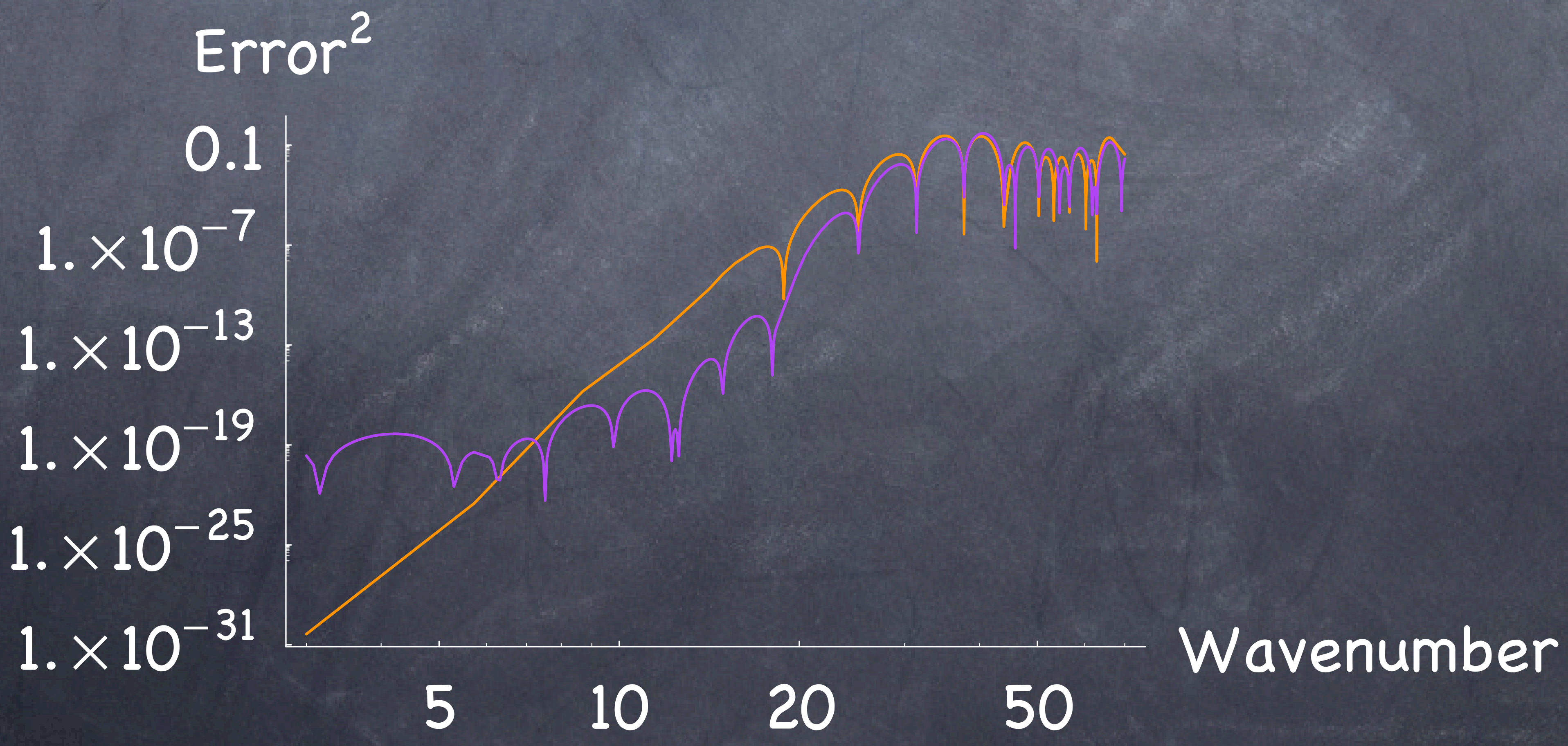
- Computed results without accuracy estimates are worthless
- It is incorrect to measure problem size by counting unknowns.
- In evaluating code efficiency, the cost of estimating the accuracy must be considered
- Low-order programs will not be tolerated

High-Order Discretizations

- Classical
  - Exact for Polynomials
  - Prototype - Gaussian Quadrature
- Neoclassical
  - Accurate for Spectrum of Sinusoids
  - Use Carefully, Don't Exhibit Classical Convergence

Square Error vs. Wavenumber

- 8 point quadrature rule - sine wave
  - > Classical
  - > Neoclassical



Well Conditioned Formulations

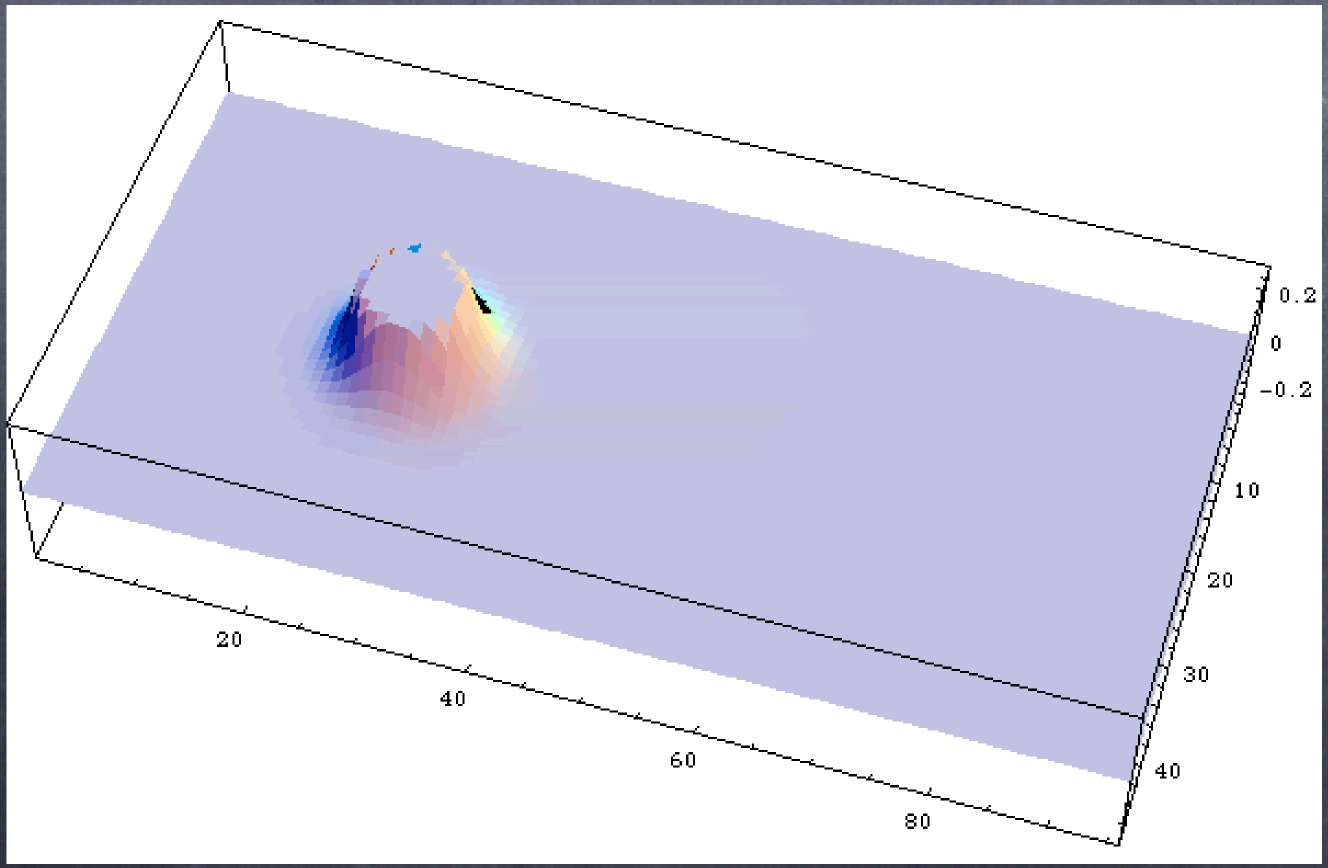
Second Kind Integral Equations and Their Close Relatives

Time Domain

- How does the Dogma apply?
  - High Order?
    - Obvious
  - Fast?
    - PWTD (= FFT(FMM))
    - BCs
  - Well Conditioned?
    - Stable (?)

Time Domain Results

- High-order, stable results
  - 2d
  - second order formulation



Current Time Domain Work

- First-order formulation
- RBCs

Wrapup

A conclusion and a couple of postscripts...

Conclusion

- Reliance on Moore's law to do bigger problems doesn't cut it, because
- As computers get bigger, the advantages of doing things carefully do also.

A Funny Thing

Nineteenth century mathematics has turned out to be more valuable that a lot of twentieth century numerical analysis.

A Cautionary Note

As the cost of computation falls, the value of programmers rises