Moreover a mathematical problem should be
difficult in order to entice us, yet not com-
pletely inaccessible, lest it mock our efforts.
It should be to us a guidepost on the mazy
path to hidden truths, and ultimately a re-
minder of our pleasure in the successful solu-
tion. ⋅⋅⋅ Besides it is an error to believe that
rigor in the proof is the enemy of simplicity.
(David Hilbert, 1900)
This lecture will make a more advanced analysis of the themes developed in Lectures 1 and 2. It will look at ‘lists and challenges’ and discuss two sets of *Ten Computational Mathematics Problems* including

\[
\int_0^\infty \cos(2x) \prod_{n=1}^\infty \cos \left( \frac{x}{n} \right) \, dx = \frac{\pi}{8}.
\]

This problem set was stimulated by Nick Trefethen’s recent more numerical *SIAM 100 Digit, 100 Dollar Challenge.*

- We start with a general description of the *Digit Challenge*† and finish with an examination of some of its components.

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*The talk is based on an article to appear in the May 2005 *Notices of the AMS*, and related resources such as [www.cs.dal.ca/~jborwein/digits.pdf](http://www.cs.dal.ca/~jborwein/digits.pdf).

†Quite full details of which are beautifully recorded on Bornemann’s website [www-m8.ma.tum.de/m3/bornemann/challengebook/](http://www-m8.ma.tum.de/m3/bornemann/challengebook/) which accompanies *The Challenge.*
Experimental Mathematics: Examples, Methods, and Implications
page 502

The Importance of MathML to Mathematics Computation
page 532

Simulating structure formation in the cosmos (see page 438)
These have a long and primarily lustrous—social constructivist—history in mathematics.

- Consider the Hilbert Problems*, the Clay Institute’s seven (million dollar) Millennium problems, or Dongarra and Sullivan’s ‘Top Ten Algorithms’.

- We turn to the story of a recent highly successful challenge.

_The book under review also makes it clear that with the continued advance of computing power and accessibility, the view that “real mathematicians don’t compute” has little traction, especially for a newer generation of mathematicians who may readily take advantage of the maturation of computational packages such as Maple, Mathematica and MATLAB._ (JMB, 2005)

*See the late Ben Yandell’s wonderful _The Honors Class: Hilbert’s Problems and Their Solvers_, A K Peters, 2001.
Numerical Analysis Then and Now

Emphasizing quite how great an advance positional notation was, Ifrah writes:

A wealthy (15th Century) German merchant, seeking to provide his son with a good business education, consulted a learned man as to which European institution offered the best training. “If you only want him to be able to cope with addition and subtraction,” the expert replied, “then any French or German university will do. But if you are intent on your son going on to multiplication and division – assuming that he has sufficient gifts – then you will have to send him to Italy. (Georges Ifrah*)

George Phillips has accurately called Archimedes the first numerical analyst. In the process of obtaining his famous estimate
\[ 3 + \frac{10}{71} < \pi < 3 + \frac{10}{70} \]
he had to master notions of recursion without computers, interval analysis without zero or positional arithmetic, and trigonometry without any of our modern analytic scaffolding ...

A modern computer algebra system can tell one that
\[ 0 < \int_0^1 \frac{(1-x)^4 x^4}{1+x^2} \, dx = \frac{22}{7} - \pi, \tag{1} \]
since the integral may be interpreted as the area under a positive curve.

We are though no wiser as to why! If, however, we ask the same system to compute the indefinite integral, we are likely to be told that
\[ \int_0^t \cdot = \frac{1}{7} t^7 - \frac{2}{3} t^6 + t^5 - \frac{4}{3} t^3 + 4 t - 4 \arctan(t). \]

Now (1) is rigourously established by differentiation and an appeal to the Fundamental theorem of calculus.
Archimedes’ method for $\pi$ with 6- and 12-gons

A random walk on one million digits of $\pi$
• While there were many fine arithmeticians over the next 1500 years, Ifrah’s anecdote above shows how little had changed, other than to get worse, before the Renaissance.

• By the 19th Century, Archimedes had finally been outstripped both as a theorist, and as an (applied) numerical analyst:

In 1831, Fourier’s posthumous work on equations showed 33 figures of solution, got with enormous labour. Thinking this is a good opportunity to illustrate the superiority of the method of W. G. Horner, not yet known in France, and not much known in England, I proposed to one of my classes, in 1841, to beat Fourier on this point, as a Christmas exercise. I received several answers, agreeing with each other, to 50 places of decimals. In 1848, I repeated the proposal, requesting that 50 places might be exceeded: I obtained answers of 75, 65, 63, 58, 57, and 52 places.* (Augustus De Morgan)

A pictorial proof

- De Morgan seems to have been one of the first to mistrust William Shanks’s epic computations of Pi—to 527, 607 and 727 places, noting there were too few sevens.

- But the error was only confirmed three quarters of a century later in 1944 by Ferguson with the help of a calculator in the last pre-computer calculations of $\pi$.*

- Until around 1950 a “computer” was still a person and ENIAC was an “Electronic Numerical Integrator and Calculator” on which Metropolis and Reitwiesner computed Pi to 2037 places in 1948 and confirmed that there were the expected number of sevens.

*A Guinness record for finding an error in math literature?
Reitwiesner, then working at the Ballistics Research Laboratory, Aberdeen Proving Ground in Maryland, starts his article with:

_Early in June, 1949, Professor John von Neumann expressed an interest in the possibility that the ENIAC might sometime be employed to determine the value of \( \pi \) and \( e \) to many decimal places with a view to toward obtaining a statistical measure of the randomness of distribution of the digits._

The paper notes that \( e \) appears to be _too random_—this is now proven—and ends by respecting an oft-neglected ‘best-practice’:

_Values of the auxiliary numbers \( \arccot 5 \) and \( \arccot 239 \) to 2035D ... have been deposited in the library of Brown University and the UMT file of MTAC._

- Just as layers of software, hardware & middleware have stabilized, so have their roles in scientific and especially mathematical computing.
Thirty years ago, LP texts concentrated on ‘Y2K’-like tricks for limiting storage demands.

– Now serious users and researchers will often happily run large-scale problems in MATLAB and other broad spectrum packages, or rely on NAG library routines.

– While such out-sourcing or commoditization of scientific computation and numerical analysis is not without its drawbacks, the analogy with automobile driving in 1905 and 2005 is apt.

– We are now in possession of mature—not to be confused with ‘error-free’—technologies. We can be fairly comfortable that Mathematica is sensibly handling round-off or cancelation error, using reasonable termination criteria etc.

– Below the hood, Maple is optimizing polynomial computations using tools like Horner’s rule, running multiple algorithms when there is no clear best choice, and switching to reduced complexity (Karatsuba or FFT-based) multiplication when accuracy so demands.*

*Though, it would be nice if all vendors allowed as much peering under the bonnet as Maple does.
About the Contest

In a 1992 essay “The Definition of Numerical Analysis”*. Trefethen engagingly demolishes the conventional definition of Numerical Analysis as “the science of rounding errors”. He explores how this hyperbolic view emerged and finishes by writing:

I believe that the existence of finite algorithms for certain problems, together with other historical forces, has distracted us for decades from a balanced view of numerical analysis. ... For guidance to the future we should study not Gaussian elimination and its beguiling stability properties, but the diabolically fast conjugate gradient iteration, or Greengard and Rokhlin’s $O(N)$ multipole algorithm for particle simulations, or the exponential convergence of spectral methods for solving certain PDEs, or the convergence in $O(N)$ iteration achieved by multigrid methods for many kinds of problems, or even Borwein and Borwein’s magical AGM iteration for determining 1,000,000 digits of $\pi$ in the blink of an eye. That is the heart of numerical analysis.

In *SIAM News* (Jan 2002), Trefethen listed ten diverse problems used in teaching *modern* graduate numerical analysis in Oxford. Readers were challenged to compute 10 digits of each, with a dollar per digit ($100) prize to the best entry. Trefethen wrote,

"*If anyone gets 50 digits in total, I will be impressed.*"

- And he was, 94 teams from 25 nations submitted results. Twenty of these teams received a full 100 points (10 correct digits for each problem).

  - They included the late John Boersma working with Fred Simons and others, Gaston Gonnet (a *Maple* founder) and Robert Israel, a team containing Carl Devore, and the current authors variously working alone and with others.

  - An originally anonymous donor, William J. Browning, provided funds for a $100 award to each of the twenty perfect teams.

  - JMB, David Bailey* and Greg Fee entered, but failed to qualify for an award.†

*Bailey wrote the introduction to the book under review.
†We took Nick at his word and turned in 85 digits!
The purpose of computing is insight, not numbers.* (Richard Hamming)

#1. What is \( \lim_{\epsilon \to 0} \int_{\epsilon}^{1} x^{-1} \cos(x^{-1} \log x) \, dx \)?

#2. A photon moving at speed 1 in the \( x-y \) plane starts at \( t = 0 \) at \( (x, y) = (1/2, 1/10) \) heading due east. Around every integer lattice point \( (i, j) \) in the plane, a circular mirror of radius \( 1/3 \) has been erected. How far from the origin is the photon at \( t = 10 \)?

#3. The infinite matrix \( A \) with entries \( a_{11} = 1, a_{12} = 1/2, a_{21} = 1/3, a_{13} = 1/4, a_{22} = 1/5, a_{31} = 1/6 \), etc., is a bounded operator on \( \ell^2 \). What is \( \|A\| \)?

#4. What is the global minimum of the function

\[
\exp(\sin(50x)) + \sin(60e^y) + \sin(70 \sin x) + \sin(\sin(80y)) - \sin(10(x + y)) + (x^2 + y^2)/4
\]

#5. Let \( f(z) = 1/\Gamma(z) \), where \( \Gamma(z) \) is the gamma function, and let \( p(z) \) be the cubic polynomial that best approximates \( f(z) \) on the unit disk in the supremum norm \( || \cdot ||_\infty \). What is \( ||f - p||_\infty \)?

#6. A flea starts at \((0, 0)\) on the infinite 2-D integer lattice and executes a biased random walk: At each step it hops north or south with probability \( 1/4 \), east with probability \( 1/4 + \epsilon \), and west with probability \( 1/4 - \epsilon \). The probability that the flea returns to \((0, 0)\) sometime during its wanderings is \( 1/2 \). What is \( \epsilon \)?

#7. Let \( A \) be the \( 20000 \times 20000 \) matrix whose entries are zero everywhere except for the primes \( 2, 3, 5, 7, \ldots, 224737 \) along the main diagonal and the number 1 in all the positions \( a_{ij} \) with \( |i - j| = 1, 2, 4, 8, \ldots, 16384 \). What is the \((1, 1)\) entry of \( A^{-1} \).
#8. A square plate $[-1, 1] \times [-1, 1]$ is at temperature $u = 0$. At time $t = 0$ the temperature is increased to $u = 5$ along one of the four sides while being held at $u = 0$ along the other three sides, and heat then flows into the plate according to $u_t = \Delta u$. When does the temperature reach $u = 1$ at the center of the plate?

#9. The integral $I(\alpha) = \int_{0}^{2} [2 + \sin(10\alpha)]x^\alpha \sin(\alpha/(2 - x)) dx$ depends on the parameter $\alpha$. What is the value $\alpha \in [0, 5]$ at which $I(\alpha)$ achieves its maximum?

#10. A particle at the center of a $10 \times 1$ rectangle undergoes Brownian motion (i.e., 2-D random walk with infinitesimal step lengths) till it hits the boundary. What is the probability that it hits at one of the ends rather than at one of the sides?

Answers correct to 40 digits are at

web.comlab.ox.ac.uk/oucl/work/nick.trefethen/hundred.html
Success in solving these problems requires a broad knowledge of mathematics and numerical analysis, together with significant computational effort, to obtain solutions and ensure correctness of the results.

- The strengths and limitations of Maple, Mathematica, Matlab (The 3Ms), and other software tools such as PARI or GAP, are strikingly revealed in these ventures.

- Almost all of the solvers relied in large part on one or more of these three packages, and while most solvers attempted to confirm their results, there was no explicit requirement for proofs to be provided.

In December 2002, Keller wrote:

To the Editor: ... found it surprising that no proof of the correctness of the answers was given. Omitting such proofs is the accepted procedure in scientific computing. However, in a contest for calculating precise digits, one might have hoped for more.

Joseph B. Keller, Stanford University
Keller’s request for proofs as opposed to compelling evidence of correctness is, in this context, somewhat unreasonable and even in the long-term somewhat counter-productive. Nonetheless, the *The Challenge* makes a complete and cogent response to Keller and much much more. The interest in the contest has extended to *The Challenge*, which has already received reviews in places such as *Science* where mathematics is not often seen.

- **Different readers, depending on temperament, tools and training will find the same problem more or less interesting** and more or less challenging.

- **Problems can be read independently**: multiple solution techniques are given, background, implementation details—variously in each of the 3Ms or otherwise—and extensions are discussed.

- **Each problem has its own chapter and lead author**: Folkmar Bornemann, Dirk Laurie, Stan Wagon and Jörg Waldvogel come from 4 countries on 3 continents and did not know each other, though Dirk did visit Jörge and Stan visited Folkmar as they were finishing up.
The book proves the growing power of collaboration, networking and the grid—both human and computational. A careful reading yields proofs of correctness for all problems except for #1, #3 and #5.

- For #5 one difficulty is to develop a robust interval implementation for both complex computation and, more importantly, for the Gamma function. Error bounds for #1 may be out of reach, but an analytic solution to #3 seems tantalizingly close.

- The authors ultimately provided 10,000-digit solutions to nine of the problems. They say that this improved their knowledge on several fronts as well as being ‘cool’.

  — success with Integer Relation Methods often demands ultrahigh precision computation.

- One (and only one) problem remains totally intractable —by this rarefied measure. As of today only 300 digits of #3 are known.
The authors* were surprised by the following:

#1. The best algorithm for 10,000 digits was the trusty *trapezoidal rule*—a not uncommon personal experience of mine.

#2. Using *interval arithmetic* with starting intervals of size smaller than $10^{-5000}$, one can still find the position of the particle at time 2000 (not just time ten), which makes a fine exercise for very high-precision interval computation.

#4. Interval analysis algorithms can handle similar problems in higher dimensions. As a foretaste of future graphic tools, one can solve this problem using current *adaptive 3-D plotting* routines which can catch all the bumps.

As an optimizer by background this was the first problem my group solved using a damped Newton method.

*Stan Wagon and Folkmar Bornemann, private communications.*
#5. While almost all canned optimization algorithms failed, differential evolution, a relatively new type of evolutionary algorithm worked quite well.

#6 This has an almost-closed form via elliptic integrals and leads to a study of random walks on hypercubic lattices, and Watson integrals.

#9. The maximum parameter is expressible in terms of a MeijerG function. Unlike most contestants, Mathematica and Maple both figure this out.

— This is another measure of the changing environment.* It is a good idea—and not at all immoral—to data-mine and find out what your one of the 3Ms knows about your current object of interest. Thus, Maple says:

The Meijer G function is defined by the inverse Laplace transform

\[
\text{MeijerG}\left(\begin{array}{c} \{a_s, b_s\} \\ \{c_s, d_s\} \end{array} \rangle, z \right) = \frac{1}{2\pi i} \int_{L} \frac{\Gamma(1-a_s+y)\Gamma(c_s-y)y}{\Gamma(b_s-y)\Gamma(1-d_s+y)} \, dx
\]

where ...

*As is Lambert W, see Brian Hayes’ Why W?
Two Big Surprises

Two solutions really surprised the authors: #7 Too Large to be Easy, Too Small to Be Hard.

Not so long ago a 20,000 × 20,000 matrix was large enough to be hard. Using both congruential and \(p\)-adic methods, Dumas, Turner and Wan obtained a fully symbolic answer, a rational with a 97,000-digit numerator and like denominator. Wan has reduced the time needed to 15 minutes on one machine, from using many days on many machines.

- While \(p\)-adic analysis is parallelizable it is less easy than with congruential methods; the need for better parallel algorithms lurks below the surface of much modern computational math.

- The surprise here, though, is not that the solution is rational, but that it can be explicitly constructed.

The chapter, like the others offers an interesting menu of numeric and exact solution strategies. Of course, in any numeric approach ill-conditioning rears its ugly head while the use of sparsity and other core topics come into play.
Problem #10: Hitting the Ends

(My personal favourite, for reasons that may be apparent.) Bornemann starts the chapter by exploring Monte-Carlo methods, which are shown to be impracticable.

- He then reformulates the problem deterministically as the value at the center of a $10 \times 1$ rectangle of an appropriate harmonic measure of the ends, arising from a 5-point discretization of Laplace's equation with Dirichlet boundary conditions.

- This is then solved by a well chosen sparse Cholesky solver. At this point a reliable numerical value of

$$3.837587979 \cdot 10^{-7}$$

is obtained.

And the posed problem is solved numerically to the requisite 10 places.

But this is only the warm up ...
**Analytic Solutions**

We proceed to develop two analytic solutions, the first using *separation of variables* on the underlying PDE on a general $2a \times 2b$ rectangle. We learn that

$$p(a, b) = \frac{4}{\pi} \sum_{k=0}^{\infty} \frac{(-1)^k}{2k + 1} \text{sech}\left(\frac{(2k + 1)\pi}{2\rho}\right)$$  \hspace{1cm} (2)

where $\rho := a/b$.

A second method using *conformal mappings*, yields

$$\arccot \rho = p(a, b) \frac{\pi}{2} + \text{arg} K\left(e^{ip(a,b)\pi}\right)$$  \hspace{1cm} (3)

where $K$ is the *complete elliptic integral* of the first kind.

- It will not be apparent to one unfamiliar with inversion of elliptic integrals that (2) and (3) encode the same solution—though they must as the solution is unique in $(0, 1)$—and each can now be used to solve for $\rho = 10$ to arbitrary precision.

*As with the trapezoidal rule, easy can be good.*
Bornemann finally shows that, for far from simple reasons, the answer is

\[ p = \frac{2}{\pi} \arcsin (k_{100}), \tag{4} \]

where

\[ k_{100} := \left( (3 - 2 \sqrt{2}) (2 + \sqrt{5}) (-3 + \sqrt{10}) (-\sqrt{2} + \frac{4}{5}) \right)^2 \]

- No one anticipated a closed form like this—a simple composition of Pi, one arcsin and a few square roots.*

▷ Let me show how to finish up the feast.

*Actually fundamental units of real (quadratic/quartic) fields; solutions to Pell’s equation.
An apt result in *Pi and the AGM* is that
\[
\sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} \operatorname{sech} \left( \frac{\pi (2n+1)}{2} \rho \right) = \frac{1}{2} \arcsin k, \tag{5}
\]

exactly when \(k \rho^2\) is parametrized by *theta functions* in terms of the *elliptic nome* as Jacobi discovered.

We have thus gotten
\[
k \rho^2 = \frac{\theta_2^2(q)}{\theta_3^2(q)} = \frac{\sum_{n=-\infty}^{\infty} q^{(n+1/2)^2}}{\sum_{n=-\infty}^{\infty} q^{n^2}} \quad q := e^{-\pi \rho}. \tag{6}
\]

Comparing (5) and (2) we see that the solution is
\[
k_{100} = 6.02806910155971082882540712292\ldots \times 10^{-7}
\]
as asserted in (4).

- The explicit form follows from 19th century *modular function theory*.

- If only Trefethen had asked for a \(\sqrt{210} \times 1\) box, or even better a \(\sqrt{15} \times \sqrt{14}\) one.

  - \(k_{15/14}\) and \(k_{210}\) share their units (*Pi & AGM*).
A Singular Interlude

Indeed $k_{210}$ is the singular value sent to Hardy in Ramanujan’s famous 1913 letter of introduction—ignored by two other famous English mathematicians.

$$k_{210} := \left(\sqrt{2} - 1\right)^2 \left(\sqrt{3} - 2\right) \left(\sqrt{7} - 6\right)^2 \left(8 - 3\sqrt{7}\right) \times \left(\sqrt{10} - 3\right)^2 \left(\sqrt{15} - \sqrt{14}\right) \left(4 - \sqrt{15}\right)^2 \left(6 - \sqrt{35}\right)$$

That is an occasion at which one would have liked to be present. Hardy, with his combination of remorseless clarity and intellectual panache (he was very English, but in argument he showed the characteristics that Latin minds have often assumed to be their own): Littlewood, imaginative, powerful, humorous. Apparently it did not take them long. Before midnight they knew, and knew for certain. The writer of these manuscripts was a man of genius. That was as much as they could judge, that night. It was only later that Hardy decided that Ramanujan was, in terms of natural mathematical genius, in the class of Gauss and Euler: but that he could not expect, because of the defects of his education, and because he had come on the scene too late in the line of mathematical history, to make a contribution on the same scale.

GH Hardy (1877–1947)

CP Snow’s description in A Mathematician’s Apology
A Modern Finale

Alternatively, armed only with the knowledge that the singular values are always algebraic we may finish with an *au courant* proof: numerically obtain the minimal polynomial from a high precision computation with (6) and recover the surds.

*Maple* allows the following

```maple
> Digits:=100:with(PolynomialTools):
> k:=s->evalf(EllipticModulus(exp(-Pi*sqrt(s))));
> p:=latex(MinimalPolynomial(k(100),12)):
> 'Error',fsolve(p)[1]-evalf(k(100)); galois(p);
```

```
-106
  Error,  4 10

"8T9", {"D(4)[x]2", "E(8):2"}, "+", 16, {"(4 5)(6 7)", 
  5)(26)(3 7)", "(1 8)(2 3)(4 5)(6 7)"}, "(2 8)(1 3)(4 6)
```

This finds the minimal polynomial for $k_{100}$, checks it to 100 places, tells us the *galois group*, and returns a latex expression ‘p’ which sets as:

$$1 - 1658904 \_X - 3317540 \_X^2 + 1657944 \_X^3 + 6637254 \_X^4$$

$$+ 1657944 \_X^5 - 3317540 \_X^6 - 1658904 \_X^7 + \_X^8,$$

and is *self-reciprocal*:
It satisfies \( p(x) = x^8 p(1/x). \)

This suggests taking a square root and we discover

\[
y = \sqrt{k_{100}} \text{ satisfies } p(y) = 1 - 1288y + 20y^2 - 1288y^3 - 26y^4 + 1288y^5 + 20y^6 + 1288y^7 + y^8.
\]

Now life is good. The prime factors of 100 are 2 and 5 prompting:

\[
\text{subs(_X=z,[op(((factor(p,{sqrt(2),sqrt(5)}))))])})
\]

The code yields four quadratic terms, the desired one being

\[
q = z^2 + 322z - 228z\sqrt{2} + 144z\sqrt{5} - 102z\sqrt{2}\sqrt{5} + 323 - 228\sqrt{2} + 144\sqrt{5} - 102\sqrt{2}\sqrt{5}.
\]

For security,

\[
w:=\text{solve}(q)[2]: \ \text{evalf}[1000](k(100)-w^2);
\]

gives a 1000-digit error check of \( 2.20226255 \cdot 10^{-998} \).

- We can work a little more to find, using one of the 3Ms, the beautiful form of \( k_{100} \) given in (4).