MAA Short Course on
Experimental Mathematics in Action
in Association with the 2006 Combined Meetings

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Abstract

The last twenty years have been witness to a fundamental shift in the way mathematics is practiced. With the continued advance of computing power and accessibility, the view that "real mathematicians don't compute" no longer has any traction for a newer generation of mathematicians that can readily take advantage of computer aided research, especially given the maturity of modern computational packages such as *Maple*, *Mathematica* and *Matlab*.

The goal in this course is to present a coherent variety of *accessible* examples of modern mathematics where intelligent computing plays a significant role and in so doing to highlight some of the key algorithms and to teach some of the key experimental approaches.

1 Overview

A coded message, for example, might represent gibberish to one person and valuable information to another. Consider the number 14159265... Depending on your prior knowledge, or lack thereof, it is either a meaningless random sequence of digits, or else

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the fractional part of pi, an important piece of scientific information.
(Hans Christian von Baeyer)[1]

The short course is in the spirit of the two recent books by Jonathan Borwein and David Bailey, *Mathematics by Experiment: Plausible Reasoning in the 21st Century* (2004) and *Experimentation in Mathematics: Computational Paths to Discovery* (2004), the latter with Roland Girgensohn. These texts will serve as a good primer for what is to be expected, though the specific topic lectures in the course are primarily new material.

A synopsis of the evolving role of computational experimentation in mathematics will constitute roughly half of the material and should be interesting to novices and experts alike. The remaining half of the material will consist of specific examples used to illustrate and amplify the issues involved in doing mathematics by experiment. These case studies will be largely self-contained and will be accessible from the background provided with each of the topics.

Time will be provided to discuss some of the philosophical, pedagogical and methodological implications. Participants should come away with a better appreciation for and ability to exercise the methods of experimental mathematics. Additional information can be found on the website `http://www.expmath.info`.

2 Level of the Material

The material will be broadly accessible to those with an undergraduate degree in mathematics. An overview of the evolving role of computational experimentation in mathematics will constitute roughly one-half of the material and should be interesting to beginners and experts alike. The course is in the spirit of the two recent books by Jonathan Borwein and David Bailey, *Mathematics by Experiment* (2004) and *Experimentation in Mathematics* (2004), the latter with Roland Girgensohn. These texts will serve as a good primer for what is to be expected, though the majority of the specific topics in the course will be new material. The remainder of the course will consist of specific examples used to illustrate and amplify the issues involved in doing mathematics by experiment. These will be largely self-contained and accessible with the background provided with each of the topics.

While a working knowledge of some mathematical computing package is an advantage, it is certainly not a prerequisite. Additionally, the course will be "hands-on" for those who wish to follow along using their laptops, via a wireless Internet connection, using tools available at `http://www.expmath.info`, a web site that has been established to support the books *Mathematics by Experiment* and*Experimentation in Mathematics*. A preliminary program is listed below. In addition, *Maple* and other software producers will assist.

[1]On page 11 of his recent book *Information The New Language of Science*, Weidenfeld and Nicolson, 2003.

3 Preliminary Course Outline

DAY ONE

9:00am–10:15am. *What is Experimental Mathematics?* (Borwein)

10:15am–10:45am. Break

10:45am–Noon. *Case Study I. Integrals and Series using Mathematica* (Moll)

Noon–2:00pm. Lunch

2:00pm–3:15pm. *Algorithms for Experimental Mathematics I* (Bailey)

3:15pm–3:45pm. Break

3:45pm–5:00pm. *Case Study II. Discrete Math and Number Theory in Maple & C^{++}* (Calkin)

5:00pm–6:30pm. Reception for participants

DAY TWO

9:00am–10:15am. *Case Study III. Inverse Scattering in Matlab* (Luke)

10:15am–10:45am. Break

10:45am–Noon. *Case Study IV. Analysis and Probability on the Computer* (Girgensohn)

Noon–2:00pm. Lunch

2:00pm–3:15pm *Algorithms for Experimental Mathematics II* (Bailey)

3:15pm–3:45pm. Break

3:45pm–5:00pm. *Concluding Examples. Putting Everything Together* (Borwein)

4 Course Description

This course will introduce the audience to the field of experimental mathematics, which we broadly define as the utilization of modern computer technology as an active tool for mathematical research. The material presented will: (1) introduce and define what is meant by "experimental mathematics"; (2) give numerous specific (and accessible) examples of experimental mathematics in action; (3) explain and give examples of some algorithms commonly used in experimental mathematics; (4) give a taste of using the general computational approach in one or two areas where computational methods heretofore have not played a major role.

Because of the highly accessible nature of much of this material, we hope to appeal to a fairly wide audience, ranging from bright undergraduates and beginning graduate students to senior research mathematicians. Indeed, we believe we will be able to convey the excitement of this field to all of our audience.

Introduction and Conclusion (Borwein). In the introductory session I shall set the context for the short course. Aided by elementary examples and using current we tools, I aim to discuss the history of experimentation in Mathematics—from the earliest times to the recent computationally solution of Kepler's problem—and to consider philosophical issues relating to the use of inductive methods in mathematics teaching and in research. To illustrate, Donald Knuth[2] recently asked for a closed form evaluation of:

$$\sum_{k=1}^{\infty} \left\{ \frac{k^k}{k!\, e^k} - \frac{1}{\sqrt{2\,\pi\, k}} \right\} = -0.084069508727655\ldots.$$

It is today easy to compute 20 or 200 digits of this sum. The 'smart lookup' facility in the *Inverse Symbolic Calculator*[3] rapidly returns

$$0.084069508727655 \approx \frac{2}{3} + \frac{\zeta\,(1/2)}{\sqrt{2\,\pi}}\,.$$

We thus have a prediction which *Maple* 9.5 on a laptop confirms to 100 places in under 6 seconds and to 500 in 40 seconds. Arguably we are done—*after all we have an evaluation!*—but even the formal proof can now be done with greater speed and confidence.

In the concluding session I shall return to these themes and explore what we have seen and learned while introducing some meatier examples—many of them also taken from the pages of the *American Mathematical Monthly.*

Algorithms I & II (Bailey). In the first algorithm session, I will give an overview of a number of basic algorithms commonly used in experimental mathematics, including the "PSLQ" integer relation algorithm, which is widely used to numerically discover new mathematical identities. I will then present several basic examples of using these algorithms, for example the 1995 discovery of the "BBP" algorithm for π:

$$\pi = \sum_{k=0}^{\infty} \frac{1}{16^k} \left(\frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6} \right), \tag{1}$$

which permits binary or hexadecimal digits of π to be calculated beginning at an arbitrary position in the expansion. Several follow-on results will be mentioned, such as the recent discovery by myself and Richard Crandall that these BBP formulas have significant implications for the question of the normality of constants such as π and $\log 2$.

[2]Posed as *MAA Problem* 10832, November 2002.

[3]Available at `http://www.cecm.sfu.ca/projects/ISC/ISCmain.html`

In the second algorithms session, I will mention a number of additional algorithms in widespread use in experimental mathematics, including: (1) a brief overview of techniques for high-precision arithmetic; (2) high-precision evaluation of common transcendental functions; and (3) high-precision evaluation of integrals and series. I will then present a variety of specific examples using these techniques to find new mathematical results. I will illustrate these methods by using computer-based tools to solve some problems "in real time."

Case Study I. Integrals and Series (Moll). The problem of evaluation of definite integrals was one of the central topics in Analysis of the $19^{th}-$century. H. J. Stephen Smith, in his retirement address as President of the London Mathematical Society stated

> ... *I will now hazard the assertion, that (after all) the advancement of the Integral Calculus is at once the most arduous and the most important task to which a mathematician can address himself.*

The evaluation of interesting definite integrals was much more popular and respected then than it is today. The appearance of symbolic languages like *Mathematica, Maple* and others has revived the quest for efficient algorithms to address this problem. This part of the course will present several classes of problems that can be solved with the current version of *Mathematica*. We will also discuss how to use integrals and symbolic languages to generate interesting mathematical problems: for example, the integrals

$$f_j = \int_0^{\pi/2} \ln^j \sin x \, dx$$

turns out to be a homogeneous polynomial (of degree $j+1$) in the "variables" $a = \ln 2$, $b = \pi$ and $x_n = \zeta(n)$ provided we assign a and b weight 1 and x_n weight n. For example,

$$f_2 = \frac{1}{2}a^2 b + \frac{1}{24}b^3 \text{ and } f_3 = -\frac{1}{2}a^3 b - \frac{1}{8}ab^3 - \frac{3}{4}bx_3.$$

We will provide a guided tour of the proofs of some of the evaluations given in the classical *Table of Integrals, Series, and Products* [5][4] and in [6].

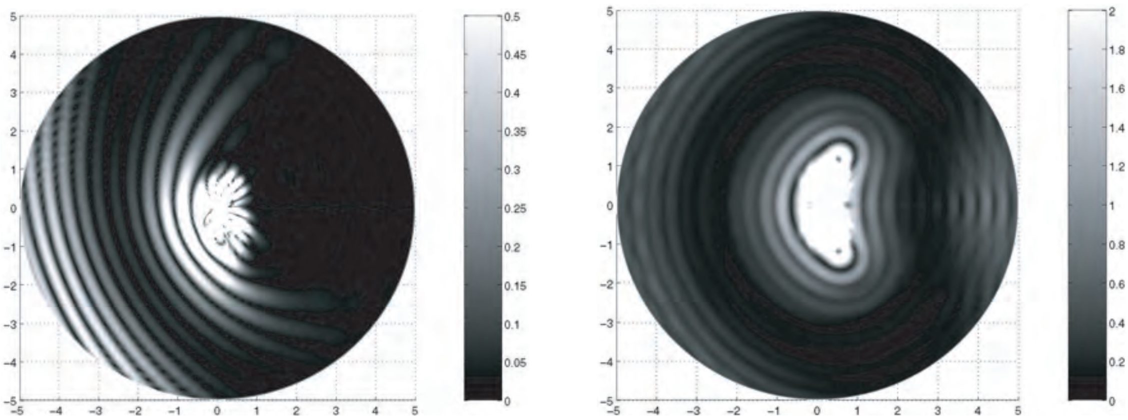
Case Study II. Discrete Mathematics and Number Theory (Calkin). *Developing and analyzing some probabilistic models for factorization algorithms.* In the past few years there has been substantial progress in the size of integers which can be factored into a product of primes. For some integers (for example, $2^n \pm 1$) there are specialized algorithms which are faster, but for general integers the best algorithms are the (simple) Quadratic Sieve and the (faster, but much more complicated) Number Field Sieve. Each of these relies upon generating a set S of vectors in Z_2^k, and finding a linear dependency in this set. Currently, the approach taken is to take $|S| > k$ to ensure that the set is linearly dependent: we discuss various probabilistic models which suggest is linearly dependent: we discuss various probabilistic models which suggest that we can speed things up by terminating with (substantially) fewer than k vectors. In particular, we will highlight

[4]See also `http://www.math.tulane.edu/~vhm/Table.html`.

some early failed models, indicating how and why they fail, and how we came to realize that the models were flawed. We will also illustrate the interplay of different computing environments (in particular, *Maple* and C/C^{++}) in the experiments we perform.

This is joint work, initiated at the Clemson Research Experience for Undergraduate (REU), 2004, with two undergraduates, Kim Bowman and Zach Cochran, two graduate students, Tim Flowers and Shannon Purvis, and the co-supervisor of the REU, Kevin James.

Case Study III. Inverse Scattering (Luke). Inverse scattering is a field that has seen dramatic changes in the last 8 years. Many of the recent advances are the fruits of mathematical analysis validated and, in some cases, lead by computer aided exploration. The key development has been the exploitation of previously undesirable properties, such as ill-posedness and ill-conditioning, in order to determine qualitative properties of some unknown specimen. We illustrate the interplay between theory, simulation and experimentation with a simple example of nonlinear inverse scattering. In this example, we seek to design algorithms for reconstructing objects from measurements of a scattered field (electromagnetic or acoustic) at an array of sensors far away from the object. This has applications from medical to military.



Reconstruction of a two dimensional nonconvex impenetrable scatterer from multiple views and multiple frequencies via qualitative optimization techniques.

Conventional optimization approaches to solving this problem were influenced by traditional uses of computers to model and *simulate* the physical processes that generate the data. The traditional optimization approach amounts to finding a closest fit, in some sense, of the model to the data. The problem to this approach is that it assumes that one knows a priori which model is appropriate. Beginning in the mid 1990's a newer generation of algorithms began to appear that had a distinctly different flavor. This newer approach uses the data to construct an oracle that, in effect, serves as an indicator function for qualitative queries about the nature of the objects, such as "how many", "where", "what shape", "what index of refraction", and so forth. The oracle requires no a priori assumption about a model for the data. These newer techniques have been very successful and can be applied in a wide variety of settings. What is vexing about them, however, is that the proof that they work is, so far, limited to a few special cases. This is an instance of the numerical experimentation leading mathematical analysis and suggesting new directions of inquiry in mathematics.

Case Study IV. Analysis and Probability (Girgensohn). *Investigating strange functions on the computer.* The computer affords an excellent tool for the visualization and analysis of "pathological" functions — such as nowhere differentiable or singular or a.e. discontinuous functions. In this case study we shall explore two examples of such an analysis. Our first example concerns the *Weierstrass functions*

$$C_{a;b}(x) = \sum_{n=0}^{\infty} a^n \cos(b^n \cdot b\pi x), \qquad S_{a;b}(x) = \sum_{n=0}^{\infty} a^n \sin(b^n \cdot b\pi x);$$

for $|a| < 1, b > 1$. Some special cases of these functions were given in 1872 by Weierstrass as the first prominent examples for *continuous but nowhere differentiable functions.* In general, these functions are nowhere differentiable when $|a|b > 1$, but only recently have simple proofs of this fact have discovered. We will show how such a proof (for integer b) can be discovered on the computer. Our second example concerns certain *infinite convolutions of the Bernoulli measure* ($P(\{+1\}) = P(\{-1\}) = \frac{1}{2}$). Their distribution functions are either purely singular or absolutely continuous, but a precise classification of these two cases is open. We will demonstrate an approach to this problem on the computer.

5 Instructors

David Bailey, Chief Technologist, Computational Research Dept., Lawrence Berkeley Lab. Dr. Bailey received a B.S. in mathematics from Brigham Young University in 1972 and a Ph.D. in mathematics from Stanford University in 1976. He worked as a computational mathematician at the U.S. Dept. of Defense, SRI International, and, for nearly 15 years, at NASA's Ames Research Center in California. Since 1998 he has been at the Lawrence Berkeley Laboratory, where he is Chief Technologist of the Computational Research Department. Dr. Bailey has received several major awards, including the Sid Fernbach Award from the IEEE Computer Society (1993) and the Chauvenet Prize from the Mathematical Association of America (1993).

Dr. Bailey's published research includes studies in numerical analysis, parallel computing, high-precision arithmetic, fast Fourier transforms, supercomputer performance, computational number theory and experimental mathematics. He is co-author with Borwein of the recently published books *Mathematics by Experiment* and *Experimentation in Mathematics.* His website is `http://crd.lbl.gov/~dhbailey`.

Jonathan Borwein, FRSC, Research Chair, Faculty of Computer Science, Dalhousie University. Dr. Borwein was Shrum Professor of Science (1993–2003) and a Canada Research Chair in Information Technology at Simon Fraser University, and was founding Director of the *Centre for Experimental and Constructive Mathematics.* In 2004, he (re-)joined the Faculty of Computer Science at Dalhousie as a Canada Research Chair in Distributed and Collaborative Research. He was born in St Andrews in 1951, and received his D Phil from Oxford in 1974, as a Rhodes Scholar. Prior to joining SFU he worked at Dalhousie (1974–91), Carnegie-Mellon (1980-82) and Waterloo (1991–93). He has received various awards including the Chauvenet Prize (93), Fellowship in the Royal Society of Canada (94), Fellowship in the American Association for the Advancement of Science (02), an honorary degree from Limoges (99), and foreign membership in the Bulgarian Academy of Sciences (03).

Dr. Borwein is Governor at large of the MAA (2004–07) and a past President of the Canadian Mathematical Society (2000–02). He is a Member of the WestGrid Executive (`http://www.westgrid.ca`) and chairs the International Math Union's Committee on Electronic Information and Communications, `http://www.ceic.math.ca`, 2002–06. His interests span pure (analysis), applied (optimization), computational (numerical and computational analysis) mathematics, and high performance computing. He has authored ten books (most recently two on Experimental Mathematics (`http://www.expmath.info` and a monograph on Variational Analysis) and over 250 journal articles, and is co-founder (1995) of a software company, MathResources (`http://www.mathresources.com`), producing highly interactive CD and Network tools primarily for school and university mathematics.

Neil Calkin, Associate Professor of Mathematical Sciences at Clemson University. Neil Calkin, Associate Professor in the Department of Mathematical Sciences at Clemson University. Dr. Calkin was educated at Cambridge University and received his Ph.D. from the Department of Combinatorics and Optimization at the University of Waterloo under the guidance of Ian Goulden. Prior to joining the faculty at Clemson University in 1997, he was the Zeev Nehari Visiting Assistant Professor of Mathematics at Carnegie Mellon University (1988-1991), and held a regular faculty position at the Georgia Institute of Technology (1991-1997). For the past three years he has co-supervised an NSF funded Research Experience for Undergraduates in Number Theory and Combinatorics, with an emphasis on the connection between experimentation and computation, conjecture and proof.

In 1994, Dr. Calkin co-founded, with Herbert S. Wilf, the Electronic Journal of Combinatorics, and served as managing editor until 2000: he continues to follow developments in the field of electronic publishing. He enjoys all areas of mathematics, but is particularly interested in the use of probabilistic methods in combinatorics and number theory. His work has appeared in a variety of journals, including the American Math. Monthly, the Electronic Journal of Combinatorics, Acta Arithmetica and Experimental Mathematics. His website is `www.math.clemson.edu/faculty/Calkin`.

Russell Luke, Assistant Professor of Mathematical Sciences at the University of Delaware. Dr. Luke received his PhD in June of 2001 under the supervision of Prof. James Burke at the University of Washington. Prior to joining the faculty at the University of Delaware, he held positions at the Institut für Numerische und Angewandte Mathematik at the Universität Göttingen (2001-2003) and the Pacific Institute for the Mathematical Sciences at Simon Fraser University (2002-2004). Dr. Luke is the recipient of a NASA/GSFC Graduate Student Fellowship (1998-2001) and a Pacific Institute for the Mathematical Sciences Postdoctoral Fellowship (2002-2004). His recent work on optical and acoustic image reconstruction has appeared in *SIAM Review*, *SIAM Journal on Control and Optimization*, *SIAM Journal on Applied Mathematics* and the *Journal of the Optical Society* *of America A*, among others.

Victor Moll, Professor of Mathematics at Tulane University, New Orleans, Louisiana received a B.S. in Mathematics from Universidad Santa Maria in Valparaiso, Chile and a Ph. D. in mathematics from the Courant Institute under the guidance of Henry McKean. He has been in the faculty at Tulane University since 1986. After some initial work on partial differential equations, he has been working on the mathematics related to the evaluation of definite integrals since 1992. This research has connections with Number Theory (many definite integrals are real numbers with interesting number-theoretical properties, for instance the special values of the Riemann zeta function), Combinatorics and (surprisingly) Dynamical Systems. The cover of the Notices of the American Mathematical Society, March 2002, volume 49 has a picture that is related to the evaluation of the integral of a rational function. *The field is full of surprises.*

He enjoys working with undergraduate and graduate students and has published several papers with them. He is also the author of two books: *Elliptic Curves* (joint with Henry McKean), on a subject orthogonal to his thesis work and *Irresistible Integrals* (joint with his former student George Boros), both published by Cambridge University Press. His website is `www.math.tulane.edu/~vhm`.

References

[1] D.H. Bailey and J.M Borwein, "Experimental Mathematics: Examples, Methods and Implications," in press , 2004. [CoLab Preprint 269].

[2] D.H. Bailey, J.M. Borwein, V. Kapoor and E. Weisstein, "Ten Problems of Experimental Mathematics," in press, 2004. [CoLab Preprint 270].

[3] J.M. Borwein and D.H. Bailey *Mathematics by Experiment: Plausible Reasoning in the 21st Century,* AK Peters Ltd, 2004.

[4] J.M. Borwein, D.H. Bailey and R.Girgensohn, *Experimentation in Mathematics: Computational Paths to Discovery,* AK Peters Ltd, 2004.

[5] I. S. Gradshteyn, I. M. Rhyzik, A. Jeffrey, D. Zwillinger, *Table of Integrals, Series, and Products*

[6] George Boros and Victor Moll *Irresistible Integrals,* Academic Press, 2004.

All papers, including an extended sample of [3, 4] are available through `www.expmath.info`.