Computer experiments in harmonic analysis

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1 Introduction

The steady march of Moore’s law—predicting the exponential increase in computing power—and the striking accretion of computer-assisted mathematical results have drawn increasing attention to the role and promise of computers in mathematics. 1 Computers have become important at many different stages of mathematical practice: they help to build intuitions, formulate conjectures, expedite computations and manipulations, and even produce proofs. Philosophical treatments of computers in mathematics have produced insights into central problems in mathematical ontology (what is mathematics about?) and epistemology (how do we know mathematical truths?). In particular, the burgeoning utility of computers has bolstered arguments against mathematics as a purely deductive science, suggesting that certain of its aspects and practices are ineluctably shaped by inductive observations and reasoning.

It is often stressed that computer methods allow mathematical researchers to explore phenomena whose initial complexity makes them effectively inaccessible to pen-and-paper modes of investigation. Computers have a great power to store and rapidly process large amounts of information in a systematic way which, with clever human insight and guidance, can yield results to varying degrees of rigor. Ever-growing databases and ever-more-sophisticated

1For an entry point into this literature, see the papers in the bibliography below and sources cited therein.
software are making more and more mathematical problems tractable for more and more mathematicians.

These computational tools lead to two broad classes of results. One type produces proofs which make direct use of computation as part of a mathematical argument, the most famous examples of which include proofs of the Four Color Theorem and Kepler’s Conjecture. Particularly within formal mathematics and mathematical logic, computer-assisted and computer-verified proofs are now commonplace, and sometimes even preferred over their more traditional counterparts. This paper describes a case study in the second type of result, where computers provide essential intuitions and aid in the formulation of problems, but do not play a role in formally establishing proofs of conclusions.

The first class might be called computer-assisted results, where the second might better be understood as computer-inspired proofs. Computers play fundamentally different roles in each case. In the first, they act as supplemental mathematicians, performing work that is instrumental to the properly mathematical reasoning of an argument or proof. In the second, they are supplements *to* mathematicians, providing essentially non-mathematical assistance to facilitate a strictly mathematical investigation or demonstration.

Yet, as supplements to mathematicians, computers used for the second purpose are not innocent bystanders to mathematical production. Computers can define new areas of inquiry and make old problems more or less important by furnishing new applications or ways of thinking. In the case considered here, the use of computers informs both the selection of problems and the range of possible solutions. So, even as their role is secondary—supplying intuitions and ruling out unpromising theoretical avenues—they have direct effects on the primary mathematical work of proving.

The work described here differs in some ways from the standard case studies in computer mathematics. The problem under consideration and the body of theorems and proofs thusfar amassed toward its solution are strictly non-computational: computers aid intuitions and suggest directions of study without entering into what is often called the ‘mathematics itself.’ At the same time, computation has been the principal tool of investigation, with formal proofs entering only at a very late stage. The research is not driven by cutting-edge computer algorithms or techniques; instead, its use of computers is in the rapid analysis of large data sets—turning patterns into formulas, which are turned into numbers, which are then used to understand
the system at hand. Thus, computers are simultaneously at the core and the periphery of the mathematical practice in play here. They are indispensable tools for creative mathematical work while remaining just that: mere tools.

2 Harmonic Analysis on Fractals

Computer exploration has long been at the center of the study of dynamical systems and fractals. Dynamical systems are systems whose states change according to a fixed set of rules. Computers can store single system states and apply their respective rules over and over to give information to varying degrees of rigor about the behavior of the system as it changes. There are two main ways of defining fractals. One, closely linked with dynamical systems, defines fractals as chaotic systems produced by deceptively simple rules. Famous examples include the Mandelbrot and Julia sets (figure 1), and a wide family of ‘strange attractors’. Computers have been indispensable in visualizing and understanding these fractals, although many of the most important results about these sets have been derived without the aid of computers. The second kind of fractal, the one considered below, is a self-similar system defined, like its chaotic cousin, by a collection of simple rules which gives the fractal a high degree of structure. These fractal objects challenge one’s typical intuitions from geometry or analysis, generally having non-integer dimensions and other unusual properties. (The ones considered below, for instance, can host entirely localized waves.)

At Cornell University, from 2006–2007, I worked with Robert Strichartz and Luke Rogers to investigate second order differential equations on the Sierpinski Gasket. Similar equations can be used to describe the propagation of waves on a string, of heat on a metal rod or sheet, or of sound through a three-dimensional medium. Because of its association with the propagation of sound and the techniques used for such studies, this area of mathematics is often called harmonic analysis. From the early 1990s, mathematics researchers have investigated how similar phenomena might work in media which are fundamentally different from the Euclidean line, plane, or space. A standard object of study is the triangular Sierpinski gasket (figure 2). The Sierpinski gasket (SG) is formed by taking a triangle and repeatedly reconstructing it out of three smaller copies of itself. The limiting object has a dimension of \( \frac{\log 3}{\log 2} \), and is made up of three smaller copies of itself.

Early in the study of harmonic analysis on SG, it was established by
Kigami and others that one can determine basic information about second
derivatives (such as are needed for second order differential equations) by
merely examining the relationship between the first and second stages of SG’s
construction. Its self-similarity properties then guarantee that any mathe-
matics performed on these crude approximations can be extended to the
actual gasket. For SG, these basic calculations can be performed by hand,
and their results can be used by computers to model the flow of waves on
the actual gasket (figure 3).

My work explored a different direction for the relation between crude
approximation and computer extension. Keeping just to the crudest approx-

Figure 1: The Mandelbrot set and an associated Julia set, from
http://aleph0.clarku.edu/~djoyce/julia/.

Figure 2: Construction of the Sierpinski Gasket.
Figure 3: ‘Sine-waves’ on the Sierpinski Gasket, generated in Matlab by Adam Allan.
imations to the fractal, I studied the relationship between second derivatives on SG and its higher dimensional analogues. The next dimension up from the triangular SG is the tetrahedral $SG_4$ (figure 4). By sequentially adding vertices and edges to the starting figures for constructing a gasket, one can produce a gasket with meaningful second derivatives with any finite number of ‘boundary vertices’. Shapes thus expand from triangles, to tetrahedra, to hyper-pyramids of increasing dimension. Our question was whether something could be said in the case where, instead of three or four boundary points, there was an infinite number of them. It was quickly established that the most straightforward way of producing second derivatives on increasingly large-boundaried gaskets gave, in the limit, a trivial outcome, one in which no theoretical wave could propagate. To explore other constructions, we turned to computers.

Figure 4: Construction of $SG_4$, a tetrahedral Sierpinski Gasket.

In the first several attempts to produce a non-trivial infinite gasket, computer computations helped to establish negative results. We started with different techniques which successfully produced variations on SG, abstracted those techniques into general patterns, and input those patterns into a computer program. This first computer program used the derived patterns to generate formulas describing increasingly large gaskets. These formulas were fed into a second computer program which performed numerical calculations to indicate whether a given technique from SG might successfully be adapted for higher-dimensional gaskets. Eventually, the first computer program was designed to generate a full sequence of commands for the second computer program, so that the two could be run in sequence with minimal input on our part. This allowed us to test variations on gaskets with full descriptions whose size meant that we could not practically write them down by hand.
with any confidence in our accuracy.

The computer thus played the role typically taken in computer-assisted proofs, processing large amounts of data behind the scenes based upon human-inputed patterns and instructions for transforming those known patterns into proper surrogates for the mathematical objects under investigation. On the one hand, our computers functioned in the same way as computer-provers. They plodded through large numbers of cases which would not be hand-checkable. On the other hand, they had a more genuinely experimental role, searching through a selected subset of possible cases for evidence to suggest whether similar cases held any promise for theoretical or further computer investigation. Transforming patterns into formulas, the computers worked as mechanical mathematicians. Testing these formulas for theoretical fruitfulness, the computers shifted into new roles as rapid handlers of large amounts of numerical data.

After a large number of possible avenues had been ruled out, our computers transitioned into a more strictly experimental usage. They still used human-inputed patterns to generate computer protocols which in turn yielded numerical information about the systems in question. But instead of testing whether a particular mathematical approach was likely to succeed, they were used to explore the details of an approach which we already believed would work, but were just not sure how. Computer analyses served to build intuitions to aid in the study of an abstract mathematical system.

The approach in this second stage of work derived from Sabot's analysis of these gaskets in terms of lower-dimensional sub-gaskets (figure 5). Sabot established that second derivatives of gaskets of the sort we were studying could be understood in terms of the fixed points of an iterative map relating two sets of parameters: the first describing the edges of the fractal and the second describing how they are scaled to produce the next level of in the fractal's construction. Iterating relationships between two sets of parameters is something computers happen to do quite well, and is a basic technique in the study of dynamical systems.

The data at hand were thus highly amenable to computation, but so too was the mathematics. The systems under consideration were known to vary continuously when perturbed, so the sorts of approximations necessitated in our computations did not unduly affect their outcomes. Moreover, enough general features of fractal gaskets were understood so as to make meaningful the scattered data generated in computation, as well as to direct future computations. It cannot be forgotten that computer-assisted or computer-
inspired mathematics requires that computers be given meaningful inputs, and in such a way as to produce meaningful outputs. Both inputs and outputs acquire their mathematical meaning not from the computer but from the mathematician. In our case, computers were used to visualize how second derivatives on various gaskets change when different parameters are modified (figure 6), as well as to test extremal conditions and conjectured formulas (figure 7).

Figure 6: Computer evidence relating to continuity in our parameter space.

In each case, the computer confirmed successful approaches and suggested general features of the systems in question. But they remained silent as to how to produce the non-computational theorems whose validity was strongly suggested by the data. The project of translating computer-aided intuitions into formal mathematics remains, for Rogers and myself, an ongoing task. In this sort of work, it is rare that the insights afforded by computation
Figure 7: Computer tests of extremal properties and conjectures.

correspond directly to the modes of reasoning required of exact proofs. This is particularly evident in our attempts to finish an existence proof. Where the computer’s ability to produce a valid result indicates existence of our desired mathematical object in the cases studied, a general existence proof requires a more mathematically robust characterization of all possible cases, not just the particular cases which are fit for computation.

3 Conclusions

What, then, can be said about the relationship between mathematics and computer experiment in the present case study? First, the type of mathematics being conducted makes a substantial difference to the role played by computers. Automated computation played a major role in studying transformations of systems of parameters, and so computers became important tools only at such points in the mathematical work as could be readily viewed in terms of these transforming parameters. Moreover, because the fractal objects of study conform to complicated but highly regular patterns, computers could be easily programmed to manipulate not only the data but the equations for their relationships themselves.

While the latter activity does not immediately seem like computer experiment (what about it is experimental?), one must at the same time hesitate to dissociate it from the more plausibly experimental work of testing outcomes from different combinations of parameters. Part of the experimental
work involves the passage from pattern to formula, a passage which does not itself become visible until after the computer-intensive trials make its effects visible. To the extent that we were studying the patterns underlying the constructions of our different gaskets, the part of our computer work typically excluded from the category of mathematical experiment must be reintegrated. This is so primarily because of the nature of the mathematical objects under investigation.

Second, computer experiments relate to mathematical proofs in a way which cannot be reduced to merely suggestion or inspiration and rigorous justification. The computational character of our computer mathematics reinforced our parameter space-based theoretical framework, closing off theoretical directions which could not be so readily adapted to computation. At the same time, the computations did not map directly onto the theory. The work of rigorous justification required an altogether different sort of mathematics than would be required to simply formalize the computer’s activity. It was neither a case of the computer supplying an answer from which an entirely different mathematical justification might spring, nor a case of the computer working in a way directly analogous to the mathematical theory. Rather, the computer modeled a defined range of finite approximations to the mathematical theory, suggesting how the infinite construction might proceed without drawing from the mathematics necessary for that final step.

Finally, computers worked as both numerical and theoretical black boxes. One might understand experimentation in the natural sciences as the attempt to produce from the results of different inputs into the black box of nature a better understanding of its inner-workings, or at least of its predictable behavior. We have cause, then, to think of the computer’s formal work, changing patterns into equations and further computer instructions, as just as much a part of the experimental function of the computer as its more conventional numerical derivations. In both cases, only the final outputted data and their relation to the initial specification of foundational patterns are practically comprehensible. The computer hides the transformations which relate the one to the other, and we as mathematicians worked from either side of the computer experiment to learn more about our objects of study.

Harmonic analysis, in opposition to more common case studies of computer experiment, neither takes the work of the computer as its object of study, nor uses computers as a merely instrumental route to an independently verifiable answer. By studying the practical aspects of this boundary case, we obtain a more complete picture of the complicated relationship be-
tween computer experiment and mathematics. Doing so might suggest a more meaningful theory of the practical workings of mathematical experiments.

Sources

Most of the following are available as preprints from David Bailey and Jonathan Borwein’s website, http://www.experimentalmath.info/papers/, or by following links therein.