Fooling the masses in 2017: Why the scientific computing community must still be vigilant

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DANGER AHEAD

Supercomputers operating on big data can generate nonsense faster than ever before!

Key concerns:

- Are the results statistically sound?
- Are the results numerically reliable?
- Have the results been validated using independent rigorous tests?
- Are the algorithms, data sources and processing methods well documented?
- Are performance results accurately and honestly reported?

Reproducibility crises in physics and cosmology

- In 2011, an international team of researchers at the Gran Sasso Laboratory in Italy announced that neutrinos had exceeded the speed of light, thus directly challenging Einstein's relativity. However, after months of careful checking, a subtle flaw was found in the measurement apparatus (a major embarrassment).
- In 2013, CERN researchers confirmed the discovery of the long-sought Higgs boson. But more recently, scientists have raised questions as to whether the particle discovered is really the Higgs – it might be some other particle or particles masquerading as the Higgs; additional research studies are required.
- In March 2014, researchers announced with considerable fanfare that they had detected the fingerprint of the long-hypothesized inflationary epoch, a tiny fraction after the big bang. Sadly, within a few weeks critics pointed out that their experimental results might well be due to dust in the Milky Way, pending better data.

Reproducibility crises in biomedicine, psychology, economics and finance

- In 2011, Bayer researchers reported that they were able to reproduce only 17 of 67 pharma studies.
- In 2012, Amgen researchers reported that they were able to reproduce only 6 of 53 cancer studies.
- In August 2015, the Reproduciblity Project in Virginia reported that they were able to reproduce only 39 of 100 psychology studies.
- In September 2015, the U.S. Federal Reserve was able to reproduce only 29 of 67 economics studies.
- In 2014-2015, "backtest overfitting" emerged as a major problem in computational finance.

Reproducibility Project staff
Credit: NY Times

These experiences have exposed at least one common flaw:
Only publicizing the results of successful trials introduces a bias into the results.

Reproducibility in scientific computing

A December 2012 workshop on reproducibility in computing, held at Brown University in Rhode Island, USA, noted that

> *Science is built upon the foundations of theory and experiment validated and improved through open, transparent communication. With the increasingly central role of computation in scientific discovery this means communicating all details of the computations needed for others to replicate the experiment. ... The "reproducible research" movement recognizes that traditional scientific research and publication practices now fall short of this ideal, and encourages all those involved in the production of computational science ... to facilitate and practice really reproducible research.*

- V. Stodden, D. H. Bailey, J. Borwein, R. J. LeVeque, W. Rider and W. Stein, "Setting the default to reproducible: Reproducibility in computational and experimental mathematics," `http://www.davidhbailey.com/dhbpapers/icerm-report.pdf`.

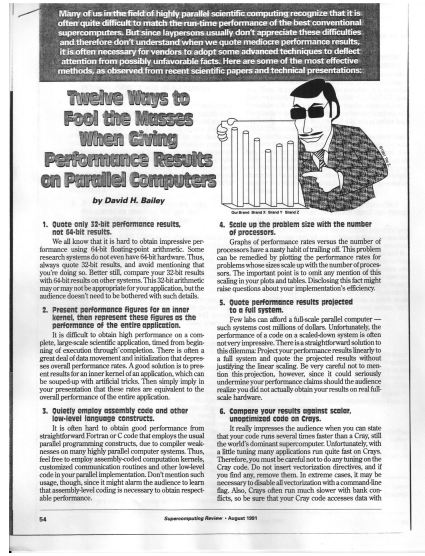
Documentation: A glaring deficiency in the scientific computing field

ICERM Report: To aid in reproducibility, computing papers should document:

- A precise statement of assertions to be made in the paper.
- A statement of the computational approach, and why it constitutes a test of hypothesis.
- Complete statements of (or references to) every algorithm employed.
- Details of auxiliary software (both research and commercial software) used.
- Details of the test environment, including hardware, system software and the number of processors utilized.
- Details of data reduction and statistical analysis methods.
- Discussion of the adequacy of parameters such as precision level and grid resolution.
- Full statement of experimental results.
- Verification and validation tests performed by the author(s).
- Availability of computer code, input data and output data.
- Instructions for repeating computational experiments described in the paper.

Parallel computing, 1991

- Many new parallel systems were offered; users were excited about potential.
- Each vendor claimed theirs was best, citing one or two selected applications.
- There were few standard benchmarks or testing methodologies — mostly Livermore Loops and original Linpack-100.
- Overall, the level of rigor and peer review in the field was disappointingly low.
- In 1991 DHB published a humorous essay Twelve Ways to Fool the Masses, poking fun at some of the abuses (authored by DHB, but with contributions from the NPB team).



Many of us in the field of highly parallel scientific computing recognize that it is often quite difficult to match the run-time performance of the best conventional supercomputers. But since laypersons usually don't appreciate these difficulties and therefore don't understand when we quote mediocre performance results, it is often necessary for vendors to adopt some advanced techniques to deflect attention from possibly unfavorable facts. Here are some of the most effective methods, as observed from recent scientific papers and technical presentations:

Twelve Ways to Fool the Masses When Giving Performance Results on Parallel Computers

by David H. Bailey

1. Quote only 32-bit performance results, not 64-bit results.

We all know that it is hard to obtain impressive performance using 64-bit floating-point arithmetic. Some research performers do not even have 64-bit hardware. Thus, always quote 32-bit results, and avoid mentioning that you're doing so. Better still, compare your 32-bit results with 64-bit results on other systems. This 32-bit arithmetic may or may not be appropriate for your application, but the audience doesn't need to be bothered with such details.

2. Present performance figures for an inner kernel, then represent these figures as the performance of the entire application.

It is difficult to obtain high performance on a complete, large-scale scientific application, timed from beginning of execution through completion. There is often a great deal of data movement and initialization that depresses overall performance rates. A good solution is to present results for an inner kernel of an application, which can be souped-up with artificial tricks. Then simply imply in your presentation that these rates are equivalent to the overall performance of the entire application.

3. Quietly employ assembly code and other low-level language constructs.

It is often hard to obtain good performance from straightforward Fortran or C code that employs the usual parallel programming constructs, due to compiler weaknesses on many highly parallel computer systems. Thus, feel free to employ assembly-coded computation kernels, customized communication routines and other low-level code in your parallel implementation. Don't mention such usage, though, since it might alarm the audience to learn that assembly-level coding is necessary to obtain respectable performance.

4. Scale up the problem size with the number of processors.

Graphs of performance rates versus the number of processors have a nasty habit of trailing off. This problem can be remedied by plotting the performance rates for problems whose sizes scale up with the number of processors. The important point is to omit any mention of this scaling in your plots and tables. Disclosing this fact might raise questions about your implementation's efficiency.

5. Quote performance results projected to a full system.

Few labs can afford a full-scale parallel computer — such systems cost millions of dollars. Unfortunately, the performance of a code on a scaled-down system is often not very impressive. There is a straightforward solution to this dilemma: Project your performance results linearly to a full system and quote the projected results without justifying the linear scaling. Be very careful not to mention this projection, however, since it could seriously undermine your performance claims should the audience realize you did not actually obtain your results on real full-scale hardware.

6. Compare your results against scalar, unoptimized code on Crays.

It really impresses the audience when you can state that your code runs several times faster than a Cray, still the world's dominant supercomputer. Unfortunately, with a little tuning many applications run quite fast on Crays. Therefore, you must be careful not to do any tuning on the Cray code. Do not insert vectorization directives, and if you find any, remove them. In extreme cases, it may be necessary to disable all vectorization with a command-line flag. Also, Crays often run much slower with bank conflicts, so be sure that your Cray code accesses data with

Twelve ways to fool the masses (paraphrased)

1. Quote 32-bit performance results, not 64-bit results, but don't mention this in paper.
2. Present performance figures for an inner kernel, then represent these figures as the performance of the entire application.
3. Quietly employ assembly code and other low-level language constructs.
4. Scale up the problem size with the number of processors, but omit any mention of this.
5. Quote performance results projected to a full system.
6. Compare your results against scalar, unoptimized code on conventional systems.
7. When run times are compared, compare with an old code on an obsolete system.
8. Base Mflop/s rates on the operation count of the parallel implementation, instead of the best practical serial algorithm.
9. Quote performance as processor utilization, parallel speedups or Mflop/s per dollar.
10. Mutilate the algorithm used in the parallel implementation to match the architecture.
11. Measure parallel run times on a dedicated system, but measure conventional run times in a busy environment.
12. If all else fails, show pretty pictures and animated videos, and don't discuss performance.

NY Times (22 Sep 1991): "Measuring How Fast Computers Really Are"

Excerpts:

- "Rival supercomputer and work station manufacturers are prone to hype, choosing the performance figures that make their own machines look best."
- "It's like the Wild West." [quoting David J. Kuck of UIUC].
- "It's not really to the point of widespread fraud, but if people aren't a little more circumspect, the entire field could start to get a bad name." [quoting DHB].

14 F THE NEW YORK TIMES, SUNDAY, SEPTEMBER 22, 1991

Technology

Measuring How Fast Computers Really Are

By JOHN MARKOFF

IN the world of scientific and technical computing, everyone agrees that computer speeds are increasing at a geometric rate. But measuring that speed is a vexing task. Rival supercomputer and work station manufacturers are prone to hype, choosing the performance figures that make their own machines look best.

"It's like the Wild West," said David J. Kuck, of the Center for Supercomputing Research and Development at the University of Illinois. "They say whatever they want to."

In fact, said David H. Bailey, a scientist at the National Aeronautics and Space Administration, "It's not really to the point of widespread fraud, but if people aren't a little more circumspect, the entire field could start to get a bad name."

The matter is complicated by a new generation of computers that have dozens, or even thousands, of separate processors. These parallel computers split problems into small parts and solve them simultaneously to reach greater speeds.

As a result, dozens of programs for determining benchmarks — measurements of computer speed — have been developed by scientists at universities and in government agencies. Some are based on how long a computer takes to solve a certain set of equations, while more sophisticated benchmarks attempt to match the operations required by real-world programs. But each benchmark generally measures only a single aspect of computer performance.

Just as a car buyer might buy a vehicle with the highest E.P.A. gas mileage rating for the price, a computer buyer could use benchmarks in deciding which machine to buy. But like their counterparts in the auto business, computer makers would do well to remind customers, "Your mileage may vary." The industry has no independent organization, analogous to the Environmental Protection Agency, to establish a single standard.

The proliferation of benchmarks is particularly problematic among the fastest scientific machines, where more than a dozen start-up companies compete to sell to university, corporate and Government laboratories.

These machines sell for hundreds of thousands of dollars or more, and the sale of only a few can mean success for a company. Supercomputers and smaller scientific work stations work on problems ranging from designing pharmaceuticals and weapons to weather modeling and the simulated crashing of automobiles.

Uneasy about the tendency for manufacturers to cite inflated claims, Mr. Bailey of NASA wrote a tongue-in-cheek indictment of performance claims for Supercomputing Review magazine in August. Titled "Twelve Ways to Fool the Masses When Giving Performance Results on Parallel Computers," it pokes fun at the tendency of computer makers to play fast and loose with speed claims.

It is common practice to "tune" computers and software to score better on benchmarks. "I know of a couple of companies who have full-time people, and all they do is optimize programs to achieve better benchmark results," said Gary Smaby, president of the Smaby Group, a consulting and market research firm in Minneapolis.

Such optimization is permissible under the rules established by benchmark designers to insure that computer makers can extract the full capability from their systems.

But some manufacturers go further and insert modules called "recognizers" into their compilers — software that translates a programmer's instructions into machine-readable form. When the recognizer finds a clue that points to a benchmark, it employs a specially written program that is designed to run a benchmark as quickly as possible.

Computer scientists say recognizers can be used to short-circuit the benchmark-measuring process and should be banned.

Today the most widely cited benchmark is Linpack. It is a set of linear algebra equations that requires a very large number of mathematical calculations to solve. Currently, the highest Linpack by a traditional supercomputer, measured in millions of mathematical calculations per second, is held by a Cray Y/MP. Its record: 403 million floating point calculations per second.

There is a similar Linpack measure for makers of massively parallel computers, and this summer the lead seesawed back and forth between Intel's Delta supercomputer and Thinking Machines' CM-200 Connection Machine. At the moment the Intel Delta has achieved the highest Linpack measure, 11.9 billion floating point calculations per second.

The Linpack benchmark results are expressed as several numbers, including the actual speed at solving the equations and another number called "theoretical peak performance," which represents a computer's absolute peak efficiency. In practice, computers generally reach only a small fraction of their theoretical peak speed.

Linpack was developed as part of an appendix to a book written by a University of Tennessee computer scientist, Jack Dongarra, in 1979. "The original benchmark was an accident," he said. "We were writing a book and were attempting to give the user a feeling for how fast particular computers could solve a problems."

The problem, Mr. Dongarra said, was chosen so that it could be run on all of the 20 machines that were being compared. There are now Linpack numbers for more than 500 machines, from laptops to supercomputers.

Mr. Dongarra acknowledges that Linpack is a limited measure, and he is working on a second-generation measure named Lapack. But a number of other researchers have developed alternative benchmarks in an effort to provide a more complete profile of computer performance.

One recently introduced benchmark is called Slalom, developed by John Gustafson, a mathematician at the Department of Energy's Ames Laboratory. "I worked in industry for several years, and I was frustrated by inaccuracy and general lack of credibility in the ways we had of measuring computer performance," he said.

Rather than measuring how quickly a computer can solve a particular problem, Slalom attempts to measure how much work a computer can complete in one minute.

The problem computers must calculate as part of the Slalom benchmark is measuring the interplay of light in a room in which each surface is painted a different color. A particularly powerful computer will obtain higher resolution in one minute of computing time than a slower one.

One strength of Slalom is that it measures several aspects of computer performance, including the time taken to set up a problem. Hightest on the Slalom scale is the experimental Intel Delta supercomputer, installed at the California Institute of Technology.

ANOTHER approach has been taken by scientists at the Center for Supercomputing Research and Development at the University of Illinois. The group, called the Perfect Club, has composed a set of speed tests it calls the Perfect Benchmarks, a set of programs that are closely patterned after real programs run by scientific computers.

These benchmarks attempt to get as close as possible to the ultimate test of a computer's performance — the actual programs that it will run. "The only important benchmark for most customers is the code they intend to run, and there is no substitute for that," Mr. Smaby said. ■

Different Benchmarks, Different Winners

The six fastest computers according to various benchmarks. The Linpack benchmark expresses the results in Mflops, or millions of floating point operations per second. Slalom, the only one of these to cover massively parallel machines, measures the amount of work accomplished in a set amount of time. The Perfect benchmark is expressed as an average of 13 different Mflop measures.

LINPACK		SLALOM		PERFECT	
Cray Y-MP/16	403	Intel Delta	5,700	Cray Y-MP/832	128.4
NEC SX-3/14	314	Siemens S600/20	5,610	Cray Y-MP/416	75.9
Cray Y-MP/832	275	Cray Y-MP/8D	5,120	Siemens S400/10	26.2
Fujitsu VP2600/10	249	Cray 2S/4	4,204	Cray 2S/4-128	22.5
Cray X-MP/416	178	nCUBE 2	3,736	NEC SX-2	18.4*
Cray 2S/4-128	129	Fujitsu VP400-EX	2,598	Hitachi S-820/80	17.1*

Sources: Oak Ridge National Laboratory, Supercomputing Review, University of Illinois, University of Tennessee

* Computed on partial data as some data points missing.

The New York Times

Examples of abuses: Scaling performance results to full-sized system

In some published papers and conference presentations, runs were performed on smaller systems, then performance rates were linearly scaled to full-sized systems, in some cases without even clearly disclosing this fact.

Example: 8,192-CPU performance results were linearly scaled to 65,536-CPU results, simply by multiplying by eight.

Typical excuse: "We can't afford a full-sized system."

- D. H. Bailey, "Misleading performance reporting in the supercomputing field," *Scientific Programming*, vol. 1., no. 2 (Winter 1992), 41–151.

Using inefficient algorithms on highly parallel systems

In many cases, inefficient algorithms were employed for highly parallel implementations, requiring many more operations, thus producing artificially high speedup figures and Mflop/s rates. Examples:

- Some researchers cited parallel PDE performance based on explicit schemes, for problems where implicit schemes were known to be significantly more efficient.
- One paper cited performance for computing a 3D discrete Fourier transform by direct evaluation of the defining formula ($8n^2$ operations), rather than by using a fast Fourier transform ($5n \log_2 n$).

Both examples violate a basic rule of parallel computing, namely to base parallel implementations and operation counts (when computing Mflop/s or Gflop/s rates) on the best practical serial algorithm.

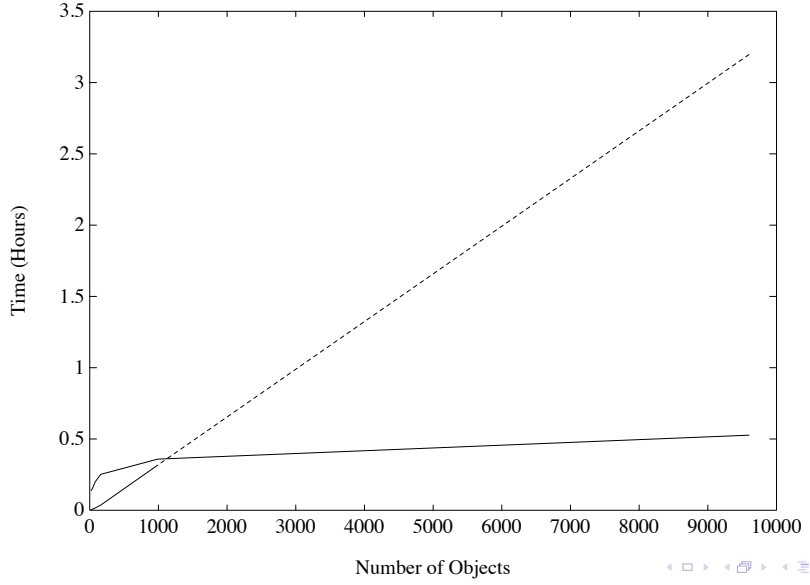
Typical excuse: Other algorithms are "more appropriate" for our parallel system.

Abstract versus details in paper

Abstract of published paper: "The current Connection Machine implementation runs at 300-800 Mflop/s on a full [64K] CM-2, or at the speed of a single processor of a Cray-2 on 1/4 of a CM-2."

- Excerpt from text: "This computation requires 568 iterations (taking 272 seconds) on a 16K Connection Machine."
  In other words, the computation was run on a 16K system, not on a 64K system; the figures cited in the abstract were merely multiplied by four.
- Excerpt from text: "In contrast, a Convex C210 requires 909 seconds to compute this example. Experience indicates that for a wide range of problems, a C210 is about 1/4 the speed of a single processor Cray-2."
  In other words, the computation mentioned in the abstract was actually run on a Convex system, and a rule-of-thumb scaling factor was used to produce the Cray-2 rate.

Performance plot: parallel run times (lower) vs vector (upper)



Data for performance plot

Problem size (x axis)	Parallel system run time	Vector system run time
20	8:18	0:16
40	9:11	0:26
80	11:59	0:57
160	15:07	2:11
990	21:32	19:00
9600	31:36	3:11:50*

Details in text of paper:

- In last entry, the 3:11:50 figure is an estimate.
- The vector system code is not optimized.

Note that the parallel system is actually slower than the vector system for all cases, except for the last (estimated) entry. Also, except for the last entry, all real data in the graph is in the lower left corner. A log-log plot should have been used instead.

Origins of the NAS Parallel Benchmarks (NPB)

- In 1991, a team of 12 researchers at the Numerical Aerodynamic Simulation (NAS) facility (now known as the NASA Advanced Supercomputing facility) formulated the "NAS Parallel Benchmarks."
- The original plan was to be a basis for an upcoming supercomputer procurement for NAS.
- A central goal of the NPB was to test algorithms of importance in computational aeronautics.
- However, the NPB team recognized from the beginning that the benchmarks should be designed to have wider usage — hopefully to help clear the hype and confusion in the field.
- The resulting paper (below) was recently awarded the 2015 "Test of Time Award" from the ACM / IEEE Supercomputing Conference.

- D. H. Bailey, E. Barszcz, J. T. Barton, D. S. Browning, R. L. Carter, L. Dagum, R. A. Fatoohi, P. O. Frederickson, T. .A. Lasinski, R. S. Schreiber, H. D. Simon, V. Venkatakrishnan and S. Weeratunga, "The NAS Parallel Benchmarks: Summary and preliminary results," *Proceedings of Supercomputing 1991*, ACM/IEEE Computer Society, 1991, 158–165.

New ways to fool the masses in high-performance computing

- Cite performance rates for a run with only one processor core active in a shared-memory multi-core node, producing artificially inflated performance (since there is no shared memory interference) and wasting resources (since most cores are idle).
  - Example: Cite performance on "1024 cores," even though the code was run on 1024 multicore nodes, one core per node, with 15 out of 16 cores idle on each node.
- Claim that since one is using a graphics processing unit (GPU) system, the most efficient algorithms must be discarded in favor of "more appropriate" algorithms (recall the experience with parallel algorithms).
- Run the test code many times, but only include the best performance rate in the paper (recall the experience of recent pharmaceutical trials).
- Employ special hardware, operating system or compiler settings that are not appropriate for real-world production usage (recall the recent Volkswagen scandal).

Numerical reproducibility

The ICERM reproducibility report further noted:

> *Numerical round-off error and numerical differences are greatly magnified as computational simulations are scaled up to run on highly parallel systems. As a result, it is increasingly difficult to determine whether a code has been correctly ported to a new system, because computational results quickly diverge from standard benchmark cases. And it is doubly difficult for other researchers, using independently written codes and distinct computer systems, to reproduce published results.*

- V. Stodden, D. H. Bailey, J. Borwein, R. J. LeVeque, W. Rider and W. Stein, "Setting the default to reproducible: Reproducibility in computational and experimental mathematics," `http://www.davidhbailey.com/dhbpapers/icerm-report.pdf`.

The growing problem of numerical reliability

Many applications routinely use either 32-bit or 64-bit IEEE arithmetic, and employ fairly simple algorithms, assuming that all is well. But problems can arise.

Particularly vulnerable are:

1. Large-scale, highly parallel simulations, running on systems with hundreds of thousands or millions of processors — numerical sensitivities are greatly magnified.
2. Certain applications with highly ill-conditioned linear systems.
3. Large summations, especially those involving cancellations.
4. Long-time, iterative simulations (such as molecular dynamics or climate models).
5. Computations to resolve small-scale phenomena.
6. Studies in computational physics or experimental mathematics often require huge precision levels.

- D. H. Bailey, R. Barrio and J. M. Borwein, "High precision computation: Mathematical physics and dynamics," *Applied Mathematics and Computation*, vol. 218 (2012), pg. 10106–10121.

Analysis of collisions at the Large Hadron Collider

- The 2012 discovery of the Higgs boson at the ATLAS experiment in the LHC relied crucially on the ability to track charged particles with exquisite precision (10 microns over a 10m length) and high reliability (over 99% of roughly 1000 charged particles per collision correctly identified).
- Software: 5 millions line of C++ and python code, developed by roughly 2000 physicists and engineers over 15 years.
- Recently, in an attempt to speed up the calculation, researchers found that merely changing the underlying math library resulted in some collisions being missed or misidentified.

Questions:

- How serious are these numerical difficulties?
- How can they be tracked down?
- How can the library be maintained, producing numerically reliable results?

Have we learned anything?

Progress has been made, but a renewed focus is needed on:

- Supporting rigorous peer review.
- Focusing on end-to-end application run time.
- Reporting full details of computational environment, so results can be reproduced.
- Reporting all results — not selecting the best run out of many.
- Basing operation counts (for performance reporting) on the best practical serial algorithm.
- Reporting performance in a realistic operating environment, with no special settings inappropriate for common production usage.
- Being careful with numerical reproducibility. With the exploding size and scope of computations, numerical round-off error is much more severe. Have the authors fully justified the numerical reliability of their results?

THANKS!

This talk is available at:
http://www.davidhbailey.com/dhbtalks/dhb-ipdps-2017.pdf