Lasting Impact Through Computation

Walter Freeman

April 18, 2021

Syracuse University PICUP

> *"The purpose of computing is insight, not numbers."*
>
> *–Richard Hamming*

Slides online:

`https://tinyurl.com/5cjtd52f`

Feel free to ask questions and discuss the material during the talk using chat.

I'll see your questions right away since I have Zoom chat up on another window.

The value of computation in the classroom

> *"The American Association of Physics Teachers urges that every physics and astronomy department provide its majors and potential majors with appropriate instruction in computational physics."*
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> –AAPT Undergraduate Curriculum Task Force, 2016

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- Integrating computation lets our students achieve the same learning objectives more efficiently and more thoroughly

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Five years ago I focused on the further idea that:

- Integrating computation lets us add new learning objectives that we couldn't teach previously

But, in the last few years, I have realized the benefits go even beyond that.

The value of computation to students

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- Integrating computation lets us add new learning objectives that we couldn't teach previously
- **Students who study computation develop a richer, more fundamental, and more empowering perspective on nature**

My experience at Syracuse

My experience teaching computational physics is colored by my career path:

- Research background: lattice QCD
- Been a teaching professor at Syracuse since 2015
- Mostly taught giant service courses + 300-level computational physics course
  - Lots of opportunities for computation in other majors classes – I haven't taught those (yet)
  - Can absolutely teach computation in intro classes – logistics prevented me from doing this (so far)
- Many students sought me out for independent study projects after computational physics course

The transition to maturity

Upper division undergraduates must transition from *receivers of knowledge* to *producers of insight*. This involves:

- **Unity and primacy of fundamental physics**: seeing physics as broad unifying principles, rather than disparate special cases
- **Universal application**: awareness that these principles apply broadly to everything, not narrowly to “textbook examples”
- **Ability and willingness to explore**: “what’s in the textbook and on the exam” -¿ “generate novel insights”
- **“Data storytelling”**: going from mathematical descriptions to coherent narratives

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- **Growth mindset, confidence, empowerment, and ownership**

The value of a physics education outside academia

Not all of our students go to grad school. But these skills are celebrated in industry, too:

"The **far-reaching expertise** that physics students develop while receiving their degrees–through exposure to a broad set of skills and techniques–makes them **exceptional problem solvers.** Moreover, their ability to **approach problems from general principles** often means that physicists can **apply their knowledge in novel contexts**, leading to innovative advances in technological development. Their intimate **understanding of the laws of the universe**, along with the ability to harness the **powerful machinery of mathematics to model and predict**, puts physics students in a unique position to tackle some of the world's biggest challenges."

–Crystal Bailey, APS Careers 2020

"As a physicist, you have scientific, technical, and problem-solving skills that are valuable in a wide range of employment sectors. You have learned to **approach problems from first principles** and can serve as a **generalist when collaborating on interdisciplinary teams**. You understand how to set up and run experiments, analyze data, and create mathematical or computational models. **Most importantly, you have the confidence to advance beyond the edge of what is known... This habit of continued learning is a hallmark of a physicist, and greatly valued in all employment sectors.**"

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0. Physics education without computation

The traditional approach, where the only way to extract meaning from the laws of nature is pencil/paper analysis:

- Go to class and talk about what the laws of physics are
- Pick a few special cases that are analytically tractable (and hopefully physically interesting)
- Follow a derivation of their properties on the ~~blackboard~~ Zoom
- Work very hard to learn that analysis inside and out
- Encounter a few other handpicked special cases that are analytically tractable in homework
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- Hope like hell you can do the math on the exam

1. Focus on general principles of physics

“In the infinitesimal scale things reduce to their definitions: $\Delta\vec{x} = \vec{v}t$. You’re seeing the laws of physics directly – and you can manipulate those laws, change them, and see their effects.You’re seeing the laws of physics directly – and you can manipulate those laws, change them, and see their effects. You can see emergent properties. You have coded in the rules directly.”

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[F]rom both mathematical and physics points of view, I feel I am much better off focusing on the conceptual aspects of these areas (what a differential equation is or does, or how gravitational orbits may look or behave between two bodies, rather than the technicalities of actually solving them).

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–Kathleen Monje (BA Physics/BS Comp Sci → film school/animation):

I am a big nerd and loved doing all the math - pen and paper. However, it wasn’t until I had to throw it into a programming code that it made total sense. It’s easy to follow steps if they just work and pop out answers, but it’s hard to throw it into code if you don’t understand each piece.

–Emily Keene, BS Environmental Resource Engineering → public health engineer

Limitations of a focus on analysis

In a standard curriculum, students' intellectual focus is often on the math: it takes time and is hard!

This means that...

- Students are often too "tired" when they finish a derivation to engage in sense-making
    - "Whew, I finally computed $V(\vec{r})$ for this system. Hope it's right. Bedtime!"
- Analysis-focused portions of a curriculum can do better, to be fair
- Lots of study time goes into making sure they know the tricks
    - "Delta function in QM? Integrate the Schrödinger equation across it..."

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But computation lends itself to a mental map based around the *physics*:

- Simulation code closely resembles the laws of physics themselves
- Similar physics gets coded in similar ways
- Taking the burden off of analytical math skills lets students focus on physics more

2. Universal applicability

With only analysis we must choose systems to study based on analytic feasibility. Unfortunately this means:

- Students don't fully appreciate the scope of physics
- Students don't fully appreciate the unity of physics
- Many very interesting topics get left out:

We study...

- Circular orbits (in intro classes)
- The Kepler problem
- Projectile motion
- The ideal gas
- The SHO
- The ideal wave equation
- Thermodynamics
- The hydrogen atom

But often students don't see...

- Elliptical orbits (in intro classes)
- Milankovitch cycles
- Air drag
- Phase changes
- Nonlinear oscillations
- Nonlinear waves
- Heat transfer and fluid flow
- The hydrogen *molecule*

Computation lifts this limitation

"[Otherwise] intractable problems seem tractable"

–Aaron Trowbridge (BS Physics/Math → grad school in HET)

Analytical solutions good for rigorous proofs, but numerical methods allow you to do things you can't do analytically – they "make impossible things possible"

...

When we studied the stable phase of damped oscillations, nobody talked about the transient – but putting this on a computer shows the transients as well.

–Nguyen Phuc Nguyen

[C]omputational physics expanded the types of problems I could solve, not limiting to only exact/approximate pen and paper solutions. When I approach problems, I check to see if it is possible analytically, but then I think if it is possible to do using a computer.

–Chris Kane, BS Bioprocess Engineering → grad school in lattice QCD

3. Students' ability to explore

"[O]nce you have working code, slight modifications can lead to being able to explore a wide variety of phenomena. This helped develop the habit of exploring and drawing conclusions based on computational 'experimentation' and explore a physical system thoroughly. This applies to almost any computational problem... "

–Chris Kane

[B]eing able to tweak more variables than before was integral (pun intended) in learning what all these things actually do. ...[T]his takes a lot of time with pen and paper. But when you have the questions, "what if I change x? What if there's more y's? What if I completely remove z?" [Y]our ability to learn and discover is increased significantly with coding. In fact, it was almost fun to "break" the code into doing something entirely weird and trying to understand what exactly went wrong."

–Emily Keene, BS Environmental Resources Engineering → public health engineer

Aaron and Nguyen both returned to the ease of exploration computer models afford several times in my interview with them.

Ready access to interesting things to explore

Computational methods let early-career students access systems that are complex enough to provoke arguments among professors!

My computational physics class gets a lot of mileage out of studying the pendulum...

4. "Data storytelling"[1]

Computation *forces* us to engage in "sense-making" from the very beginning:

The result of a computational physics solution usually involves plots and tables of data. I have to choose what is the best plot to show or the best way to plot it in order to explain the major results of the calculation. Even before deciding on what plot to show, we have to make lots of plots in order to understand what is happening in our calculation.

–Chris Kane

The sense-making skills in computation are readily transferrable to *professional* communication to other scientists and the public:

[C]omputational work in general lends itself more readily to visualization of any kind than analytical work. This is wonderful for me since I'm a very visual thinker, and it's also great for science outreach to the public.

–Patrick Miles

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[1] ... a brilliant term coined by Christopher Oakley of Spelman College at a PICUP institute

The computer as a pontifex

Computational tools provide a powerful way to connect physical laws to their consequences:

- Visualization (especially animation) takes students directly to physical consequences
- ... but computational work is not a “one-and-done” path to meaningful results

Computational projects leave a lot of room for students to explore *how to use a simulation* to extract physical meaning:

- What parameters do I use?
- How do I vary them?
- How do I visualize the data?
- How do I distinguish physical results from numerical artifacts?

Computational work can help develop analytic sense-making skills as well!

- Analysis-also approach: “Let’s simulate this system and compare it to an analytic solution”
- Analyze-back approach: Use pencil-and-paper math to interpret data from simulations and reconnect them to fundamental laws

Is this our world?

Analytically tractable
(use a pencil)

- Simple harmonic oscillator
- The Kepler problem
- The proton mass
- Ideal gas
- Infinite square well

Analytically intractable
(use a computer)

- Driven damped pendulum
- Three-body gravitation
- Hydrogen atom
- Phase transitions
- Highly nonlinear oscillations

Is this our world?

Analytically tractable (use a pencil)

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Perturbatively accessible (think carefully)

- Ordinary pendulum
- Earth/Sun/Jupiter
- Helium atom
- van der Waals gas
- $g-2$
- The guitar string
- Zeeman effect
- Fine structure
- Multipole expansions
- Effective field theories
- ...

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Doing computer simulations gives you a better sense that 'physics is a model' rather than 'physics is the gospel'. When you are taught physics [analytically] you are given rules in a very arbitrary way – 'here are the equations, they work' – they don't stress enough that it's something that we chose *because* they work, it's a convention – we don't stress enough that physics, as it is right now, is built to convention.

–Nguyen Phuc Nguyen

Flaws in the usual handling of teaching approximation

- It happens too late (undergrad quantum perturbation theory)
- They don't get to drive until even later
  - Students need practice with the whole perturbative reasoning process, not just "calculate this matrix element to second order"
- They rarely get to look beyond approximations and compare to the full thing
- They often mistake the approximation for the real thing

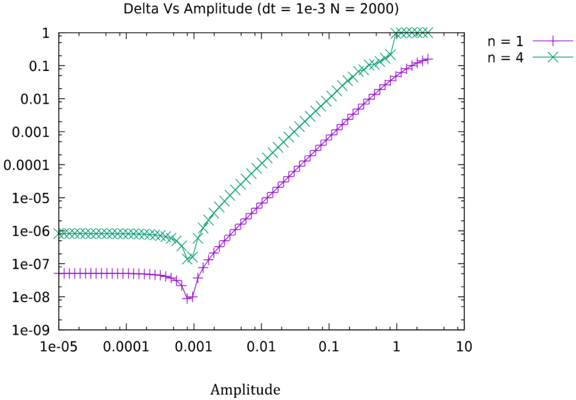
Using "perturbative reasoning" to create expectations for, and to analyze the results of, a nonperturbative simulation is an excellent opportunity!

Example: the guitar string at nonvanishing amplitude

How do identical vibrating strings in the $n = 1$ mode at different amplitudes differ?

It is seen that for small amplitudes, the error calculated is constant and insignificant. This tells us that the small angle approximation is being obeyed.... The error rises steadily for both normal modes as the square of the amplitude.... This error is caused by the violation of the small angle approximation. In more mathematical terms, the 2^{nd} *term in the power series expansion of* $\sin(x)$ *can no longer be ignored and hence the small angle approximation fails. If one looks closely at the highest amplitude for the* 1^{st} *normal mode, the error trend changed. Here the* 3^{rd} *term in the expansion can no longer be ignored...*

–Chris Kane (class work)



The value of a physics education, revisited

"The far-reaching expertise that physics students develop while receiving their degrees–through exposure to a broad set of skills and techniques–makes them exceptional problem solvers. Moreover, their ability to approach problems from general principles often means that physicists can apply their knowledge in novel contexts, leading to innovative advances in technological development. Their intimate understanding of the laws of the universe, along with the ability to harness the powerful machinery of mathematics to model and predict, puts physics students in a unique position to tackle some of the world's biggest challenges."

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Education is not just about knowledge.

It's about **empowerment, confidence, and agency**.

Does the use of computation affect students' growth mindset and self-efficacy?

"I feel that one of the biggest problems in education today is the immense pressure students feel to succeed. So much so that failure doesn't feel like an option. Yet failure is an integral part of the learning process. What makes your [computational physics] class unique is that my worth isn't based on the end result but rather my willingness to push onward despite failing again and again. I used to ask for help the moment I encountered an error because, in my mind, writing the perfect code was all that mattered. I slowly realized that wasn't the point. With each project, I allowed myself a bit more time to figure it out on my own and surprised myself every time. Now, I'm no longer afraid to be wrong after the first, second, or even twentieth attempt. You taught me that failure isn't something to be avoided at all costs but embraced as an opportunity to learn. I'm walking away from this class a much more self-sufficient and resilient person, not just in comp sci but in all areas of my life."

–Diane Portugal, physics/architecture major

> ... [M]aybe it’s because I’m a big nerd, but learning concepts with a new tool that’s challenging enough to suck you in but simple enough to keep you from being discouraged is vital in a society where learning is fairly independent and digital. (I’m sure there are statistics out there about visual and kinesthetic learners and ... [computational physics] combines both strategies).
>
> –Emily Keene

“I’ve grown so much as a physicist since (and because of) taking [computational physics] with you and doing our n-body independent study that I can barely remember or imagine my perspective on physics from before those experiences. It feels like I went from egg to chicken; blind, then suddenly I could see. And run! Studying computational physics ... broadened my perspective on physics, and science as a whole, more than any other experience I had in my undergrad career. I now feel like I have the tools to learn anything I want. In fact, I’ve been working with/reading about smoothed-particle hydrodynamics code recently, and just today I realized those codes have a ton in common with the n-body program we wrote! Realizing this has made SPH feel so much more accessible to me. That n-body independent study put me so far ahead in my growth as a physicist than I would have been without it.... This comp phy experience has been and will continue to be invaluable to me!”

–Patrick Miles

Computation as part of a balanced breakfast

My experience has been that computation:

- **... allows students an approach that emphasizes the fundamental principles, not only special cases**
- **... gives them tools to freely apply these principles universally to a variety of situations**
- **... encourages them to explore and generate novel/interesting insights**
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- **... centers the process of sense-making from simulation results and behavior**
- **... provides a powerful on-ramp to the notion of physics as a set of interlocking models**
- **... has tremendous effects on students' self-efficacy, growth mindset, and empowerment!**

Recommendations

- Computational integration should be done with an eye toward broad advantages for student growth
- Numerics are not a substitute for analytic math; they are a **complementary** approach.
    - "Analysis-also" and "analyze-back" approaches let students use numerics and analysis in tandem to gain extra insight

- Computational integration gives us the flexibility to design a curriculum that **reinforces all the benefits from physics training** that we celebrate
- ... we should keep those benefits in mind when integrating computation!

Questions

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