The Computationally-Trained Physicist

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https://tinyurl.com/rwrdyxa

The value of computation in the classroom

The value of computational physics in our work has become widely known.

"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."

-AAPT Undergraduate Curriculum Task Force, 2016

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A few years ago I focused on the further idea that:

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

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- Students who study computation develop a richer, more fundamental, and more empowering perspective on nature

Why is the study of physics so respected as an avenue for intellectual growth?

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The standard lore: physics training helps students...

- ... explain diverse phenomena from the same basic laws of nature
- ... solve problems from the ground up starting with broad principles
- ... use mathematical modeling to analyze consequences of those broad principles
- ... be an expert at "data storytelling", extracting meaning from data
- ... "connect the dots" between technical fields
- ... work with confidence even beyond the frontier of "things that are well understood" to expand that frontier

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"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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Incorporating computation as part of physics training consolidates and extends these benefits that our discipline celebrates!

Physics education without computation

The traditional approach, where the only way to extract meaning from the laws of nature is pages of 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
- 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

Limitations, I: focus on analysis

In an analysis-only curriculum, students' intellectual focus is often on the analysis:

- Analysis takes time
- Analysis is *hard* and often requires specialized skills

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 Schroedinger equation across it..."

Since this is hard and takes time, students' mental map of physics is shaped by it:

- Students' intellectual organization is shaped by "what math trick did I need?"
- Sometimes this is a good thing (symmetry/geometry), but not exclusively

Computation can rebalance students' intellectual attention:

- Taking the burden off of analytical math skills lets students focus on physics more
- Simulations naturally focus attention on sense-making ("I wrote this thing, now let me see what it does")

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

- Simulation code centers the laws of physics themselves
- Similar physics gets coded in similar ways

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Important to ensure that coding itself doesn't become a huge intellectual burden:

- Make sure coding doesn't become an end in itself
- Assess physical interpretation, not "did you build the simulation?"
- Choose tools/algorithms/etc. that minimize burden of CS knowledge when appropriate
- Segregate CS focus when possible so nobody mistakes hash tables and binary trees for physics

Limitations, II: the math barrier to entry

If pen and paper analysis is the only tool you have to make meaning out of the laws of nature, students have to master it or miss out.

Usual assignment: "Here's an interesting system, go calculate something, and then learn from it"

- Analytic math is hard; so is the crucial "sense-making" step after it's done
- Students often neglect the latter ("calculate $\psi(x)$, then think about what it means")
- Lots of failure modes:
 - Student makes uncaught error in analysis \rightarrow result isn't physical
 - Student unable to interpret/visualize result \rightarrow no physics learning
 - Made worse by the fact that analysis is usually solitary
 - Analytic activities should try to catch these

Having computational tools as another way to connect physical laws to their consequences can tunnel through this barrier:

- Visualization (especially animation) takes students directly to physical consequences
- Computation is much more friendly with "iterate until works":
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 - Analysis-also approach: "Let's simulate this system and see how it compares to the analytic solution"
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Caution: don't want coding skill to become a *new* barrier to entry!

- Nature of computation makes this less likely but still possible
- Programming skill rarely limiting factor in my comp phys class (even in C)
- Relying on high school/CS 101 instruction probably not the right thing

Limitations, III: biased choice of systems

Currently we cherry-pick systems to study based on analytic tractability.

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
- 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
- Milankovitch cycles
- Air drag
- Phase changes
- Nonlinear oscillations
- Nonlinear waves
- Heat transfer and fluid flow
- The hydrogen molecule

Limitations, III: biased choice of systems

We should structure our curriculum to serve *physics*, not be a thrall to tools.

More flexible tools mean a curriculum that serves student growth in physics better.

Using computation:

- We can address more interesting systems
- We can address them earlier (Elliptical orbits! Air resistance!)
- Numerics give more flexibility to choose systems that are tailored to the *physics* we want students to learn

An example: molecular dynamics and phase changes

(running in realtime on this laptop)

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• This is a crucial skill and students need to learn it even earlier and in greater depth

Flaws in our handling of teaching approximation

- It happens too late (undergrad quantum perturbation theory)
- They don't get to drive until even later (perturbative reasoning, not just "calculate this")
- They rarely get to look beyond approximations and compare to the full thing
- There is little consideration of philosophy behind approximations (power counting)
- 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!

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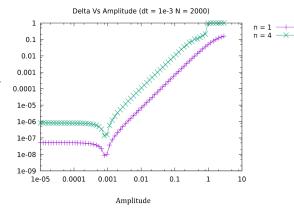
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- Examine departure from expected period as angle gets big
- Do "data storytelling" to understand what is going on
- "Analyze-back": use perturbative logic to understand why $T(\theta) = T_0 + \mathcal{O}(\theta^2)$

Mutual reinforcement between numeric and analytic approach to math

Sample work: nonlinearities in the guitar string

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 2nd 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 3rd term in the expansion can no longer be ignored...

-Chris Kane, bioprocess engineering (now PhD candidate in LQCD)



The value of a physics education, revisited

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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?

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I'll let them speak for themselves.

"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 wasnt 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 isnt 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 major, aiming for grad school in architecture

"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. If anything I learned more about math in this class than I anticipated. (TAYLOR SERIES) (capitalization original)

... [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).

[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, environmental resources engineer (graduated)

"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, physics major at Syracuse, now PhD student

Conclusions

Students with computational training as part of their study:

- ... have a sharper focus on fundamental laws of nature
- ... have a greater awareness of the *scope* and *unity* of the physical perspective
- ... have more experience on sense-making, modeling, and "data storytelling"
- ... can find physics study more accessible
- ... can study the most interesting or illuminating systems, less confined by their tools
- ... access high-level problem-solving skills (especially reasoning with approximation) earlier in their careers
- ... have more of the skills industry celebrates in physicists

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- ... access high-level problem-solving skills (especially reasoning with approximation) earlier in their careers
- ... have more of the skills industry celebrates in physicists
- ... show remarkable enthusiasm, self-efficacy, and agency in learning by discovery!

Recommendations

- Computational integration should be done with an eye toward its 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!