PHY 604: Computational Methods in Physics and Astrophysics II

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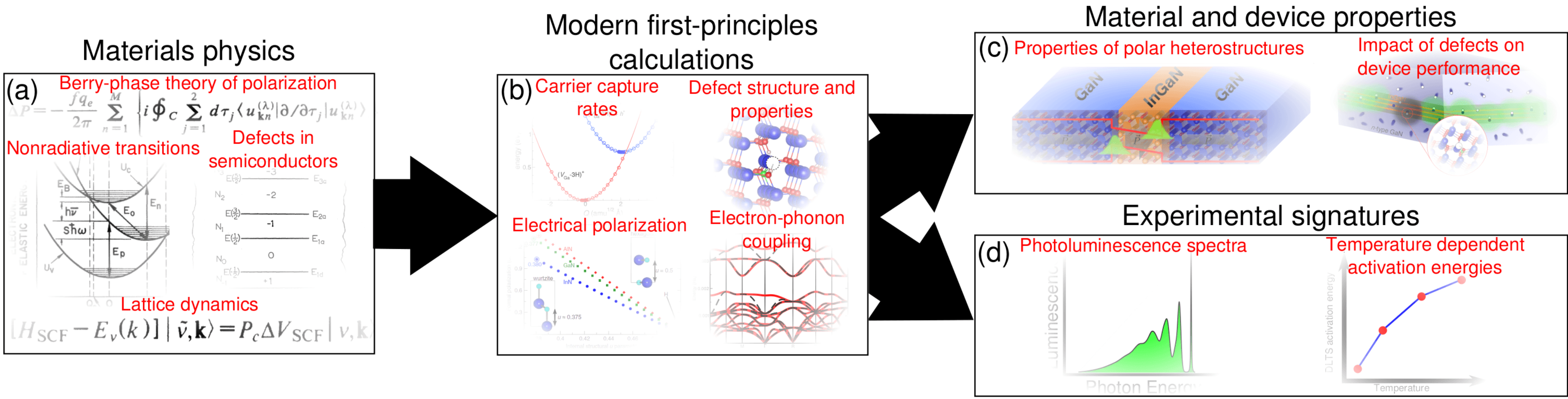
My research interests: Computational condensed matter physics

Stony Brook University

FLATIRON INSTITUTE

Center for Computational Quantum Physics

https://www.simonsfoundation.org/flatiron/



https://you.stonybrook.edu/cdreyer/

Goals of the course:

- Learn how to solve problems in physics computationally
- Understand the limitations of numerical methods
- Have the ability to interpret numerical results presented in the literature
- Have exposure to computational tools
- Understand basic idea behind algorithms for performing common computational tasks

Technical points about the class: Programming Languages

- The assignments will involve writing computer programs
- You may use the programming language of your choice.* I would prefer:
  - Fortran
  - C++
  - Matlab
  - **Python (recommended)**
- * In general, and especially if your language is not on the list, you should provide some help for how to compile (if necessary) and run your code
- Examples will be given mostly in python

Technical points about the class: Topics covered

- Basics of computation and programming constructions
- Good programming practices
- Numerical differentiation and integration
- Interpolation and root finding
- Ordinary differential equations
- Linear algebra
- Fast Fourier transforms
- Fitting
- Partial differential equations
- Monte Carlo techniques
- Genetic algorithms
- Parallel computing
- Machine learning

Technical points about the class: Class location

- Vote: Move the class to Physics building (likely B131)

Technical points about the class: Assignments

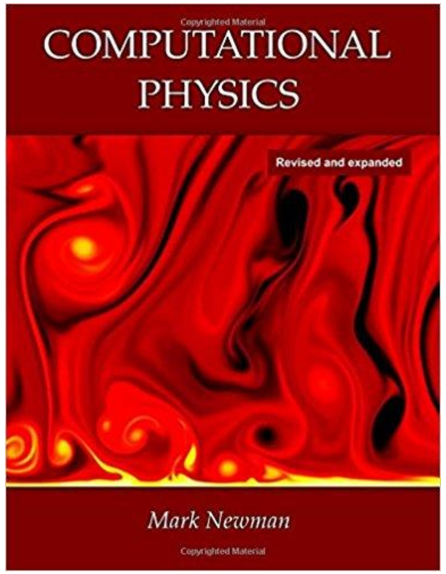
- Coding homework will be assigned roughly every two weeks
  - Homeworks will be 50% of the final grade
  - Will involve code and written analysis
  - **Recommendation** (not required)**: Use Jupyter notebooks**

- Office hours: By appointment
  - Please feel free to come to me for help!

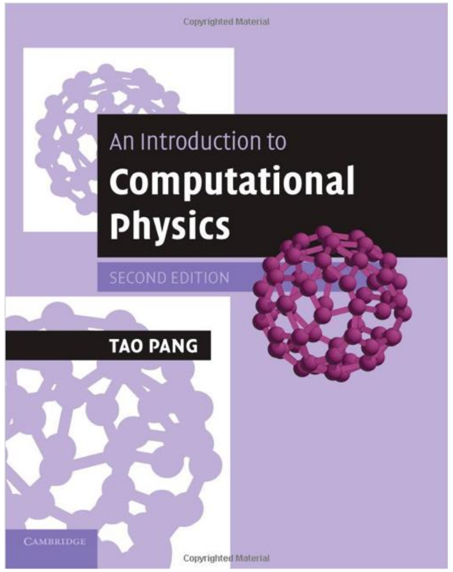
- There will be a final project at the end of the semester
  - Solve a physics problem computationally
  - Write up a short report, and present to the class
  - Final project is 50% of the final grade

Technical points about the class: Textbooks

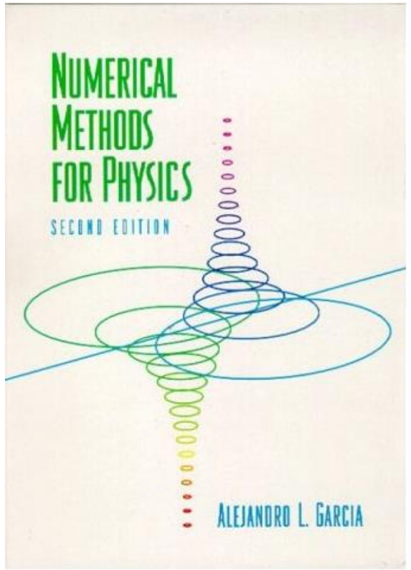
- **No textbook is required for this course**
  - Some recommended texts for further reading:



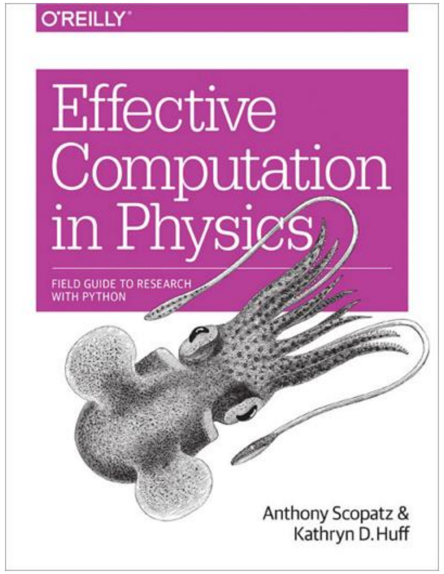
***Computational Physics*, by Mark Newman**
- Generally good coverage on most of the topics we'll discuss
- Lots of physics examples
- Inexpensive
- Main recommended book



***An Introduction to Computational Physics*, by Tao Pang**
- Also good coverage of the topics (up to PDEs)
- Lots of physics examples
- Inexpensive



***Numerical Methods for Physics* by Alejandro Garcia**
- Broad coverage
- More PDE stuff than Pang



Effective Computation in Physics by Scopatz & Huff
- Introduces linux/unix shell
- Covers programming practices
- Introduces parallel programming

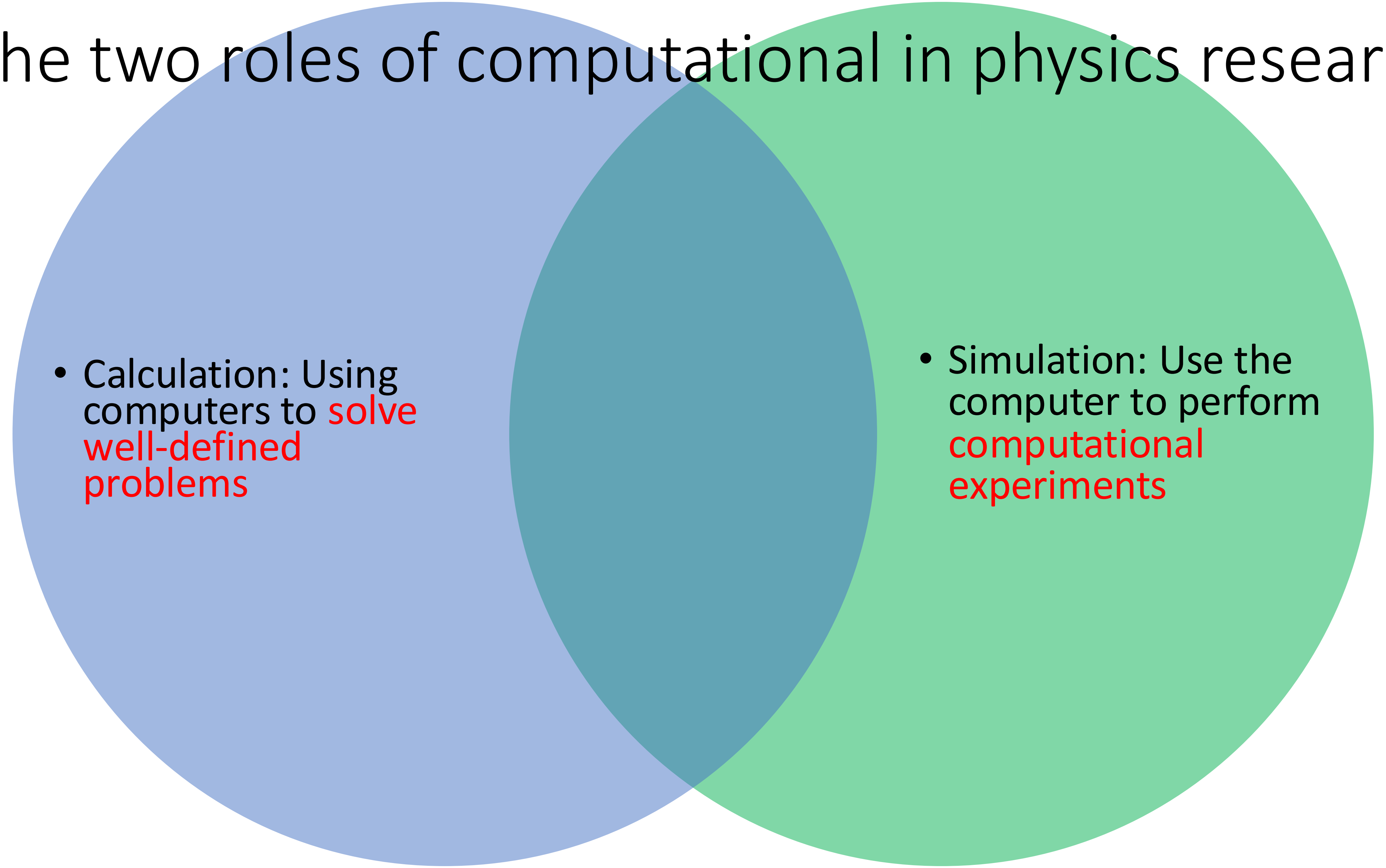
Why computation?

"Computational science now constitutes what many call the third pillar of the scientific enterprise, a peer alongside theory and physical experimentation."

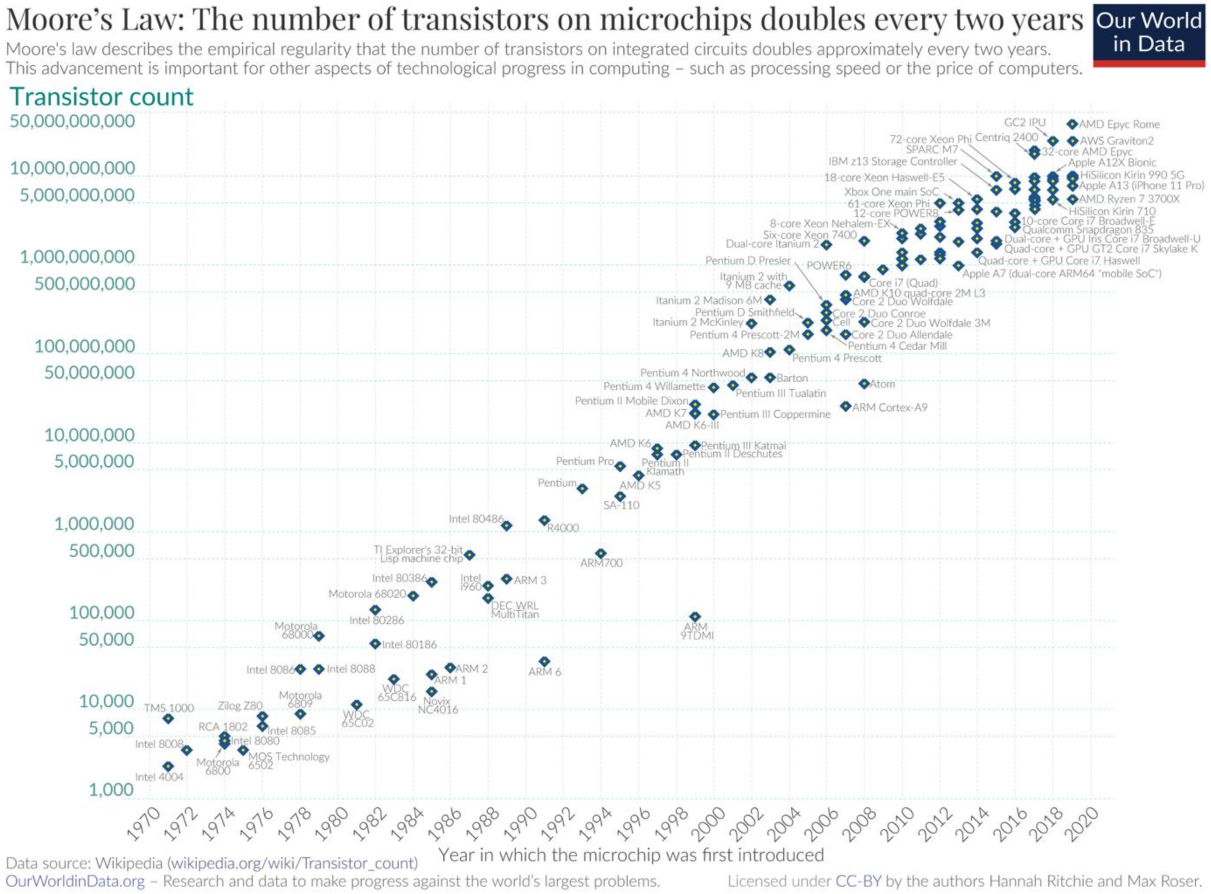
—President's information technology advisory committee (2005)

- Computation allows us to go beyond analytically solvable problems
- Computers allow us to perform repetitive tasks efficiently
- Computers allow us to generate and analyze large amounts of data

The two roles of computational in physics research



Computational science is driven by **more powerful computers**



Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**El Capitan** - HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8GHz, AMD Instinct MI300A, Slingshot-11, TOSS, HPE DOE/NNSA/LLNL United States	11,039,616	1,742.00	2,746.38	29,581
2	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE Cray OS, HPE DOE/SC/Oak Ridge National Laboratory United States	9,066,176	1,353.00	2,055.72	24,607
3	**Aurora** - HPE Cray EX - Intel Exascale Compute Blade, Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU Max, Slingshot-11, Intel DOE/SC/Argonne National Laboratory United States	9,264,128	1,012.00	1,980.01	38,698
4	**JUPITER Booster** - BullSequana XH3000, GH Superchip 72C 3GHz, NVIDIA GH200 Superchip, Quad-Rail NVIDIA InfiniBand NDR200, RedHat Enterprise Linux, EVIDEN EuroHPC/FZJ Germany	4,801,344	793.40	930.00	13,088
5	**Eagle** - Microsoft NDv5, Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR, Microsoft Azure Microsoft Azure United States	2,073,600	561.20	846.84	

Computational science is driven by **better methods/algorithms**

$$\hat{H} = -\frac{\hbar}{2m_e}\sum_i \nabla_i^2 - \sum_{i,I}\frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} - \sum_I \frac{\hbar^2}{2M_I}\nabla_I^2 + \frac{1}{2}\sum_{I\neq J}\frac{Z_I Z_J}{|\mathbf{R}_I - \mathbf{R}_J|}$$

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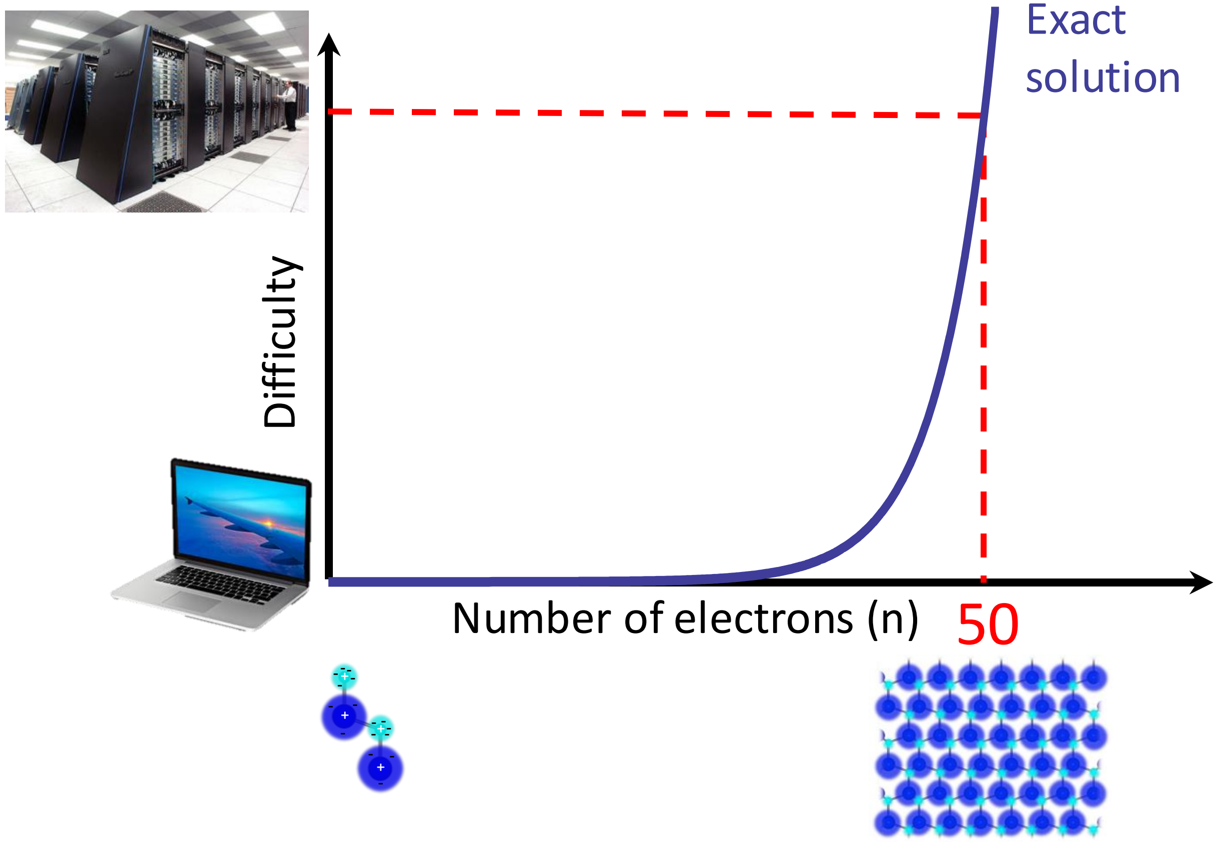

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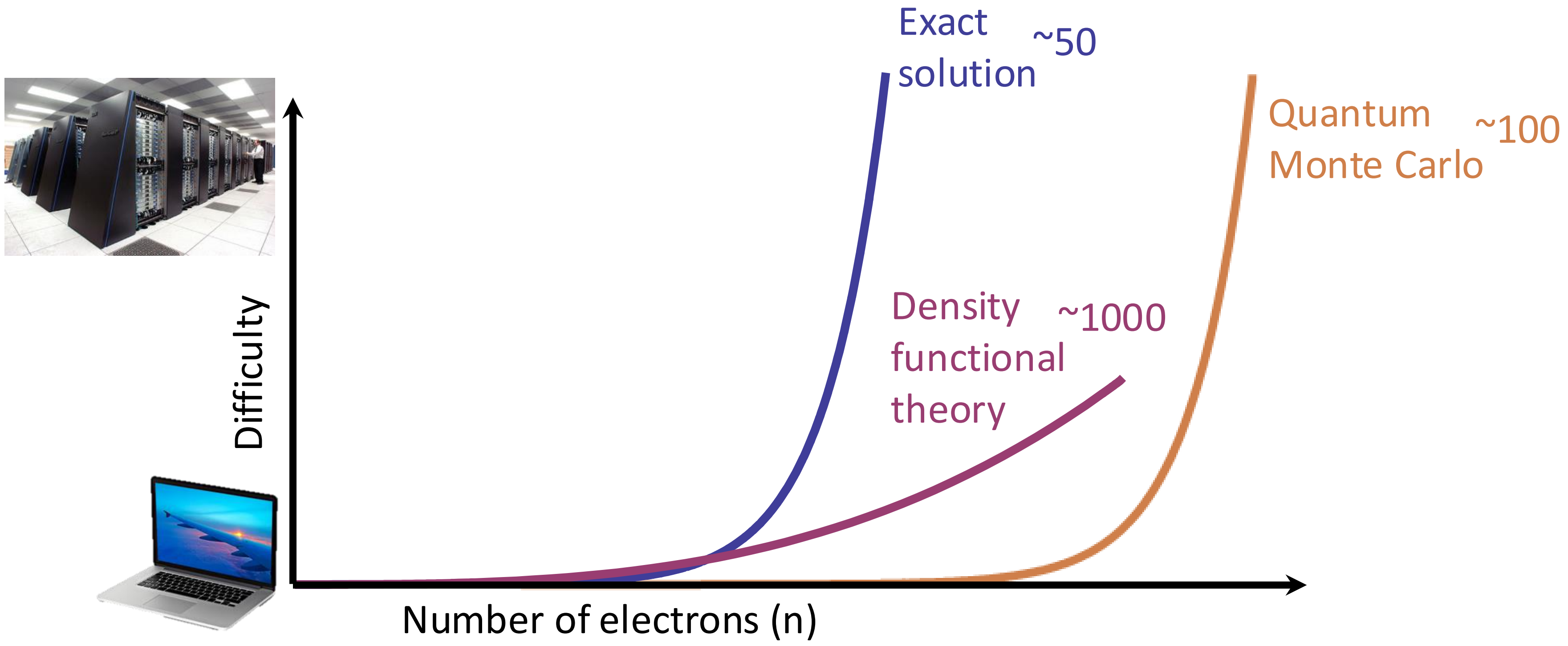

Goals for (the rest of) this lecture

- Representing numbers on the computer
  - Types
  - Finite precision of floating points
  - Comparing real numbers

Information in computer programs categorized by “**Type**”

C++ Type	**Fortran Equivalent**	**Description**	**Example**
`short` (also called `short int`)	`integer(4)`	Positive or negative number with no decimal places.	`56478, 3, -278`
`int`	`integer`		
`long` (also called `long int`)	`integer(8)`		
`float`	`real`	Positive or negative number with decimal places.	`3.0, 1.67e10, -3.2234e-20`
`double`	`real(8)`		
`long double`	`real(16)`		
`char`	`character(1)`	Single or multiple letters, numbers, symbols with no special interpretation	`a, abj3a, gh_&w`
`string` (string type implemented as a container in C++ standard library)	`character(len=*)` (as of Fortran 2008 standard)		
`bool`	`logical`	True or False	`.True., False`
`complex` (complex type implemented as a Template class in C++ standard library)	`complex`	Complex numbers	`3.0+5.6i`

All information in a computer stored as **bits**

- Basic unit of information in a computer is a bit: **0 or 1**
    - 8 bits = 1 byte

- All types must be converted into some number of bytes

- Finite storage limits, e.g., the size or precision of a number

Binary data representation

- "Human" representation: Base ten (decimal)
    - Each digit multiplies a power of 10

10^0 = 1's place

10^1 = 10's place

10^2 = 100's place

$$137_{10} = 1x10^2 + 3x10^1 + 7x10^0$$

- "Computer" representation: Base two (binary)
    - Each digit multiplies a power of 2:

2^0 = 1's place

2^1 = 2's place

2^2 = 4's place

$$101_2 = 1x2^2 + 0x2^1 + 1x2^0$$

$= 5_{10}$ (in base 10 representation)

The amount of memory allocated to an integer determines largest number that can be stored

- E.g., 1 byte: | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | $= 1x2^6 + 1x2^5 + 1x2^4 + 1x2^3 + 1x2^2 + 1x2^1 + 1x2^0 = 127_{10}$

  Sign bit; 0 if positive integer
  1 if negative integer

- 2-byte:
  - This can store 2^{15}-1 distinct values: -32,768 to 32,767 (signed)
  - Or it can store 2^{16} values: 0 to 65,535 (unsigned)

- Standard in many languages is 4-bytes
  - This can store 2^{31}-1 distinct values: -2,147,483,648 to 2,147,483,647 (signed)
    - C/C++: int (usually) or int32_t
    - Fortran: integer or integer(4)
  - Or it can store 2^{32} distinct values : 0 to 4,294,967,295 (unsigned)
    - C/C++: uint or uint32_t
    - Fortran (as of 95): unsigned

- For very big integers, 8-byte allows for 2^{64}
  - Fotran: integer(8)
  - C++: long

Overflow: Trying to put more information in a type than will fit

- What happens when you try to store an integer that too large for the memory allocated?
  - **Depends on the language!**

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- Fortran: Just gives you the wrong result

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- Fortran: Just gives you the wrong result

- Python: Allows the size of the integer to scale with the size of the number

Another aspect of integers to keep in mind: **Integer division**

- Multiplication of integers results in an integer; addition/subtraction of integers result in an integer; division of integers does not always result in an integer!!

- What happens if we divide two integers like: `1/2`?

Another aspect of integers to keep in mind: **Integer division**

- Multiplication of integers results in an integer; addition/subtraction of integers result in an integer; division of integers does not always result in an integer!

- What happens if we divide two integers like: `1/2`?
  - In some codes, 1/2 gives 0, in others it converts to real and give 0.5
  - Common source of bugs!!

Integers versus real/floating-point: Mind the decimal place

- Keep in mind that in many languages, `2` and `2.0` (or `2.`) are interpreted differently
  - `2` is taken to be an integer
  - `2.` or `2.0` is taken to be real

- This can be important in a variety of contexts:
  - Integers are stored exactly, floats are approximate
  - Integer and floating-point division are different
  - Exponentiating negative numbers can be problematic `(-3.5)**(2)` is safer than `(-3.5)**(2.0)`
  - Integers must be used for, e.g., array indices

Real/Floating point numbers are more complicated

- Infinite real numbers on the number line need to be represented by a finite number of bits

- Finite memory results in limited **size and precision** of floating point numbers
  - Not all real numbers (even simple ones) can be stored in a finite number of digits in a base-2 representation
  - Example: $1/10=0.1_{10} = 0.0001100110011..._2$ does not have a finite representation in base 2 just as $1/3=0.333333..._{10}$ has no finite representation in base 10

- This means that even simple floating point numbers are often approximated with some small error
  - This means that floating point arithmetic is not exact! (on all computers and programming languages)

- Errors can compound if not treated carefully!

Real (a.k.a. floating point) data

- IEEE 754 mantissa-exponent form:

$$\underbrace{\text{mmmmmmmmmmmmmmmmmmmmmmmm}}_{\text{24 bit mantissa}}\underbrace{\text{eeeeeeee}}_{\text{8 bit exponent}}$$

- Value = mantissa x 2 $^{\text{exponent}}$
- Single precision:
  - Sign: 1 bit; exponent: 8 bits; significand: 24 bits (23 stored) = 32 bits
  - Range: 2^7-1 in exponent (because of sign) = 2^{127} multiplier ~ 10^{38}
  - Decimal precision: ~6 significant digits
- Double precision:
  - Sign: 1 bit; exponent: 11 bits; significand: 53 bits (52 stored) = 64 bits
  - Range: 2^{10}-1 in exponent = 2^{1023} multiplier ~ 10^{308}
  - Decimal precision: ~15 significant digits

Finite precision of floating points

- This means that most real numbers do not have an exact representation on a computer.
  - Spacing between numbers varies with the size of numbers
  - Relative spacing is constant

$$\text{relative roundoff error} = \frac{|\text{true number} - \text{computer number}|}{|\text{true number}|} \leq \epsilon$$

Overflows/underflows with reals

- Overflows and underflows can still occur when you go outside the representable range.
  - The floating-point standard will signal these (and compilers can catch them)
- Some special numbers:
  - `NaN` = 0/0 or $\sqrt{-1}$
  - `Inf` is for overflows, like 1/0
  - Both of these allow the program to continue, and both can be trapped (and dealt with)
- `−0` is a valid number, and `−0 = 0` in comparison
- Floating point is governed by an IEEE standard
  - Ensures all machines do the same thing
  - Aggressive compiler optimizations can break the standard

A result of finite precision: Need to be careful when comparing floats/reals

- Floating point numbers involve rounding and imprecision, which propagate in different ways under different operations
- Mathematically analogous expressions may yield slightly (or significantly as we will see!) different results
- In principle, this can be accounted for since floating point operations follow specific rules
  - see reading "What Every Computer Scientist Should Know About Floating-Point Arithmetic," by David Goldberg
- In practice, it best to do an "epsilon check"

Epsilon check for comparing floats

- Take two real numbers `a` and `b`
- We take `a==b` if `abs(a-b) < epsilon`

- Have to be very careful with this!!! We should think about:
  - The choice of `epsilon` based on the precision we require/expect for `a` and `b`
  - The choice of `epsilon` based on the magnitude of `a` and `b`
  - What will happen in special cases (`0, NaN, inf`)
  - …

OTB: Round-off error example

- Imagine that we can only keep track of 4 significant digits
- Compute $\sqrt{x+1} - \sqrt{x}$
- Take *x* = 1984. Keeping only 4 digits each step of the way:

$$\sqrt{x+1} - \sqrt{x} = 44.55 - 44.54 = 0.01$$

- We've lost a lot of precision
- Instead, consider:

$$\sqrt{x+1} - \sqrt{x} = (\sqrt{x+1} - \sqrt{x}) \left(\frac{\sqrt{x+1} + \sqrt{x}}{\sqrt{x+1} + \sqrt{x}} \right) = \frac{1}{\sqrt{x+1} + \sqrt{x}}$$

- Then

$$\sqrt{1985} - \sqrt{1984} = \frac{1}{\sqrt{1985} + \sqrt{1984}} = \frac{1}{44.55 + 44.54} = 0.01122$$

Truncation errors are different from roundoff

- Translating continuous mathematical expressions into discrete forms introduces truncation error
- For example: $e^x \simeq S(x) = 1 + \frac{x}{1!} + \frac{x^2}{2!} + ... + \frac{x^n}{n!}$
- Error: $\frac{|x|^{n+1}}{(n+1)!} \max\{1, e^x\}$
- Or $f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$ vs. $D_h(x) = \frac{f(x+h) - f(x)}{h}$

Floating point arithmetic not associative

- Adding lots of numbers together can compound round-off error
- One solution: sort and add starting with the smallest numbers
- Kahan summation (see reading list)
  - Algorithm for adding sequence of numbers while minimizing roundoff accumulation
  - Keeps a separate variable that accumulates small errors
  - Requires that the compiler obey parenthesis

Floating point arithmetic not associative:

$$(1.0 - 1.0) + 1.0^{-9} \stackrel{?}{=} 1.0 + (-1.0 + 1.0^{-9})$$

```
! Purpose:  Test the precision of reals
! Author:    Cyrus Dreyer
! Date:        2/4/2019
program test_prec_reals
  implicit none          ! Turn off implicit typing
  ! Variable dictionary
  real :: factor1     ! Variable for factor 1
  real :: factor2     ! Variable for factor 2
  real :: prec_test_lhs ! Variable for result
  real :: prec_test_rhs ! Variable for result

  factor1 = 1.0           ! Assign a value to factor1
  factor2 = 1.0d-9        ! Assign a value to factor2

  prec_test_lhs = (factor1-factor1) + factor2 ! LHS of inequality on slide
  prec_test_rhs = factor1 + (-factor1 + factor2) ! RHS of inequality on slide

  ! Output
  write(*,'(a20,e20.12e2,a20,e20.12e2)') "Prec_test_lhs:",prec_test_lhs, &
       "Prec_test_rhs:", prec_test_rhs

  stop 0                 ! Stop execution of the program
end program test_prec_reals
```

Further reading

- Readings:
  - What every computer scientist should know about floating-point arithmetic
  - Wikipedia page on the Floating Point
  - Wikipedia page on the Kahan Summation Algorithm