Introduction

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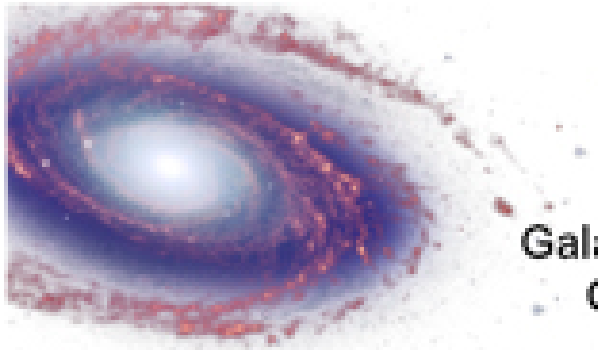
TALENT School on Nuclear Quantum Monte Carlo Methods
North Carolina State University (NCSU), July 11-29 2016.

The Quantum Ladder



Galaxy clusters
Galaxies

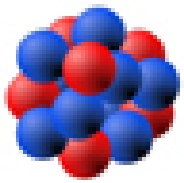
Stars
Planets

Living Organisms,
Man-made Structures

Cells,
Materials

Molecules

Atoms



Atomic
Nuclei

Quarks and
Leptons

Baryons and mesons

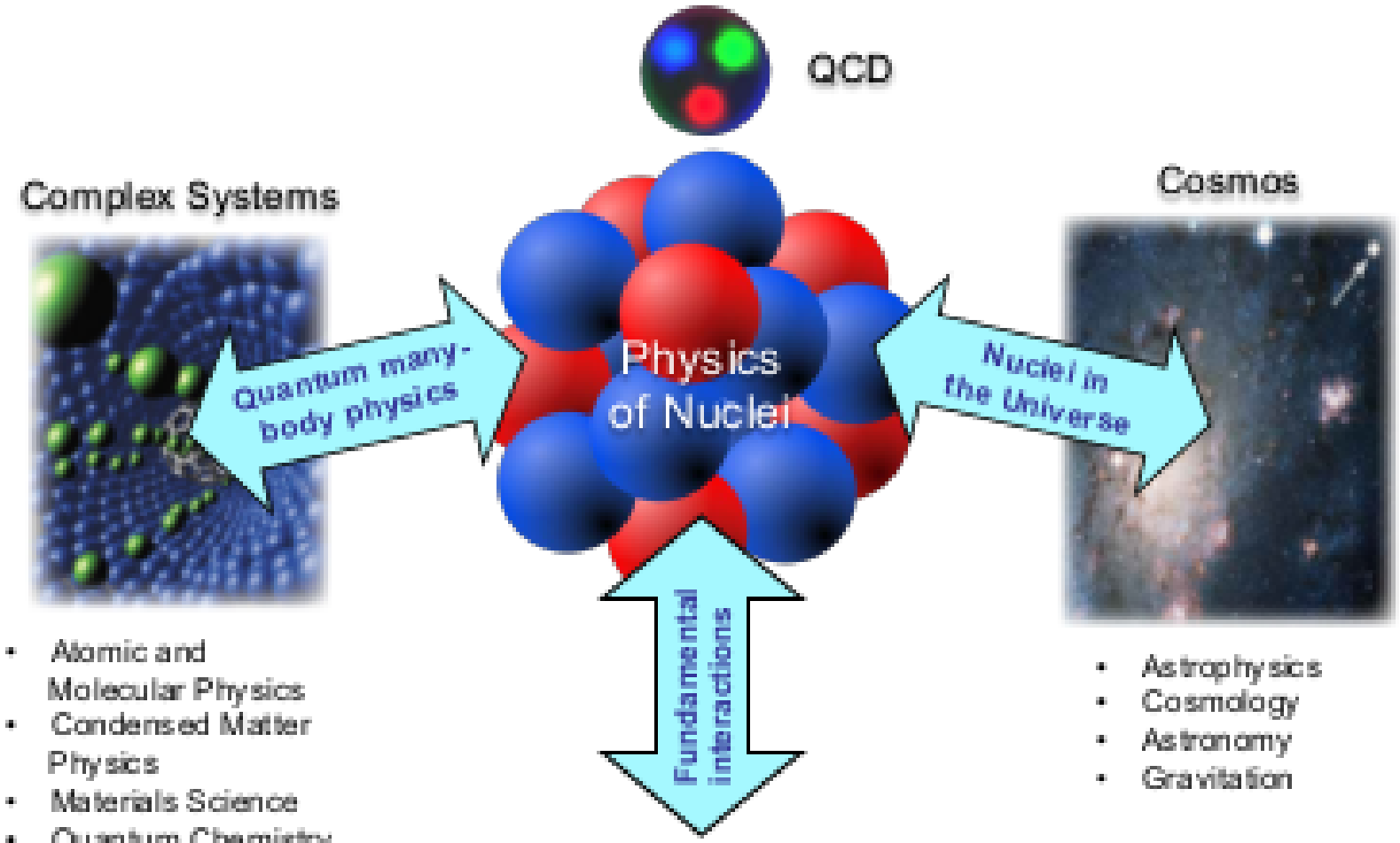
???

Superstrings ?

subatomic atomic macroscopic

reduction

complexity


QCD
Complex Systems
Cosmos
Quantum many-body physics
Physics of Nuclei
Nuclei in the Universe
Fundamental interactions
• Atomic and Molecular Physics
• Condensed Matter Physics
• Materials Science
• Quantum Chemistry
• Particle Physics
• Cosmology
• Astrophysics
• Cosmology
• Astronomy
• Gravitation

Fundamental questions in nuclear physics

Physics of nuclei:

- How do nucleons interact?
- How are nuclei formed? How can their properties be so different for different A?
- What's the nature of closed shell numbers, and what's their evolution for neutron rich nuclei?
- What is the equation of state of dense matter?
- Can we describe simultaneously 2, 3, and many-body nuclei?

Nuclear astrophysics:

- What's the relation between nuclear physics and neutron stars?
- What are the composition and properties of neutron stars?
- How do supernovae explode?
- How are heavy elements formed?

Very incomplete list...

The goal of this school is to provide you **some** machinery to address problems related to those fundamental questions!

About this school

This is one of the many different TALENT schools, covering broadly nuclear physics. For more info: http://www.nucleartalent.org/

Teachers:

- Joe Carlson, carlson@lanl.gov (LANL)
- Joaquin Drut, drut@email.unc.edu (UNC)
- Stefano Gandolfi, stefano@lanl.gov (LANL)
- Dean Lee, dean_lee@ncsu.edu (NCSU)

This school:

- Three weeks
- About 7 one-hour lectures by the above speakers. Several hours on exercises/coding
- Talks related to the school. Speakers: Alex Gezerlis (Guelph), David Dean (ORNL), Shailesh Chandrasekharan (Duke), and Lubos Mitas (NCSU)

Requirements

What we expect from you

- Basic knowledge of a computer language (most of the examples will be given in Fortran and Python). For coding, you are very welcome to use any language that you like (but our help will be depending on that!)
- Know how to compile and run a simple code
- Have your laptop ready to compile Fortran codes. We can help if you use a Linux or Mac distribution
- Have basic libraries installed (Lapack, Blas, random numbers generator, ...)
- Install some MPI library. We recommend OpenMPI, https://www.open-mpi.org/ (we can help installing on Linux and Mac)
- Have fun while learning!!!

Why (quantum) Monte Carlo?

Monte Carlo: solve multi-dimensional integrals by using random numbers.

Quantum Monte Carlo: solve quantum mechanical problems using Monte Carlo methods.

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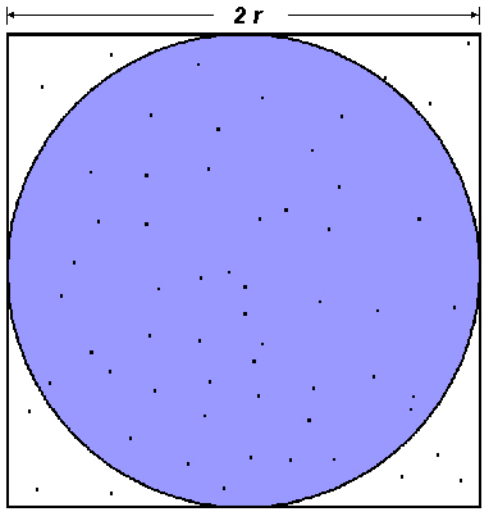
From Wikipedia, "Monte Carlo algorithm":

> *In computing, a Monte Carlo algorithm is a randomized algorithm whose running time is deterministic, but whose output may be incorrect with a certain (typically small) probability.*
>
> *The name refers to the grand casino in the Principality of Monaco at Monte Carlo, which is well-known around the world as an icon of gambling.*

The first example

The first, older, example that I found on literature to calculate something by mean of random events, the **dartboard method:**

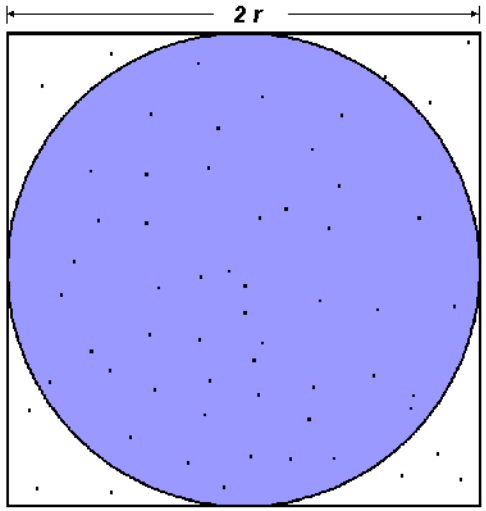
Throw darts, i.e. choose points randomly within a rectangular box with some area inside to integrate on:



$$A_{\text{box}} = 4\,r^2\,, \qquad A_{\text{area}} = \pi\,r^2\,, \qquad \pi = 4\frac{A_{\text{area}}}{A_{\text{box}}}$$

$$\frac{A_{\text{area}}}{A_{\text{box}}} = P(\text{hit inside the area}) = \frac{\#\text{ hits inside the area}}{\#\text{ hits inside the box}}$$

The first example



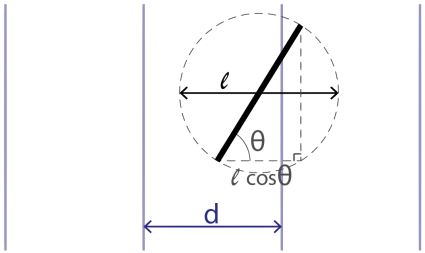
The first code!

```
npt=10000
count=0
do j=1,npt
  x=random1
  y=random2
  if (sqrt(x**2+y**2).lt.radius) count=count+1
enddo
pi=4.0*count/npt
```

Another example, π

Buffon's Needle Problem (1733):

What is the probability that a needle of length l will land on a line, given a floor with equally spaced parallel lines a distance d apart?



Let's define $x = l/d$. For a short needle ($l < d$):

$$P(x) = \int_0^{2\pi} \frac{l|\cos\theta|}{d}\frac{d\,\theta}{2\pi} = \frac{2l}{\pi d} \rightarrow \pi \approx \frac{2lN}{dH}$$

where N is needles thrown, and H is the time for a needle to cross a line.

One possible exercise for later:
throw many needles, or write a MC code for this!

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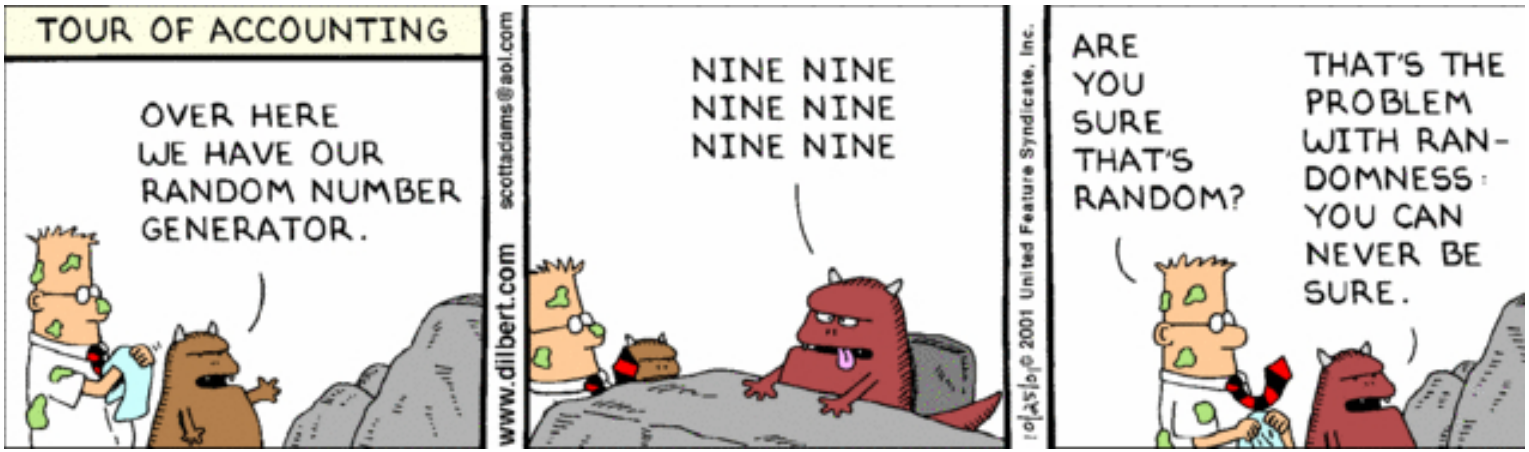

Brute force integration

Suppose that we want to calculate some integral of dimension D. The easiest thing to do is a sum over discrete intervals h, something like

$$I = \int_a^b dx_1 \ldots \int_a^b dx_D f(x_1 \ldots x_D) \approx h^D \sum f(x_1 \ldots x_D)$$

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so, for $\epsilon = 0.1$ and a system with 20 particles ($D = 60$) we have to sum $N = 10^{60}$ points.

With the best available supercomputers the time needed is greater that the age of the universe!

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... for now :-)