Physics and Computers

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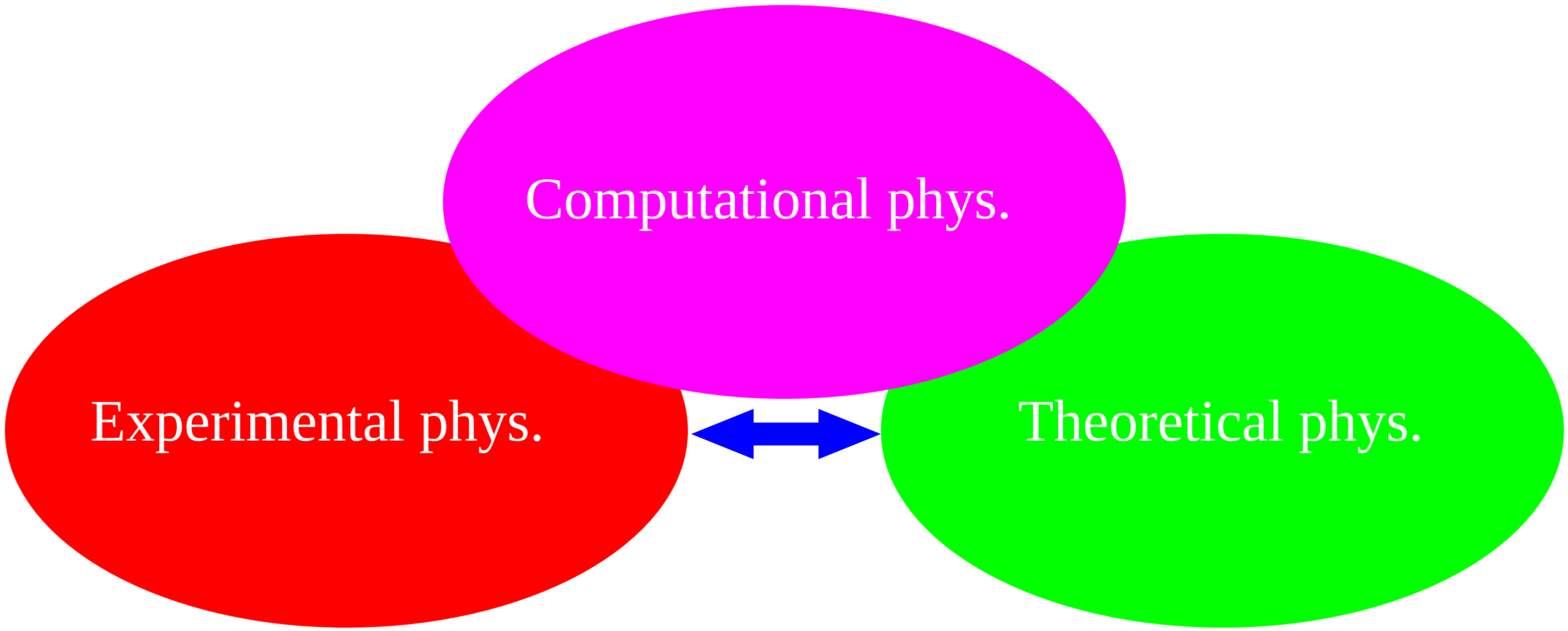
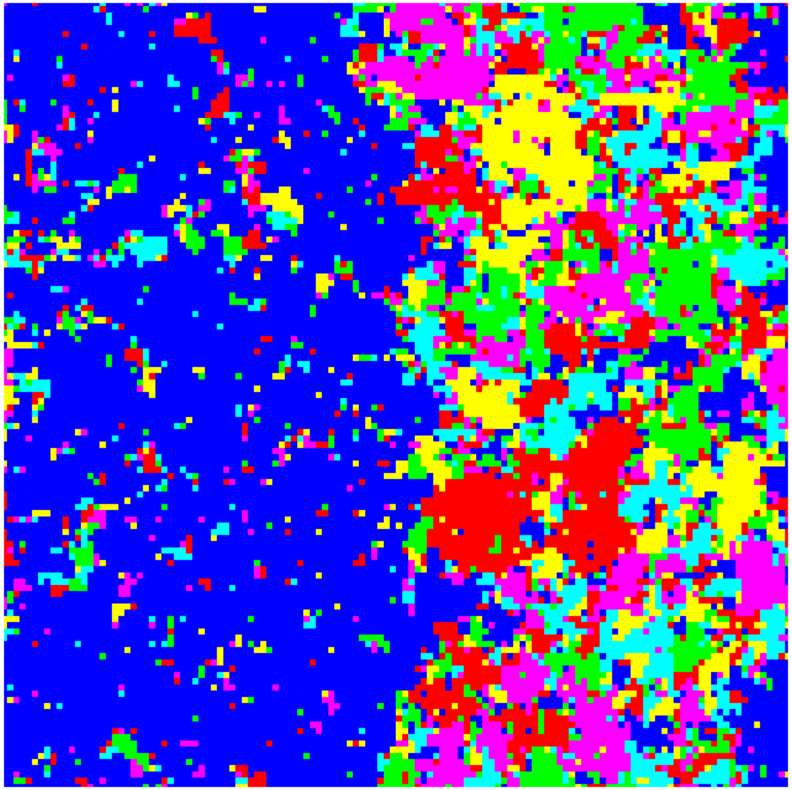
Computers in physics, used for:

- monitoring of experiments
- data acquisition
- data analysis
- evaluation of mathematical expressions
- computational physics



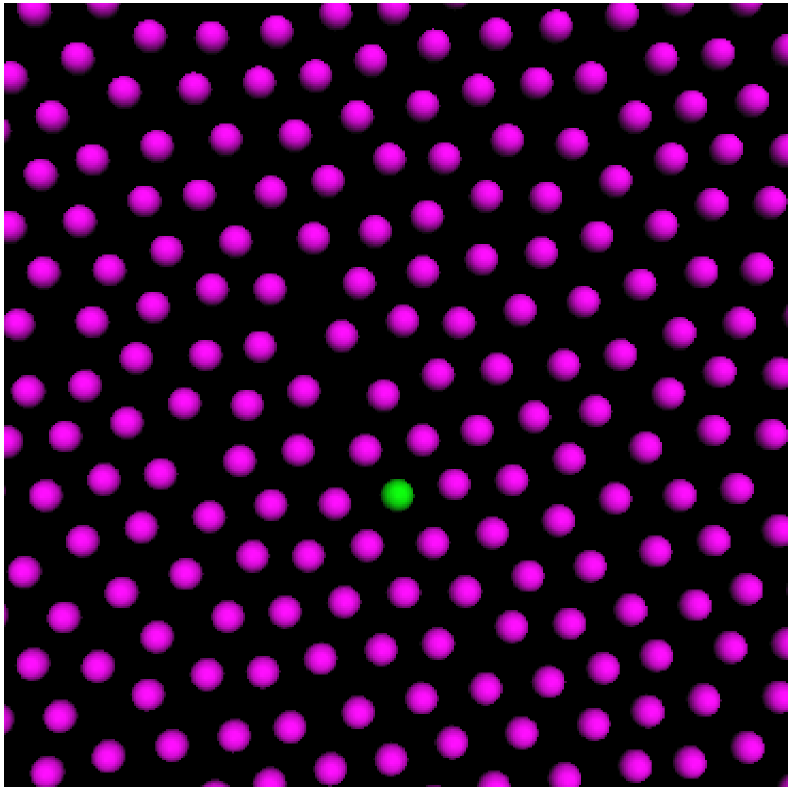
Computational physics is a methodology to derive predictions from theoretical assumptions by numerical techniques: it parallels and complements the traditional methods of theoretical and experimental physics, is not a substitute for either.



Early applications:

statistical mechanics

Phase structure in a Potts model simulation.



Early applications:

molecular dynamics and

fluid dynamics

Atoms with Lennard-Jones

interaction.

Applications of computational physics:

- condensed matter physics
- particle physics
- astrophysics
- gravitation
- plasma physics
- hydrodynamics
- biophysics
- and many more

Computational physics at its best proceeds hand in hand with theoretical analysis.

New challenges for computational physics

Over the years the powers of computers has increased by many orders of magnitude ($> 10^8$)

1970: CDC-7600, delivered $\sim$1 MFlops

2005: IBM BlueGene at LLNL, peak 183 TFlops (366 TFlops when fully configured), delivers 137 TFlops

New challenges for computational physics

The dramatic increase of computer power has widened enormously the scope of computational science, but this is forcing a change in its M.O.

Forefront investigations today require:

- algorithm development
- software engineering
- integration of graphics
- advanced data management
- team work

The U.S. DOE SciDAC program

SciDAC

Scientific Discovery through Advanced Computing

Mission (from the DOE web page):

- Create a new generation of Scientific Challenge Codes for terascale computers
- Create the enabling Mathematical and Computing Systems Software
- Create the appropriate Collaboratory Software Infrastructure

SciDAC Program areas

- Fusion Energy Sciences
- High-Energy & Nuclear Physics
- Biology & Environmental Research: Global Climate Research
- Basic Energy Sciences: Chemical Sciences
- Advanced Scientific Computing: National Collaboratories & Networking
- Advanced Scientific Computing: Integrated Software Infrastructure Centers

SciDAC funded projects in High-Energy & Nuclear Physics

- Advanced Computing for 21st Century Accelerator Science and Technology
- National Computational Infrastructure for Lattice Gauge Theory
- The Particle Physics Data Grid
- Shedding New Light on Exploding Stars: Terascale Simulations of Neutrino-Driven SuperNovae and their NucleoSynthesis
- SciDAC Center for Supernova Research

National Computational Infrastructure for Lattice Gauge Theory

Quantum Chromodynamics (QCD) explains structure and interactions of nuclear components (hadrons: proton, neutron, π mesons ...) in terms of quarks kept together by a gluon field.

Asymptotic freedom: $g \longrightarrow 0$ for $E \longrightarrow \infty$, $d \longrightarrow 0$

g increases as $E \longrightarrow 0$ or $d \longrightarrow \infty$

Low energy phenomena in QCD:

- confinement, hadron spectrum, weak matrix elements ...

To study a quantum field theory with large g we formulate it on a space-time lattice (Wilson, 1974) and then simulate the quantum fluctuations by computer

Lattice QCD

The variables of the theory:

- quark fields ψ defined over the sites of the space-time lattice, they carry spin and the intrinsic "color" degree of freedom ($4 \times 3 \times 480000 = 5.76\mathrm{M}$ on a $20^3 \times 60$ lattice)

- gluon fields U defined over the oriented links of the space-time lattice, they carry two color indices ($4 \times 9 \times 480000 = 17.28\mathrm{M}$ on a $20^3 \times 60$ lattice)

QCD observables

$$\langle \mathcal{O} \rangle = Z^{-1} \int dU \int d(\bar{\psi}\psi) \mathcal{O} e^{-S_g(U) - \bar{\psi} D(U) \psi}$$

where $D(U)$ stands for the discretized Dirac operator, i.e. a matrix operating on all space-time, spin and color components of the quark field

$D(U) = 5.76M \times 5.76M$ matrix on a $20^3 \times 60$ lattice

QCD observables, cont'd

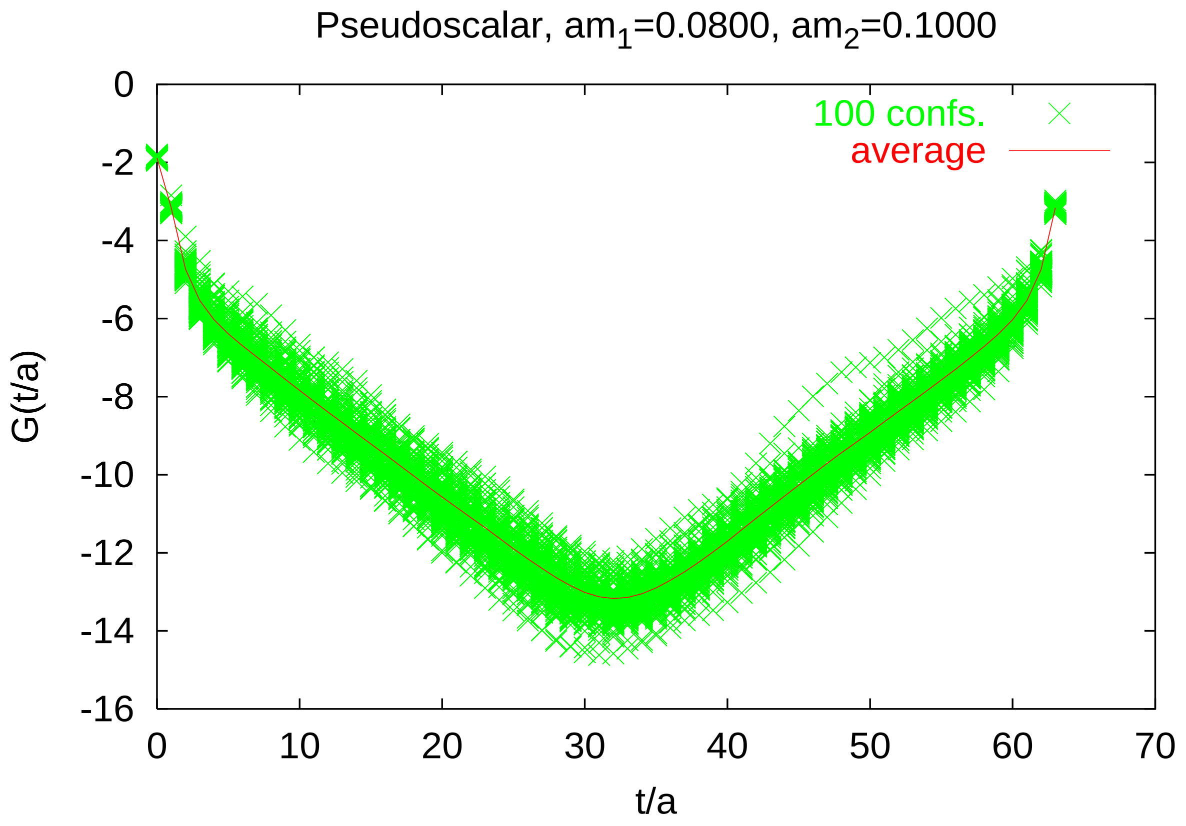
The Gaussian integration over quark field can be performed, yielding e.g. for $\mathcal{O} = \bar{\psi}\psi(x)\bar{\psi}\psi(y)$ (a meson propagator)

$$\langle\bar{\psi}\psi(x)\bar{\psi}\psi(y)\rangle = Z^{-1}\int dU\, D^{-1}(x,y)D^{-1}(y,x)e^{-S_g(U)}\mathrm{Det}\,D(U)$$

Advanced linear algebra algorithms are used together with sophisticated stochastic sampling techniques to generate a large sample of gauge field configurations U and to calculate the value of the meson propagator $\Pi(x,y) = D^{-1}(x,y)D^{-1}(y,x)$ configuration per configuration.

The exact quantum mechanical expectation value $\langle\bar{\psi}\psi(x)\bar{\psi}\psi(y)\rangle$ is then approximated by its average over the sample of gauge field configurations.

Meson correlation function (example)

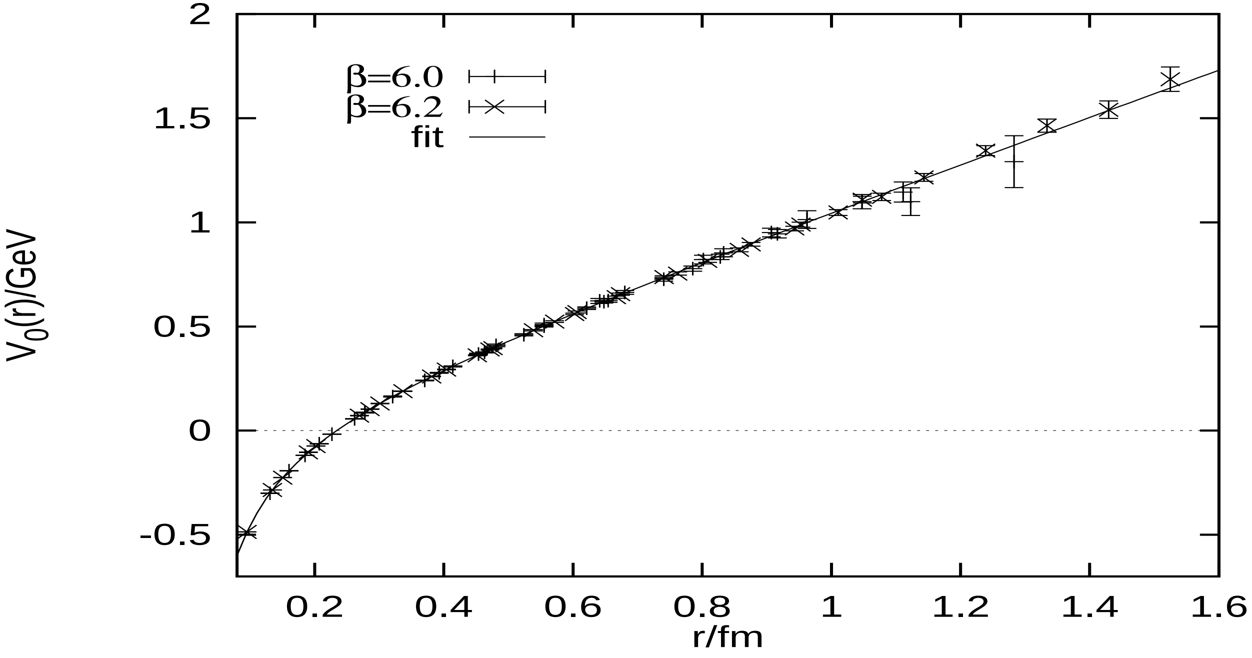


From the rate of decay of the meson correlator one can extract the meson mass.

Lattice QCD calculations

Lattice QCD simulations were first performed in the early 80’s. Since then there has been constant progress in the scope and accuracy of the calculations.

- E.g. the confining potential, from Bali, Schilling and Wachter (1997):



Lattice QCD calculations, cont'd

The power of today's supercomputers has opened the possibility of using lattice simulations not only for a validation of QCD as the theory of strong interactions, but, for the first time, to produce a determination of many quantities (weak matrix elements, parameters of the quark-gluon plasma, form factors, moments of structure functions ...) which play a crucial role for the interpretation of experimental results.

However, this requires the deployment of dedicated supercomputers (QCDOC, ApeNext, specialized clusters) as well as the development of algorithms, software, visualization and data handling tools.

The US LQCD collaboration http://www.usqcd.org/

National Computational Infrastructure for Lattice Gauge Theory

Overview Software Hardware Science Contacts and Links Strategic Plan! News

Overview

Scientific Goals

Project Goals

Distributed Terascale Facility

Impact

Objective

Create the software and hardware infrastructure needed for terascale simulations of Quantum Chromodynamics (QCD).

Scientific Goals

Non-perturbative Study of QCD

- **Calculation of Weak Decays of Strongly Interacting Particles**
  - **Determination of least-well-known parameters of the Standard Model**
  - **Precision tests of the Standard Mode**
- **Investigation of Matter under Extreme Conditions**
  - **Mapping the phase diagram of strongly interacting matter**
  - **Determining the properties of the Quark-Gluon Plasma**
- **Understanding the Structure and Interaction of Hadrons**
  - **Calculation of spectrum of hadrons existing in nature, and exploration of**

Conclusions

- Computers offer enormous potential for basic physics research, extending the methods of theoretical physics.

- The ever increasing power of supercomputers continues to augment the scope and depth of computational investigations.

- This requires some fundamental changes in the mode of operation of computational physics, which should be brought about without losing its strong intellectual focus.