UC RIVERSIDE | 2023 National Nuclear Physics Summer School

July 10-22, 2023

Lattice QCD (selected topics)

Lecture 1

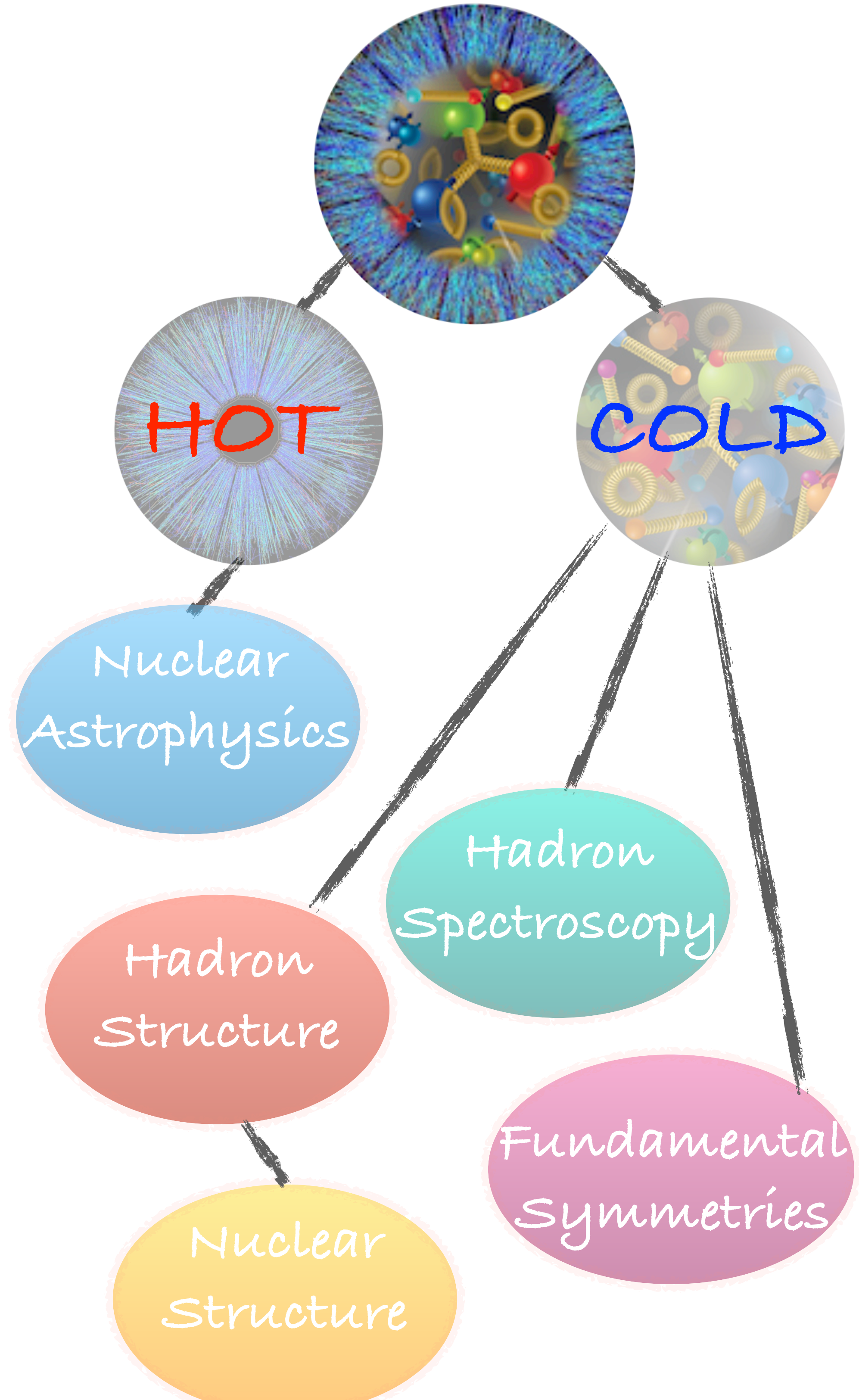
Martha Constantinou

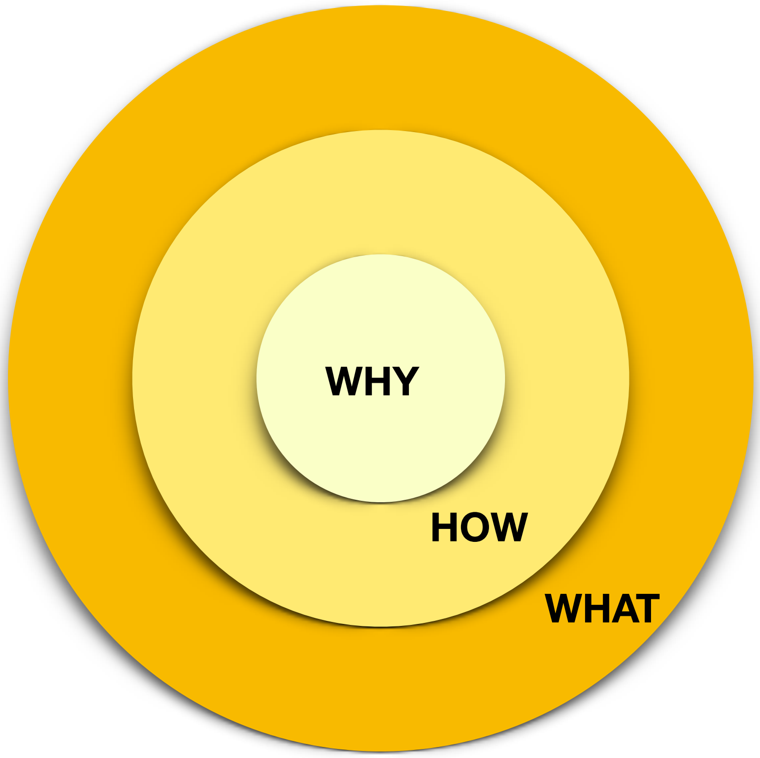
Temple University

July 10, 2023

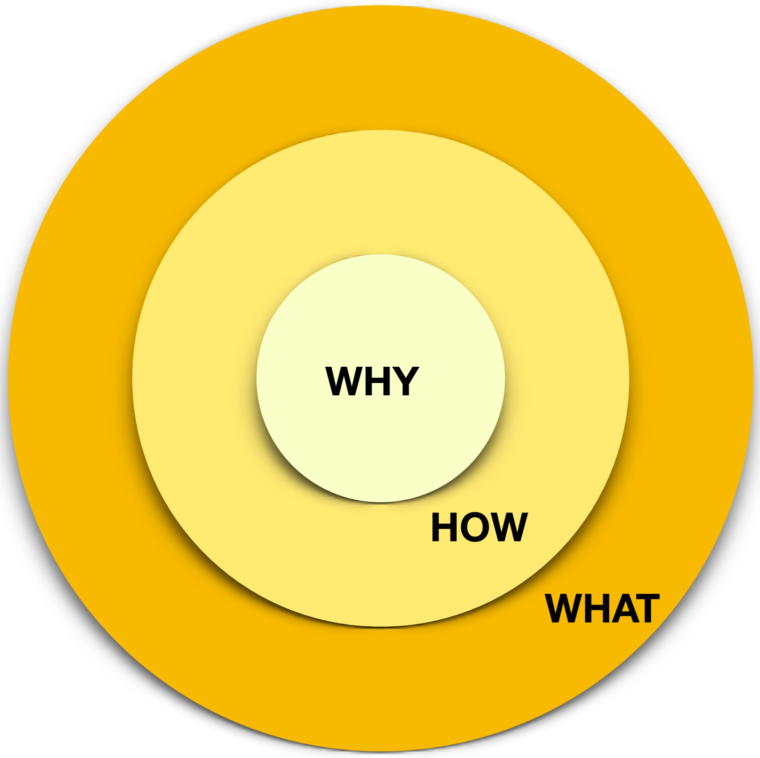
USQCD Nuclear Physics Program

- ★ Important Lattice QCD contributions that complement the experimental program in both Hot and Cold QCD




WHY
HOW
WHAT

What is the physics we are after?



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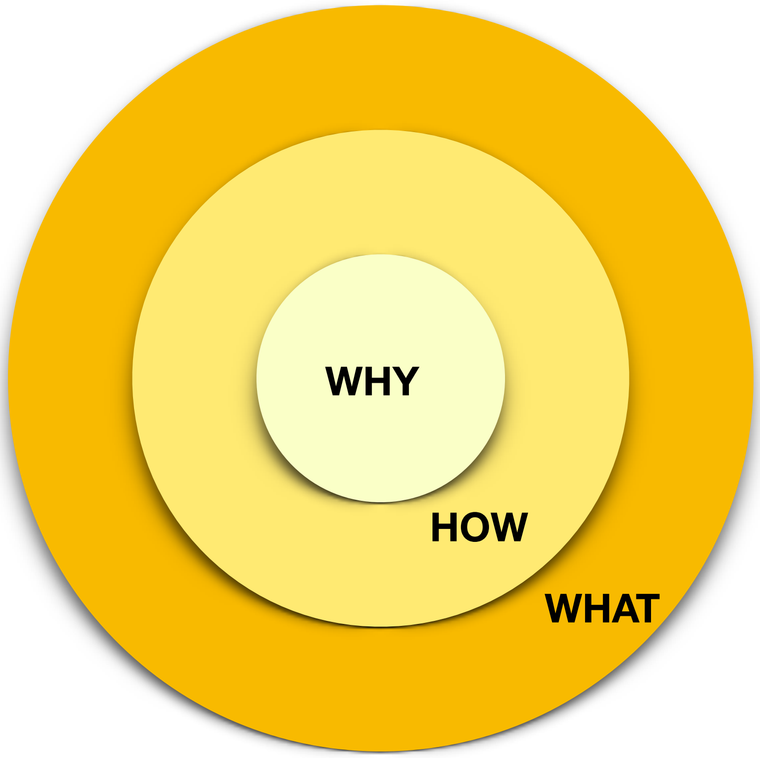

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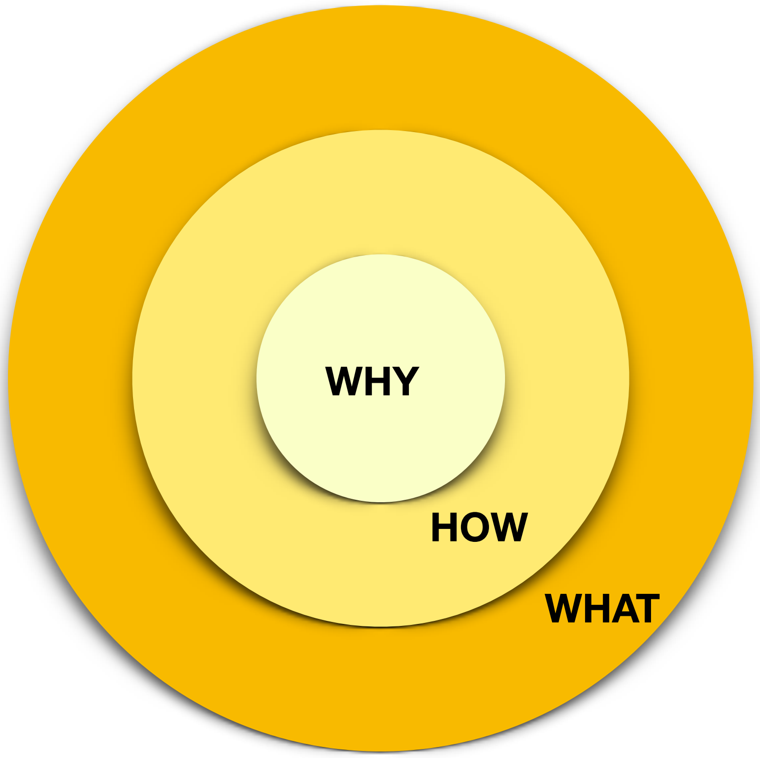

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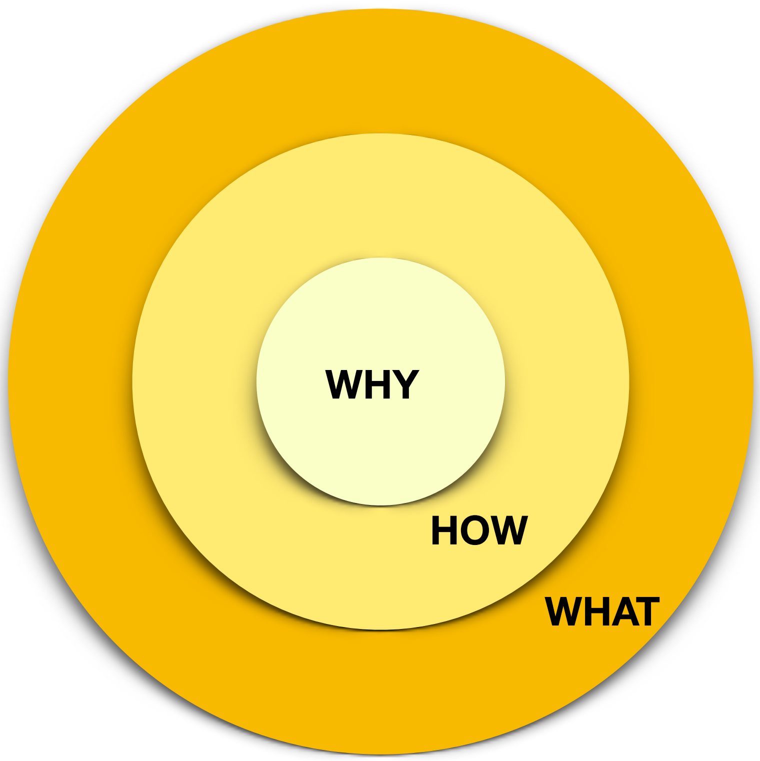

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- ★ Hadron spectroscopy - Exotic states
- ★ Hadron structure
- ★ Nuclear Forces and Nuclei
- ★ Nuclear Astrophysics
- ★ Beyond the Standard Model Physics
- ★ Hot QCD (quark-gluon plasma, QCD phase diagram)

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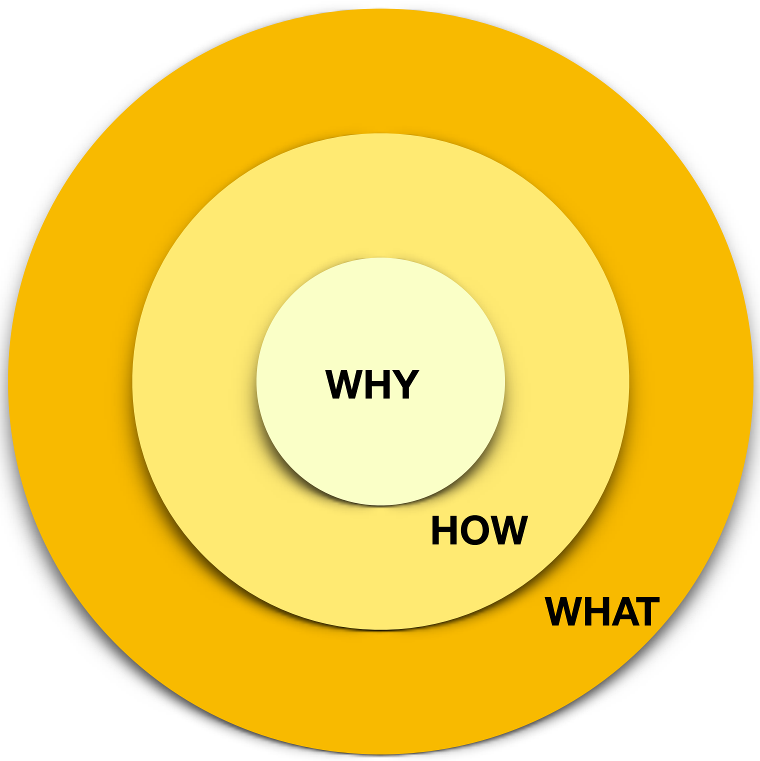

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  — billions of degrees of freedom
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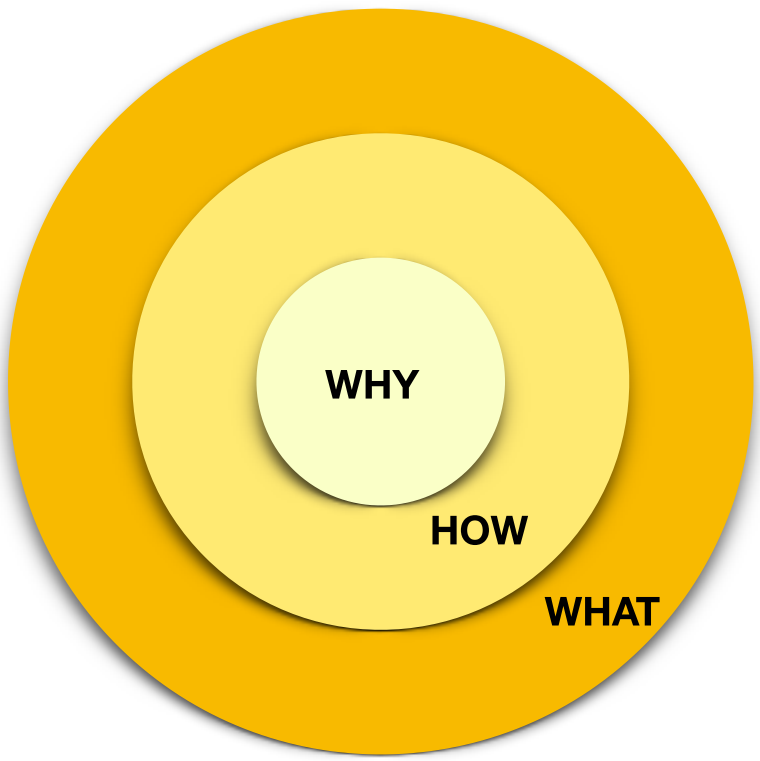

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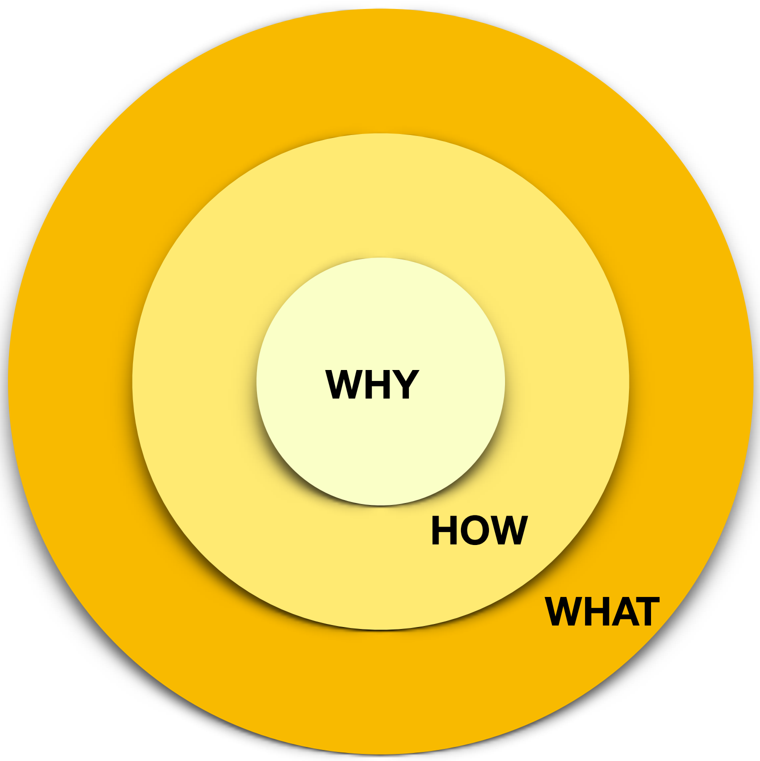

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Numerical simulations of QCD address aspects of key questions

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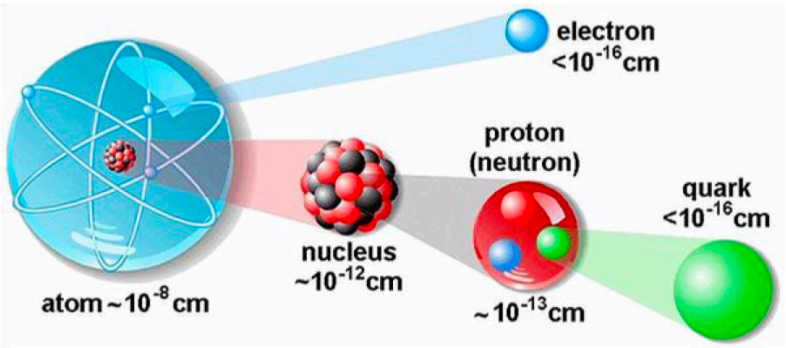

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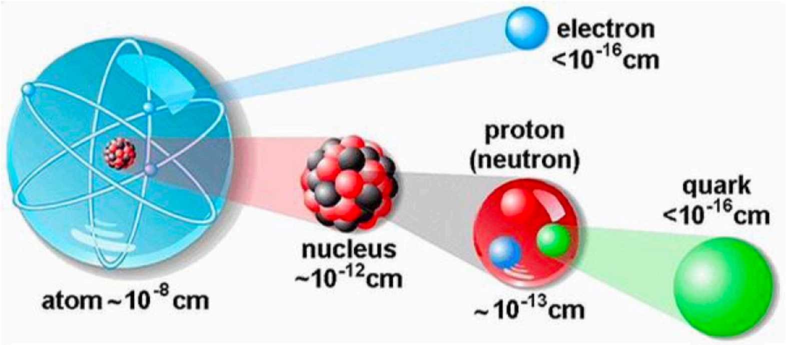
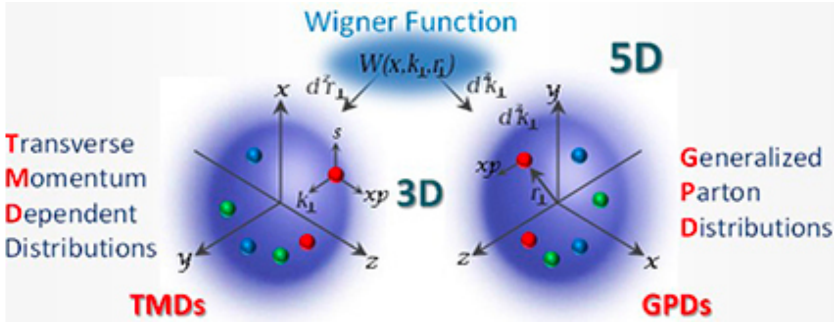


What is the 3-D tomographic mapping of nucleons (p,n)?



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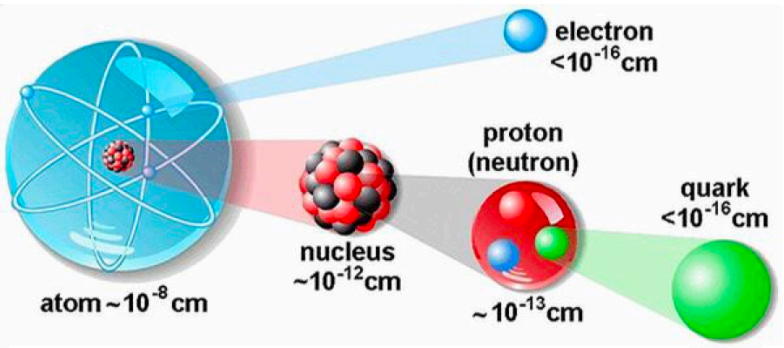

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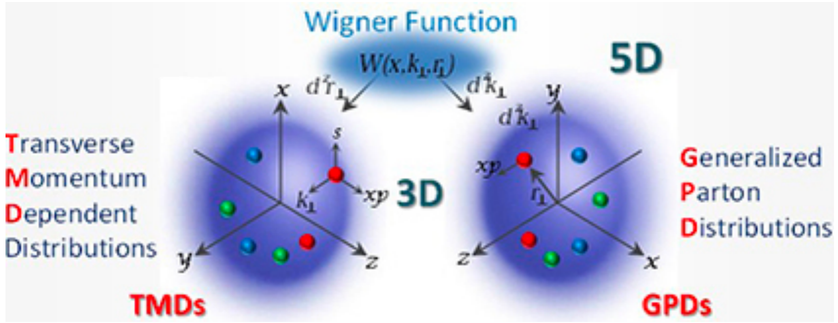
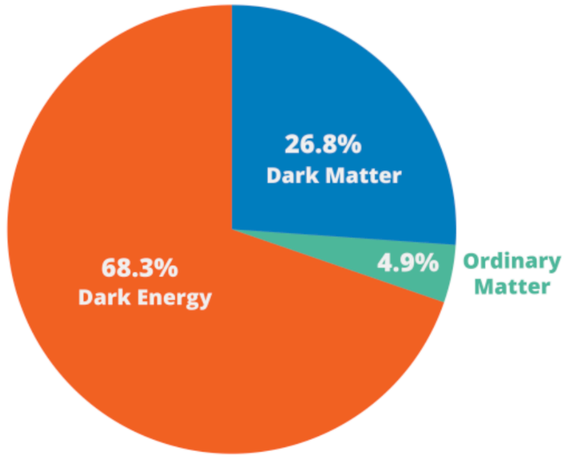


To what extent do we understand matter and energy? Is there New Physics to be discovered?



OUTLINE OF LECTURES

★ **Monday, July 10:**
Motivation and Formulation of Lattice QCD

★ **Tuesday, July 11:**
Renormalization and Hadron Spectroscopy

★ **Wednesday, July 12:**
Hadron Structure - EIC physics

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  ~~Renormalization~~ and Hadron Spectroscopy
  Proton mass?

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OUTLINE OF LECTURE 1

★ Quantum Chromodynamics in a nutshell

★ Path Integral Formalism

★ Lattice QCD formulation

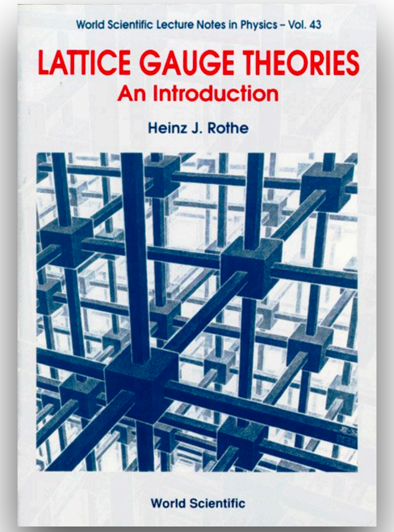
★ Fermion and Gluon fields on the lattice

★ Landscape of numerical simulations

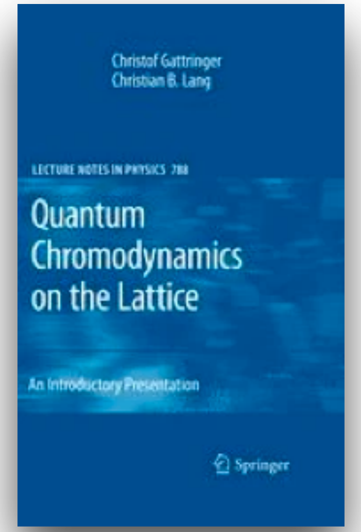
★ Key points of Lecture 1

Useful Reading Material

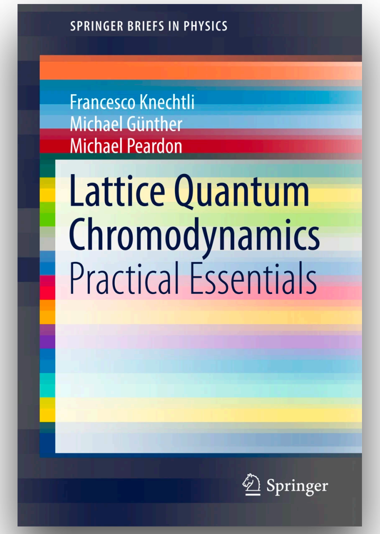
★ Lattice Gauge Theories: An Introduction
H. J. Rothe
https://www.worldscientific.com/worldscibooks/10.1142/1268



★ Quantum Chromodynamics on the Lattice
An Introductory Presentation
C. Gattringer and C. Lang
https://www.springer.com/us/book/9783642018497



★ Lattice quantum chromodynamics: practical essentials
Knechtli, Günther & Peardon
https://link.springer.com/book/10.1007/978-94-024-0999-4



Useful Reading Material

Review article for the European Physical Journal C (EPJ C)

50 Years of Quantum Chromodynamics

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arXiv: 2212.11107
https://inspirehep.net/literature/2617065

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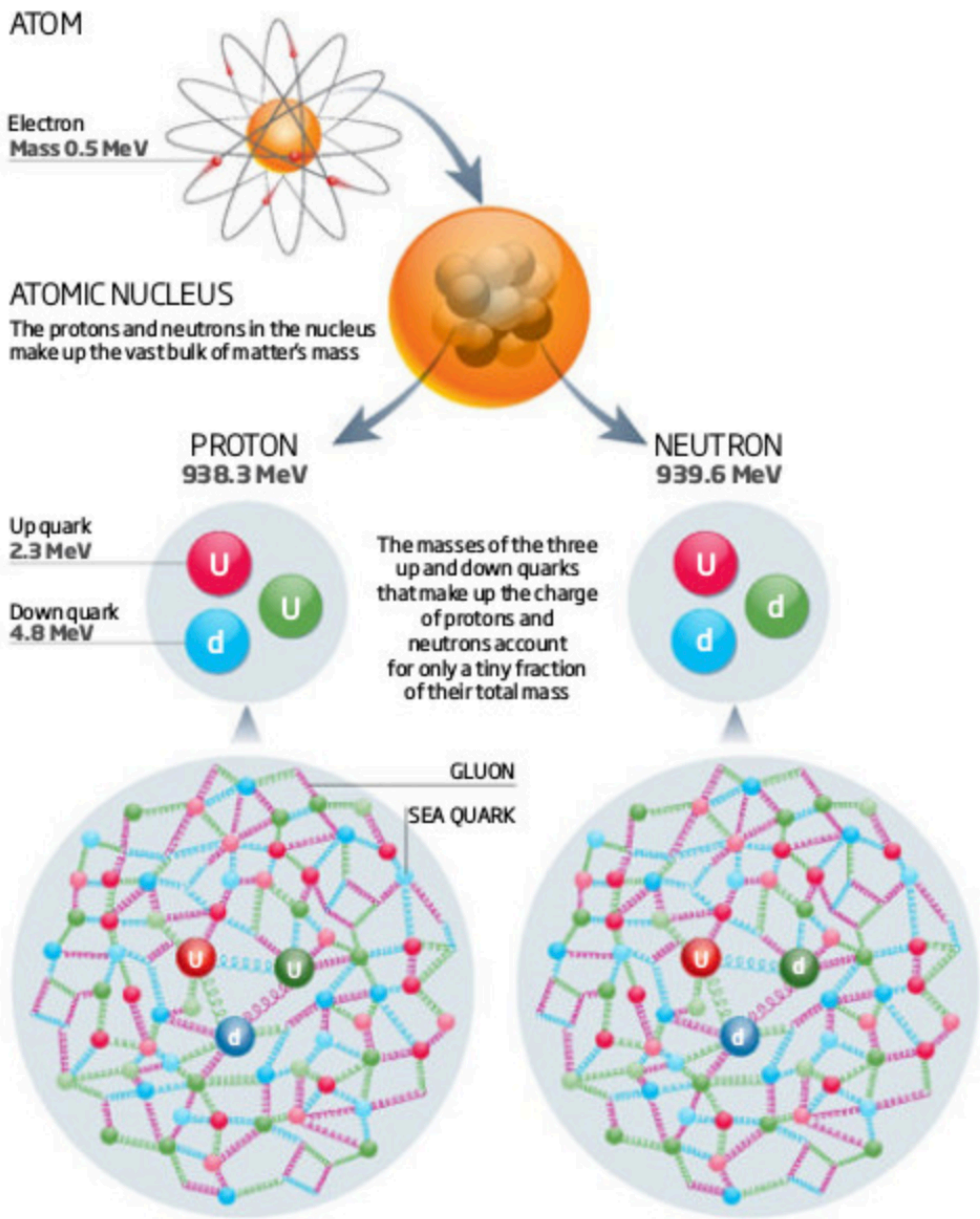
Characteristics of QCD and role in nature

Strong Interactions:
Evolution from Big Bang to present Universe and beyond

- **Quark-Gluon plasma at t~10^{-32} s**
  studied in heavy ion collisions at RHIC and LHC
- **Hadron formation at t~10^{-6} s**
  studied in experimental facilities wordwide e.g. CERN, JLab, Mainz,…
- **Primordial nucleosynthesis between 10s to 20 min**

Quantum Chromodynamics (QCD)

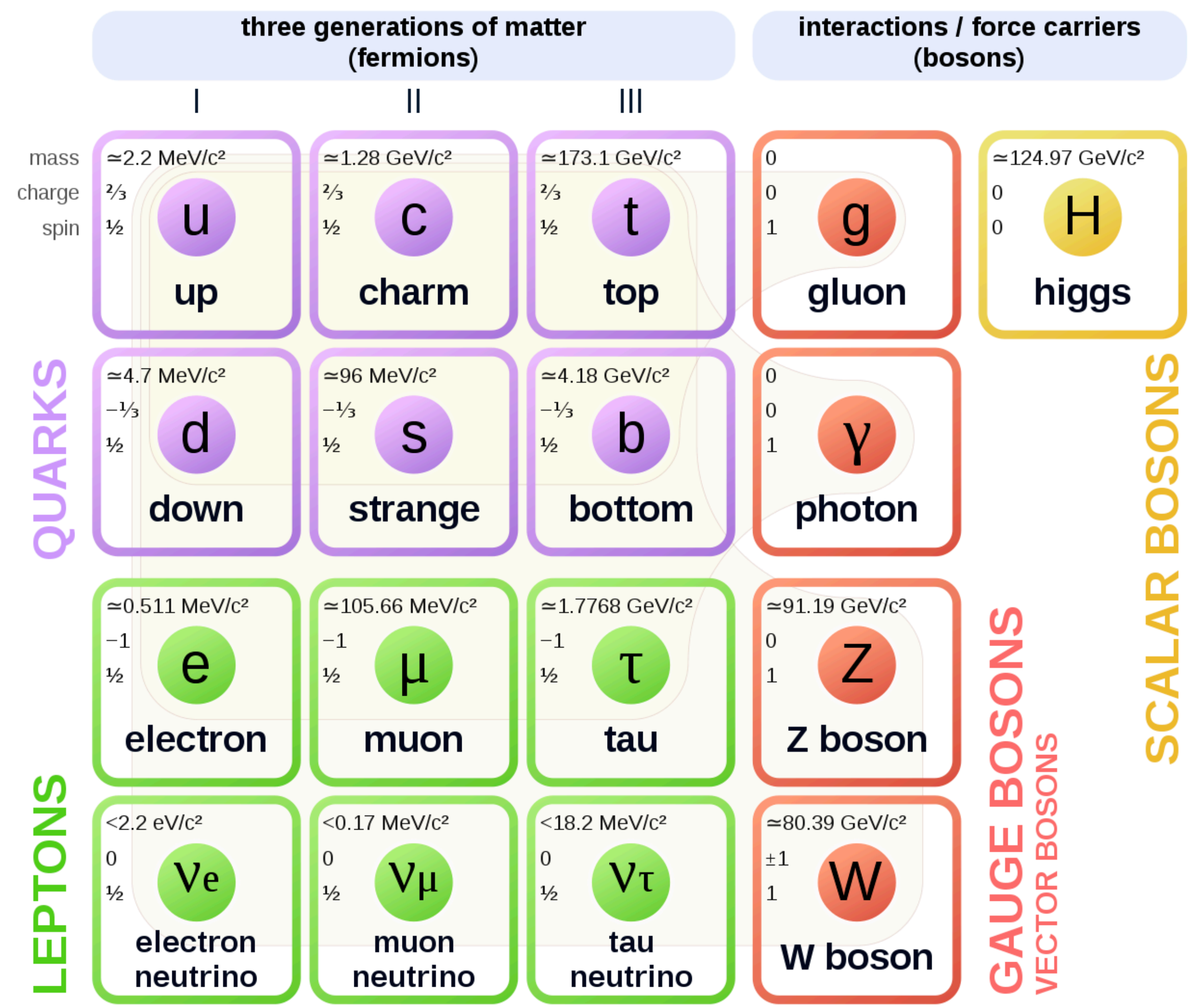
Structure of Matter



★ **Theory of the strong interactions**

★ **Fundamental constituents: 6 quark and 8 gluons**

★ **Included in elementary particles**



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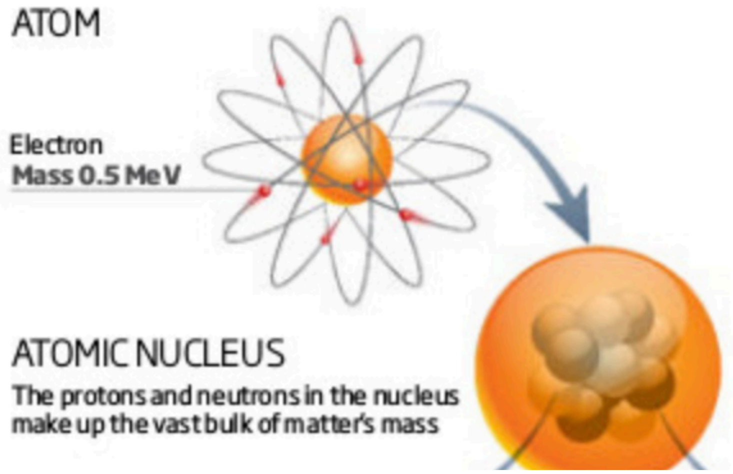

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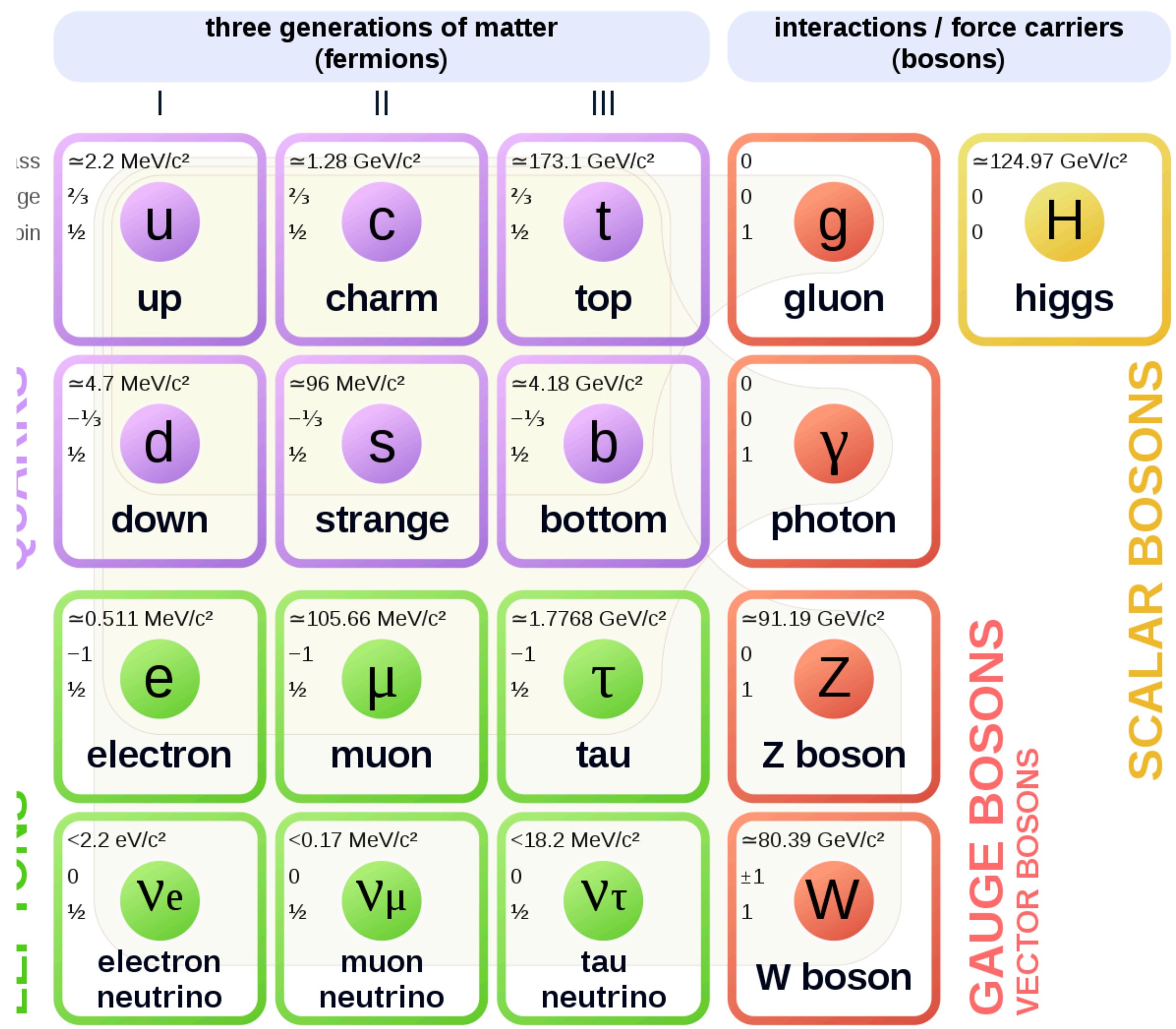
July 4, 2012 at CERN



Theory of QCD

★ Quarks & gluons carry a color quantum number
- quarks: 3 colors (red, blue, green)
- gluons interact with gluons (force mediators)

★ Only a few parameters needed to describe QCD
- quark masses
- coupling constant

★ QCD successfully describes a wide range of complex processes
- fusion and fission processes that power the sun
- formation and explosion of stars
- the state of matter at the birth of the universe

QCD Lagrangian

QCD is a non-abelian gauge theory with symmetry group SU(3):

— 8 generators of SU(3) gauge group
— dimensionality of transformation space: 3

QCD Lagrangian density:

$$\mathscr{L}_{\mathrm{QCD}} = \sum_f \bar{\psi}_f \left(i\gamma^\mu D_\mu - m_f \right) \psi_f - \frac{1}{4} F^a_{\mu\nu} F^{a\,\mu\nu}$$

$$\gamma^\mu D_\mu = \gamma^\mu \partial_\mu + i g G^a_\mu \gamma^\mu T^a$$

$$F^a_{\mu\nu} = \partial_\mu G^a_\nu - \partial_\nu G^a_\mu - g f_{abc} G^b_\mu G^c_\nu$$

f_{abc} : structure constants of SU(3)

T^α : SU(3) generators, α : 1,2,...,8

$F^\alpha_{\mu\nu}$: field tensor operator

G^α_μ : gluon field

$\psi^{s,c}_f(x)$: quark field, 4 component spinors, 3 component color, 6 flavors

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Quark kinetic & mass terms
quark-gluon terms

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Huge increase of complexity level to solve QCD (compared to QED)

Features of QCD: The running coupling

Confinement

- ⇨ low energies/large distances
- ⇨ strong coupling
- ⇨ non-perturbative tools
- ⇨ hadrons and glue balls

Asymptotic freedom

- ⇨ high-energies/short distances
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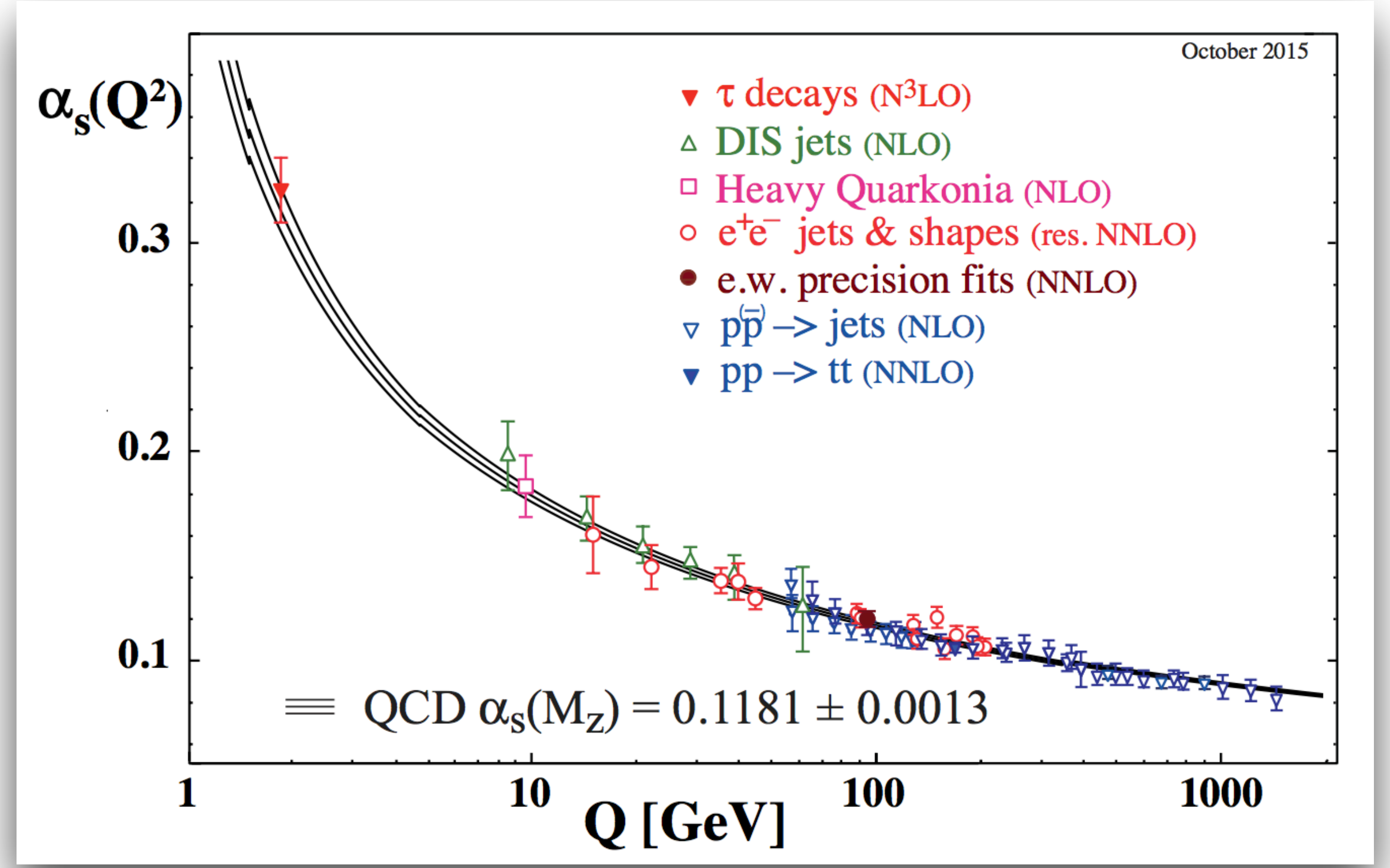

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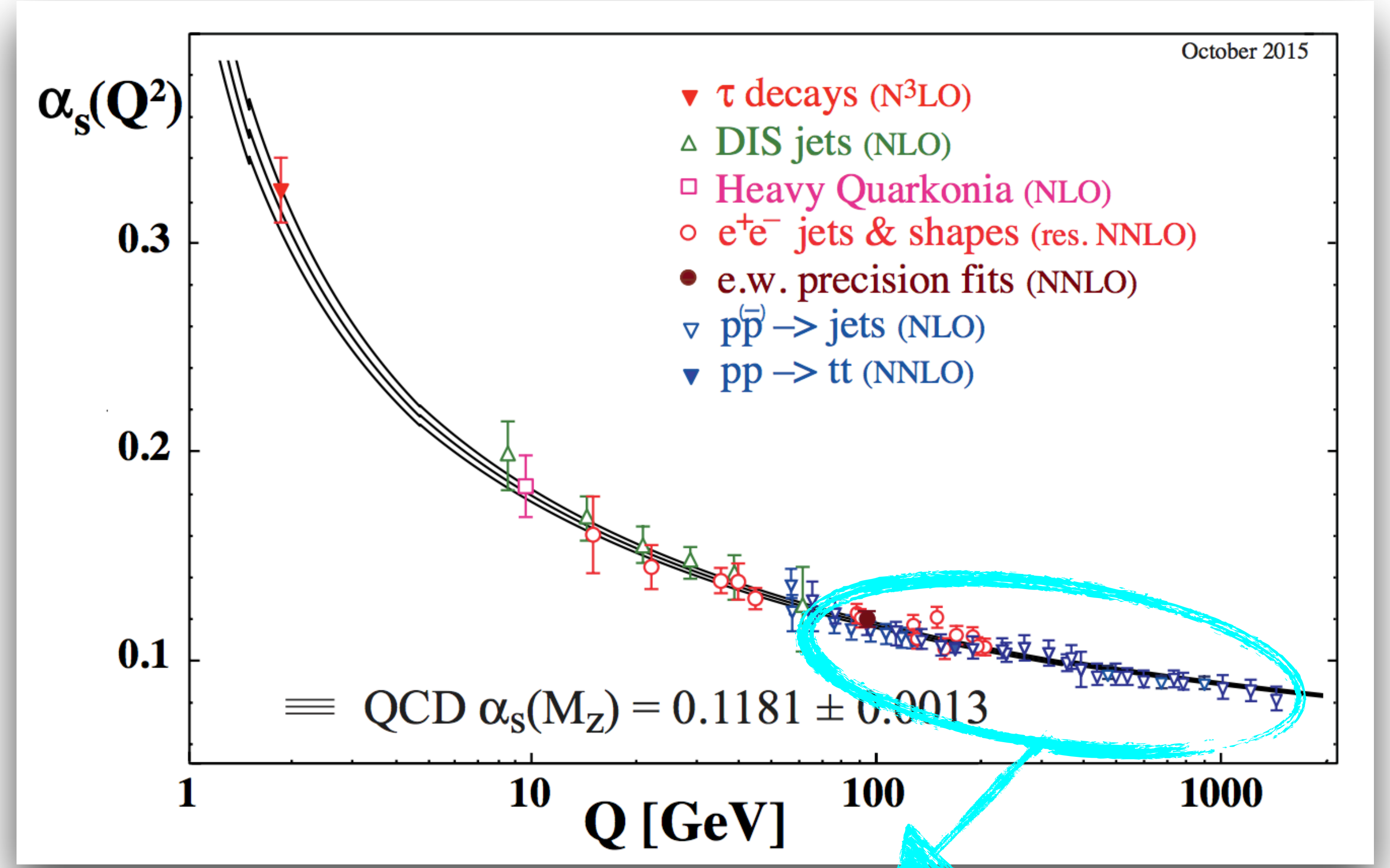

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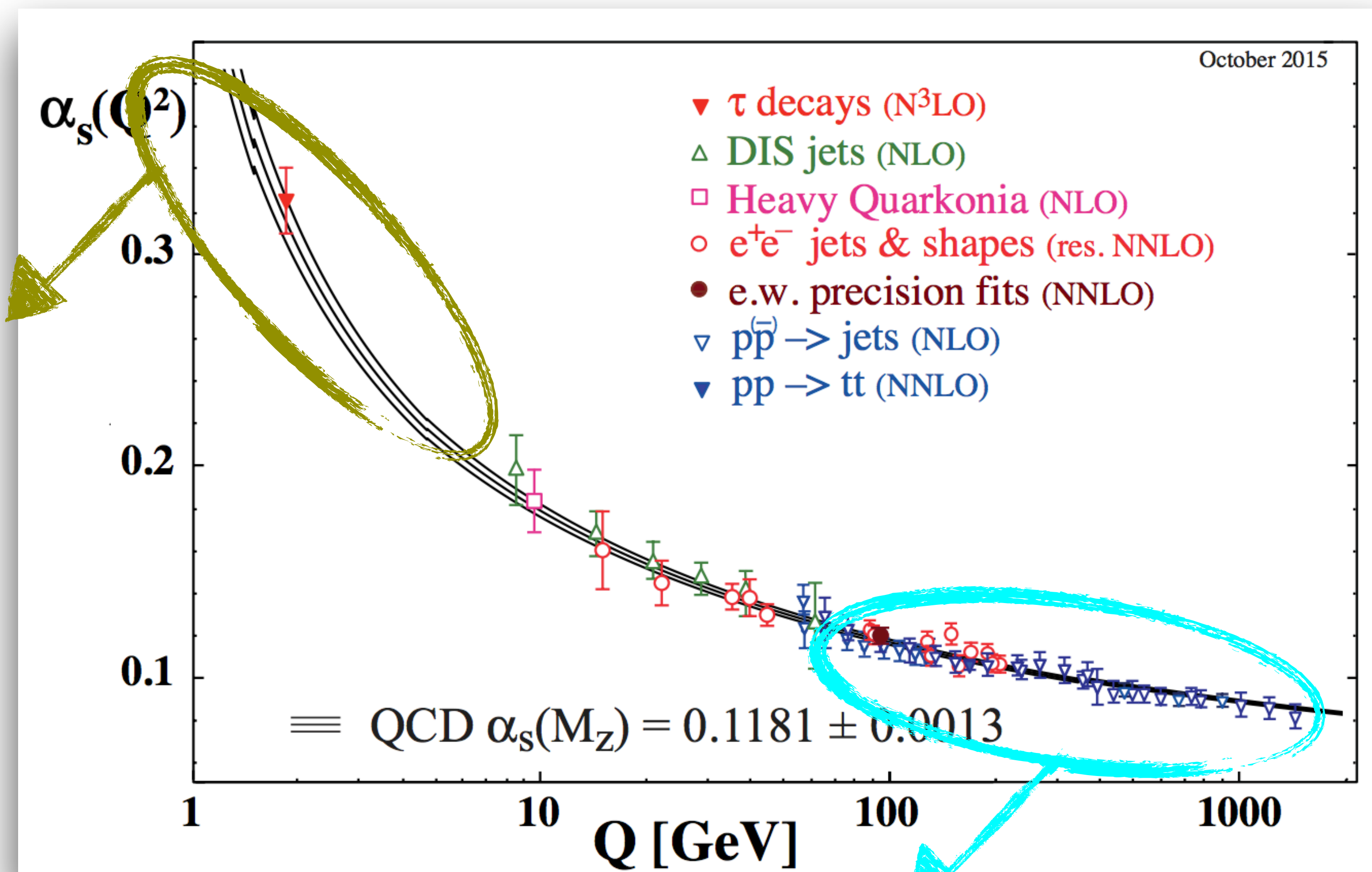

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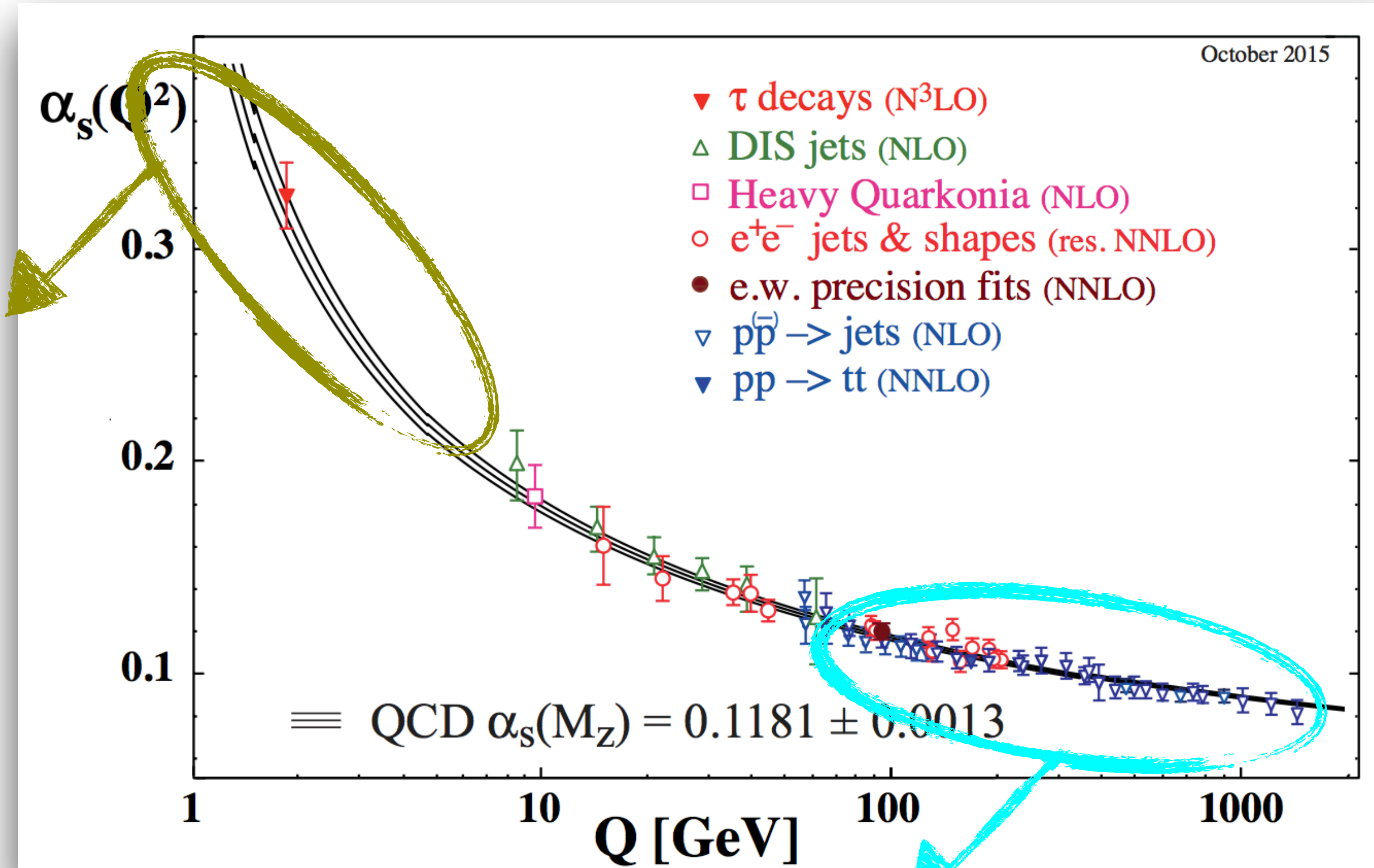

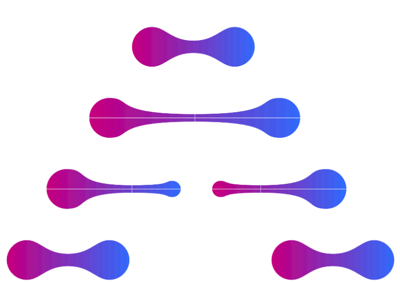

Quark confinement

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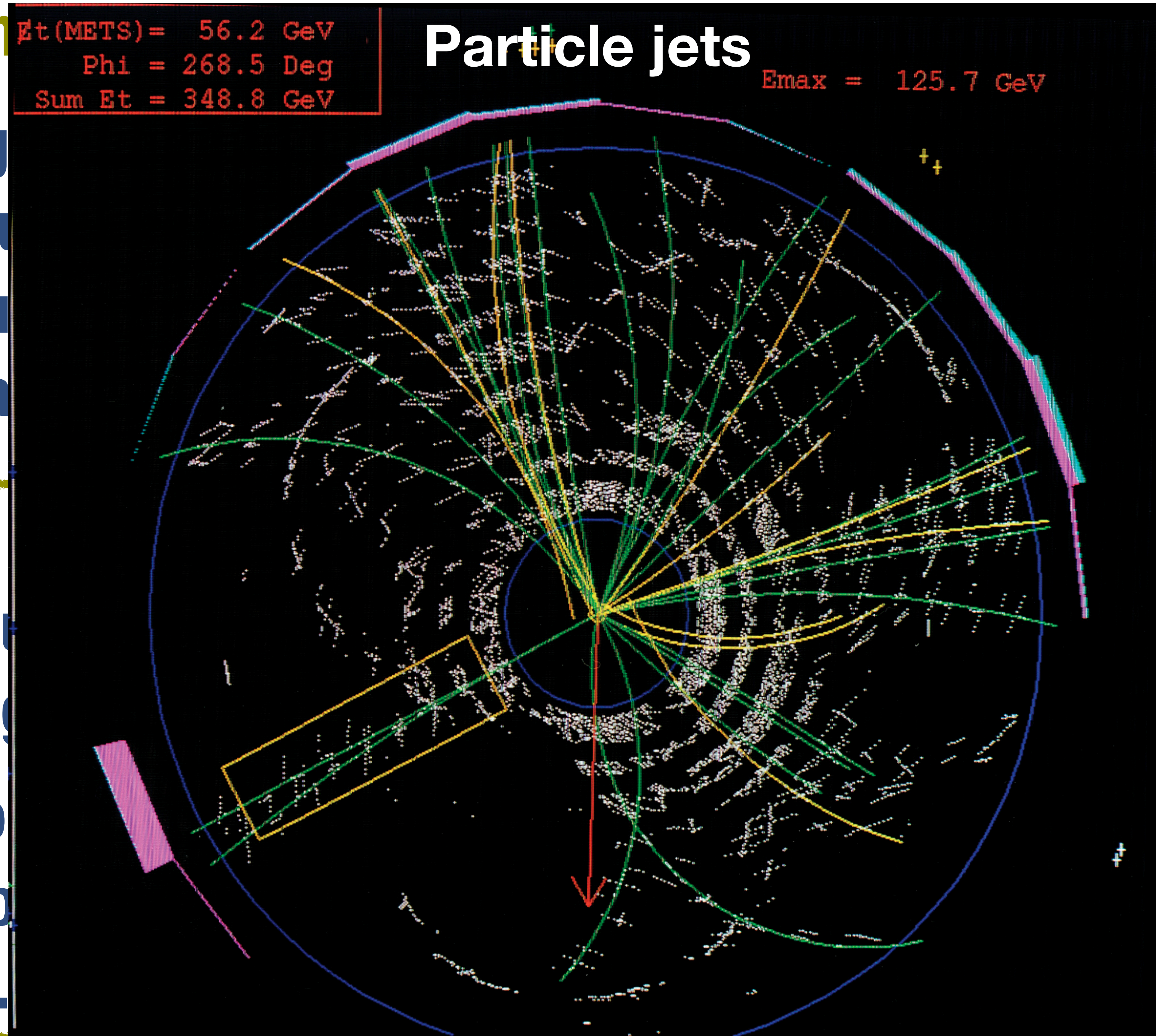

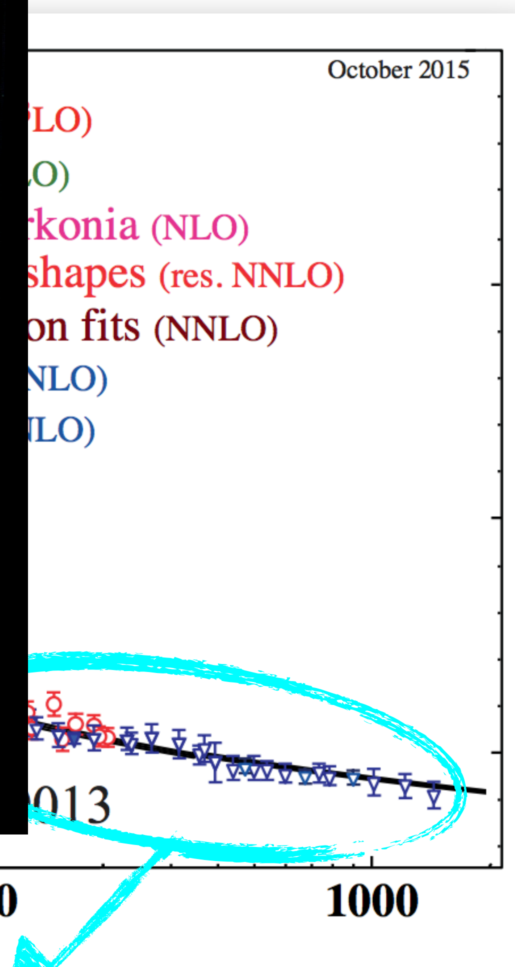

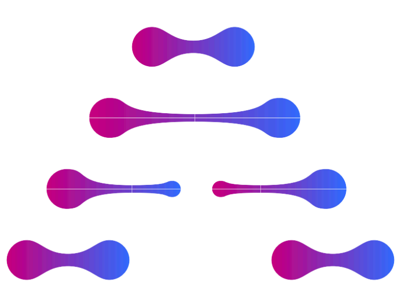

Quark confinement

Perturbative tools are successful

QCD vs QED

QED:

- ★ Description of interaction between light and matter
- ★ Two types of electric charge: positive & negative
- ★ Force mediated by exchange of photons
- ★ Photons: no electric charge and do not self-interact

Hydrogen Atom: $$m_{hydr} = \underbrace{0.51 MeV}_{m_{e^-}} + \underbrace{938.29 MeV}_{m_{p^+}} - \underbrace{13.6 eV}_{E_{binding}}$$

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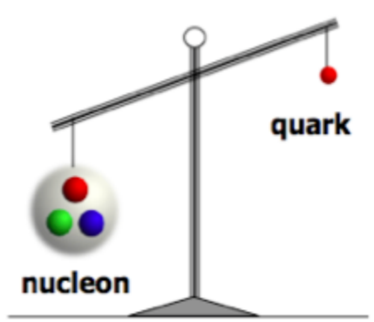
Proton: $m_p = \underbrace{4.4 MeV}_{2\times m_u} + \underbrace{4.7 MeV}_{m_d} + \underbrace{929.2 MeV}_{interaction}$



99% of the mass is due to interactions

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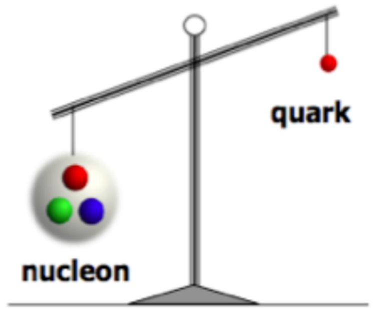

99% of the mass is due to interactions

Origin of the hadron mass is yet to be fully understood

Emergence is the key …

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Individual starlings

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Individual starlings

murmuration of starlings

How do we study QCD?

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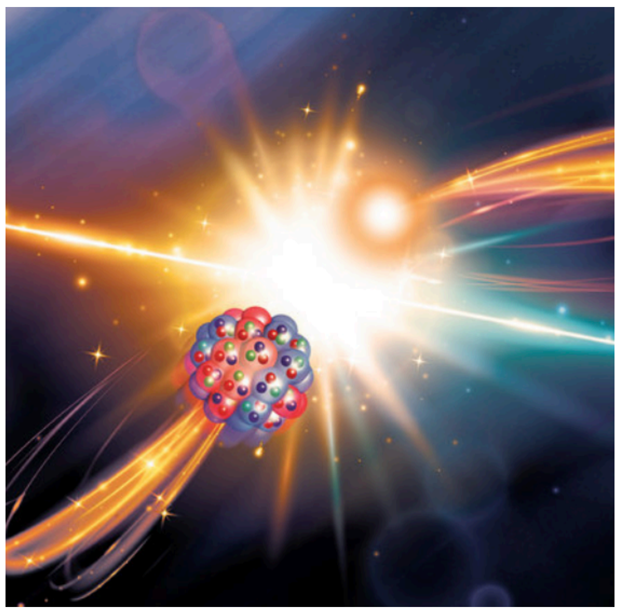
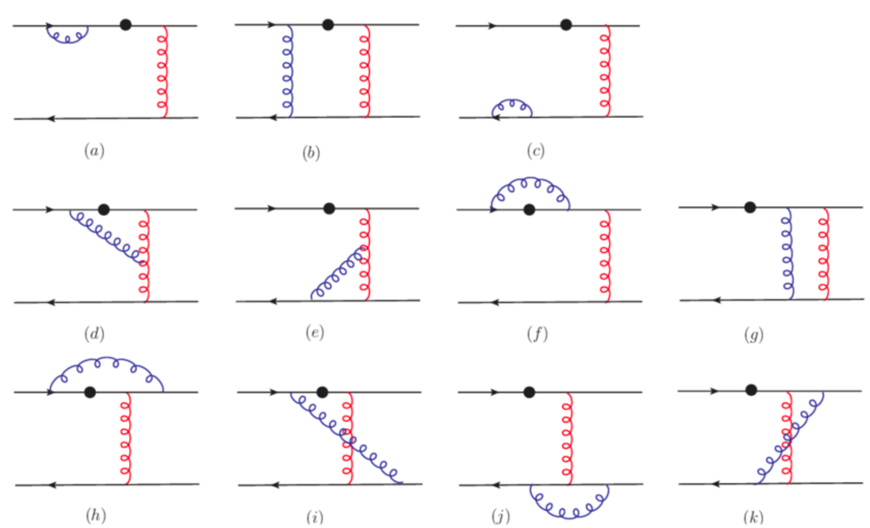
High-energy collisions



Perturbative QCD / phenomenology



First principles (Simulations on supercomputers)

How do we study QCD?

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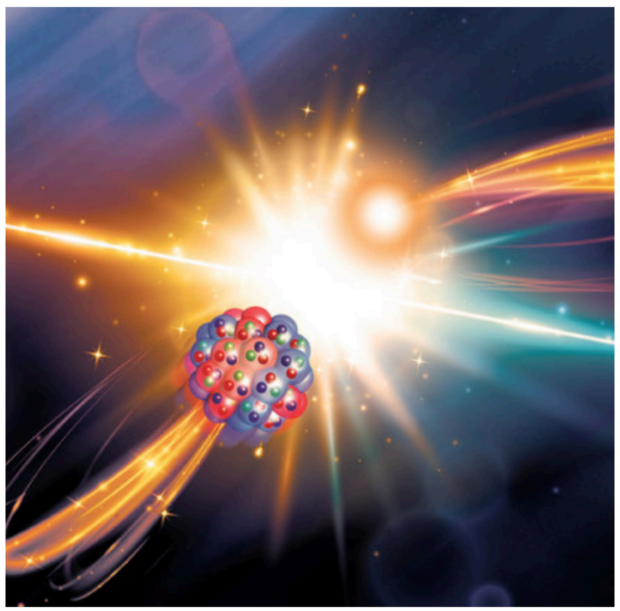

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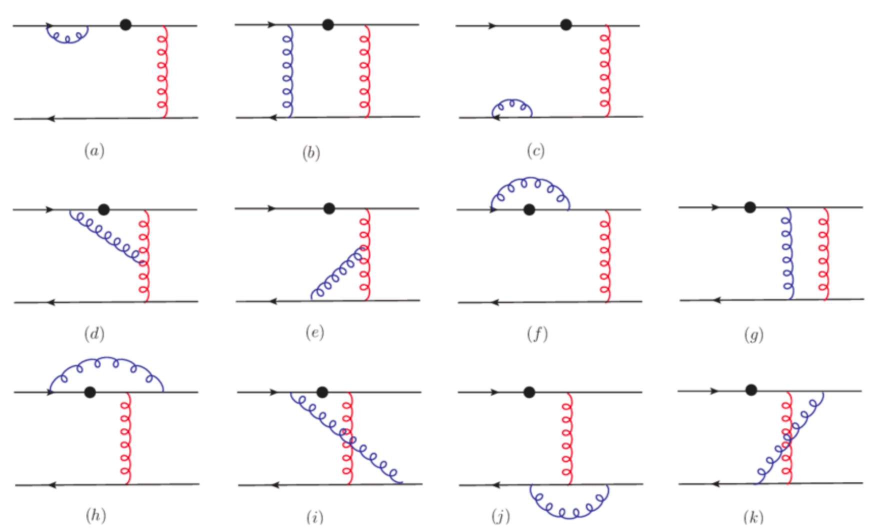

First principles (Simulations on supercomputers)

Wealth of information from each approach

Synergistic research activities critical!

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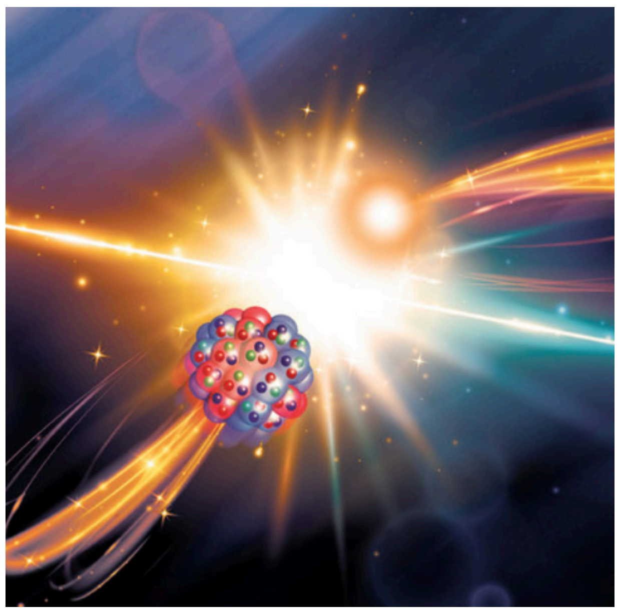

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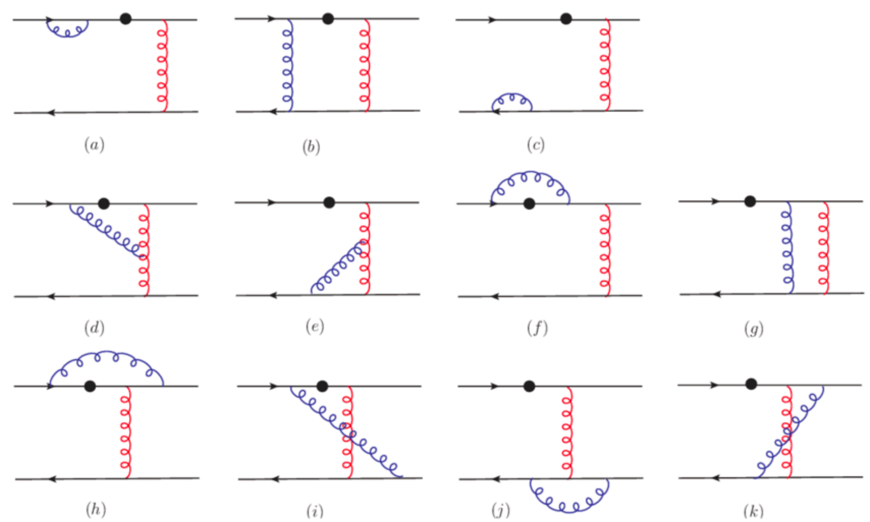

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Oak Ridge National Lab

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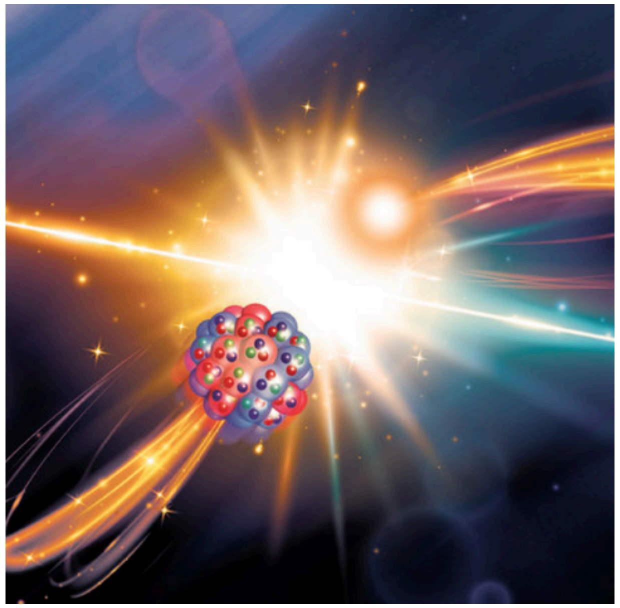

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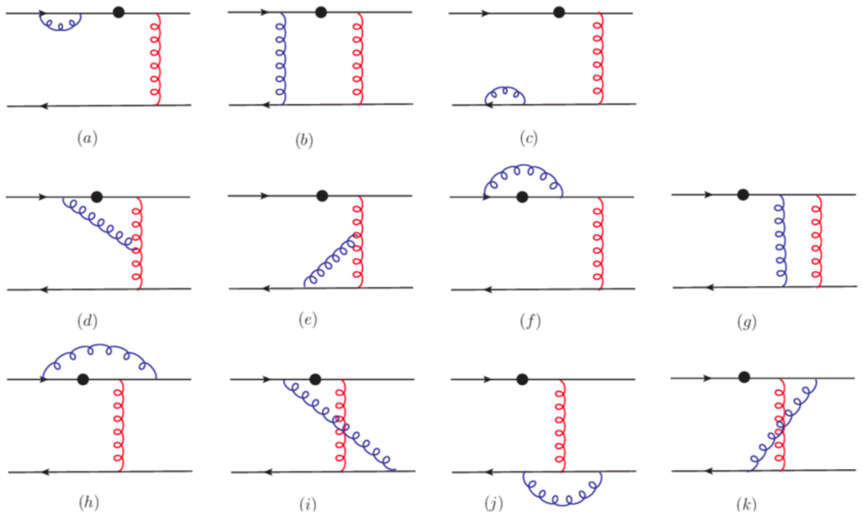

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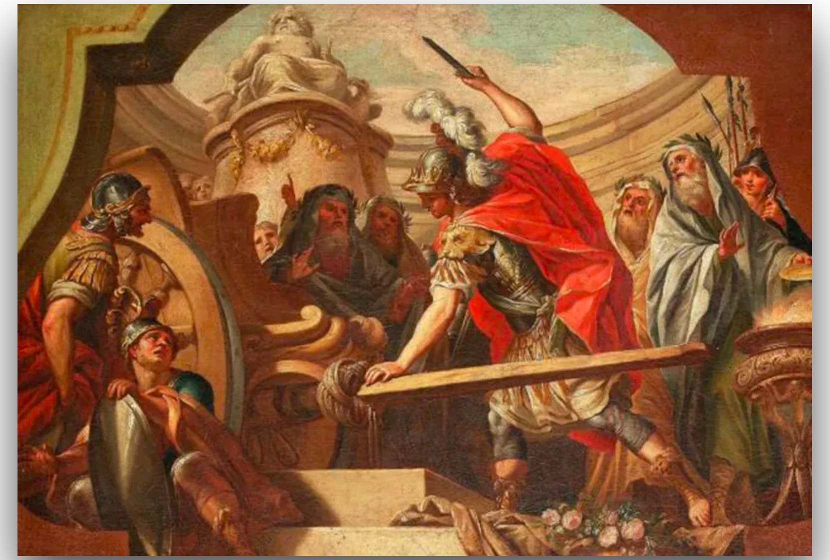
Let's start from the basics

In the quest of solving complex problems



“Ότι δεν λύνεται, κόβεται”

Alexander the Great while cutting the Gordian knot

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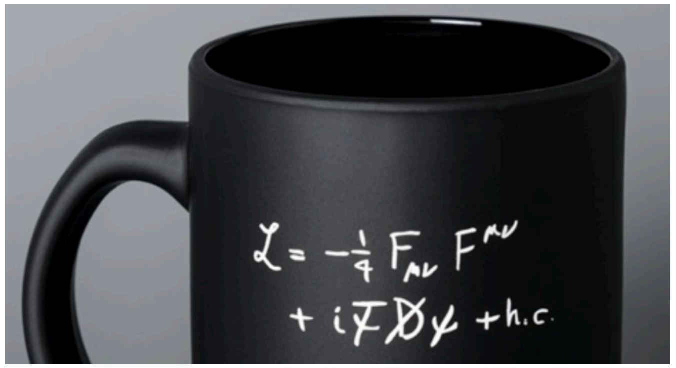

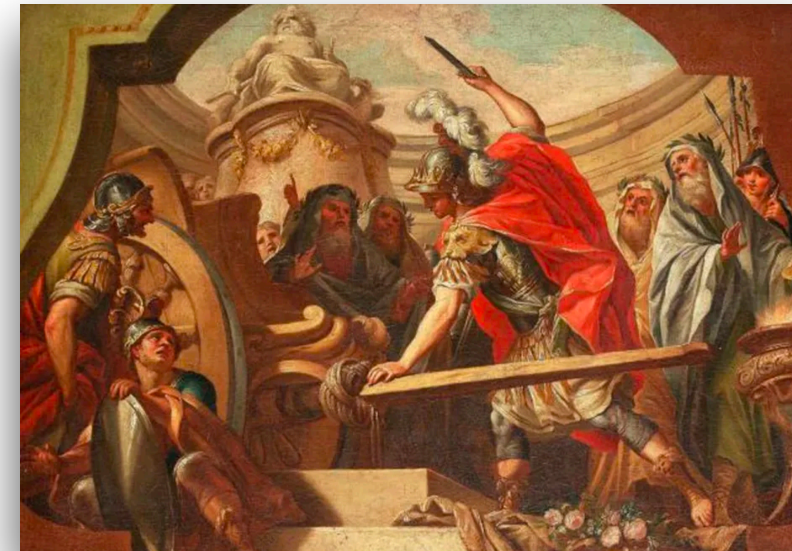

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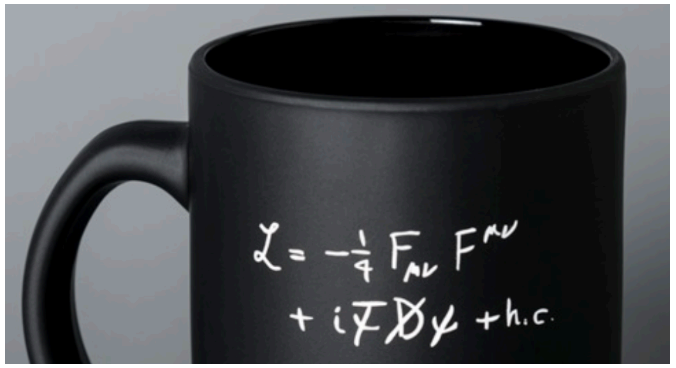

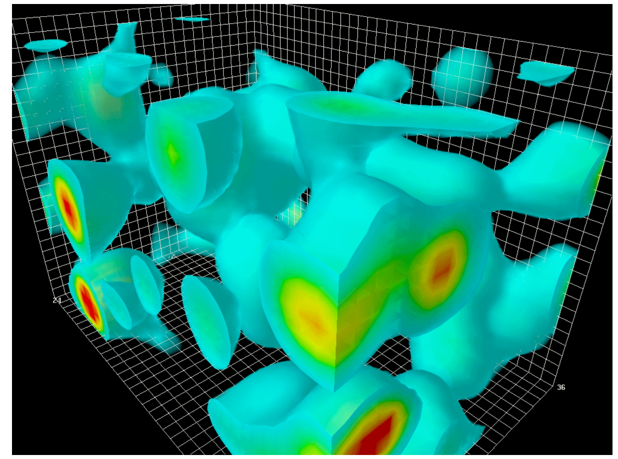

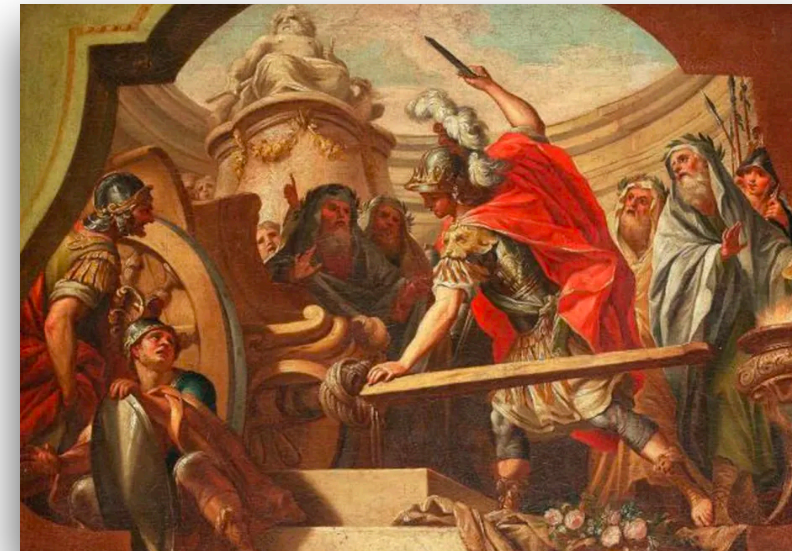

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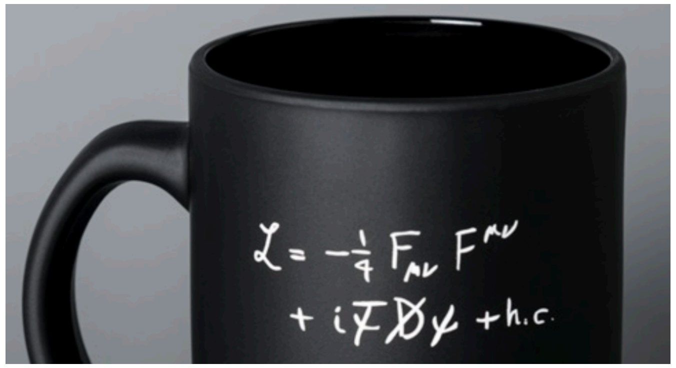
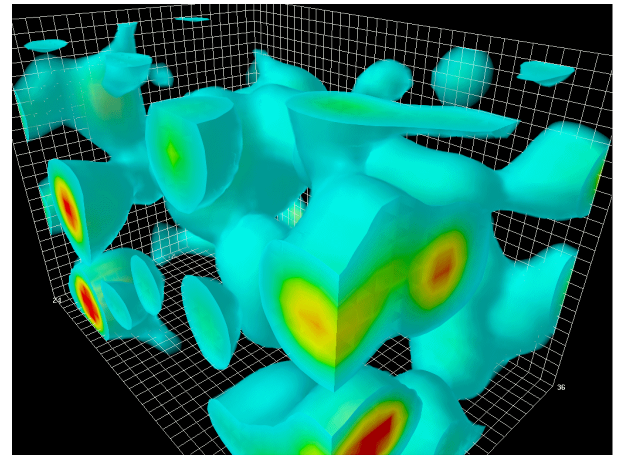
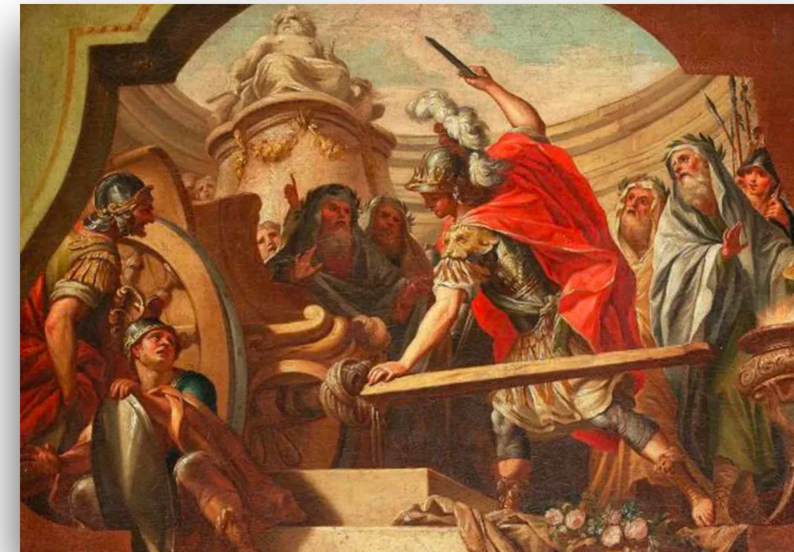




“Simulate non-analytical systems”



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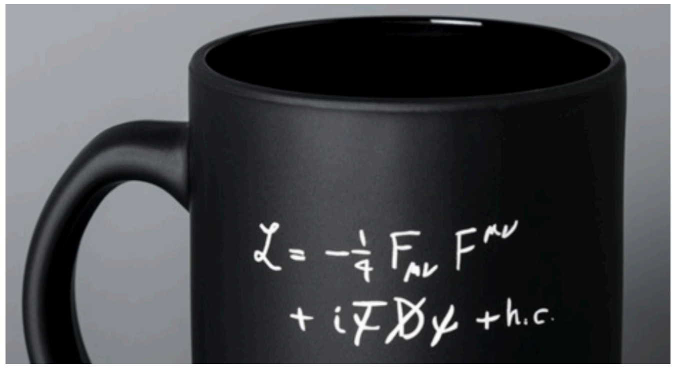

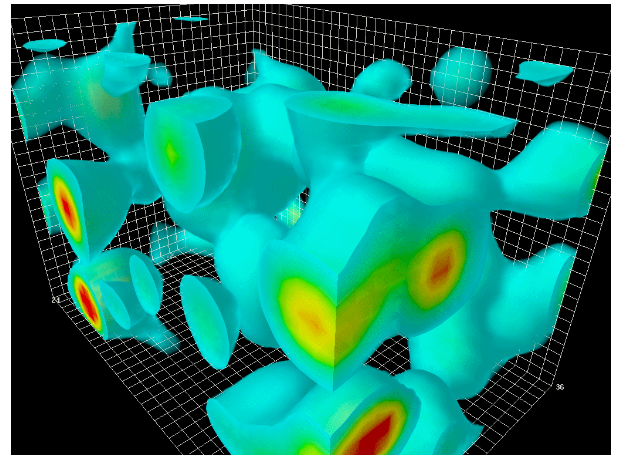

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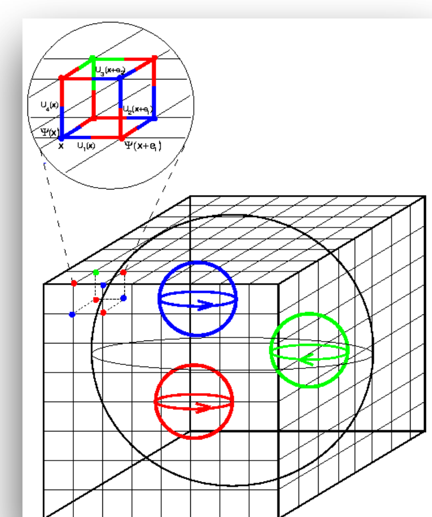
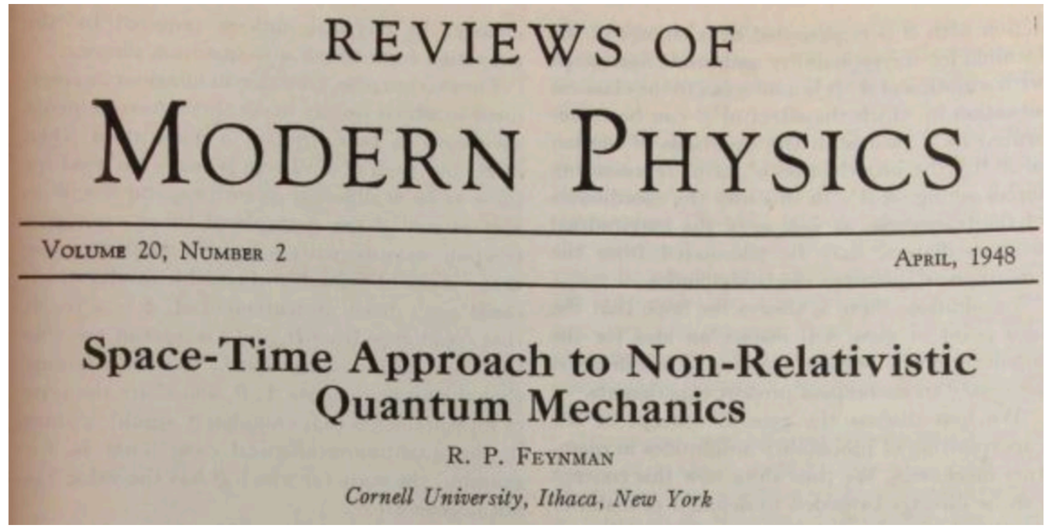
QCD and beyond



Path Integral Formalism


REVIEWS OF
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Cornell University, Ithaca, New York

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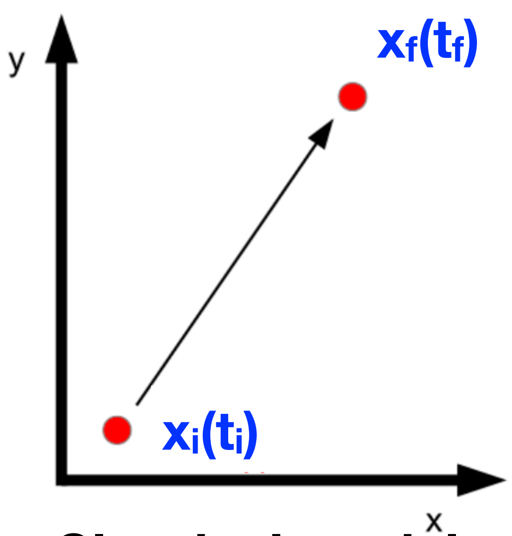
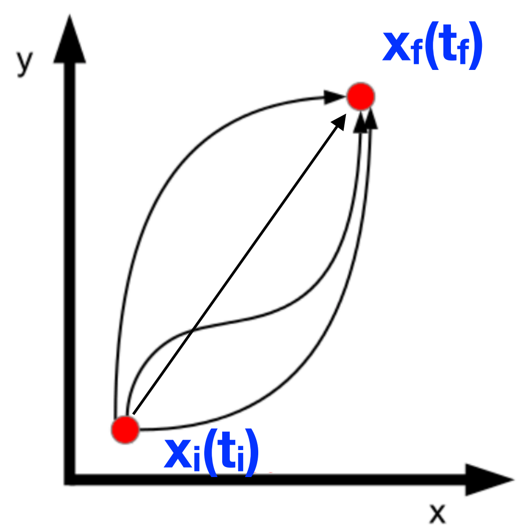


Classical particle



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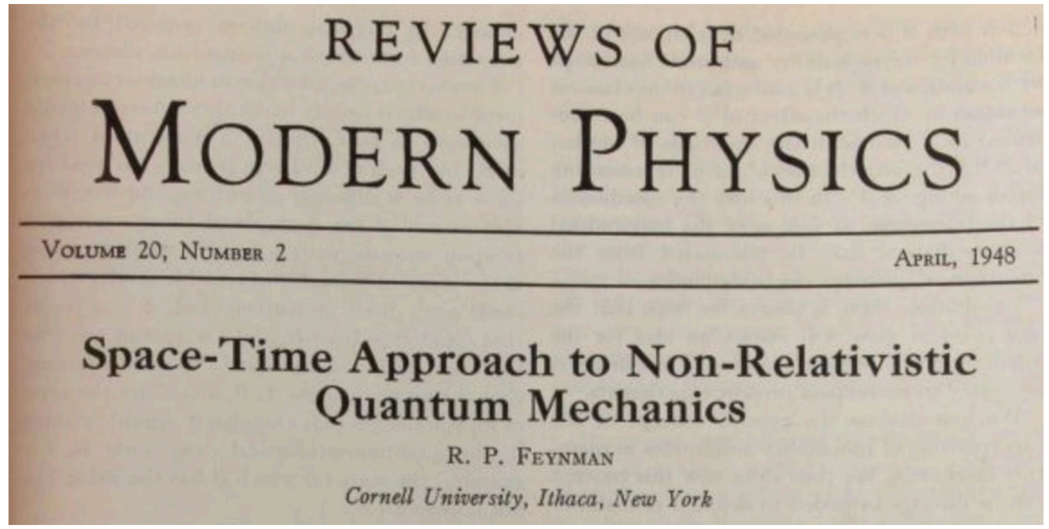
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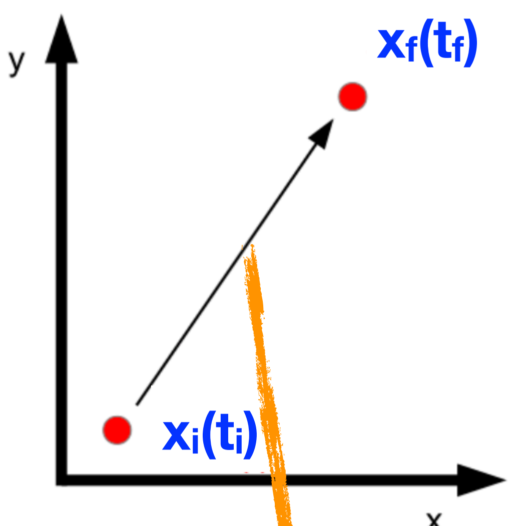

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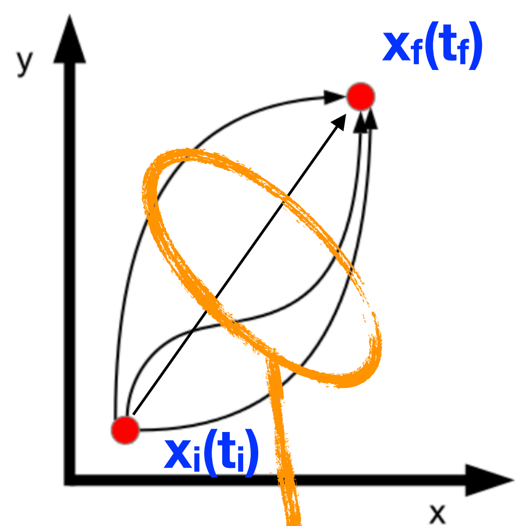

Quantum particle

All possible trajectories (weighted)

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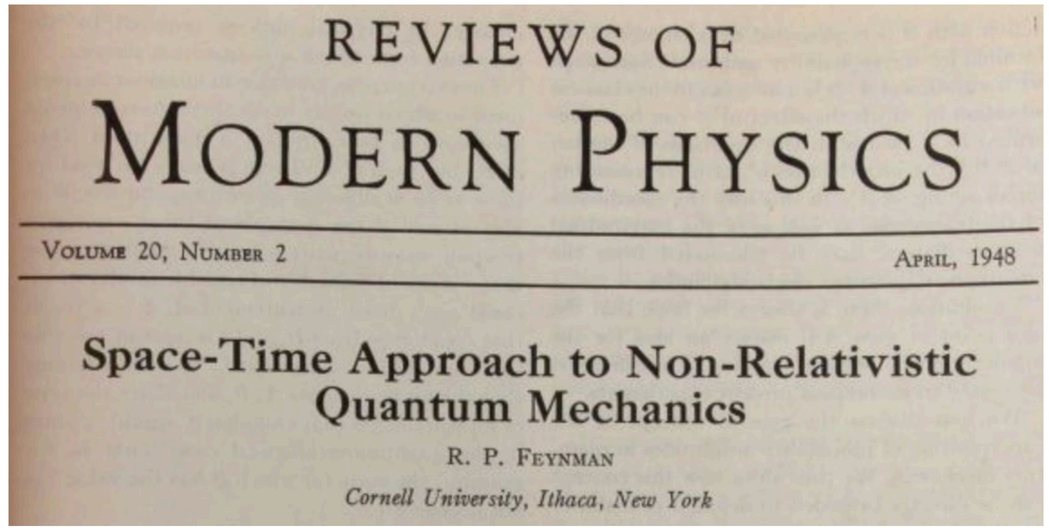
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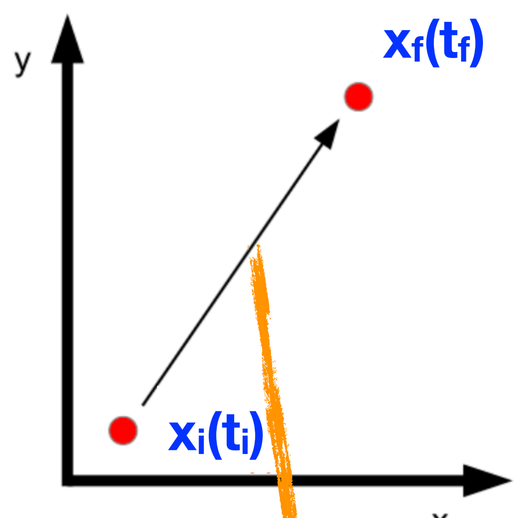

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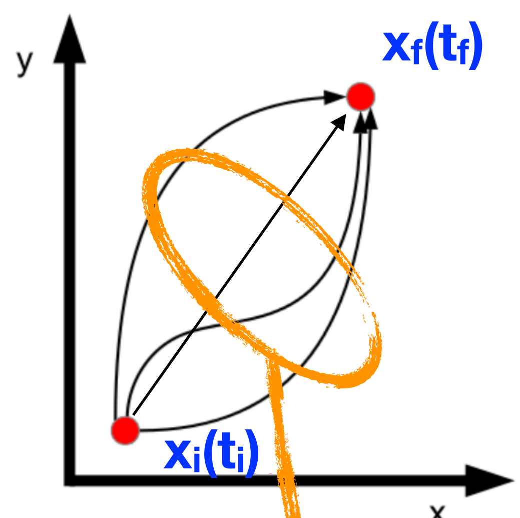

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Propagator

$$U(x_f, t_f; x_i, t_i) = \langle \psi(x_f, t_f) \,|\, \psi(x_i, t_i) \rangle$$
$$= \langle \psi(x_f) \,|\, e^{-\frac{i}{\hbar}\hat{H}(t_f - t_i)} \,|\, \psi(x_i) \rangle$$

Path integral "language" (sum of all paths weighted by action)

$$U(x_f, t_f; x_i, t_i) = \int \mathscr{D}x(t) e^{\frac{i}{\hbar}S[x(t)]}$$

$\int \mathscr{D}x(t)$: measure

$S[x(t)]$: action

Path Integral Formalism

- ★ Equivalent to the Schrödinger formalism - more intuitive in interpretation
- ★ Very practical for quantum mechanics (weighted sum over all paths)
- ★ Critical for quantum field theories (weighted sum over all field values)
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$$\mathcal{Z} = \int D[U] D[\bar{\psi}]\, D[\psi]\, e^{i\, S_{\rm QCD}[U,\bar{\psi},\psi]} = \int D[U]\, det(D[U])^{N_f}\, e^{i\, S_{\rm QCD,G}[U]}$$

Fermion degrees of freedom integrated out
(anticommuting Granssmann variables)

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Functional volume element for corresponding fields

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Complex action problem: makes weight sampling impossible
(oscillatory phase factors)

Euclidean metric & Discretization

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(temporal and spatial components same sign in invariant length)

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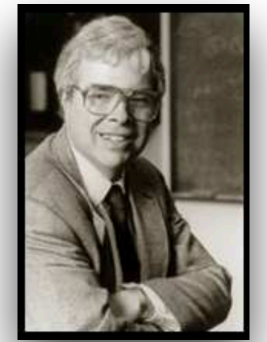
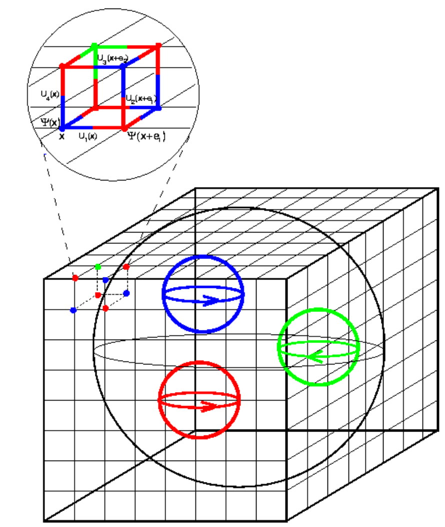
★ Path integral has infinite degrees of freedom:

Need to introduce a space-time discretization


K. Wilson

Lattice formulation of QCD


M. Creutz



★ Space-time discretization on a finite-size 4-D grid

★ Serves as a regulator of theory:

– UV (hard momentum) cut-off (finite integrals):
  inverse lattice spacing (α^{-1})
  momentum and energy < |π/α|

$$\int_{-\infty}^{\infty} dp \;\rightarrow\; \int_{-\pi/a}^{\pi/a} \frac{dp}{2\pi}$$

– IR cut-off (finite number of d.o.f): inverse lattice size ($V^{-1/4}$)

$$\int dp F(p) \;\rightarrow\; \sum_{n}^{N_{\max}} \frac{2\pi}{L} F(p_0 + \frac{2\pi n}{L})$$

★ Removal of regulator $L \rightarrow \infty\,,\;\; a \rightarrow 0$

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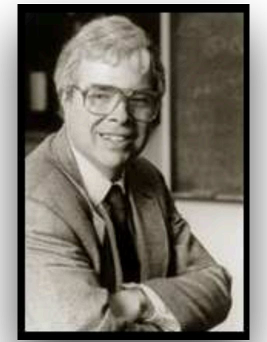
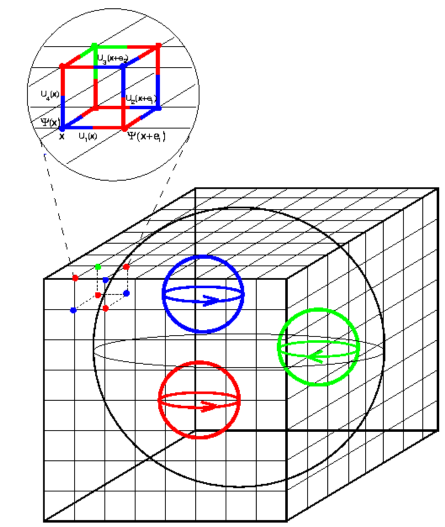


K. Wilson

M. Creutz

First principle (ab initial) formulation



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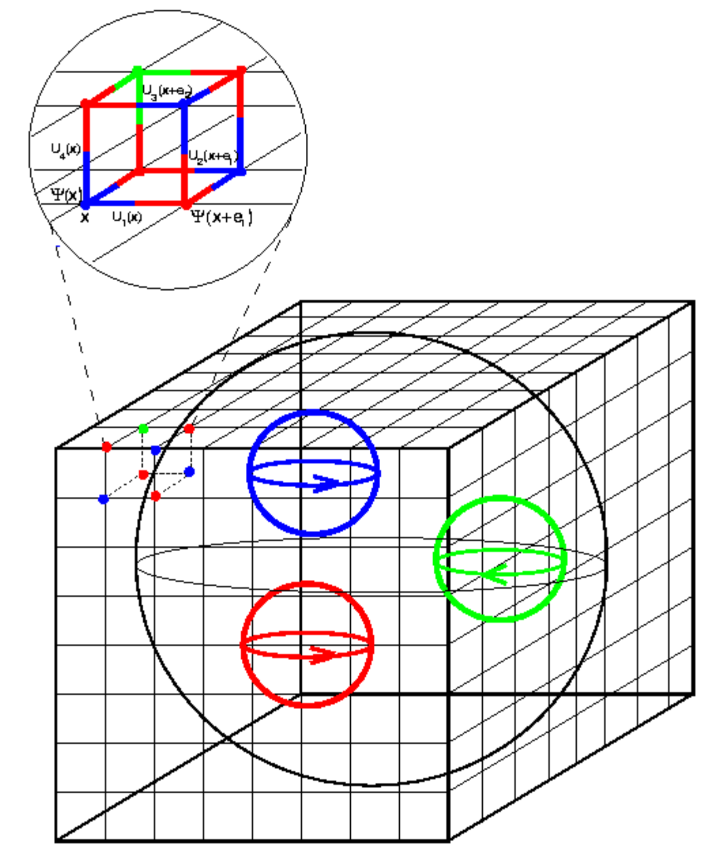
Technical Aspects



★ **Parameters (define cost of simulations):**

- quark masses (aim at physical values)
- lattice spacing* (ideally fine lattices)
- lattice size (need large volumes)

★ **Discretization not unique**

- clover improved fermions
- Domain wall fermions
- Overlap fermions
- Staggered fermions
- Twisted mass fermions

* In practice, the coupling is set in simulation and α is defined by comparing lattice results and values of physical quantities, e.g., proton mass

Monte Carlo Methods for Lattice QCD

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One needs to invert the Dirac matrix (~ $10^8 \times 10^8$)

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★ Discretization in a lattice of volume:
e.g., $48^3 \times 96$: 340 Million degrees of freedom!

Monte Carlo Methods for Lattice QCD

★ Direct evaluation of (finite d.o.f.) path integral is unfeasible:
One needs to invert the Dirac matrix (~ $10^8 \times 10^8$)

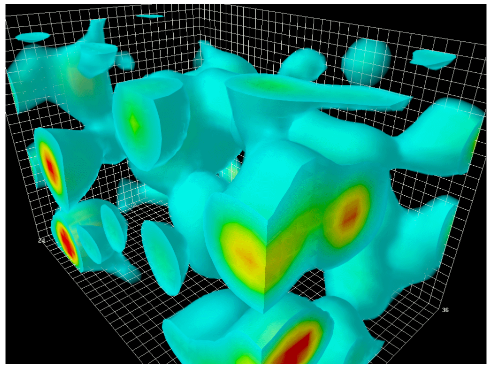
★ Solution: Stochastic estimation of path integral

★ Discretization in a lattice of volume:
e.g., $48^3 \times 96$: 340 Million degrees of freedom!

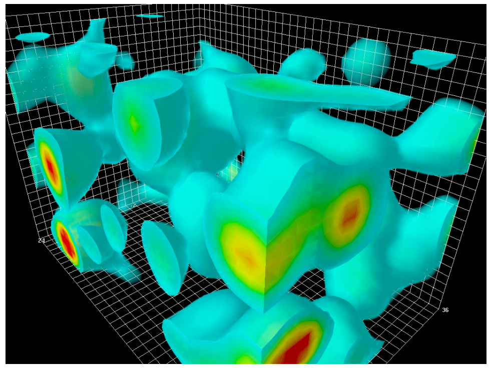
↓

Monte Carlo Methods
for Numerical Simulations

Monte Carlo Methods for Lattice QCD



Monte Carlo Methods for Lattice QCD

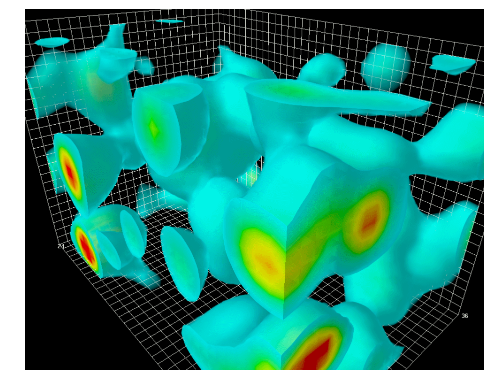


Monte Carlo Methods for Lattice QCD

★ Representative ensemble of gauge field configurations of the vacuum with acceptance probability

$$e^{-S[U]+N_f \log(det(D[U]))}$$

- Metropolis Algorithm:
  Very slow due to sequential repetition of updating variables
- Hybrid MC, important sampling, use of Markov process:
  update all variables at once, better scaling behavior in volume



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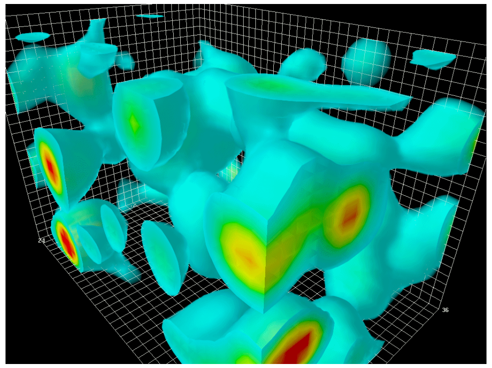

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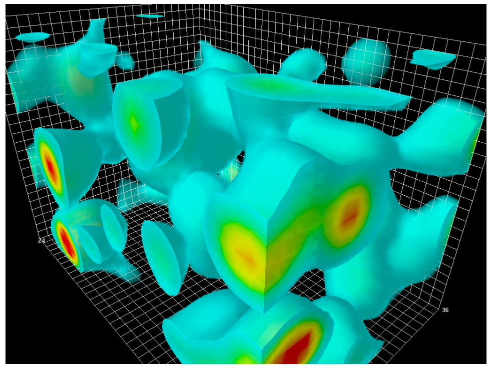

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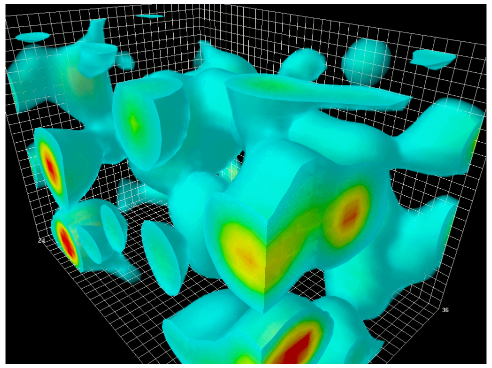

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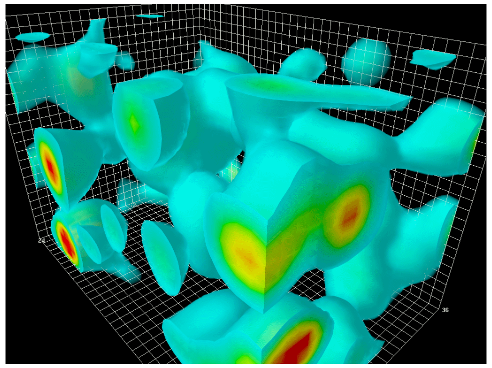

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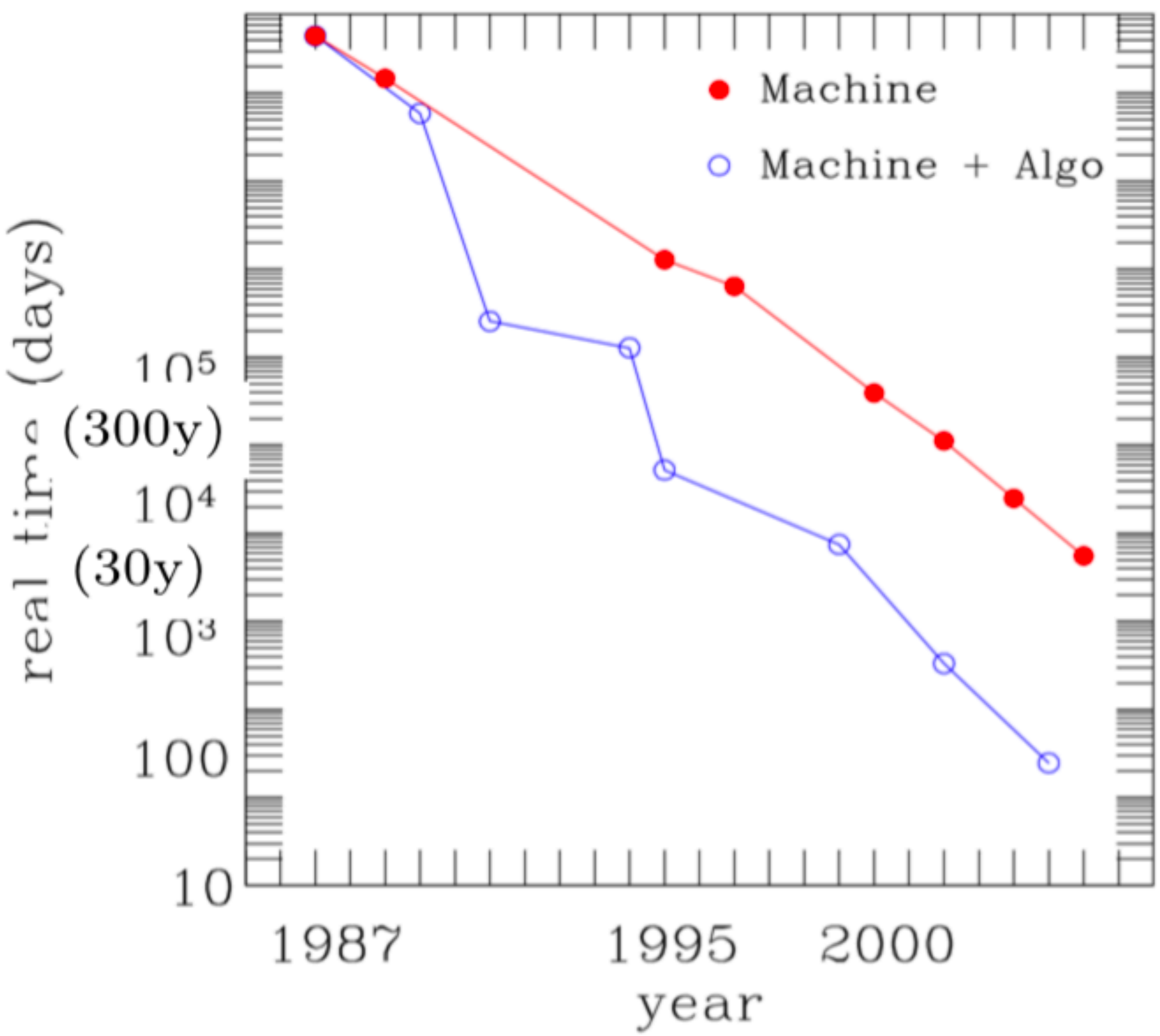
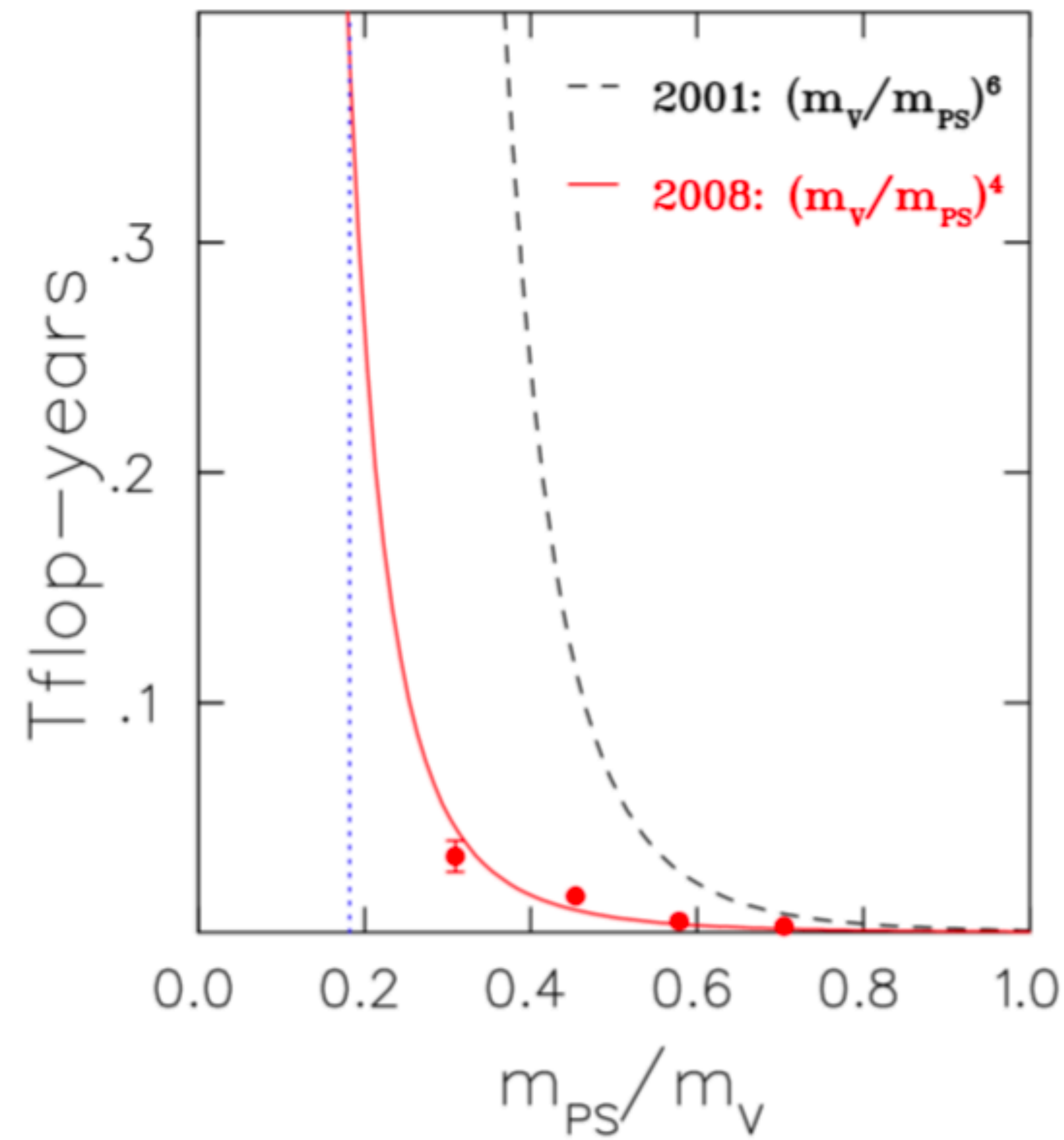
★ Statistical errors (jackknife, bootstrap) decrease as $\sigma(\overline{O}) \propto 1/\sqrt{N}$

Challenges of numerical simulations





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★ Modern calculations (physical parameters) require TFlops x years

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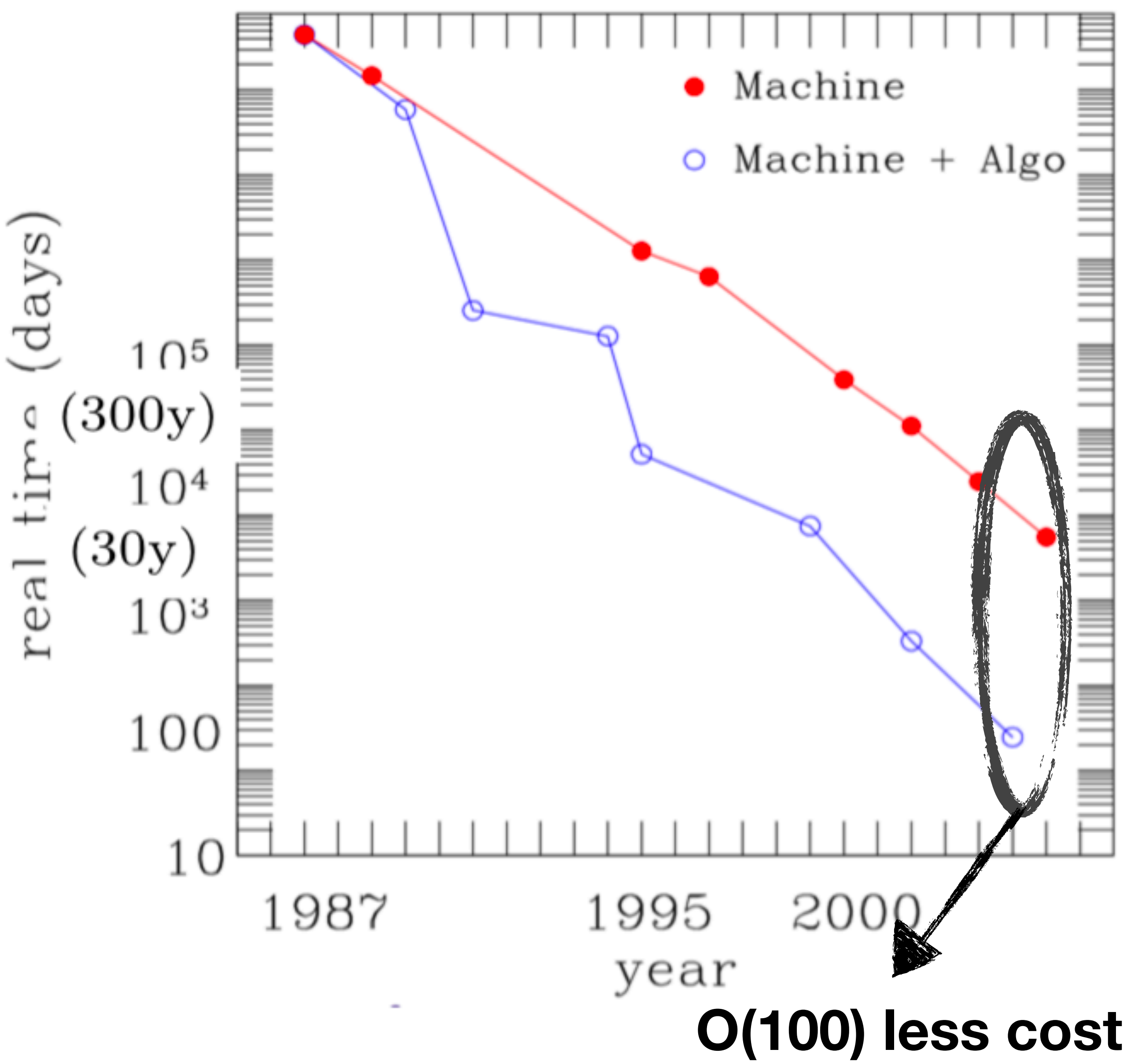

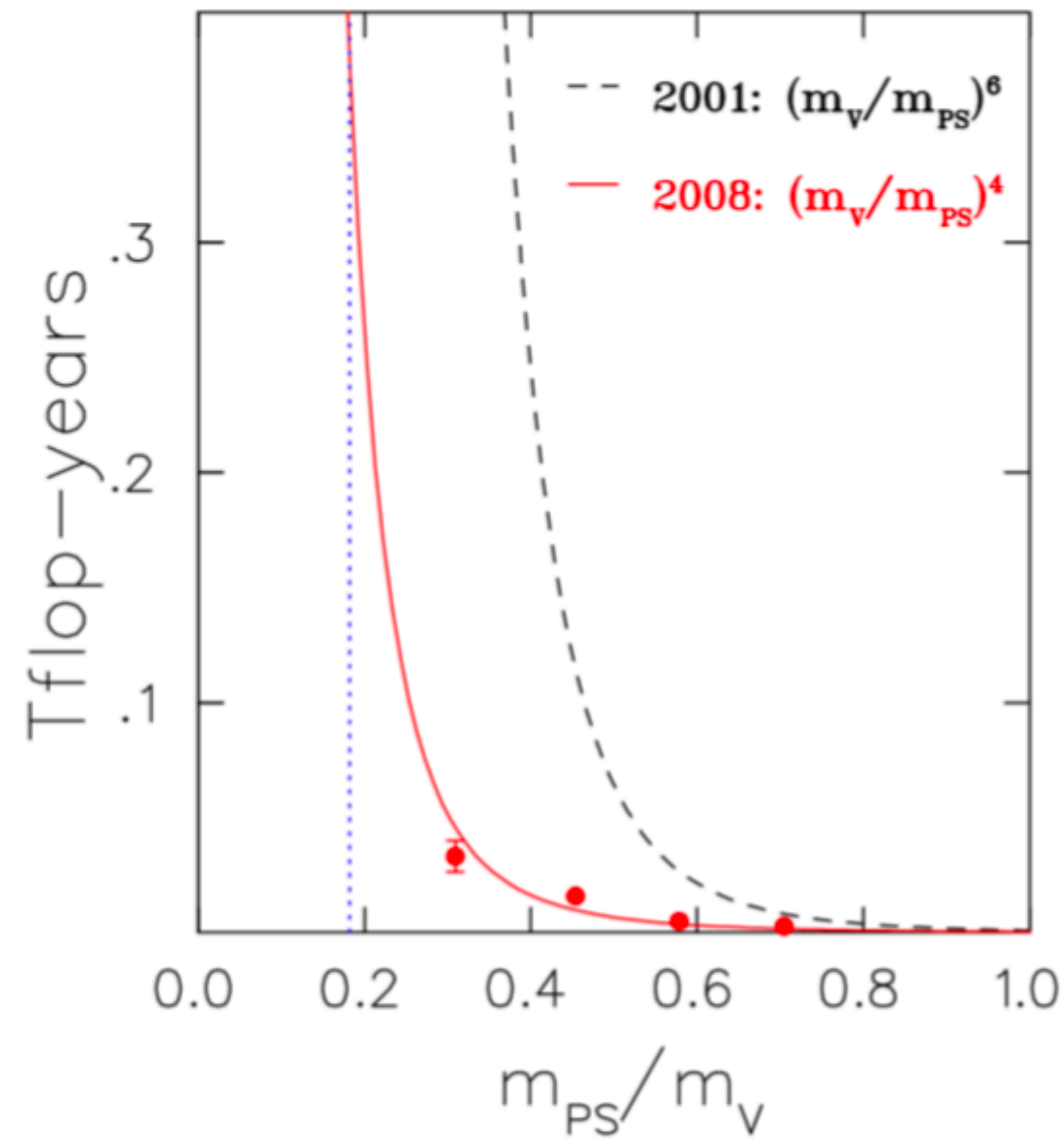

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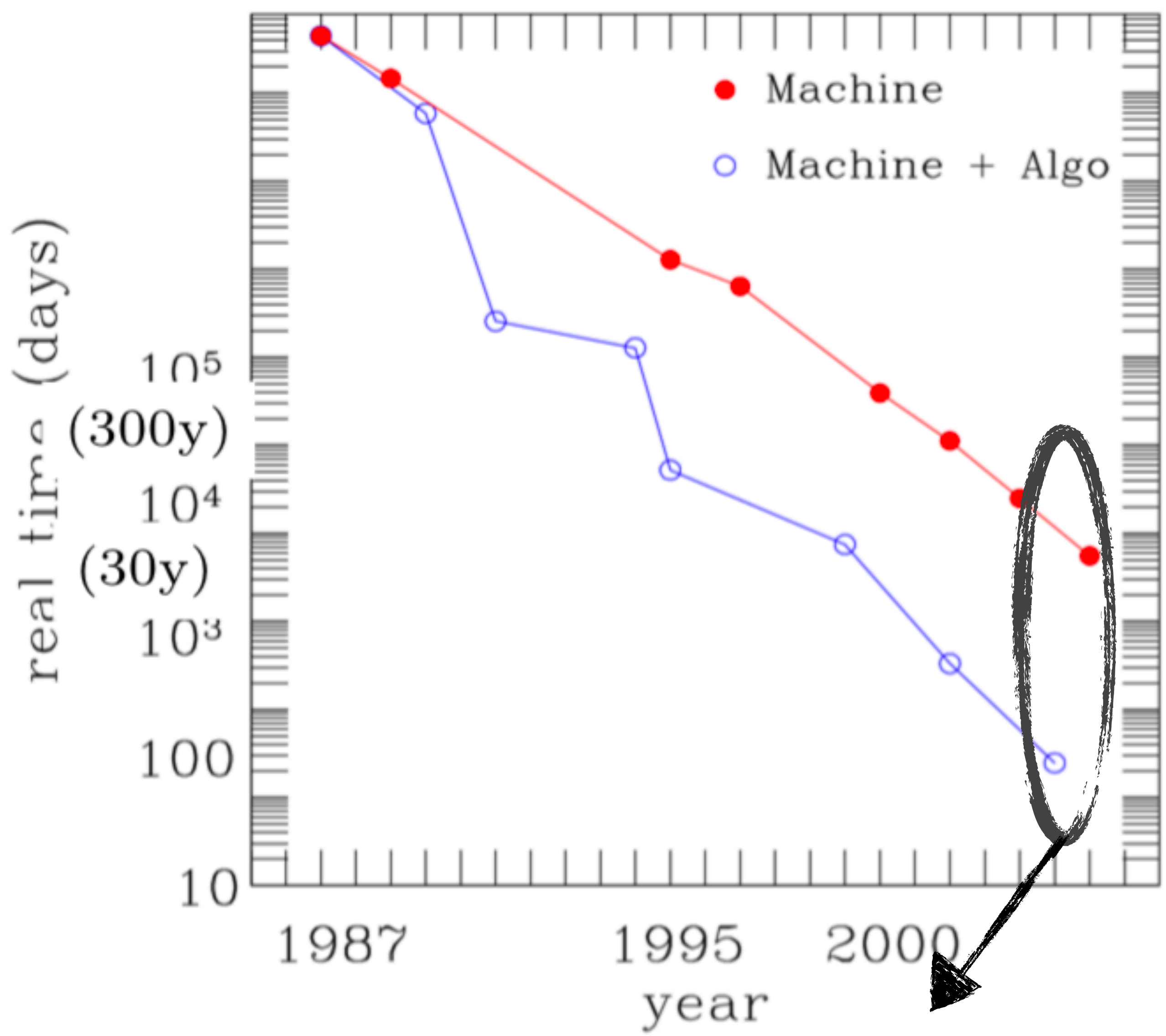

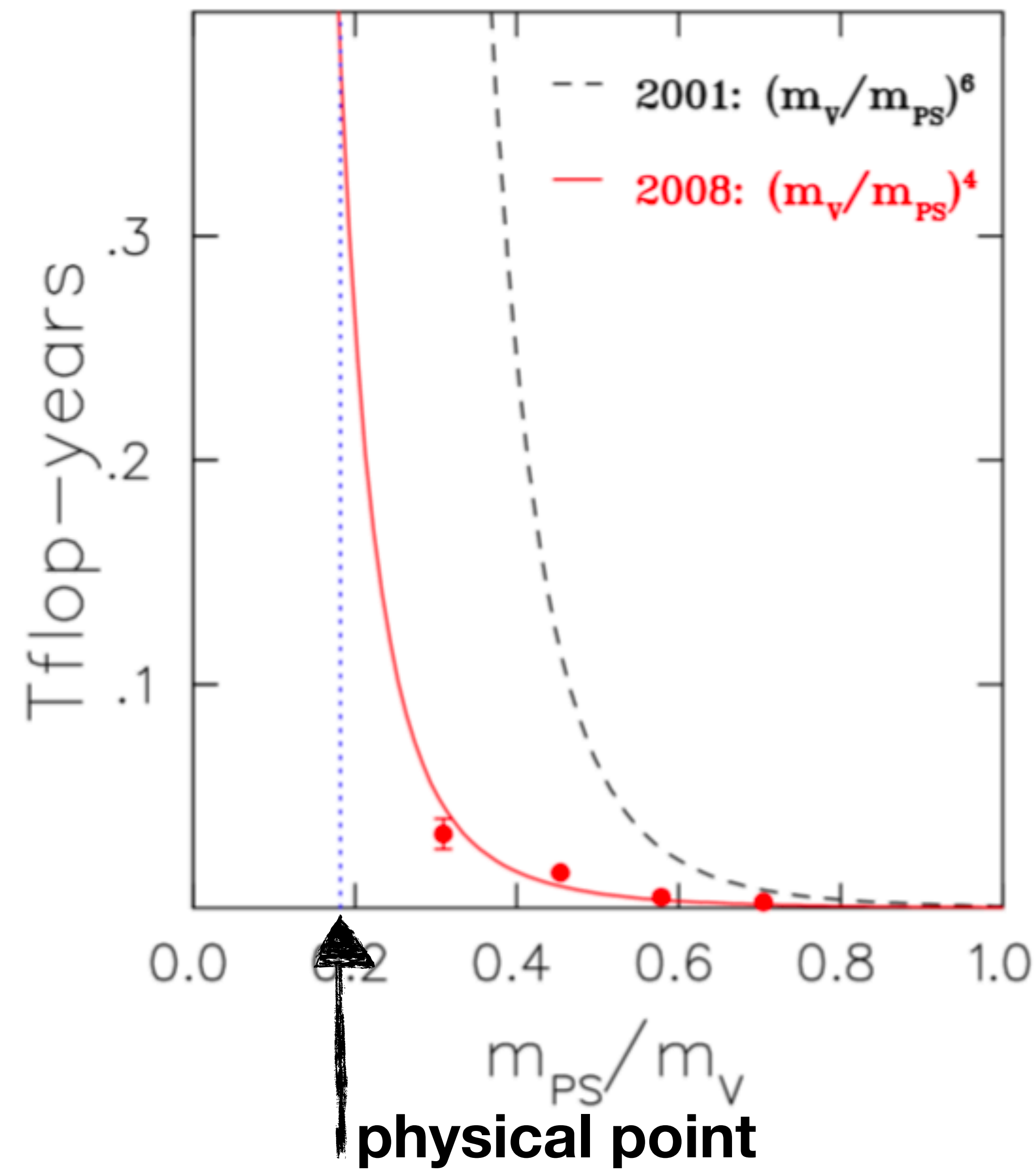

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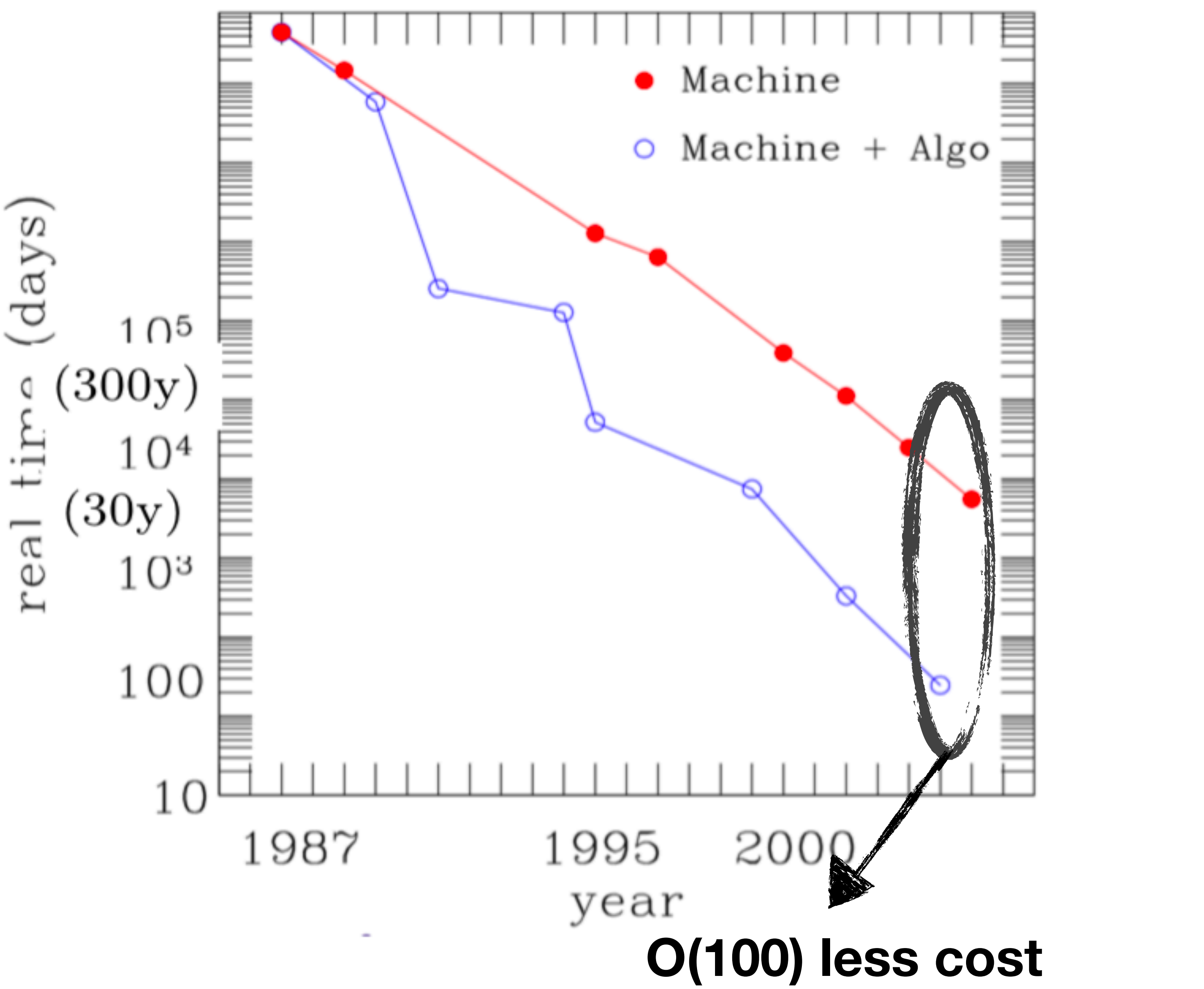

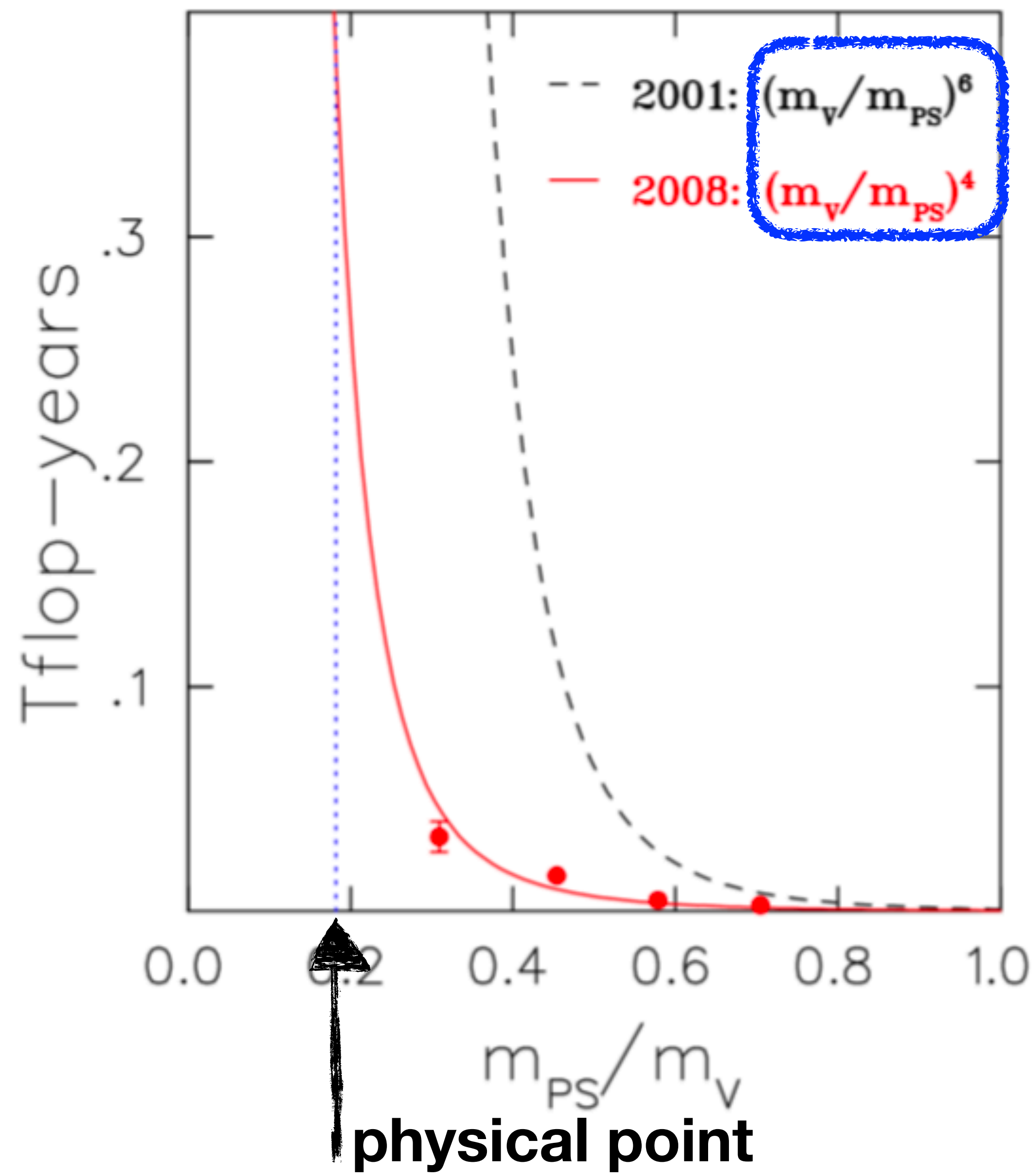

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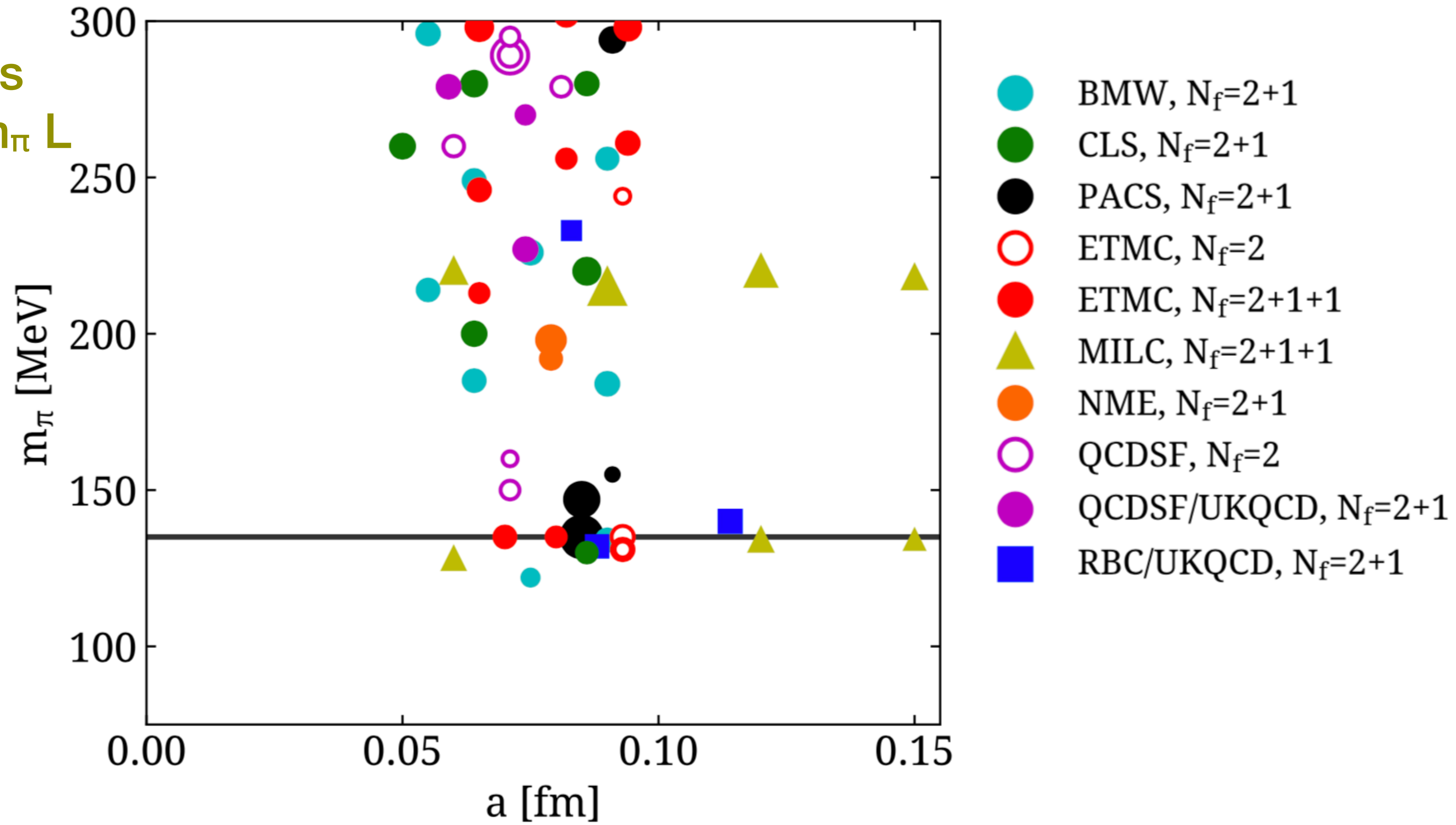
Landscape of numerical simulations

Lattice (fermion) formulations employed by various groups:

Wilson, Clover, Twisted Mass, Staggered, Overlap, Domain Wall, Mixed actions

Size of symbols proportional to $m_\pi L$



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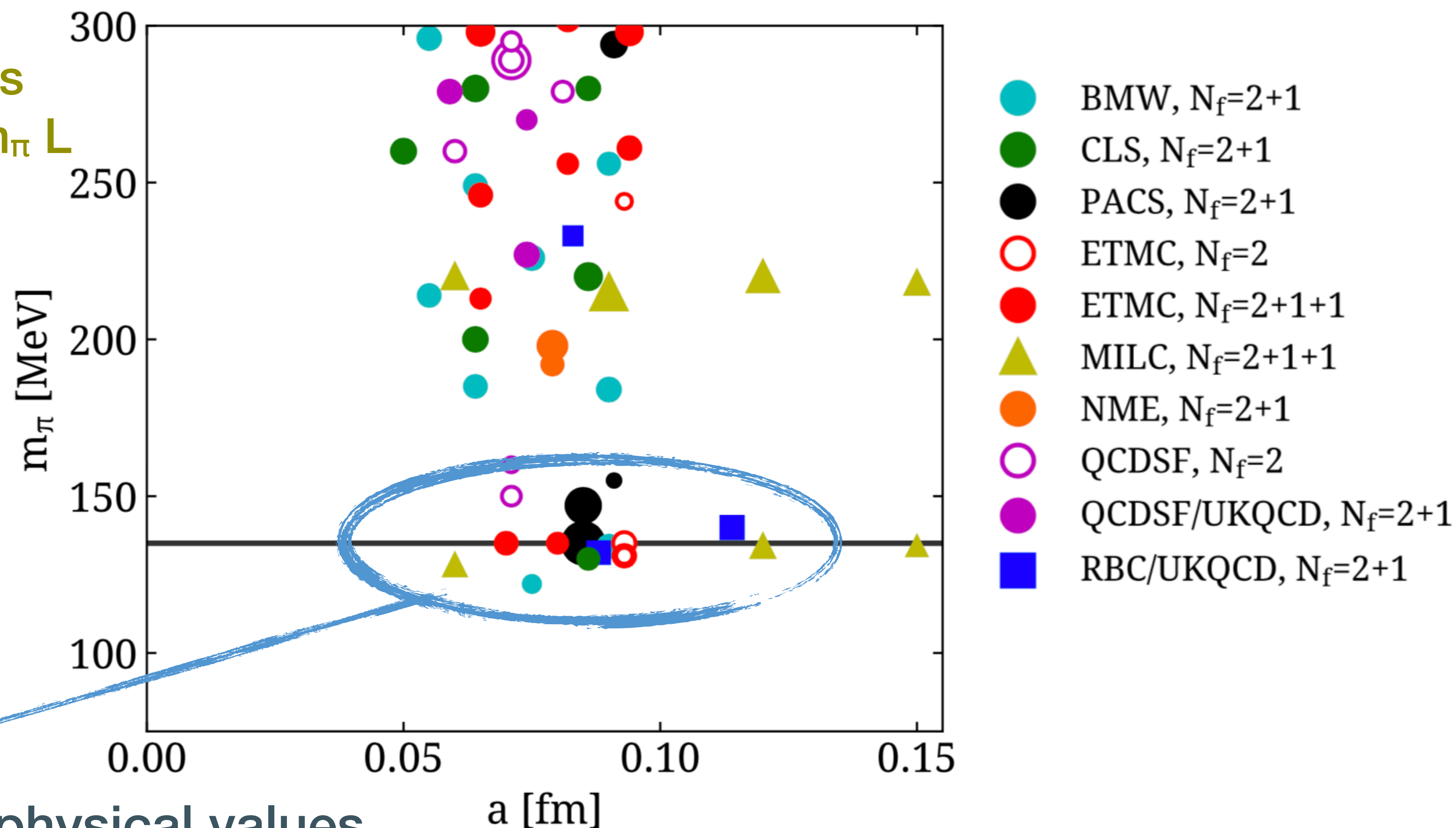

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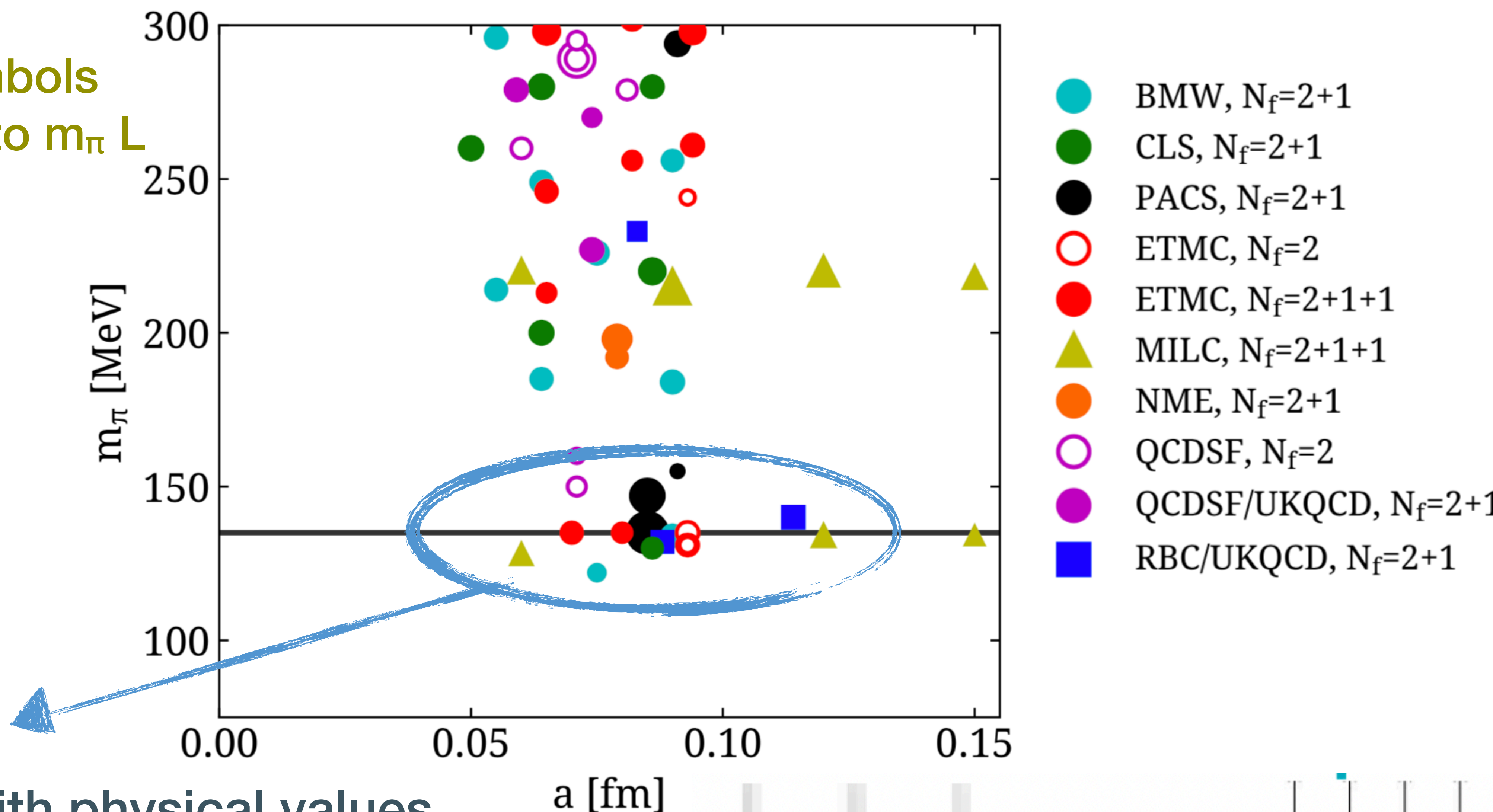

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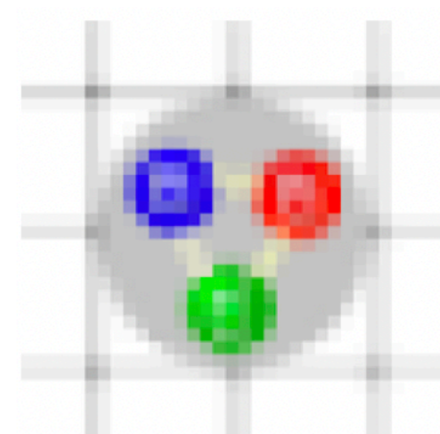

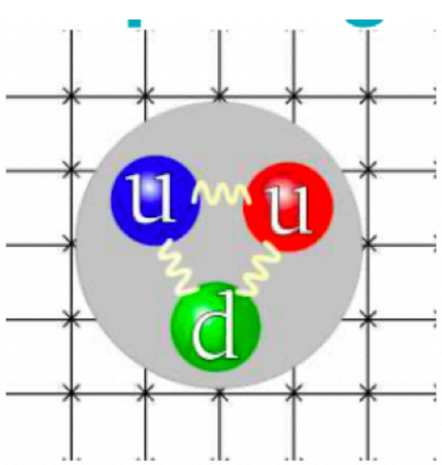

Theoretical aspects of lattice QCD

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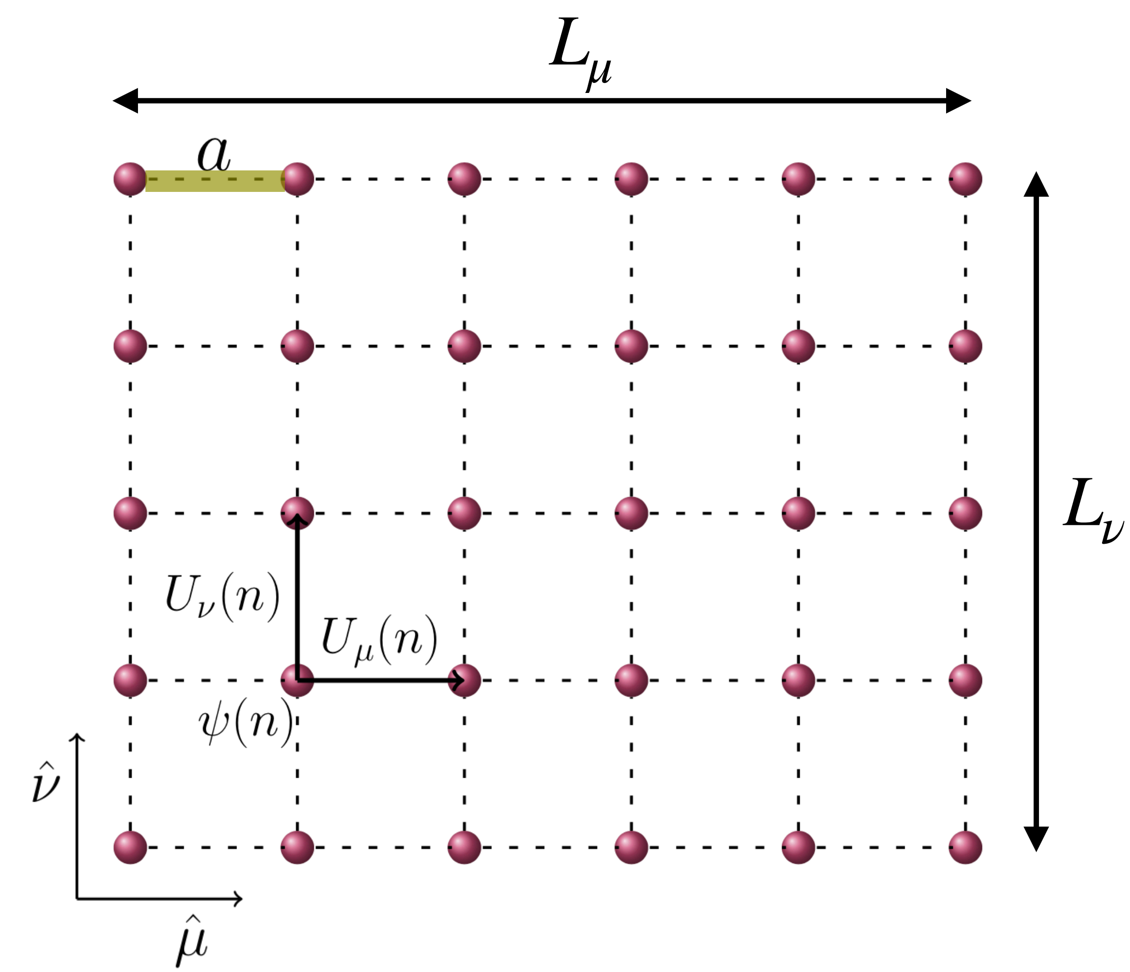
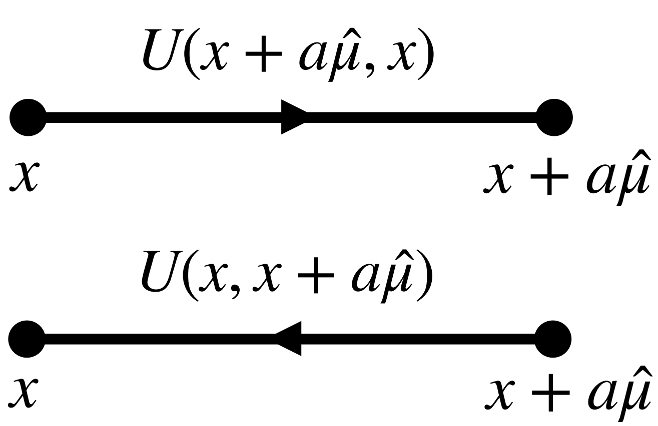
The boring stuff…

Fermions and Gluons on the Lattice



Link variable U_μ relates to gauge field G_μ

$$U(x+a\hat{\mu};x) = U_\mu(x) = \mathcal{P}e^{-ig\int_x^{x+a\hat{\mu}} dx G_\mu^b(x) T_b} \simeq e^{-igaG_\mu^b(x)T_b} \qquad x = na$$



$\Psi(x)$: anticommuting Grassmann variables

Fermions and Gluons on the Lattice

★ Lattice formulation "must" be invariant under SU(3) local gauge transformation

$$\psi(x) \to V(x)\psi(x)\,, \qquad \bar{\psi}(x) \to \bar{\psi}(x)V^\dagger(x)$$

$$U_\mu(x) \to V(x)U_\mu(x)V^\dagger(x+\hat{\mu}a)$$

$$V(x) = e^{-i\theta_a(x)\frac{\lambda_a}{2}}$$

★ Giving up gauge invariance would create a series of problems:

– More parameters to tune
(couplings for quark-gluon, 3- & 4-gluon interactions, the gluon mass,…)

– More operators at any given order in α, thus increase of discretization errors

– Proofs of renormalizability within perturbation theory rely on strict gauge invariance
[T. Reisz & H. Rothe, Nucl.Phys. B575 (2000) 255]

★ Gauge invariant quantities:

– Products of Ψ(x), Ψ(x') and gauge links connecting x and x'

– Closed gluonic loops

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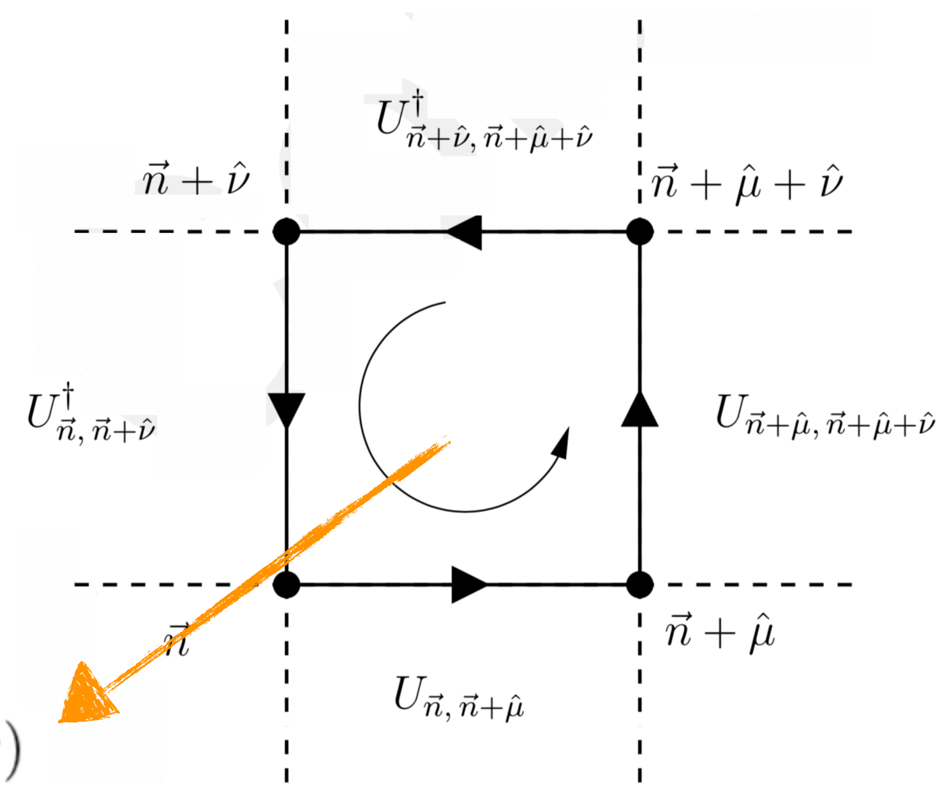


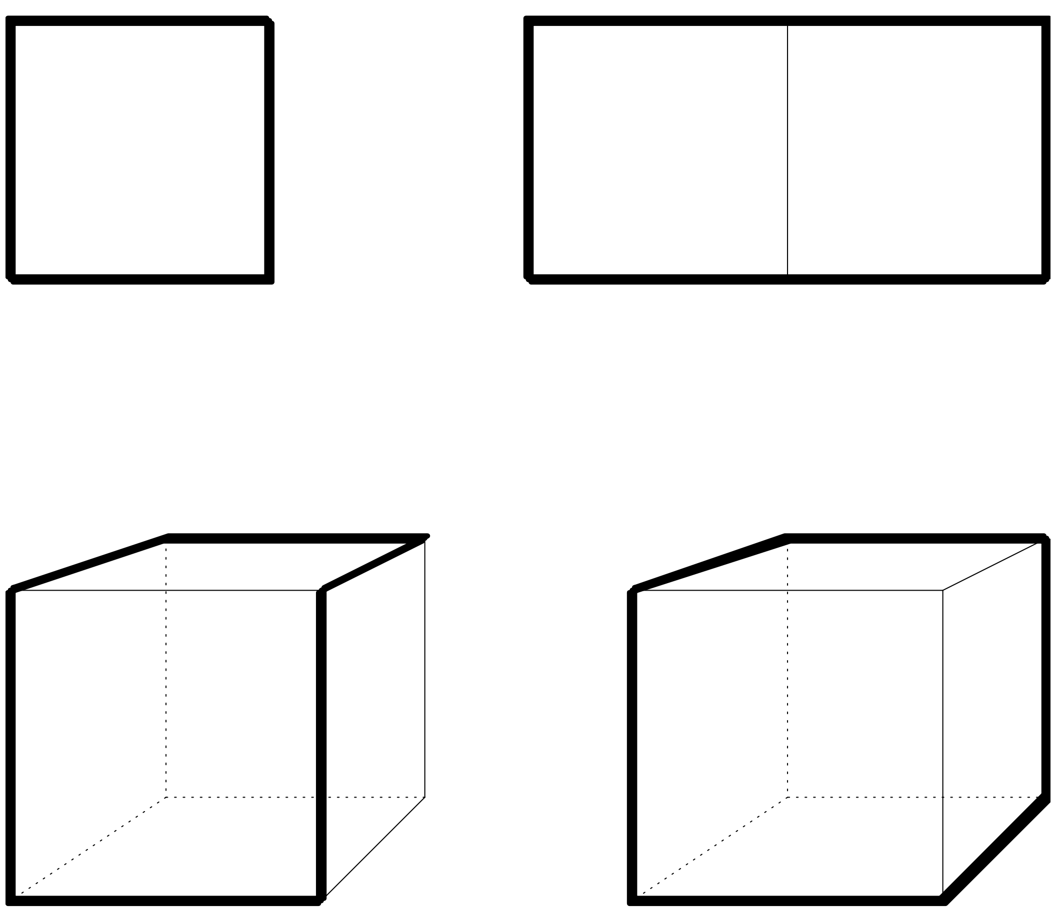
$$P_{\mu\nu} \equiv U_\mu(x)U_\nu(x+a\hat\mu)U^\dagger_\mu(x+a\hat\nu)U^\dagger_\nu(x)$$

Gluons on the Lattice

Gluon Actions:

$$S_G = \frac{2}{g^2}\Big[c_0 \sum_{\text{plaquette}} \mathrm{Re\,Tr}\,\{1 - U_{\text{plaquette}}\} + c_1 \sum_{\text{rectangle}} \mathrm{Re\,Tr}\,\{1 - U_{\text{rectangle}}\}$$
$$+ c_2 \sum_{\text{chair}} \mathrm{Re\,Tr}\,\{1 - U_{\text{chair}}\} + c_3 \sum_{\text{parallelogram}} \mathrm{Re\,Tr}\,\{1 - U_{\text{parallelogram}}\}\Big]$$

plaquette rectangle



chair parallelogram

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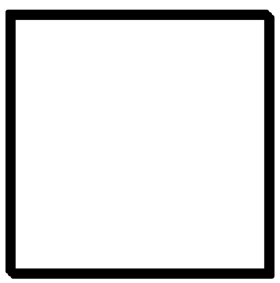
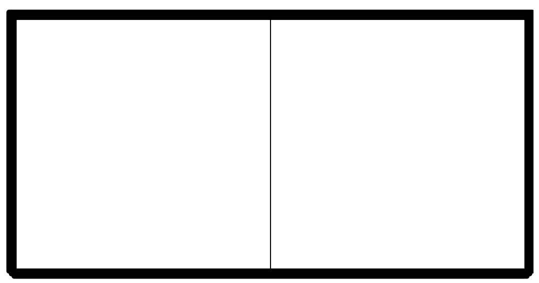
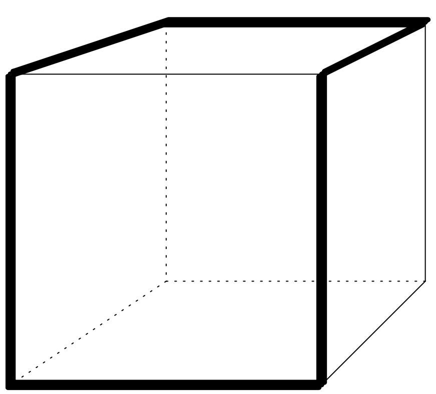
plaquette

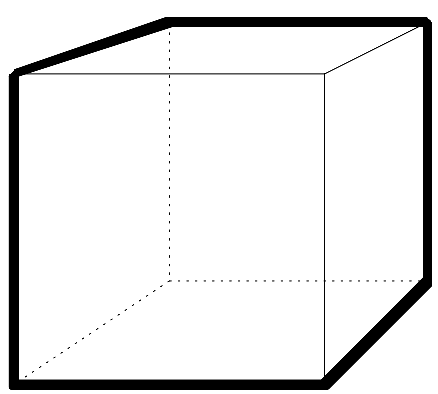


rectangle





chair



parallelogram

★ Choice of discretization not unique

Action	c_0	c_1	c_3
Plaquette	1.0	0	0
Symanzik	1.6666667	-0.083333	0
TILW, $\beta c_0 = 8.60$	2.3168064	-0.151791	-0.0128098
TILW, $\beta c_0 = 8.45$	2.3460240	-0.154846	-0.0134070
TILW, $\beta c_0 = 8.30$	2.3869776	-0.159128	-0.0142442
TILW, $\beta c_0 = 8.20$	2.4127840	-0.161827	-0.0147710
TILW, $\beta c_0 = 8.10$	2.4465400	-0.165353	-0.0154645
TILW, $\beta c_0 = 8.00$	2.4891712	-0.169805	-0.0163414
Iwasaki	3.648	-0.331	0
DBW2	12.2688	-1.4086	0

★ $O(\alpha^2)$ improved actions: approach better continuum limit

Fermions on the Lattice

★ Discretization of fermionic action complicated

★ Naive discretization preserves gauge invariance, but results in fermion doubling problem: appearance of spurious states and continuum limit wrongly leads to 2^4 fermions instead of one.

$$S_F^{naive} = a^4 \sum_x \frac{1}{2a}\gamma^\mu[\bar{\psi}(x)U_\mu(x)\psi(x+a\hat{\mu}) - \bar{\psi}(x)U_\mu^\dagger(x-a\hat{\mu})\psi(x-a\hat{\mu})] + m\bar{\psi}(x)\psi(x)$$

Fermion propagator (in momentum space upon Fourier Transform):

$$\langle\psi(x)\overline{\psi}(y)\rangle = \lim_{a\to 0}\int_{-\pi}^{\pi}\frac{d^4k}{(2\pi)^4}\, e^{ik(x-y)}\,\frac{-i\sum_\mu \gamma_\mu sin(k_\mu) + m_0}{\sum_\mu sin^2(k_\mu) + m_0^2}$$

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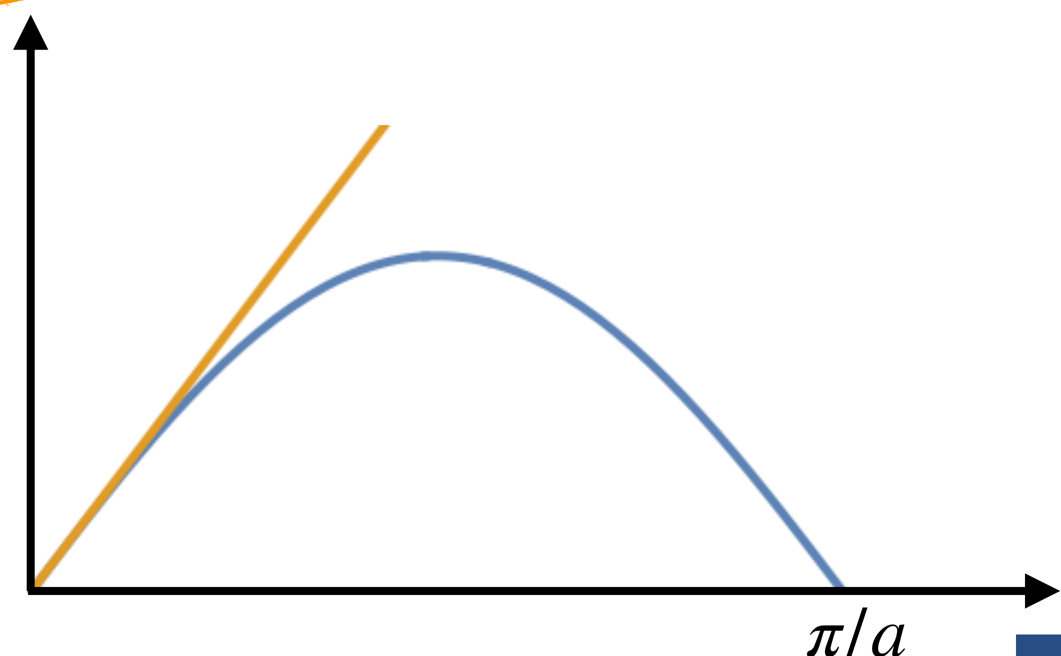
Additional poles:
Vanishes at the ends of Brillouin zone [-π/α,π/α].
In 4-dim these are sixteen regions instead of p~0 only, thus 16 species of fermions



Fermions on the Lattice

★ Wilson action to avoid doubling problem [Kenneth G. Wilson, Phys. Rev. D10 2445 (1974)]

$$S_F^W = \quad a^4 \sum_{x,\mu} \bar{\psi}(x)\gamma^\mu D_\mu \psi(x) - a\frac{r}{2}\bar{\psi}(x) D_\mu D^\mu \psi(x) + m\bar{\psi}(x)\psi(x)$$

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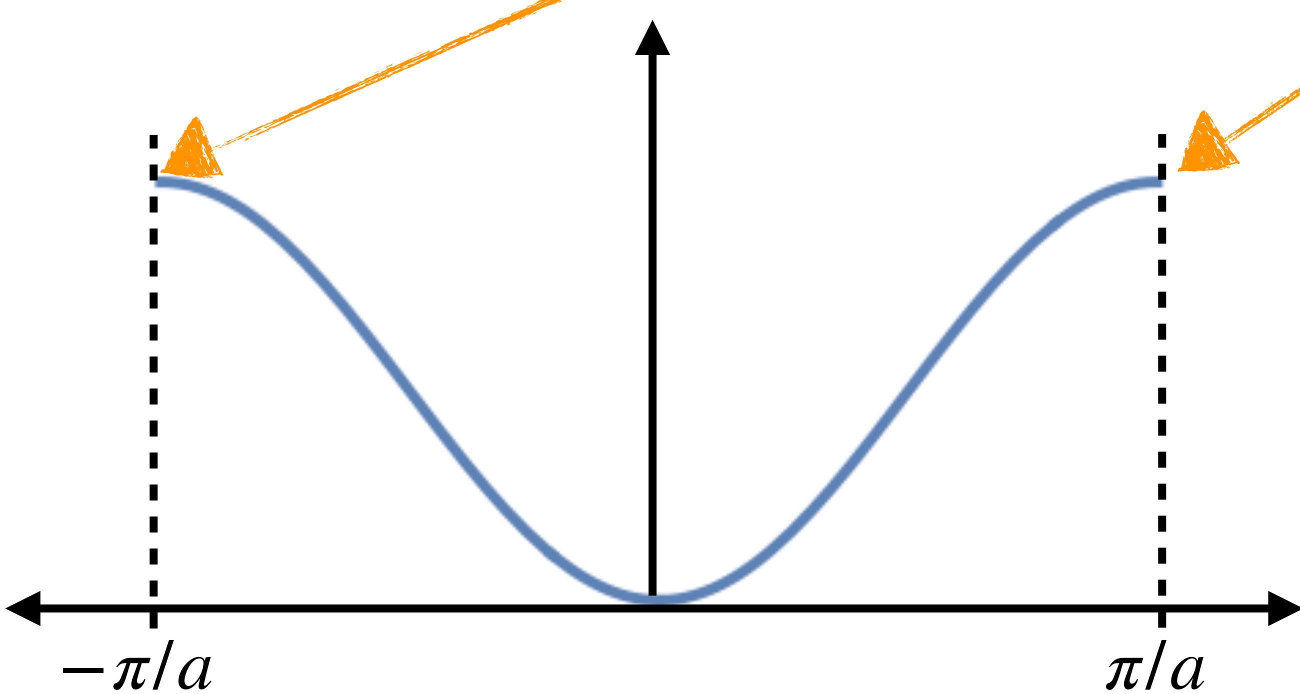

No poles at the edge of B.Z.

Properties of Wilson fermion action

- ★ Gauge invariant
- ★ Translational invariance
- ★ Invariant under charge conjugation (C), parity (P) and time reversal (T) transformations
- ★ Only nearest neighbors interactions (useful for lattice pert. theory)
- ★ Wilson-Dirac operator has γ_5-hermicity: $\gamma_5 D_W \gamma_5 = D^\dagger$

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- ★ Wilson-Dirac operator, D_W+m is not protected against zero modes (quark mass: additive and multiplicative renormalization)
- ★ Chiral symmetry is explicitly broken at O(α) by Wilson term
- ★ O(α) Discretization effects
- ★ Axial current transformations are not exact symmetry and nonsinglet axial current requires renormalization

Nielsen-Ninomiya (No-Go) theorem

It is not possible to define a local, translationally invariant, hermitian lattice action that preserves chiral symmetry and does not have doublers

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break chiral symmetry & require operator improvement

Twisted Mass:
computationally fast & automatic improvement
break chiral symmetry & violation of isospin

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Domain Wall
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All these formulations are used to understand aspects of QCD (hadron structure, spectroscopy, etc)

Recap of Lecture 1

Key points of Lecture 1

- ★ Theoretical study of strong interactions is closely related to understanding the properties of the visible matter
- ★ QCD Lagrangian is compact, but extremely difficult to solve
- ★ Several models of QCD provide intuitive understanding, and can reliable results to high energy scales
- ★ Lattice QCD is the ideal non-perturbative formulation to study QCD from first principle
- ★ Lattice regularization is a well-formulated 4-D discretization
- ★ Several discretizations proposed for fermion and gluon action, with different advantages disadvantages
- ★ Computational cost is among the challenges of numerical simulations

Thank you

Exercise

Prove that the plaquette: $P_{\mu\nu} \equiv U_\mu(x) U_\nu(x + a\hat{\mu}) U_\mu^\dagger(x + a\hat{\nu}) U_\nu^\dagger(x)$

has the correct continuum limit for the gluon part of L_{QCD}: $\int d^4x \frac{1}{4} F_{\mu\nu}^b F_b^{\mu\nu}$