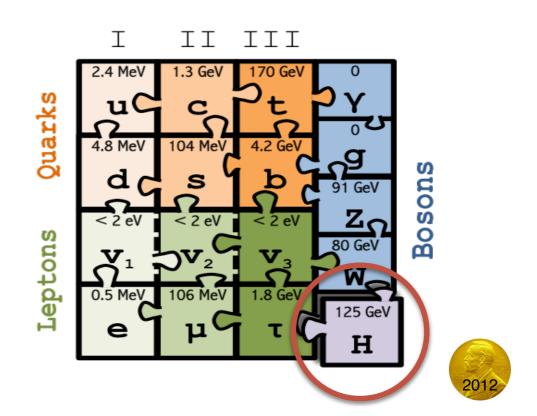
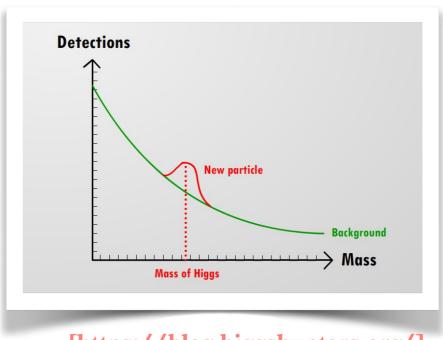


Four fundamental interactions:

- Electromagnetism
- → Weak
- → Strong
- Gravity

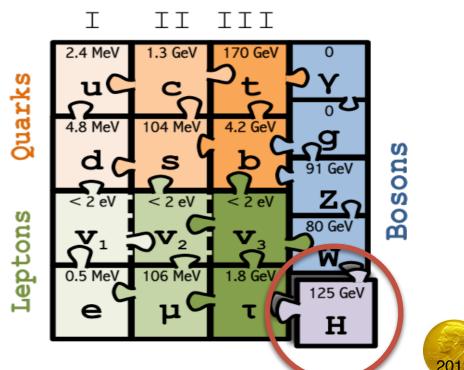




Four fundamental interactions:

- Electromagnetism
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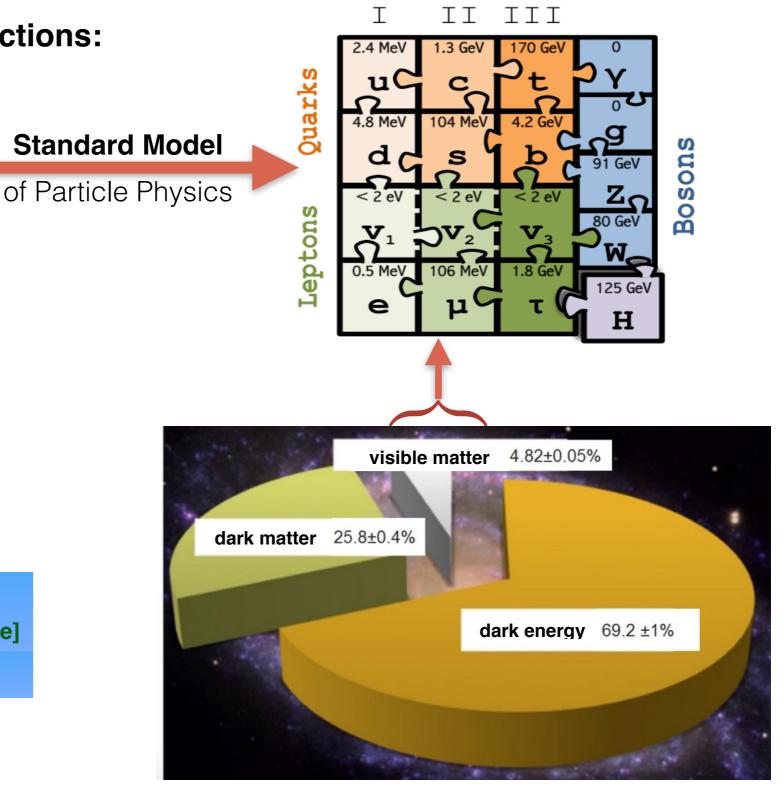


Four fundamental interactions:

- Electromagnetism
- → Weak
- Strong
- Gravity

See lectures in this school:

[Ronald Garcia Ruiz, Week1, Mon-Tue]
[Maria Piarulli, Week1, Mon-Wed]



The strong interaction

- Commonly accepted theory of strong interaction is Quantum Chromodynamics (QCD)
- Fundamental parameters of QCD:
 - gauge coupling: q
 - ightharpoonup quark masses: m_u, m_d, m_s, \dots



- color confinement
- asymptotic freedom

Strong coupling "constant":

$$\alpha_s(Q^2) = \frac{\bar{g}^2(Q^2)}{4\pi}$$

The strong interaction

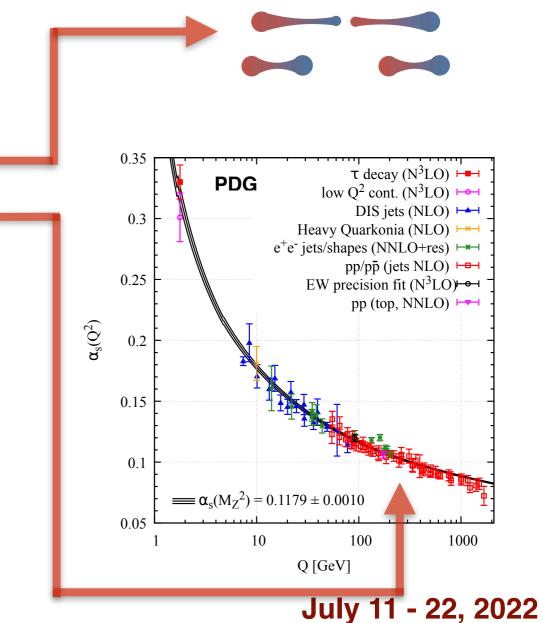
- Commonly accepted theory of strong interaction is Quantum Chromodynamics (QCD)
- Fundamental parameters of QCD:
 - gauge coupling: g
 - ightharpoonup quark masses: m_u, m_d, m_s, \dots
- Two exciting properties of QCD:
 - color confinement
 - asymptotic freedom

[D. Gross, F. Wilczek; D. Politzer (1973)]

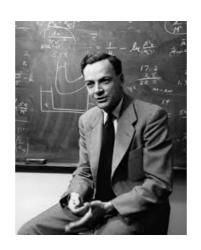


Strong coupling "constant":

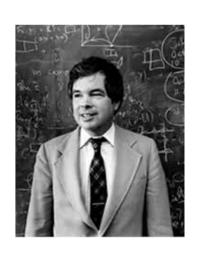
$$\alpha_s(Q^2) = \frac{\bar{g}^2(Q^2)}{4\pi}$$



[R. P. Feynman, "Space-Time Approach to Non-Relativistic Quantum Mechanics" Rev. Mod. Phys. 20, 367 (1948)]

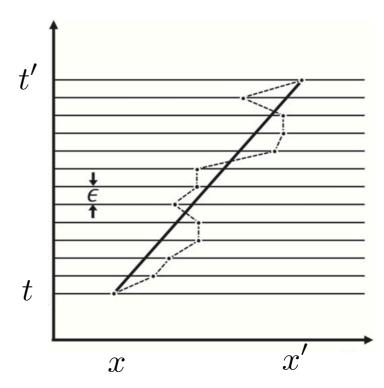


[K. Wilson, "Confinement of quarks" *Phys. Rev.D.* **10** (8): 2445–245 (1974)]



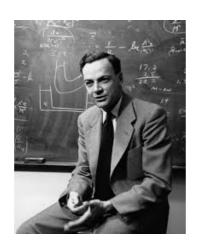
- (1) Path Integral quantization
- (2) Continuation to Euclidean time
- (3) Lattice regularization

$$\langle x'|U(t',t)|x\rangle = \int dx_1 \langle x'|U(t',t_1)|x_1\rangle \langle x_1|U(t_1,t)|x\rangle$$

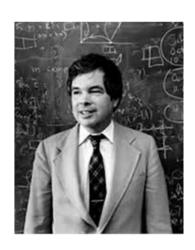


$$\langle x'|U(t',t)|x\rangle = \int \mathcal{D}x \,e^{\frac{i}{\hbar}S[x]}$$

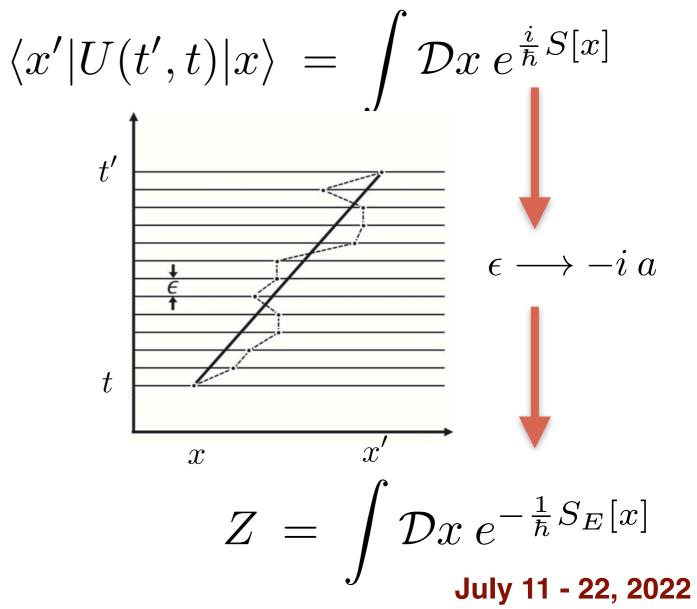
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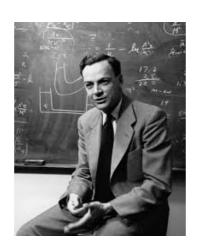
[K. Wilson, "Confinement of quarks" Phys. Rev.D. 10 (8): 2445-245 (1974)]



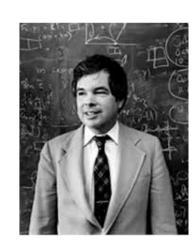
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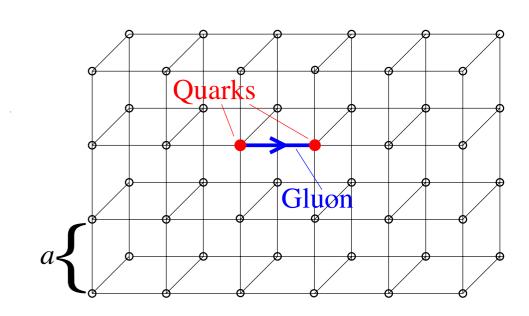
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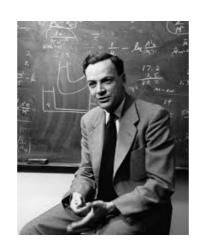
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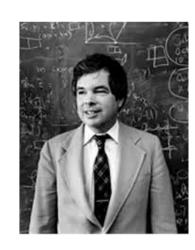
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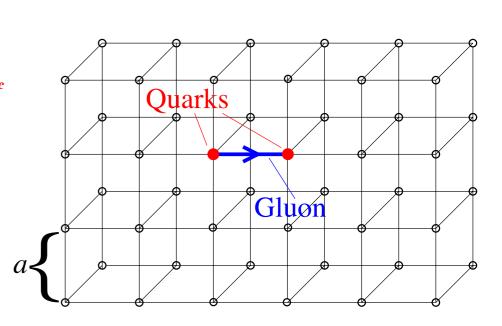


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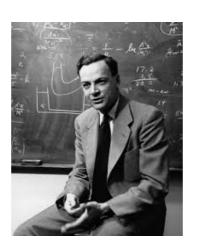


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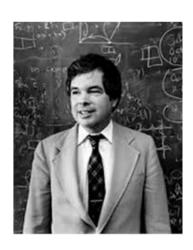
$$\begin{split} \mathcal{L}^{E}_{QCD} &= \frac{1}{2g} \; F^{a}_{\mu\nu} F^{a}_{\mu\nu} + \sum_{f=u,d,s,...} \overline{\psi}_{f} \; \left\{ \; \gamma_{\mu} \; (\partial_{\mu} + i A^{a}_{\mu} T^{a}) + m_{f} \; \right\} \; \psi_{f} \\ S^{E}_{QCD} &= \int d^{4}x \; \mathcal{L}^{E}_{QCD} \end{split}$$



[R. P. Feynman, "Space-Time Approach to Non-Relativistic Quantum Mechanics" Rev. Mod. Phys. 20, 367 (1948)]



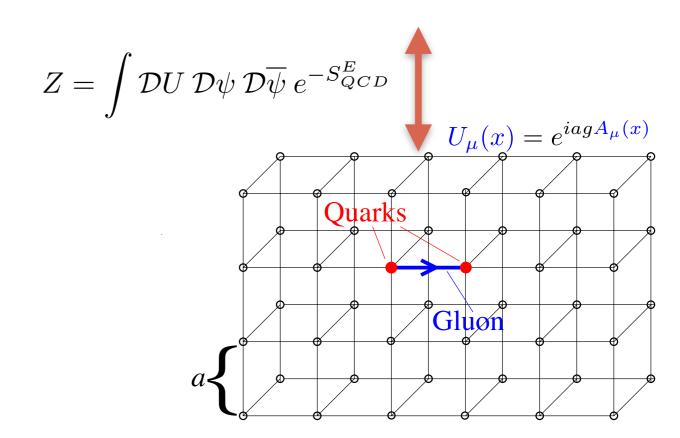
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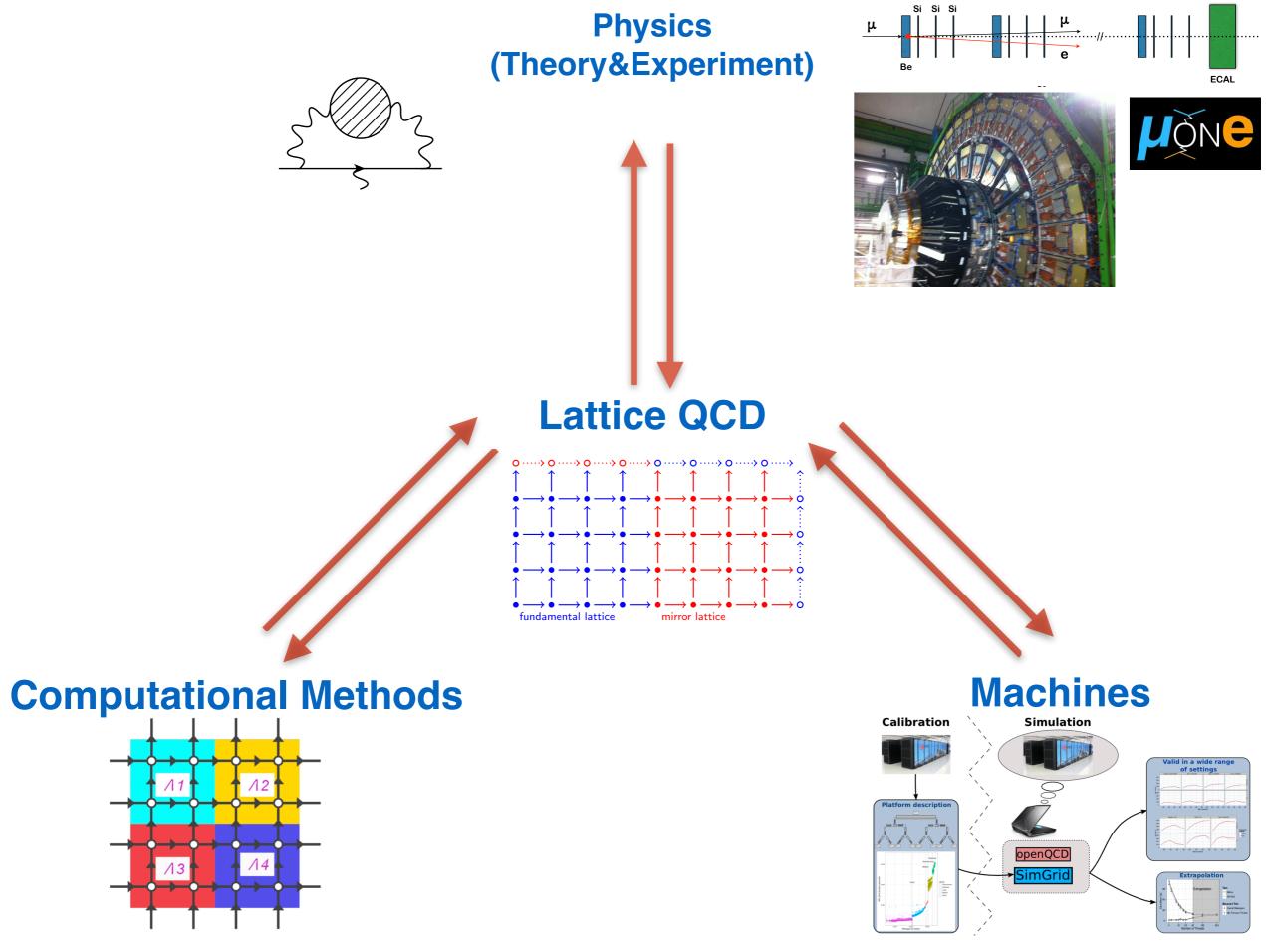


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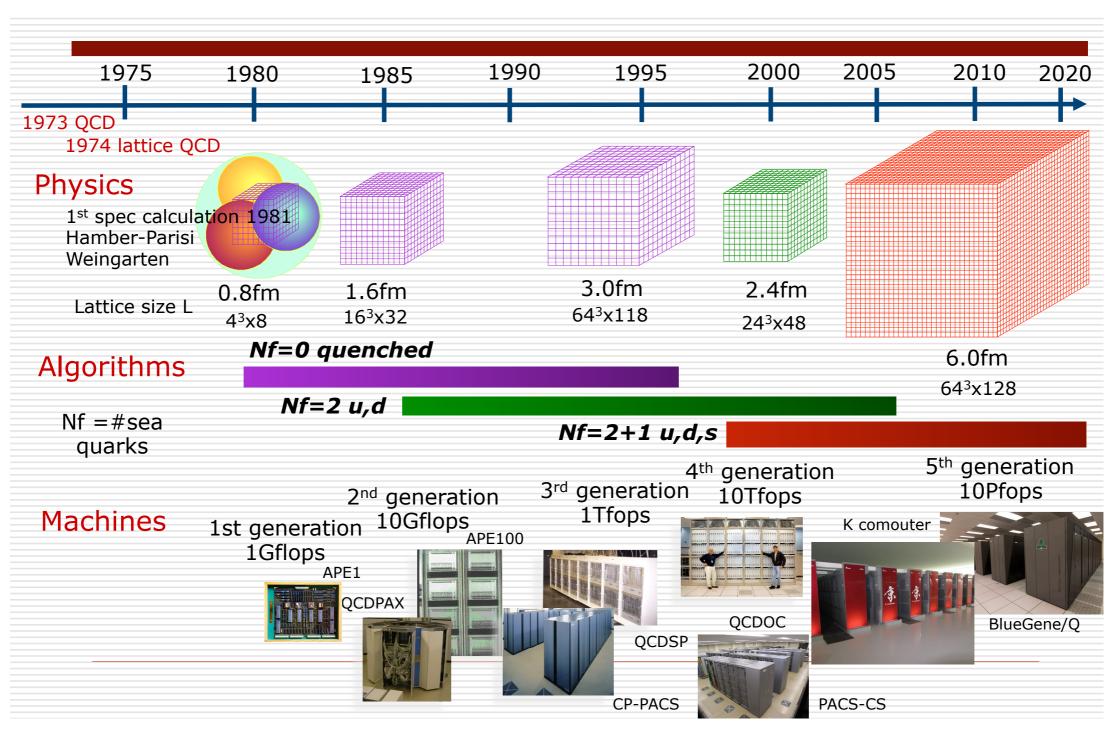


CLASSICAL STATISTICAL MECHANICS

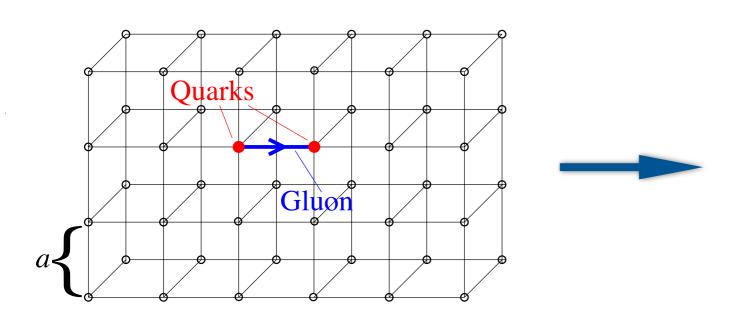




Development of Lattice QCD



Typical Lattice QCD Computation



- physical lattice size: ~6fm, spacing 0.05-0.1fm
- 643 x 128 lattice —> 34 x 106 points
- Operator dimensions: **10⁷ x 10⁷** matrices
- Advanced computational methods are needed
- Large computer resources: multiple TFlop years!



Altamira@IFCA, Santander

Wilson Cluster at Mainz U.

Backstage of LGT Calculations



[bbc tyne in pictures backstage at theatre royal; image by www.bbc.co.uk]

Plan of the Lectures:

- Lecture 1: Path Integral Quantization and scalar fields on the lattice; Why do we need to consider discrete space/time?
- Lecture 2: QCD on the lattice; Computational methods for lattice field theories; Why is LQCD so comp. expensive? What are the limitations?
- Lecture 3: Lattice QCD phenomenology: selected topics (Muon g-2, flavor physics, machine learning, quantum computing applications and more) Where can we move the needle with LQCD?

Part 1:

Path Integral Quantization and scalar fields on the lattice

Outline

- Point Mechanics vs. Classical Field Theory
- Path Integral in Quantum Mechanics (real and Euclidean time)
- Scalar Field Theory on the lattice
- Analogy with Statistical Mechanics and continuum limit
- Spectrum of the lattice Scalar Theory

Classical Point Mechanics

Point Mechanics — 2nd Newton's law:

$$m\frac{d^2x}{dt^2} = m \,\partial_t^2 x = F(x) = -\frac{dV(x)}{dx}$$

 $m\hspace{0.1cm}$ — mass of the classical non-relativistic point particle

V(x) — external potential

• The principle of least action:

$$S[x] = \int dt \ \mathcal{L}(x, \partial_t x)$$

• Lagrange function:

$$\mathcal{L}(x, \partial_t x) = \frac{m}{2} (\partial_t x)^2 - V(x)$$

• Euler-Lagrange equation:

$$\partial_t \frac{\delta \mathcal{L}}{\delta(\partial_t x)} - \frac{\delta \mathcal{L}}{\delta x} = 0$$

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Classical Field Theory

- Generalization to systems with infinitely many d.o.f. (field values $\phi(\vec{x})$)
- Classical field e. o. m. for neutral scalars Klein-Gordon eq.: $\partial_{\mu}\partial^{\mu}\phi = -\frac{dV(\phi)}{d\phi}$
- Again, the classical e. o. m obtained by minimizing the action:

$$S[\phi] = \int d^4x \ \mathcal{L}(\phi, \partial_{\mu}\phi)$$

$$\partial_{\mu} \frac{\delta \mathcal{L}}{\delta(\partial_{\mu} x)} - \frac{\delta \mathcal{L}}{\delta x} = 0$$

 $_{ullet}$ A simple example of interacting scalar field theory (' ϕ^4 — <code>theory</code> ')

$$V(\phi) = \frac{m^2}{2}\phi^2 + \frac{\lambda}{4!}\phi^4$$

 ${\it m}$ – mass of the scalar field

 λ - coupling strength of its self-interaction

Classical Field Theory

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Point Mechanics vs. Classical Field Theory

Point Mechanics	Field Theory
time t	space-time $x = (t, \vec{x})$
particle coordinate x	field value ϕ
particle path $x(t)$	field configuration $\phi(x)$
action $S[x] = \int dt \ L(x, \partial_t x)$	action $S[\phi] = \int d^4x \mathcal{L}(\phi, \partial_{\mu}\phi)$
Lagrange function	Lagrangian
$L(x, \partial_t x) = \frac{m}{2} (\partial_t x)^2 - V(x)$	$\mathcal{L}(\phi, \partial_{\mu}\phi) = \frac{1}{2}\partial_{\mu}\phi\partial^{\mu}\phi - V(\phi)$
equation of motion	field equation
$\partial_t \frac{\delta L}{\delta(\partial_t x)} - \frac{\delta L}{\delta x} = 0$	$\partial_{\mu} \frac{\delta L}{\delta(\partial_{\mu} \phi)} - \frac{\delta L}{\delta \phi} = 0$
Newton's equation	Klein-Gordon equation
$\partial_t^2 x = -\frac{dV(x)}{dx}$	$\partial_{\mu}\partial^{\mu}\phi = -\frac{dV(\phi)}{d\phi}$
kinetic energy $\frac{m}{2}(\partial_t x)^2$	kinetic energy $\frac{1}{2}\partial_{\mu}\phi\partial^{\mu}\phi$
harmonic oscillator potential $\frac{m}{2}\omega^2x^2$	mass term $\frac{m^2}{2}\phi^2$
anharmonic perturbation $\frac{\lambda}{4}x^4$	self-interaction term $\frac{\lambda}{4}\phi^4$

[Credit: U.-J. Wiese https://inspirehep.net/literature/946884]

Point Mechanics vs. Classical Field Theory

Path Integral in Quantum Mechanics: real time (I)

Time-dependent Schrödinger Eq.

$$i\hbar\partial_t |\Psi(t)\rangle = H |\Psi(t)\rangle$$

Time evolution operator

$$U(t',t) = e^{-\frac{i}{\hbar}H(t'-t)}; \quad |\Psi(t')\rangle = U(t',t)|\Psi(t)\rangle$$

 $H\,$ — time independent Hamilton operator

• Transition amplitude of a non-relativistic point particle — a propagator:

$$\langle x'|U(t',t)|x\rangle$$

Contains information about the energy spectrum of the theory.

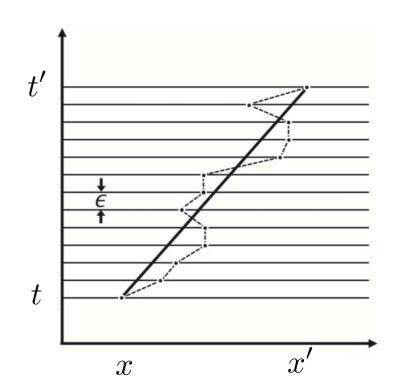
Path Integral in Quantum Mechanics: real time (II)

Propagator from x to x'

$$\langle x'|U(t',t)|x\rangle = \int dx_1 \langle x'|U(t',t_1)|x_1\rangle \langle x_1|U(t_1,t)|x\rangle$$

Divide time interval into N elementary steps of size

$$[t', t]; \qquad t' - t = N \epsilon$$



Repeat previous procedure at all intermediate times

$$\langle x'|U(t',t)|x\rangle = \int dx_1 \int dx_2 \dots \int dx_{N-1} \langle x'|U(t',t_{N-1})|x_{N-1}\rangle \times \dots \times \langle x_2|U(t_2,t_1)|x_1\rangle \times \langle x_1|U(t_1,t)|x\rangle$$

• Take factor $\langle x_{i+1}|U(t_{i+1},t_i)|x_i\rangle$; assume single non-relativistic point particle

$$H = \frac{p^2}{2m} + V(x)$$

• Insert complete set of states + BCH formula:

$$\langle x_{i+1}|U(t_{i+1},t_i)|x_i\rangle = \frac{1}{2\pi} \int dp \ e^{-\frac{i\epsilon p^2}{2m\hbar}} \ e^{-\frac{i}{\hbar}p(x_{i+1}-x_i)} \ e^{-\frac{i\epsilon}{\hbar}V(x_i)}$$

Path Integral in Quantum Mechanics: real time (III)

$$\langle x_{i+1}|U(t_{i+1},t_i)|x_i\rangle = \frac{1}{2\pi} \int dp \ e^{-\frac{i\epsilon p^2}{2m\hbar}} \ e^{-\frac{i}{\hbar}p(x_{i+1}-x_i)} \ e^{-\frac{i\epsilon}{\hbar}V(x_i)}$$

ullet $\int dp$ ill-defined: integrand rapidly oscillating f-on

For it to be well-defined:

- 1. replace: $\epsilon \longrightarrow \epsilon i a; \quad a \in \mathbb{R}$
- 2. evaluate $\int dp \dots$
- 3. take $a \rightarrow 0$ limit, one gets:

$$\langle x_{i+1}|U(t_{i+1},t_i)|x_i\rangle = \sqrt{\frac{m}{2\pi i\hbar\epsilon}} e^{\frac{i}{\hbar}\epsilon \left[\frac{m}{2}\left(\frac{x_{i+1}-x_i}{\epsilon}\right)^2 - V(x_i)\right]}$$

Insert into original propagator:

$$\langle x'|U(t',t)|x\rangle = \int \mathcal{D}x \, e^{\frac{i}{\hbar}S[x]}$$

$$\int \mathcal{D}x = \lim_{\epsilon \to 0} \sqrt{\frac{m}{2\pi i\hbar \epsilon}}^{N-1} \int dx_1 \int dx_2 \dots \int dx_{N-1}$$

Path Integral in Quantum Mechanics: real time (IV)

$$\langle x'|U(t',t)|x\rangle = \int \mathcal{D}x \, e^{\frac{i}{\hbar}S[x]}$$

$$\int \mathcal{D}x = \lim_{\epsilon \to 0} \sqrt{\frac{m}{2\pi i\hbar \epsilon}}^{N-1} \int dx_1 \int dx_2 \dots \int dx_{N-1}$$

• The action is continuum limit of the discretised action:

$$S[x] = \int dt \left[\frac{m}{2} (\partial_t x)^2 - V(x) \right] = \lim_{\epsilon \to 0} \sum_i \epsilon \left[\frac{m}{2} \left(\frac{x_{i+1} - x_i}{\epsilon} \right)^2 - V(x_i) \right]$$

- Summary:
 - (i) Integrate over all particle positions for each intermediate time t_i
 - (ii) Amounts to integrating over all possible paths of a particle starting at x and ending at x^\prime
 - (iii) Each path weighted with oscillating phase
 - (iv) Classical path: the smallest oscillations \Rightarrow largest contribution to the P.I. ($\hbar \to 0$ class. limit)
- Note: definition of the path integral required an analytic continuation in time!

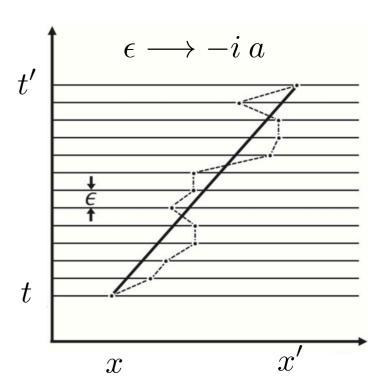
Euclidean Path Integral in Quantum Mechanics

• Statistical partition function: $Z = e^{-\beta H}; \quad \beta = \frac{1}{T}$

$$\beta = \frac{i}{\hbar}(t'-t) \implies e^{-\beta H} \Leftrightarrow U(t,t')$$

System at finite temperature T

System propagating in purely imaginary time



- Repeat all the steps from the derivation in real time:
 - (i) Divide Euclidean time interval into N time steps: $\beta = \frac{Na}{\hbar}$
 - (ii) Insert complete set of position eigenstates
- The Euclidean Path Integral:

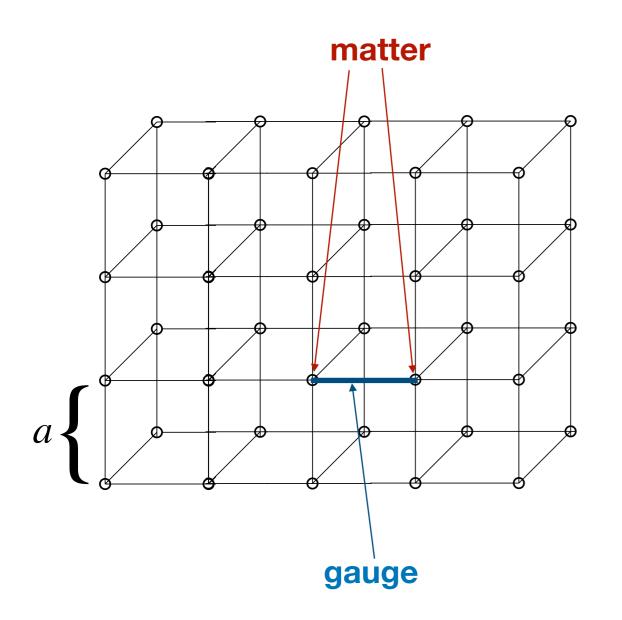
$$Z = \int \mathcal{D}x \, e^{-\frac{1}{\hbar}S_E[x]}$$

$$S_E[x] = \int dt \left[\frac{m}{2} (\partial_t x)^2 + V(x) \right] = \lim_{a \to 0} \sum_i a \left[\frac{m}{2} \left(\frac{x_{i+1} - x_i}{a} \right)^2 + V(x_i) \right]$$

$$\int \mathcal{D}x = \lim_{a \to 0} \sqrt{\frac{m}{2\pi i \hbar a}}^N \int dx_1 \int dx_2 \dots \int dx_N$$

Scalar fields on the lattice

- Quantum field theories beyond tree level are plagued by UV divergencies
- Defining the theory on a lattice introduces a minimum length



ullet Lattice spacing acts as an UV cut-off: $\Lambda \sim rac{1}{a}$

$$Z = \int \mathcal{D}\phi \ e^{-S_E[\phi]}$$

$$\int \mathcal{D}\phi = \prod_{x} \int d\phi(x)$$

$$S_E[\phi] = \int d^D x \left[\frac{1}{2} (\partial_\mu \phi)^2 + \frac{1}{2} m^2 \phi^2 + \frac{\lambda}{4!} \phi^4 \right]$$

Scalar field theory

Discretize space-time and define matter fields on the sites of the lattice:

$$x \longrightarrow an = (an_1, an_2, an_3, an_4); n_{\mu} \in \mathbb{Z}$$

 $\phi(x) \longrightarrow \phi(an)$

• Momentum integrals are restricted to the first Brillouin zone:

$$\int d^4x \longrightarrow a^4 \sum_{n_\mu} \equiv \sum_x$$

$$\int \frac{d^4k}{2\pi} \longrightarrow \int_{|k| < \frac{2\pi}{a}} \frac{d^4k}{2\pi} \equiv \int_k$$

Discretize the derivatives:

$$\partial_{\mu}\phi(x) \longrightarrow \nabla_{\mu}\phi(x) = \frac{1}{a} \left[\phi(x + a\hat{\mu}) - \phi(x) \right]$$
$$\longrightarrow \nabla_{\mu}^{*}\phi(x) = \frac{1}{a} \left[\phi(x) - \phi(x - a\hat{\mu}) \right]$$

Lattice action

Discretized action (bare parameters)

$$S[\phi] = \sum_{x} \left[\frac{1}{2} \nabla_{\mu} \phi(x) \nabla_{\mu} \phi(x) + \frac{1}{2} m_0^2 \phi(x)^2 + \frac{\lambda_0}{4!} \phi(x)^4 \right]$$

Scalar propagator

$$\Delta(k)^{-1} = \sum_{\mu} \left[\frac{2}{a} sin(\frac{k_{\mu}a}{2}) \right]^{2} + m_{0}^{2}$$
$$= k^{2} + m_{0}^{2} + \mathcal{O}(a^{2})$$

ullet Space time symmetry: $O(4) \longrightarrow H(4)$

Rotation symmetry recovered in the continuum limit

From P.I. in Quantum Mech. to Statistical Stat. Mech.

Quantum mechanics	Classical statistical mechanics
Euclidean time lattice	d-dimensional spatial lattice
elementary time step a	crystal lattice spacing
particle position x	classical spin variable s
particle path $x(t)$	spin configuration s_x
path integral $\int \mathcal{D}x$	sum over configurations $\prod_x \sum_{s_x}$
Euclidean action $S_E[x]$	classical Hamilton function $\mathcal{H}[s]$
Planck's constant \hbar	temperature T
quantum fluctuations	thermal fluctuations
kinetic energy $\frac{1}{2}(\frac{x_{i+1}-x_i}{a})^2$	neighbor coupling $s_x s_{x+1}$
potential energy $V(x_i)$	external field energy $\mu B s_x$
weight of a path $\exp(-\frac{1}{\hbar}S_E[x])$	Boltzmann factor $\exp(-\mathcal{H}[s]/T)$
vacuum expectation value $\langle \mathcal{O}(x) \rangle$	magnetization $\langle s_x \rangle$
2-point function $\langle \mathcal{O}(x(0))\mathcal{O}(x(t))\rangle$	correlation function $\langle s_x s_y \rangle$
energy gap $E_1 - E_0$	inverse correlation length $1/\xi$
continuum limit $a \to 0$	critical behavior $\xi \to \infty$

[Credit: U.-J. Wiese https://inspirehep.net/literature/946884]

From Statistical Mech. to Quantum Field Theories

Classical Statistical Mechanics	Quantum Field Theories
Partition $Z_{eta} = \sum_{\sigma} e^{-eta H(\sigma)}$	Feynman $\mathcal{Z} = \int D[U] e [(-1 / g^2) S(U)]$ Path Integral
Inverse temperature $\beta \sim 1/T$	Inverse gauge coupling ~1/g ²
Correlation functions $< \sigma(x) \sigma(y) > \sim e^{- x-y /\xi}$	2-point functions $< Tr(U(p)_x) TrU(p)_y > \sim e^{- x-y r}$
Inverse correlation length $1/\xi$	Particle mass: m
2nd order phase transition $\xi/a \rightarrow \infty$ with a fixed	Continuum limit: $m \rightarrow 0$ with m fixed

2-d spatial lattice with physical lattice spacing *a*

4-d space-time lattice with unphysical cut-off *a*

 Monte Carlo: a numerical method for estimating high-dimensional integrals by random sampling

JOURNAL OF THE AMERICAN STATISTICAL ASSOCIATION

Number 247

SEPTEMBER 1949

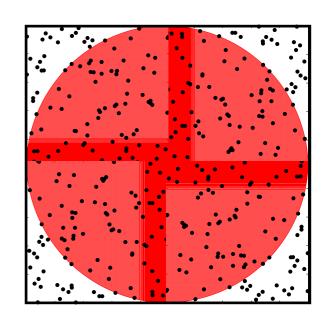
Volume 44

THE MONTE CARLO METHOD

NICHOLAS METROPOLIS AND S. ULAM

Los Alamos Laboratory

We shall present here the motivation and a general description of a method dealing with a class of problems in mathematical physics. The method is, essentially, a statistical approach to the study of differential equations, or more generally, of integro-differential equations that occur in various branches of the natural sciences.





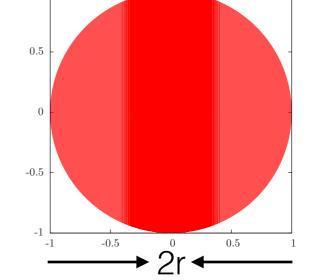


Ratio of the surface area of the circle and the square:

$$\frac{S_{circle}}{S_{square}} = \frac{\pi r^2}{4r^2}$$

We can then express:

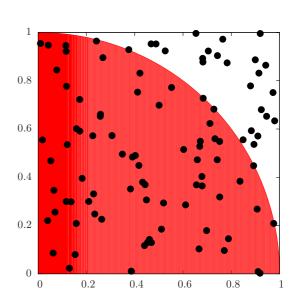
$$\pi = \frac{4S_{circle}}{S_{square}}$$



- $_{\bullet}~$ If we know S_{circle}/S_{square} , we know the value of π
- Throw N random points on the surface of the square

$$\pi = \frac{4S_{circle}}{S_{square}} \approx \frac{N_{inside}}{N}$$

 \bullet For N - large, the value of π will be very well approximated



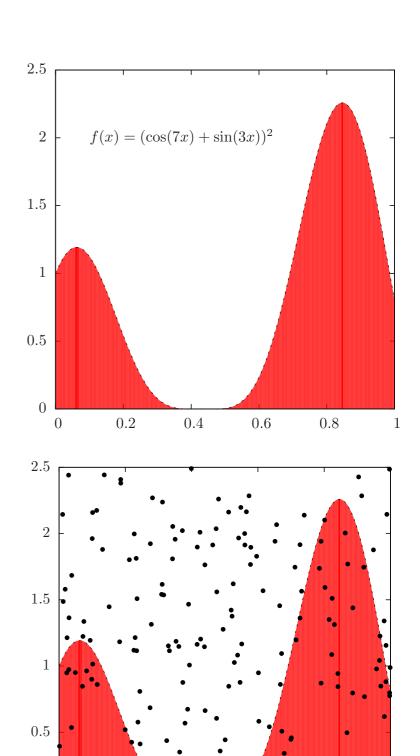
Calculating 1-dim integral:

$$I = \int_0^1 f(x) dx$$

- Again, throw N random points on the rectangular surface:
- Count those under the value of the function f(x)
- Then the value of the integral is obtained by:

$$I \approx \langle I \rangle_N = 2.5 \times 1 \times \frac{N_{inside}}{N}$$

- For larger N, better and better approximation of the integral
- Monte Carlo error in d-dim:
- Monte Carlo error in d-dim: $pprox rac{1}{\sqrt{N}}$ Numerical integration error in d-dim: $pprox rac{1}{N^{2/d}}$
- For d>4, Monte Carlo is better than Numerical Integration!



0.2

0.4

0.8

0.6

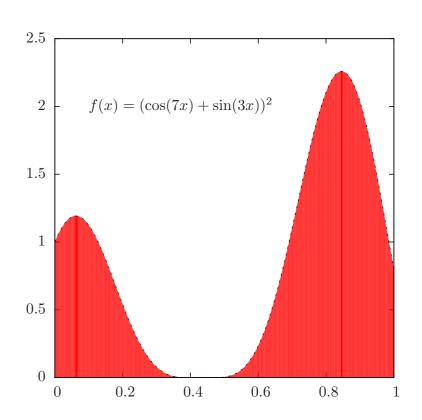
Calculating 1-dim integral:

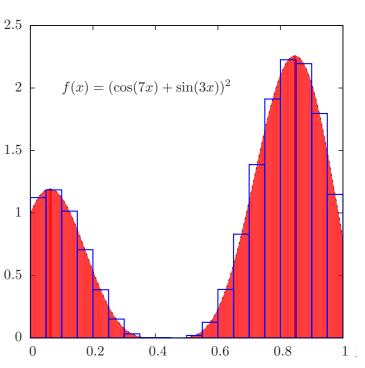
$$I = \int_0^1 f(x) dx$$

- Again, throw N random points on the rectangular surface:
- **©** Count those under the value of the function f(x)
- Then the value of the integral is obtained by:

•
$$I \approx \langle I \rangle_N = 2.5 \times 1 \times \frac{N_{inside}}{N}$$

- For larger N, better and better approximation of the integral
- Monte Carlo error in d-dim: $pprox rac{1}{\sqrt{N}}$
- ullet Numerical integration error (midpoint rule) in d-dim: $pprox rac{1}{N^{2/d}}$
- For d>4, Monte Carlo is better than Numerical Integration!





Expectation values in Monte Carlo

Ising model Hamiltonian (without external magnetic field):

$$H = J \sum_{\langle x,y \rangle} s_x s_y; \quad \langle x,y \rangle$$
 — nearest neighbours

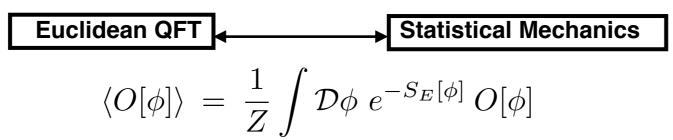
- Generate configurations of spins with probability $\sim e^{-\frac{H}{T}}$ (importance sampling)
- Expectation value of the observables as averages over ensemble of spin configurations

$$\langle O \rangle \approx \bar{O} = \frac{1}{N_{cnfg}} \sum_{k=1}^{N_{cnfg}} O[\bar{s}_k] + \mathcal{O}(\frac{1}{\sqrt{N_{cnfg}}})$$

• How do we generate the ensemble $\{\bar{s}_k\}$?

Numerical Simulations

• Numerical approach exploits the analogy:



Path integrals are computed by importance sampling

$$\mathcal{P}[\phi_i] \propto e^{-S_E[\phi]}$$

- ullet Generate ensemble of field configurations $\{\phi_i\}$
- \bullet Expectation values $\langle O[\phi] \rangle$ are averages over the ensemble

$$\langle O \rangle \approx \bar{O} = \frac{1}{N_{cnfg}} \sum_{i=1}^{N_{cnfg}} O[\phi] + \mathcal{O}(\frac{1}{\sqrt{N_{cnfg}}})$$

ullet How do we generate ensemble $\{\phi_i\}$ with the correct probability distribution?

Markov processes

ullet Recursive procedure that generates $\{\phi_i\}$ with specific algorithm s.t. aimed distribution is asymptotically obtained

$$\{\phi_0\} \longrightarrow \{\phi_1\} \longrightarrow \{\phi_2\} \longrightarrow \cdots \longrightarrow \{\phi_i\} \longrightarrow \{\phi_{i+1}\} \longrightarrow \cdots$$

- Markov chains that converge exponentially to the equilibrium distr.
- ullet The configurations $\{\phi_i\}$ are correlated by construction

$$Var\left[\bar{O}\right] = Var\left[O\right] \left(\frac{2\tau_O}{N_{cnfq}}\right)$$

- integrated autocorrelation time

- \bullet The error of the estimator scales as $~\frac{1}{\sqrt{N_{cnfg}}}~$ (Monte Carlo)
- The variance of the actual observable

$$Var\left[O\right] \,=\, \langle \left(O-\langle O\rangle\right)^2\rangle$$
 property of QFT itself, should not depend of the Markov chain.

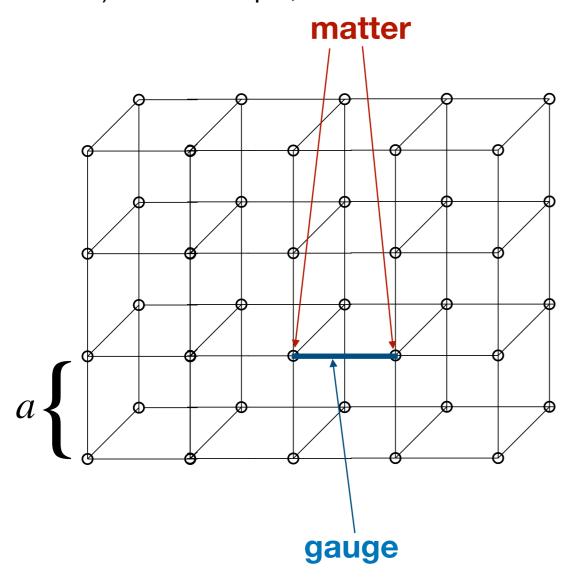
QFT on the lattice: symmetries

Translational Symmetry:

Broken to discrete symmetry, but nicely restored in the continuum limit

Rotational Symmetry:

Similar to translational symmetry. Finite number of irreducible representations (quantum numbers) instead of spin, but correct states are obtained in the continuum limit





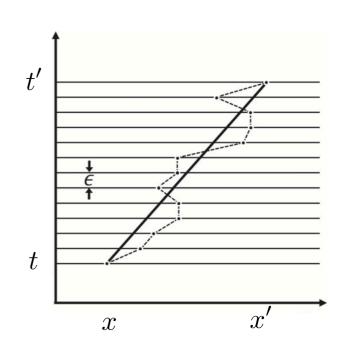
In today's lecture:

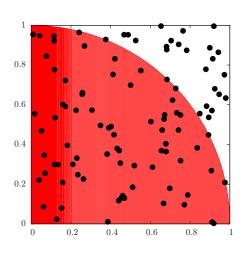
- We have learned/reminded ourselves how to quantize:
 - Quantum Mechanics
 - Scalar Field Theory





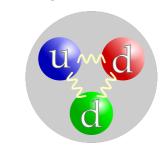






In tomorrow's lecture:

- We shall generalize this approach to Quantum Chromodynamics (QCD)
- We shall see how the numerical sampling is done in practice



- **→** for scalar field theory
- **→** for QCD





- Why is QCD numerically so expensive?
- Practical examples

