Lessons from lattice QCD

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We would like for you to give a "challenge talk" to the quantum gravity community at large. We would like to hear from you, as a practitioner in lattice gauge theories with oscillating / alternating contributions, how to tackle such challenges in numerical simulations...

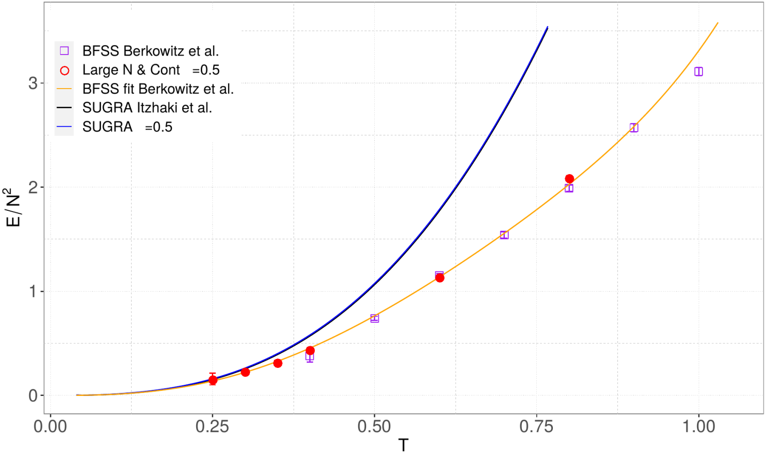
... *different methods to overcome problems, in particular when dealing with complex, oscillating amplitudes.*

... *next challenges and obstacles might be that quantum gravity has to face when increasing the scale and costs of simulations.*

My expertise:

- Main contributions: BSM lattice studies, gauge/gravity duality
- Contributions to: finite temperature and density, vacuum structure and confinement, algorithms and machines, QCD precision measurements, theoretical developments, quantum computing
- Worked with several code packages, including own developments

Quantum gravity and gauge/gravity duality



[S. Pateloudis et al. [MCSMC] (2023)]

$\Rightarrow$ not topic of this talk

Goal of this talk

- explain concepts and challenges of Lattice QCD
- find some generic messages, relevant for QG
- explain generic challenges with code developments and scaling up without reference to specific algorithms
- some parts are based on personal opinions

1. What is lattice gauge theory? A brief summary.
2. History: 50 years of lattice QCD
3. Current status and practice with notes on code development
4. Beyond the limits: sign problem and quantum computing
5. Conclusions

What is lattice gauge theory? A brief summary.

1. Wick rotation: Euclidean path integral
2. Discretize field space: finite (large) number of integrations
3. Stochastic estimation of path integral: importance sampling with Makov chain Monte Carlo

- introduce a regulator without breaking gauge invariance/ gauge fixing
- scaling window given by box size and lattice spacing: $1/L \ll |k| \ll 1/a$
- $SO(3,1) \to SO(4) \to$ cubic group, full $SO(4)$ is accidentally recovered
- lattice theory corresponds to a classical statistical system with Boltzmann weight $e^{-S[\phi]}$

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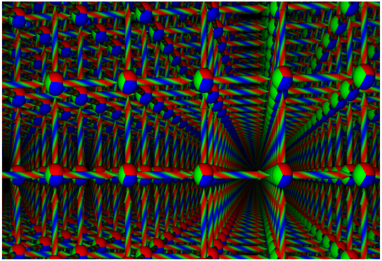
QCD on the lattice: the path integral

$$Z = \int \mathcal{D}\phi \; e^{-S[\phi]} = \int \prod_i d\phi_i \; e^{-S_L[\phi]}$$

- field on lattice points $\phi_i = \phi(an)$
- derivative operators:
  $\partial_\mu \phi(x) \to \frac{1}{2a}(\phi(a(n+\hat{\mu})) - \phi(a(n-\hat{\mu}))) + \mathcal{O}(a^2)$
- discretization not unique

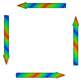


gauge fields
$A_\mu \to e^{igaA_\mu} = U_\mu$:

matter fields ψ, ϕ:

QCD on the lattice: the action

$$S_L = \beta \sum_p \left(1 - \frac{1}{N_c}\Re(\mathrm{Tr}\, U_p)\right) + \sum_{f,n} \bar{\psi}_f(\mathrm{D[U]} + m_f)\psi_f$$

- plaquette $U_p =$  ; $\beta = \frac{2N_c}{g^2}$
- integral of group elements: Haar measure dU
- Grassmann fields: integrated out

$$Z = \int \prod_i dU_i \prod_f \det(D[U] + m_f)\exp(-S_g[U])$$

- importance sampling: configurations $U^{(k)}$ with distribution $\exp(-S_L)$

$$\langle O \rangle = \frac{1}{Z}\int \prod_i dU_i O[U] \ldots \approx \frac{1}{N_{\mathrm{conf}}}\sum_k^{N_{\mathrm{conf}}} O[U^{(k)}] + \mathcal{O}\left(\frac{1}{\sqrt{N_{\mathrm{conf}}}}\right)$$

QCD on the lattice: fermions

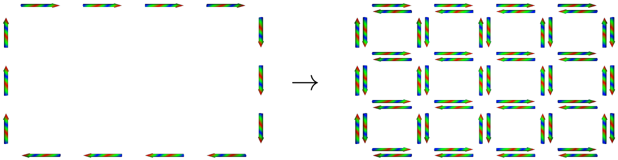
$$\sum_x \bar{\psi}(x)(\mathrm{D}-m)_{x,y}\psi(y) = \sum_x \Big[(m+4r)\bar{\psi}(x)\psi(x)$$

$$+\frac{1}{2}\sum_\mu \bar{\psi}(x)\big((\gamma_\mu - r)U_\mu(x)\psi(x+\hat{\mu}) + (\gamma_\mu + r)U^\dagger_\mu(x-\hat{\mu})\psi(x-\hat{\mu})\big)\Big]$$

- lattice Dirac operator D: derivatives replaced by gauge invariant difference operators
- fermion doubling: $r = 0$ leads to 16 fermion species
- Wilson-Dirac operator: additional momentum dependent mass term $\Rightarrow$ chiral symmetry breaking
- Nielsen-Ninomiya theorem: No-Go for chiral symmetry on the lattice, but can only be represented in a modified way

Static quark-antiquark potential in strong coupling limit

average Wilson loop:



$$\propto \left(\frac{\beta}{2N_c^2}\right)^{\mathcal{R}\mathcal{T}}$$

- first contribution: Loop filled with plaquettes
- confinement:
  $V(\mathcal{R}) = -\lim_{\mathcal{T}\to\infty} \frac{1}{\mathcal{T}} \log\langle W\rangle = -\sigma\mathcal{R}; \quad \sigma = -\log(\frac{\beta}{2N_c^2})$
- strong coupling expansion: $O = \sum_n O_n \beta^n$
- in certain region convergent series, but not connected to the continuum limit

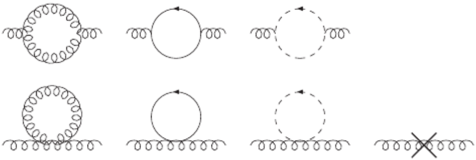
Weak coupling and continuum limit

Lattice spacing determined by gauge coupling g^2:

- asymptotic freedom implies: $g \to 0$ in continuum limit
- Gaussian UV fixed point

Weak coupling expansion:

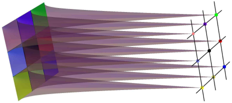
- same techniques as in continuum perturbation theory: gauge fixing, Feynman rules, etc.
- painfully more complicated: propagators with $p^2 \to (\sin(p))^2$, additional vertices, ...
- proves convergence to and matching of continuum perturbation theory



[Capitani (2003)]

Perfect lattice QCD

$$e^{-S_L[\phi]} = \int d\varphi \, e^{-R[\varphi,\phi]-S[\varphi]}$$



- derivation based on a renormalization group step (integrating out the continuum degrees of freedom)
- shows how to implement symmetries on the lattice: Ginsparg-Wilson relation for chiral symmetry
- modified symmetry relation: $\bar{\gamma}_{5,\mathrm{def}}\mathcal{D} + \mathcal{D}\gamma_{5,\mathrm{def}} = 0$ replaces naive symmetry: $\{\gamma_5, \mathcal{D}\} = 0$
- resembles relevant properties of the symmetry on the lattice

Lessons to be learned from general setup.

- implementation of symmetries, especially gauge symmetries, essential
- analytic expansions (no numerics) show: confinement possible, contact to continuum theory (UV fixed point)
- symmetries broken by regulator:
  - implemented in Ginsparg-Wilson relation
  - recovered accidentally
  - fine-tuned
- "Ms RG is a good physics teacher" (P. Hasenfratz)

History: 50 years of lattice QCD (I)

Origins statistical physics:

- Spin models: statistical methods and exact solutions
- Wegner: Ising lattice gauge theory
- Wilson: Considerations on Ising models and RG

Early QCD:

1960s Quark model, low energy effective field theories: nuclear physics, hadron physics

1970s non-Abelian gauge theories

1973 Gross, Wilczek, Politzer: asymptotic freedom

Missing gap between low and high energy description: How does confinement and hadrons follow from the fundamental theory?

1974 Wilson's seminal paper: *Confinement of Quarks*

- similar developments by Smit and Polyakov

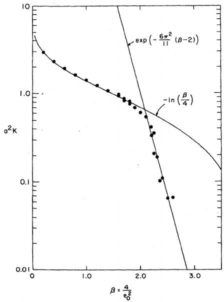
History: 50 years of lattice QCD (II)

Analytic calculations and establishing the theory (1974-1980)

- strong coupling expansions: confinement
- weak coupling expansion: continuum limit

First numerical simulations

- [M. Creutz (1981)] SU(2) gauge theory
- development of algorithms:
  Z_2, U(1), SU(2), SU(3), SU(N)
- QCD without fermion determinant (quenched)
- Hybrid Monte Carlo
  [Duane, Kennedy, Pendelton, Roweth (1987)]



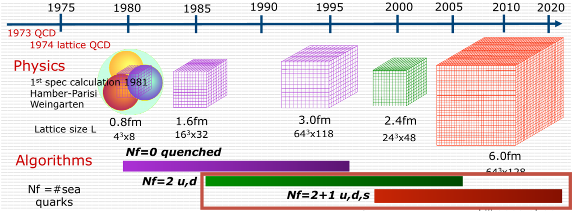
Scaling up, algorithmic and theoretical improvements:

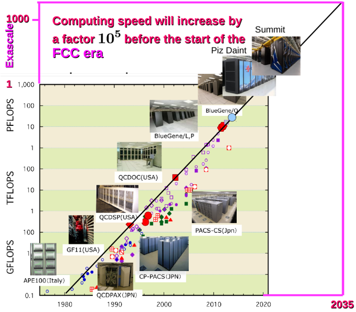
- implementation of Symanzik improvement program:
  compensate leading order lattice artefacts
- Domain-Wall and overlap fermions for chiral symmetry

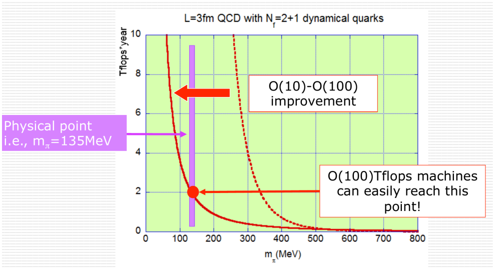
$\Rightarrow$ around 2010: lattice QCD competitive with experimental data

[See Lepage *40 Years of Lattice QCD* (2015)]

Major breakthroughs







[Credit: A. Ukawa Talk at CERN 2013, update F. Karsch CERN 2018]

Lessons to be learned from history of lattice QCD.

Lattice QCD:

- bridge the gap between UV and IR physics: first principles proof of fundamental theory
- show that path integral is a meaningful description, not just another way to derive perturbation theory
- controlled UV: connections to perturbation theory

Lessons to be learned from history of lattice QCD.

Quantum Gravity:

- discover while building
- can build upon established QFT methods, but need to be reconsidered for QG
- hope for asymptotic safety and well defined continuum limit

Lessons to be learned from history of lattice QCD.

- even naive attempts can lead in the right direction
- universality and connection between different approaches essential
- it takes a long time (40 years) to arrive at physical relevant results
- 20 years to establish the main approaches, 20 years to make it working
- don't try to solve everything just by scaling up compute power; estimate costs

Current status and future of lattice QCD

Some directions followed by current research:

- Precision physics:
  QCD contributions as input for experiments
- QCD phase transitions:
  nature of deconfinement and chiral transition
- Understanding of confinement:
  identify possible pictures of QCD vacuum
- Beyond QCD:
  solid state physics, dark matter, Higgs models, etc.

Reaching/extending limits of lattice calculations:

- sign problems: QCD at finite density, real time dynamics
- supersymmetry, conformal theories, etc.

Current scale of lattice QCD investigations

- lattice spacings down to 0.03 fm; lattice sizes: $m_\pi L \sim 5$
- physical fermion masses
- sub-percent accuracy: isospin breaking, QED corrections
- using largest available HPC clusters
- computing time 10-100 Mio Core-h / 10000 EXAFLOP
- obtaining 1-100 TFlops/s performance
- collaborations: MILC, BMW, ETMC, Hot-QCD, CLS ...
- national initiatives: USQCD, UKQCD,...
- order of 10-100 people involved
- software packages: MILC, Chroma, Gird, openQCD, QUDA...
- collaborations with hardware vendors (Nvidia, Intel,...) / computing centers

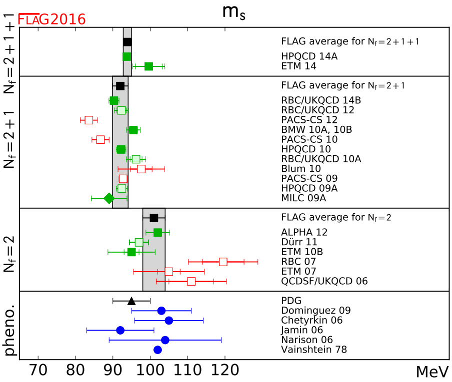
Current scale lattice QCD: development process

- Low level optimizations (CPU, GPU, etc.):
  - *Welcome to the Jungle* [H. Sutter]
- algorithms for linear algebra etc.
  - generic but strongly adapted and optimized
- physics inspired parameter setting and optimizations
  - guided by analytic estimates, RG, discretizations, phase transitions
- statistical data analysis
  - clever composition of observables, autocorrelations
- extrapolations and systematic uncertainty estimation
  - based on EFT, modeling, model averaging,. . .
- final data interpretation
  - What do we learn from it?

42

FLAG report

- combine values from different collaborations
- rate according quality criteria
- provide reference estimates



Current scale lattice QCD: comments on code development

Ideal case:

- reusable, reliable, maintainable, modularized, scalable code
- development principles: review, testing, refactoring, version control
- reproducibility: software available, data release, documentation (Initiatives: open Science, FAIR, ILDG)

"Successful" anti-patterns:

- Don't reuse, write new code for every project.
- Don't use any third parity software. Write everything from scratch.
- Don't share any data.
- only 1 person understands core parts of the code

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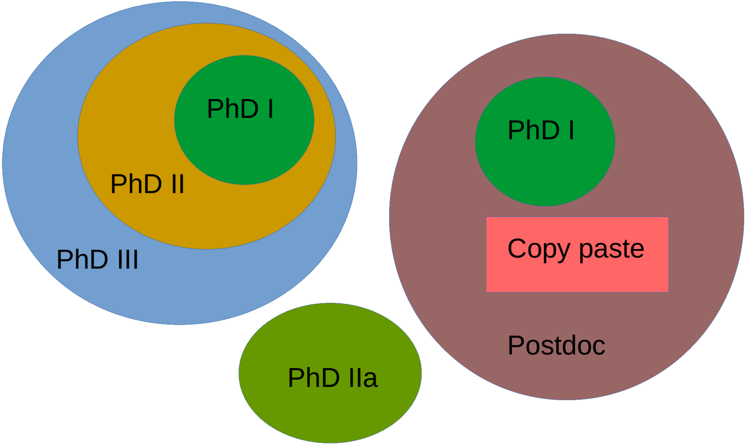
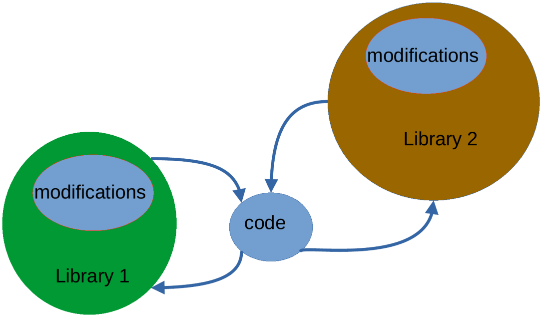
How your project might end up



Library usage in projects

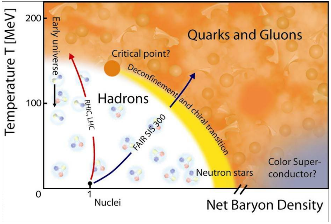


Final thoughts

- before developing new code: be aware what is already available, discuss with similar projects
- be aware of the challenges on large scale supercomputers:
  - documentation ? support ?
  - availability of compilers/libraries, bugs
  - claimed $\neq$ delivered performance
  - multi-paradigm parallelism, heterogeneous
  - developments for specific machine obsolete in next iterations
  - consider not developing for the highest scale / performance
- need to consider reward for programmers/developers (publications, hiring)
- manage knowledge: only 1-3 people understand core code
- goals/problems/failures are changing frequently: ensure clear communication

Lattice QCD, finite density, and the sign problem

$$Z(T,\mu) = \mathrm{Tr}(e^{-(H-\mu Q)/T})$$



- continuum physics: extra term $\mu\bar{\psi}\gamma_0\psi$
- on the lattice modification of D

$$\bar{\psi}(x)((\gamma_0 - r)e^{a\mu}U_0(x)\psi(x+\hat{0}) + (\gamma_0 + r)e^{-a\mu}U_\mu^\dagger(x-\hat{0})\psi(x-\hat{0}))$$

- $\gamma_5\mathrm{D}(\mu)^\dagger\gamma_5 = \mathrm{D}(-\mu^*) \Rightarrow \det(\mathrm{D}(\mu)) = \det(\mathrm{D}(-\mu^*))^*$
- complex determinant
- other sign problems: real time dynamics, QCD with θ term (CP violation)

$\Rightarrow$ much important physics beyond reach of MC

Possible solutions to the sign problem on the lattice

Brute force:

- reweighting
- Taylor expansion
- analytic continuation

Model specific

- effective theories
- dual variables

Non Monte-Carlo simulations:

- Complex Langeving

Path optimizations in complexified space

- Lefschetz thimbles
- holomorphic flow
- machine learning

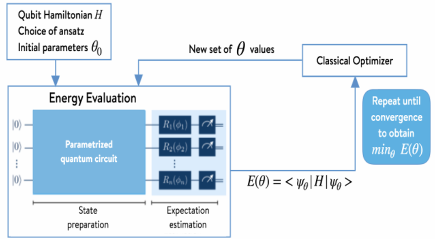
Hamiltonean formulation

- Tensor networks
- Quantum computing

Currently progress in many different directions, good results in 1+1 dimensions. However, no clear winner for 4D QCD.

Quantum computing

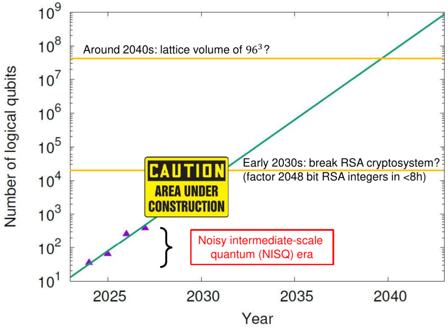
- Many believe only quantum computing can solve the (NP-hard) sign problem.
- Problem seems to be well suited for a quantum computer, if discretized only in spacial direction
- Can apply Variational Quantum Eigensolver, standard technique also for quantum chemistry etc.



[Credit: K. Jansen QCHSC 2024]

Quantum computing roadmap

- Much effort is now put into quantum computing: ambitious road maps, may technologies currently under development
- Still in NISQ (Noisy Intermediate-scale Quantum) era
- Analog or digital approaches



[Credit: L. Funcke Lattice 2022]

Lattice QCD on a quantum computer

Standard approach Kogut-Susskind Hamiltonean ($A_0 = 0$):

$$\hat{H} = \frac{g^2}{2a} \sum_l \hat{E}_l \hat{E}_l + \frac{1}{2g^2 a} \sum_p \mathrm{Tr}\left[2I - \hat{U}_p - \hat{U}_p^\dagger\right]$$

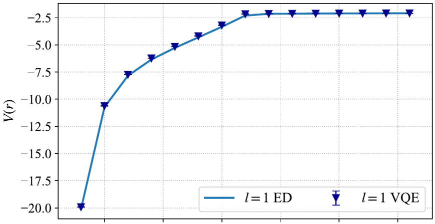
Need to consider:

- implementation of operators/ state preparation
- select a basis
- gauge constraint
- truncate to represent by a finite number of qubits/qudits

Lattice QCD on a quantum computer

Some first results:

- currently different alternative formulations under investigation
- many studies of Schwinger model, theories in 1+1 D
- first investigations of real time dynamics
- at the moment: tests of algorithms and methods
- currently main problem: missing error correction



[K. Jansen, E. Rinaldi QCHSC 2024]

Conclusions

- Numerical quantum gravity might be similar to LQCD some decades ago, but there are also clear distinctions
- Need to find safe ground at the conceptual level, not only numerical methods
- Different levels of scaling up in history of LQCD:
  - show method might be working
  - invent numerical algorithms
  - improve and scale up
- be aware of challenges when scaling up projects
- considering quantum computing: high risk/ high gain

Get connected

Plenty of opportunities to discuss:

- this workshop
- Lattice conference (2025 in Mumbai)
- Sign Workshop (2025 in Bern)
- Open data and reproducibility: see panel discussion at Lattice 2024 (E. Bennett et al.)
- workshops on quantum computing
- ...