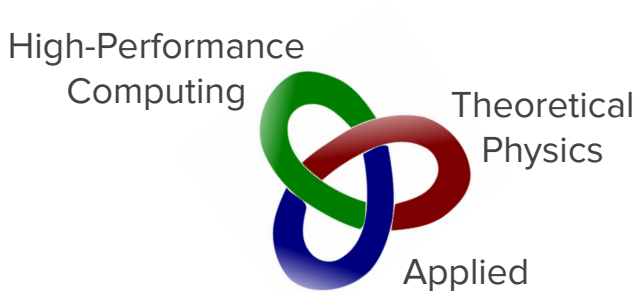
High-Performance Computing (HPC)

for Fundamental Physics: Lattice QCD



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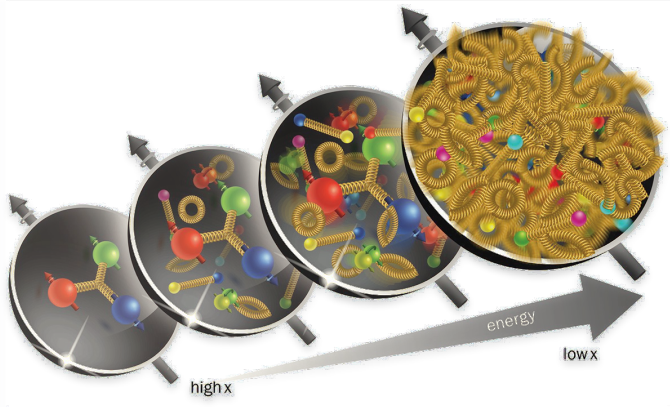
CaSToRC, The Cyprus Institute



30/09/26 – AQTIVATE Conference, Larnaca, Cyprus

Outlook

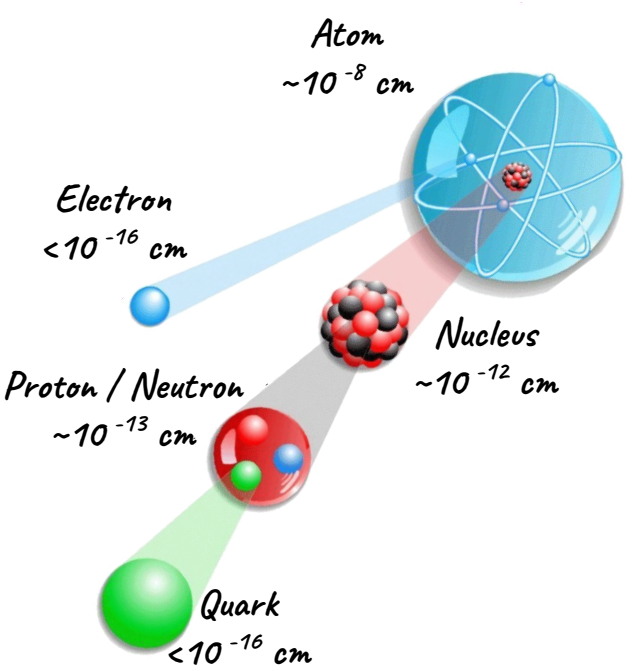
Numerical Challenges

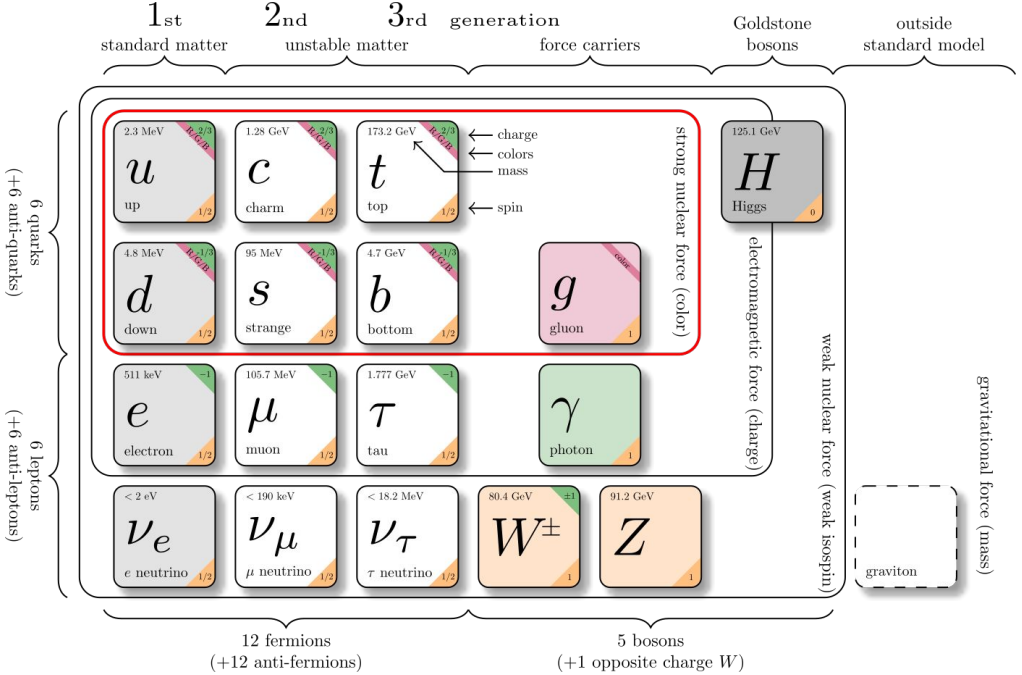
1. Simulating fermions (at light mass)
$$\langle \mathcal{O} \rangle = \lim_{\vec{\mu}_f \to \vec{m}_f} \langle \mathcal{O} \rangle_{a,V,\vec{\mu}_f}$$
2. High-dimensional integral
$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathrm{D}[U]\, \mathcal{O}(U)\, \exp(-S(U))$$
3. Continuum and infinite volume limit
$$\langle \mathcal{O} \rangle = \lim_{a \to 0\ V \to \infty} \langle \mathcal{O} \rangle_{a,V}$$
4. High-precision results
$$\langle \mathcal{O} \rangle = \lim_{N \to \infty} \frac{1}{N} \sum_i^N \mathcal{O}(U_i)$$

State-of-the-art Solutions

- Krylow solvers and Multigrid methods
  E.g. DD-αAMG developed by BUW
- Importance Sampling and Hybrid Monte Carlo (HMC)
  $\langle \mathcal{O} \rangle = \frac{1}{N} \sum_i^N O(U_i)$ *with* $p(U) = \frac{1}{\mathcal{Z}} \exp(-S(U))$
- High-Performance Computing
  Parallelizable and scalable problem
- Noise reduction techniques
  E.g. low-mode averaging

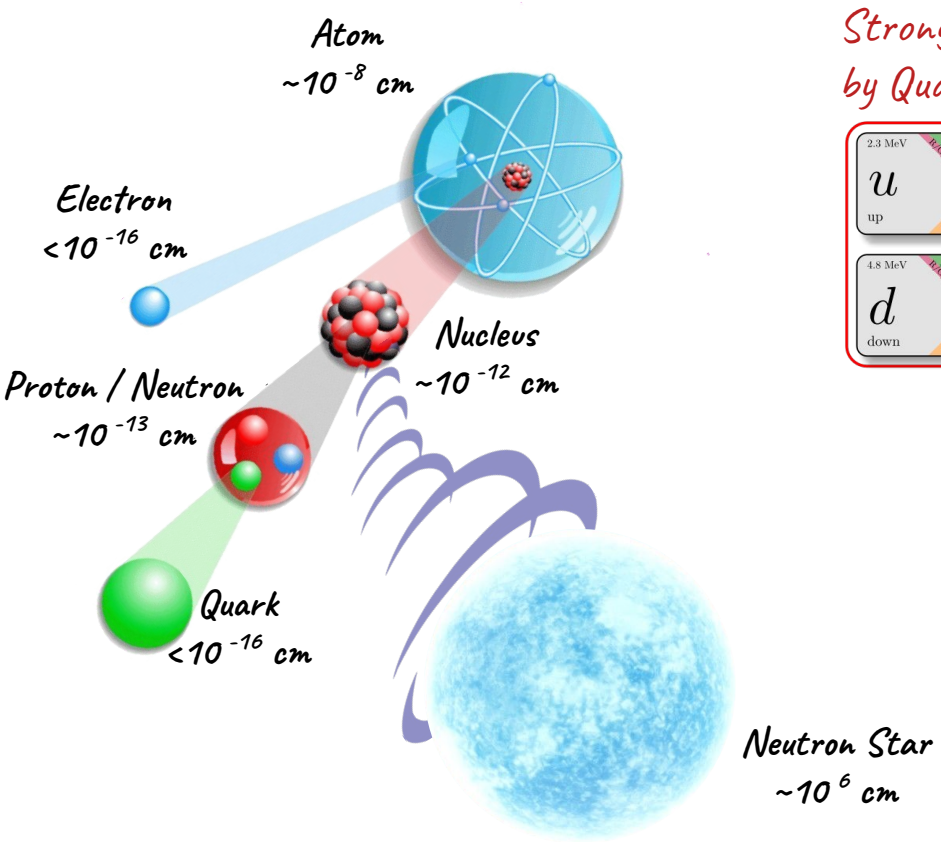
Standard Model of Particle Physics



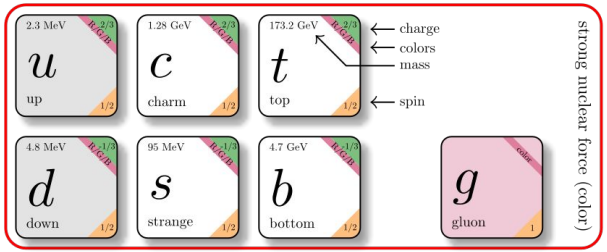


Developed in the early 1970s

Standard Model of Particle Physics



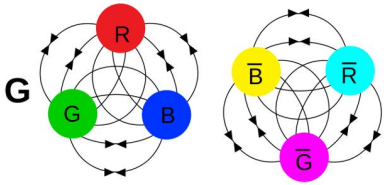
Strong Nuclear Force described
by Quantum ChromoDynamics (QCD)



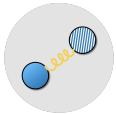
Baryons



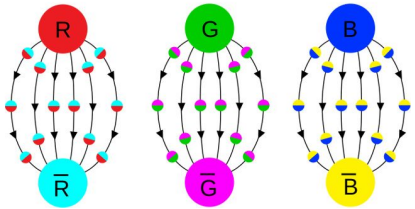
Proton, Neutron, ...



Mesons



Pion, Kaon, ...



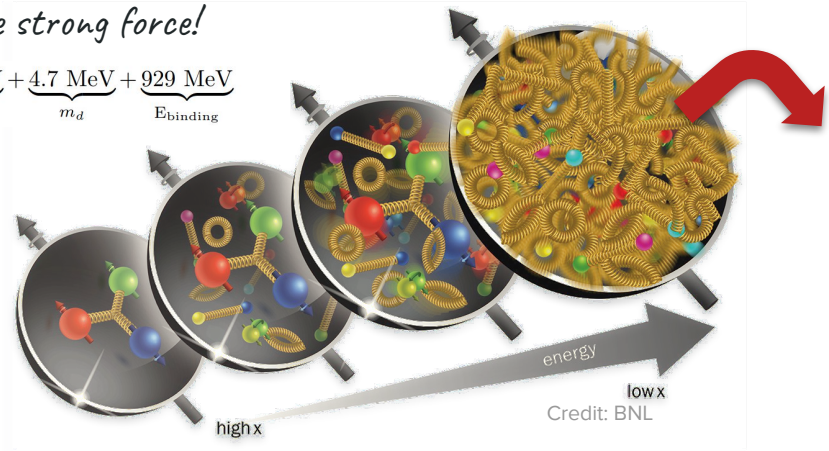
Lattice QCD: Why? How?

Why? **The Lattice formulation** is a non-perturbative, systematically-improvable approach to regularize a quantum field theory; it provides a fundamental framework for the study of QCD at low energies

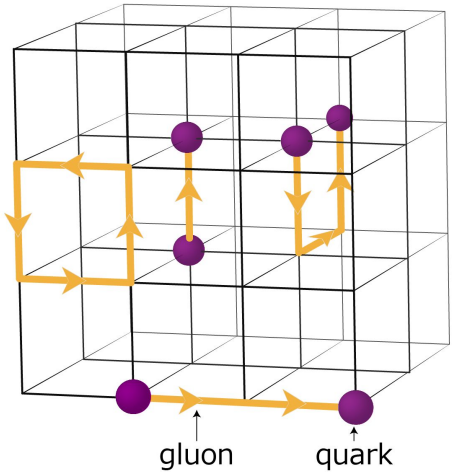
$$\mathcal{L}_{\mathrm{QCD}} = -\frac{1}{4} F^a_{\mu\nu} F_a^{\mu\nu} + \sum_f \bar{\psi}_f \left(i\gamma^\mu D_\mu - m_f \right) \psi_f$$

99% of our mass comes from the strong force!

$$m_p = \underbrace{2.3\ \mathrm{MeV}}_{2\times m_u} + \underbrace{4.7\ \mathrm{MeV}}_{m_d} + \underbrace{929\ \mathrm{MeV}}_{\mathrm{E_{binding}}}$$



Numerical approaches required!



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How?



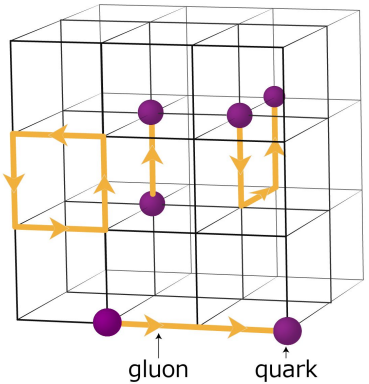
K. G. Wilson
1974

From QCD

- Continuous space-time
- Minkowski space-time
- Lie algebra $A_\mu(x)$
- Lagrangian $\mathcal{L}_{\mathrm{QCD}}(g, m_f)$

To Lattice QCD

- 4D hypercubic lattice a, V
- Euclidean space-time
- Lie group $U_\mu(x) = e^{igaA_\mu(x)}$
- Lattice action $S(a, \mu_f)$



$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[U]\mathcal{D}[\psi\bar{\psi}] O(U, \psi, \bar{\psi})\, e^{-S(U,\psi,\bar{\psi})}$$

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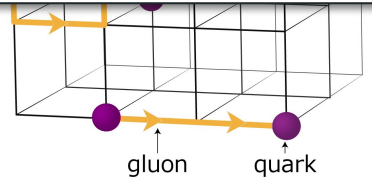
$$\langle \mathcal{O} \rangle = \lim_{\substack{\mu_f \to m_f \\ V \to \infty \\ a \to 0}} \langle \mathcal{O} \rangle_{a,V,\mu_f}$$



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How to simulate QCD? … many challenges!

$$\langle \mathcal{O} \rangle_{a,V,\vec{\mu}_f} = \frac{1}{\mathcal{Z}} \int \mathrm{D}[U]^V \, \mathrm{D}[\psi\bar{\psi}]^{V n_f} \, \mathcal{O}(U,\psi,\bar{\psi}) \, e^{-S(a,\vec{\mu}_f;U,\psi,\bar{\psi})}$$

1. Simulating fermions (at light mass)

$$\langle \mathcal{O} \rangle = \lim_{\vec{\mu}_f \to \vec{m}_f} \langle \mathcal{O} \rangle_{a,V,\vec{\mu}_f}$$

- Krylow solvers and Multigrid methods

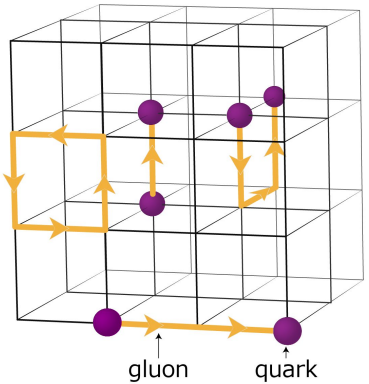
  E.g. DD-αAMG developed by BUW

QCD has two fundamental ingredients:

- $U_\mu(x)$ gauge field: "*lives on the links*"
- $\psi(x)$ fermion: "*lives on the sites*"

$$\psi(x+\vec{\mu}) = U_\mu(x)\psi(x)$$

Grassmann variables: $\psi_i\psi_j = -\psi_j\psi_i \;\Rightarrow\; \psi^2 = 0$

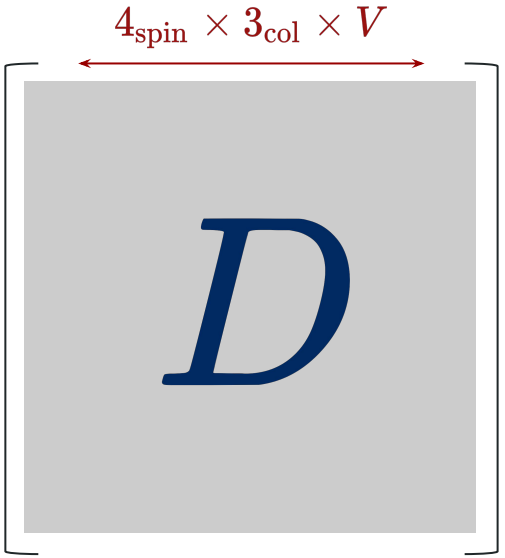


1st challenge: Fermions on the Lattice

$$\langle \mathcal{T}\psi_j\bar{\psi}_i\rangle = \frac{1}{Z}\int \mathcal{D}[U]\mathcal{D}[\psi\bar{\psi}]\,\psi_j\bar{\psi}_i\, e^{-S_{YM}(U)-\bar{\psi}D\psi}$$
$$= \frac{1}{Z}\int \mathcal{D}[U]\, D^{-1}_{ji}\,\det D\, e^{-S_{YM}(U)}$$

with $D \equiv D(U,m) \underset{a\to 0}{\longrightarrow} (i\gamma^\mu\partial_\mu - m)$

- Many possible discretizations of the Dirac operator
  - *Wilson, Twisted-Mass, Domain-Wall, Overlap, etc.*
- Fermions require the inverse of the Dirac operator
- **BUT** practically <u>impossible to be inverted directly</u>
  - *V^2 problem: size of the matrix (V x 4 x 3)^2*
  - *e.g. 100 EB required for a single inversion*
  - *Impossible to compute the complete inverse of D*



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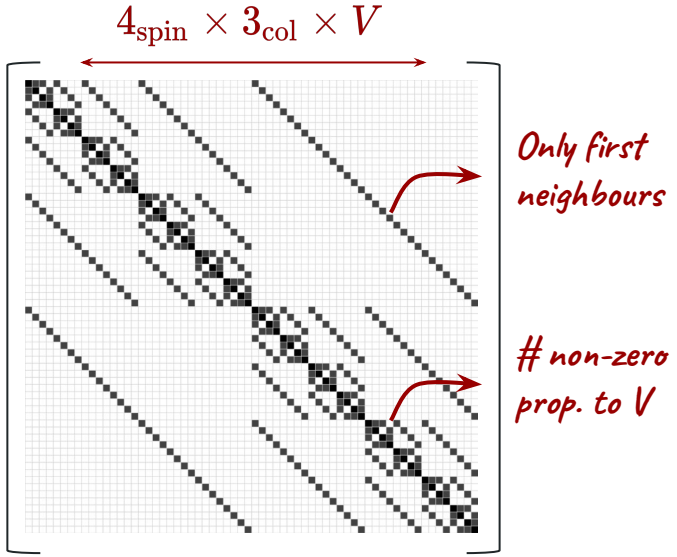
- Many possible discretizations of the Dirac operator
  - *Wilson, Twisted-Mass, Domain-Wall, Overlap, etc.*
- The Dirac operator is a **sparse matrix** (first-neighbors only)
  - *Krylov methods are used to solve:* $D\vec{x} = \vec{b}$
  - e.g. $D\vec{x} = \vec{e}_i \implies x_j = D^{-1}_{ji}$
  - e.g. $D\vec{x} = \vec{\eta} \implies |\vec{x}|^2 \approx \mathrm{Tr}(D^{-1})$



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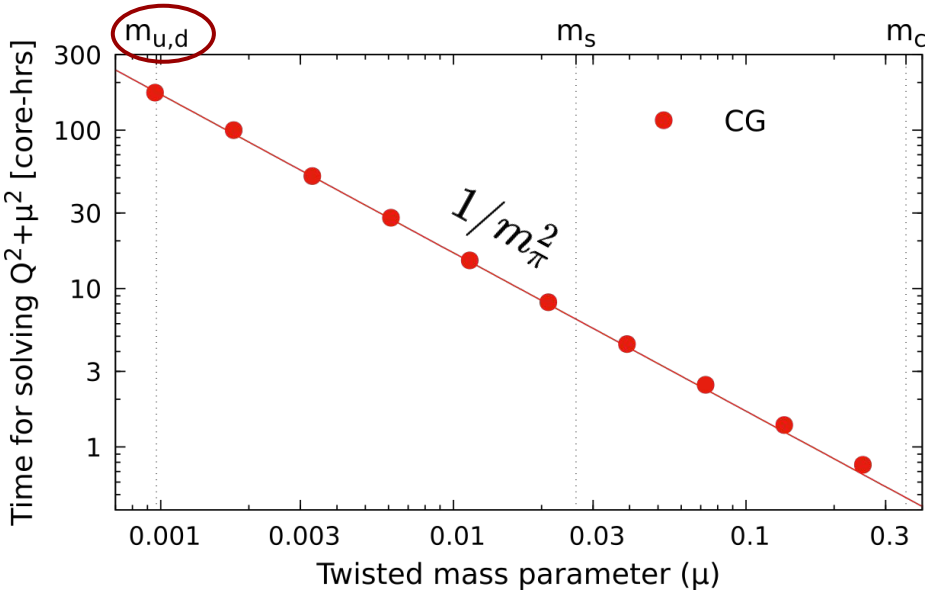
- Dirac operator is singular at $\mu=0$
  - *Critical slowing down, e.g.*
  - *Light quark masses 100x more expensive than strange mass*
  - *Common to all discretizations*

~ **Simulations at larger pion mass**



1st challenge: Fermions on the Lattice

$$\langle \mathcal{O} \rangle = \lim_{\cancel{\vec{\mu}_f \to \vec{m}_f}} \langle \mathcal{O} \rangle_{a,V,\vec{\mu}_f}$$ ✔

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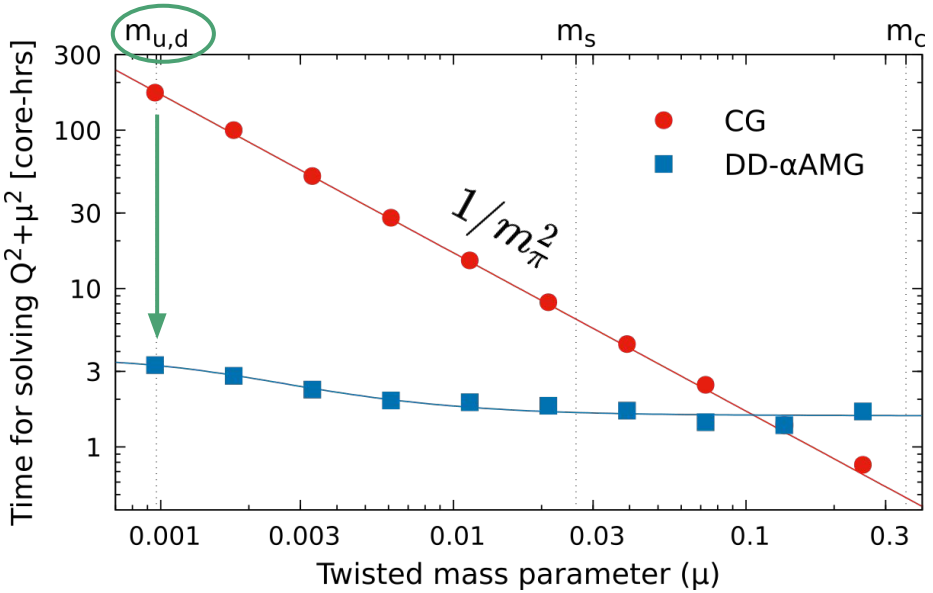
✓ **Resolved by multigrid methods**



1st Solution: Multigrid Solvers

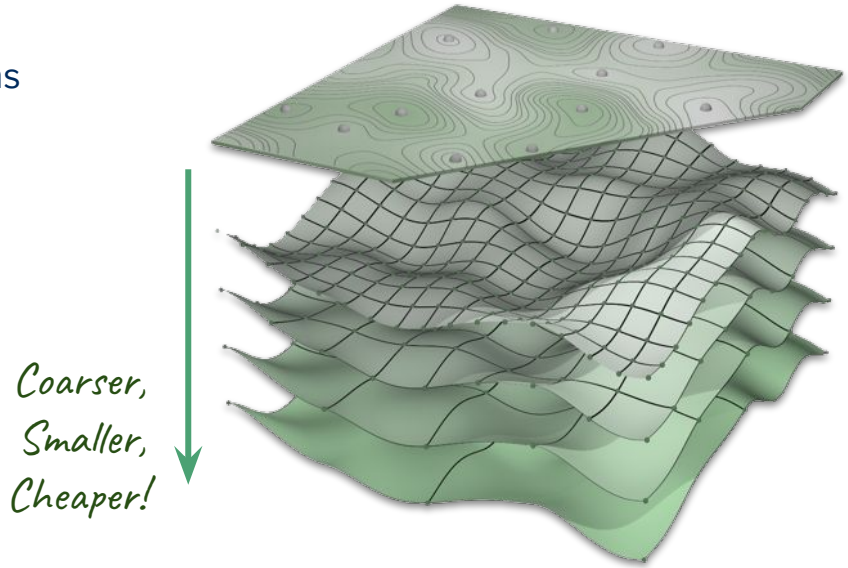
Idea: Use multiple layers of coarsening for accelerating the inversions.

On the coarse grid computations are less intensive and faster.

The goal is also to tackle errors of different wavelengths more effectively. Coarse grids reduce low-frequency errors, while fine grids refine the solution.

But in **Lattice QCD,** it took more than 20 years to develop a successful multigrid approach due to

- Highly oscillatory gauge fields
- Very ill-conditioned Dirac operator



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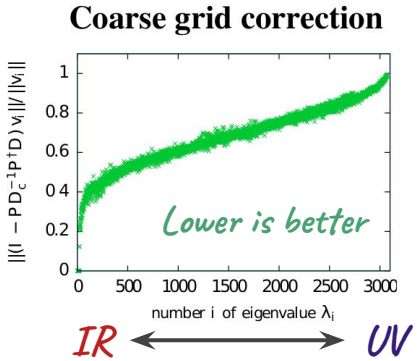
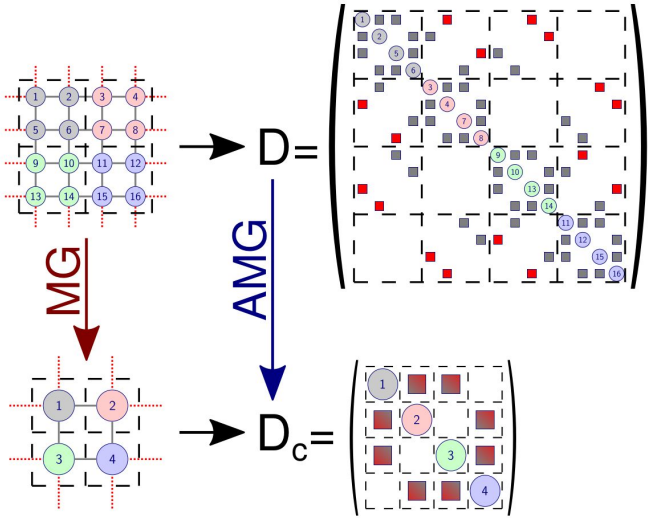
The coarse Dirac operator is define via algebraic approach: $D_c = RDP.$ [A. Frommer et al., 2013]

Information about the low-modes of the Dirac operator are preserved thanks to the property of **local coherence** [M. Lüscher, 2007]



$$P = \begin{pmatrix} \blacksquare & & \\ & \ddots & \\ & & \blacksquare \end{pmatrix}$$



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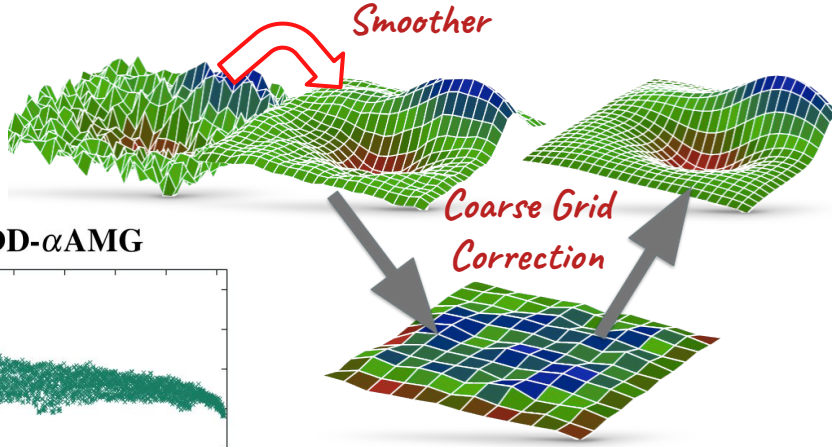
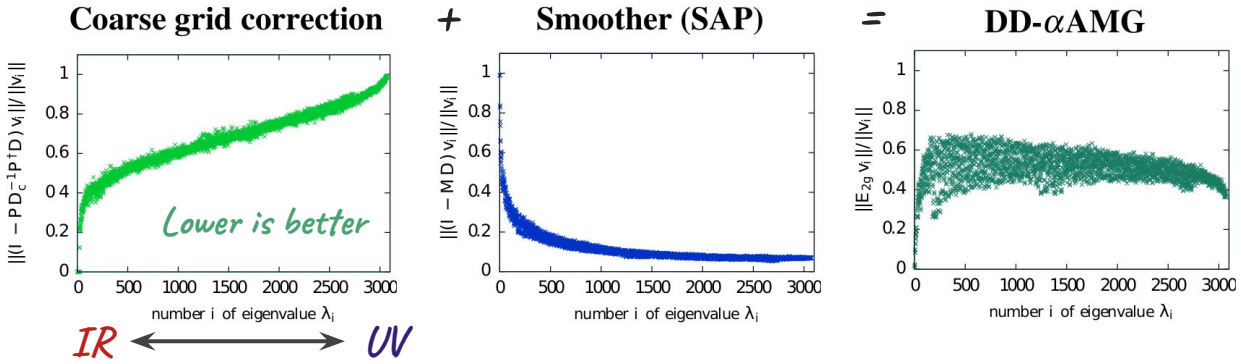
A **smoother (e.g. SAP)** is used to remove high-modes fluctuations on the fine grid.
The resulting **DD-αAMG** is efficient on all modes.





[C. Alexandrou, **S. B.**, *et al.*. "Adaptive Aggregation-based Domain Decomposition Multigrid for Twisted Mass Fermions". Phys.Rev.D 94 11, 114509, 2016]

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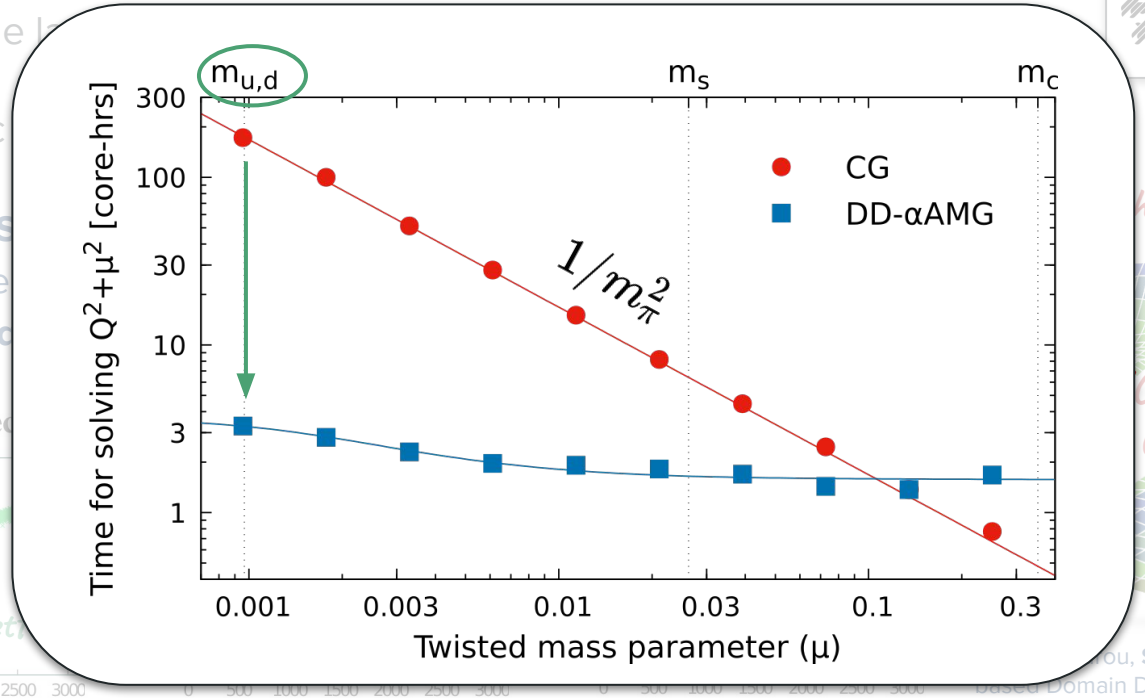

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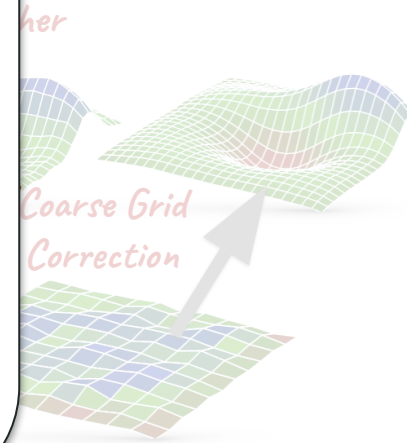

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How to simulate QCD? … many challenges!

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↳ Singularity at $\mu=0$

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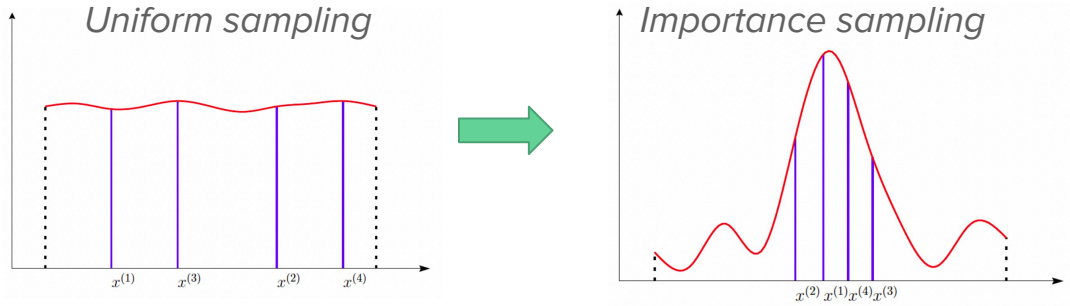
2. High-dimensional integral

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathrm{D}[U]\, \mathcal{O}(U)\, \exp(-S(U))$$

4x8xV dofs

→
- Importance Sampling and Hybrid Monte Carlo (HMC)

$$\langle \mathcal{O} \rangle = \frac{1}{N} \sum_i^N O(U_i) \quad \textit{with} \quad p(U) = \frac{1}{\mathcal{Z}} \exp(-S(U))$$



Metropolis algorithm and Hybrid Monte Carlo (HMC)

Metropolis algorithm:

1. Propose a new configuration with symmetric prob.: $P(U \to U') = P(U' \to U)$
2. Accept the new configuration with a prob.: $P_{\text{acc}}(U \to U') = \min[1, e^{-S(U')+S(U)}]$

➔ The resulting Markov chain is distributed with prob.: $P_{\text{eq.}}(U) = e^{-S(U)}$

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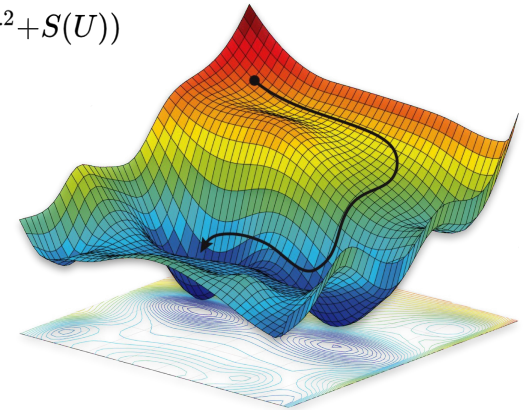
Hybrid (or Hamiltonian) Monte Carlo:

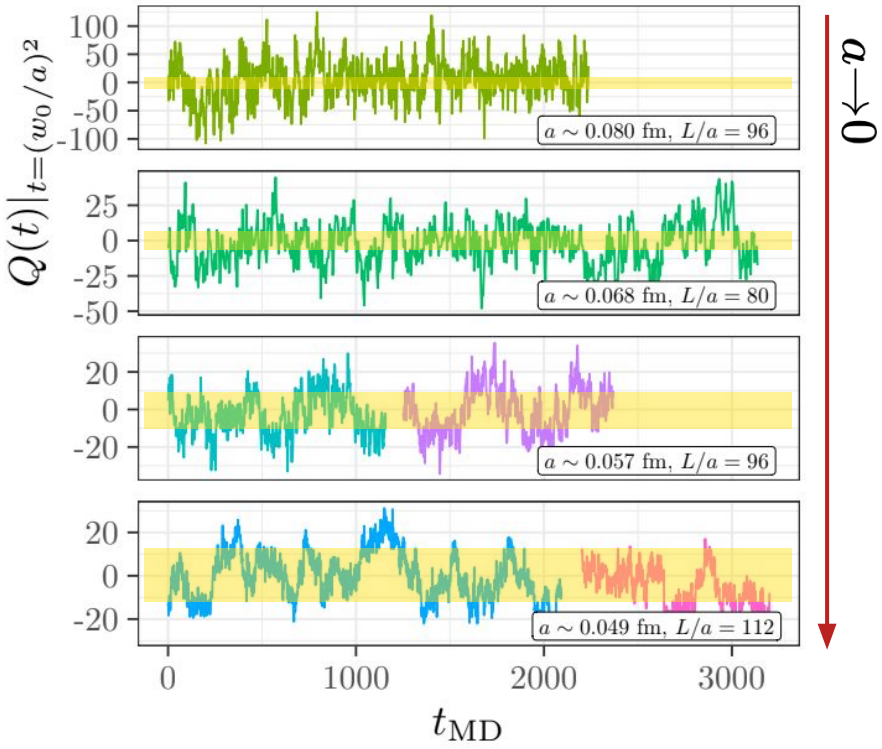
$$\frac{1}{\mathcal{Z}} \int D[U]^V \mathcal{O}(U)\, e^{-S(U)} \longrightarrow \frac{1}{\mathcal{Z}\mathcal{Z}_\pi} \int D[U]^V D[\pi]^V \mathcal{O}(U)\, e^{-(\pi^2+S(U))}$$

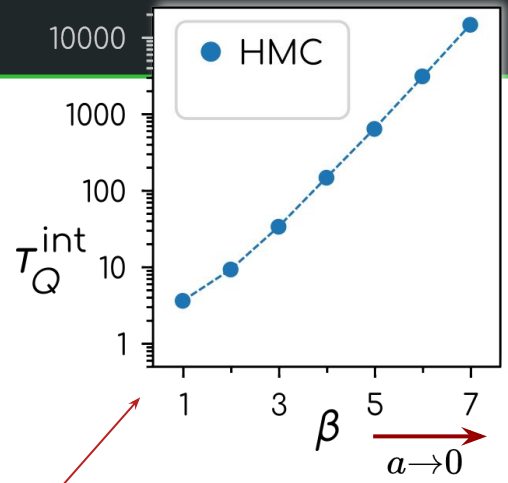
$$H(\pi, U) = \pi^2 + S(U) \xrightarrow[\text{MD}]{} H(\pi', U') = H(\pi, U)$$

$$\Longrightarrow \quad P_{\text{acc}}(\pi, U \to \pi', U') \equiv 1$$



Yet, another challenge: Critical slowing down





$$\langle \mathcal{O} \rangle = \frac{1}{N} \sum_i^N O(U_i)$$

$$\mathrm{Err}[\langle \mathcal{O} \rangle] = \sqrt{\frac{2\,\tau_{\mathrm{int}}\,\mathrm{Var}[\langle \mathcal{O} \rangle]}{N}}$$

$$\mathrm{Var}[\langle \mathcal{O} \rangle] = \langle \mathcal{O}^2 \rangle - \langle \mathcal{O} \rangle^2$$

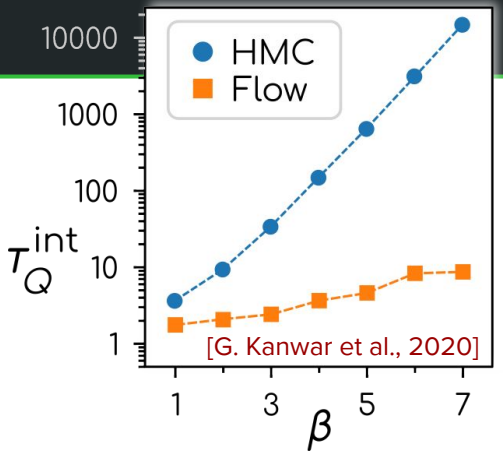
And a solution?! Generative flows

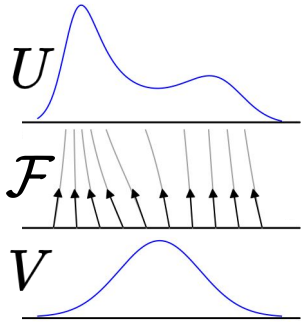
Ongoing research directions: *J. Finkenrath, Tuesday*

$$U = \mathcal{F}(V)$$

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int D[U]\, \mathcal{O}(U)\, e^{-S(U)}$$

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int D[V]\, \mathcal{O}(\mathcal{F}(V))\, e^{-S(\mathcal{F}(V)) + \log\det \mathcal{F}_*(V)}$$





If we find an $\mathcal{F}$ such that $S_{\mathcal{F}}(V) = S(\mathcal{F}(V)) - \log\det \mathcal{F}_*(V) = \text{const.}$

⇒ $\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int D[V]\, \mathcal{O}(\mathcal{F}(V))$ ⇒ V is uniformly distr.

Very promising! but also very challenging!!

... no applications yet beyond toy models (?)

How to simulate QCD? … many challenges!

$$\langle \mathcal{O} \rangle_{a,V,\vec{m}_f} = \frac{1}{\mathcal{Z}} \int D[U]^V \mathcal{O}(U)\, e^{-S(a,\vec{m}_f;U)}$$

$$\langle \mathcal{O} \rangle_{a,V,\vec{m}_f} = \frac{1}{N} \sum_i^N \mathcal{O}(U_i) \quad \text{with} \quad p(U) = \frac{1}{\mathcal{Z}} e^{-S(a,\vec{m}_f;U)}$$

1. ✔ Simulating fermions (at light mass)

$$\langle \mathcal{O} \rangle = \lim_{\vec{\mu}_f \to \vec{m}_f} \langle \mathcal{O} \rangle_{a,V,\vec{\mu}_f}$$

- Krylow solvers and Multigrid methods

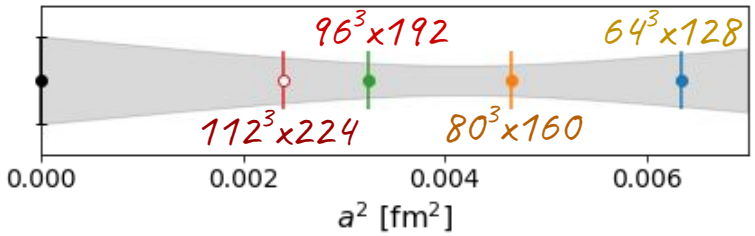
  E.g. DD-αAMG developed by BUW

2. ✔ High-dimensional integral

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathrm{D}[U]\, \mathcal{O}(U)\, \exp(-S(U))$$

- Importance Sampling and Hybrid Monte Carlo (HMC)

$$\langle \mathcal{O} \rangle = \frac{1}{N} \sum_i^N O(U_i) \;\; \textit{with} \;\; p(U) = \frac{1}{\mathcal{Z}} \exp(-S(U))$$



We can simulate lattice spacings between 0.09 fm to 0.05 fm.

Sufficient for current accuracy since discretization effects are $O(a^2)$

How to simulate QCD? … many challenges!

$$\langle \mathcal{O} \rangle_{a,V,\vec{m}_f} = \frac{1}{N} \sum_i^N \mathcal{O}(U_i) \quad \text{with} \quad p(U) = \frac{1}{\mathcal{Z}} e^{-S(a,\vec{m}_f;U)}$$

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3. Continuum and infinite volume limit
$$\langle \mathcal{O} \rangle = \lim_{a \to 0\; V \to \infty} \langle \mathcal{O} \rangle_{a,V}$$
→
- High-Performance Computing
  Parallelizable and scalable problem

$$V = L^4 \quad \& \quad a\,L = \text{const}$$

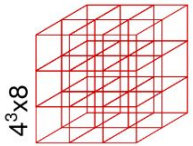


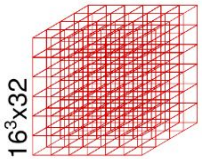
50 year of using HPC in Lattice QCD



K. G. Wilson
1974

1980 1990 2000 2010 2020

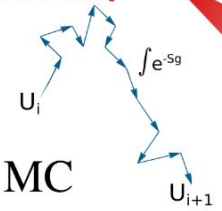




$$\langle \mathcal{O} \rangle_{a,V,\vec{\mu}_f} = \frac{1}{\mathcal{Z}} \int \mathrm{D}[U]^V \, \mathrm{D}[\psi\bar{\psi}]^{V n_f} \, \mathcal{O}(U,\psi,\bar{\psi}) \, e^{-S(a,\vec{\mu}_f;U,\psi,\bar{\psi})}$$

N_f=0 quenched
[Creutz 1980]

Algorithms



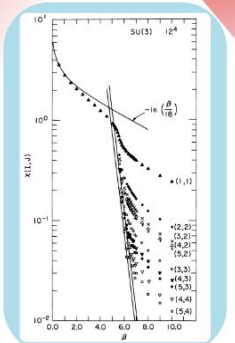
Machines



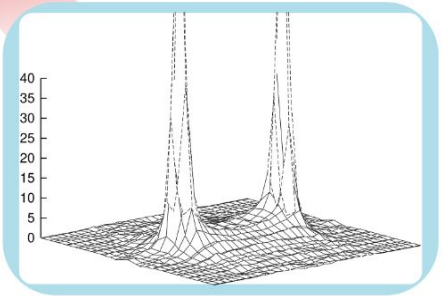
QCDPAX
12.5 GFlops



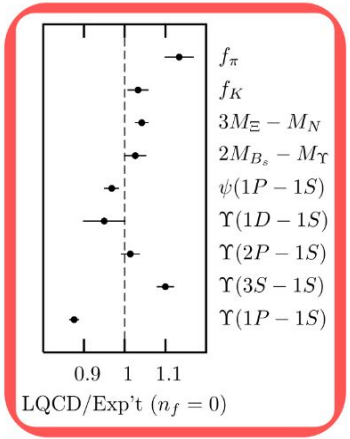
APE100
6.4 GFlops



[Barkai et al. 1984]



[Bali et al. 1994]



50 year of using HPC in Lattice QCD



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1980 1990 2000 2010 2020

4^3x8 16^3x32 28^3x28

N_f=0 quenched [Creutz 1980]

N_f=2 u,d

Algorithms

MC: U_i → U_{i+1}, $\int e^{-Sg}$

HMC: U_t → $U_{t+\tau}$, $\int \det(D^2)\, e^{-Sg}$, $\delta\tau$

Machines



APE100
6.4 GFlops



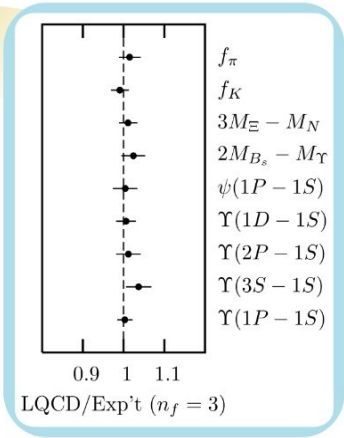
QCDPAX
12.5 GFlops



CP-PACS
600 GFlops



QCDOC
10 TFlops

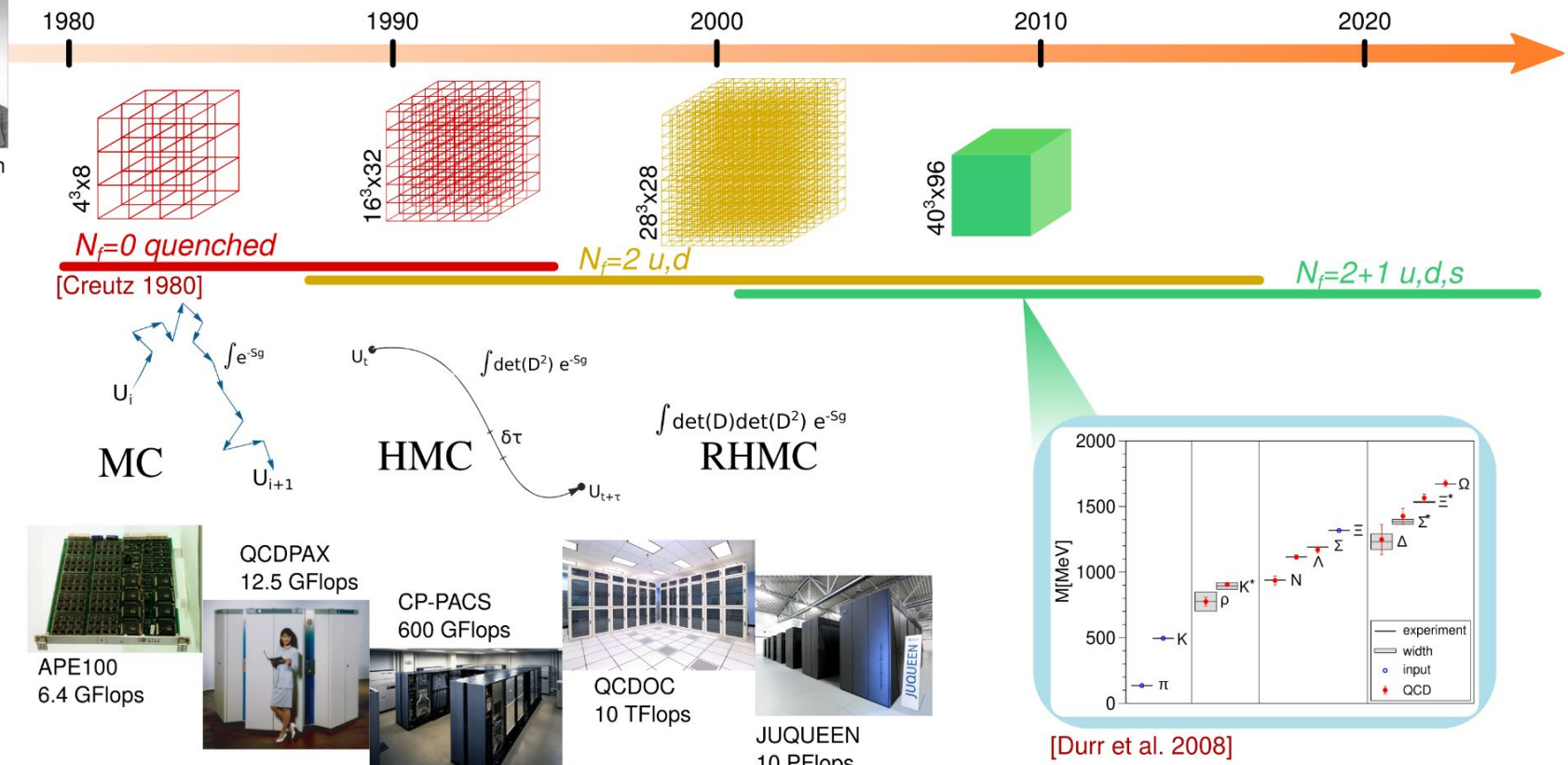


[Davies et al. 2004]

50 year of using HPC in Lattice QCD



K. G. Wilson
1974



[Durr et al. 2008]

50 year of using HPC in Lattice QCD



K. G. Wilson
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1980 1990 2000 2010 2020

4^3x8 16^3x32 28^3x28 40^3x96 64^3x128

N_f=0 quenched
[Creutz 1980]

N_f=2 u,d

N_f=2+1 u,d,s

N_f=2+1+1 u,d,s,c

Algorithms

MC

HMC

RHMC

AMG

Machines

APE100
6.4 GFlops

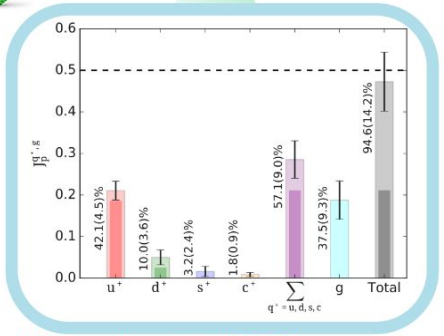
QCDPAX
12.5 GFlops

CP-PACS
600 GFlops

QCDOC
10 TFlops

JUQUEEN
10 PFlops

Summit
200 PFlops



[Alexandrou et al. 2020]

50 year of using HPC in Lattice QCD



K. G. Wilson
1974

1980 1990 2000 2010 2020

4^3x8 16^3x32 28^3x28 40^3x96 64^3x128 128^3x256

N_f=0 quenched
[Creutz 1980]

N_f=2 u,d

N_f=2+1 u,d,s

N_f=2+1+1 u,d,s,c

Algorithms

U_i $\int e^{-Sg}$ U_{i+1}
MC

U_t $\int \det(D^2)\, e^{-Sg}$ $\delta\tau$ $U_{t+\tau}$
HMC

$\int \det(D)\det(D^2)\, e^{-Sg}$
RHMC

AMG

$r(z)$ g_1^{-1} ... g_l^{-1}
ML

Machines



APE100
6.4 GFlops



QCDPAX
12.5 GFlops



CP-PACS
600 GFlops



QCDOC
10 TFlops



JUQUEEN
10 PFlops



Summit
200 PFlops



LUMI
400 PFlops

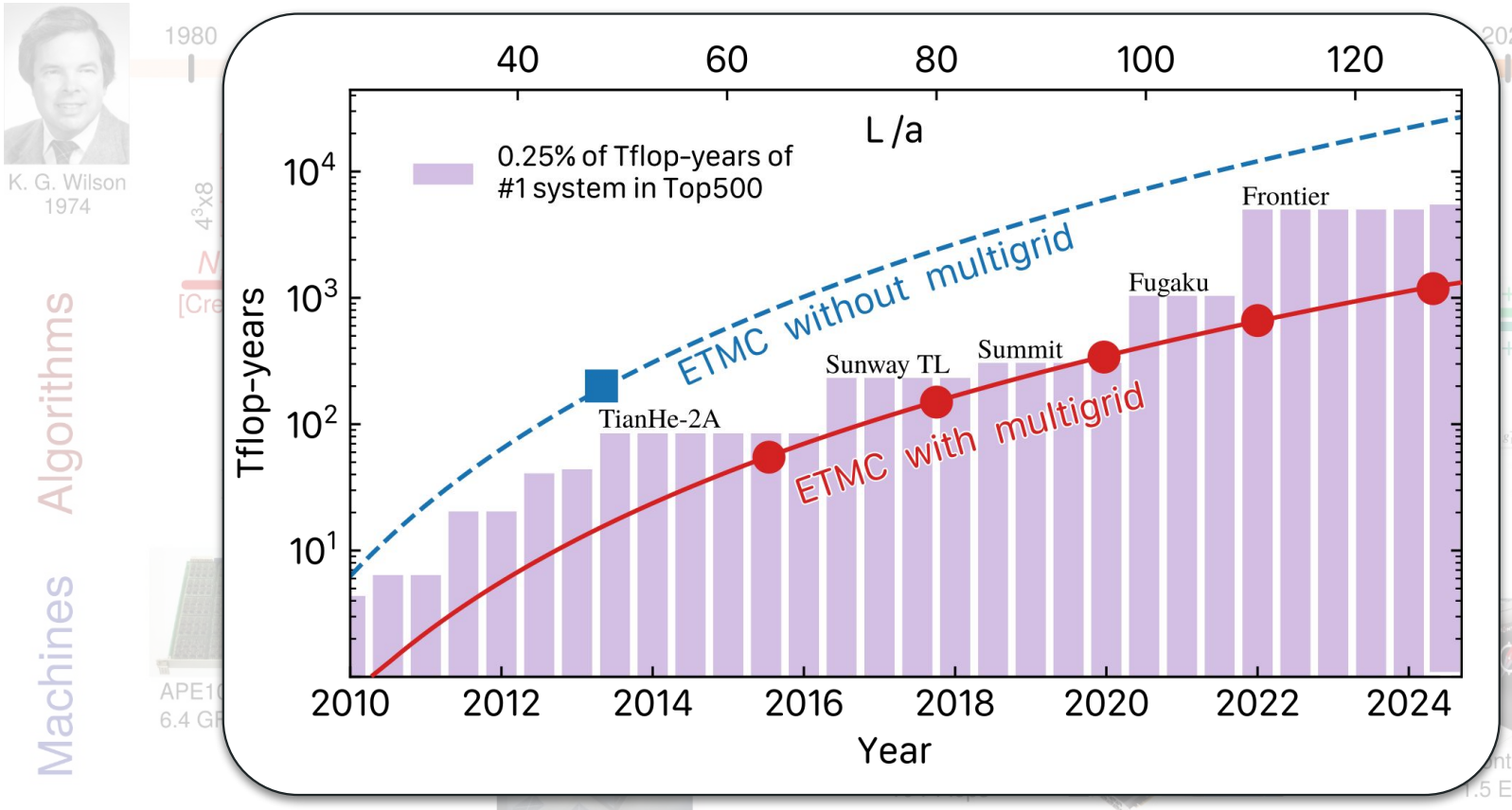


Frontier
1.5 EFlops



IBM
400 Qubits

50 year of using HPC in Lattice QCD



How to simulate QCD? … many challenges!

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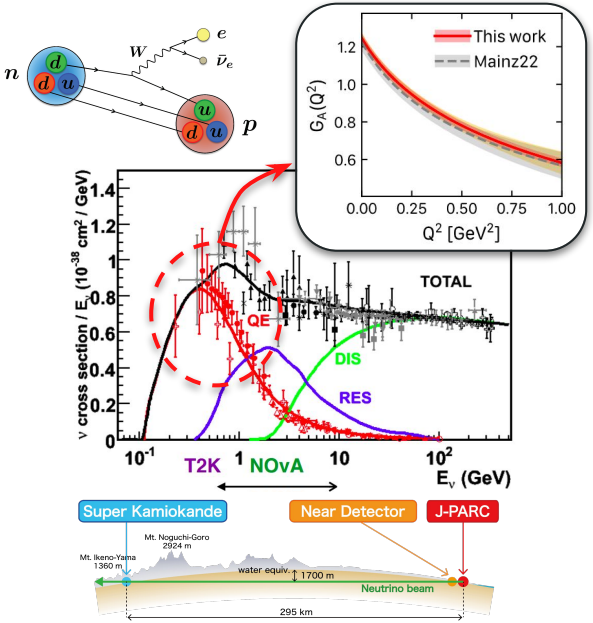
$$\langle \mathcal{O} \rangle = \lim_{a \to 0\ V \to \infty} \langle \mathcal{O} \rangle_{a,V}$$
→ High-Performance Computing
Parallelizable and scalable problem

4. High-precision results
$\langle \mathcal{O} \rangle = \lim_{N \to \infty} \frac{1}{N} \sum_i^N \mathcal{O}(U_i)$
→ Noise reduction techniques
E.g. low-mode averaging

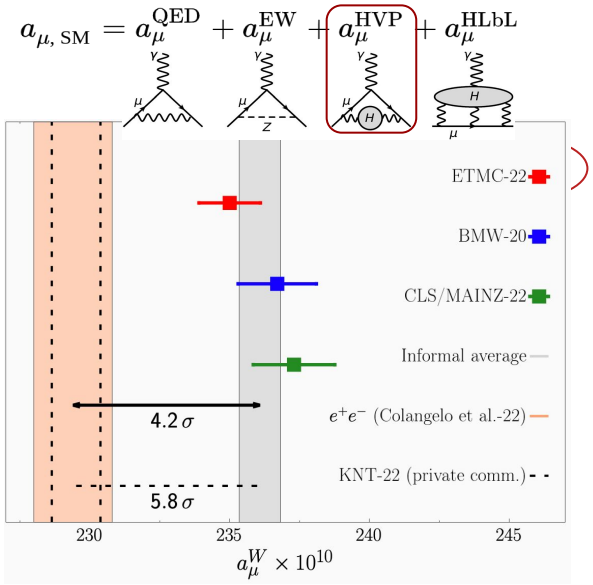
Main Research Directions

Input to Experiments & Complementary Results



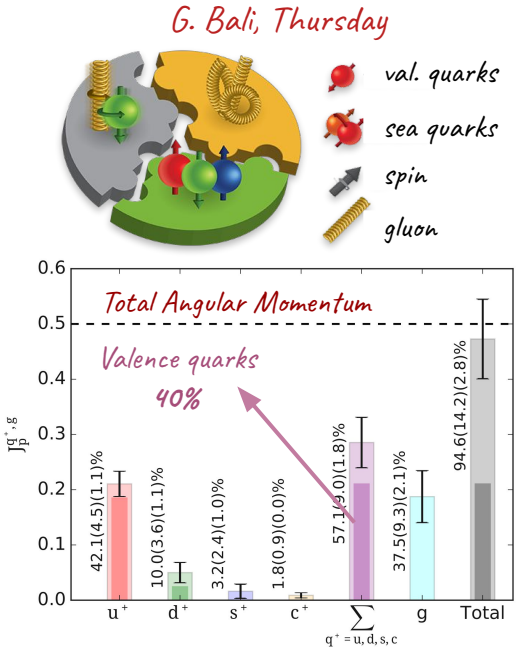
[C. Alexandrou, **S. B.**, et al. "Nucleon axial and pseudoscalar form factors using twisted-mass fermion ensembles at the physical point". Phys. Rev., D109(3), 2024]

Precision Physics & Searches for New Physics



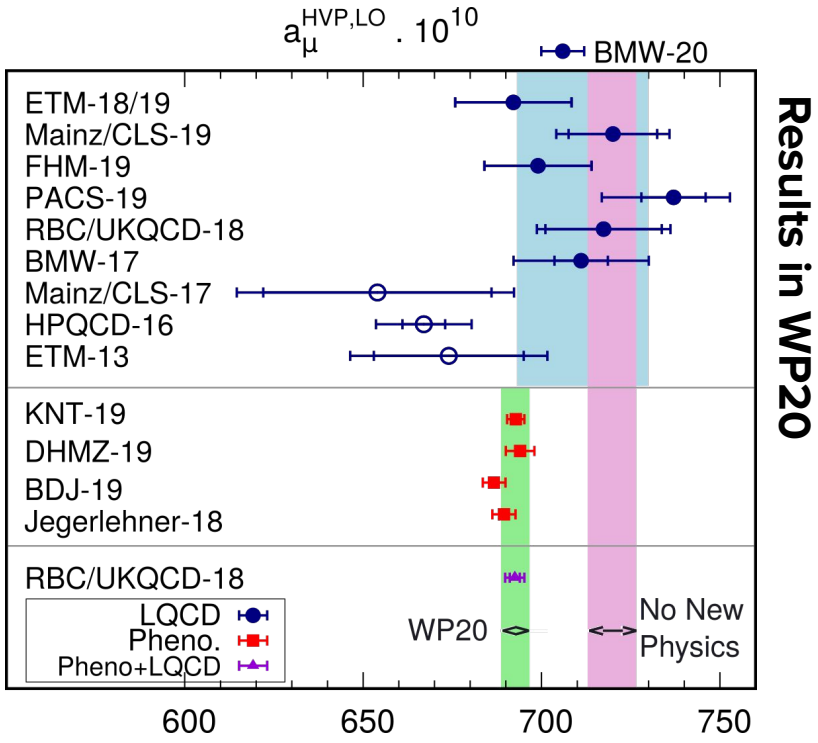
[C. Alexandrou, **S. B.**, et al. "Lattice calculation of the short and intermediate time-distance hadronic vacuum polarization contributions to the muon...". Phys. Rev., D107(7), 2023]

Revealing Nucleon Structure & Constituents of Matter

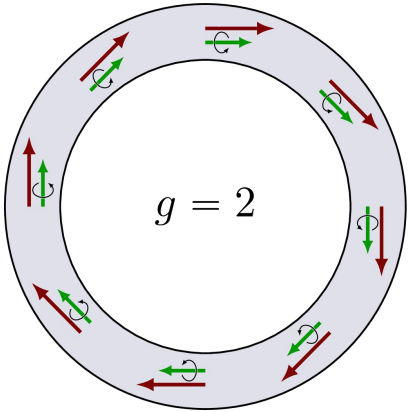


[C. Alexandrou, **S. B.**, et al. "Complete flavor decomposition of the spin and momentum fraction of the proton using lattice QCD simulations at physical pion mass". Phys. Rev., D101(9), 2021]

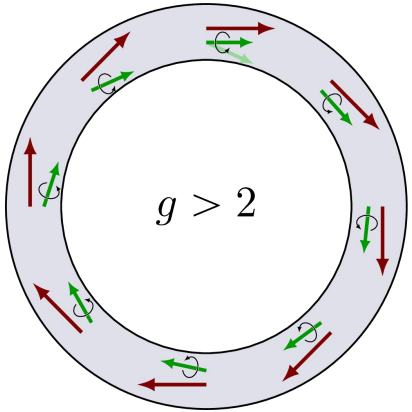
Example Muon g-2 Anomaly



Results in WP20



$\odot\, \mathbf{B}$



A. Evangelista, Thursday

$$a = \frac{g-2}{2}$$

$$a_{\mu,\,\mathrm{exp}} = 0.001\,165\,920\,61(41)$$

$$a_{\mu,\,\mathrm{SM}} = 0.001\,165\,918\,10(43)$$

Challenge: Large-Distance Correlation

The correlation function between two electromagnetic currents:

$$C_{2pt}(t) \equiv \langle J_{em}(t) J_{em}(0) \rangle = \langle J_{em} | T^t | J_{em} \rangle = \sum_n \underbrace{\langle J_{em} | n \rangle \langle n | J_{em} \rangle}_{\sim \text{HVP} \sim \ \rho^{\text{HVP}}(\omega)} e^{-E_n t}$$

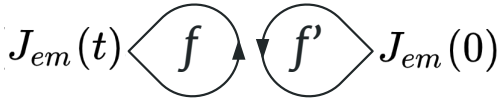
$T^t \to e^{-H}$

→ Exponential suppression!

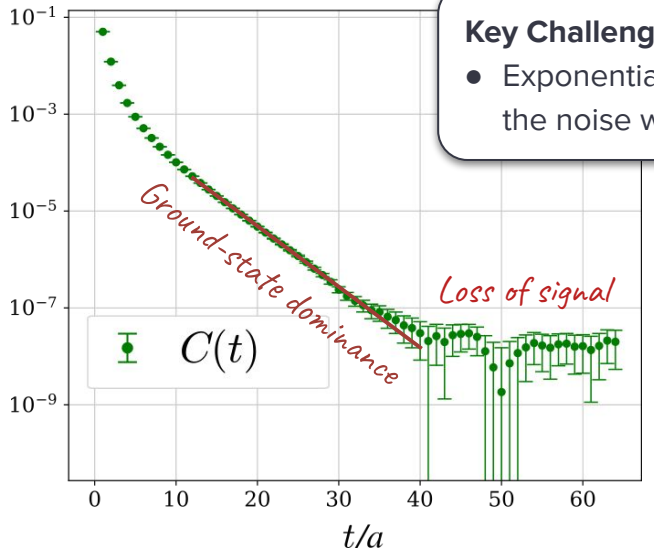
$$J^i_{\text{em}} = \frac{2}{3}\bar{u}\gamma^i u - \frac{1}{3}\bar{d}\gamma^i d - \frac{1}{3}\bar{s}\gamma^i s + \frac{2}{3}\bar{c}\gamma^i c$$



Connected



Disconnected



Key Challenge:

- Exponential growth of the noise with distance

Key technique: Low-Mode Averaging (LMA)

Concept: Low-modes dominate at large distance in correlation functions!

IR contribution

UV contribution

$$S_r(x,y) = |P_{\mathrm{IR}} Q_r^{-1} P_{\mathrm{IR}} \eta(x)\rangle \langle \eta(y)| \gamma_5 + |P_{\mathrm{UV}} Q_r^{-1} P_{\mathrm{UV}} \eta(x)\rangle \langle \eta(y)| \gamma_5$$

Quark Propagator

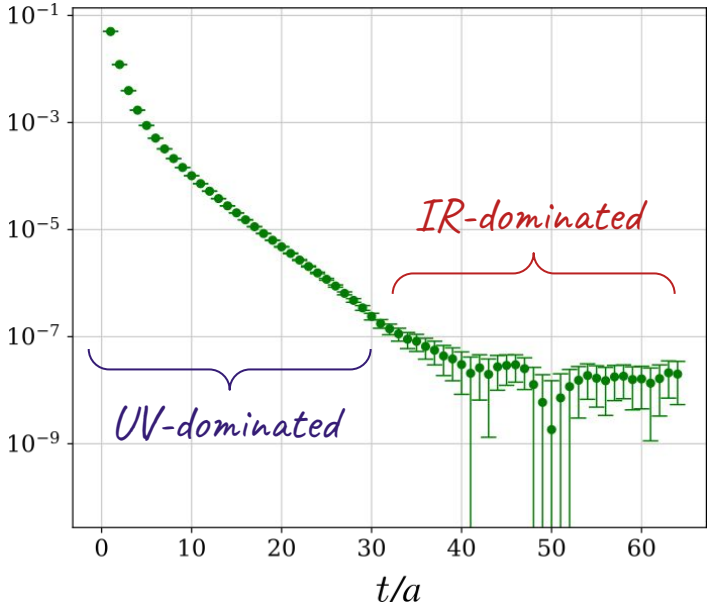
$$= \sum_{j=1}^{K} \frac{|v_j(x)\rangle \langle v_j(y)| \gamma_5}{\lambda_j + i r \mu} + \frac{1}{N} \sum_{\eta} |\widetilde{\phi}_r^{\eta}(x)\rangle \langle \eta(y)| \gamma_5 \Big|_{N \gg 1} ,$$

Computed Exactly

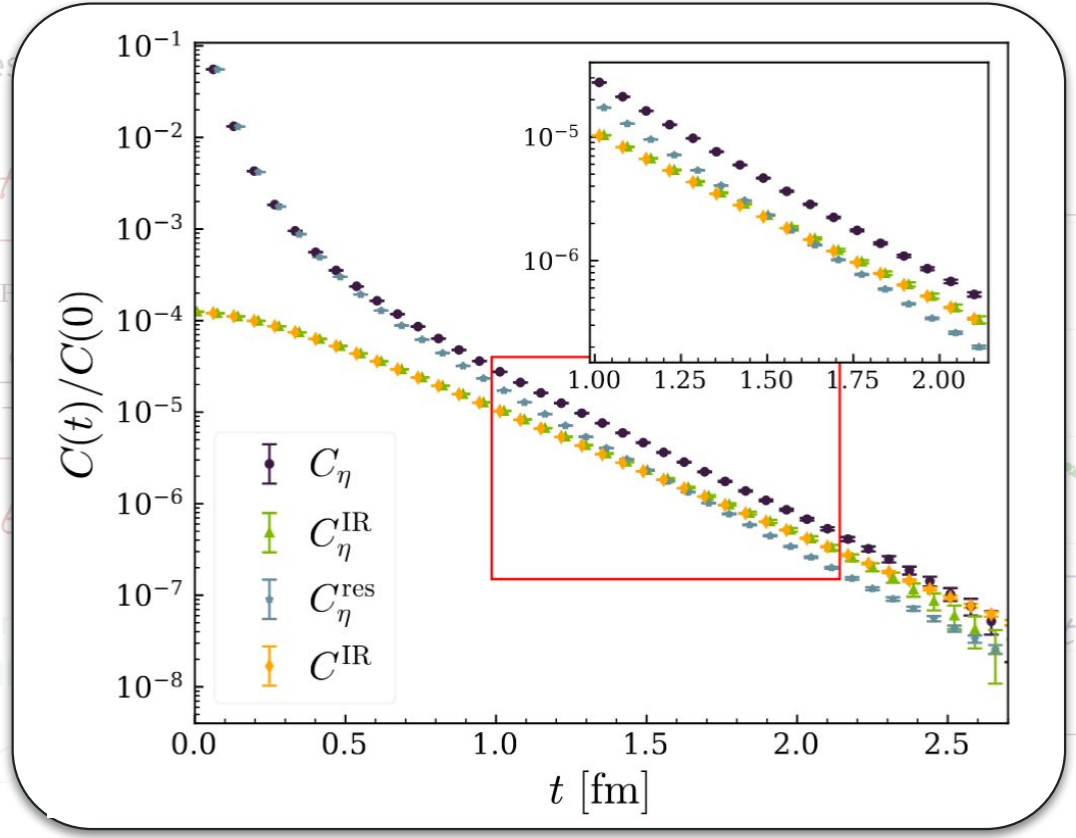
Computed Stochastically

- In the correlation function computed stochastically, we replace the IR part with an **exact** knowledge of it

$$C_{\mathrm{LMA}}(t) = C_{\mathrm{stoch.}}(t) - C^{\mathrm{IR}}_{\mathrm{stoch.}}(t) + C^{\mathrm{IR}}_{\mathrm{exact.}}(t)$$



Key technique: Low-Mode Averaging (LMA)



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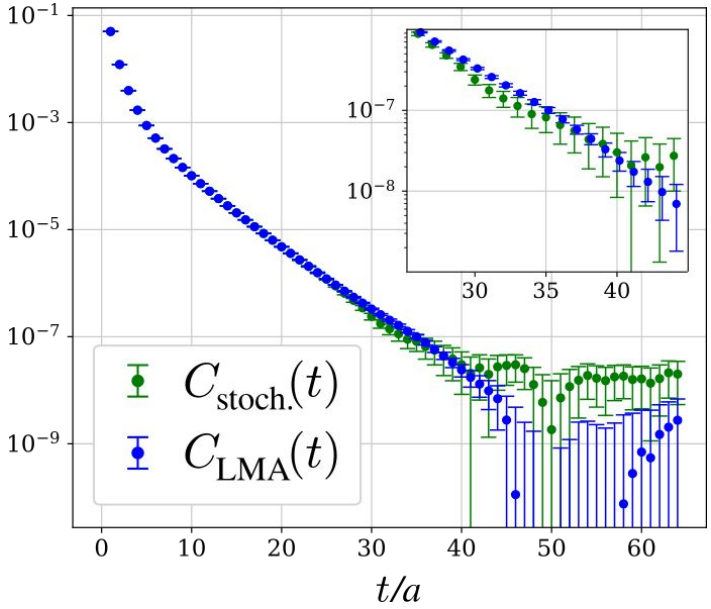

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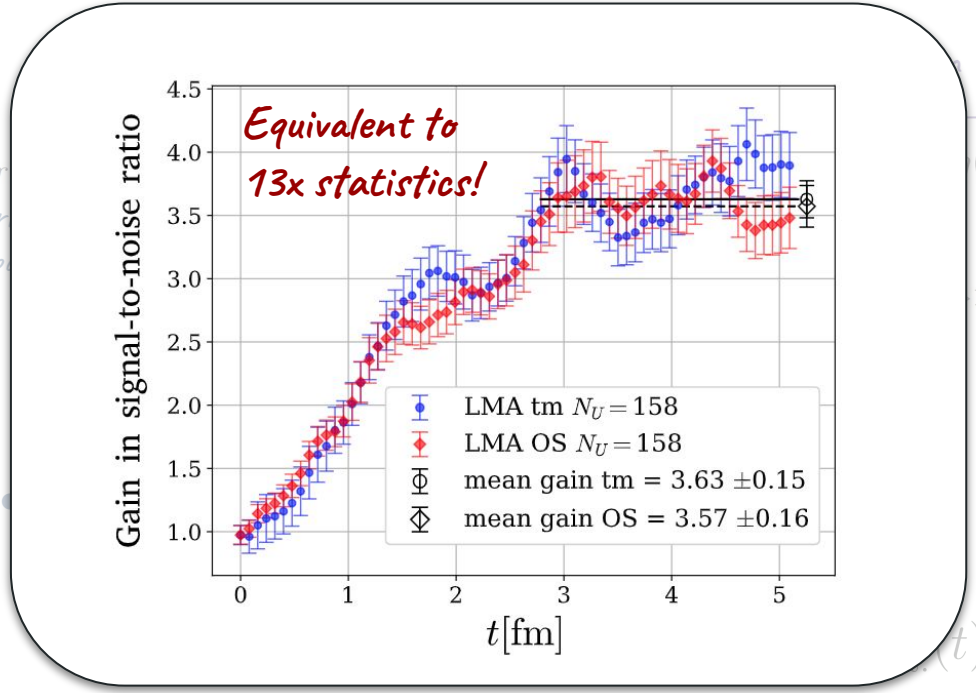
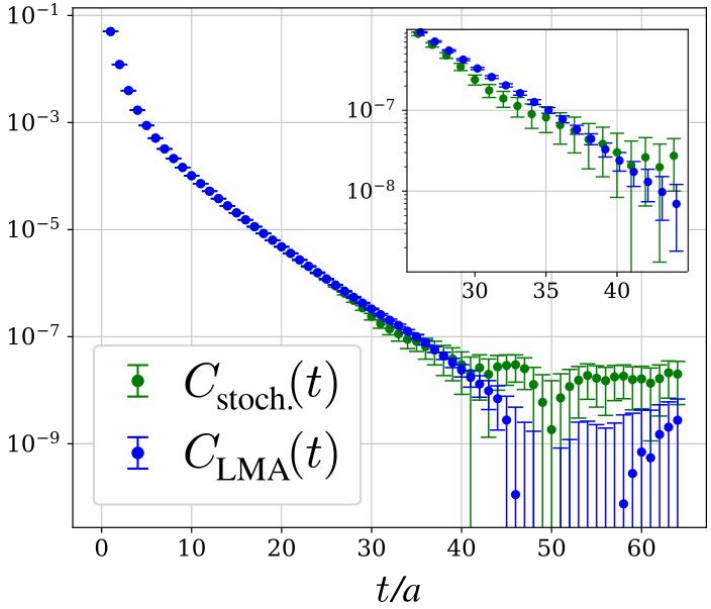
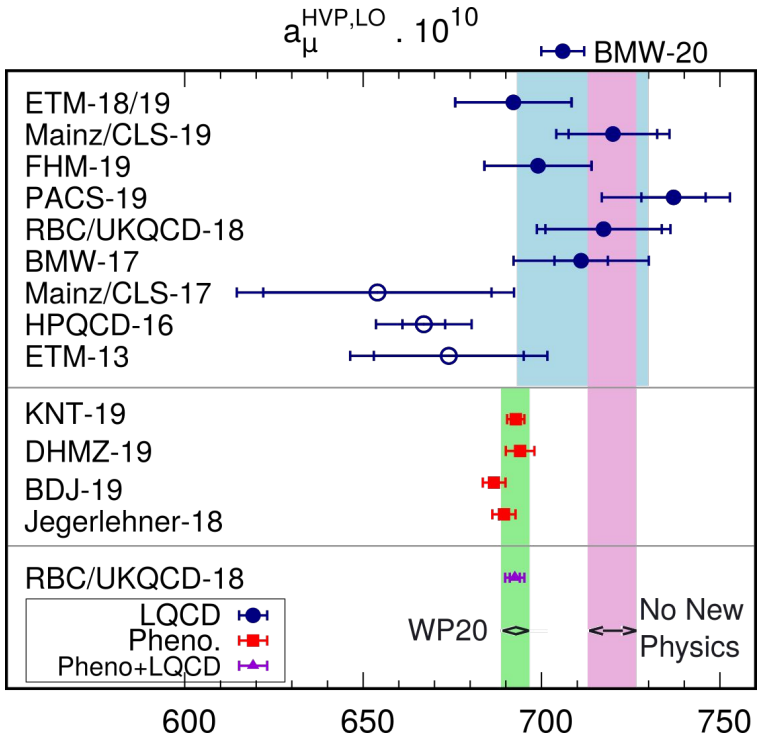




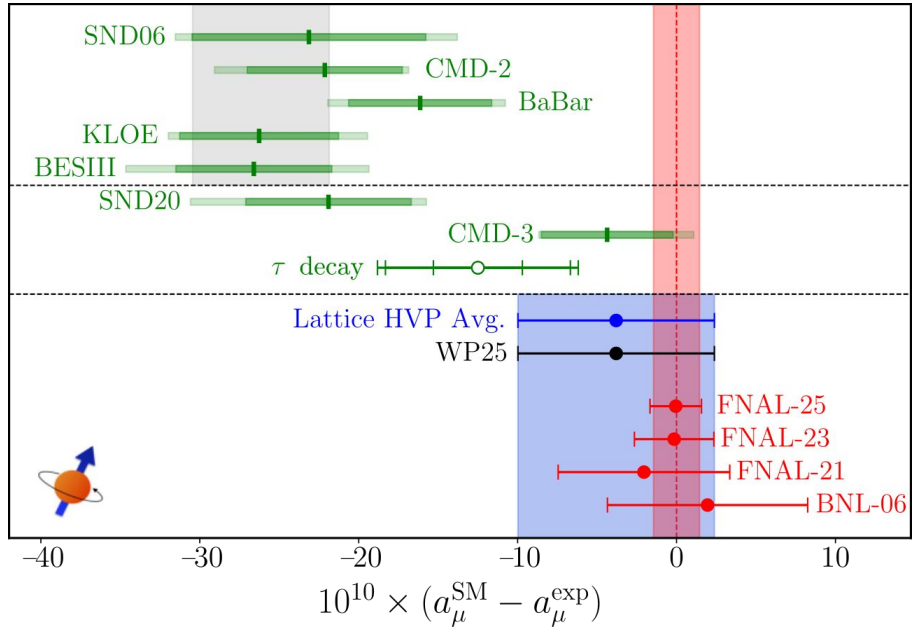
From Anomaly to Agreement



Results in WP20

- **BMW20:** first precise lattice QCD calculation [Sz. Borsanyi *et al.*, 2020]

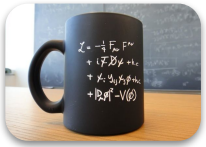
Results in WP25

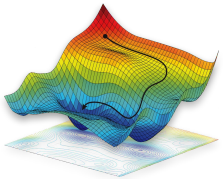


Summary

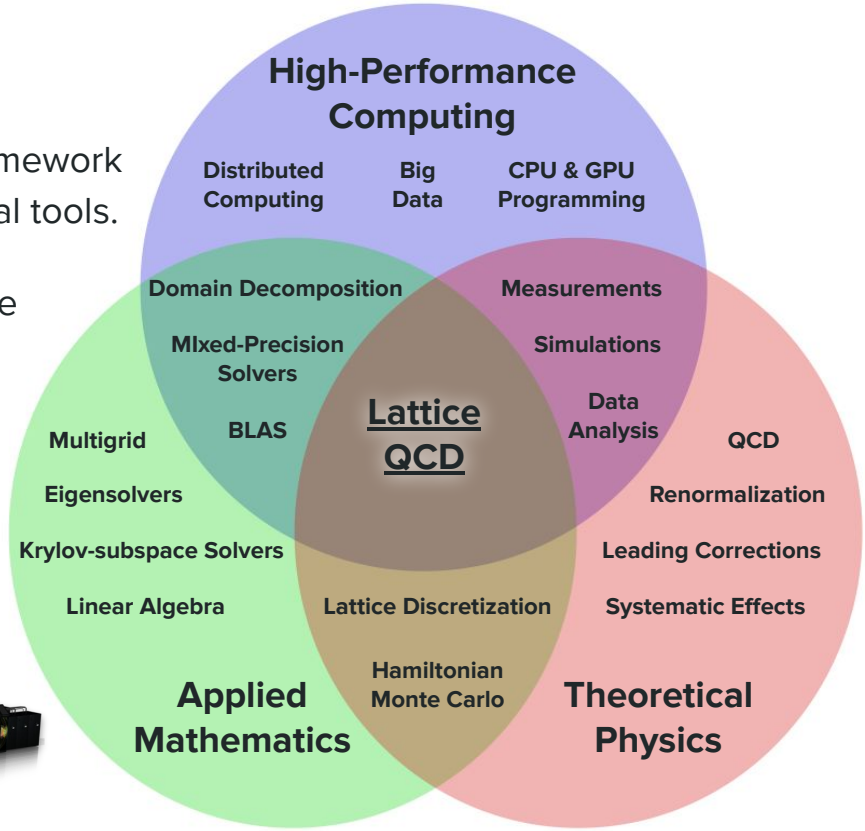
Lattice QCD is a highly interdisciplinary field!

- **Theoretical Physics:** Provides the fundamental framework and principles, quantum field theory, and theoretical tools.
- **High-Performance Computing:** Enables large-scale numerical simulations of quark and gluon interactions on discretized space-time lattices.
- **Applied Mathematics:** Develops and refines algorithms and numerical methods essential for accurate and efficient lattice QCD computations.





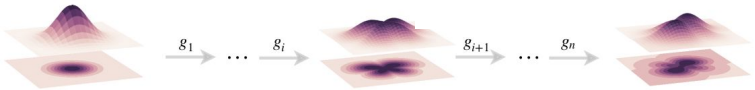




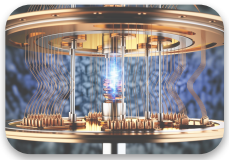
Future Directions

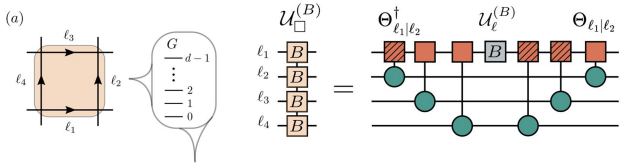
New technologies ➜ New Solutions!

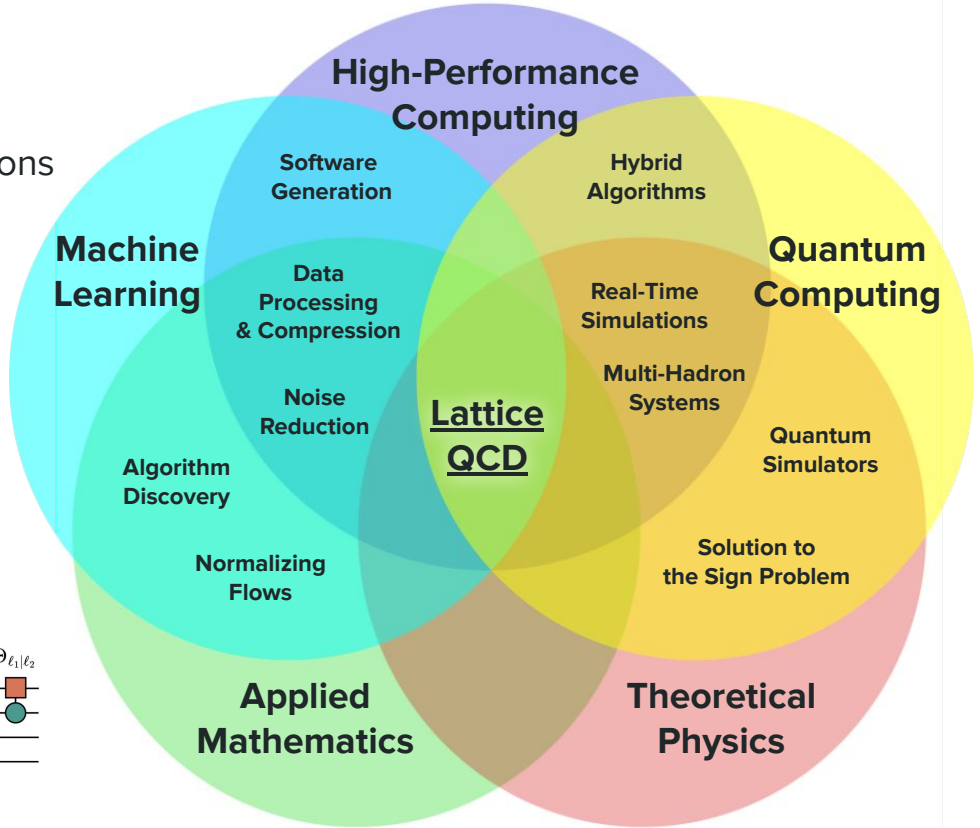
- **Machine Learning:** Aims to accelerate simulations and improve data analysis by optimizing algorithms and extracting patterns from data.



- **Quantum Computing:** Offers the potential to simulate quantum field theories more naturally and efficiently than classical methods.







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Thank you for your attention!



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