ETH zürich

Institute for Theoretical Physics, HPCP lab

Introduction to Lattice QCD

Prof. Marina Krstic Marinkovic, ETH Zurich

11-22 July 2022, NNPSS, MIT

Part 3:
Lattice QCD phenomenology: selected results and challenges

The cost of dynamical fermions

$$\langle O[\psi, \overline{\psi}, U] \rangle = \frac{1}{Z} \int \mathcal{D}\, U \; e^{-S_G[U]} \, \underline{[det\,(\gamma_\mu D_\mu + m_q)]}^{N_f} \; O[\psi, \overline{\psi}, U]$$

$$\int \mathcal{D}\, \phi \; \mathcal{D}\, \phi^\dagger \; e^{-\phi^\dagger \, (D^\dagger(m_q) D(m_q))^{-1} \, \phi} \quad \propto \quad \underline{[det\,(\gamma_\mu D_\mu + m_q)]^2}$$

- Determinant: non-local object on the lattice —> virtually impossible to compute exactly!

- Computational cost of solving:

$$\chi = (\gamma_\mu D_\mu + m_q)^{-1} \Phi$$

grows for: small quark masses m_q, and large $\dfrac{L}{a}$

- $k = \text{cond}\,(M) \;\; \propto \;\; \dfrac{\lambda_{max}}{\lambda_{min}}$

The cost of dynamical fermions

$$\langle O[\psi, \overline{\psi}, U] \rangle = \frac{1}{Z} \int \mathcal{D}\, U\, \mathcal{D}\, \phi\, \mathcal{D}\, \phi^\dagger\ e^{-S_G[U] - \phi^\dagger\ (D^\dagger(m_q) D(m_q))^{-\frac{N_f}{2}}\ \phi}\ O[U, \phi, \phi^\dagger]$$

$$\int \mathcal{D}\, \phi\, \mathcal{D}\, \phi^\dagger\ e^{-\phi^\dagger\ (D^\dagger(m_q) D(m_q))^{-1}\ \phi} \quad \propto \quad [det\,(\gamma_\mu D_\mu + m_q)]^2$$

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The cost of dynamical fermions

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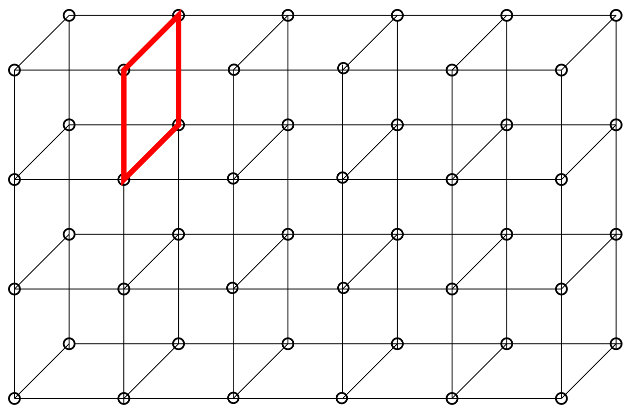
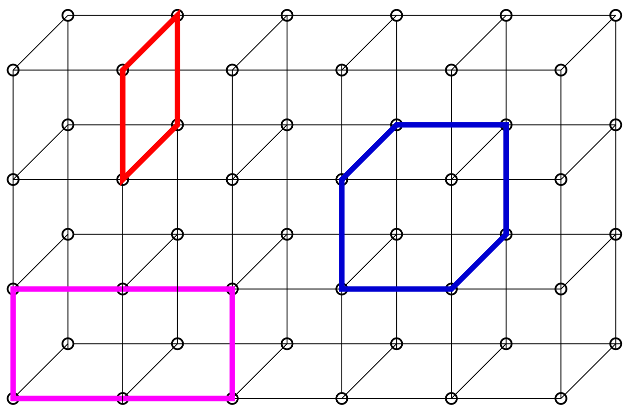
S_G Wilson



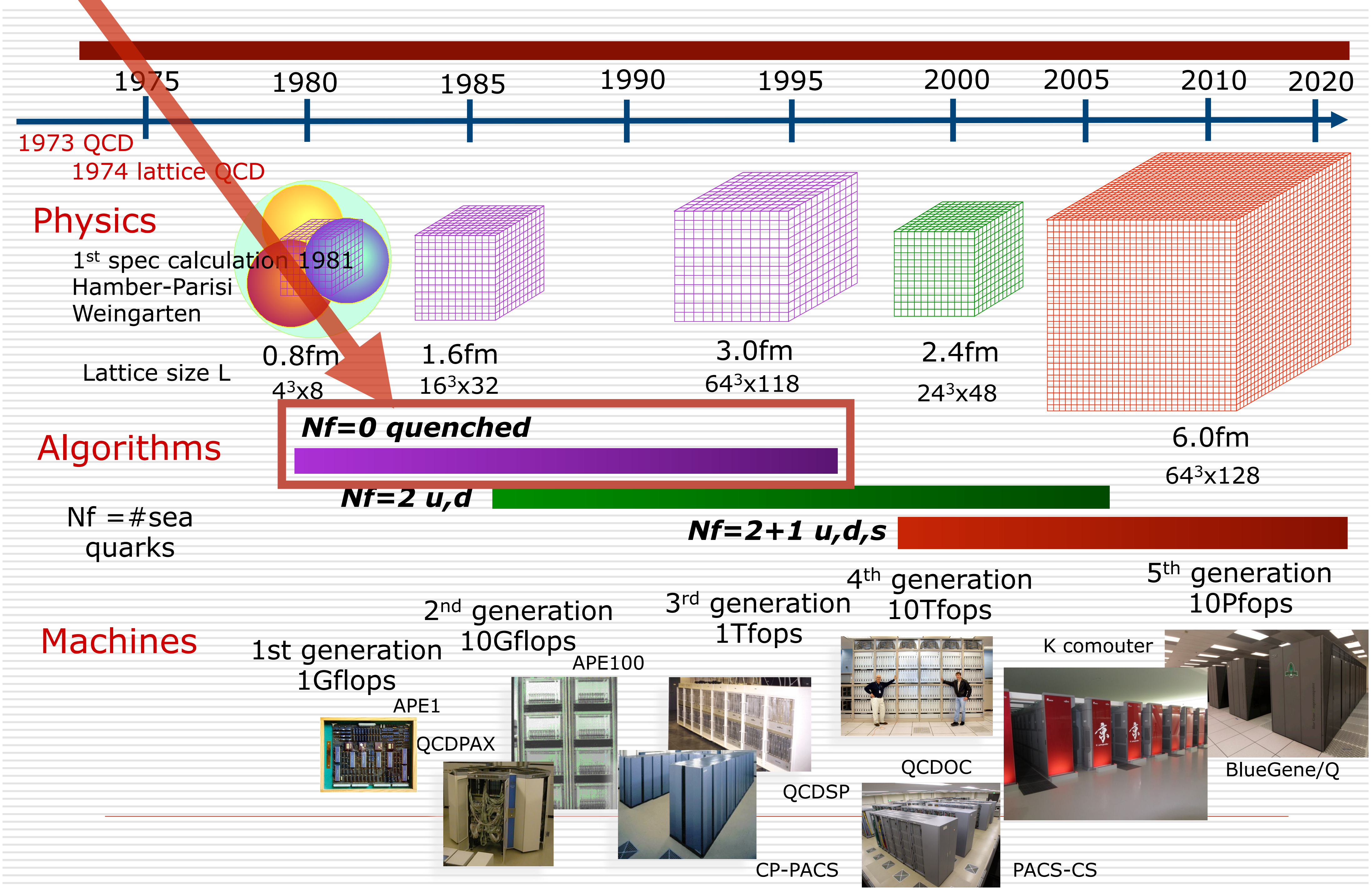
Luscher-Weisz



- Local objects: plaquettes, extended plaquettes (rectangles, chairs …)
- Rate of convergence towards continuum limit: $O(a), O(a^2), \ldots$
- Monte Carlo algorithms with local updates sufficient in the approximation: $\boxed{\det\,(\gamma_\mu D_\mu + m_q) \equiv 1}$

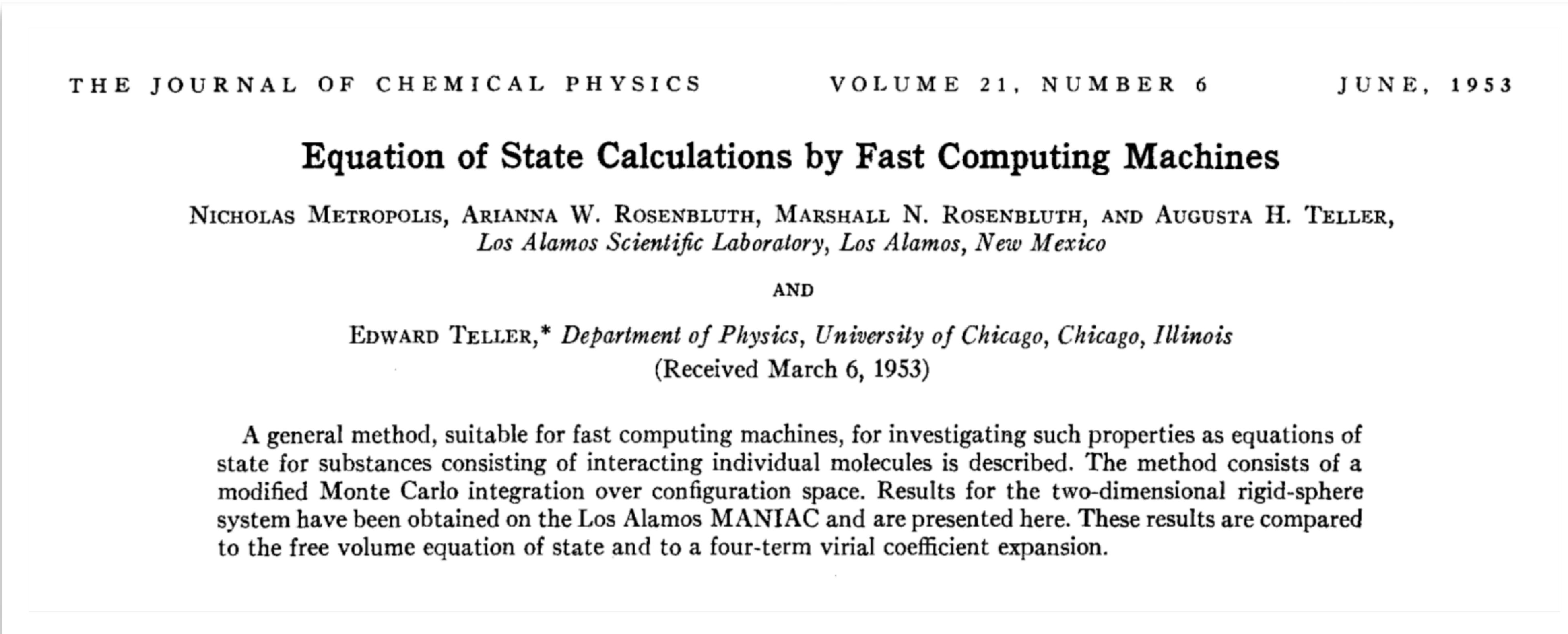
Development of Lattice QCD

$$\det(\gamma_\mu D_\mu + m_q) \equiv 1$$



[Credit: A. Ukawa, HPC Summer School (2013)]

The Metropolis algorithm



THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

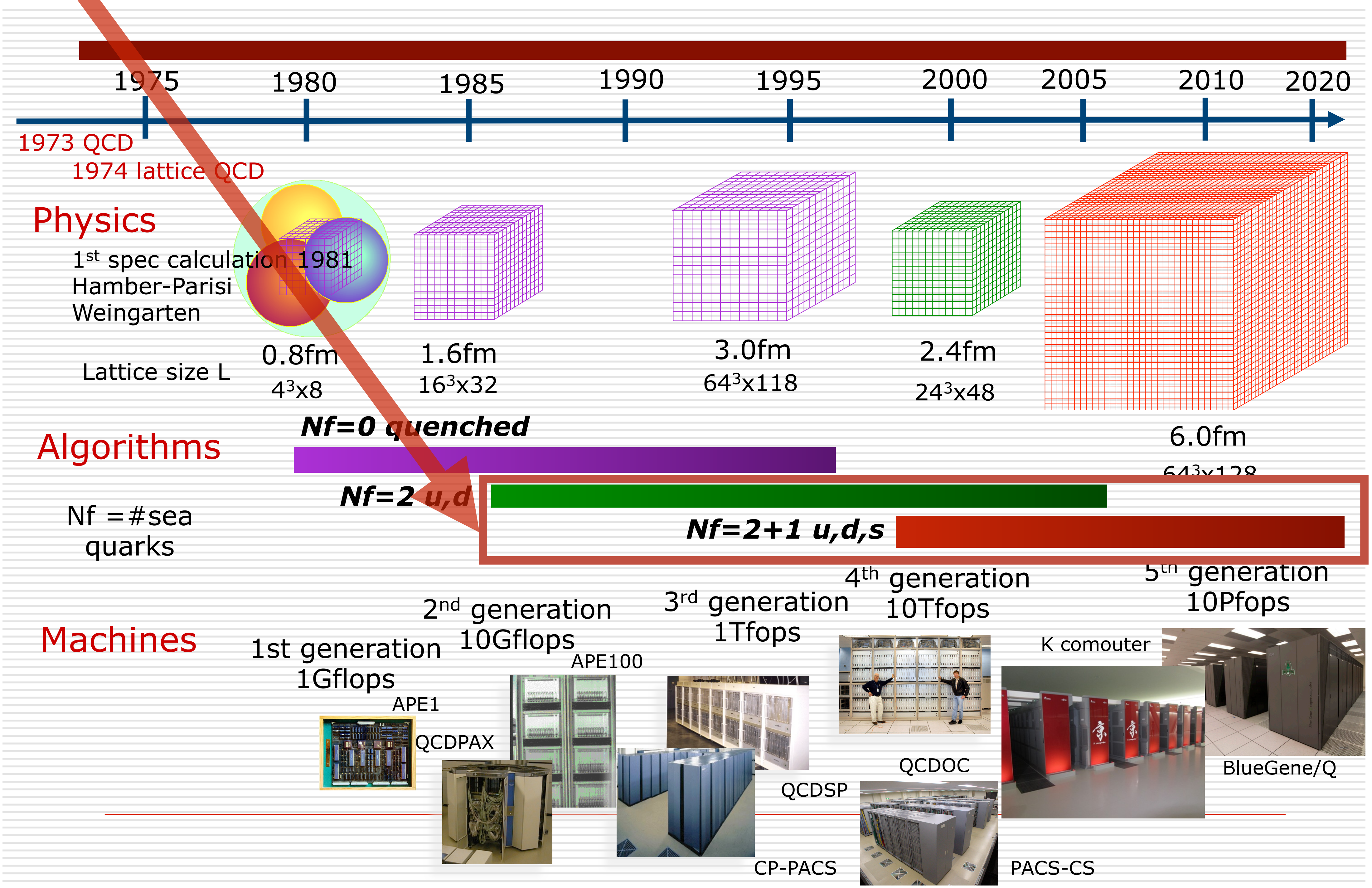
A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

- The Metropolis Algorithm:
- Given $\{U\}$, propose $\{U'\}$ in a reversible, area-preserving way
- Accept the proposal as new entry with probability p,

  otherwise add $\{U\}$ to the chain again.
- $p = \min\left(1, \dfrac{\pi(U')}{\pi(U)}\right)$

Development of Lattice QCD

$$\det(\gamma_\mu D_\mu + m_q) \neq 1$$



[Credit: A. Ukawa, HPC Summer School (2013)]

Hybrid Monte Carlo algorithm for QCD

- Most widely used exact method for lattice QCD [Duane, Kennedy, Pendleton, Roweth, Phys. Lett. B, 195 (1987)]

- Introduce momenta $\pi_\mu(n)$ conjugate to fundamental fields $U_\mu(n)$ and the Hamiltonian

$$\mathscr{H} = \frac{1}{2}\sum_{n,\mu} \pi^2_{n,\mu} + S[U]$$

- **Momentum Heat-bath**: refresh momenta π (Gaussian random numbers)

- **Molecular Dynamics (MD)** evolution of π and U

  ➡ numerically integrating the corresponding equations of motion (fictitious time τ):

$$(\pi, U) \longrightarrow (\pi', U')$$

reversible, area-preserving scheme such as leap-frog, Omelyan…

- **Metropolis accept/reject step**

  ➡ correcting for discretization errors of the numerical integration

$$P_{acc} = min\{1, e^{-(\mathscr{H}(\pi', U') - \mathscr{H}(\pi, U))}\}$$

Recipe for Lattice QCD Computation

(1) Generate ensembles of field configurations using Monte Carlo

(2) Average over a set of configurations: $\langle O \rangle \approx \bar{O} = \frac{1}{N_{cnfg}} \sum_{i=1}^{N_{cnfg}} O[U] + \mathcal{O}(\frac{1}{\sqrt{N_{cnfg}}})$

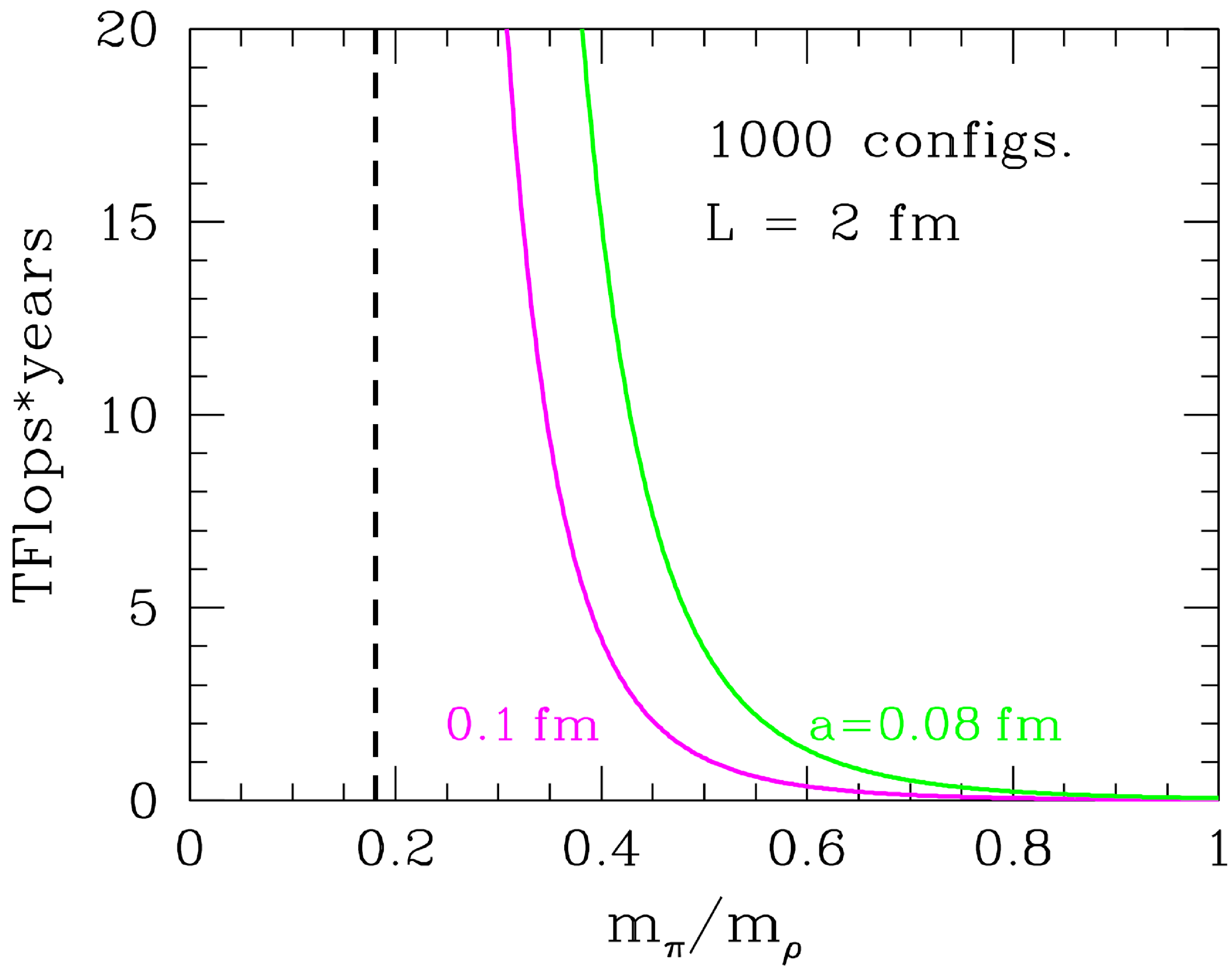
- Compute correlation function of fields, extract Euclidean matrix elements or amplitudes
- Computational cost dominated by quarks: inverses of large, sparse matrix

(3) Extrapolate to continuum, infinite volume, physical quark masses (now directly accessible)

- Lattice QCD path integrals are computed by **importance sampling**: $\mathcal{P}[U_i] \propto e^{-S_E[U]}$
- Markov chain: $\{U_0\} \longrightarrow \{U_1\} \longrightarrow \{U_2\} \longrightarrow \cdots \longrightarrow \{U_i\} \longrightarrow \{U_{i+1}\} \longrightarrow \ldots$
- The configurations are correlated by construction: $Var\,[\bar{O}] = Var[O]\,(\frac{2\tau_O}{N_{cnfg}})$

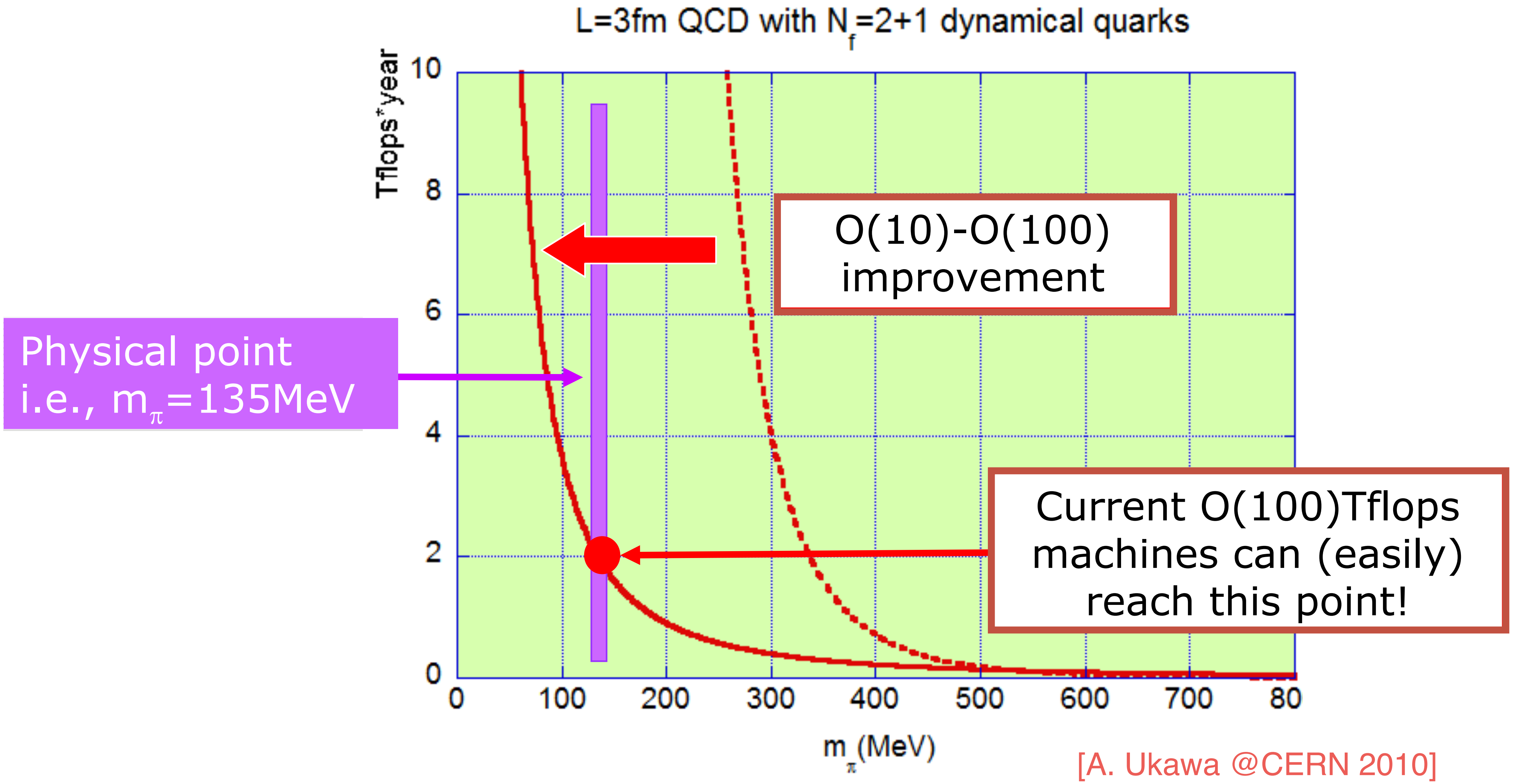
"Berlin Wall"

[Lattice 2001 (Berlin)]



- Status in 2001: [A. Ukawa (2001)]
  - ➡ quarks 16x heavier than in nature; coarse lattices $a \approx 0.1$ fm (typical length scale is 1fm)
  - ➡ Cost of a simulation: $C\left[\frac{\#conf}{1000}\right]\left[\frac{m_q}{16 m_{phys}}\right]^{-3}\left[\frac{L}{3\mathrm{fm}}\right]^5\left[\frac{a}{0.1\mathrm{fm}}\right]^{-7}; \quad C \approx 2.8$

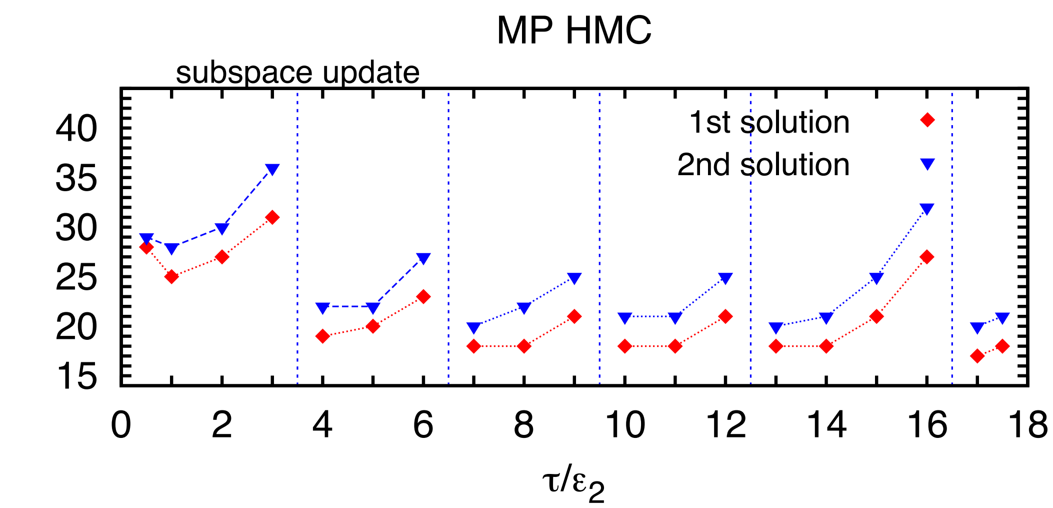
Berlin Wall update



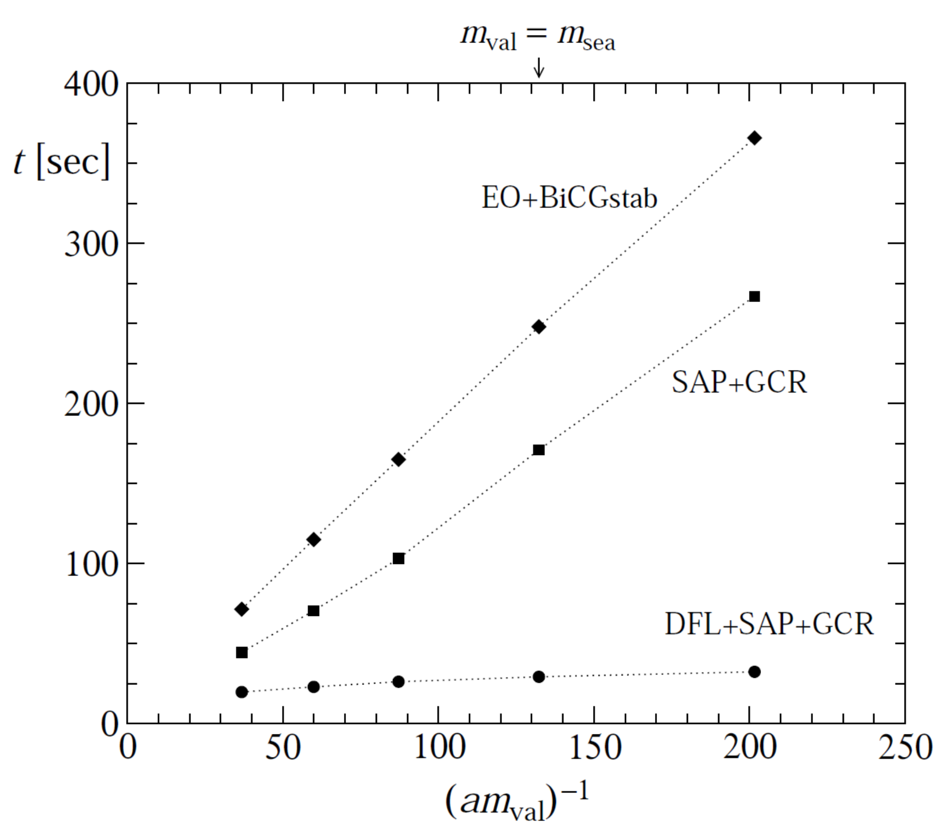
Simulating physical quark masses becomes reality!

Action and Solver Preconditioning

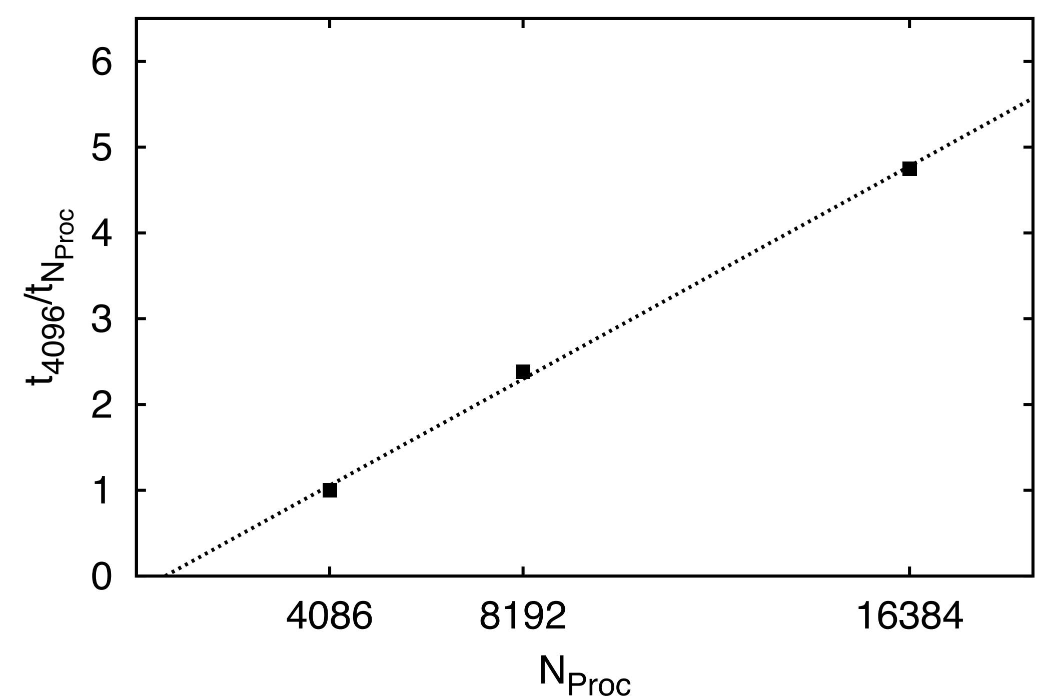
- DD-HMC program package [**M. Lüscher** (2006)]
  - ➡ domain decomposition, deflated SAP-GCR solver
- MP-HMC program package [**M.M., S. Schaefer** (2010)]
  - ➡ mass preconditioning, deflated SAP-GCR solver



[M.K.M., S. Schaefer, arXiv: arXiv:1011.0911]



[M. Lüscher, arXiv:1002.4232]



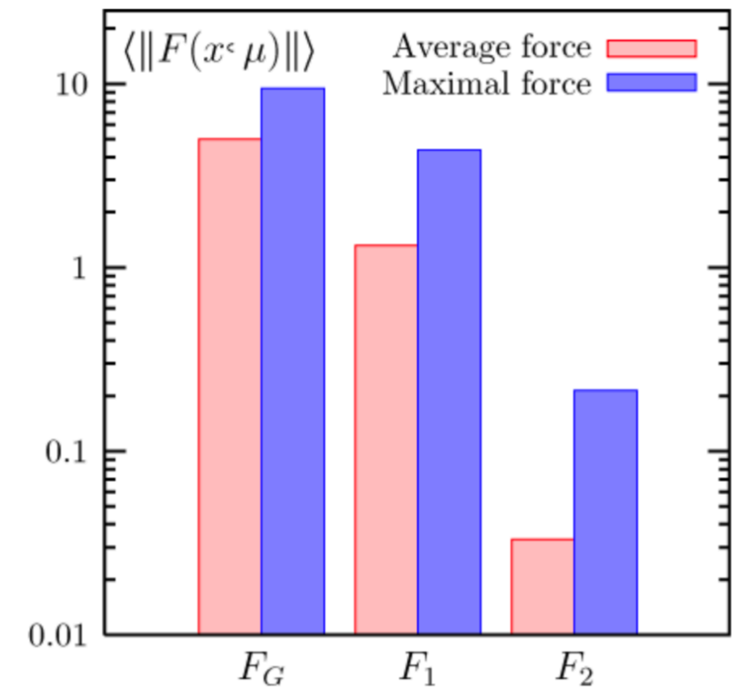
[M. Marinkovic, PhD Thesis https://edoc.hu-berlin.de/handle/18452/17597]

Action and Solver Preconditioning

- Mass preconditioning [M. Hasenbusch (2001)]

  ➡ $$\det D(m) = \boxed{\det \frac{D(m)}{D(m_1)}}\ \boxed{\det D(m_1)}$$

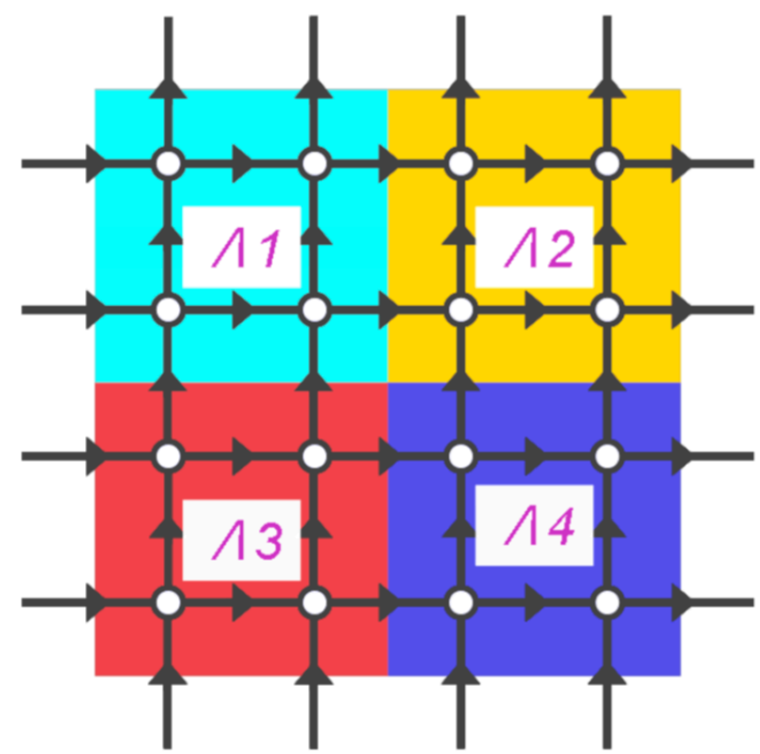
  IR modes UV modes



[C.Urbach, K.Jansen, A.Shindler, U.Wenger, CPC 174 (2006)]

- Domain-decompositioning [M. Lüscher (2003)]

  ➡ practical limitations on the parallelization and lattices that can be simulated



- Deflation acceleration (preconditioning of the Dirac solver) **[M. Lüscher (2007)]**

  ➡ removing low eigenmodes from the spectrum $\Rightarrow$ improved convergence

  ➡ inexact deflation: efficiently suppresses the eigenspace associated to the low-lying modes of D

  ➡ "Local Coherence": low modes can be well approximated by few blocked basis vectors

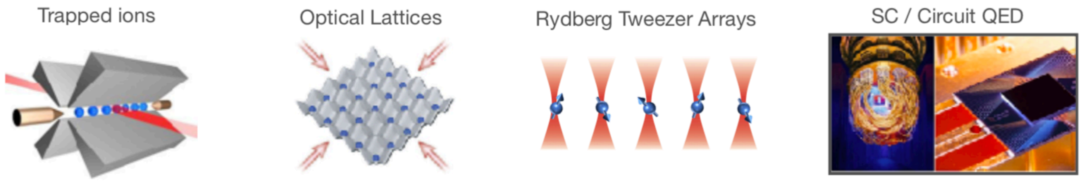
Exascale Computing Era

- Simulating physical quark masses became reality, still computationally expensive
- Recent progress in employing Machine Learning algorithms in configuration generation

[Hacket et al. 2020 2107.00734 [hep-lat]]

[Albergo et al. 2020 2106.05934 [hep-lat]]

- Quantum algorithms for quantum computers/simulators

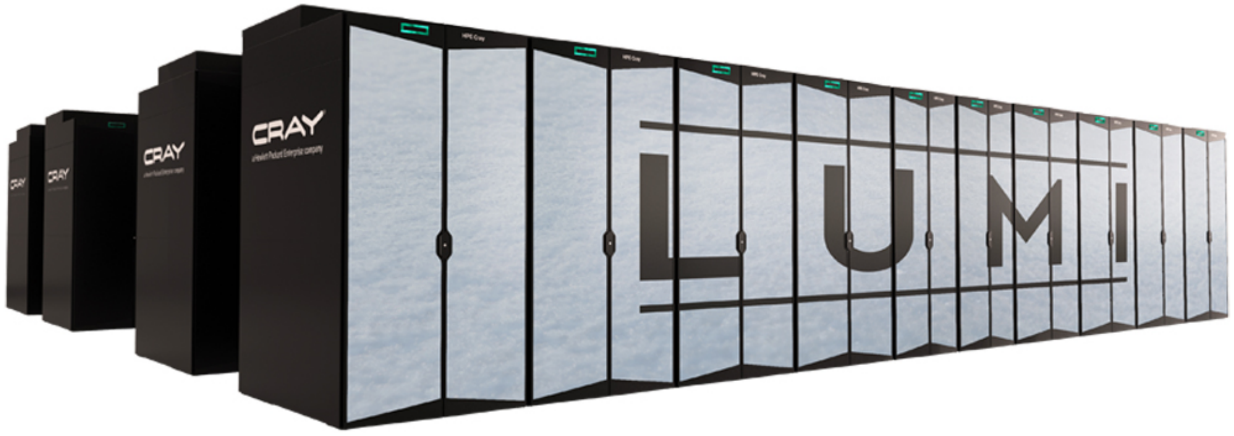


[Davoudi et al. 2104.09346 [quant-ph]]

[Farrell et al. 2020 2207.01731 [quant-ph]]

- Classical algorithms on Exascale supercomputers (10^{18} floating point operations per sec.)

[Credit: Riken Center for Computational Science]



[Credit: Hewlett Packard Enterprise]

In previous lecture:

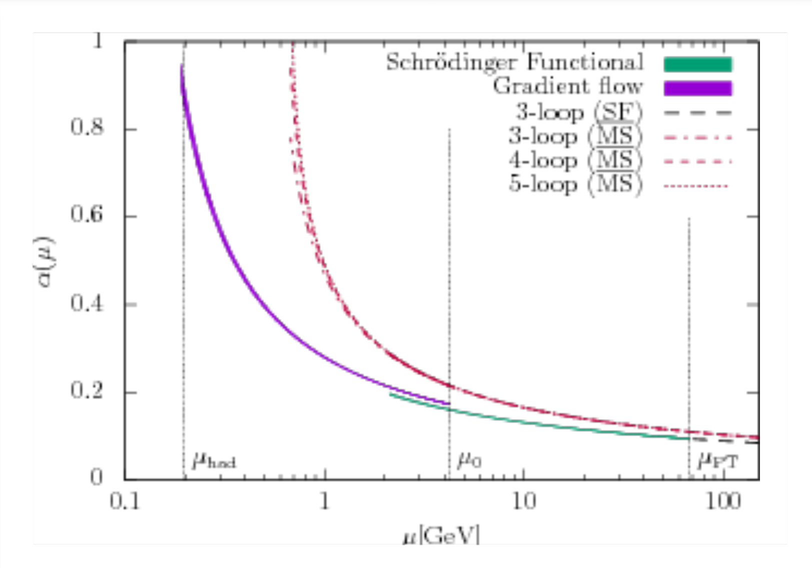
- QCD can be formulated on a Euclidean space time lattice **in a gauge invariant way**

- Quantization amounts to summing over all gauge configurations; this can again be computed by Monte Carlo methods

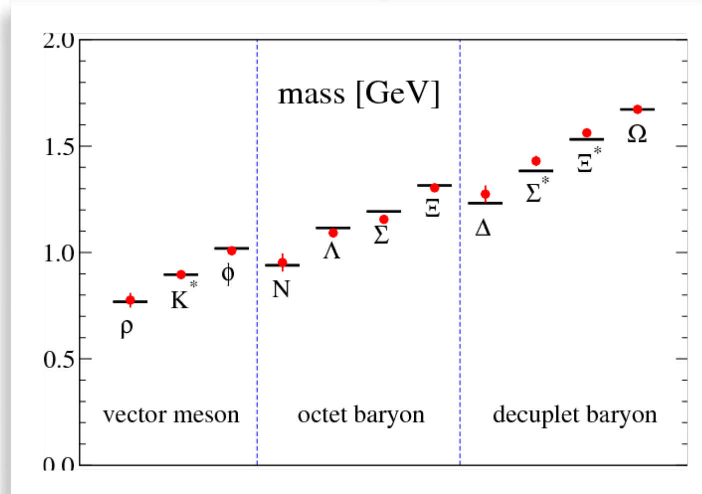
- Different discretizations give different lattice artefacts
  - ➡ **universal in continuum limit!**

- Simulations with dynamical fermions computationally costly; many tricks in algorithms need to be applied
  - ➡ precise predictions of hadron spectrum, non-pert. renormalization, muon g-2, CKM matrix elements, QCD phase diagram etc.

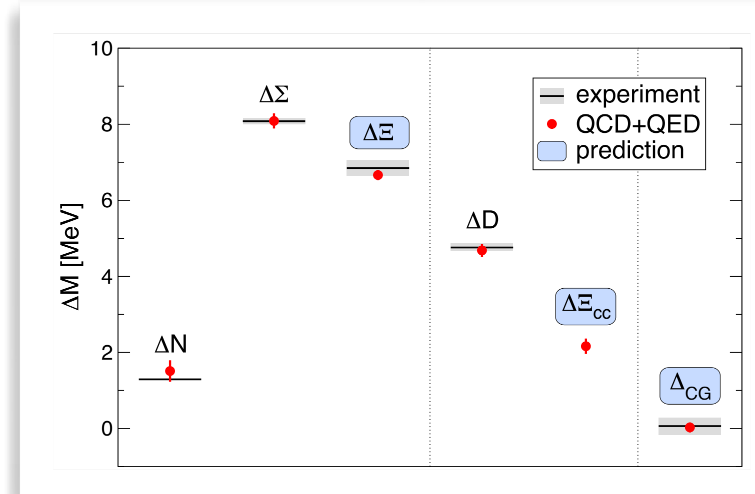
In today's lecture:



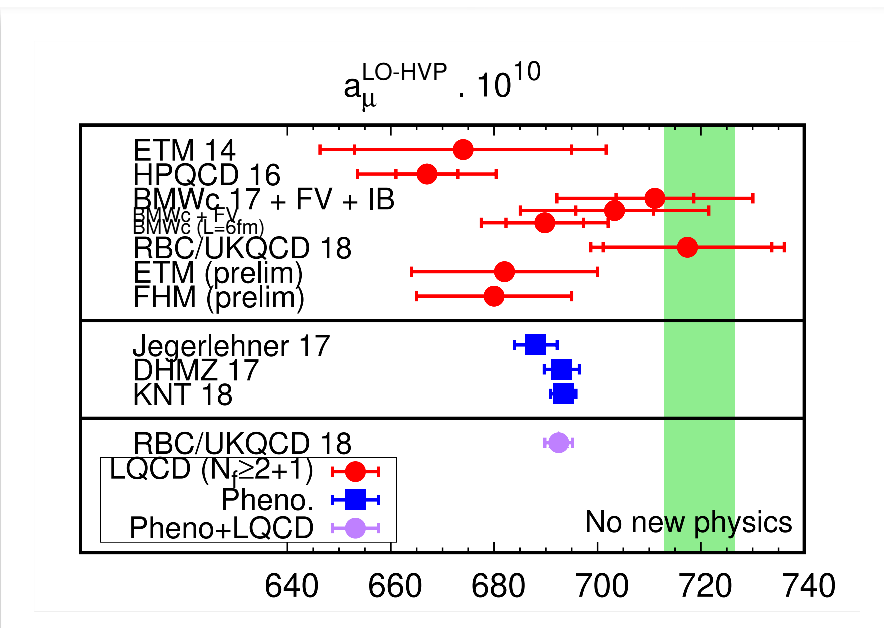
Strong coupling [Bruno et. al 2017]



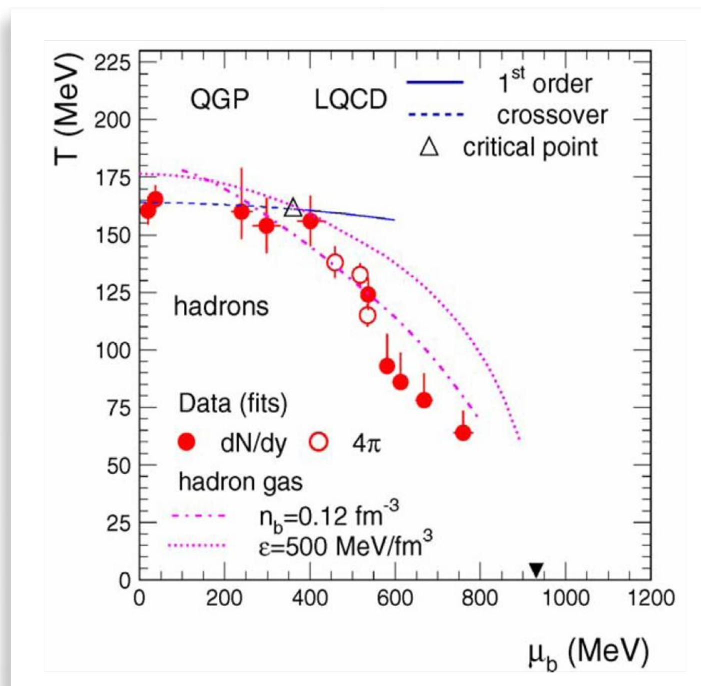
Hadron Spectrum [Aoki et. al 2008]



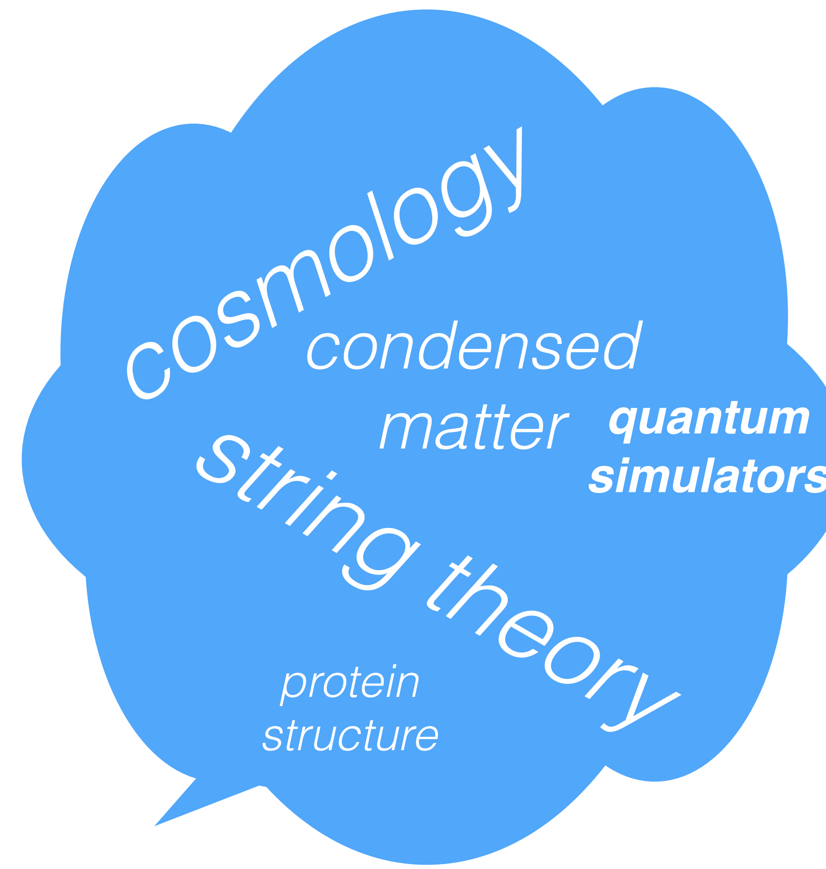
M_p-M_n [Borsanyi et. al 2014]



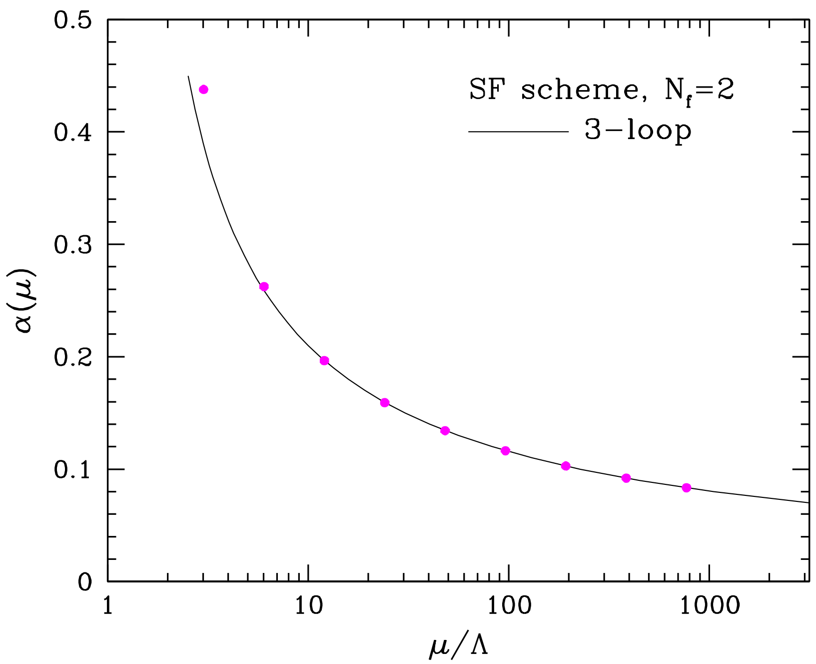
muon g-2: leading had. contib.
K. Miura @LATTICE2018



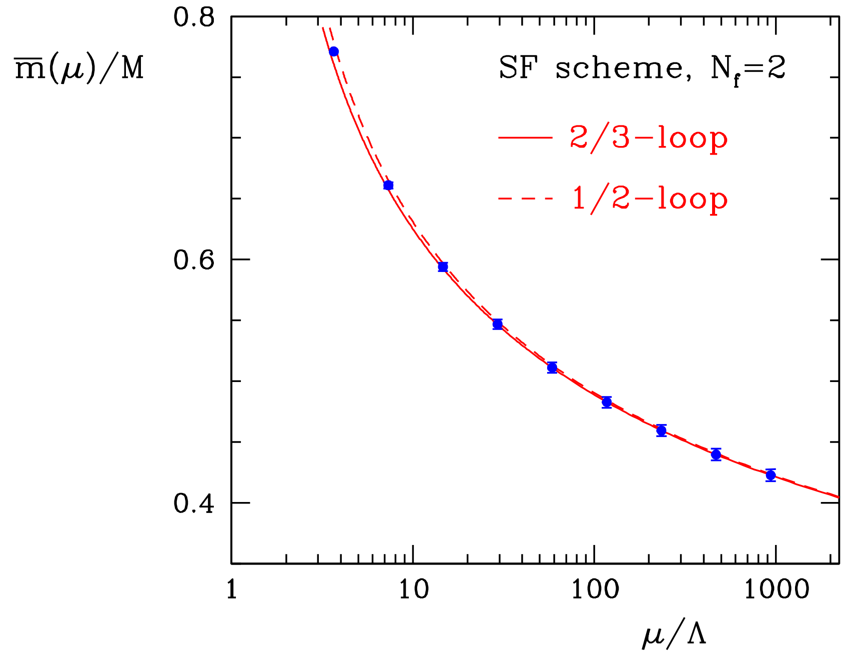
QCD Phase diagram
[Hohne et. al 2009]



Fundamental parameters of QCD: $N_f = 2$



[ALPHA Collaboration, 2004]



[ALPHA Collaboration, 2005]

- Dimensionless quantities aQ measured (Q-dimensionful obs.)
- calibration of the lattice spacing needed

$$a^{-1}\,[\mathrm{MeV}] = \frac{Q[\mathrm{MeV}]}{aQ}$$

$$Q = M_N, m_\rho, f_\pi, f_K, \ldots$$

- Lambda parameter:

$$\Lambda^{(2)}_{\overline{MS}} \; = \; 310(20)\;\mathrm{MeV}$$

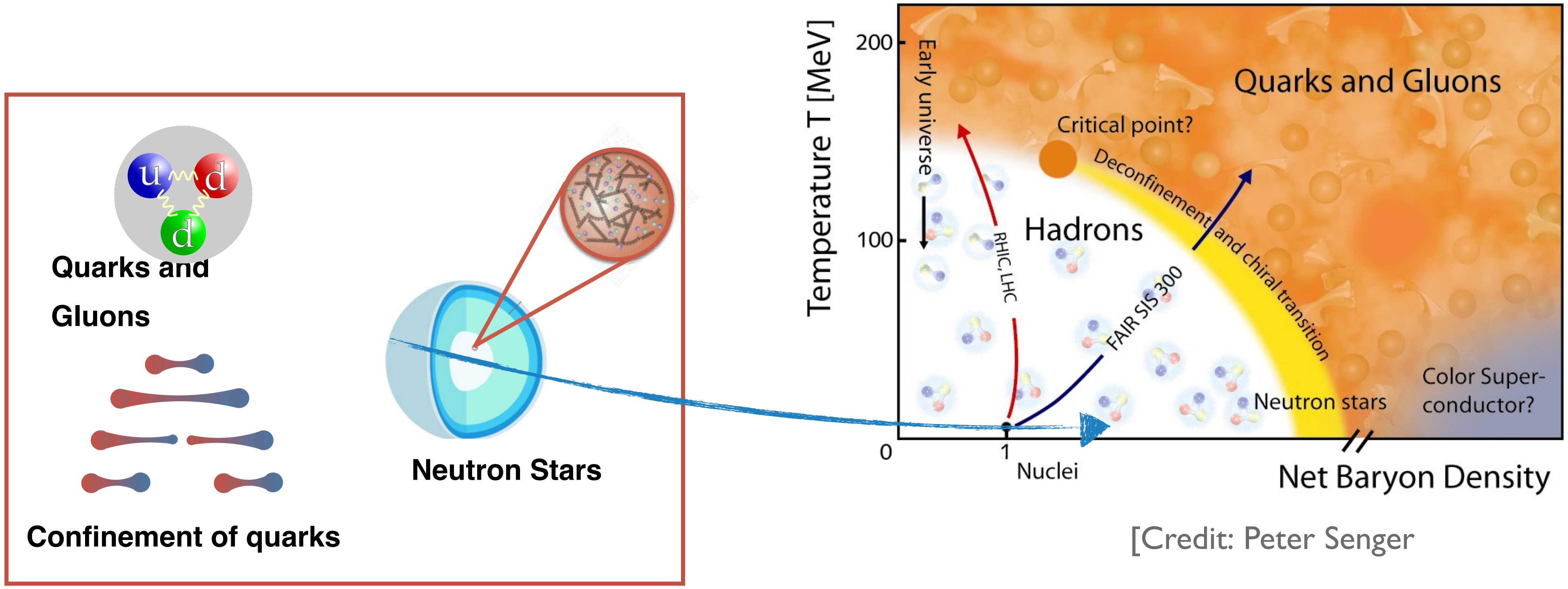
- Strange quark mass:

$$\overline{m}_s^{\overline{MS}}(\mu = 2\;\mathrm{GeV}) \; = \; 102(3)(1)\;\mathrm{MeV}$$

FLAG 2019 Flavour Lattice Averaging Group

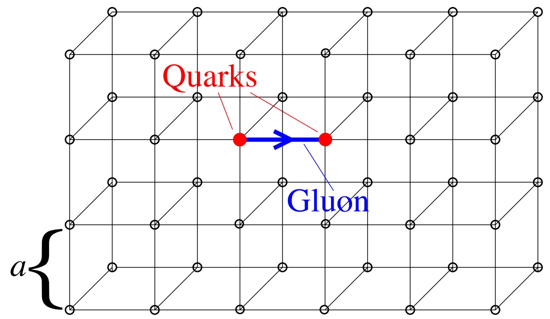
[Fritzsch, Knechtli, Leder, M.K.M., Schaefer, Sommer, Virotta, Nucl.Phys.B865 (2012)]

Lattice QCD at nonzero baryon density



[Credit: Peter Senger

Sign Problem at finite baryon densities

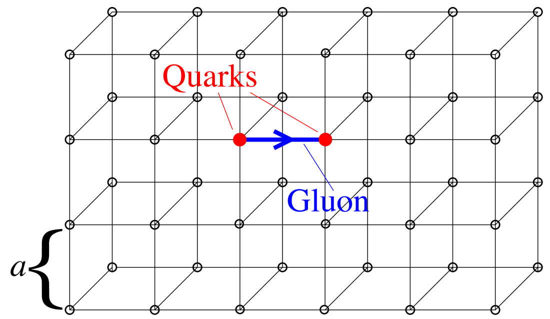


Lattice QCD: Monte Carlo Simulations

$$\langle O \rangle = \frac{1}{Z} \int D[U]\ O[U]\ det[D]\ e^{-S_G[U]}$$

113

Sign Problem at finite baryon densities



Lattice QCD: Monte Carlo Simulations

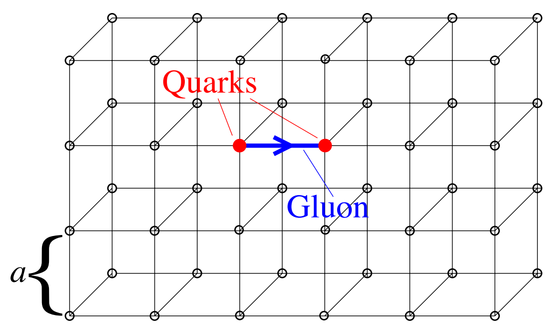
$$\langle O \rangle = \frac{1}{Z} \int D[U]\; O[U]\; \boxed{det[D]\; e^{-S_G[U]}}$$

$$\langle O \rangle = \frac{\sum_C O_C \cdot W_C}{\sum_C W_C}$$

Boltzmann Weight W → real and positive

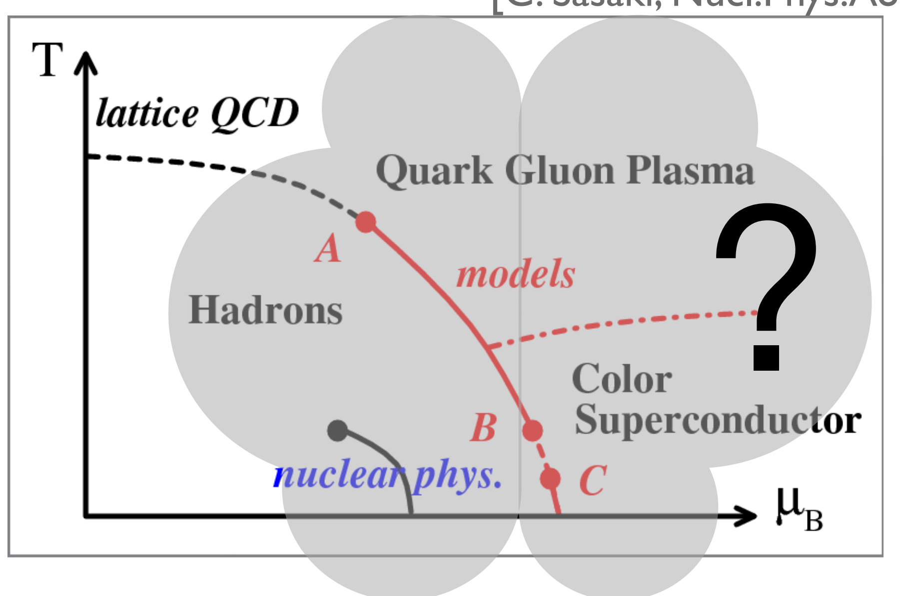
114

Sign Problem at finite baryon densities



Lattice QCD: Monte Carlo Simulations

[C. Sasaki, Nucl.Phys.A830 (2009)]



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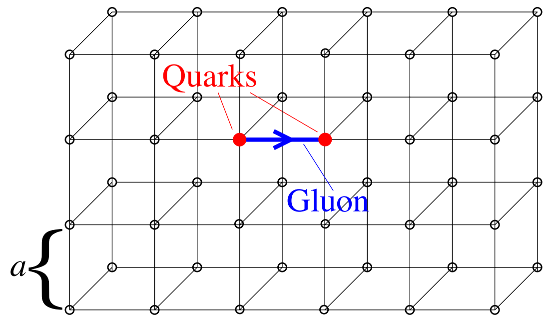

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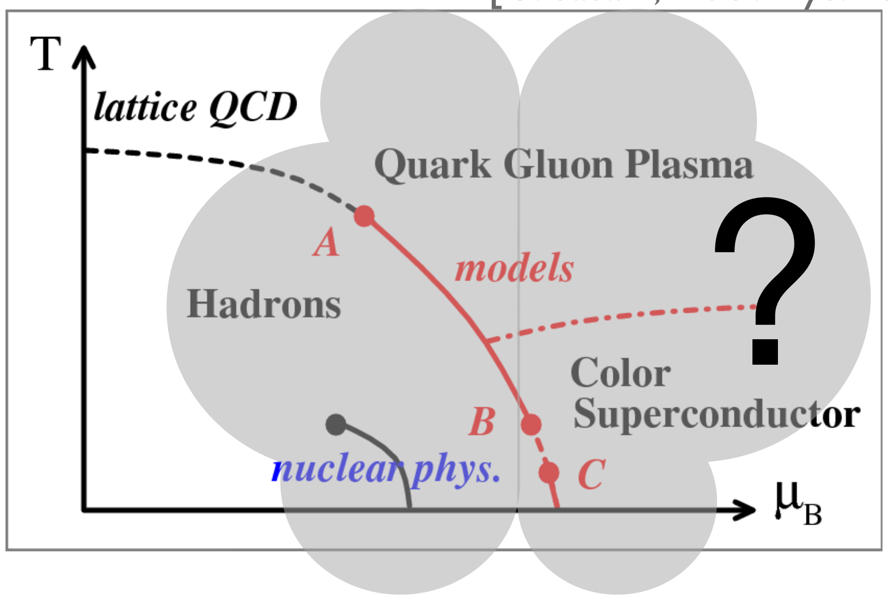


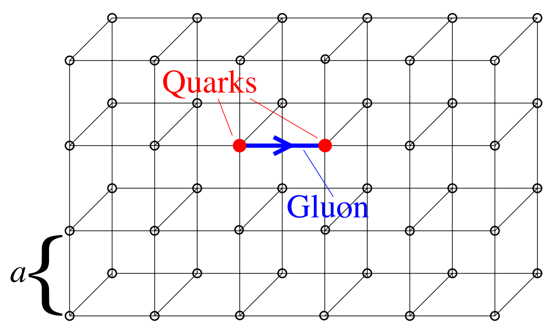
$$\langle O \rangle = \frac{1}{Z} \int D[U]\, O[U]\, \boxed{det[D]\, e^{-S_G[U]}}$$

Complex Weight W → SIGN PROBLEM

$$\langle O \rangle = \frac{\sum_C O_C \cdot W_C}{\sum_C W_C} = \frac{\sum_C O_C \cdot \mathrm{sign}(W_C) \cdot |W_C|}{\sum_C \mathrm{sign}(W_C) \cdot |W_C|}$$

$$= \frac{\langle \mathrm{sign} \cdot O \rangle_{|W|}}{\langle \mathrm{sign} \rangle_{|W|}}$$

Sign Problem at finite baryon densities



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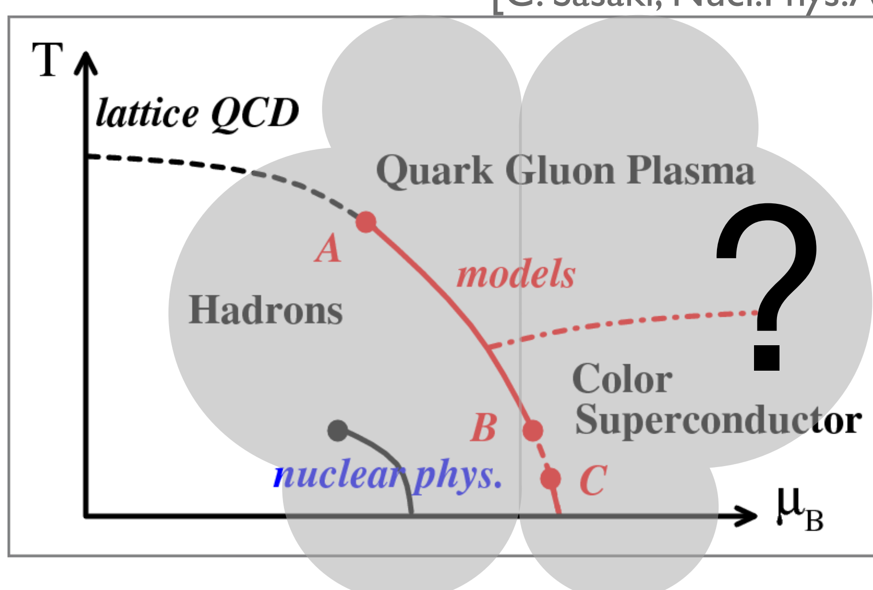

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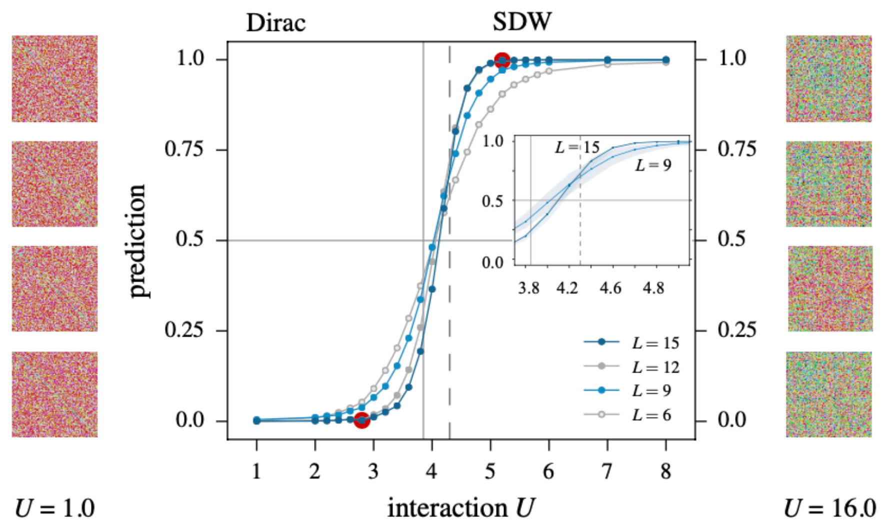
- Use Quantum Technologies and Machine Learning to enhance our fundamental understanding of the phases of matter

Why would ML work at finite densities?

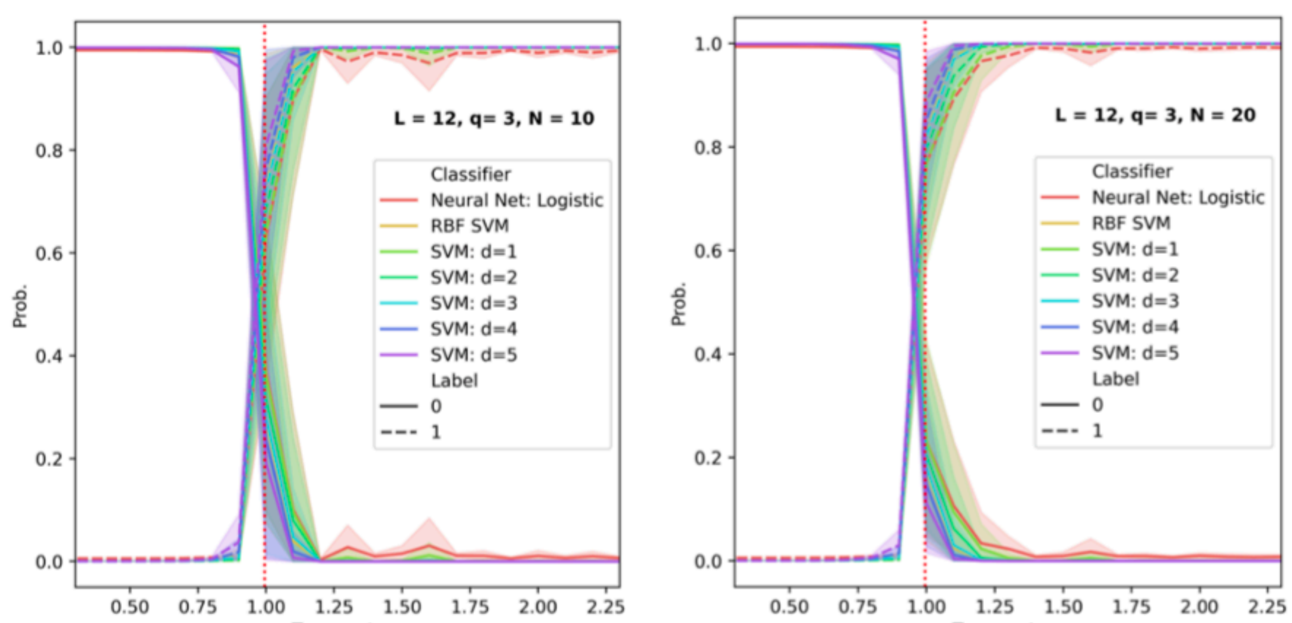
[Shiina et. al, Scientific Reports 10 (2020)]
[Giannetti et al. Nucl. Phys. B (2019)]
[Carrasquilla, Melko, Nature Physics (2017)]
[Broecker, Carrasquilla, Melko, Trebst, Sci.Rept.7 (2017)]



[Broecker, Carrasquilla, Melko, Trebst, Sci.Rept.7 (2017)]

ML has proven successful in classifying phases of matter in two and three dimensions

also in theories with sign problem



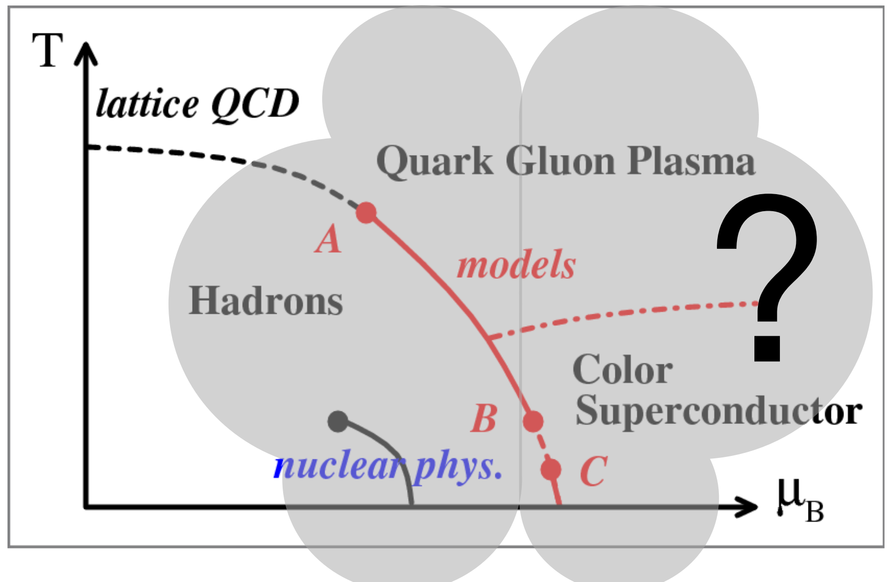
training for temperatures far away from the critical region (T=0.5 and T=5.0) gives precise predictions of the critical parameters

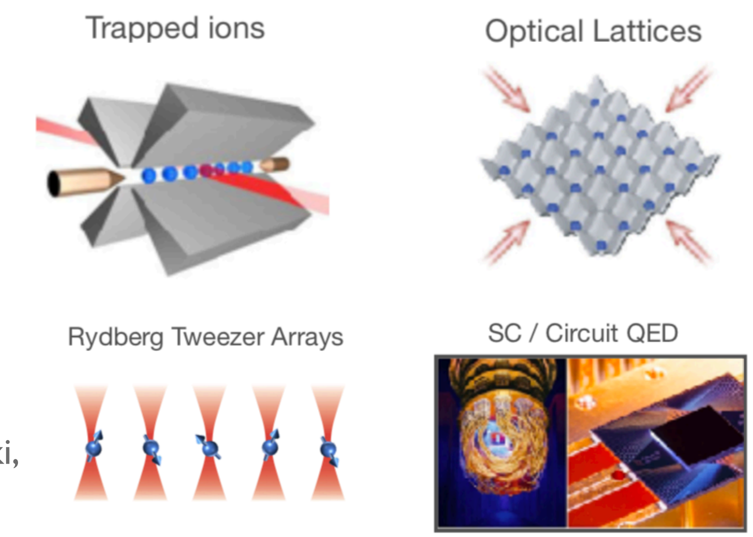
[De Giorgi, MKM, LATTICE21]

Could Quantum computing solve the Sign Problem?

polynomial time needed to obtain aimed precision

Bazavov et al., Eur. Phys. J. A55 (2019)
Ratti Rept. Prog. Phys. 81 (2019)
Borsanyi et al. Nature 539 (2016)





[Modified figure from C. Sasaki,

Classical algorithms:

Alternative methods for finite densities $\longrightarrow$ difficult to generalise

NP-hard [Troyer, Wiese Phys. Rev. Lett. 94 (2005)]

At finite μ_B: exponential time needed to obtain the aimed precision

World-line type of representations [Gattringer, Langfeld, Int.J.Mod. Phys. A31 (2016)]

Density of states approach [Körner et al. Phys.Rev. D102 (2020)]

Langenvin dynamics [Attanasio et al. Eur. Phys. J. A 56 (2020)]

Fermion bag approach [Chandrasekharan, Phys. Rev. D82 (2010)]

Reweighting the phase [Danzer, MKM et. al, Phys. Lett. B682 (2009)]

. . .

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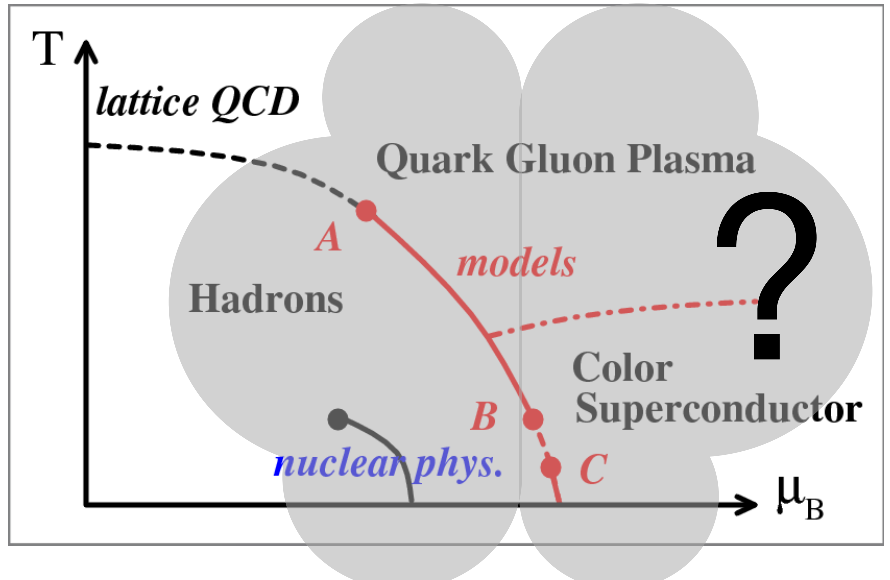
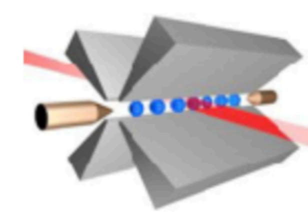
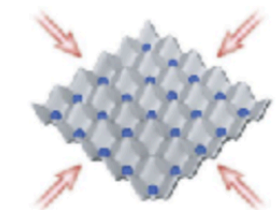


[Modified figure from C. Sasaki,

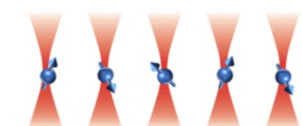
Trapped ions



Optical Lattices



Rydberg Tweezer Arrays



SC / Circuit QED

Classical algorithms:

Alternative methods for finite densities ⟶ difficult to generalise

NP-hard [Troyer, Wiese Phys. Rev. Lett. 94 (2005)]

At finite μ_B: exponential time needed to obtain the aimed precision

World-line type of representations [Gattringer, Langfeld, Int.J.Mod. Phys. A31 (2016)]

Density of states approach [Körner et al. Phys.Rev. D102 (2020)]

Langenvin dynamics [Attanasio et al. Eur. Phys. J. A 56 (2020)]

Fermion bag approach [Chandrasekharan, Phys. Rev. D82 (2010)]

Reweighting the phase [Danzer, MKM et. al, Phys. Lett. B682 (2009)]

. . .

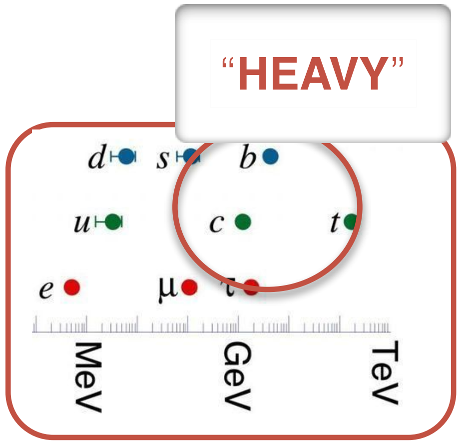
Quantum algorithms:

Quantum link models [Chandrasekharan, Wiese Nucl. Phys. B 492 (1997), Wiese Nucl.Phys.A 931 (2014)]

Analogue quantum simulations [Banuls Eur. Phys. J. D74 (2020), Paulson et al. PRX Quantum 2 (2021)]

Digital Simulations of the Schwinger Model [Chakraborty et al. Phys.Rev.D 105 (2022) 9, 094503]

Indirect New Physics Searches

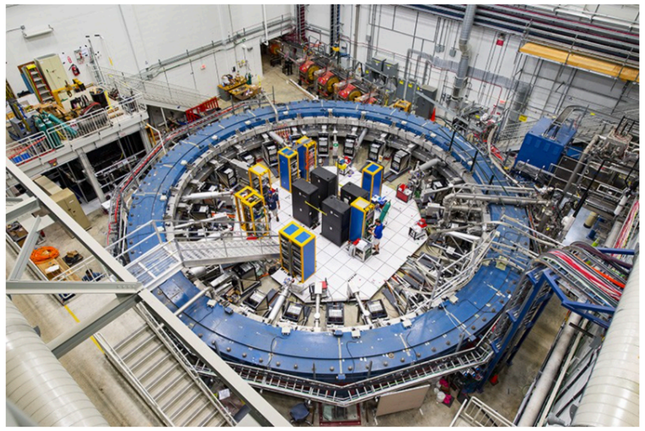


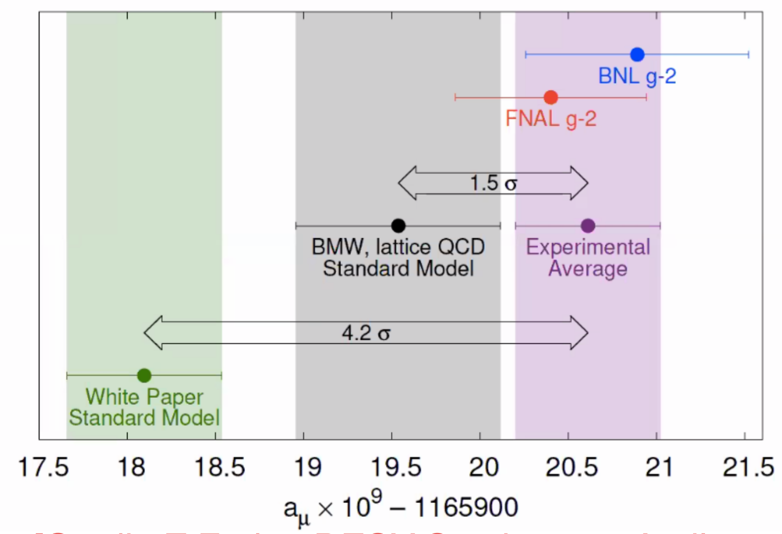
[Credit: Hitoshi Murayama]

- Searches for rare processes and for tiny deviations from Standard model expectations

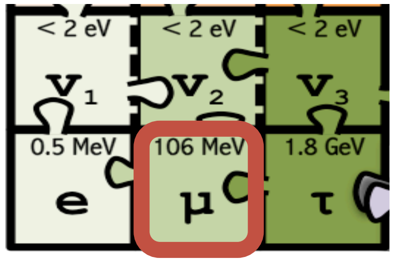
- **Heavy flavour physics**
  - ➡ Experimental measurement (**BaBar, Belle, LHCb, CMS**) vs. **SM** prediction > 3σ
  - ➡ Recent result by **LHCb** on $B_s \to \phi\mu^+\mu^-$ br. fract. and angular analysis **[LHCb Collab, FPCP21 arXiv:2105.14007]**
  - ➡ Recent result by **LHCb** on $D_0 - \bar{D}_0$ neutral charm meson oscillations **[R. Aaij et al., arXiv:2106.03744]**
  - ➡ Recent result by **LHCb** on $B_s{}^0 - \bar{B}_s{}^0$ oscillation frequency **[R. Aaij et al., arXiv:2104.04421]**
  - ➡ Recent result by **LHCb** on probing Lepton Flavour Universality **[R. Aaij et al., arXiv:2103.11769] …**

- **Muon anomalous magnetic moment**


[Credit: https://vms.fnal.gov/]



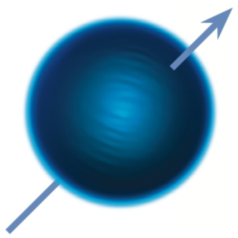
[Credit: Z.Fodor, DESY Seminar, 13 April 2021]



The magnetic moment of the lepton: $\boxed{a_l = \frac{g_l - 2}{2}}$

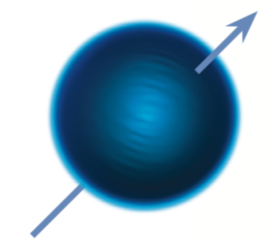
- Intrinsic magnetic moment of any spinning particle

$$\vec{\mu} = g_l \frac{e\hbar}{2m_l c} \vec{S}$$



- For leptons, $s = \frac{1}{2}$, the giromagnetic factor from Dirac theory: $g_l = 2$

The magnetic moment of the lepton: $\boxed{a_l = \frac{g_l - 2}{2}}$



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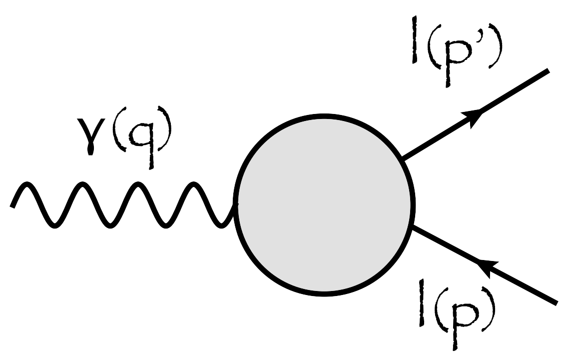
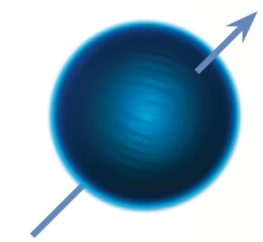


$$g_l = 2 + \underbrace{\begin{matrix}\text{quantum}\\ \text{corrections}\end{matrix}}$$

Standard Model:

(1) Q.E.D.
(2) Electroweak
(3) Hadronic

The magnetic moment of the lepton: $\boxed{a_l = \frac{g_l - 2}{2}}$



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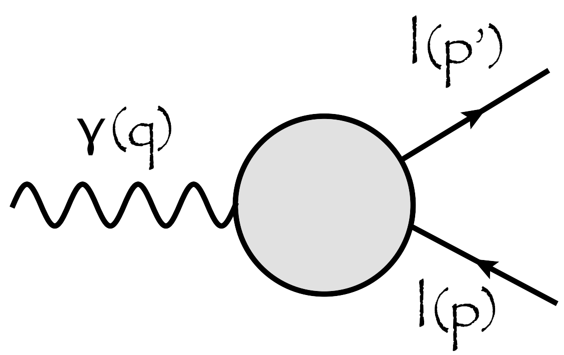


$$g_l = 2 + \underbrace{\text{quantum corrections}}_{} \overset{?}{+}$$

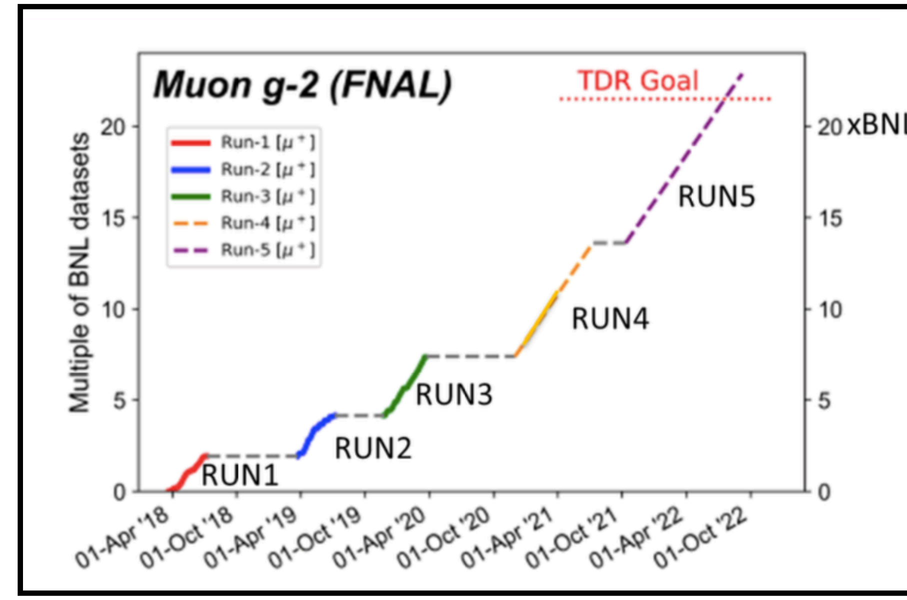
additional BSM heavier particles or contrib. from higher energy scales:

$$\frac{\delta a_l}{a_l} \propto \frac{m_l^2}{M_{NP}^2}$$

Standard Model:

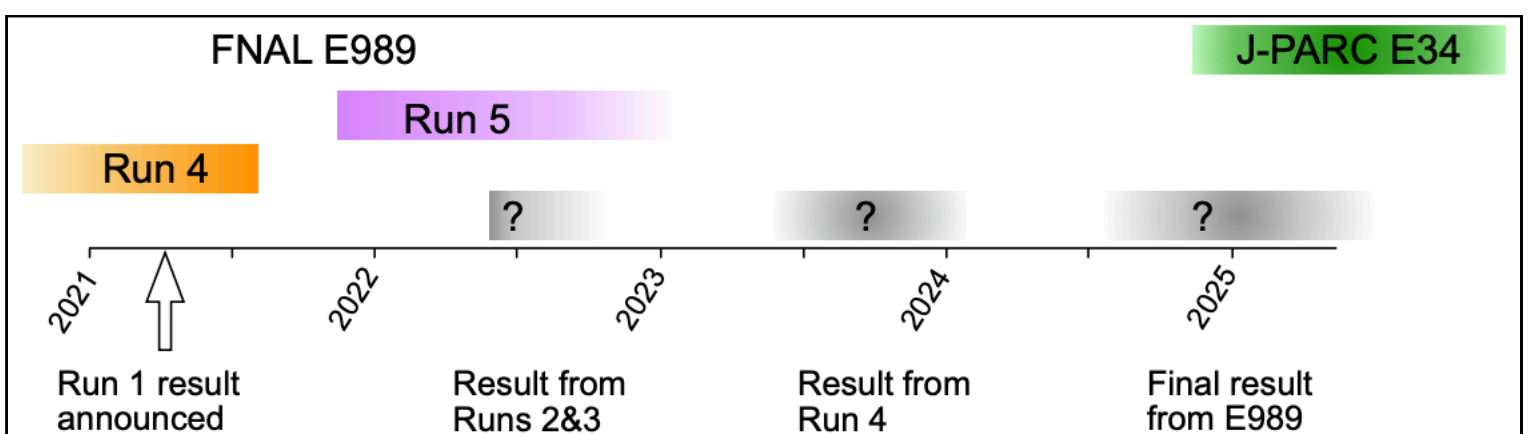
(1) Q.E.D.
(2) Electroweak
(3) Hadronic

a_μ from experiment: FNAL E989, J-PARC

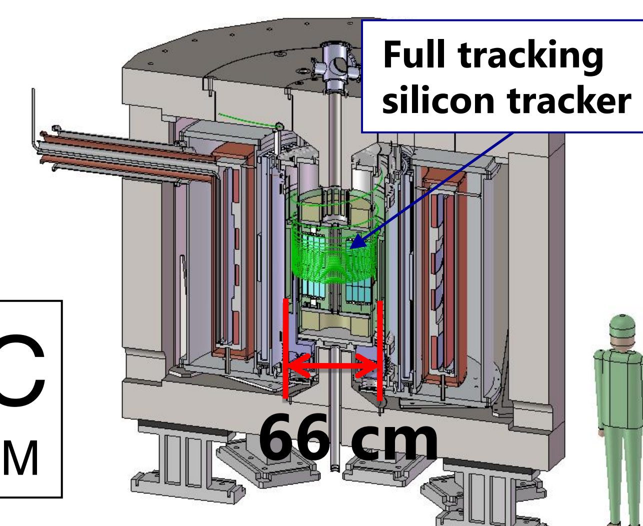


- a_μ^{exp}= 11659208.0(6.3) × 10 $^{-10}$ (0.54ppm) [BNL, 2006-2008]
- a_μ^{exp}= 11659204.0(5.4) × 10 $^{-10}$ (0.46ppm) [Fermilab, 2018-2021]

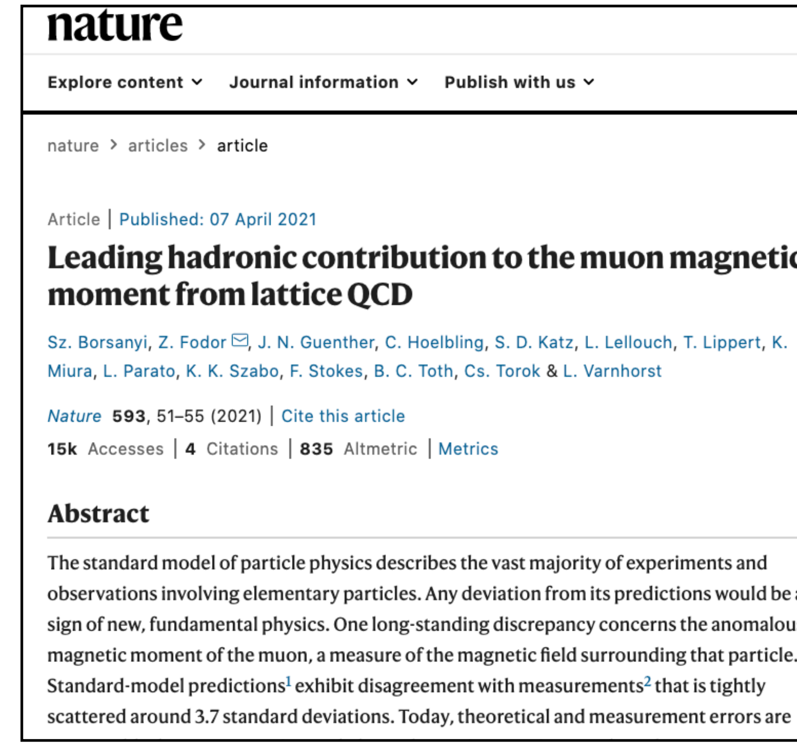
D. B. Abi *et al.* (Muon g–2 Collaboration) Phys. Rev. Lett. 126, 141801 – Published 7 April 2021



J-PARC
Muon g-2/EDM



a_μ from experiment: FNAL E989



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Article | Published: 07 April 2021

Leading hadronic contribution to the muon magnetic moment from lattice QCD

Sz. Borsanyi, Z. Fodor, J. N. Guenther, C. Hoelbling, S. D. Katz, L. Lellouch, T. Lippert, K. Miura, L. Parato, K. K. Szabo, F. Stokes, B. C. Toth, Cs. Torok & L. Varnhorst

Nature **593**, 51–55 (2021) | Cite this article

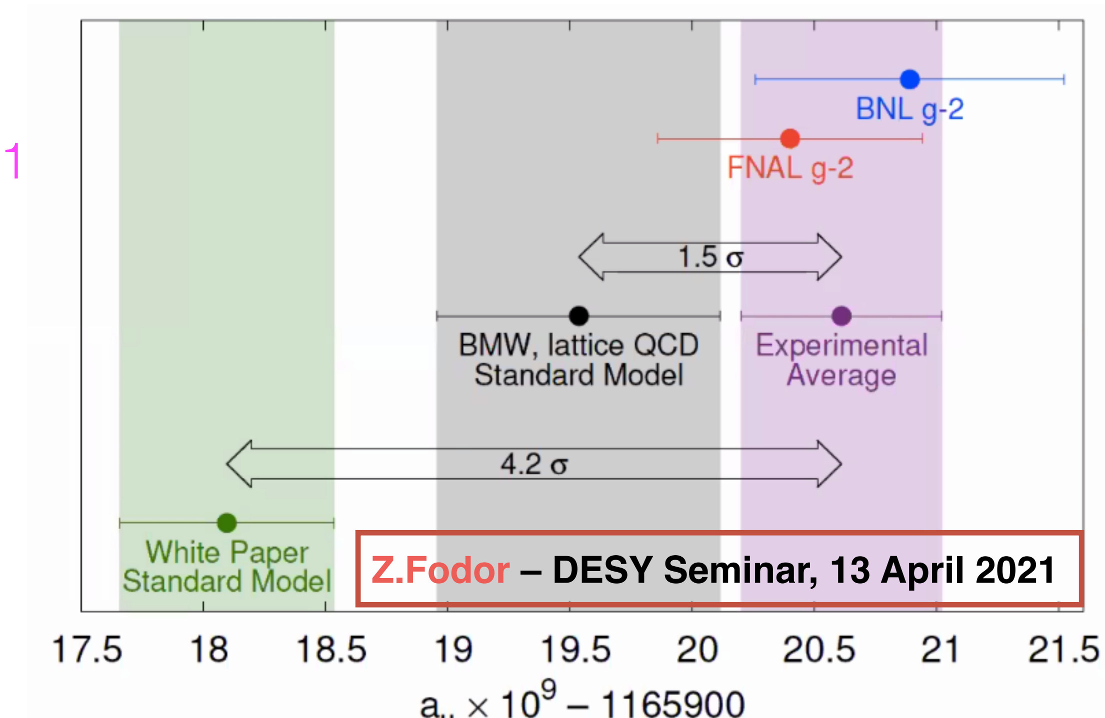
15k Accesses | **4** Citations | **835** Altmetric | Metrics

Abstract

The standard model of particle physics describes the vast majority of experiments and observations involving elementary particles. Any deviation from its predictions would be a sign of new, fundamental physics. One long-standing discrepancy concerns the anomalous magnetic moment of the muon, a measure of the magnetic field surrounding that particle. Standard-model predictions[1] exhibit disagreement with measurements[2] that is tightly scattered around 3.7 standard deviations. Today, theoretical and measurement errors are

- a_μ^{exp} = 11659208.0(6.3) × 10 $^{-10}$ (0.54ppm) [BNL, 2006-2008]
- a_μ^{exp} = 11659204.0(5.4) × 10 $^{-10}$ (0.46ppm) [Fermilab, 2018-2021

- New experiments (FNAL E989) expected to perform 4× more precise measurement, J-PARC for crosscheck of systematics
- Improved precision of the theoretical estimates with dominating uncertainty required



The magnetic moment of the muon: $\boxed{a_\mu = \frac{g_\mu - 2}{2}}$

EXPERIMENT:

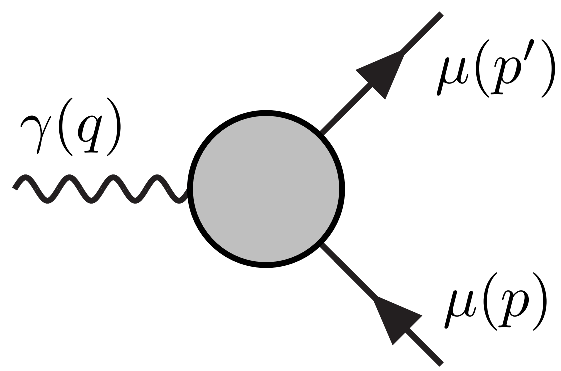
a_μ^{exp} = 11659208.0(6.3) × 10 $^{-10}$ (0.54ppm) [BNL E821, 2006-2008]

a_μ^{exp} = 11659204.0(5.4) × 10 $^{-10}$ (0.46ppm) [Fermilab Muon g-2, 2018-2021]

THEORY:

a_μ^{th} = 11659181.0(4.3) × 10 $^{-10}$ (0.37ppm) [Muon g-2 Theory Initiative, Phys.Rept. 887 (2020), 1-166]

TENSION: **4.2 σ**



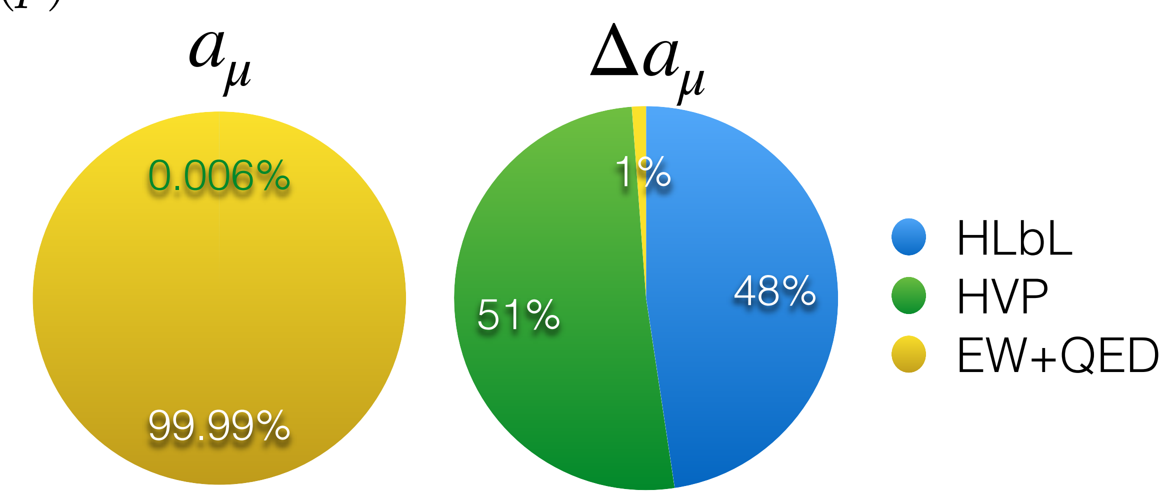
$$a_\mu = \frac{g_\mu - 2}{2}$$

Standard Model:

(1) Q.E.D.

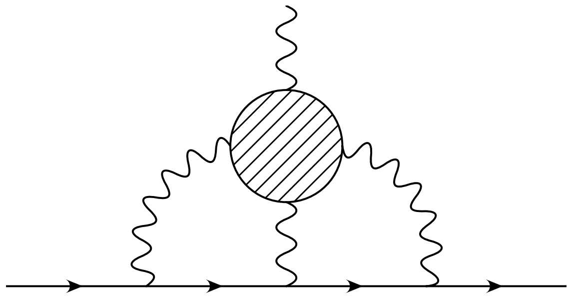
(2) Electroweak

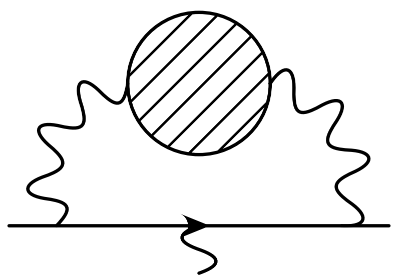
(3) Hadronic



Muon g-2 from Theory and Experiment

	2011		**2020**	
QED	11658471.81 (0.02)	$\longrightarrow$	11658471.89 (0.01)	**[WP20]**
EW	15.40 (0.20)	$\longrightarrow$	15.36 (0.10)	**[WP20]**
LO HLbL	10.50 (2.60)	$\longrightarrow$	9.20 (1.90)	**[WP20]**
NLO HLbL			0.20 (0.10)	**[WP20]**
	HLMNT11		**KNT18**	
LO HVP	694.91 (4.27)	$\longrightarrow$	693.1 (4.0)	**[WP20]**
NLO HVP	-9.84 (0.07)	$\longrightarrow$	-9.83 (0.07)	**[Phys.Rev. D 97 (2018) 114025]**
NNLO HVP			1.24 (0.01)	**[Phys. Lett. B 735 (2014) 90]**
Theory total	11659182.80 (4.94)	$\longrightarrow$	11659181.0 (4.3)	**[WP20]**
Experiment			11659206.1 (4.1)	world avg
Exp - Theory	26.1 (8.0)	$\longrightarrow$	25.1 (5.9)	**April 2021: WP20/exp.**
Δa_μ	3.3σ	$\longrightarrow$	$4.2\ \sigma$	**April 2021: WP20/exp.**





[WP20] **T. Aoyama et al, arXiv:2006.04822, Phys. Repts. 887 (2020) 1-166**
White Paper Muon g-2 Theory Initiative: https://muon-gm2-theory.illinois.edu

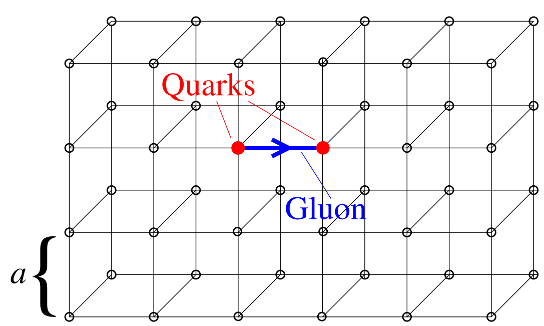
Recipe for Lattice QCD Computation

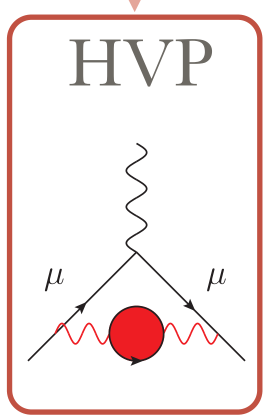
(1) Generate ensembles of field configurations using *Monte Carlo*

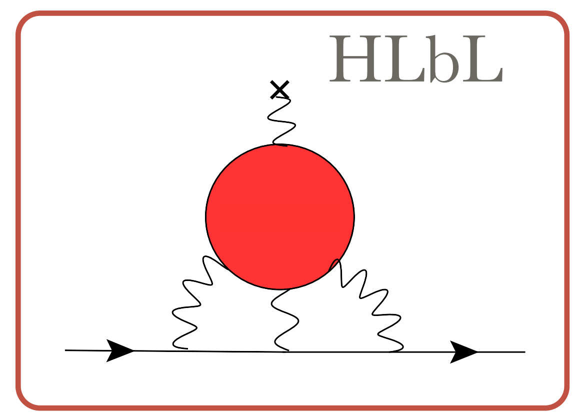
(2) Average over a set of configurations:

- Compute $\underbrace{\text{correlation function of fields,}}$ extract Euclidean matrix elements or amplitudes
- Computational cost dominated by quarks: inverses of large, sparse matrix

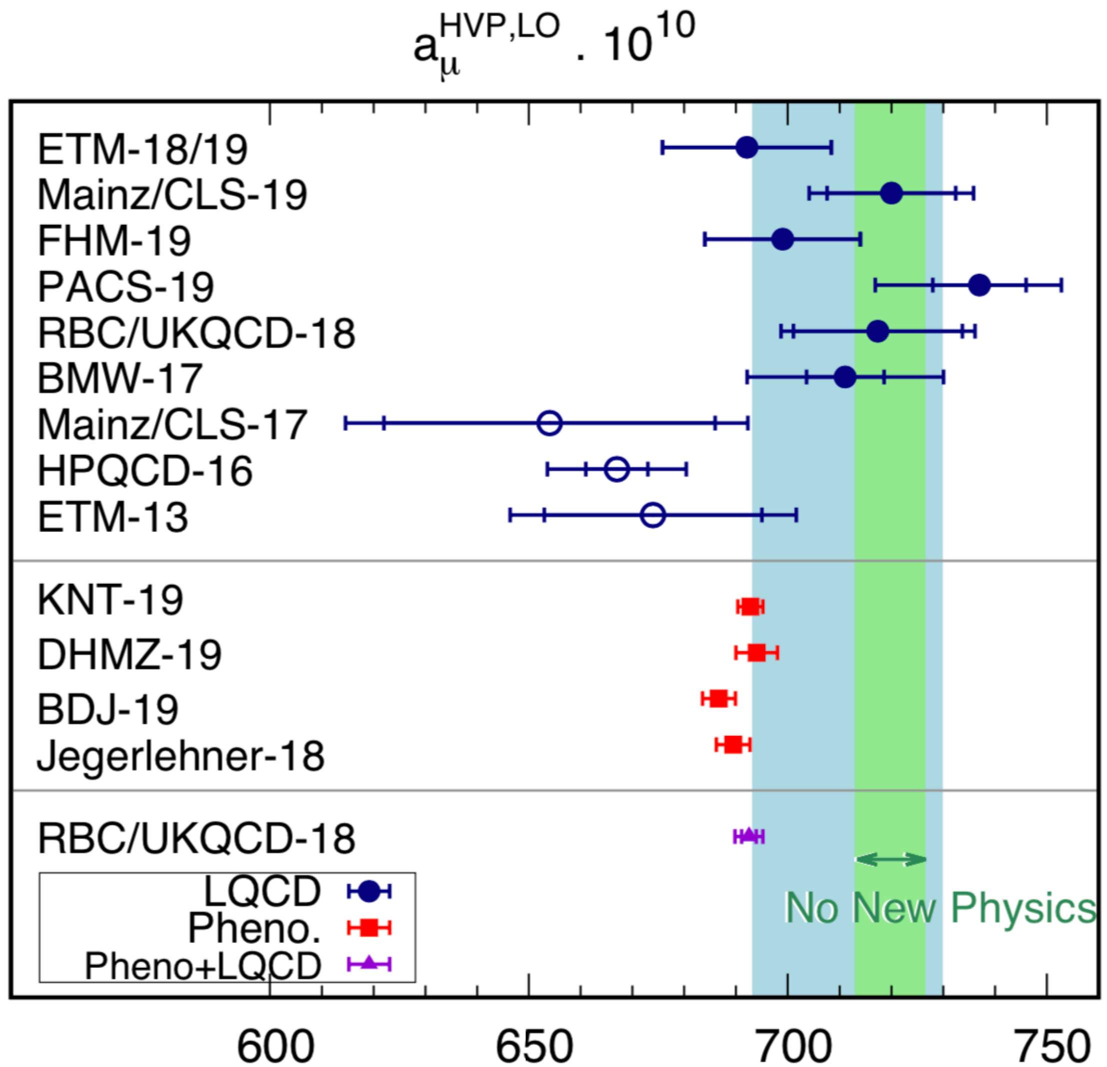
(3) Extrapolate to continuum, infinite volume, physical quark masses (now directly accessible)



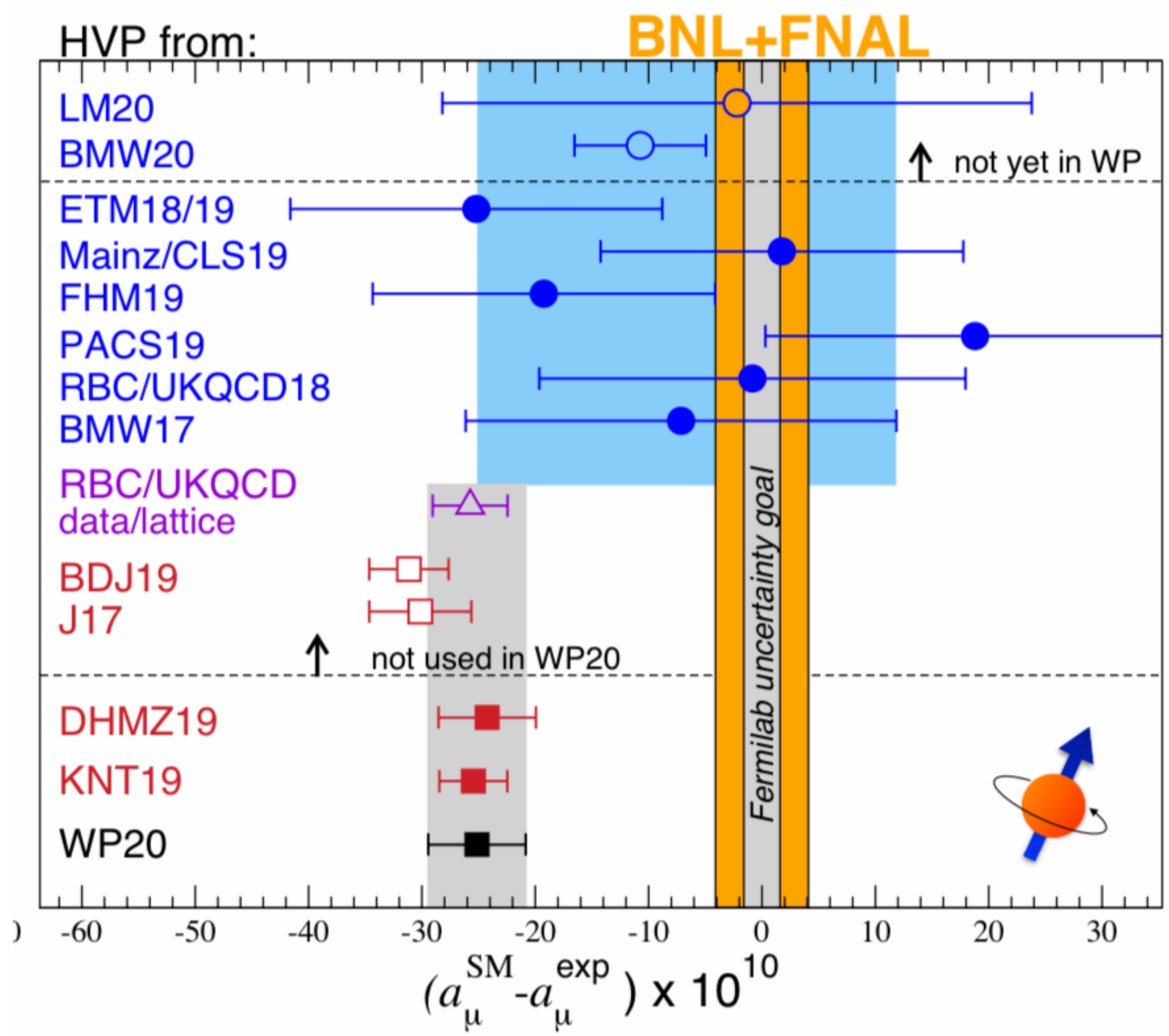




Challenging lattice computation of $a_\mu^{\rm HVP,LO}$



[Muon g-2 theory Initiative, White Paper 2006.04822 [hep-ph]]



[Snowmass22 2203.15810 [hep-ph]]

Summary & Outlook

- Exciting time for lattice QCD computations: mature and innovative!
- Large computing power and advanced (clever) algorithms needed
- **Muon anomalous magnetic moment (muon g-2):** good quantity for constraining new physics
  - ➡ **Lattice QCD(+QED)** gives an independent theory prediction of **HVP and HLbL**
- Exascale classical comp. resources will help better control systematics in next 5 years
- Solving the sign problem requires a paradigm shift: AI, quantum computing, reformulating the theory …
- Lattice computations instrumental also for other NP searches (e.g. heavy flavour, kaon physics, BSM simulations)