Lattice Field Theory
Session 84: Computational Requirements & Opportunities

Snowmass Community Planning Meeting
October 7, 2020 — Rich Brower

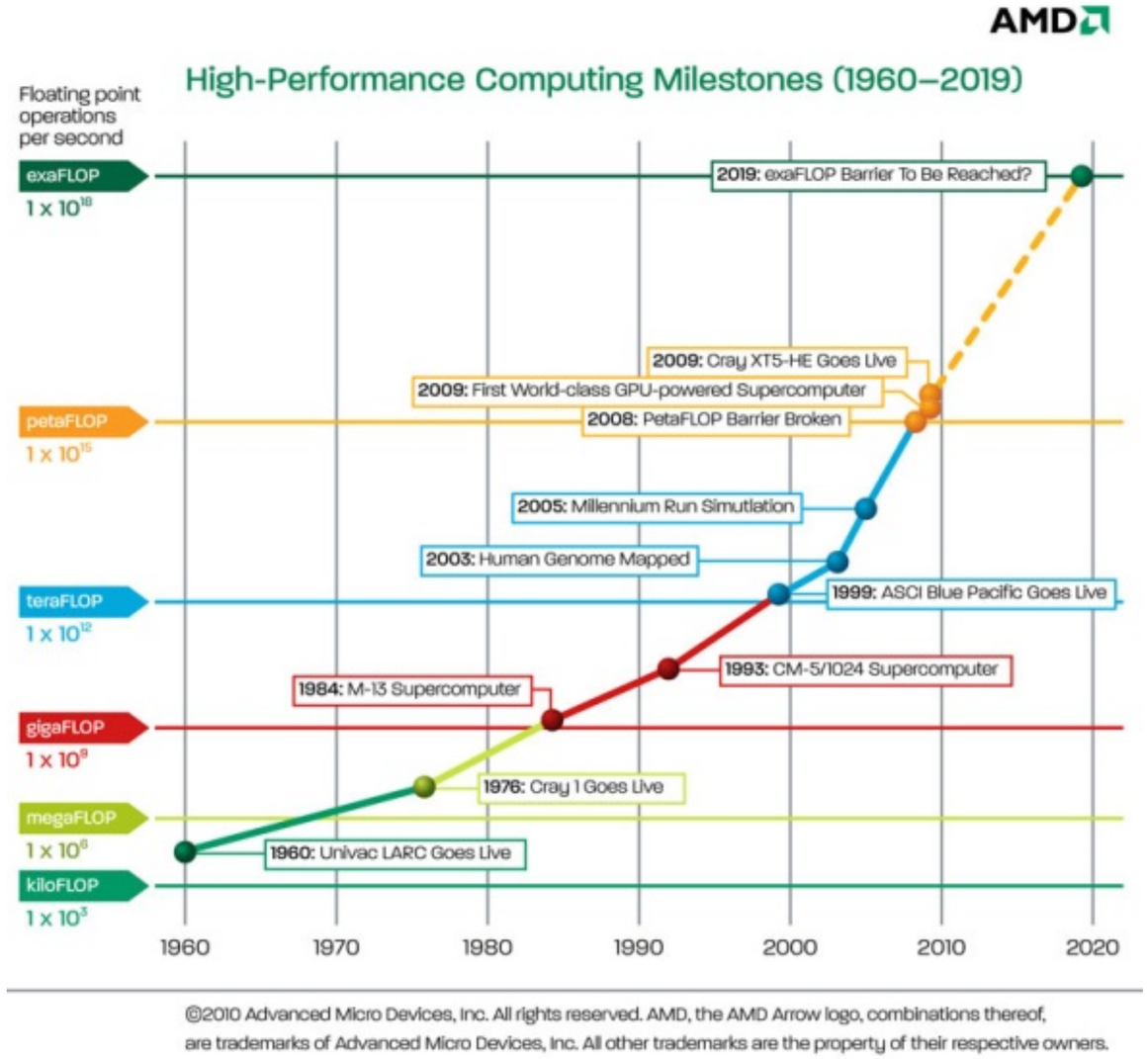
LOI in Computational Lattice Field Theory

Algorithms and Software in Support of Computational HEP and NP at the Exascale and Beyond	Carleton DeTar
Chiral Lattice Fermions and the Computational Frontier	Peter Boyle
Multiscale QCD algorithms Beyond the Exascale	Rich Brower
Machine Learning and Lattice QCD *Machine Learning for sampling in lattice quantum field theory*	Akio Tamayo Phiala Shanahan

See also White Paper: ***Status and Future Perspectives for Lattice Gauge Theory Calculations to the Exascale and Beyond*** *(B. Joó, C. Jung, N.H. Christ, W. Detmold, R.G. Edwards, M. Savage, P.E. Shanahan)*
https://arxiv.org/abs/1904.09725v2

50 years: Wilson LQCD(1970) to Exascale (2023)

roughly $\mathcal{O}(10^3)$ *per decade in hardware* $\implies \mathcal{O}(10^{18})$



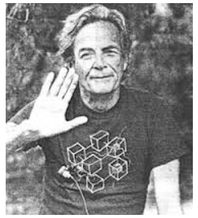
$\leftarrow 10^{18}$

$\leftarrow 10^3$

All numerical predictions from Quantum Field Theory require "Algorithms"

Z = Path Integral exp[- Action]

Feynman Diagrams



'tHooft Dim Reg

Quantum Computing and Sign Problem

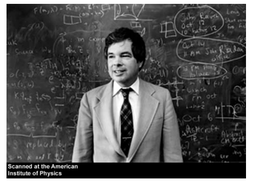
Conformal Bootstrap

AdS/CFT

OPE & Renormalization Group

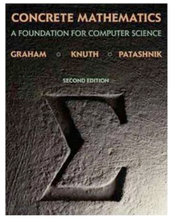
Curved Simplicial Lattices & Regge Gravity

Wilson Lattice QCD

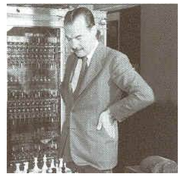


Domain Wall

Wilson Flow



Finite Elements Schwartz Schurs



HMC (Monte Carlo +fermions)

Multi-Grid

Machine Learning

Status approaching Exascale

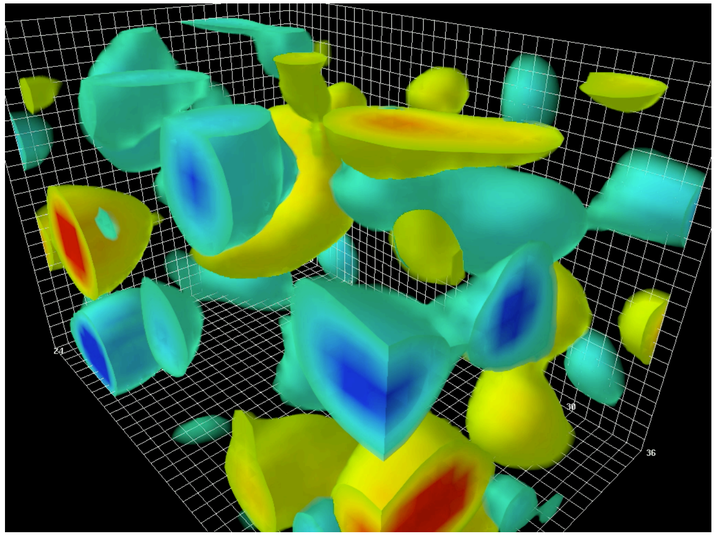
- *LQCD now provides **ab initio** test the Standard Mode*
  - *high precision due in "equal parts"*
    - *advances in hardware/software*
    - *advance in algorithms and theory*

- *The Exascale Computing Project (ECP) gives crucial support to*
  - *Acceleration for statistical independent gauge configuration*
  - *Combinatoric for multi-quark graphs.*
  - *Solvers for 3 Dirac discretization:*
    - *Wilson, Staggered and Domain Wall (extra 5th dimension)*

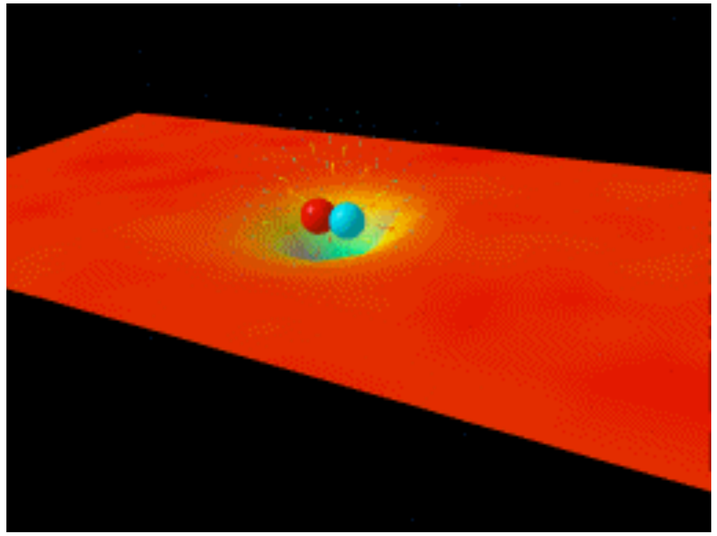
Virtuous Cycle:
Hardware Advance <==> Algorithms Advances

Increased Resolution causes "critical slowing down"
BUT also expose new scale for algorithms to exploit

Vacuum Scale

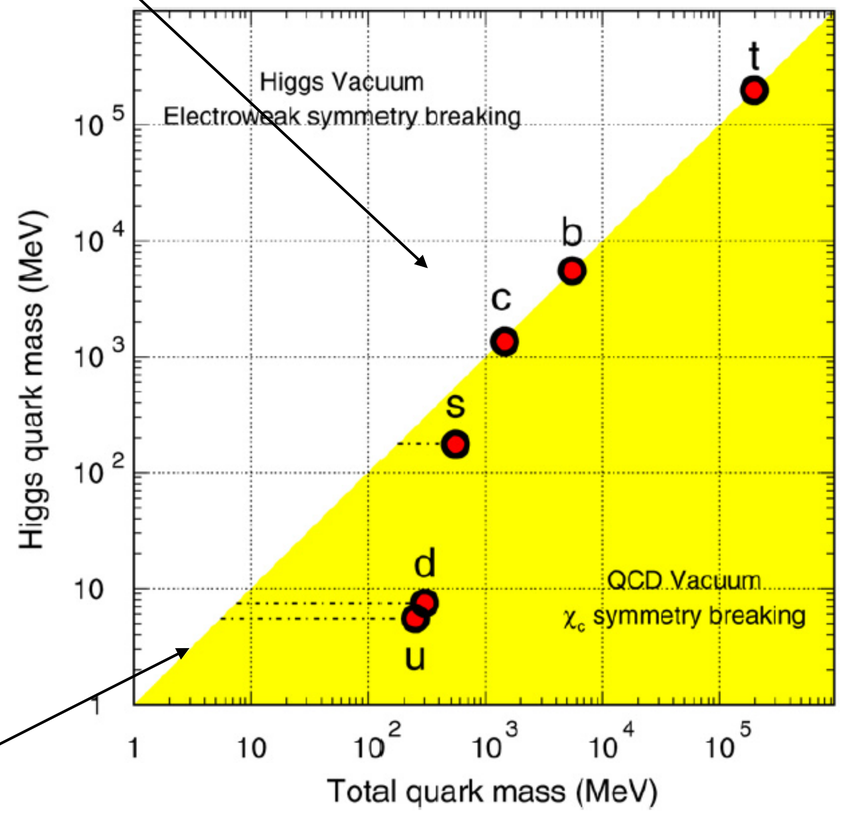


Confinement Scale



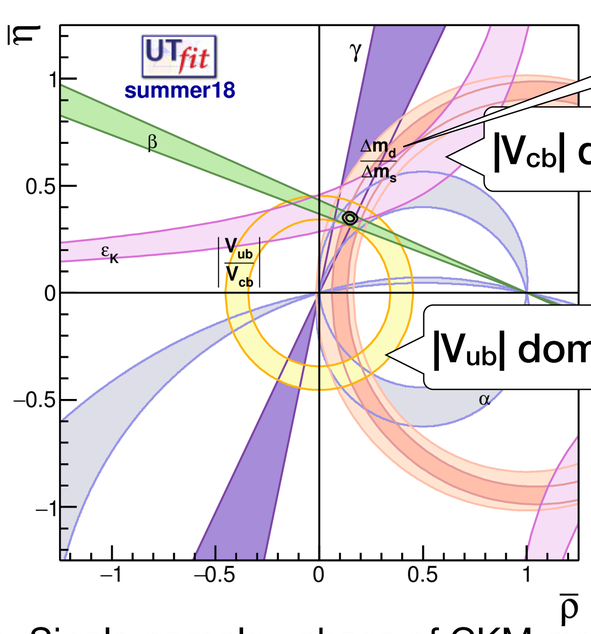
Heavy quark effective theory

Quark Mass probes



Chiral effective theory

One Example of Precision QCD: CKM Matrix



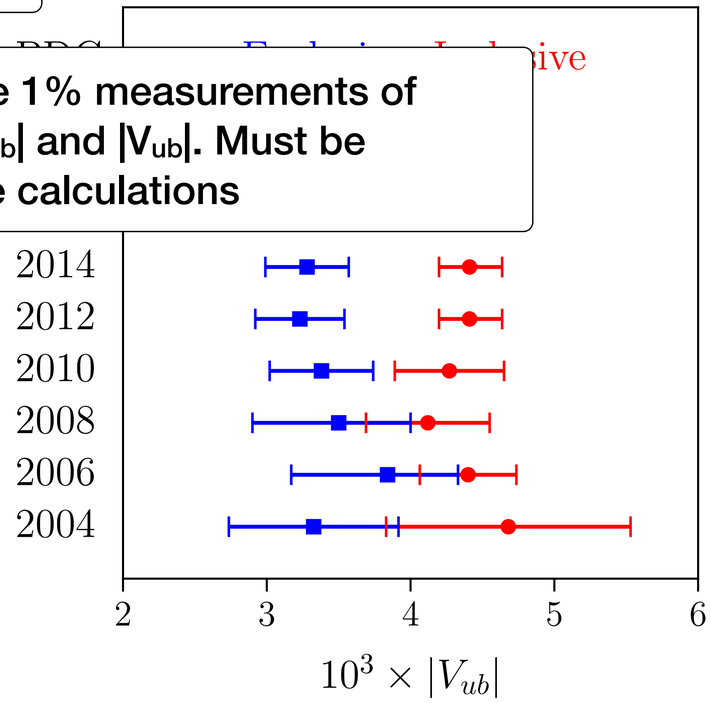
neutral B meson mixing

$|V_{cb}|$ dominates uncertainty

$|V_{ub}|$ dominates uncertainty

- Discrepancy between exclusive $B \to \pi \ell \bar{\nu}$ and inclusive determinations of $|V_{ub}|$
- Interesting ideas for inclusive on lattice

Belle II will provide 1% measurements of decay rates for $|V_{cb}|$ and $|V_{ub}|$. Must be matched by lattice calculations



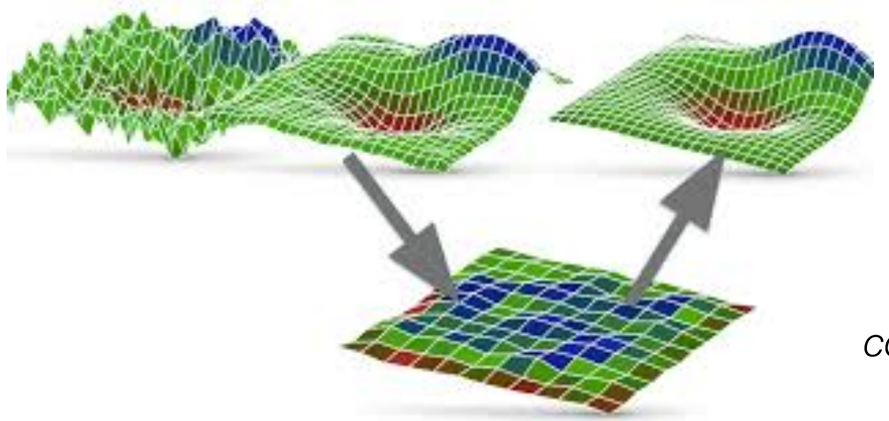
- Single complex phase of CKM matrix only source of CP violation in the SM.
- All curves must intersect at apex of unitarity triangle
- Experiments LHCb, Belle II, BESIII, KOTO, NA62, … to test whether all can be explained by single unitary matrix.

One Example: Multigrid Solvers

- *MG solvers required long term commitment:*
  Sustained Effort for 30 years continues

- *Wilson MG began in* *1990*
- *First successful adaptive approach* *2010*
- *WilsonIntegration in HMC evolution* *2015-2020*
- *Staggered first success in* *2018*
- *Domain Wall very active research* *2019- 2020*

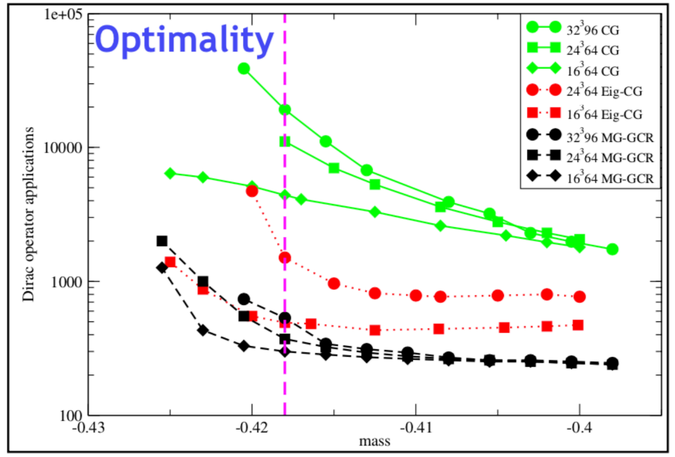
Gauge Covariant Adaptive Multigrid



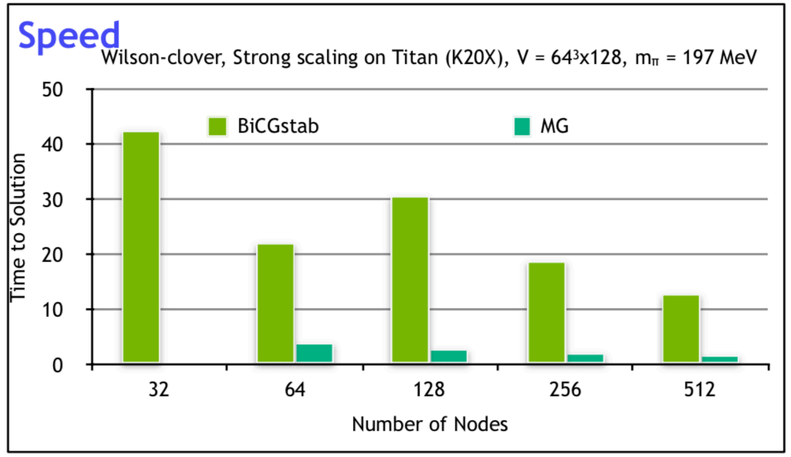
fine operator

coarse operator

Machine Learning: The computer discovers MG the coarse scale operators adapted to the gauge background



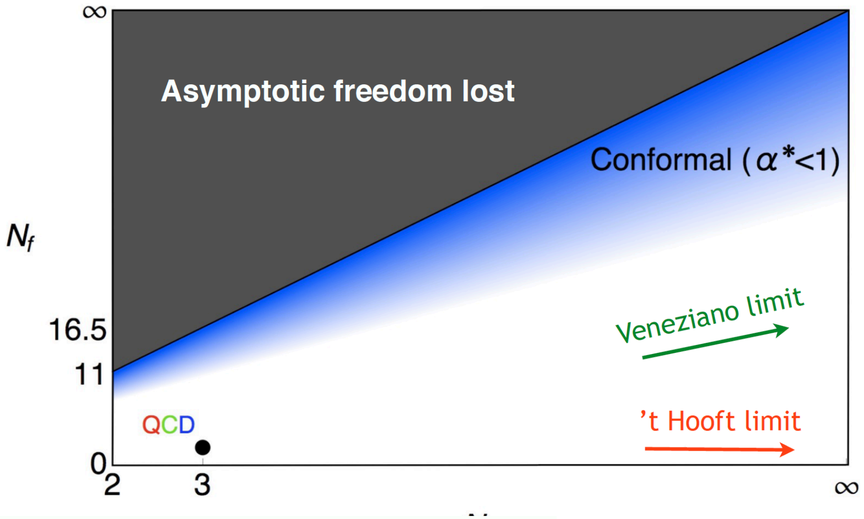
2010



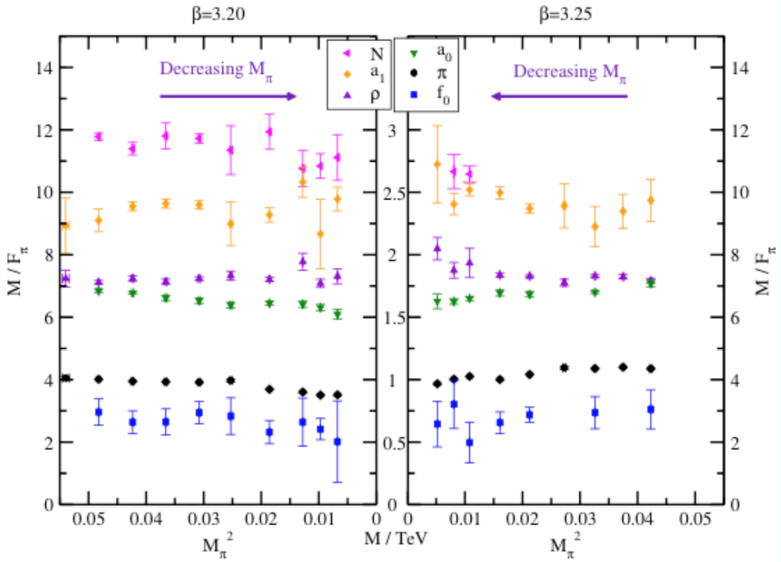
2016

BSM Gauge Theories for Higgs or Dark Matter

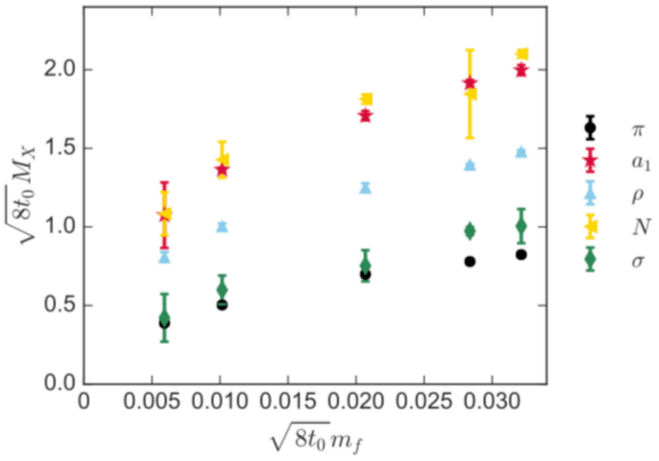
- *Exploit and Extend lattice QCD Algorithms*
  - *Framework to Change Gauge and Fermion Reps*
  - *Better Algorithms near Conformity with divergent scales*



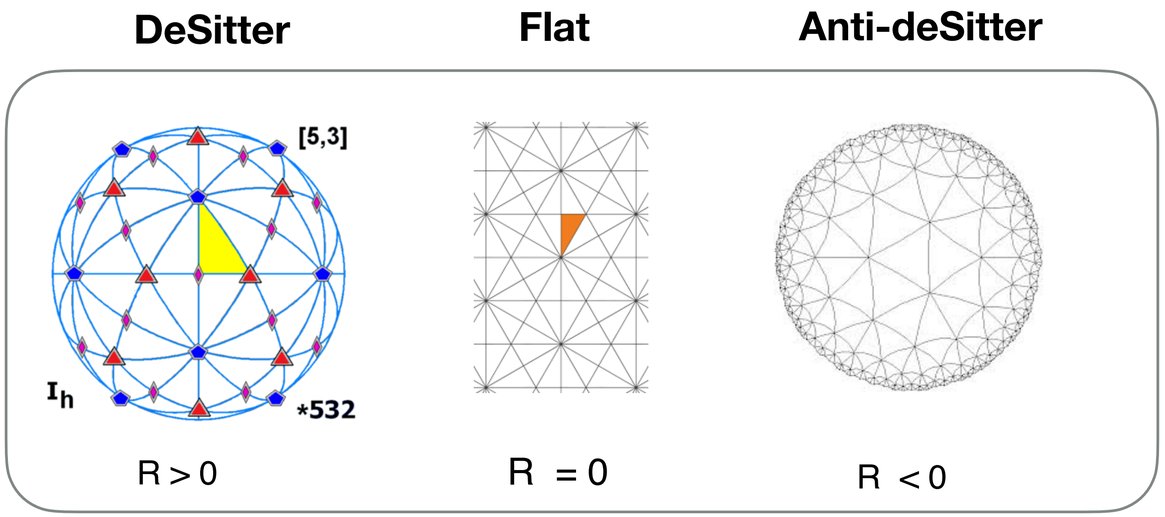
Fodor, Holland, Kuti, Wong (**LatHC collab**), arXiv:1901.06324)



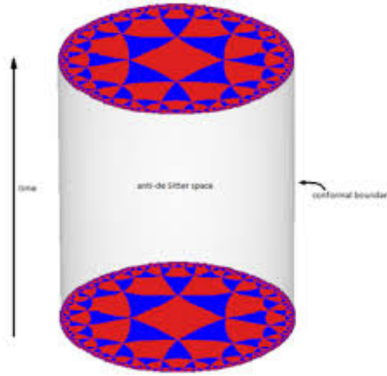
T. Appelquist et al (**LSD collab**), arXiv:1807.0841

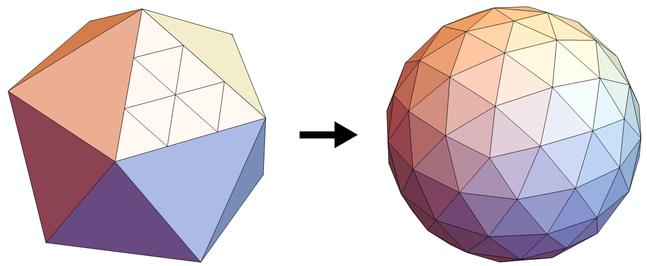


Curved Riemann (Simplicial) Lattices: CFT on the Boundary of Anti-deSitter Space.

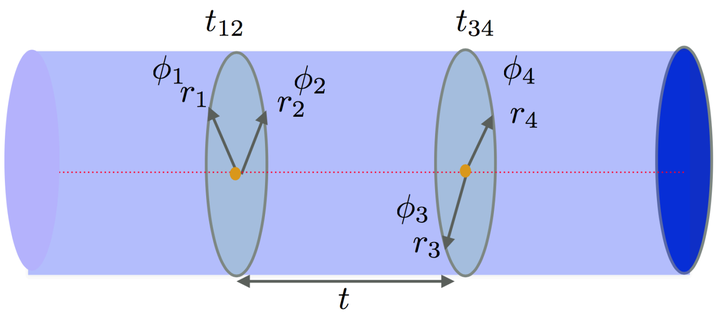


$$\mathbb{H}^d \quad \rightarrow \quad \mathbb{A}d\mathbb{S}^{d+1}$$

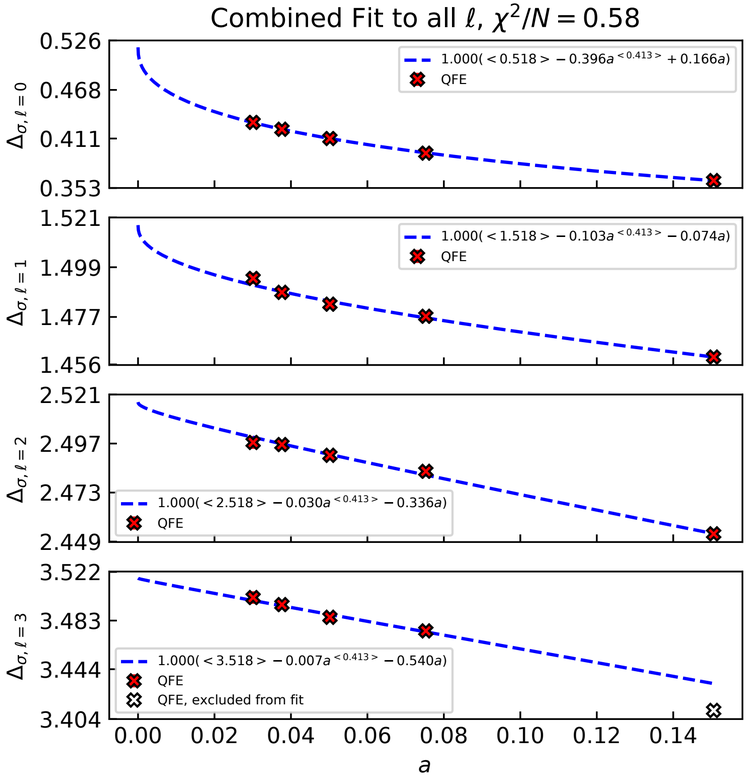




Spheres



Cylinder



Integer Descendant Spectra

Radial Quantization: Conformal map to cylinder

$$\mathbb{R}^d \implies \mathbb{R} \times \mathbb{S}^{d-1}$$

Auto-tuning & Machine Learning

- *Complexity of algorithms and target architecture outstripping "by hand parameter optimization" .*

- ***Auto tuning of control parameters is one software solution.***
  - *Algorithms are introducing 100s parameter to map algorithms to highly complex memory hierarchies.*
  - *CUDA library for NVIDIA GPUs autotunes each GPU*
  - *Autotuning across the full software stack is important.*

- ***Accelerating the Monte Carlo evolution is central challenge.***
  - *Under ECP very substantial progress is being achieve to reduce Critical slowing down in lattice evolution.*
  - *Very important to continue post ECP to explore large landscape of methods: Fourier acceleration, Riemann Manifolds etc.*
  - *Machine Learning is being pursed but the cost step to enforce an unbiased estimator is still a major challenge.*

Recommendations beyond ECP

- *Key recommendations from ECP/Transition ASCAC report*

- *Recommendation A.3. "Collaborative application support" "Transition ECP application into SciDAC-like … joint funding from ASCR and application home organizations". Past SciDAC program was critical to create components of current LQCD codes.*

- *Recommendation C.2. "Retain the current workforce"*

- *Recommendation C.3. "Strengthen ties to universities and the ecosystem" Here "ecosystem" refers to software technology experts and vendor system engineers. Universities are the pipeline for providing the young talent needed to sustain the software effort.*

- *Recommendation C.4. "Create career paths for scientific software professionals" For Lattice QCD, lab professionals at ANL, BNL, Fermilab, and JLab have been the backbone for expertise and continuity in LQCD software development.*

- *See recommendations "ECP/Transitions" ASCAC subcommittee chaired by Prof. Roscoe Giles of Boston University provide a crucial template to sustain lattice field theory beyond 2023.*
- *https://science.osti.gov/-/media/ascr/ascac/pdf/meetings/202001/EXASCALE_Transition_Presentation.pdf?*