EXASCALE COMPUTING PROJECT

Brookhaven National Laboratory

Progress towards an improved lattice calculation of Standard Model direct CP-violation in kaon decays

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(RBC & UKQCD collaborations)

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Motivation

- Likely explanation for matter/antimatter asymmetry in Universe, baryogenesis, requires violation of CP.
- Amount of CPV in Standard Model appears too low to describe measured M/AM asymmetry: tantalizing hint of new physics.
- Direct CPV first observed in late 90s at CERN (NA31/NA48) and Fermilab (KTeV) in $K^0 \rightarrow \pi\pi$:

$$\eta_{00} = \frac{A(K_L \rightarrow \pi^0\pi^0)}{A(K_S \rightarrow \pi^0\pi^0)}, \qquad \eta_{+-} = \frac{A(K_L \rightarrow \pi^+\pi^-)}{A(K_S \rightarrow \pi^+\pi^-)}.$$

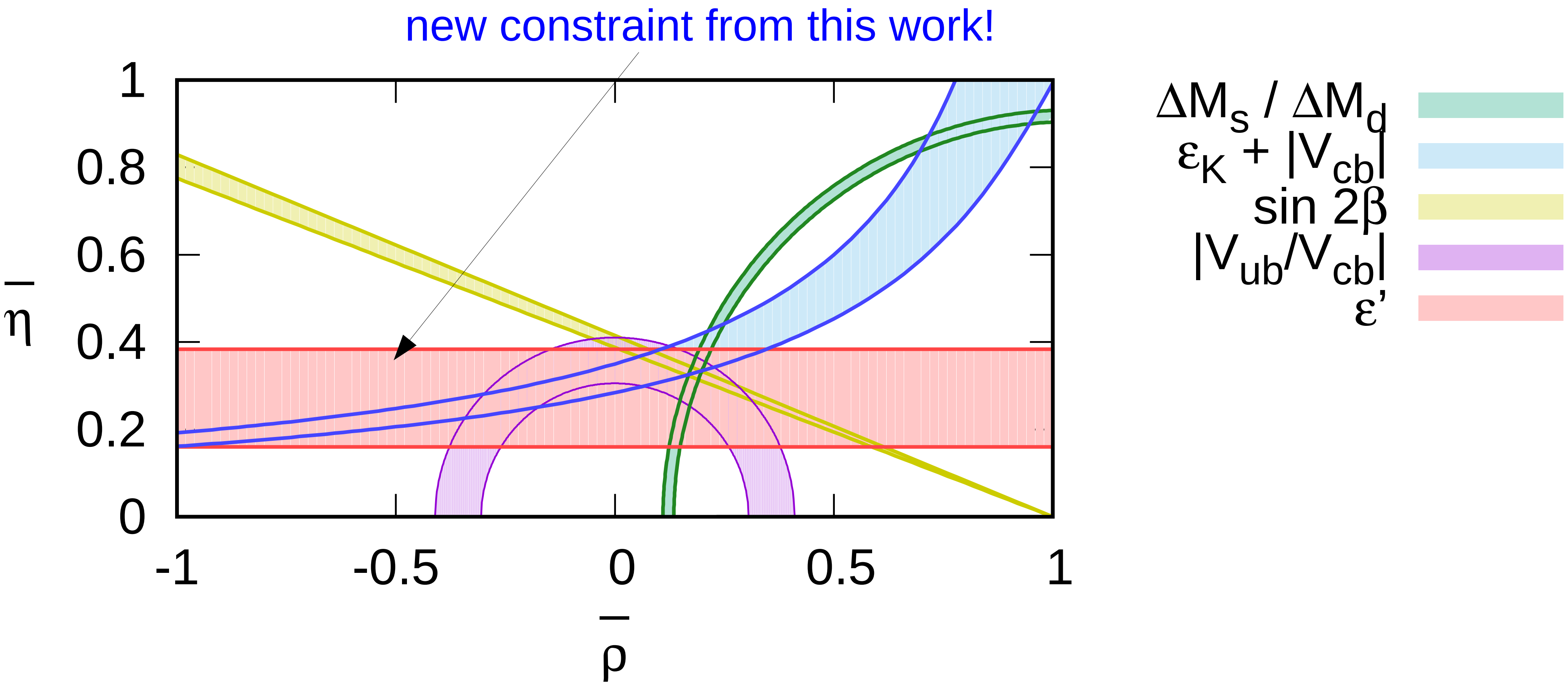
$$\mathrm{Re}(\epsilon'/\epsilon) \approx \frac{1}{6}\left(1 - \left|\frac{\eta_{00}}{\eta_{\pm}}\right|^2\right) = 16.6(2.3) \times 10^{-4} \quad \text{(experiment)}$$

measure of direct CPV

measure of indirect CPV

- Small size of ε' makes it particularly sensitive to new direct-CPV introduced by many BSM models.
- Looking for deviations from experiment may help shed light on origin of M/AM asymmetry.

- A Standard Model prediction of ε' also provides a new horizontal band constraint on CKM matrix in ρ-η plane:


new constraint from this work!

- While underlying weak process occurs at high energies ~M_W=80 GeV, K → ππ decays receive large corrections from low-energy hadronic physics O(Λ_{QCD})~250 MeV.
- Lattice QCD is the only known *ab initio*, **systematically improvable** technique for studying non-perturbative QCD.

Overview of calculation

$$A(K^0 \to \pi^+\pi^-) = \sqrt{\frac{2}{3}} A_0 e^{i\delta_0} + \sqrt{\frac{1}{3}} A_2 e^{i\delta_2} \,,$$
$$A(K^0 \to \pi^0\pi^0) = \sqrt{\frac{2}{3}} A_0 e^{i\delta_0} - 2\sqrt{\frac{1}{3}} A_2 e^{i\delta_2} \,.$$

$$\Longrightarrow \quad \epsilon' = \frac{i\omega e^{i(\delta_2-\delta_0)}}{\sqrt{2}} \left(\frac{\mathrm{Im}A_2}{\mathrm{Re}A_2} - \frac{\mathrm{Im}A_0}{\mathrm{Re}A_0} \right)$$

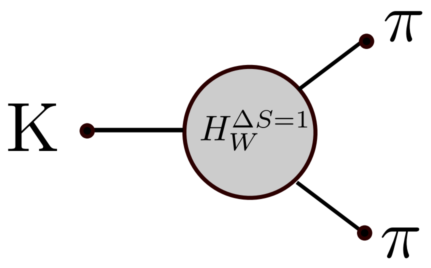
ππ phase shifts

$$\boxed{\omega = \mathrm{Re}A_2/\mathrm{Re}A_0}$$

I=2 decay

I=0 decay

- **Hadronic energy scale << M_W – use weak effective theory (3 flavors)**



renormalization
matrix (mixing)
Use RI-SMOM
convert to MSbar
perturbatively

LL finite-volume correction

$$A^I = F \frac{G_F}{\sqrt{2}} V_{ud}^* V_{us} \sum_{i=1}^{10} \sum_{j=1}^{7} \left[\left(z_i(\mu) + \tau y_i(\mu) \right) Z_{ij}^{\mathrm{lat}\to\overline{\mathrm{MS}}} M_j^{I,\,\mathrm{lat}} \right]$$

perturbative Wilson coeffs.

$$M_j^{I,lat} = \langle (\pi\pi)_I | Q_j | K \rangle$$ (lattice)

10 effective four-quark operators

$$\tau = -\frac{V_{ts}^* V_{td}}{V_{us}^* V_{ud}} = 0.0014606 + 0.00060408i$$

Imaginary part solely responsible for CPV
(everything else is pure-real)

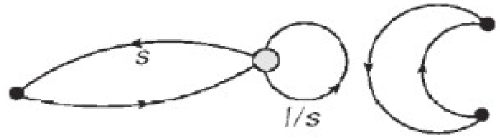
I=2 calculation

[Phys.Rev. D91 (2015) no.7, 074502]

- A_2 can be measured very precisely using “standard” lattice techniques.
- Most recent result (2015):
  - Computed with large, ~ (5.5 fm)^3 volumes
  - Physical quark masses
  - Two lattice spacings (2.36 GeV and 1.73 GeV) → Continuum limit taken.
- <1% statistical error!
- 10% and 12% total errors on Re(A_2) and Im(A_2) resp.
- Dominant sys. errors due to truncation of PT series in computation of renormalization and Wilson coefficients.

I=0 Calculation

- A_0 is more difficult than A_2, primarily because I=0 ππ state has *vacuum quantum numbers.*
- *“Disconnected diagrams”* dominate statistical noise

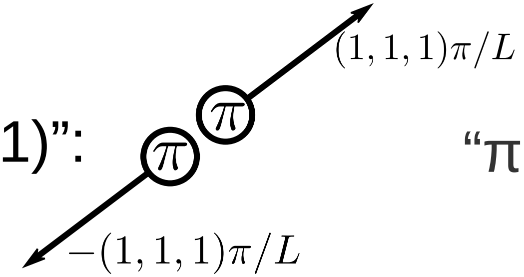


“type4”

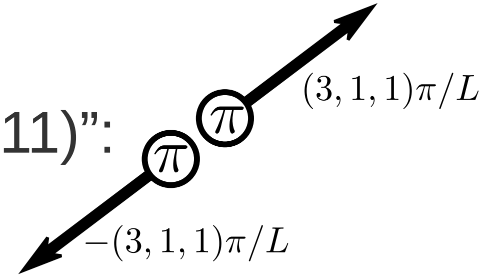
2020 calculation [arXiv:2004.09440]

- Physical quark masses on single, coarse lattice (a^{-1}= 1.38 GeV) but with large (4.6 fm)^3 physical volume to control FV errors.
- G-parity boundary conditions remove dominant unphysical contribution from stationary ππ state.
- 3x ππ operators allow clean isolation of physical decay component.

“ππ(111)”:



“ππ(311)”:



$$\boxed{\sigma} = \frac{1}{\sqrt{2}}(\bar{u}u + \bar{d}d)$$

- Achieved O(10%) statistical precision on both Re(A_0) and Im(A_0)!
- O(20%) systematic errors

Current result for ε’

$$\mathrm{Re}\left(\frac{\varepsilon'}{\varepsilon}\right) = \mathrm{Re}\left\{\frac{i\omega e^{i(\delta_2-\delta_0)}}{\sqrt{2}\varepsilon}\left[\frac{\mathrm{Im}A_2}{\mathrm{Re}A_2} - \frac{\mathrm{Im}A_0}{\mathrm{Re}A_0}\right]\right\}$$

$$= 0.00217\underbrace{(26)}_{\text{stat}}\underbrace{(62)}_{\text{sys}}\underbrace{(50)}_{\text{IB + EM}}$$

Consistent with experimental result:

$$\mathrm{Re}(\epsilon'/\epsilon)_{\mathrm{expt}} = 0.00166(23)$$

- In order to match precision of experiment we must focus on addressing the systematic errors.
- Primary systematic errors:
  - Wilson coefficients: 12%
  - Isospin breaking + electromagnetic effects: 23%
  - Finite lattice spacing: 12%

Wilson coefficients

- Perturbative Wilson coefficients incorporate high-energy physics and running down to 3-flavor theory.
- Currently computed in $\overline{\text{MS}}$ scheme to NLO

  [Buchalla *et al.* Rev. Mod. Phys. 68, 1125]
- Matching to renormalied lattice calculation is performed at high energy (4 GeV)
- However PT is still used internally to cross the charm threshold at m_c=1.3 GeV → significant systematic error ~12%
- Progress towards a complete NNLO calculation is underway which can be expected to significantly improve this error.

  [Cerda-Sevilla *et al.* Acta Phys.Polon.B 4 (2018) 1087-1096]
- We are also investigating a direct non-perturbative calculation of the 4f → 3f matching
  - Directly compare 4f and 3f matrix elements on a 3f background gauge field
  - Position space technique reduces mixing with irrelevant operators
  - Preliminary demonstration on 16^3x32, a^{-1}=1.78 GeV DWF ensemble shows promising potential in approach

    [M. Tomii, PoS LATTICE2019 (2020)]
- In longer term a direct 4f calculation will largely eliminate this error but requirement for high statistics, large volume and fine lattice spacing make this presently unfeasible.

Isospin breaking + EM effects

- Simulation does not include isospin breaking or EM effects.
- Typically these effects are O(1%)
- However $\epsilon' \propto \mathrm{Re}(A_2)/\mathrm{Re}(A_0) \approx 1/22.45$ small due to "ΔI=1/2 rule", a non-perturbative QCD effect.
- Thus relative of EM+IB on A_2 and hence ε' expected O(20%).
- Current best determination uses NLO χPT and $1/N_c$ expansion, predicts 23% correction → separate sys err.

[Cirigliano *et al*, JHEP 02 (2020) 032]

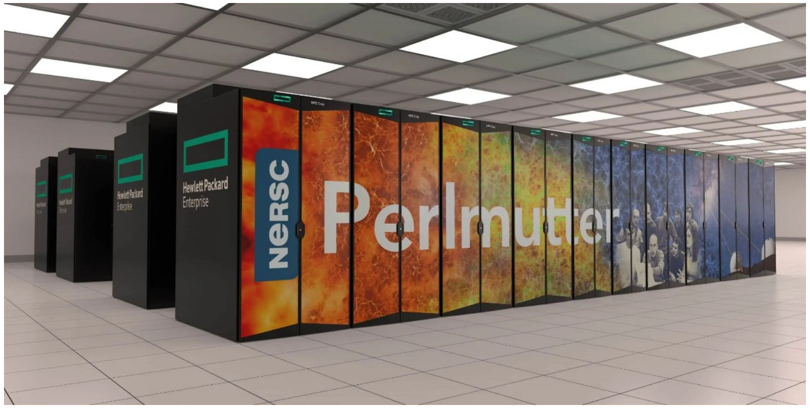
- Developing approaches to measuring using lattice QCD. Challenging:
  - Need to reconcile long-distance nature of QED with the local interaction assumptions of the Luscher FV formalism
  - The mixing of final state two-pions by isospin breaking
  - Soft-photon emission introducing additional final states
- Promising start in this direction: A complete demonstration of calculation of (dominant) Coulomb correction to $\pi^+\pi^+$ scattering

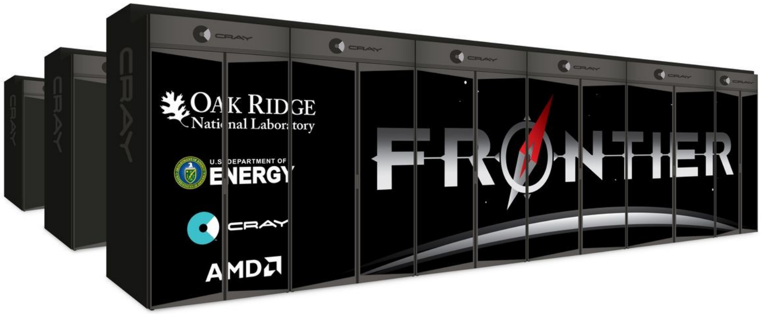
[Christ *et al.* PRD 106 (2022) 1, 014508]

- Additional challenges remain including computing transverse radiation contribution.

Discretization errors

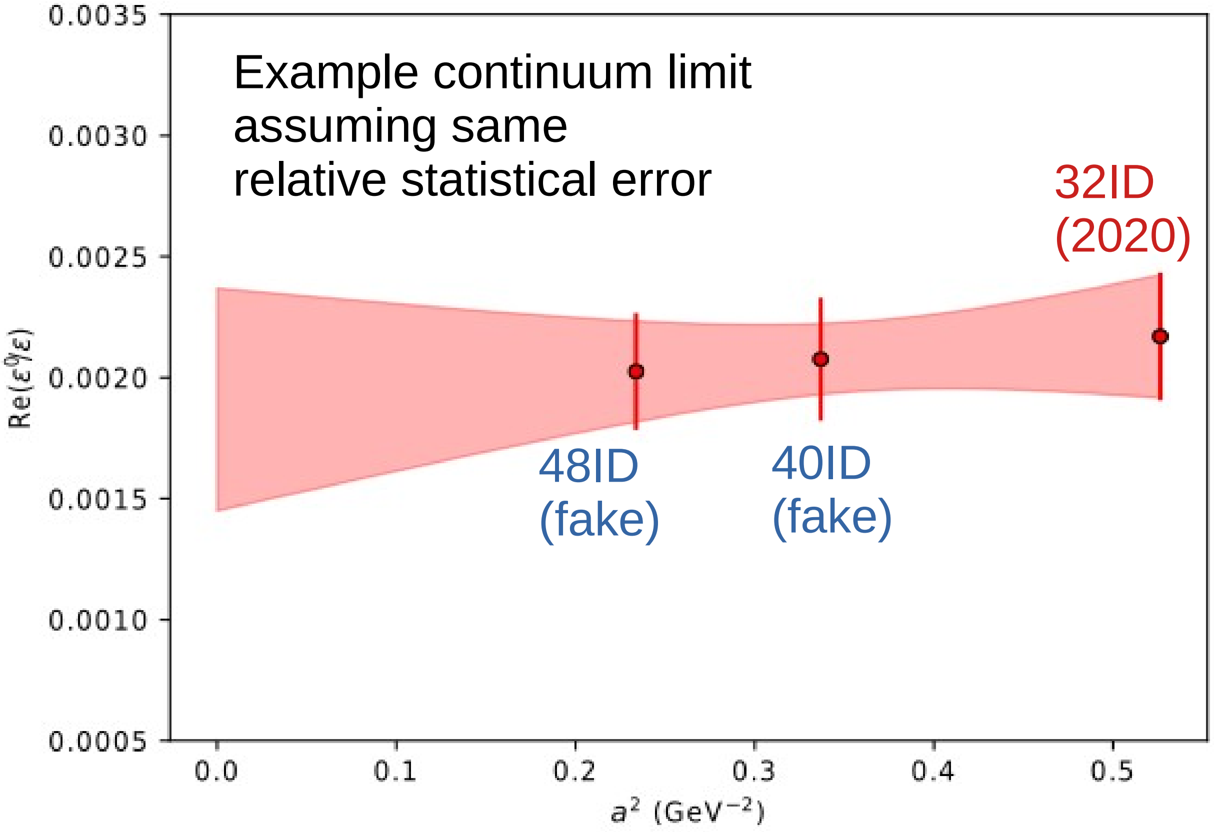
- Primary pure-lattice error (~12%) and “easiest” to address
- Currently estimated using scaling of I=2 ops. but may be significant “error on the error”.
- Exploit new exascale and pre-exascale hardware to perform continuum limit.
- Extensive effort in porting measurement code to Intel, NVidia and AMD GPUs almost complete.
- G-parity BCs requires us to also generate new lattices.





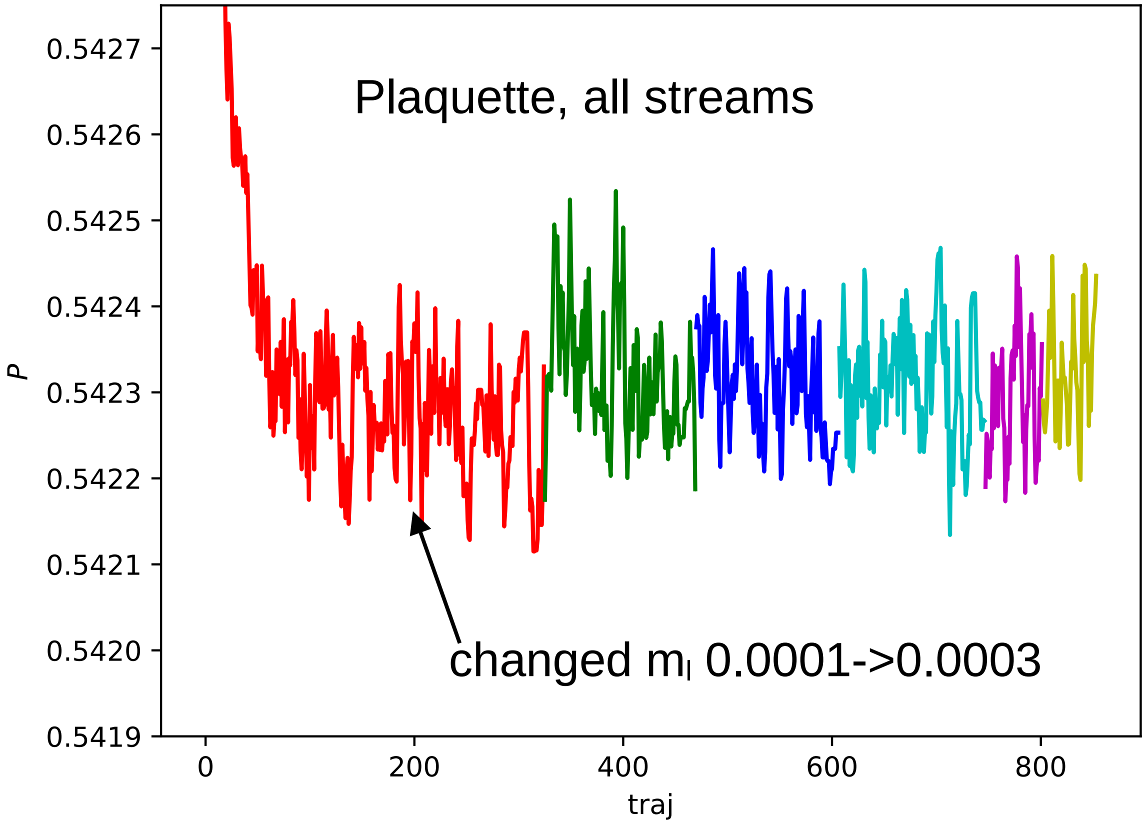
Continuum extrapolation lever-arm

- Utilizing and expanding on HMC capacities of Grid framework to run efficiently on GPUs
- Two new lattices:
  - 40ID: 40^3x64x12 DWF+ID
    a^{-1}=1.723 GeV
  - 48ID: 48^3x64x12 DWF+ID
    a^{-1}=2.068 GeV
- Physical pion masses
- GPBC in 3 directions
- Same physical volume (4.6 fm)^3 →
  ππ energy remains the same as before and interaction remains physical.



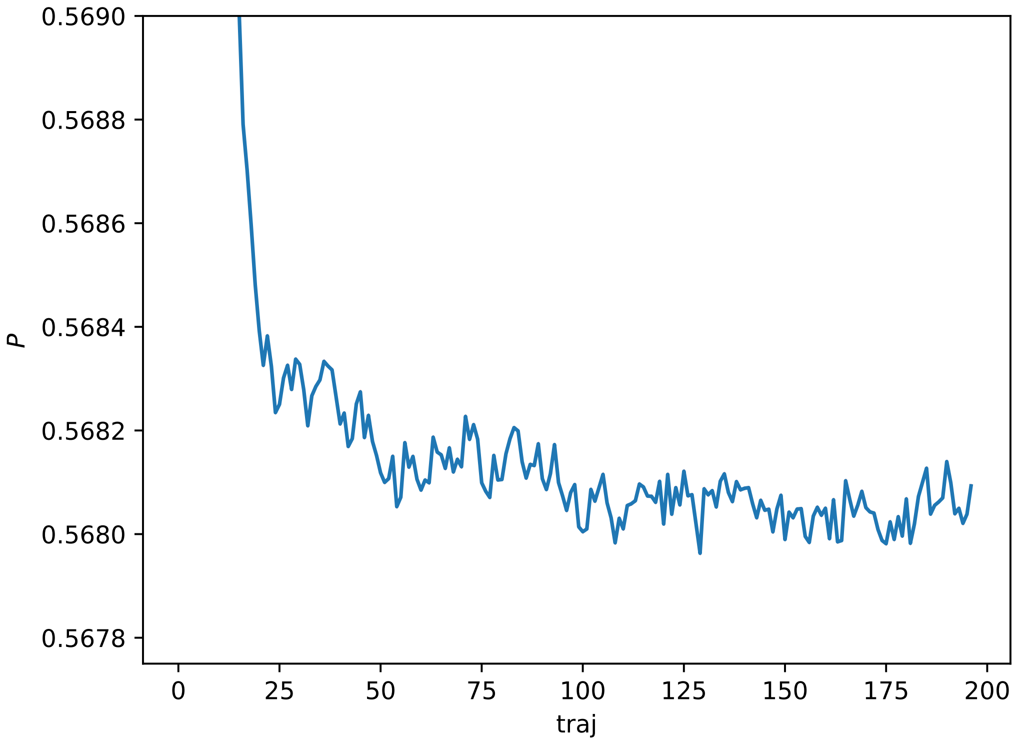
40ID status

- Tuning and running performed on Perlmutter machine.
- Thermalized with 1 initial stream.
- 5 additional streams started from thermalized configs.
- Job time ~6hrs on 32 nodes (128 NVidia A-100 GPUs)
- Severely hampered by Slingshot 10 network
  - Expect significant improvements with new phase 2 (Slingshot 11) network.



48ID status

- Tuning progress hampered by wall-clock time limits on Perlmutter and weak network
- Expect significant improvement with Slingshot 11 network



K→ππ without G-parity

- Independent calculation of ϵ’ using multiple operators to extract on-shell matrix elements as excited-state contributions in a periodic lattice is well under way.
    - Avoid complications of using G-parity BCs
    - Uses existing MDWF+I ensembles with physical pion masses
    - 2 lattice spacings allowing continuum limit

[See Masaaki Tomii’s talk - next!]

Conclusions

- Result for ε’ consistent with experimental value but total error is still ~3.6x that of experiment.
- ε’ remains a promising avenue to search for new physics, but greater precision is required.
- RBC & UKQCD are working to improve all 3 primary systematic errors:
  - Attempt to address EM+IB errors through lattice calculation (hard!).
  - Investigating direct lattice calculation of 3f-4f matching in Wilson coefficients.
  - (Potential for NNLO calculation of EM+IB in near future may reduce urgency.)
  - Addressing discretization error by introducing two finer lattices
  - Independent calculation with different systematics using periodic BCs.