PACS10 project

– larger than $(10\text{fm})^4$ volume simulation at physical point –

Takeshi Yamazaki

University of Tsukuba

Center for Computational Sciences

Challenges and opportunities in Lattice QCD simulations and related fields

@ Riken CCS, February 15-17 2023

PACS10 project

PACS Collaboration

Tsukuba

N. Ishizuka, Y. Kuramashi, K. Sato, E. Shintani,
T. Taniguchi, N. Ukita, T. Yamazaki, T. Yoshié

Hiroshima

K.-I. Ishikawa, N. Namekawa

Kyoto

H. Watanabe

Riken-CCS

Y. Aoki, Y. Nakamura

Tohoku

S. Sasaki, R. Tsuji

PACS10 project

PACS Collaboration

Tsukuba	N. Ishizuka, Y. Kuramashi, K. Sato, E. Shintani, T. Taniguchi, N. Ukita, T. Yamazaki, T. Yoshié
Hiroshima	K.-I. Ishikawa, N. Namekawa
Kyoto	H. Watanabe
Riken-CCS	Y. Aoki, Y. Nakamura
Tohoku	S. Sasaki, R. Tsuji

Larger than $(10\ \mathrm{fm})^4$ volume

PACS10 project

PACS Collaboration

Tsukuba	N. Ishizuka, Y. Kuramashi, K. Sato, E. Shintani, T. Taniguchi, N. Ukita, T. Yamazaki, T. Yoshié
Hiroshima	K.-I. Ishikawa, N. Namekawa
Kyoto	H. Watanabe
Riken-CCS	Y. Aoki, Y. Nakamura
Tohoku	S. Sasaki, R. Tsuji

Larger than (10 fm)^4 volume

Purpose of PACS10 project

Removing main systematic uncertainties in lattice QCD

three $N_f = 2 + 1$ ensembles at physical m_π on (10 fm)^4 volume

Outline

- PACS10 project
  - PACS10 configuration
- Results with PACS10 configuration
  - Light meson spectrum
  - Hadron vacuum polarization
  - Electromagnetic meson form factors
- Kaon semileptonic decay form factor
- Summary

PACS10 project since 2016

	PACS10 configuration		
$L^3 \cdot T$	128^4	160^4	256^4
L [fm]	10.9	10.2	∼10
a [fm]	0.08	0.06	0.04
m_π [GeV]	0.135	0.138	∼0.135
m_K [GeV]	0.497	0.505	∼0.497
Machine	OFP	OFP	OFP→Fugaku
Node	512	512	2048→16384

OFP: Oakforest-PACS (KNL machine)

PACS10 configuration

$N_f = 2+1$ nonperturbatively $O(a)$ improved Wilson clover quark action with 6-stout smeared link + Iwasaki gauge action

same actions as HPCI Field 5 project using K computer [PoS LATTICE2015 (2016) 075]

a^{-1} determined from Ξ baryon mass

Fugaku co-design outcome:

QCD Wide SIMD (QWS) Library for Fugaku [Ishikawa *et al.*:CPC(2023)]

PACS10 project since 2016

	PACS10 configuration			
$L^3 \cdot T$	128^4	160^4	256^4	64^4
L [fm]	10.9	10.2	∼10	5.5
a [fm]	0.08	0.06	0.04	0.08
m_π [GeV]	0.135	0.138	∼0.135	0.138
m_K [GeV]	0.497	0.505	∼0.497	0.498
Machine	OFP	OFP	OFP→Fugaku	OFP
Node	512	512	2048→16384	128

OFP: Oakforest-PACS (KNL machine)

PACS10 configuration

$N_f = 2+1$ nonperturbatively $O(a)$ improved Wilson clover quark action with 6-stout smeared link + Iwasaki gauge action

Removing main systematic uncertainties in $N_f = 2+1$ lattice QCD

- chiral extrapolation
- finite volume effect

  Coarsest lattice spacing: finite volume study using 128^4 and 64^4
- finite lattice spacing effect

Results of PACS10 project

precise determination of physical quantity from lattice QCD

I. quantitatively understand property of hadrons

reproduce experimental values in high accuracy

- Hadron spectrum
- Nucleon form factor Sasaki
- Light meson electromagnetic form factor

II. search for new physics beyond the standard model

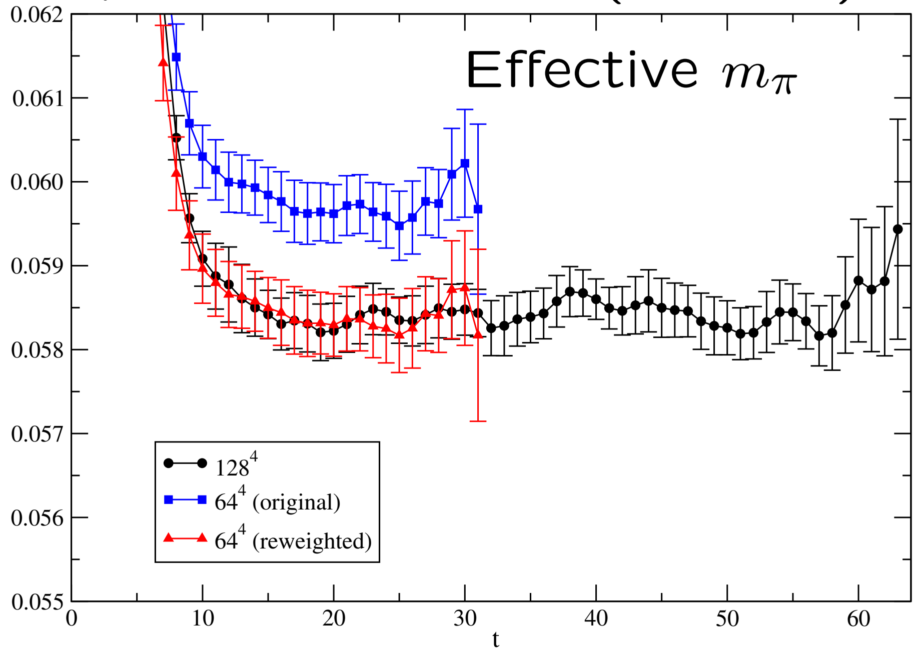
discrepancy between theoretical calculation and experiment

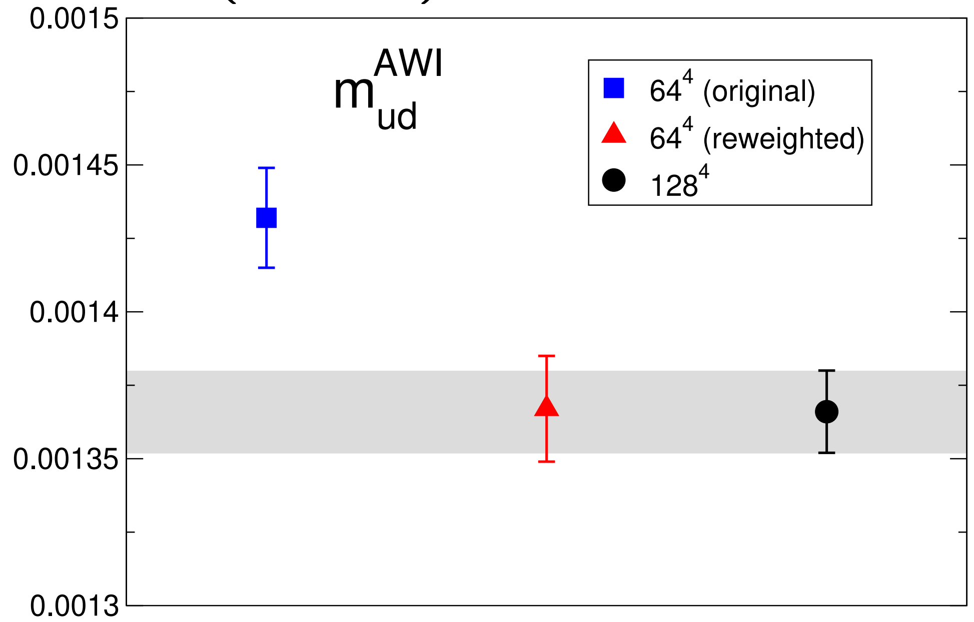
- Nucleon charge Tsuji
- Proton decay matrix element
- Hadron vacuum polarization
- Kaon semileptonic decay form factor

Finite volume study of m_π

[PACS:PRD99(2019)]

Comparison with 128^4 $(10.8\ \text{fm})^4$ and 64^4 $(5.5\ \text{fm})^4$





fixed κ_{ud}: 128^4 and 64^4 (original)

- m_π on 64^4 (original) is 3 MeV larger than 128^4
- similar behavior in $m_{\text{ud}}^{\text{AWI}}$

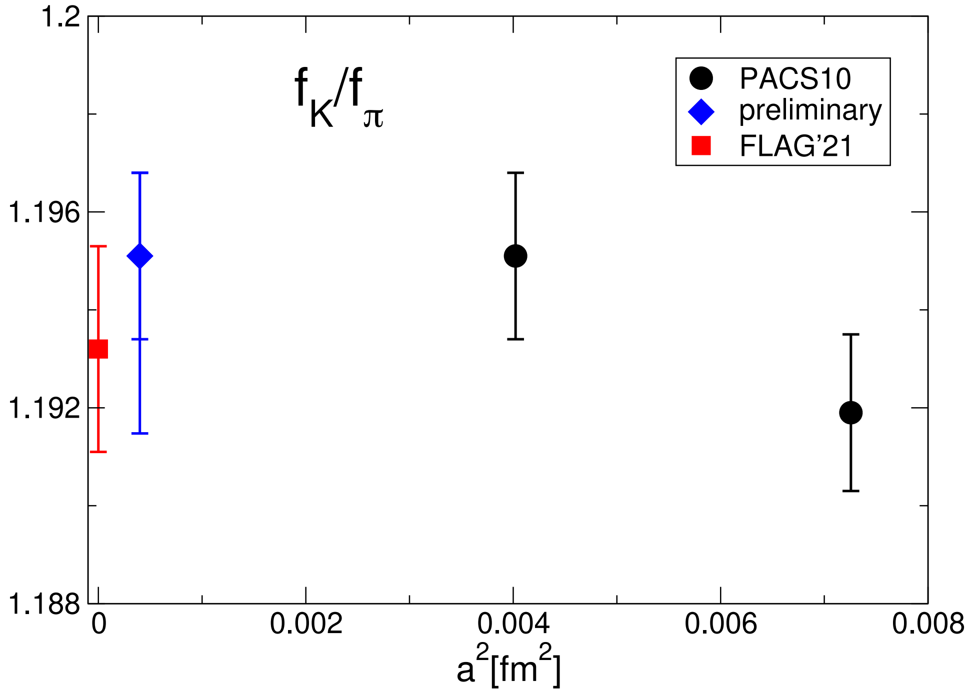
fixed $m_{\text{ud}}^{\text{AWI}}$: 128^4 and 64^4 (reweighted)

- discrepancy disappears

$\rightarrow$ discrepancy not physical finite V effect, but due to shift of κ_c

less than 0.7(3)% finite V effect in m_H and f_H [PACS:PRD99(2019);PRD100(2019)]

Ratio of decay constants [Preliminary result]



$L^3 \cdot T$	128^4	160^4
a [fm]	0.08	0.06
m_π [GeV]	0.135	0.138
m_K [GeV]	0.497	0.505

Short m_π and m_K extrapolation to physial point

using m_π and m_K dependences determined from 64^4 reweigted data

Two a results are consistent with FLAG'21 value

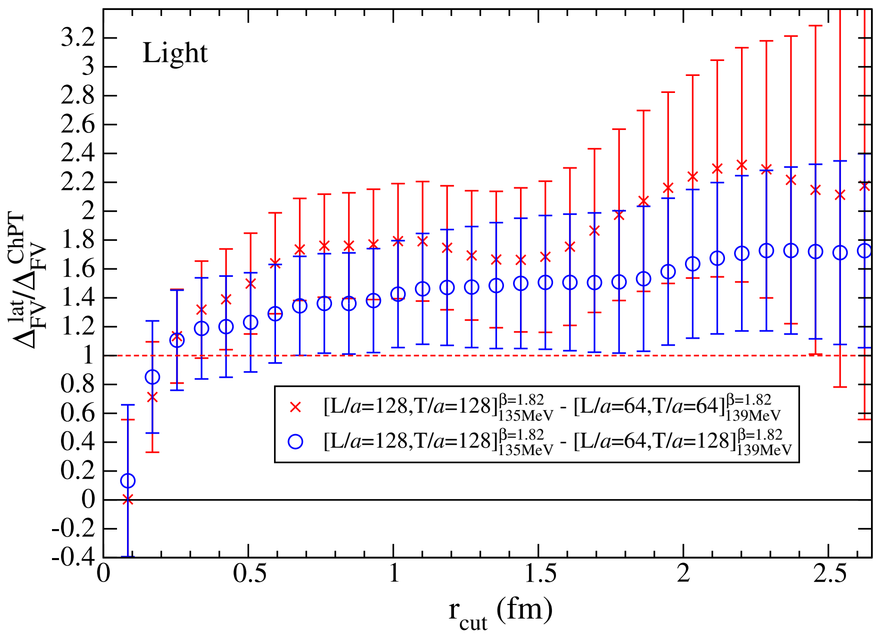
Slight upward dependence towards $a \to 0$

3rd PACS10 configuration is importand for $a \to 0$ extrapolation

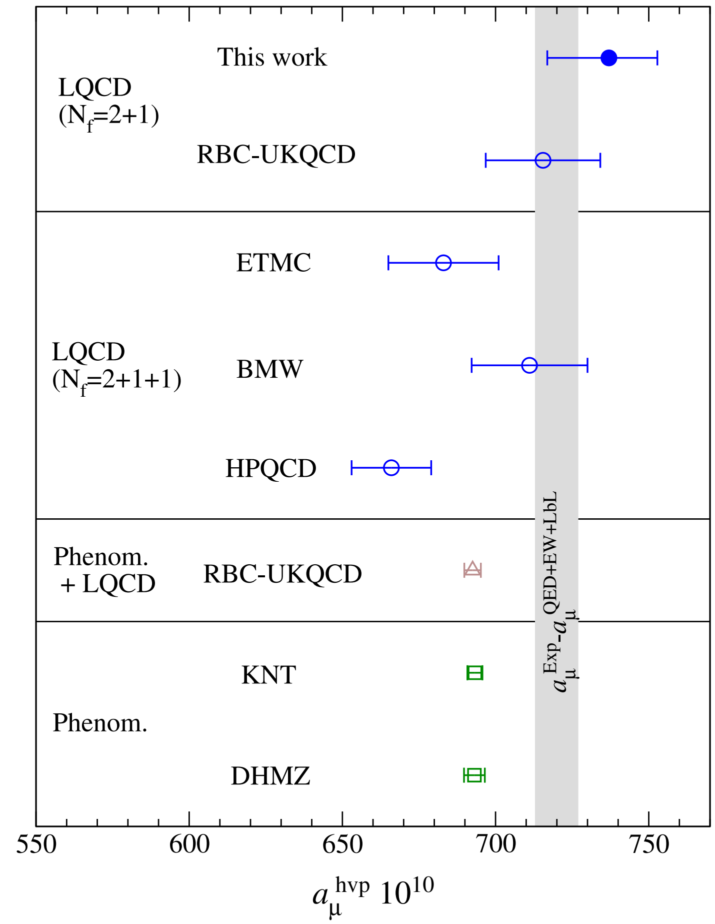
Preliminary result: Central value and statistical error from 160^4
systematic error from difference between 160^4 and 128^4

Hadron vacuum polarization

[PACS:PRD98(2018);PRD100(2019)]



r_{cut}: cut of coordinate space summation



About twice larger finite volume effect than NLO ChPT

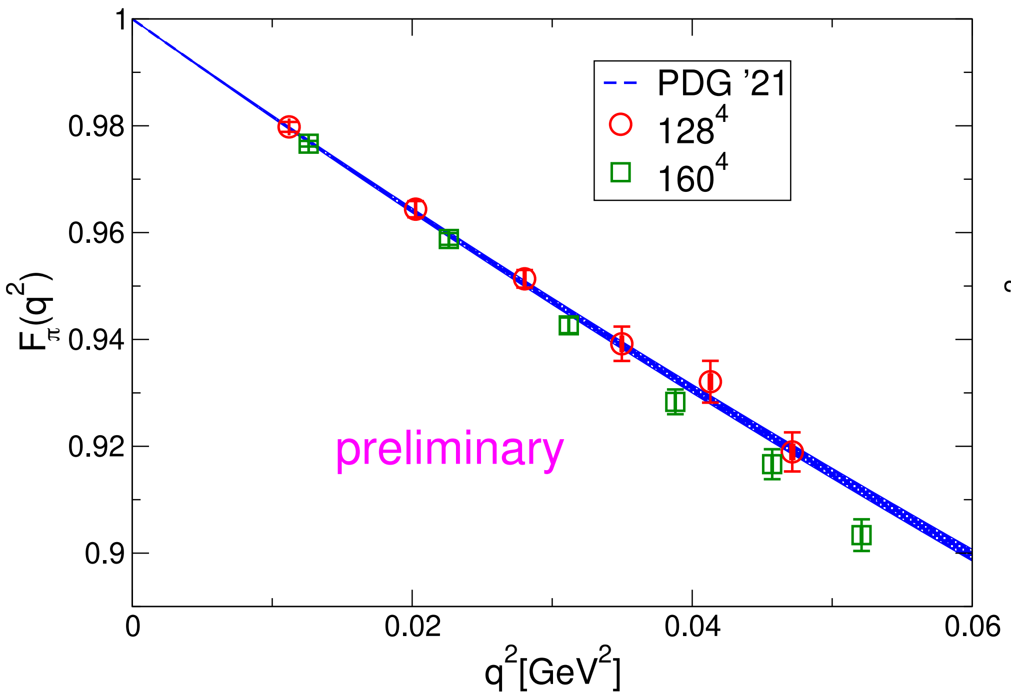
comparing between 128^4 and 64^4

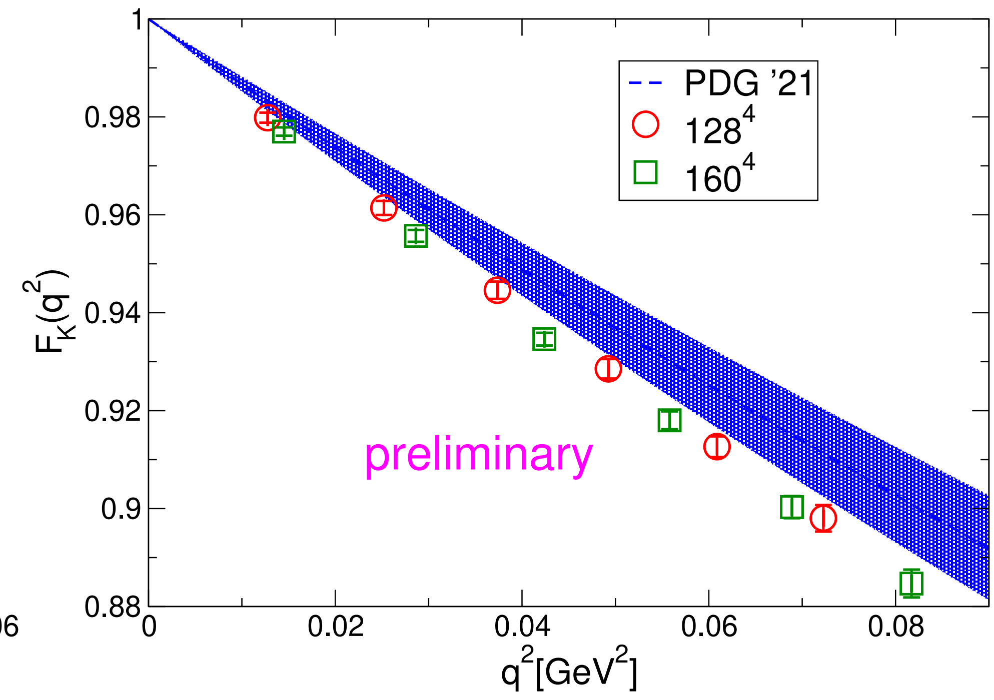
Linear continuum extrapolation using 128^4 and 160^4 w/o disconnected, IB effect

comparable with other groups and consistent with experiment

also consistent with BNL+FNAL result [Snowmass 2021:arXiv:2203.15810]

Electromagnetic meson form factors [Preliminary result]





[blue lines: PDG'21 values with monopole form]

Access to tiny q^2 thanks to huge L

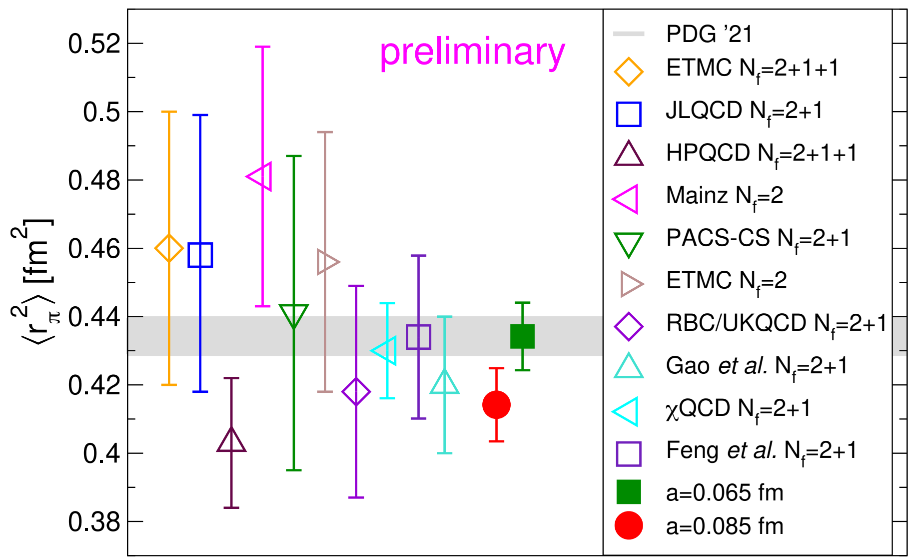
Two a data reasonably agree with PDG w/o chiral extrapolation

Seem to be small a effect in $F_K(q^2)$

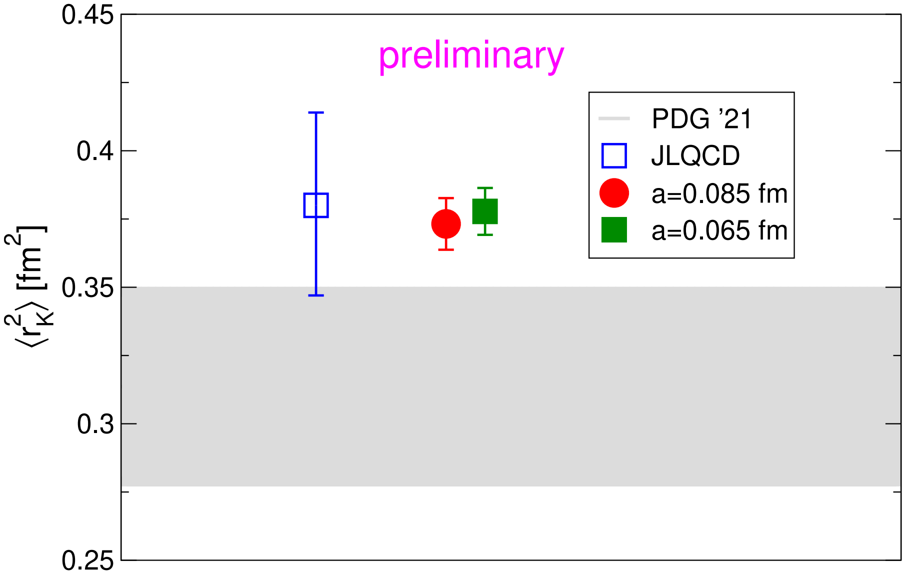
Pion and kaon charge radii [Preliminary result]

Charge radius $F(q^2) = 1 - \frac{1}{6} q^2 \langle r^2 \rangle + \cdots$

$F_\pi(q^2)$ with SU(2) NLO ChPT fit



$F_K(q^2)$ with Monopole fit



only statistical error in our results

Good agreement with other lattice results and PDG values (gray bands)

$\langle r_K^2 \rangle$: smaller error than PDG value

Direct calculation of derivative of form factor

model-independent calculation: [Sato *et al.*:PoS(Lattice2022)]; cf) [Feng *et al.*:PRD101(R)(2020)]

Kaon semileptonic ($K_{\ell 3}$) decay form factor

Introduction

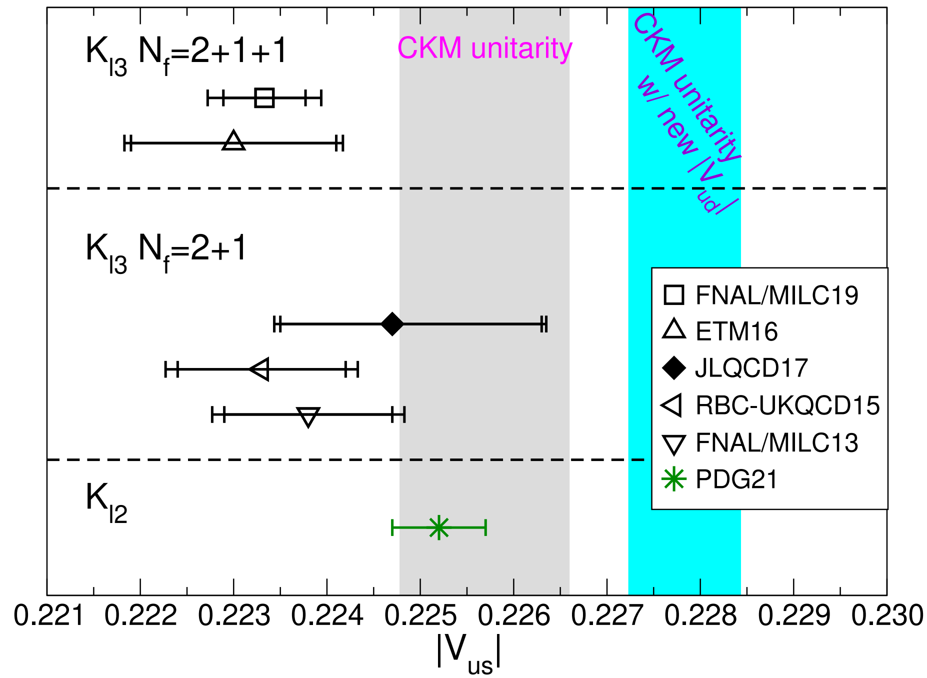
$|V_{us}|$: $\gtrsim 2\sigma$ discrepancy between experiment and standard model
$\rightarrow$ a candidate of BSM signal

Most accurate $|V_{us}|$ from $K_{\ell 3}$ decay
[FNAL/MILC19]

$\sim 2\sigma$ from SM (gray band)
using CKM unitarity $|V_{us}| \approx \sqrt{1 - |V_{ud}|^2}$

$\sim 5\sigma$ from SM w/ new $|V_{ud}|$ (cyan band)
[Seng *et al.*:PRL121,241804(2018)]

$\sim 2\sigma$ from $K_{\ell 2}$ (green star)



Important to confirm by several independent calculations

Introduction

$|V_{us}|$: $\gtrsim 2\sigma$ discrepancy between experiment and standard model
$\rightarrow$ a candidate of BSM signal

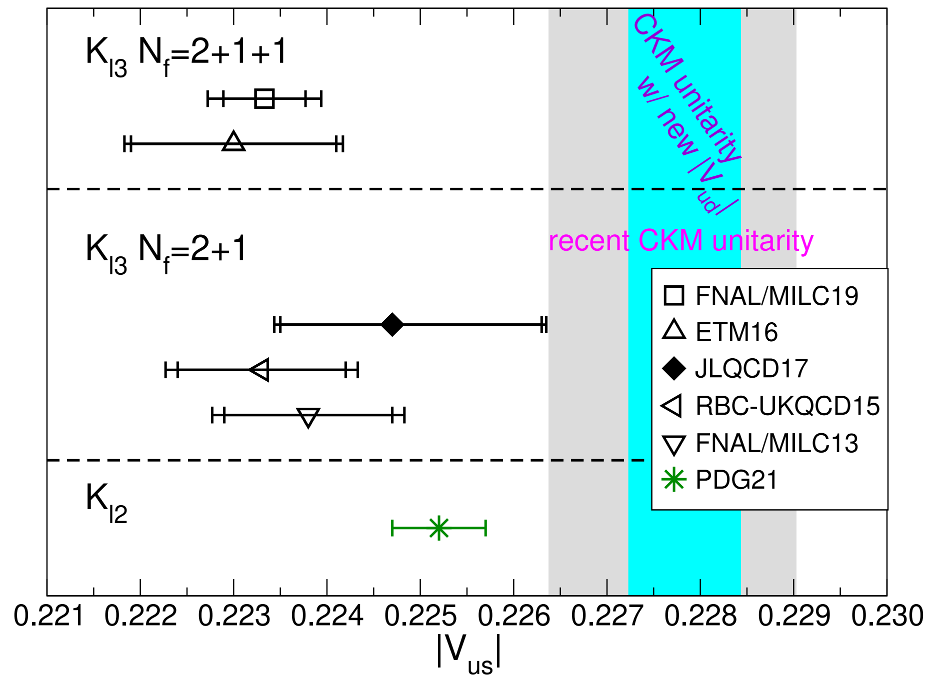
Most accurate $|V_{us}|$ from $K_{\ell 3}$ decay [FNAL/MILC19]

using CKM unitarity $|V_{us}| \approx \sqrt{1 - |V_{ud}|^2}$

$\sim 5\sigma$ from SM w/ new $|V_{ud}|$ (cyan band) [Seng *et al.*:PRL121(2018)]

$\sim 3\sigma$ from SM w/ recent $|V_{ud}|$ (gray band) [Hardy and Towner *et al.*:PRC102(2020)]

$\sim 2\sigma$ from $K_{\ell 2}$ (green star)



Important to confirm by several independent calculations

$K_{\ell 3}$ form factors with PACS10 configurations [PACS20,21]

$L = 10.9$[fm] at physical point

Negligible finite L effect, tiny q^2 region, without chiral extrapolation

Simulation parameters

[PACS:PRD101(2020);PRD106(2022)]

PACS10 configurations: $L \gtrsim 10$[fm] at physical point

β	$L^3 \cdot T$	L[fm]	a[fm]	a^{-1}[GeV]	M_π[MeV]	M_K[MeV]	$N_{\rm conf}$
1.82	128^4	10.9	0.085	2.3162	135	497	20
2.00	160^4	10.2	0.063	3.1108	138	505	20

Parameters for $K_{\ell 3}$ form factors $f_+(q^2)$ and $f_0(q^2)$

β	source	$t_{\rm sep}$[fm]	current
1.82	R-local	3.1, 3.6, 4.1	local, conserved
2.00	R-local	3.2, 3.7, 4.1	local, conserved
	R-smear	2.3, 2.7, 3.1, 3.5	local, conserved

R-local: $Z(2) \times Z(2)$ random source spread in spatial volume, spin, color spaces

R-smear: R-local + exponential smearing

[RBC-UKQCD:JHEP07,112(2008)]

Combined analysis with two source data at $\beta = 2.00$

Matrix element from $t_{\rm sep}$ dependence

Two vector currents at each β

$K_{\ell 3}$ form factors $f_+(q^2)$ and $f_0(q^2)$

$K_{\ell 3}$ form factors $f_+(q^2), f_0(q^2)$

$$\langle \pi(p)|V_\mu|K(0)\rangle = (p_K + p_\pi)_\mu f_+(q^2) + (p_K - p_\pi)_\mu f_-(q^2)$$

$$f_0(q^2) = f_+(q^2) - \frac{q^2}{M_K^2 - M_\pi^2} f_-(q^2)$$

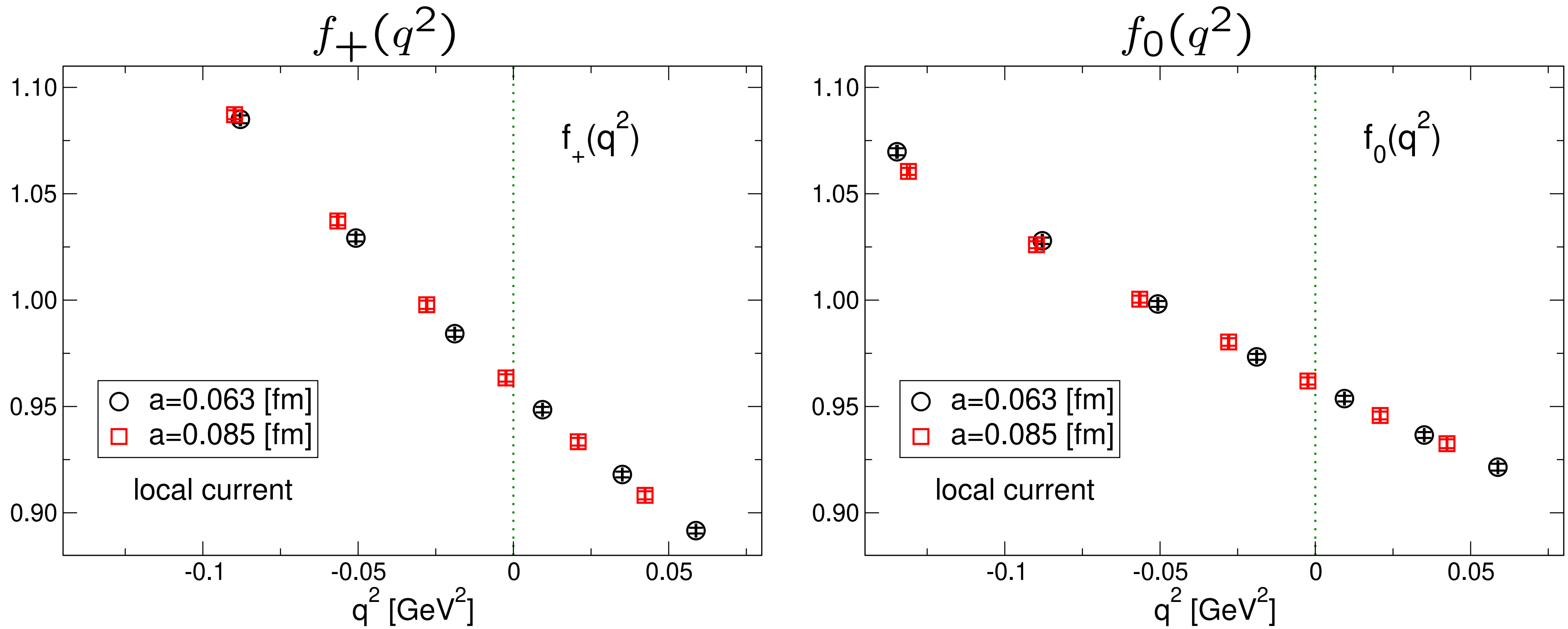
$p_K = (M_K, \mathbf{0}), p_\pi = (E_\pi, \vec{p})$
$q^2 = -(M_K - E_\pi)^2 + p^2$

$q^2 \to 0$ interpolation + $a \to 0$ extrapolation for $f_+(q^2), f_0(q^2)$
with two current data at two a

Physical quantities from $f_+(q^2), f_0(q^2)$

1. $f_+(0)\,(= f_0(0)) \to |V_{us}|$ $\quad |V_{us}|f_+(0) = 0.21654(41)$ [Moulson:PoS(CKM2016)]
2. slope and curvature
$$\lambda_+^{(n)} = \frac{M_{\pi^-}^{2n}}{f_+(0)} \frac{d^n f_+(0)}{d(-q^2)^n}, \ \lambda_0^{(n)} = \frac{M_{\pi^-}^{2n}}{f_+(0)} \frac{d^n f_0(0)}{d(-q^2)^n}$$
3. Phase space integral

$f_+(q^2)$ and $f_0(q^2)$ at two lattice spacings



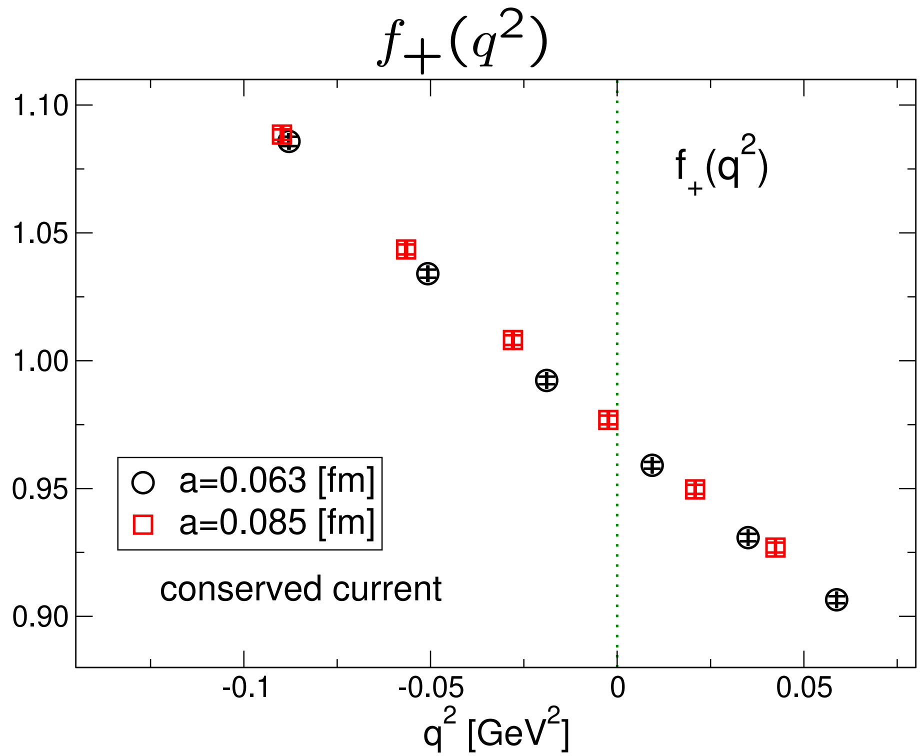
Access tiny q^2 region thanks to $L \sim 10$ [fm]

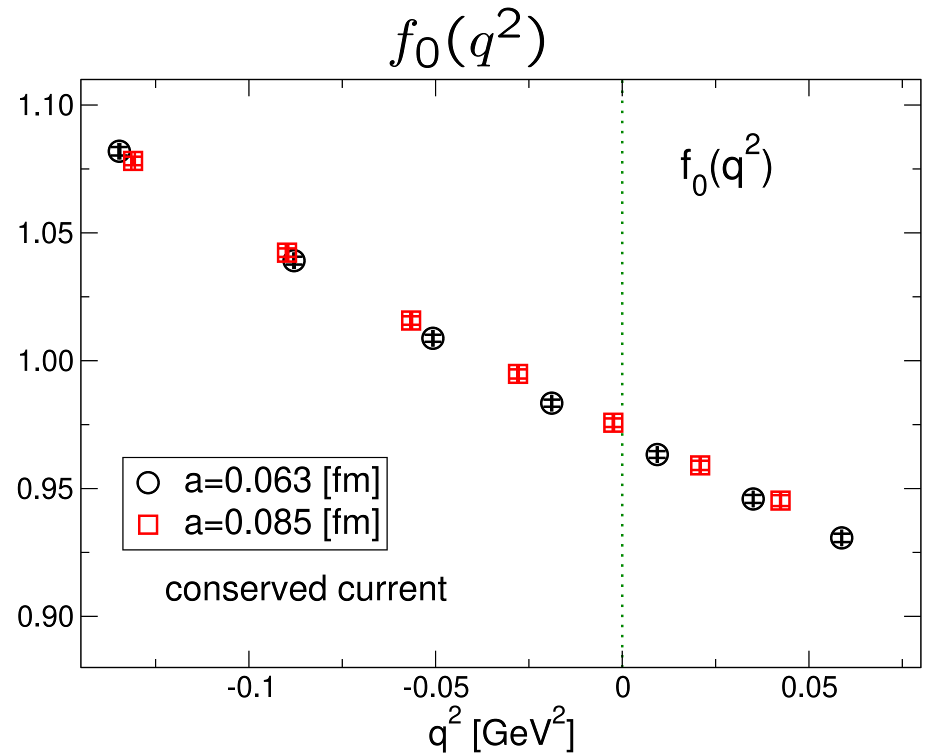
$f_+(q^2)$: No visible difference in all q^2

$f_0(q^2)$: Little difference in small q^2

$\rightarrow$ Small a effect in $q^2 \sim 0$ in local current data

$f_+(q^2)$ and $f_0(q^2)$ at two lattice spacings





Access tiny q^2 region thanks to $L \sim 10$ [fm]

Larger a effect in conserved current data

q^2 interpolation + $a \to 0$ extrapolation

Fit based on SU(3) NLO ChPT with $f_+(0) = f_0(0)$ [PACS:PRD106(2022)]

$$f_+(q^2) = 1 - \frac{4}{F_0^2} L_9(\mu) q^2 + K_+(q^2, M_\pi^2, M_K^2, F_0, \mu) + c_0 + c_2^+ q^4 + g_+^{\text{cur}}(a, q^2)$$

$$f_0(q^2) = 1 - \frac{8}{F_0^2} L_5(\mu) q^2 + K_0(q^2, M_\pi^2, M_K^2, F_0, \mu) + c_0 + c_2^0 q^4 + g_0^{\text{cur}}(a, q^2)$$

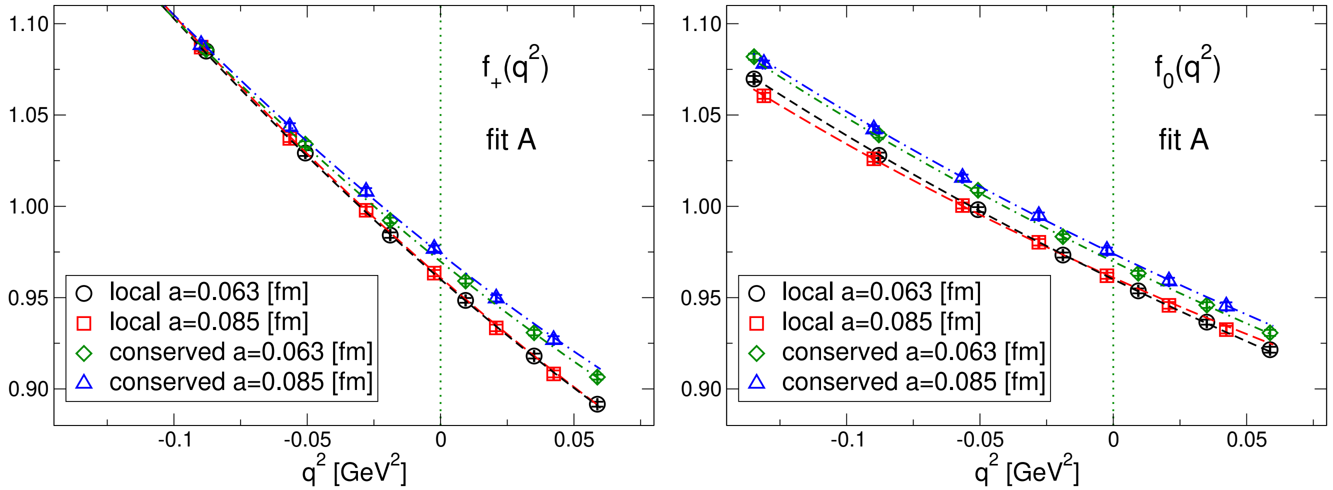
K_+, K_0: known functions ['85 Gasser, Leutwyler]

$g_{+,0}^{\text{cur}} = \sum_{n,m} e_{+,0}^{\text{cur},nm} a^n q^{2m}$, cur = local, conserved: 3 types (fit A,B,C) investigated

free parameters: $L_5(\mu), L_9(\mu), c_0, c_2^+, c_2^0 + e_{+,0}^{\text{cur},nm}$

fixed parameters: $\mu = 0.77$ GeV, $F_0 = 0.11205$ GeV

F_0 estimated from FLAG $F^{SU(2)}/F_0$ w/ $F^{SU(2)} = 0.129$ GeV



Simultaneous fit for (f_+, f_0) with (local,conserved) works well.

Tiny extrapolation to physical M_{π^-} and M_{K^0} using same formulas

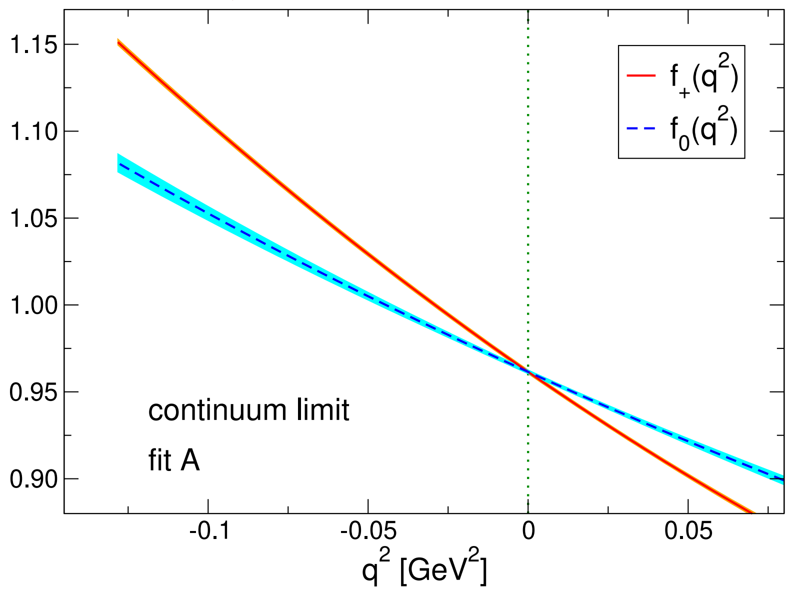
q^2 interpolation + $a \to 0$ extrapolation

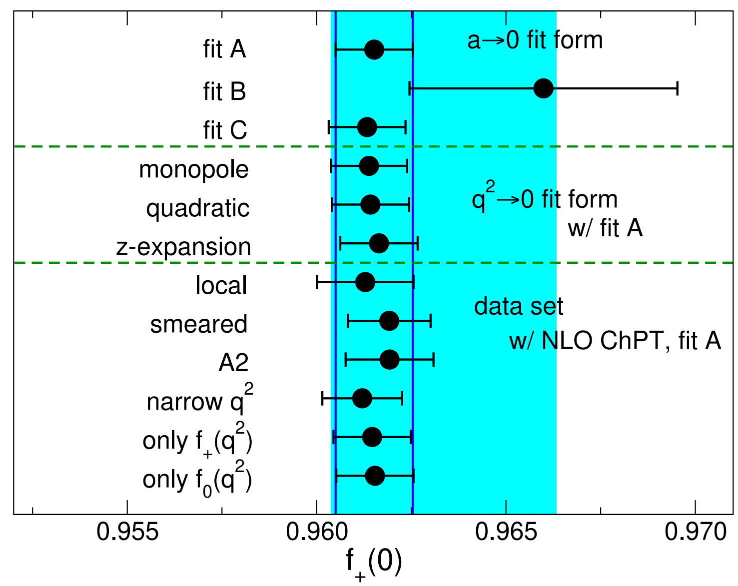
Fit based on SU(3) NLO ChPT with $f_+(0) = f_0(0)$ [PACS:PRD106(2022)]

$$f_+(q^2) = 1 - \frac{4}{F_0^2} L_9(\mu) q^2 + K_+(q^2, M_\pi^2, M_K^2, F_0, \mu) + c_0 + c_2^+ q^4 + g_+^{\rm cur}(a, q^2)$$

$$f_0(q^2) = 1 - \frac{8}{F_0^2} L_5(\mu) q^2 + K_0(q^2, M_\pi^2, M_K^2, F_0, \mu) + c_0 + c_2^0 q^4 + g_0^{\rm cur}(a, q^2)$$

$g_{+,0}^{\rm cur} = \sum_{n,m} e_{+,0}^{{\rm cur},nm} a^n q^{2m}$, cur = local, conserved: 3 types (fit A,B,C) investigated

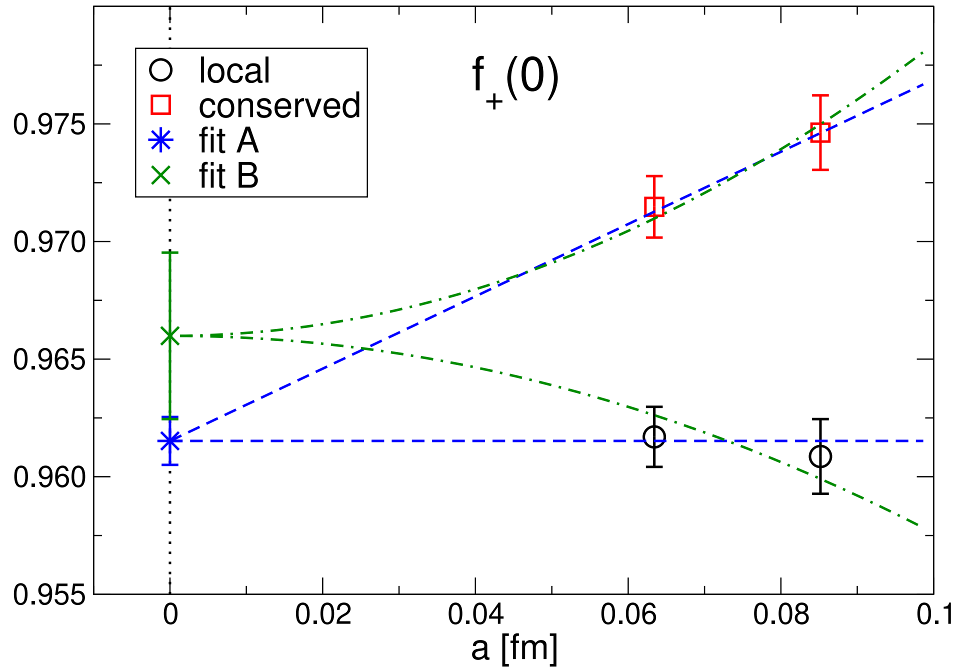




$$f_+(0) = 0.9615(10)\left({}^{+47}_{-2}\right)(5)$$

uncertainty: 1st statistical, 2nd fit form + data, 3rd isospin breaking w/ NLO ChPT

Continuum extrapolation at $q^2 = 0$



local current: almost flat

conserved current: clear a dependence

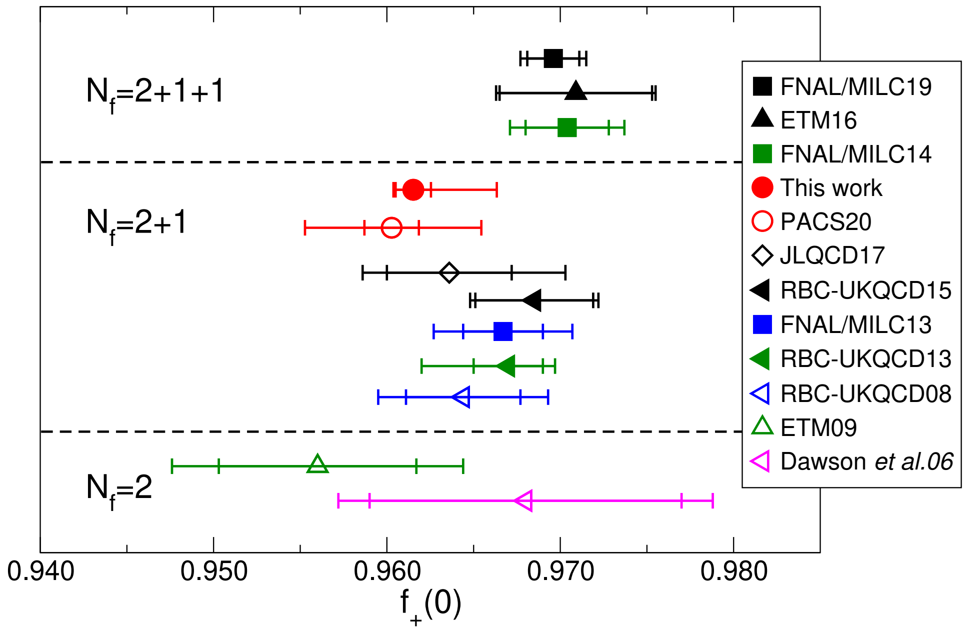
Similar trend seen in HVP calculation ['19 PACS]

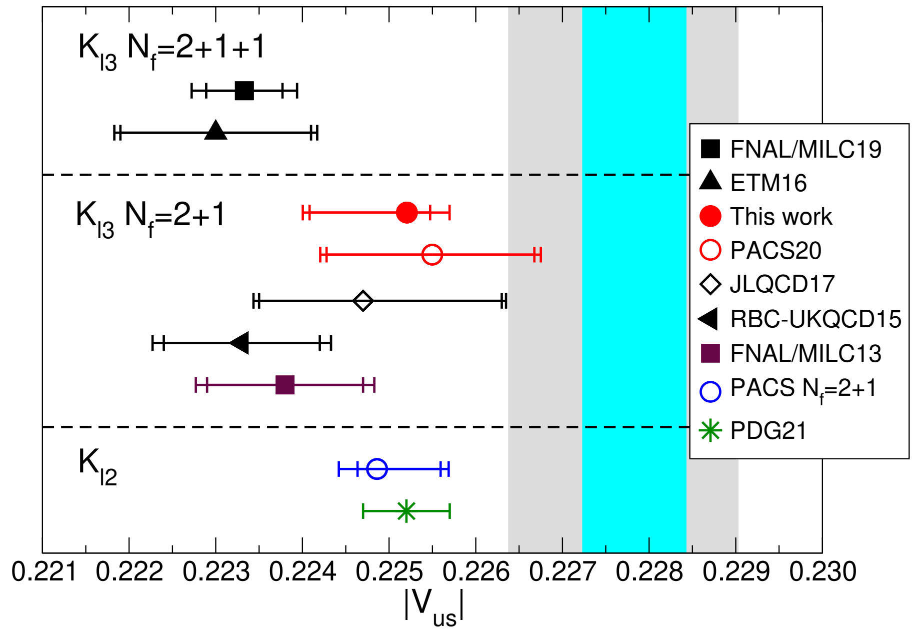
fit form	local	conserved
fit A	C_0	$C_0 + C_1' a$
fit B	$C_0 + C_2 a^2$	$C_0 + C_2' a^2$

$\rightarrow$ large systematic error from $a \rightarrow 0$ fit form

Smaller a data will improve $a \rightarrow 0$ extrapolation.

$f_+(0)$ and $|V_{us}|$





inner, outer = statistical, total(stat.+sys.) inner, outer = lattice, total(lat.+exp.)

Standard model cyan band: ['18 Seng *et al.*]; grey band: ['20 Hardy, Towner]

$f_+(0)$: Reasonably agree with previous lattice calculations $\lesssim 2\sigma$

$|V_{us}|$ using $|V_{us}|f_+(0) = 0.21654(41)$ ['17 Moulson]

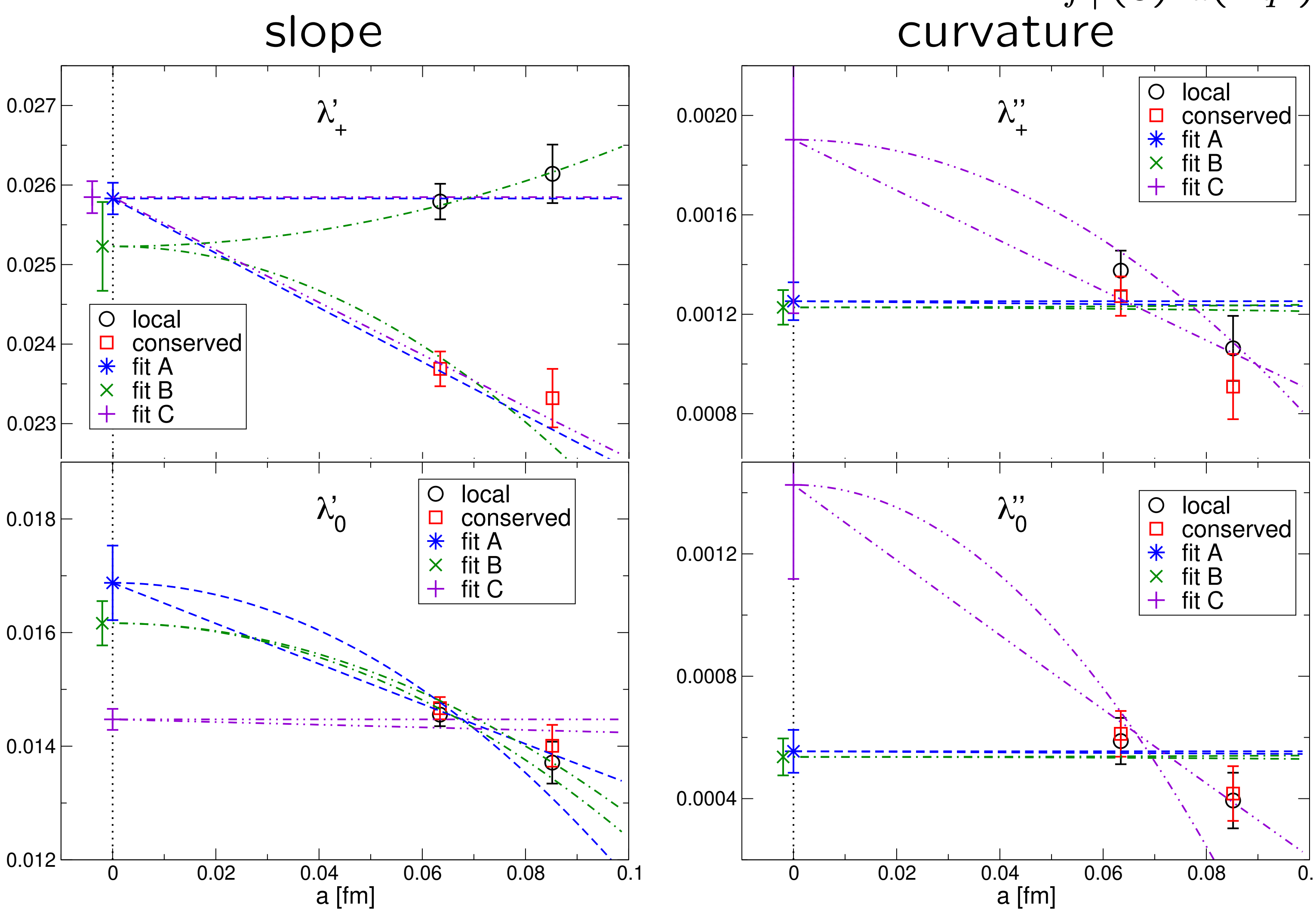
agree with $|V_{us}|$ from $K_{\ell 2}$ using f_K/f_π

$2 \sim 3\sigma$ difference from CKM unitarity (grey and cyan bands)

Future work: $a \to 0$ extrapolation with 3rd PACS10 configuration

Shape of $f_+(q^2), f_0(q^2)$ at $q^2 = 0$

$$\lambda_{+,0}^{(n)} = \frac{M_{\pi^-}^{2n}}{f_+(0)} \frac{d^n f_{+,0}(0)}{d(-q^2)^n}$$



local and conserved data degenerate at each a, except for λ'_+

$\rightarrow$ large dependence on choice of $g_{+,0}^{\mathrm{cur}}$

Smaller a data will improve $a \rightarrow 0$ extrapolation.

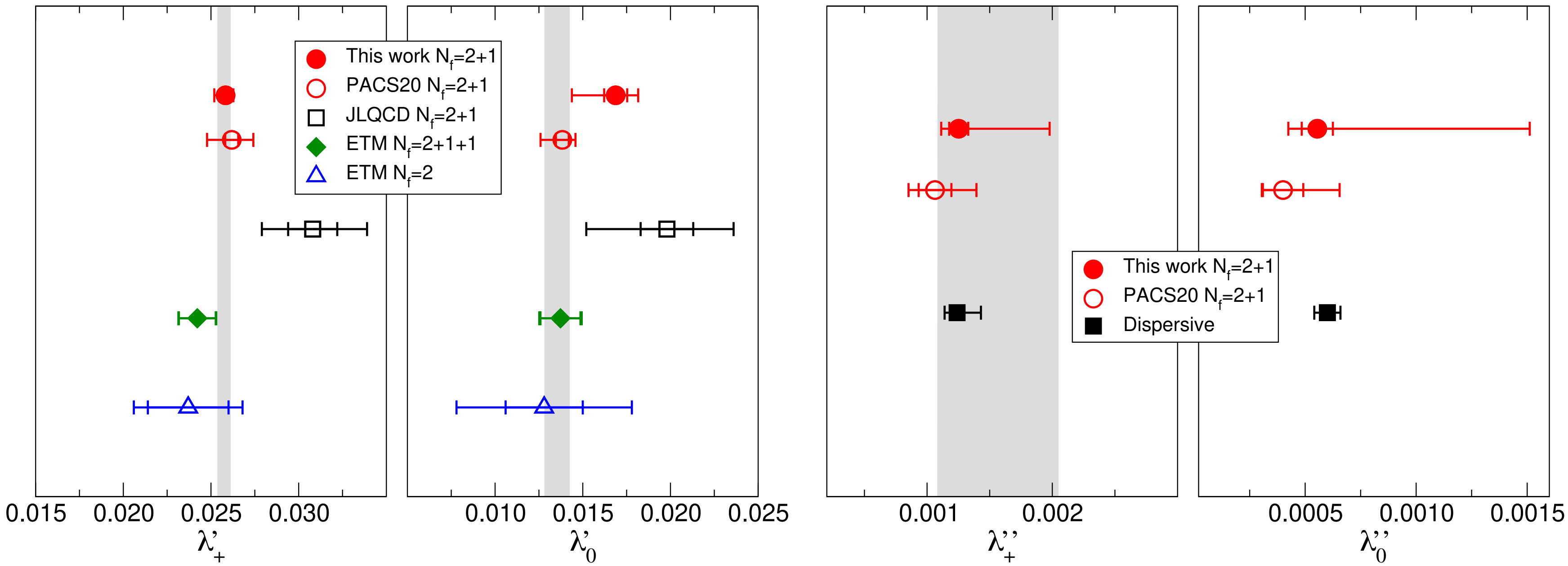
Shape of $f_+(q^2), f_0(q^2)$ at $q^2 = 0$

slope

$$\lambda'_{+,0} = \frac{M_{\pi^-}^2}{f_+(0)} \frac{df_{+,0}(q^2)}{d(-q^2)}$$

curvature

$$\lambda''_{+,0} = \frac{M_{\pi^-}^4}{f_+(0)} \frac{d^2 f_{+,0}(q^2)}{d(-q^2)^2}$$



Large uncertainty from fit form of $a \to 0$

Comparable with experiment (grey band), dispersive representation,

['10 Antonelli *et al.*; '17 Moulson; '09 Bernard *et al.*]

and also previous lattice calculations ['09, '16 ETM; '17 JLQCD, '20 PACS]

Phase space integral I_K^ℓ

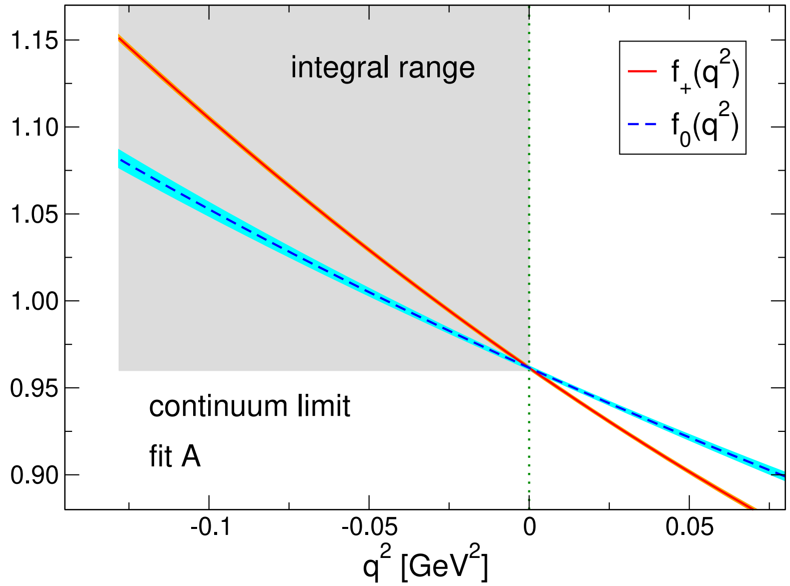
$\Gamma_{K_{\ell 3}} = C_{K_{\ell 3}}(|V_{us}|f_+(0))^2 I_K^\ell$ $\Gamma_{K_{\ell 3}}$: decay width, $C_{K_{\ell 3}}$: known factor, $\ell = e, \mu$

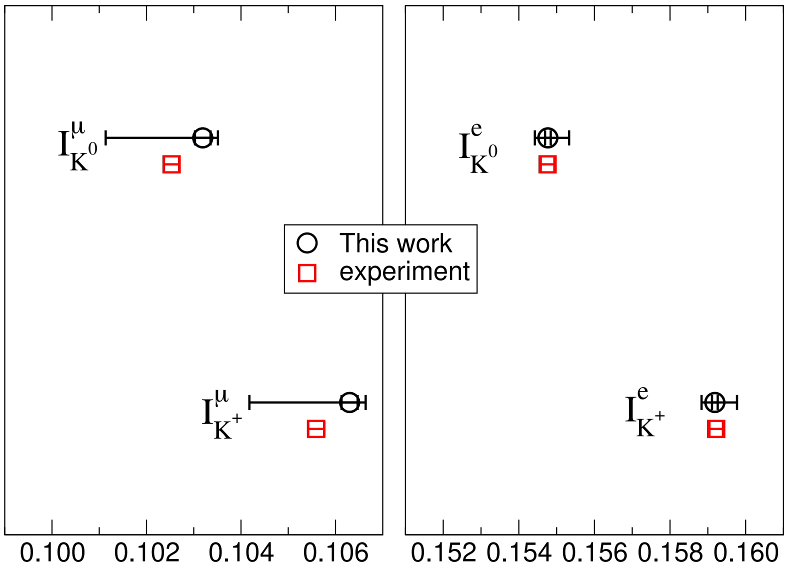
$|V_{us}|f_+(0) = 0.21654(41)$ ['17 Moulson]

$\leftarrow$ I_K^ℓ from dispersive representation of experimental $\overline{F}_{+,0}(t)$

$$I_K^\ell = \int_{m_\ell^2}^{(M_K - M_\pi)^2} dt \left(J_+(t)\overline{F}_+^2(t) + J_0(t)\overline{F}_0^2(t) \right), \quad \overline{F}_{+,0}(t) = \frac{f_{+,0}(-t)}{f_+(0)}$$

$J_{+,0}(t)$: known function ['84 Leutwyler, Roos]





inner: stat. error; outer: (stat.+sys.) error

Reasonably agree with experimental values ['10 Antonelli *et al.*]

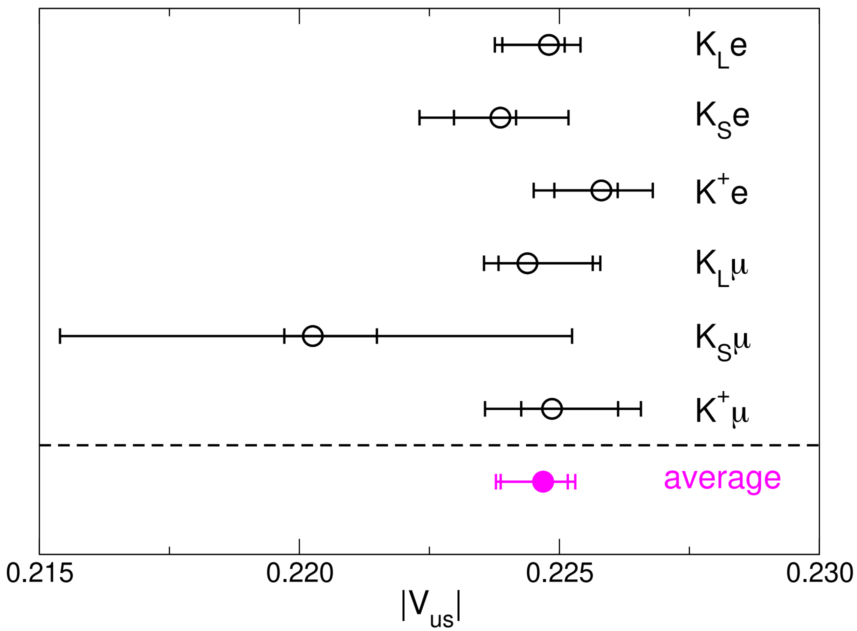
Large uncertainty from fit form of $a \to 0$

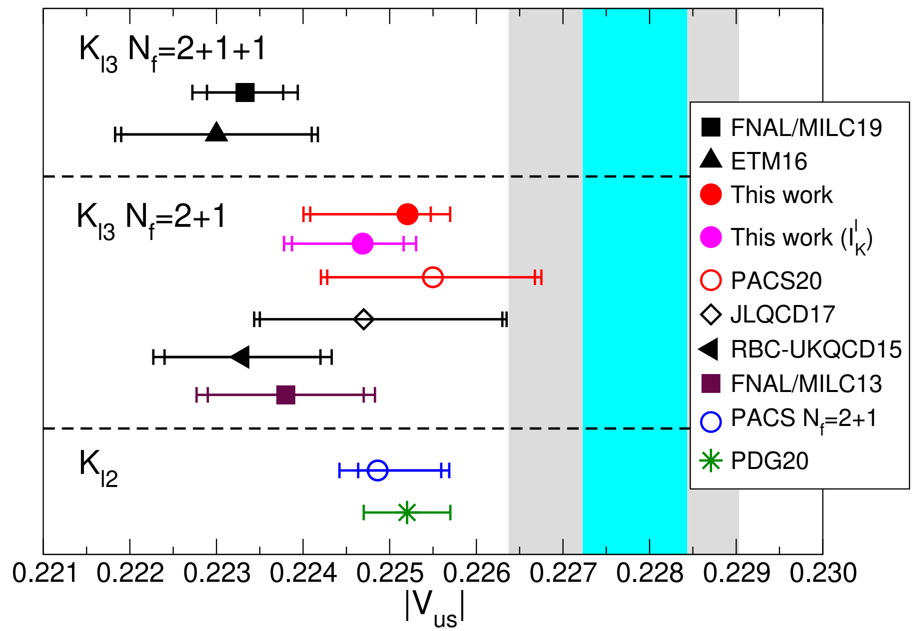
$|V_{us}|$ using I_K^ℓ

$$|V_{us}| = \sqrt{\frac{\Gamma_{K_{\ell 3}}}{C_{K_{\ell 3}}(f_+(0))^2 I_K^\ell}}$$

Two parts calculated from lattice QCD

$\Gamma_{K_{\ell 3}}, C_{K_{\ell 3}}$ ['10 Antonelli *et al.*, '18 Seng *et al.*, '20 Seng *et al.*]





inner: lattice error, outer: (lat.+exp.) error

Weighted average of 6 decay processes using experimental errors

Good agreement with $|V_{us}|$ using only $f_+(0)$

Summary

PACS10 Project

calculation w/o three main systematic uncertainties in lattice QCD

PACS10 configuraiton:

$V \gtrsim (10\text{fm})^4$ in physical point at three lattice spacings

various calculations w/ 2 lattice spacings

- Hadron spectrum
- Nucleon charge and form factor
- Light meson electromagnetic form factor
- Proton decay matrix element
- Hadron vacuum polarization
- Kaon semileptonic decay form factor

Future works

Calculations with 3rd PACS10 configuration

more reliable $a \to 0$ extrapolations