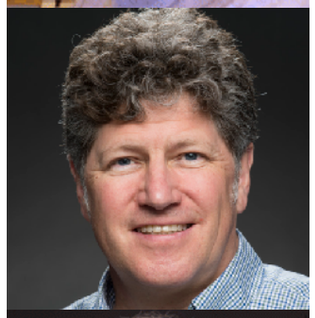
Lattice QCD: 2020 and beyond

Andreas Kronfeld with input from Ruth Van de Water and Mike Wagman

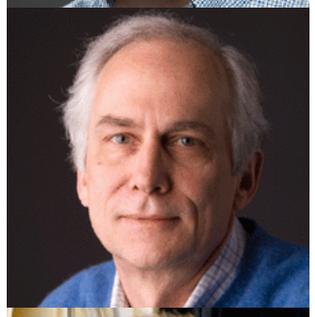
Scientists, Research Associates, and Students

Ruth Van de Water
2012–????
also RA 2005–2008

James Simone (SCD)
1998–present
also RA 1993–1996



Andreas Kronfeld
1988–present
RA 1988–1989

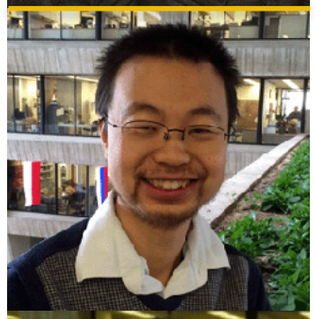


Paul Mackenzie
1986–2019
also RA 1981–1984

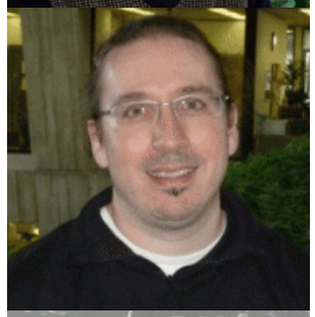
Estia Eichten
1982–2019

Ciaran Hughes
2017–2019

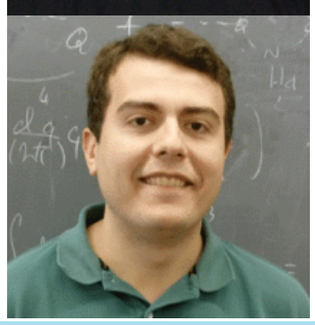
Aarti Veernala
2016–2018



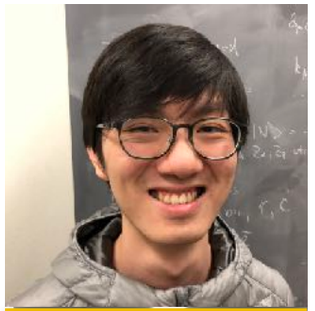
Ran Zhou
2014–2017
data scientist
Xilinx Corp.



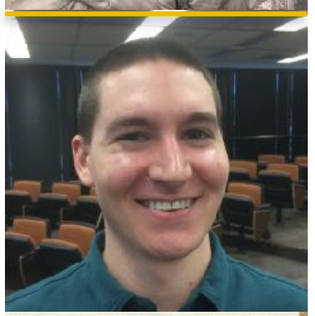
Daniel Mohler
2013–2016
postdoc
U. Mainz



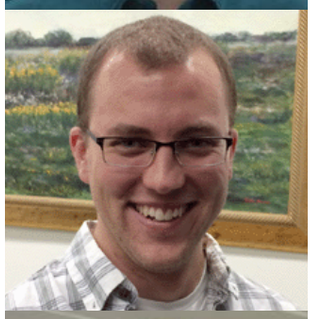
Ethan Neil
2011–2014
ass't prof.
U. Colorado



Yin Lin
2017–present
Chicago

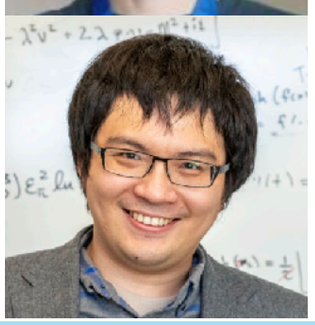


Zech Gelzer
2014–2017
Iowa
now UIUC



Aaron Meyer
2013–2017
Chicago
now BNL

James Gloudemans
2015–2016
UIUC



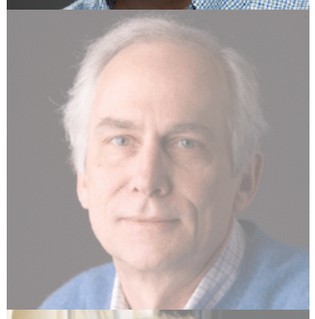
Chia Cheng Chang
2011–2015
UIUC
now LBNL/RIKEN

Scientists, Research Associates, and Students

Ruth Van de Water
2012–????
also RA 2005–2008

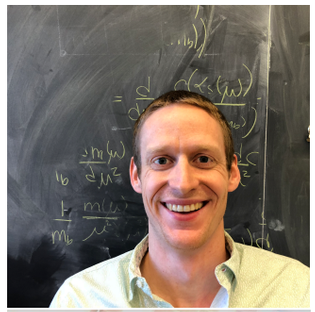
James Simone (SCD)
1998–present
also RA 1993–1996

Andreas Kronfeld
1988–present
RA 1988–1989

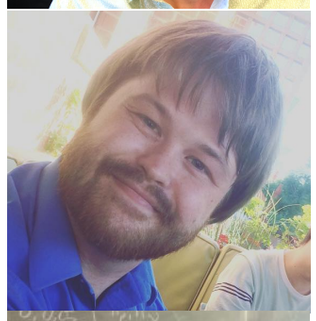


Paul Mackenzie
1986–2019
also RA 1981–1984

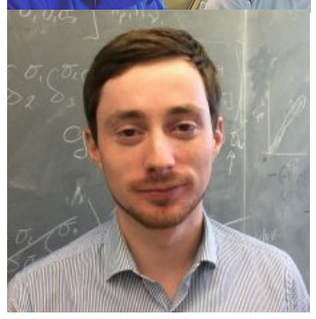
Estia Eichten
1982–2019



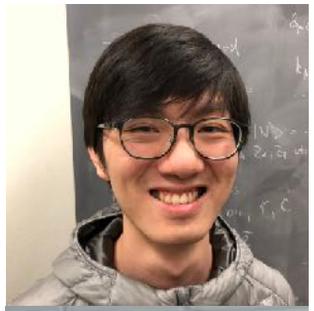
William Jay
2018–present



Hank Lamm
2019–present
(QIS)



Ciaran Hughes
2019–present
(QIS)



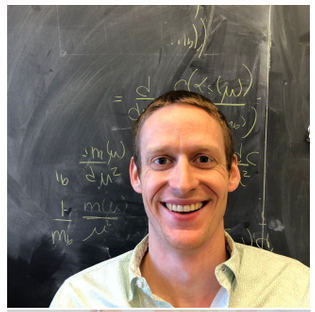
Yin Lin
2017–present
Chicago

Shaun Lahert
2019–present
UIUC

Scientists, Research Associates, and Students

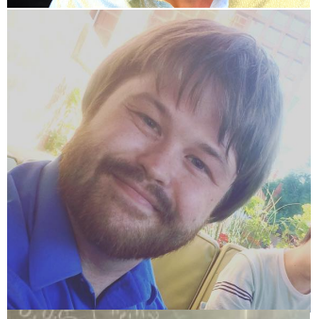
Ruth Van de Water
2012–????
also RA 2005–2008

James Simone (SCD)
1998–present
also RA 1993–1996

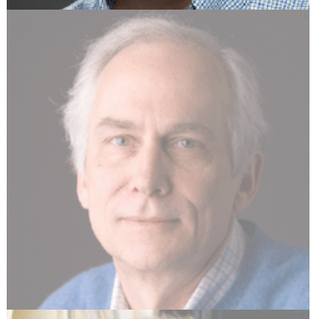


William Jay
2018–present

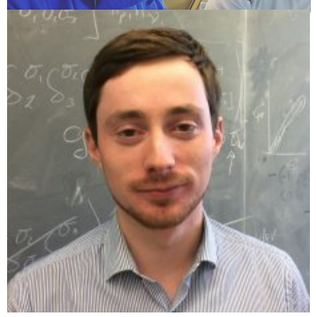
Andreas Kronfeld
1988–present
RA 1988–1989



Hank Lamm
2019–present
(QIS)

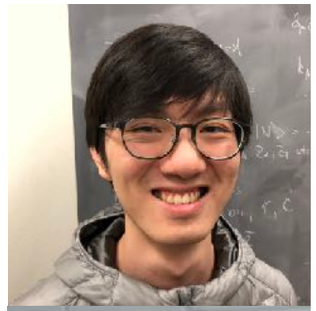


Paul Mackenzie
1986–2019
also RA 1981–1984



Ciaran Hughes
2019–present
(QIS)

Estia Eichten
1982–2019



Yin Lin
2017–present
Chicago

Shaun Lahert
2019–present
UIUC

Associate Scientist
Michael Wagman
12/2019–∞

Uncertainty Analysis

(adapted from summer 2018)

- Paul: will he retire during the next four years? Yes.
- Ruth: how will teaching affect her physics productivity?
  - Asymptotically free.
- Andreas: how will USQCD spokesperson (2018–2021) and ECP PI (2018–2023) duties affect physics productivity?
  - life is one long zoom meeting, with breaks for BlueJeans.
  - charging 0.25FTE to ECP grant.
- Jim and Andreas: will they retire during the coming five years?

Computing Activities

USQCD

- Spokesperson of the USQCD Collaboration and Chair of its Executive Committee (April 2018–sometime 2021):
    - USQCD is a federation of science collaborations, working together to secure and coordinate computing resources for lattice QCD;
    - INCITE allocation process (2019 🙂, 2020 😬);
    - DOE-HEP funding for clusters at Fermilab & BNL (FY2020–24 😁); DOE-NP funding for computing at JLab;
        - time on institutional clusters are funding for five FYs;
        - Fermilab leadership in computing, management, and science required for national success in lattice gauge theory.

Exascale Computing Project

- Principal Investigator of the Lattice QCD Exascale Computing Project (April 2018–June 30, 2023 = end date):
  - manage budget distributed over 4 nat'l labs and 7 universities;
  - software, solvers, critical slowing down, tensor contractions.
- There are ~20 other projects; funding from DOE-ASCR and NNSA.
- Lots of PR: youtube.
- Discussions afoot (beyond my pay grade) on what follows ECP: after huge effort to create codes for exascale computers, how will the codes be maintained?

OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

IBM CPU, NVIDIA GPU, CRAY

NERSC National Energy Research Scientific Computing Center

AMD CPU, NVIDIA GPU, CRAY

NERSC PERLMUTTER

Argonne NATIONAL LABORATORY | Leadership Computing Facility

AMD CPU & accelerator, CRAY

intel CPU & accelerator, CRAY

Flavor Physics

HISQ Ensembles: 2+1+1

MILC, arXiv:1212.4768 + further runs

a (fm)	size	$am'_l/am'_s/am'_c$	# confs	# sources	notes
≈ 0.15	$16^3\times 48$	0.0130/0.065/0.838	1020	4	
≈ 0.15	$24^3\times 48$	0.0064/0.064/0.828	1000	4	
≈ 0.15	$32^3\times 48$	0.00235/0.0647/0.831	1000	4	physical
≈ 0.12	$24^3\times 64$	0.0102/0.0509/0.635	1040	4	
≈ 0.12	$32^3\times 64$	0.00507/0.0507/0.628	1020	4	also 24^3, 40^3
≈ 0.12	$48^3\times 64$	0.00184/0.0507/0.628	999	4	physical
≈ 0.12	$24^3\times 64$	0.0102/0.03054/0.635	1020	4	$m'_s < m_s$
≈ 0.12	$24^3\times 64$	0.01275/0.01275/0.640	1020	4	$m'_s = m'_l$
≈ 0.12	$32^3\times 64$	0.00507/0.0304/0.628	1020	4	$m'_s < m_s$
≈ 0.12	$32^3\times 64$	0.00507/0.022815/0.628	1020	4	$m'_s < m_s$
≈ 0.12	$32^3\times 64$	0.00507/0.012675/0.628	1020	4	$m'_s \ll m_s$
≈ 0.12	$32^3\times 64$	0.00507/0.00507/0.628	1020	4	$m'_s = m'_l$
≈ 0.12	$32^3\times 64$	0.0088725/0.022815/0.628	1020	4	$m'_s < m_s$
≈ 0.09	$32^3\times 96$	0.0074/0.037/0.440	1005	4	
≈ 0.09	$48^3\times 96$	0.00363/0.0363/0.430	999	4	
≈ 0.09	$64^3\times 96$	0.0012/0.0363/0.432	484	4	physical
≈ 0.06	$48^3\times 144$	0.0048/0.024/0.286	1016	4	
≈ 0.06	$64^3\times 144$	0.0024/0.024/0.286	572	4	
≈ 0.06	$96^3\times 192$	0.0008/0.022/0.260	842	6	physical
≈ 0.042	$64^3\times 192$	0.00316/0.0158/0.188	1167	6	
≈ 0.042	$144^3\times 288$	0.000569/0.01555/0.1827	429	6	physical
≈ 0.03	$96^3\times 288$	0.00223/0.01115/0.1316	724	4	

HISQ Ensembles: 2+1+1

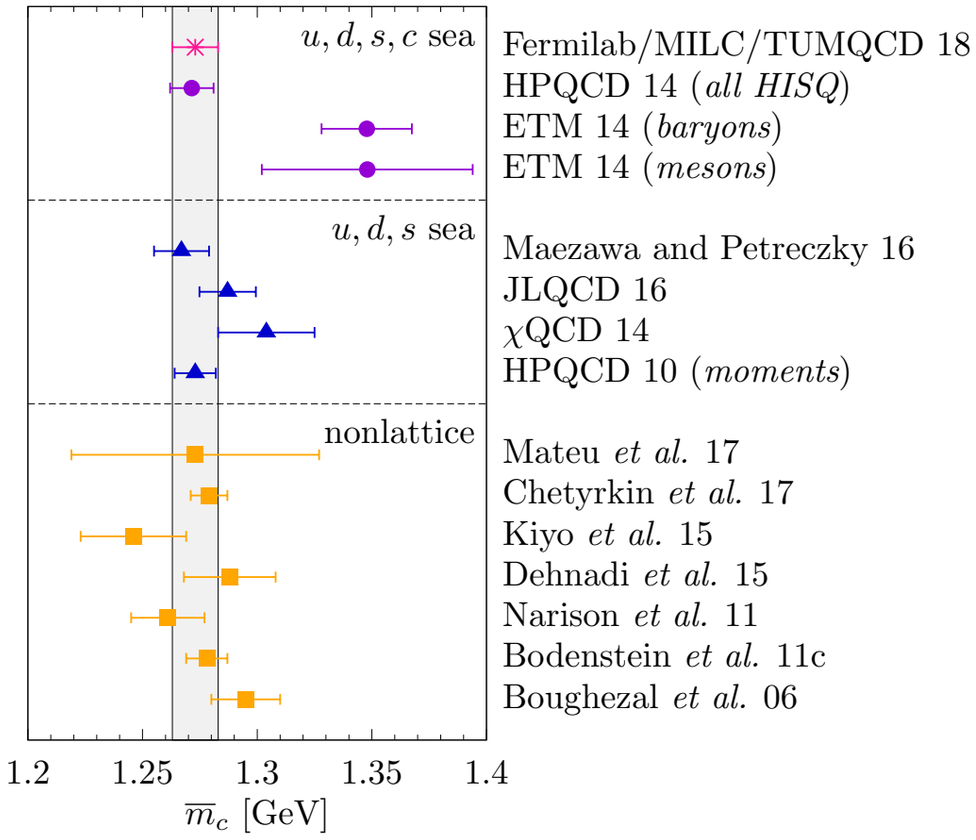
MILC, arXiv:1212.4768 + further runs

a (fm)	size	$am_l'/am_s'/am_c'$	# confs	# sources	notes
≈ 0.15	$16^3\times 48$	0.0130/0.065/0.838	1020	4	
≈ 0.15	$24^3\times 48$	0.0064/0.064/0.828	1000	4	
≈ 0.15	$32^3\times 48$	0.00235/0.0647/0.831	1000	4	physical
≈ 0.12	$24^3\times 64$	0.0102/0.0509/0.635	1040	4	
≈ 0.12	$32^3\times 64$	0.00507/0.0507/0.628	1020	4	also 24^3, 40^3
≈ 0.12	$48^3\times 64$	0.00184/0.0507/0.628	999	4	physical
≈ 0.12	$24^3\times 64$	0.0102/0.03054/0.635	1020	4	$m_s' < m_s$
≈					
≈					
≈					
≈					
≈					
≈					
≈					
≈ 0.09	$48^3\times 96$	0.00363/0.0363/0.430	999	4	
≈ 0.09	$64^3\times 96$	0.0012/0.0363/0.432	484	4	physical
≈ 0.06	$48^3\times 144$	0.0048/0.024/0.286	1016	4	
≈ 0.06	$64^3\times 144$	0.0024/0.024/0.286	572	4	
≈ 0.06	$96^3\times 192$	0.0008/0.022/0.260	842	6	physical
≈ 0.042	$64^3\times 192$	0.00316/0.0158/0.188	1167	6	
≈ 0.042	$144^3\times 288$	0.000569/0.01555/0.1827	429	6	physical
≈ 0.03	$96^3\times 288$	0.00223/0.01115/0.1316	724	4	

Huge slab in (a, L, m_x, m_l, m_s, m_h) parameter space!

Results & Comparisons

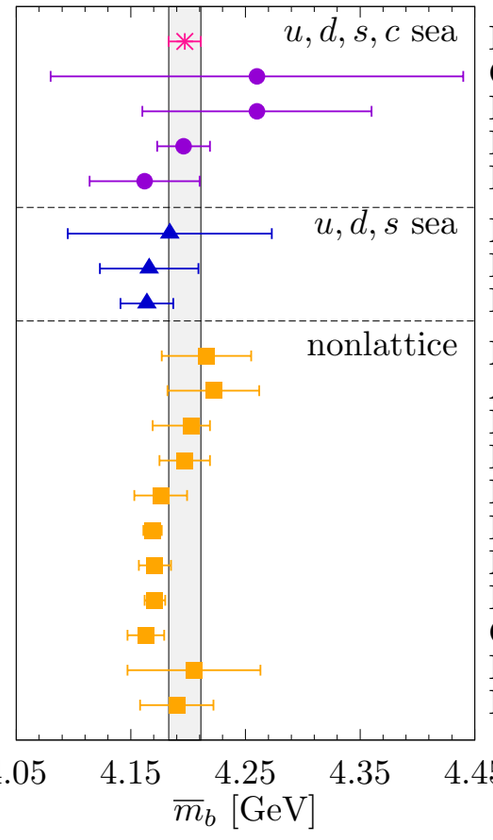
- Results form arXiv:1802.04248:



Fermilab/MILC/TUMQCD 18
HPQCD 14 (*all HISQ*)
ETM 14 (*baryons*)
ETM 14 (*mesons*)

Maezawa and Petreczky 16
JLQCD 16
χQCD 14
HPQCD 10 (*moments*)

Mateu *et al.* 17
Chetyrkin *et al.* 17
Kiyo *et al.* 15
Dehnadi *et al.* 15
Narison *et al.* 11
Bodenstein *et al.* 11c
Boughezal *et al.* 06



Fermilab/MILC/TUMQCD 18
Gambino *et al.* 17
ETM 16
HPQCD 14 (*NRQCD b*)
HPQCD 14 (*all HISQ*)

Maezawa and Petreczky 16
HPQCD 13 (Υ *splittings*)
HPQCD 10 (*moments*)

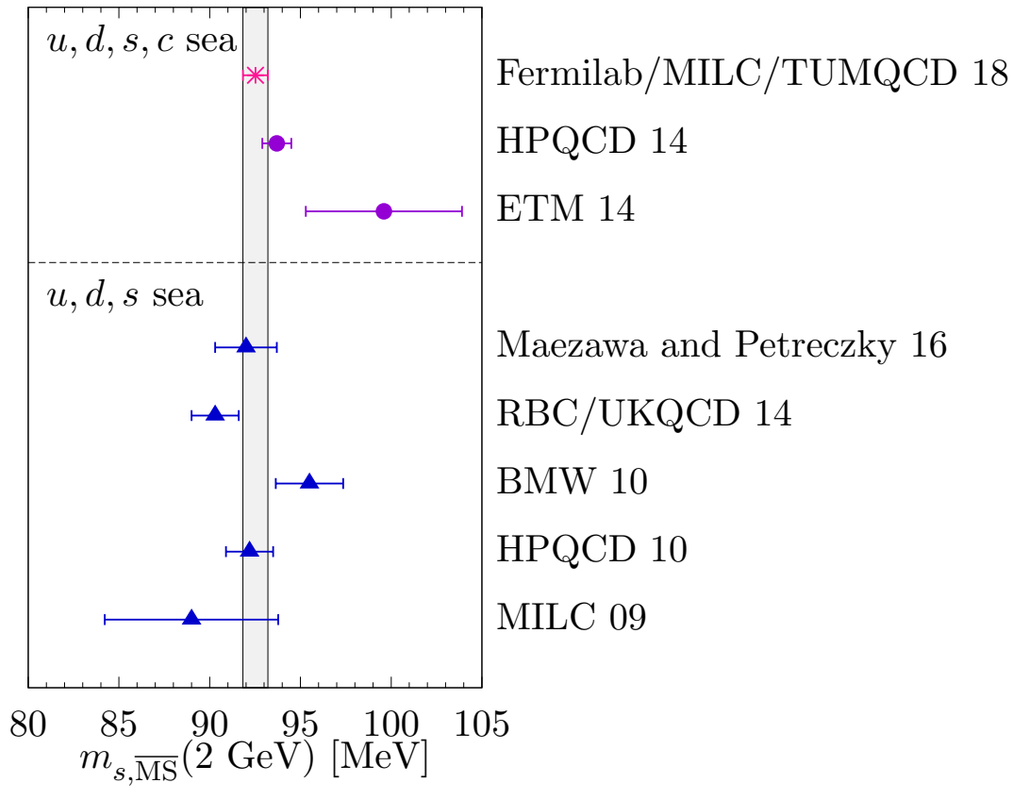
Mateu *et al.* 17
Ayala *et al.* 16
Beneke *et al.* 16
Kiyo *et al.* 15
Dehnadi *et al.* 15
Penin *et al.* 14
Narison *et al.* 11
Bodenstein *et al.* 11b
Chetyrkin *et al.* 09
Boughezal *et al.* 06
Brambilla *et al.* 01

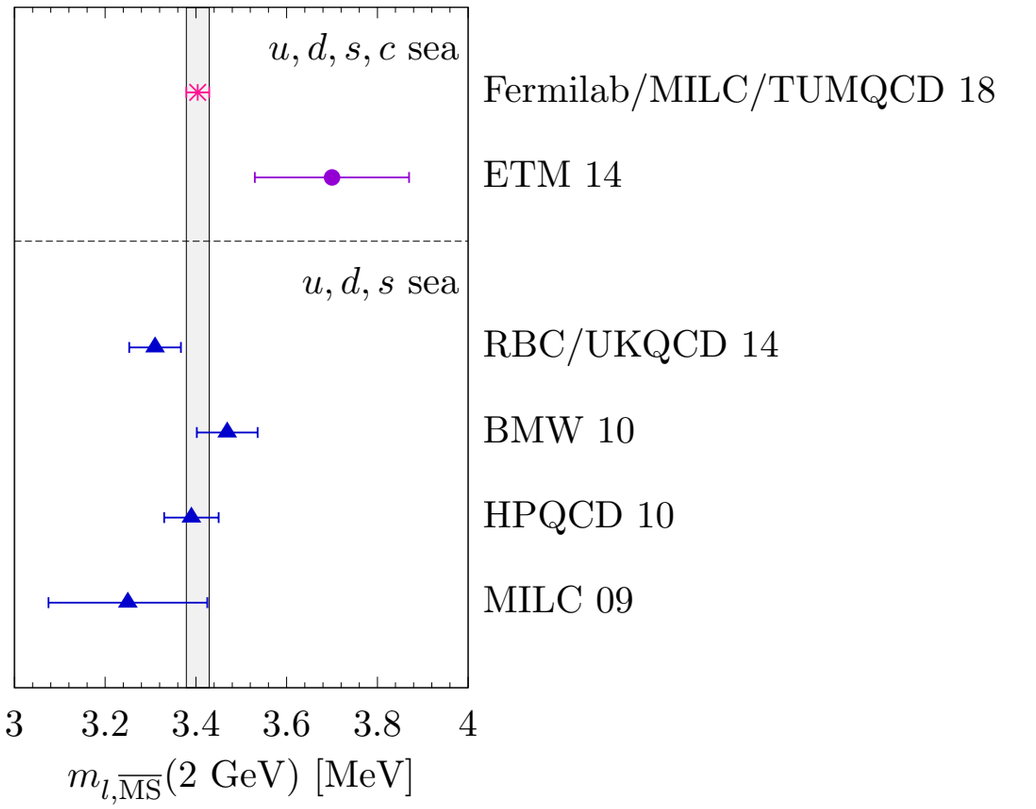
- To our knowledge, first results w/ order-α_s^5 running & order-α_s^4 matching.

- Precision: 0.3% for bottom to 0.5% for charm.

Results & Comparisons 2

- With mass ratios from light pseudoscalar mesons:





- Most precise strange and “light” quark masses to date.
- Most (~) precise quark masses for all quarks except top ($m_u > 50\sigma$).

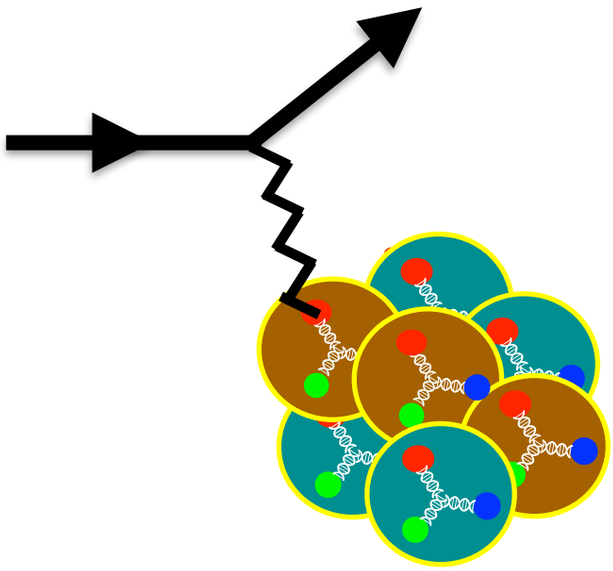
Future Projects

- Use these methods to gain sub-percent level uncertainty for semileptonic B decays: synergy with the set of flavor anomalies (LHCb, Belle, Belle II).
    - Will Jay; postdocs at collaborators' institutions.
- B^0-$\bar{B}^0$ mixing will require new ideas (Laiho, El-Khadra, Lahert)—level of effort here unclear.
- Muon anomalous magnetic moment:
    - HVP will continue with Ruth's leadership and strong effort from HPQCD and from MILC;
    - HLbL not on the horizon.

from Mike Wagman

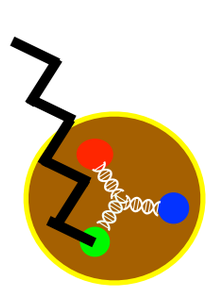
Neutrinos and nucleons

Cross-section governed by vector and axial structure functions including 0 - few GeV momentum transfer

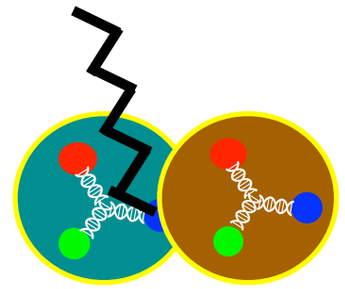


Ongoing LQCD efforts

- Single-nucleon coupling
- Single-nucleon form factors
- Hadron tensor (exploratory)
- Two/three-nucleon couplings (exploratory)



g_A



L_{1A}

Future directions

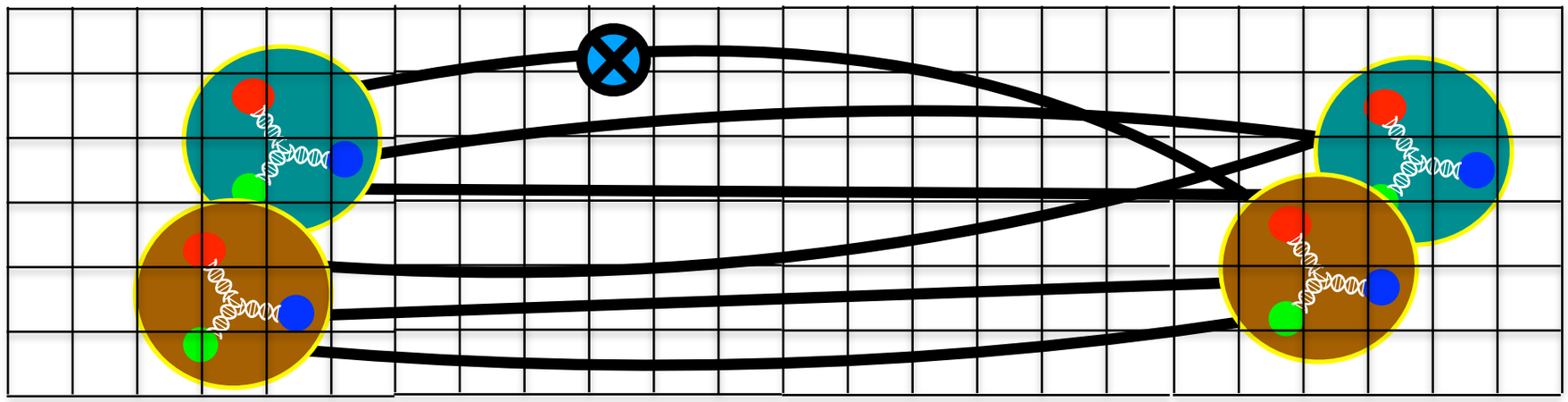
- Exclusive inelastic reactions on nucleons

  pion production, especially in Delta resonance region

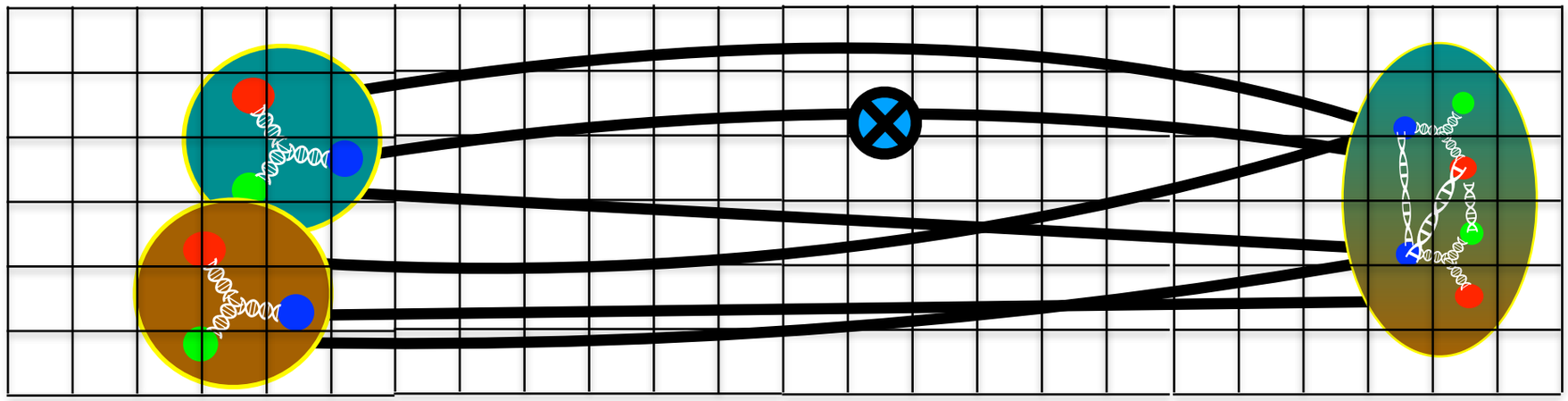
- Two-nucleon form factors

Schematic *NN* interpolators

Ideal interpolating operator basis would include baryon-baryon molecules/ scattering states



With point-to-all propagators, limited to hexaquark source operators



Problematic if current injects momentum, overlaps onto excited-to-ground state transition from factors as well as ground-to-ground

Variational methods needed, in development with NPLQCD collaboration

Less schematic *N* interpolators

Local nucleon interpolator:

$$B_P^{\pm}(x) = \varepsilon_{ijk}\left[q_i^+(x)q_j^-(x) - q_i^-(x)q_j^+(x)\right]q_k^{\pm}(x) \qquad q_i^{\pm}(x) = \left(\frac{1+\gamma_4}{2}\right)(1 \pm i\gamma_3\gamma_5)q(x)$$

Isolates G_{1g} cubic irrep

See e.g. Basak et al [LHPC] PRD 72 (2005)

General building blocks:

Spin-color indices

$S_{a'a}(\mathbf{x},\mathbf{y})$ $w^{\alpha}_{a_1a_2a_3}$ $\psi_n(\mathbf{x})$

Propagators **Weights** **Wavefunctions**

$$C^B_{n'n}(t) = \sum_{\text{perms } p}\sum_{\alpha,\alpha'}\sum_{\mathbf{x},\mathbf{y}} w^{\alpha'}_{a'_{p(1)}a'_{p(2)}a'_{p(3)}}\psi_{n'}(\mathbf{x})S_{a'_{p(1)}a_1}(\mathbf{x},\mathbf{y})$$
$$\times S_{a'_{p(2)}a_2}(\mathbf{x},\mathbf{y})S_{a'_{p(3)}a_3}(\mathbf{x},\mathbf{y})w^{\alpha}_{a_1a_2a_3}\psi_n(\mathbf{y})$$

Less schematic *NN* interpolators

Analogous building blocks:

$$S_{a'a}(\mathbf{x},\mathbf{y}) \qquad w^{\alpha}_{a_1a_2a_3a_4a_5a_6} \qquad \psi_n(\mathbf{x}_1),\ \psi_n(\mathbf{x}_2)$$

Simple spin algebra on baryon weights, e.g. $\frac{1}{\sqrt{2}}(\uparrow\downarrow \pm \downarrow\uparrow)$ gives correct weights for cubic group

$$G_{1g} \otimes G_{1g} = T_{1g} \oplus A_{1g}$$

$$C^{BB}_{n'n}(t) = \sum_{\text{perms } p} \sum_{\alpha,\alpha'} \sum_{\mathbf{x}_1,\mathbf{x}_2,\mathbf{y}_1,\mathbf{y}_2} w^{\alpha'}_{a'_{p(1)}a'_{p(2)}a'_{p(3)}a'_{p(4)}a'_{p(5)}a'_{p(6)}} \psi_{n'}(\mathbf{x}_{p(1)})\psi_{n'}(\mathbf{x}_{p(2)})$$

$$\times S_{a'_{p(1)}a_1}(\mathbf{x}_{p(1)},\mathbf{y}_1) S_{a'_{p(2)}a_2}(\mathbf{x}_{p(1)},\mathbf{y}_1) S_{a'_{p(3)}a_3}(\mathbf{x}_{p(1)},\mathbf{y}_1) S_{a'_{p(4)}a_4}(\mathbf{x}_{p(2)},\mathbf{y}_2)$$

$$\times S_{a'_{p(5)}a_5}(\mathbf{x}_{p(2)},\mathbf{y}_2) S_{a'_{p(6)}a_6}(\mathbf{x}_{p(2)},\mathbf{y}_2) w^{\alpha}_{a_1a_2a_3a_4a_5a_6} \psi_n(\mathbf{y}_1)\psi_n(\mathbf{y}_2)$$

Factorizes into baryon blocks:

Doi, Endres, Comput. Phys. Commun. 184 (2013)

Detmold, Orginos, PRD 87 (2013)

Fermion schemes?

Weight construction simple for Wilson-like fermions, generic multi-hadron systems (*pi-pi, N-N-N*, *N-pi*, …)

To a naive outsider, staggered seems both more complicated and more computationally expensive (12 component -> 48 component?)

But MILC ensembles are a valuable resource…

Mixed action?

— clover on HISQ (e.g. PNDME) cheap but have to worry about exceptional, smearing / gradient flow on fine lattices ok?

— domain wall on HISQ (e.g. CalLatt) avoids exceptionals at a price

Possible testing ground: *pi - pi* studies in collaboration with NPLQCD

Connections to QIS

- Expertise in classical simulation could inform quantum simulation.
- Existence of a strong numerical lattice-gauge-theory effort makes Fermilab attractive (senior hire target, private communication).
- The two QIS theory postdocs have a background in lattice gauge theory.
- Connection at Fermilab should become stronger:
  - Wagman has relevant work on, e.g., sign problems in QFT;
  - my efforts could go beyond “hobby”;
  - management might stop bypassing us as partners in QIS.

Future Hiring

- This year's hire doesn't offset retirements and (likely) departure.
- Another Associate Scientist hire will be needed in theory; another in computing.
- That said, time is not *right* now:
  - other pressing issues in the department;
    - RSV's departure only likely, not certain;
    - growth of QIS group may by synergistic enough to address these needs.
- Still, another lattice-QCD hire over the next five years should in the strategic plan (with what Eisenhower said about plans).