Lattice QCD with O(a) improved Wilson quarks

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on behalf of

Coordinated Lattice Simulations — CLS

European Lattice Community HPC Access Town-Hall Meeting
Trinity College Dublin
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HIM Helmholtz-Institut Mainz

PRISMA

SFB 1044 THE LOW-ENERGY FRONTIER OF THE STANDARD MODEL

CLS Consortium

Denmark: Odense

Germany: Berlin (HU), DESY-Zeuthen, Mainz, Münster, Regensburg, Wuppertal

Italy: Milano Bicocca, Roma 1

Spain: Madrid (UAM), Valencia

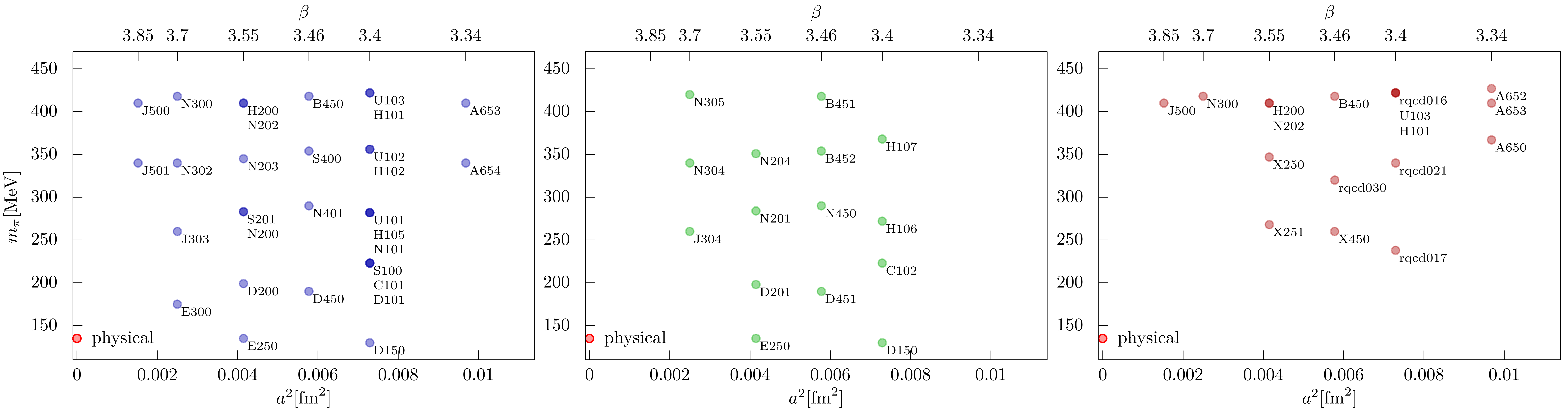
Switzerland: CERN

* Common set of gauge ensembles
* Sharing of computational resources
* Collaboration on specific projects

Computational Framework

Lattice action and parameters

- $\mathrm{O}(a)$-improved Wilson quarks; tree-level Lüscher-Weisz gauge action
- Six values of the lattice spacing: $a \approx 0.035 - 0.1\,\mathrm{fm}$
- Pion masses and volumes: $m_\pi^{\mathrm{min}} \approx 135\,\mathrm{MeV}, \quad m_\pi L \geq 4$



$m_u + m_d + m_s \approx \mathrm{const}$ $\qquad$ $m_s \approx \mathrm{const}$ $\qquad$ $m_u = m_d = m_s$

Calculational Framework

Simulation code

openQCD code suite;

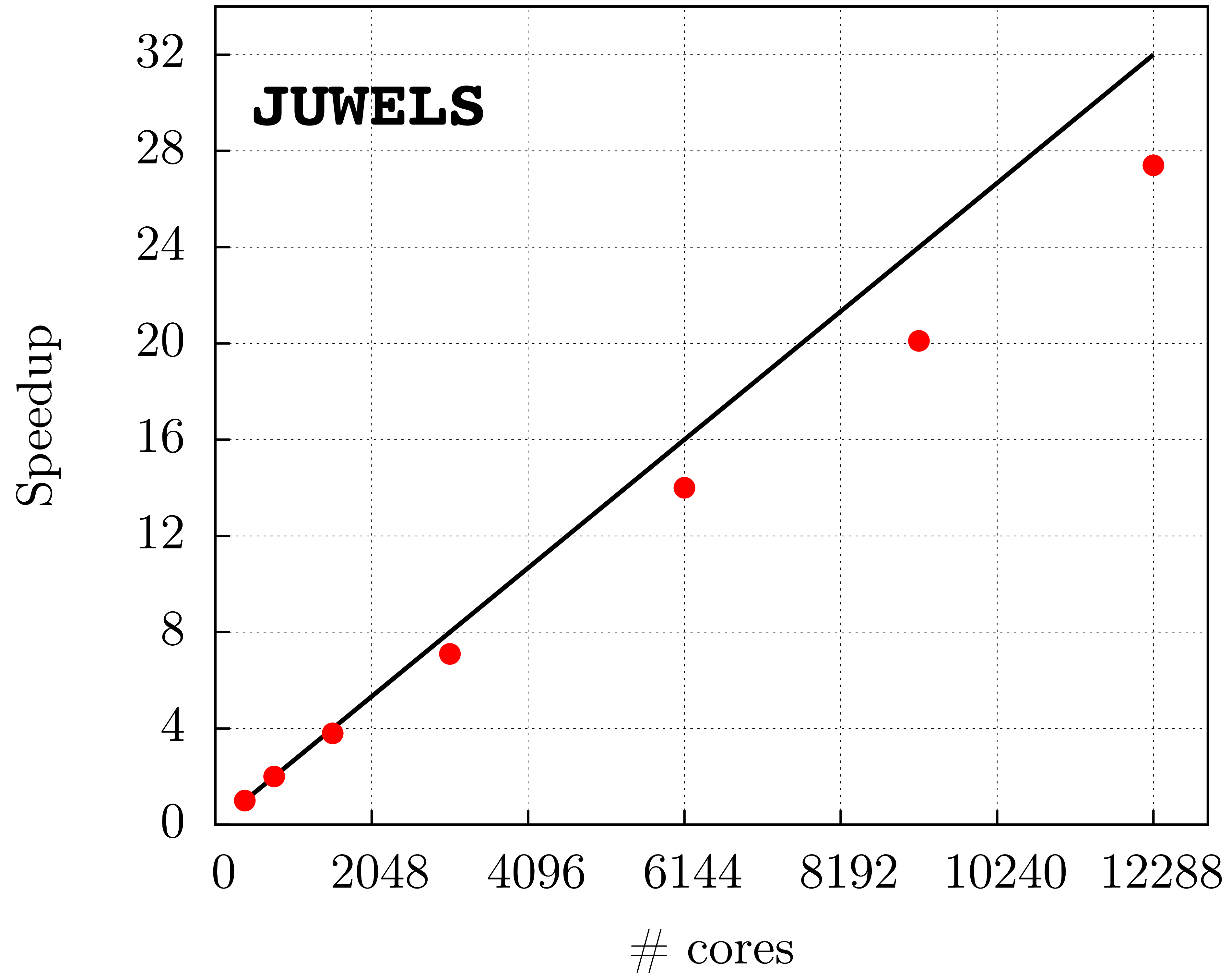
`http://luscher.web.cern.ch/luscher/openQCD/index.html`

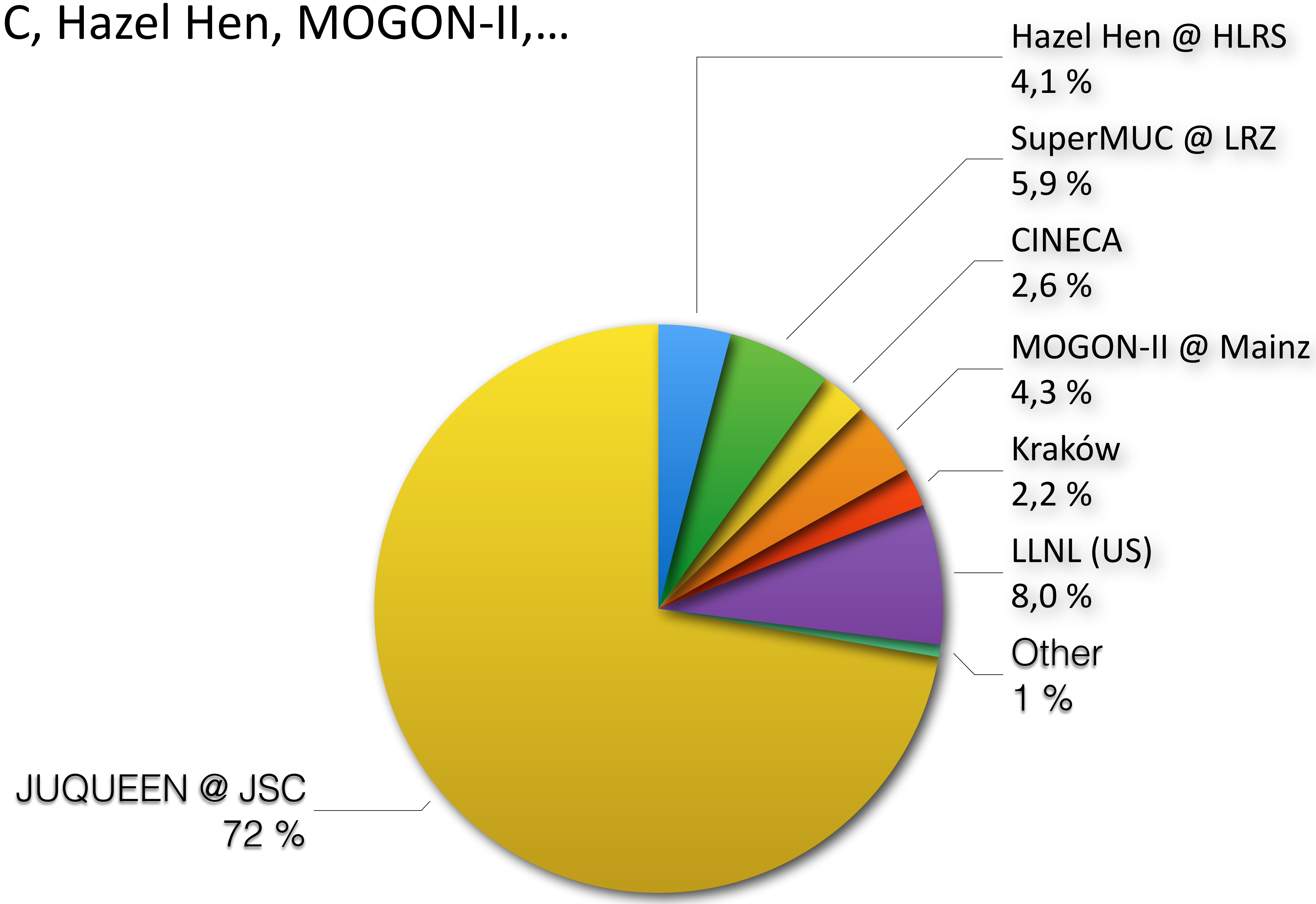
- Twisted-mass determinant reweighting
- Hasenbusch mass factorisation
- Boundary conditions in time: open, SF, periodic
- Single quark flavours simulated using the Rational HMC (RHMC) algorithm
- Nested hierarchical integrators for Molecular Dynamics equations
- Variety of solvers: SAP-GCR, CGNE, MSCG
- Plain C code (ISO C89); parallelisation via MPI
- Extension to include AVX-512 vector instructions
- Other extensions / derivatives: **openQCD-FASTSUM**; **openQxD** — QCD+QED simulations

Computing Platforms and Code Performance

* Cluster architectures: JUWELS, SuperMUC, Hazel Hen, MOGON-II,…
* BlueGene/Q: JUQUEEN

Application of even-odd-preconditioned Wilson-Dirac operator; $96^3 \cdot 192$





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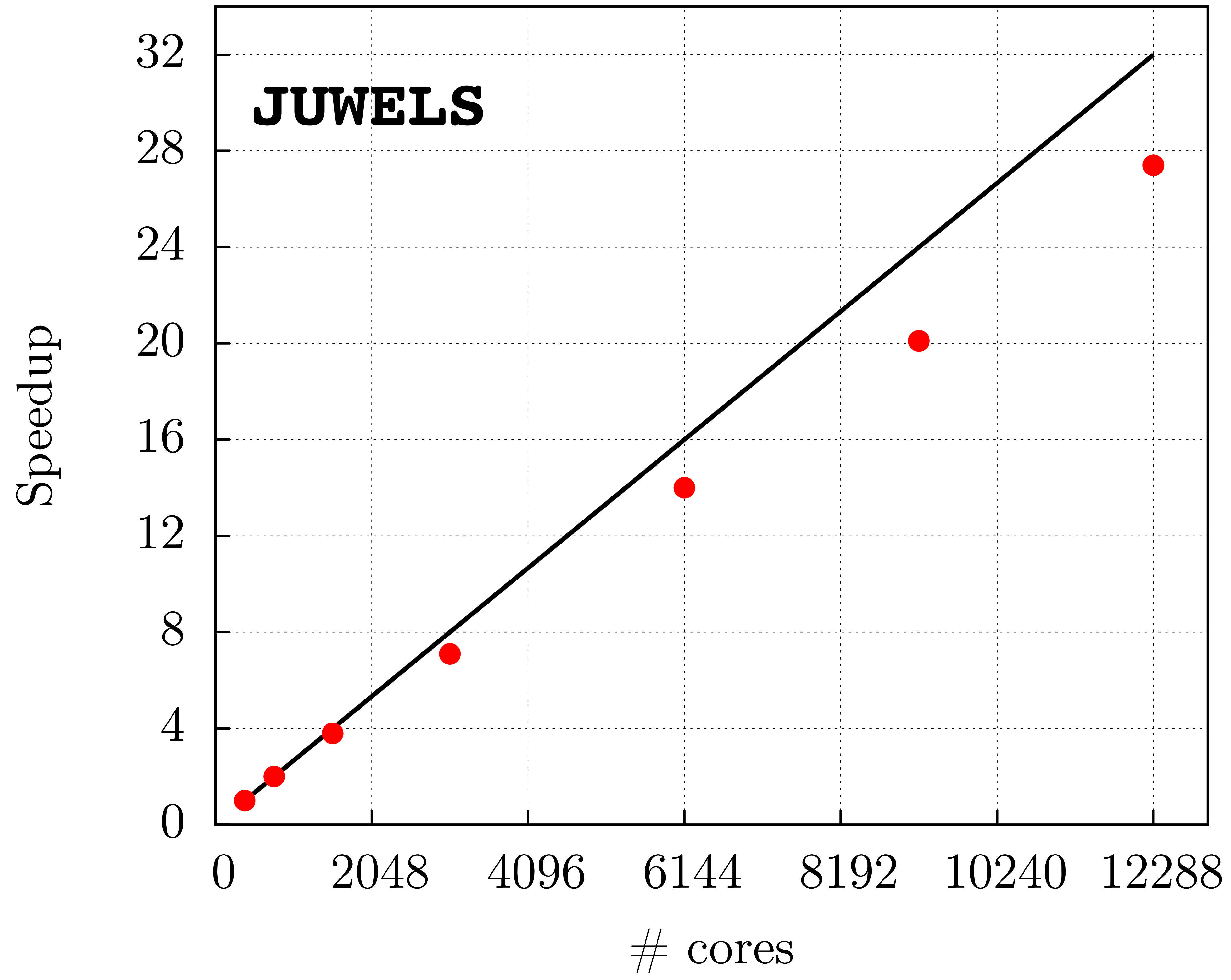

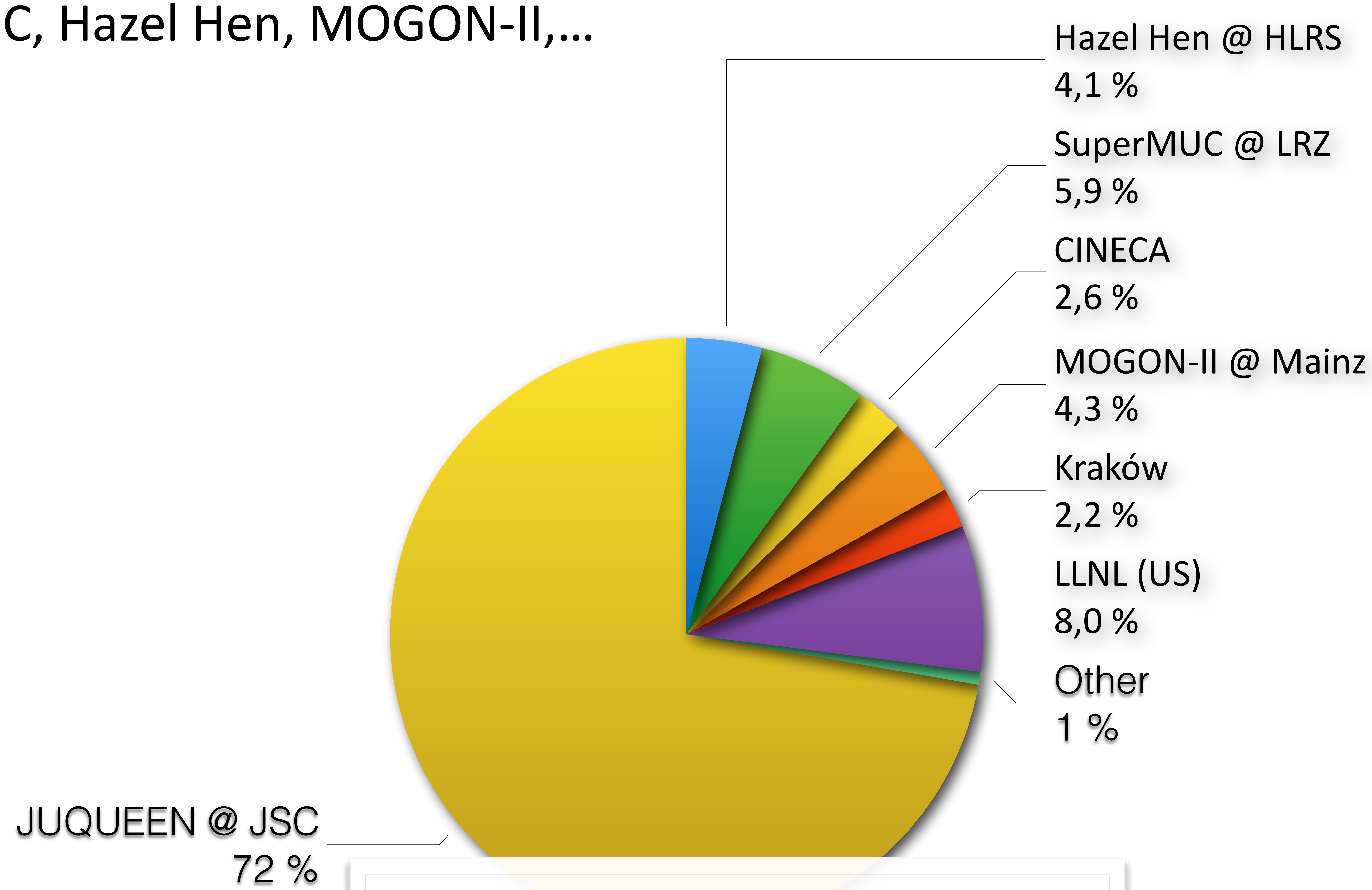

Total CPU usage (**gauge ensembles**):
1.36 Gcore-hrs

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Carbon footprint

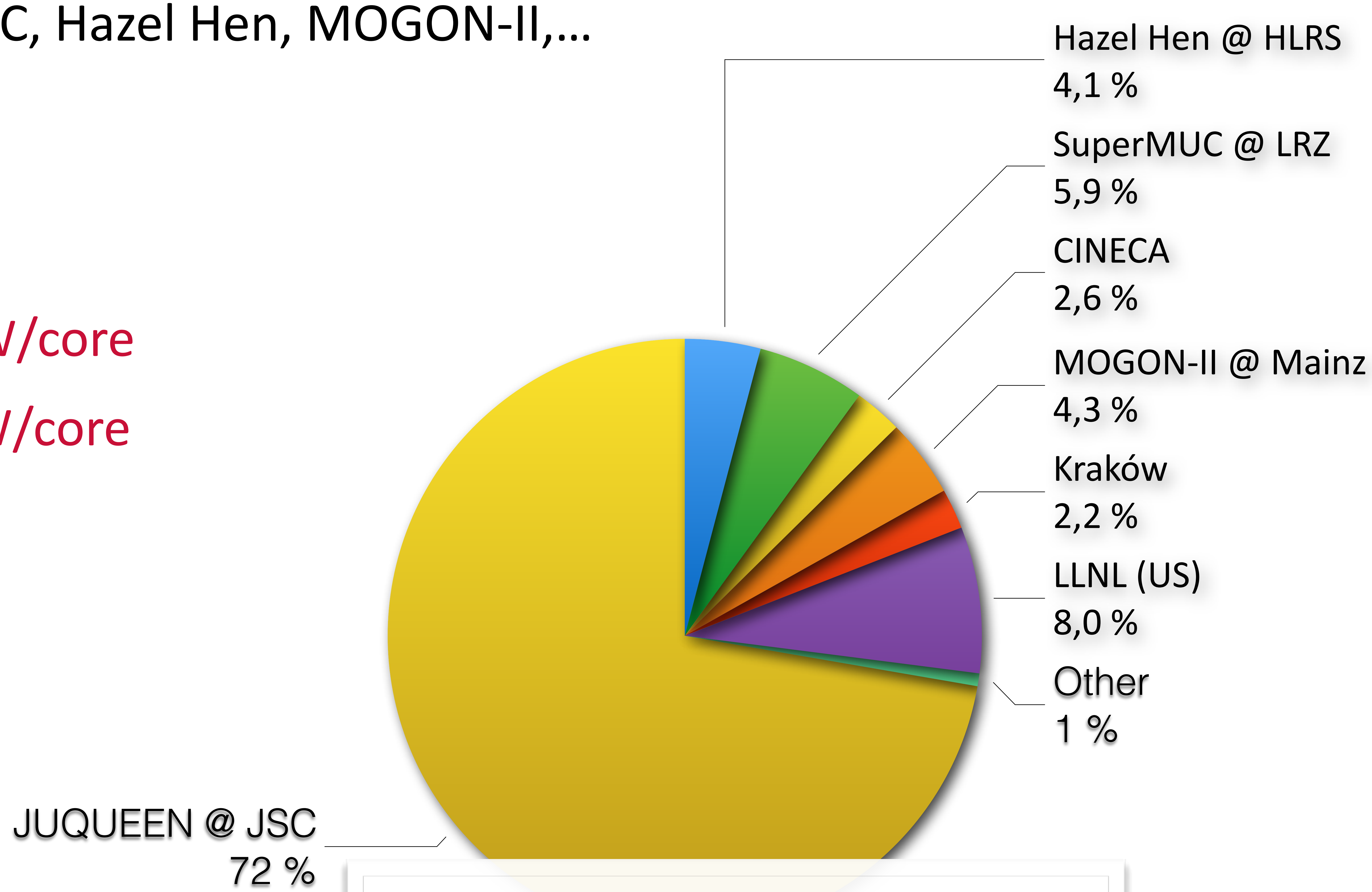
- 1.10 Gcore-hrs on BG/Q systems; 5 W/core
- 0.263 Gcore-hrs on cluster systems; 10 W/core

⇒ **8.13 GWh**

assuming 0.527 kg CO_2 / kWh yields

≈ **4300 tons** of CO_2

(excluding calculation of observables…)



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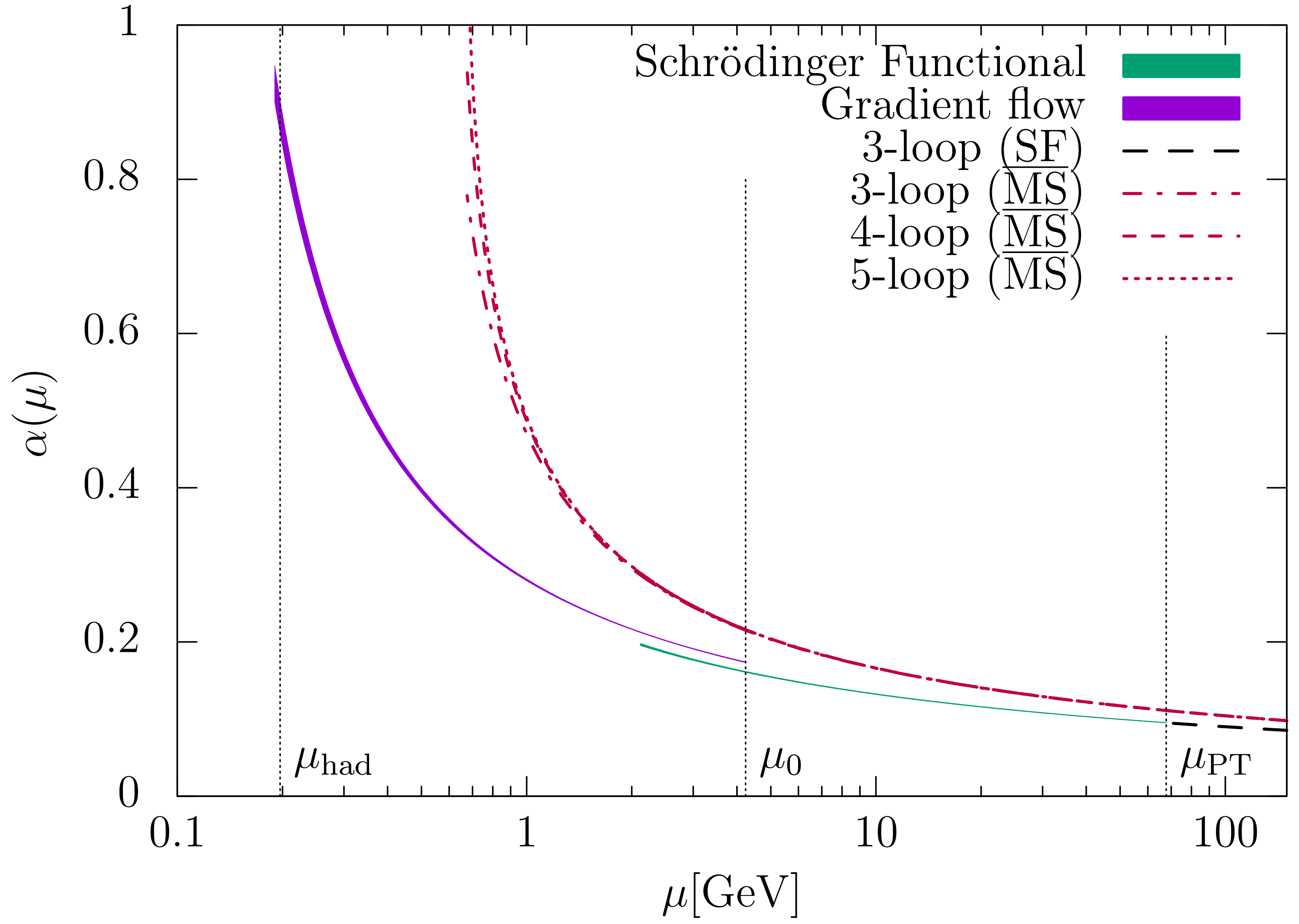
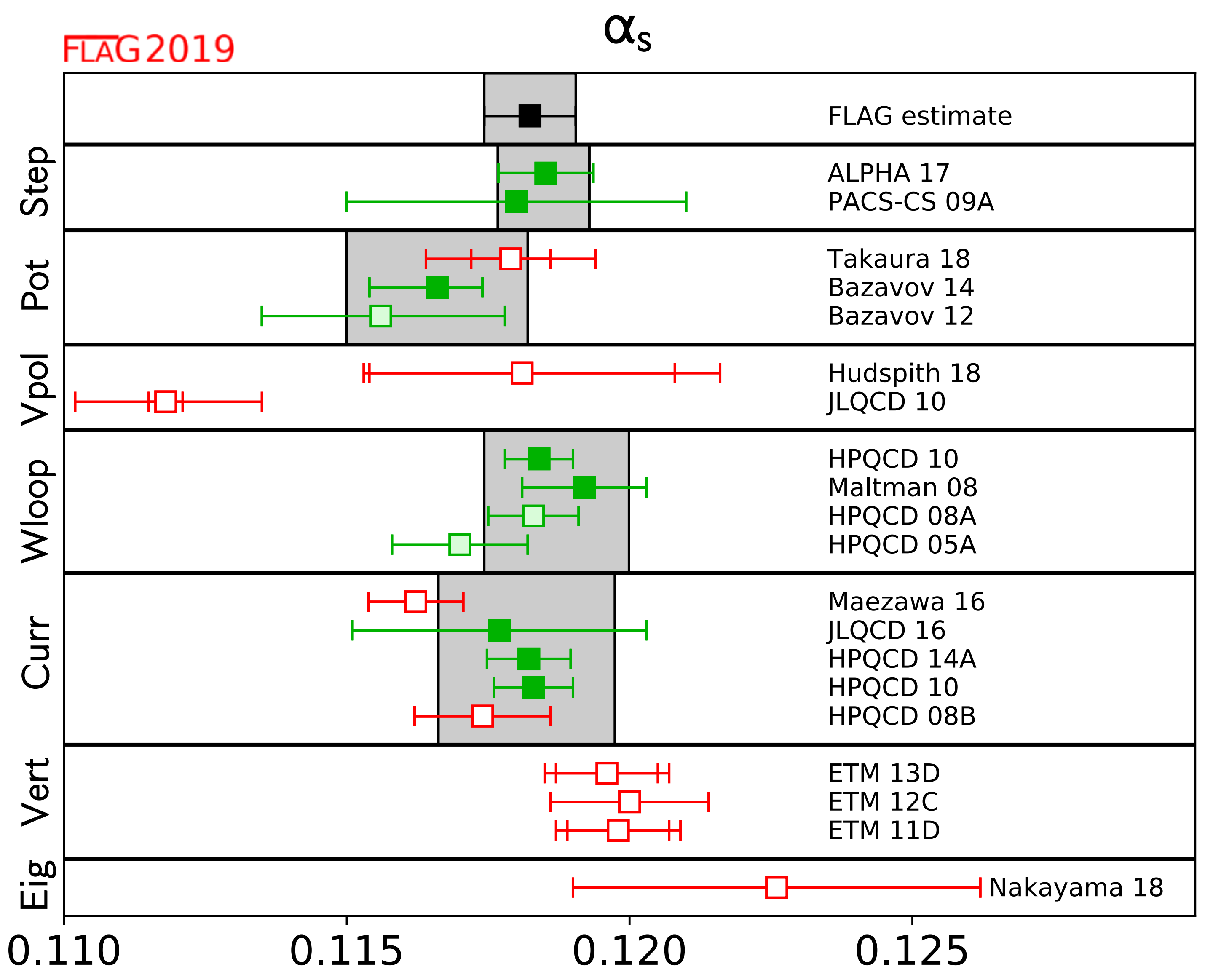
Research Highlights

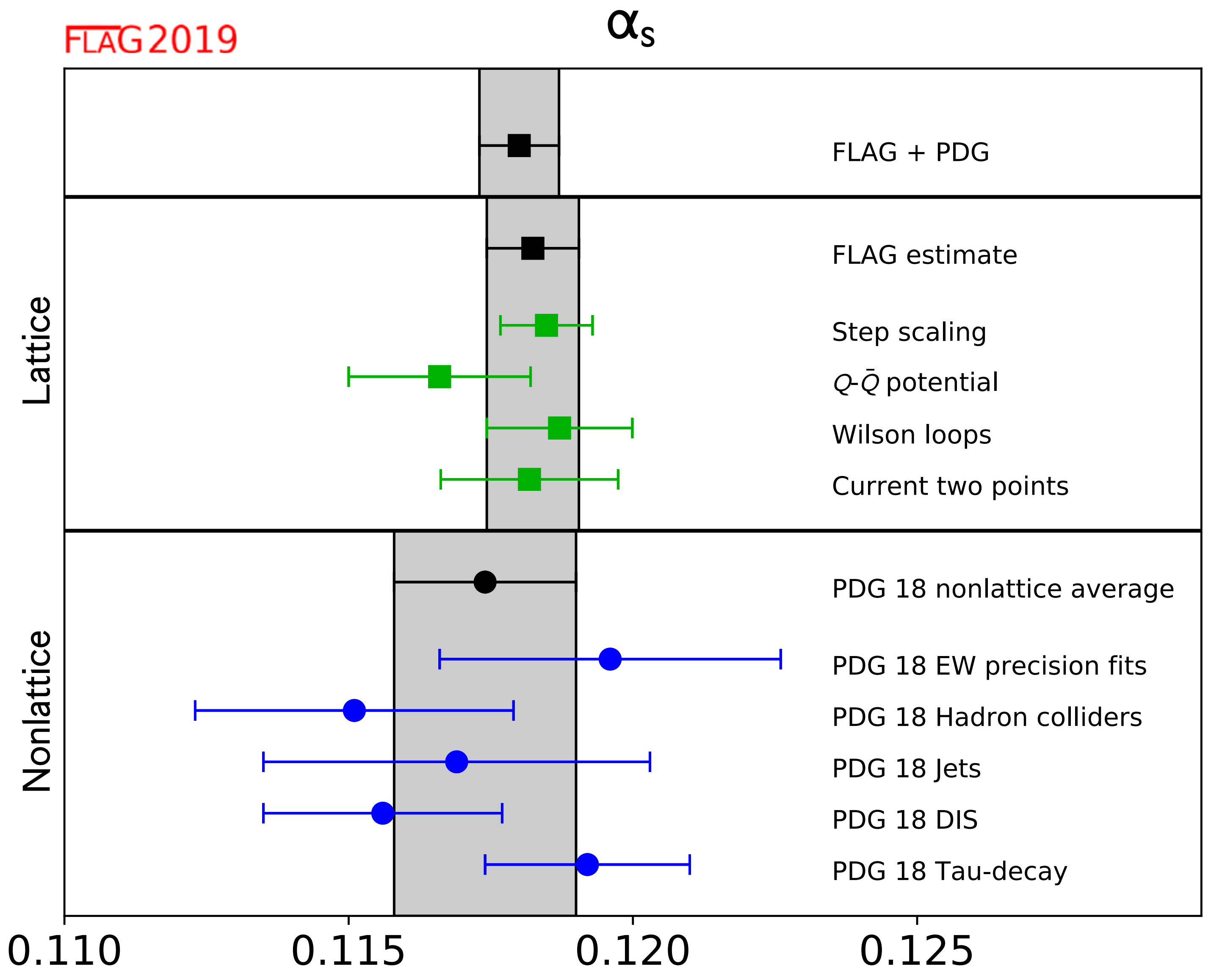
Running coupling: $\alpha_s(q)$

[Bruno et al., Phys Rev Lett 119 (2017) 102001]

- Strong coupling: fundamental parameter of the Standard Model
- ALPHA Collaboration: determination of α_s via step scaling / finite-volume scheme
- Express running scale in terms of low-energy quantity: $f_{\pi K} \equiv \frac{2}{3}(f_K + \frac{1}{2} f_\pi)$







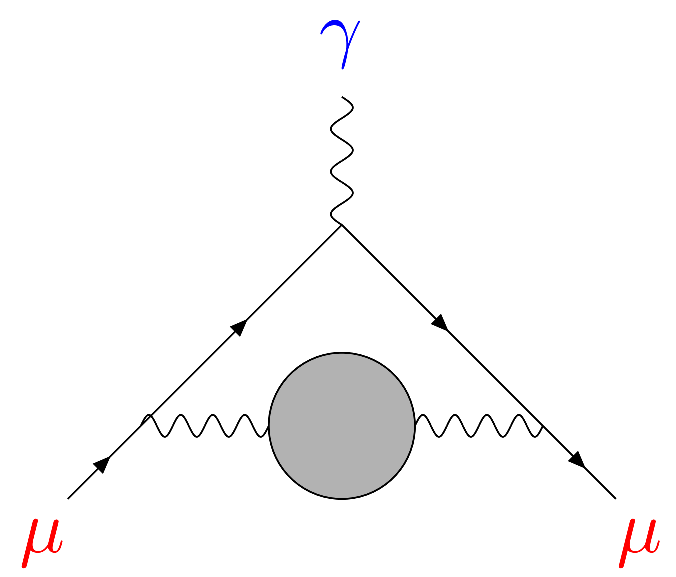
- Final result: $\alpha^{(5)}_{\overline{\rm MS}}(m_Z) = 0.11852(84)$ — dominates FLAG 2019 estimate and PDG value

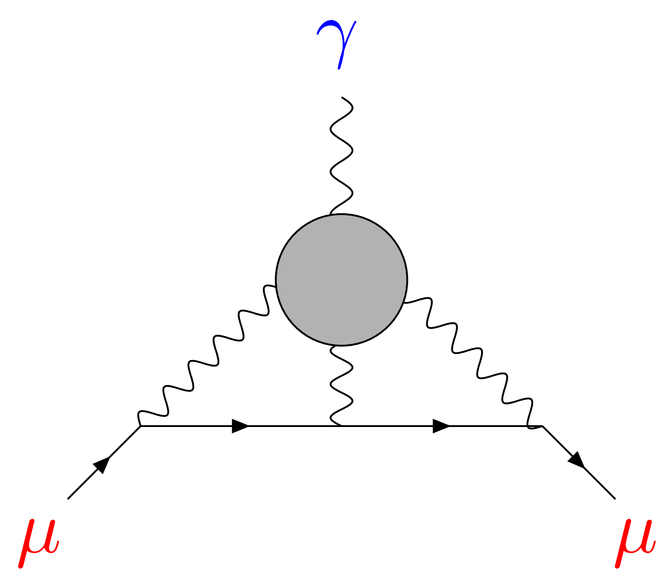
Research Highlights

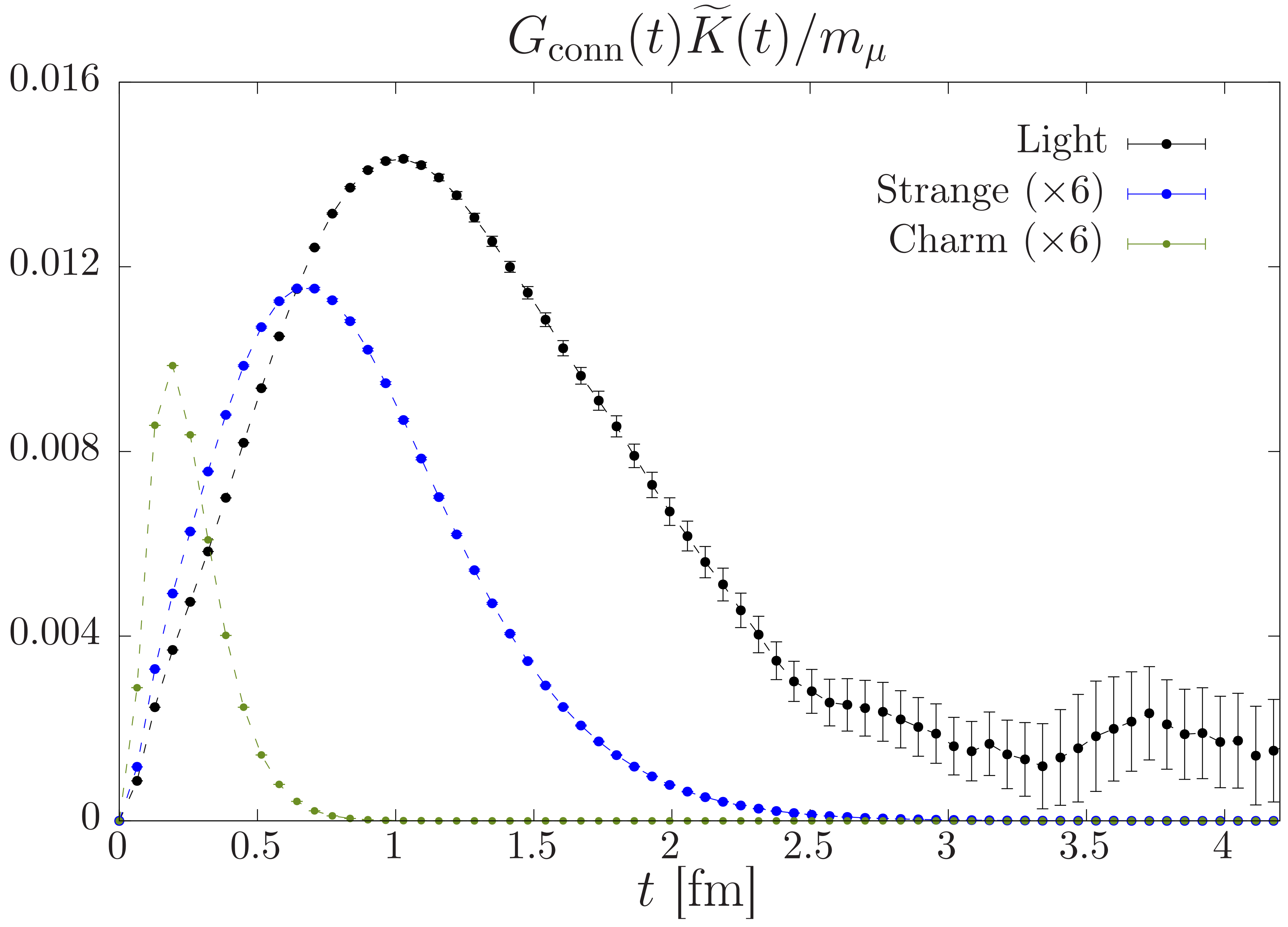
Hadronic contributions to the muon $(g-2)_\mu$

[Gérardin et al., Phys Rev D 100 (2019) 014510]

- Discrepancy of $\approx 3.5\sigma$ between SM prediction and experiment: $a_\mu^{\text{exp}} - a_\mu^{\text{SM}} = (26.9 \pm 7.3) \cdot 10^{-10}$
- Theory error dominated by hadronic contributions
- Determine HVP and HLbL contributions in lattice QCD







$m_\pi \approx 135\,\text{MeV}, \quad 96^3 \cdot 192$

- Must control infrared regime of vector correlator
- Quantify finite-volume corrections
- Evaluate quark-disconnected contributions
- Include isospin-breaking effects

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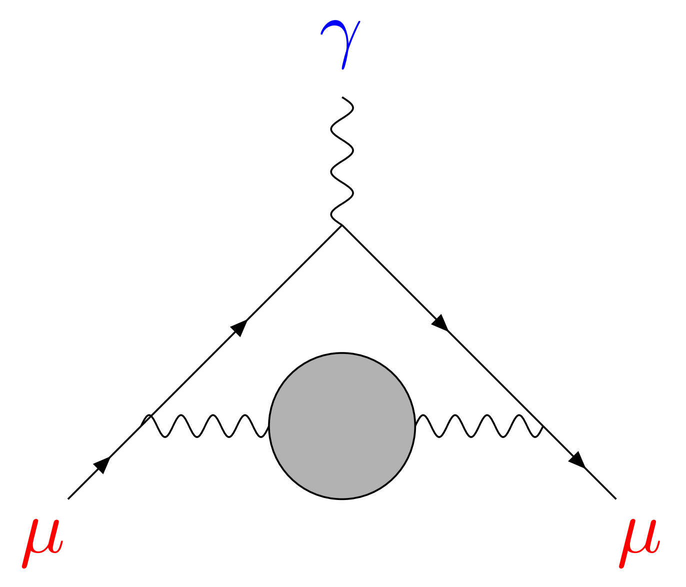

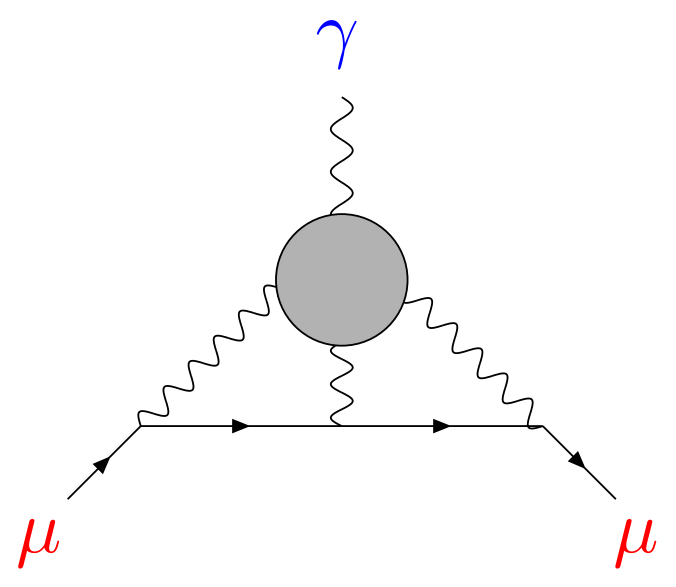

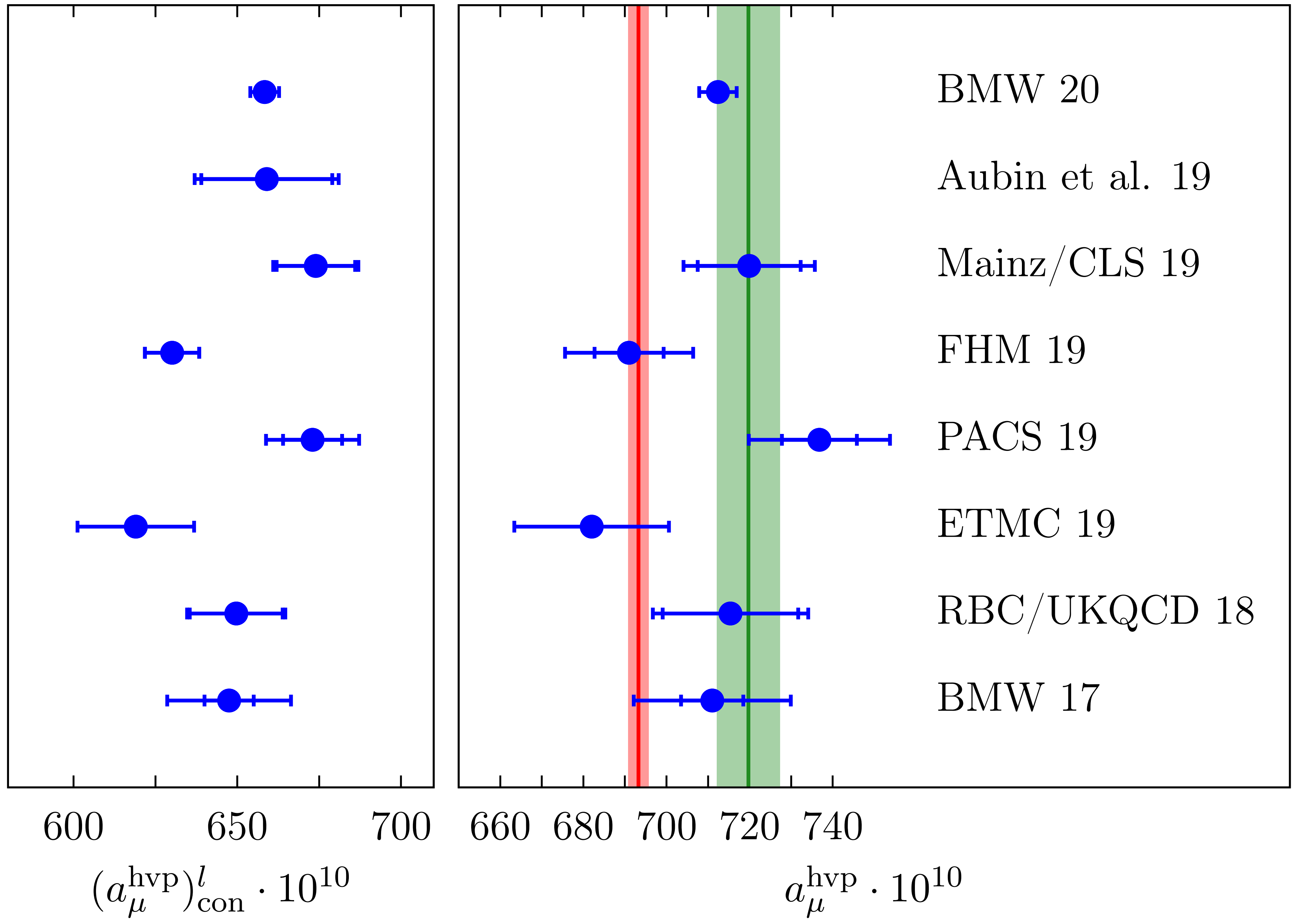

- Must control infrared regime of vector correlator
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$$a_\mu^{\rm hvp} = (720.0 \pm 12.4 \pm 9.9)\cdot 10^{-10}$$

Research Highlights

Hadronic contributions to the muon $(g-2)_\mu$

[Gérardin et al., Phys Rev D 100 (2019) 034520]

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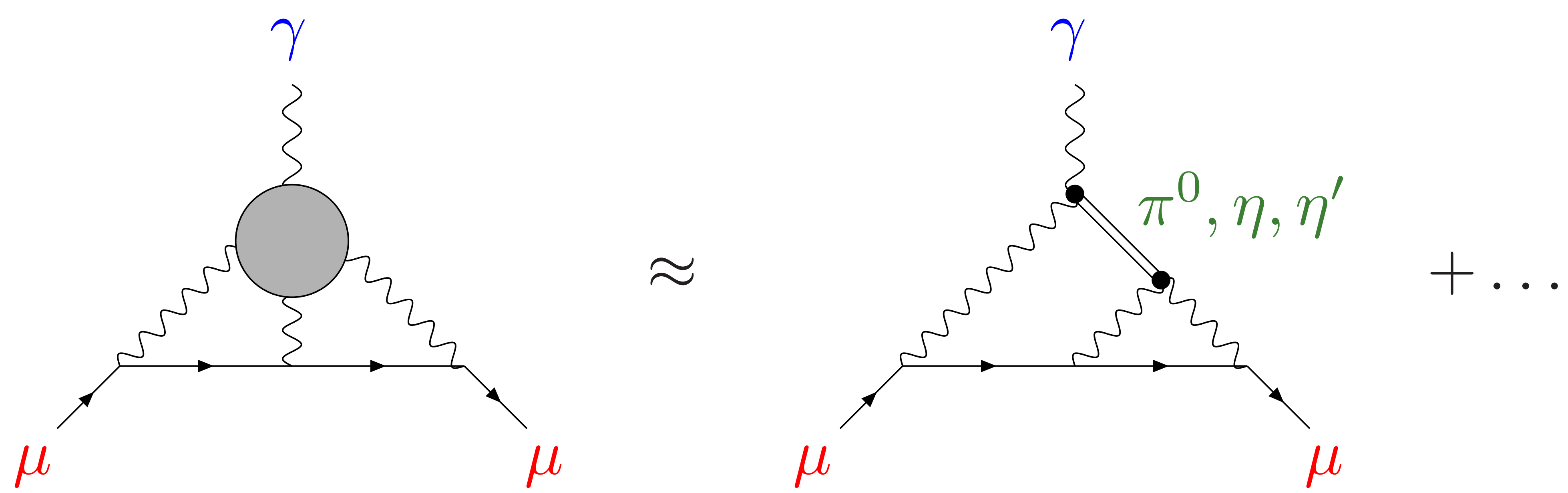
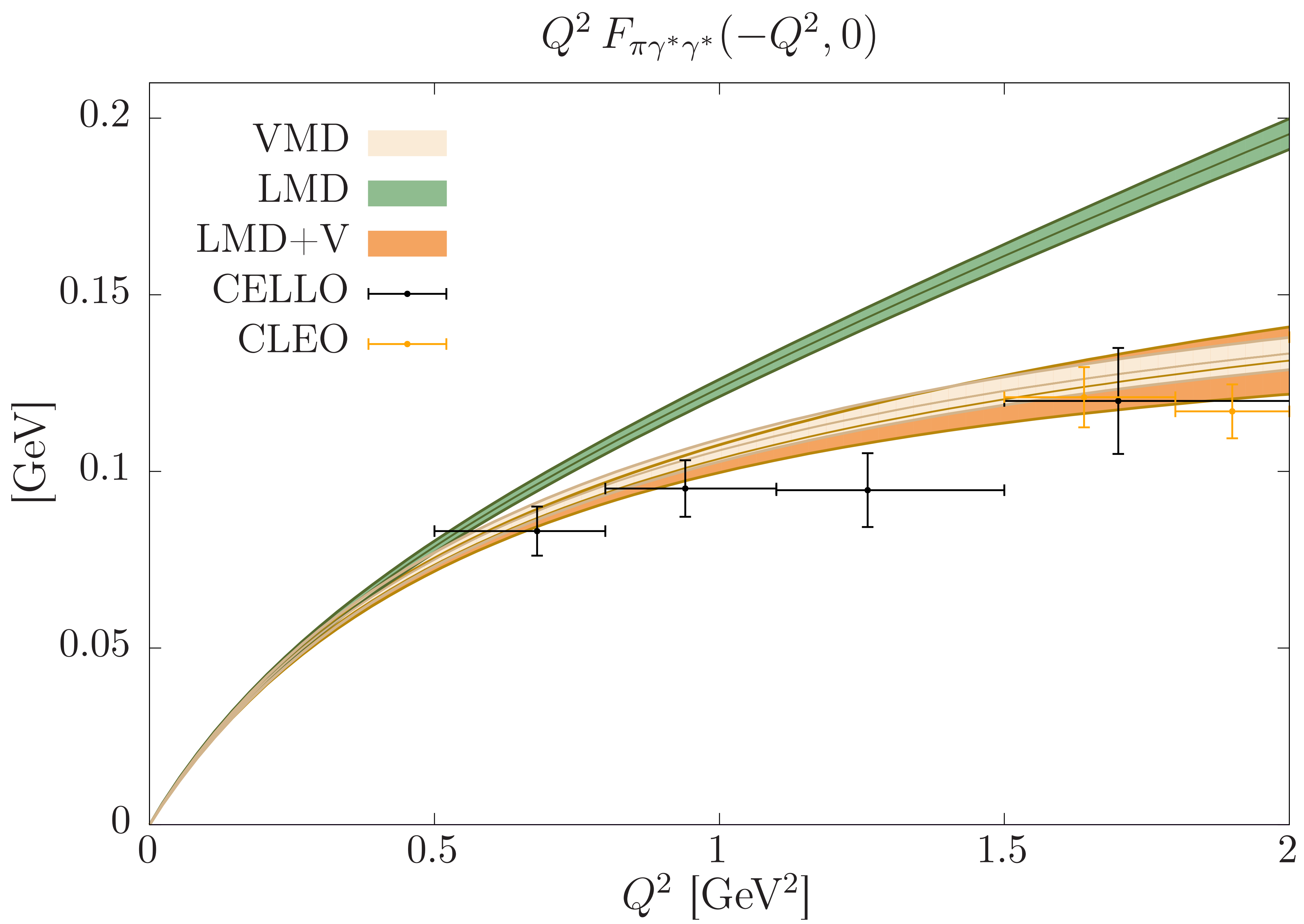




- Pion pole dominates light-by-light scattering
- Compute transition form factor $\pi^0 \to \gamma^*\gamma^*$
- Compare with result from dispersion theory

$$(a_\mu^{\text{hlbl}})_{\pi^0} = \begin{cases} (5.97 \pm 0.36) \cdot 10^{-10} & \text{Lattice QCD} \\ (6.26\,^{+0.30}_{-0.25}) \cdot 10^{-10} & \text{Dispersion theory} \end{cases}$$

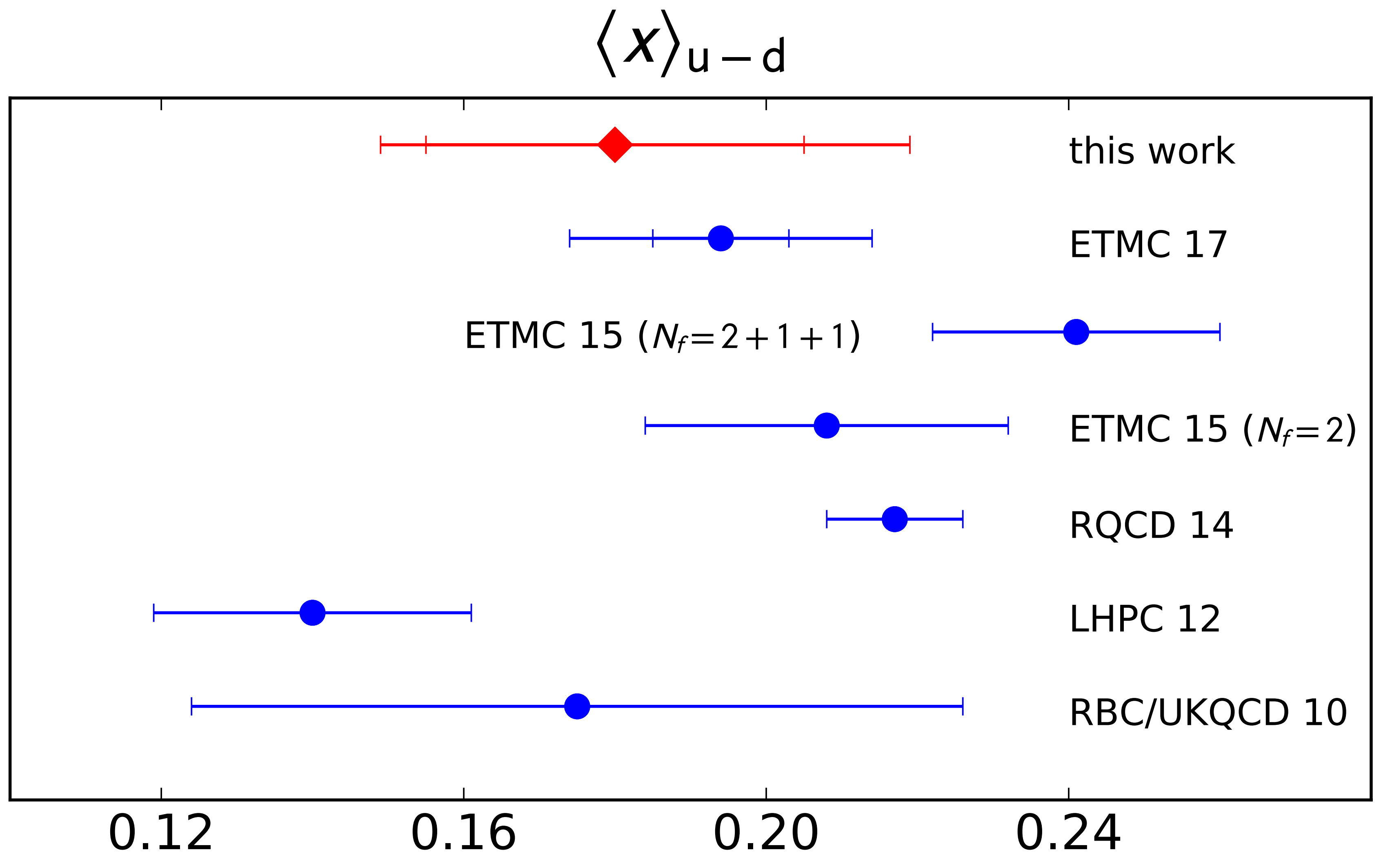
Research Highlights

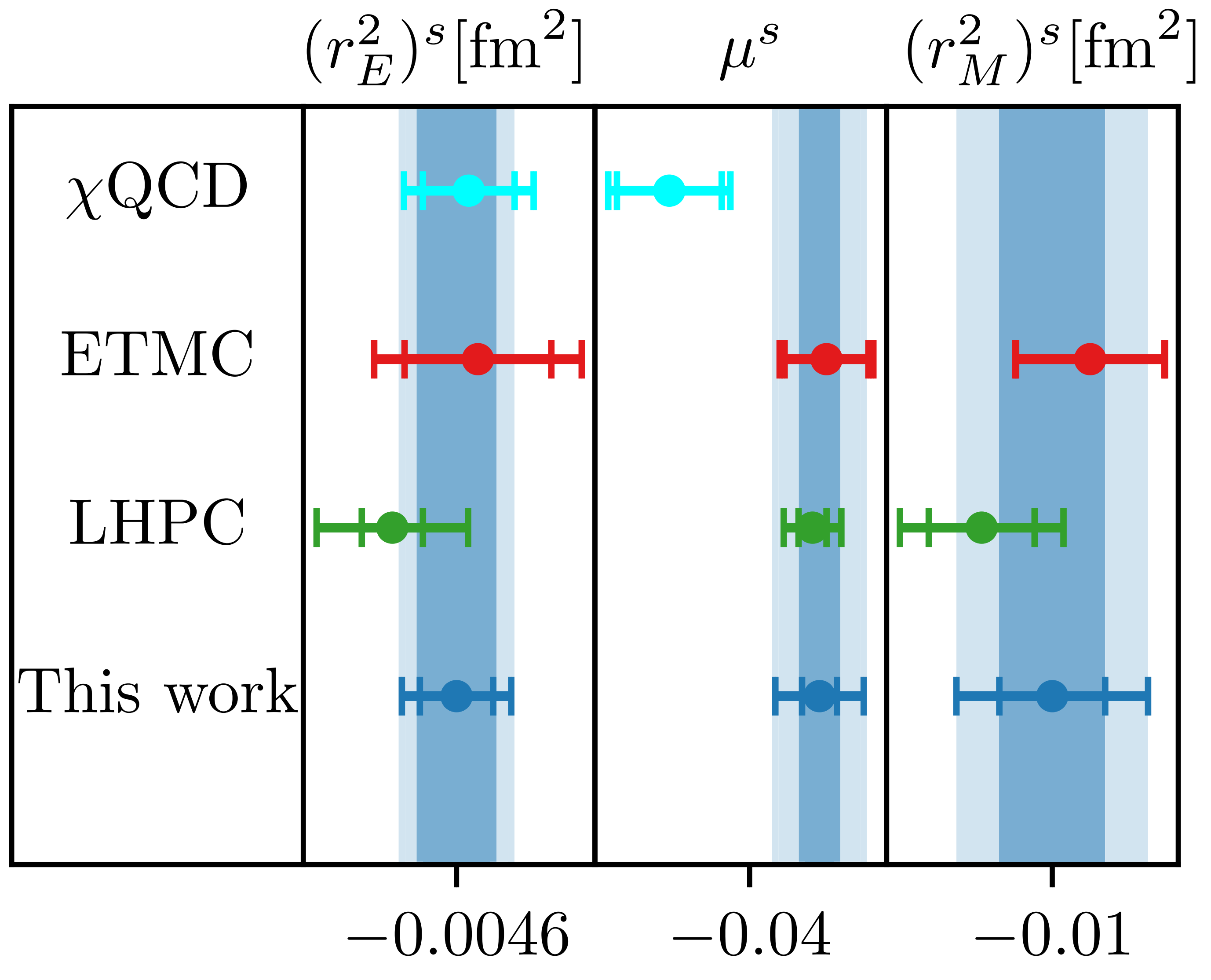
Nucleon structure observables

[Djukanovic et al., Phys Rev Lett 123 (2019) 212001, Harris et al., Phys Rev D 100 (2019) 034513]

- Axial, tensor & scalar charges: nucleon β-decay, constraints on contact interactions (BSM physics)
- Moments of parton distributions functions, helicity / transversity moments
- Electromagnetic, axial and strangeness form factors

  ⇒ "Proton radius puzzle", ν-nucleon interactions, weak charge of the proton



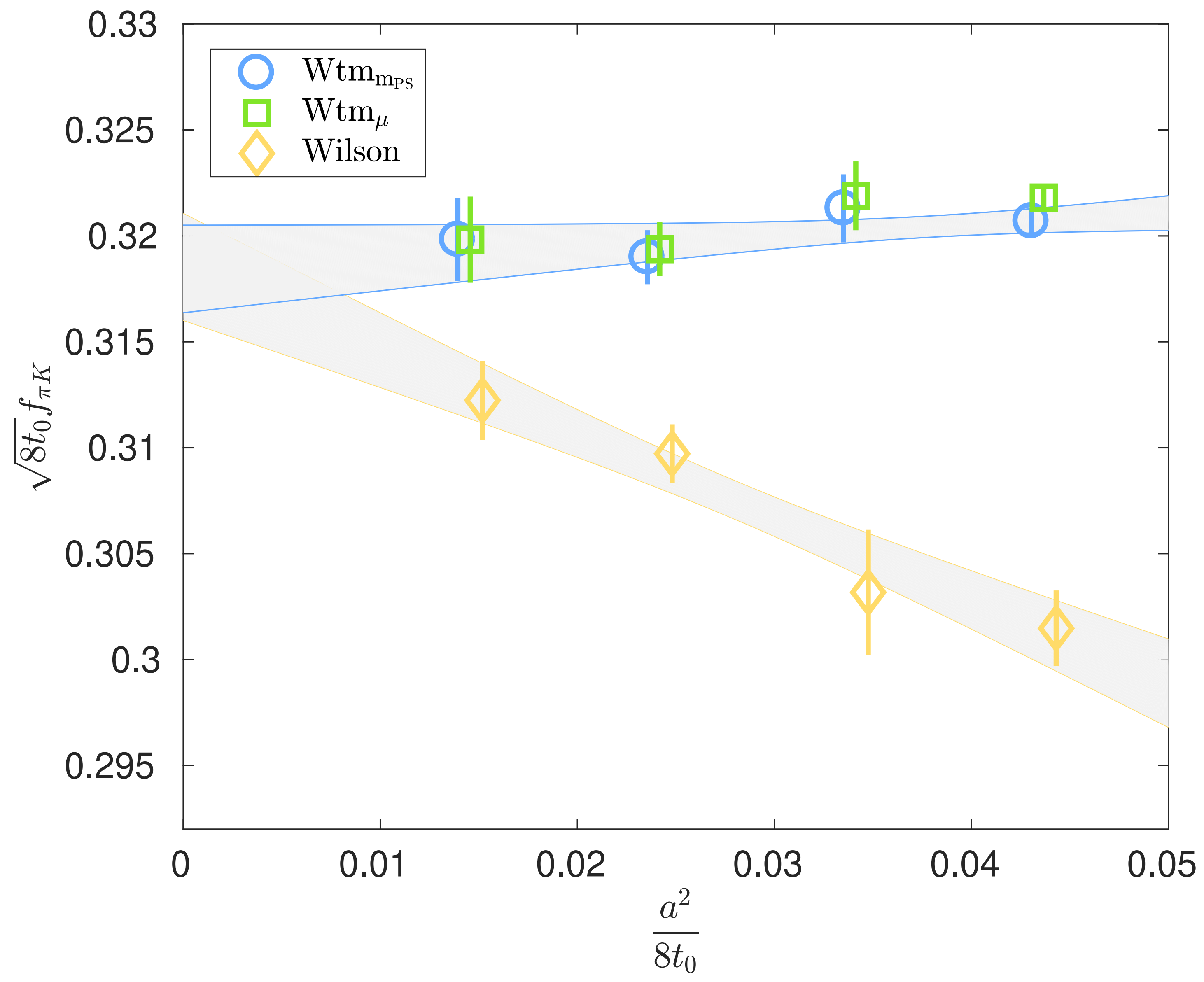


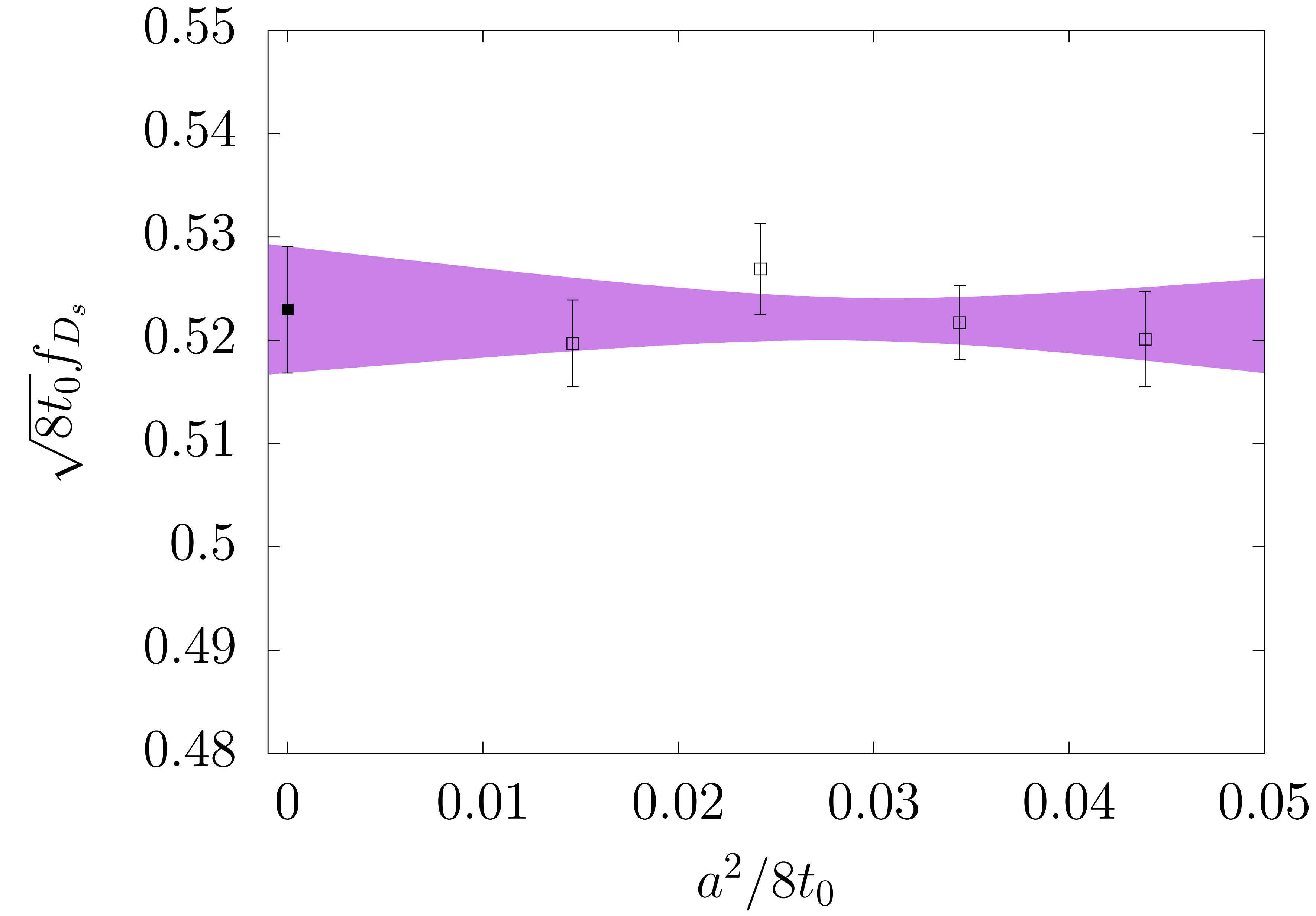
- Huge numerical effort: high statistics, quark-disconnected diagrams

Research Highlights

Flavour physics

- Determination of SM parameters: quark masses, CKM matrix elements
- Supports experimental programme at Belle-II, LHC-b, BESIII, NA62: searches for BSM physics
- Leptonic and semi-leptonic decays of heavy-light mesons
- Leptonic decays of quarkonia and final-state resonances
- Mixed action setup: twisted mass Wilson fermions on CLS configurations





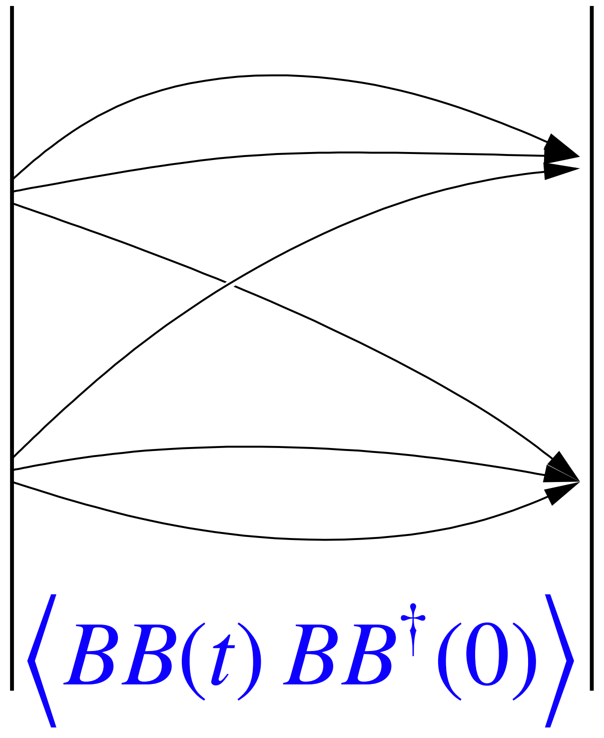
Research Highlights

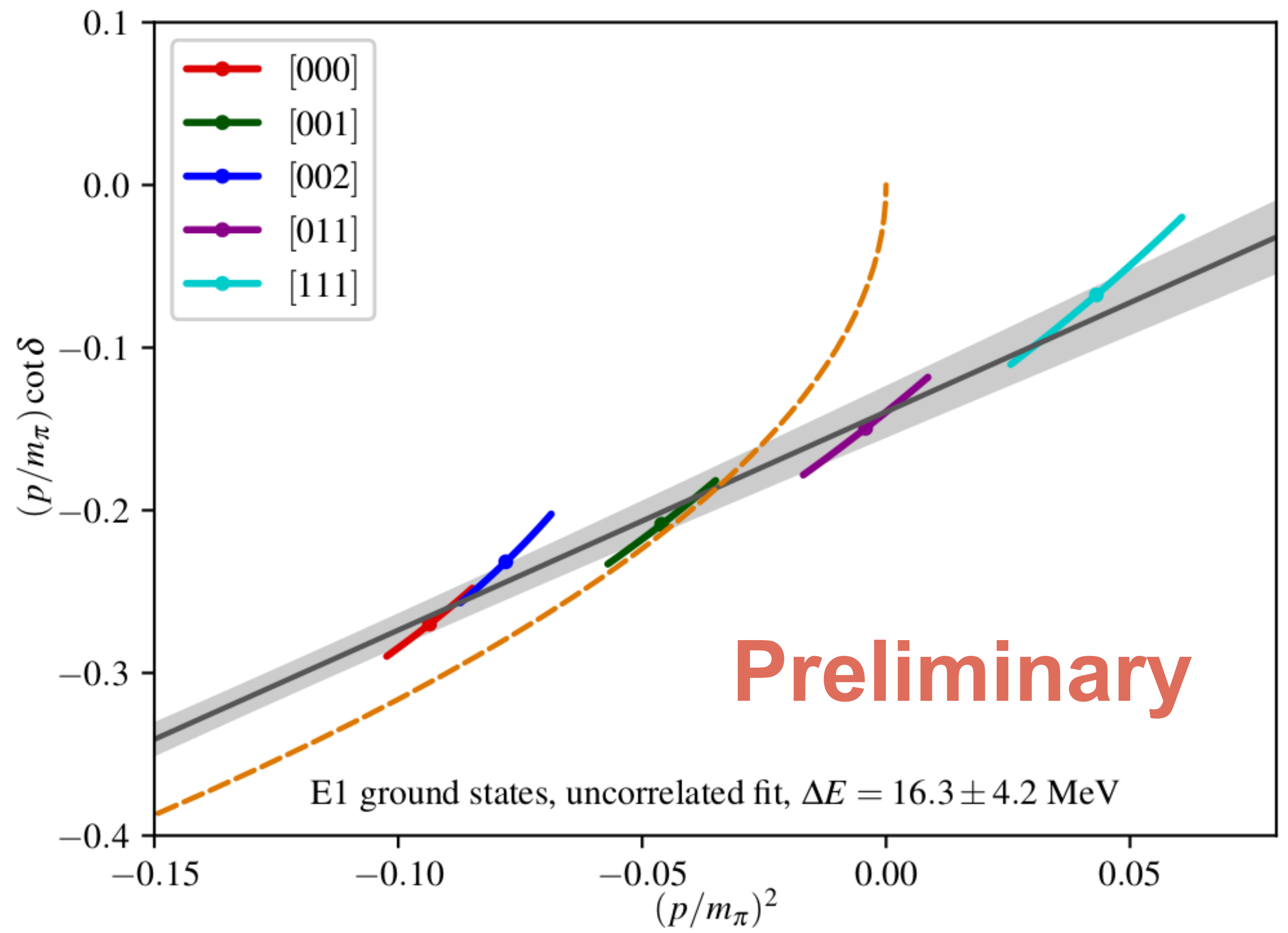
Baryon-baryon interactions

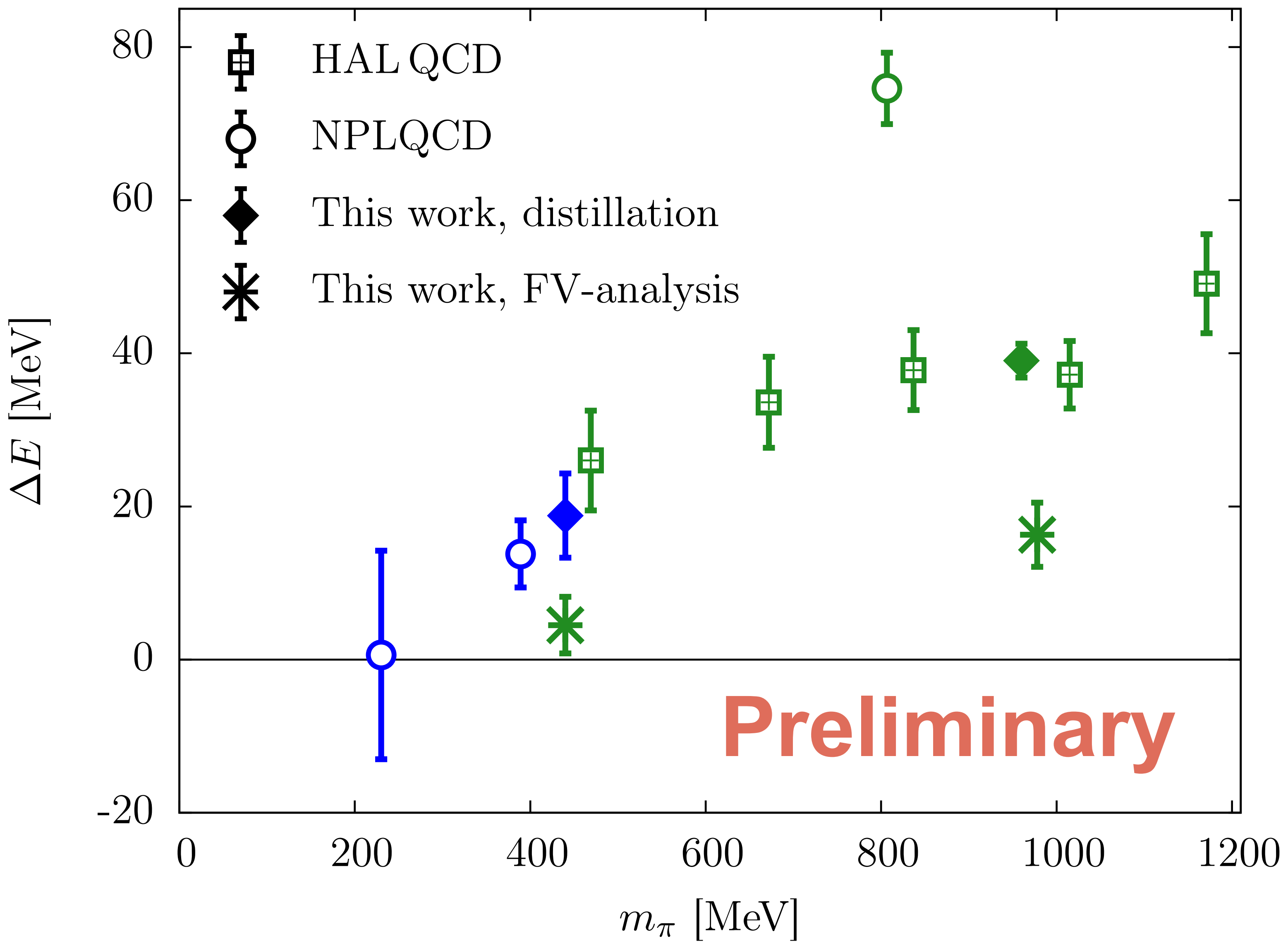
[Francis et al., Phys Rev D 99 (2019) 074550]

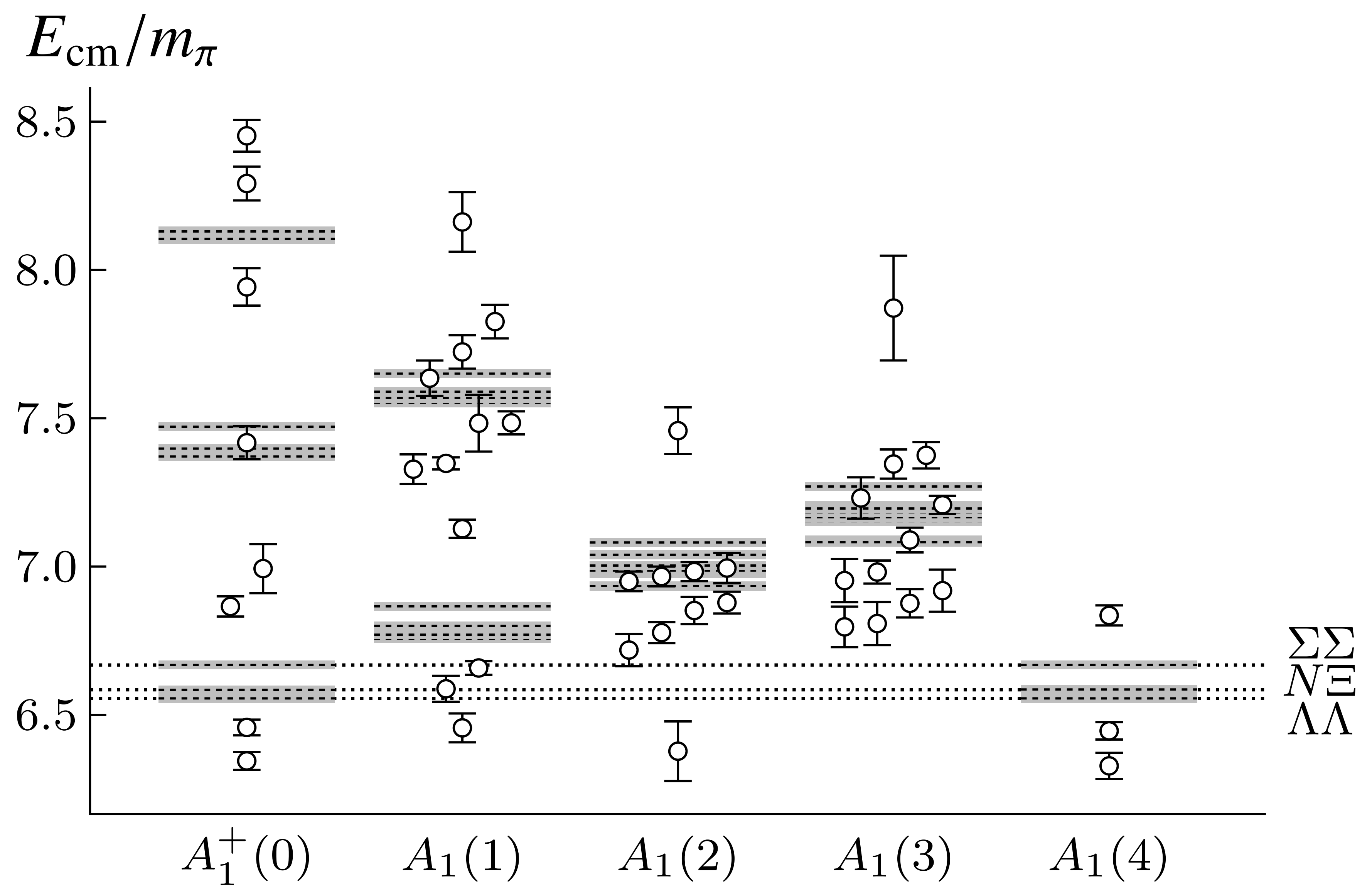
- Does a bound state of two Λ baryons (*H* dibaryon) exist?
- Use distillation and GEVP to determine energy levels
- Binding energy from pole in the scattering amplitude via Lüscher formalism

$$p \cot\delta_0(p) = A + Bp^2 + \ldots \stackrel{!}{=} -\sqrt{-p^2}$$







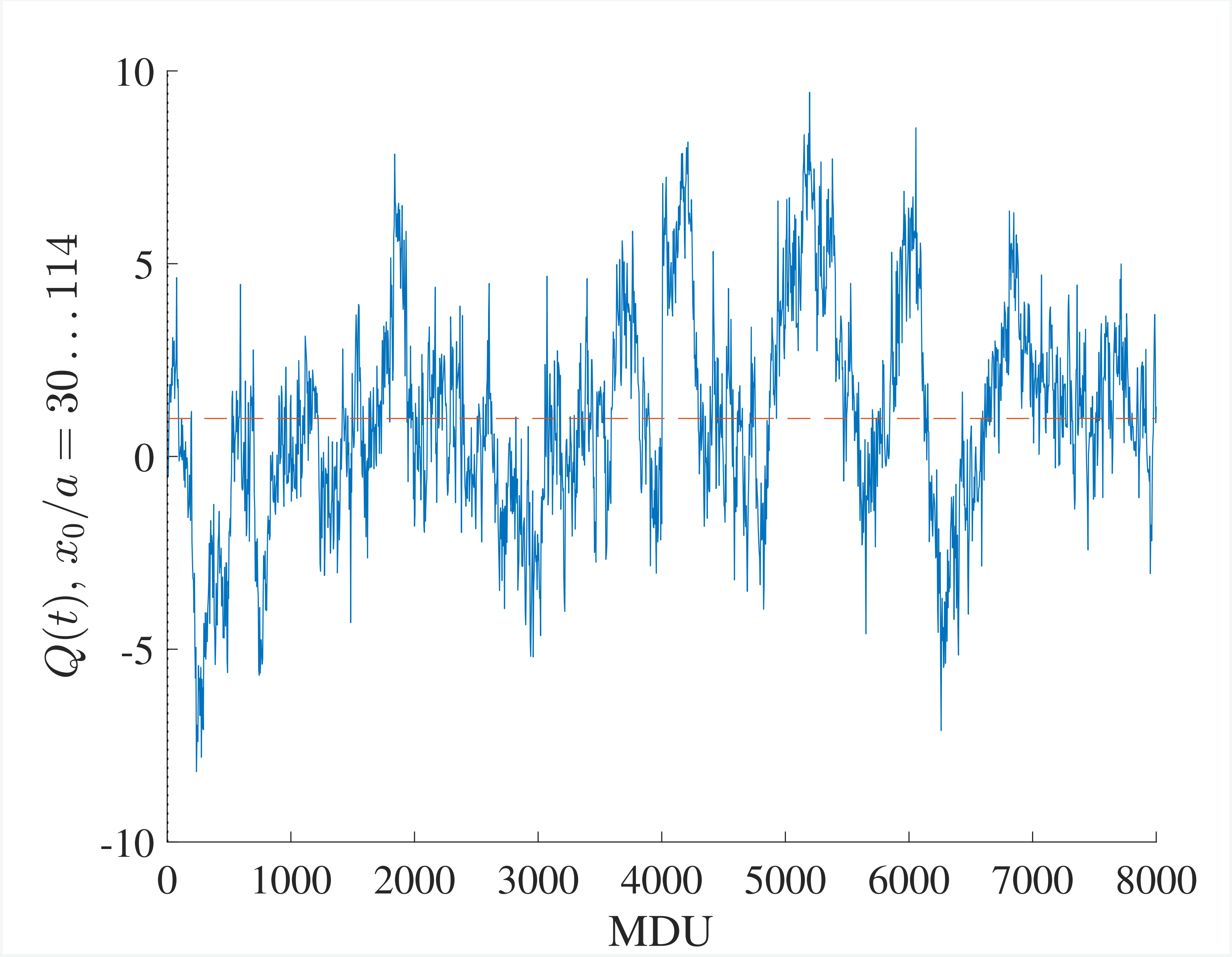


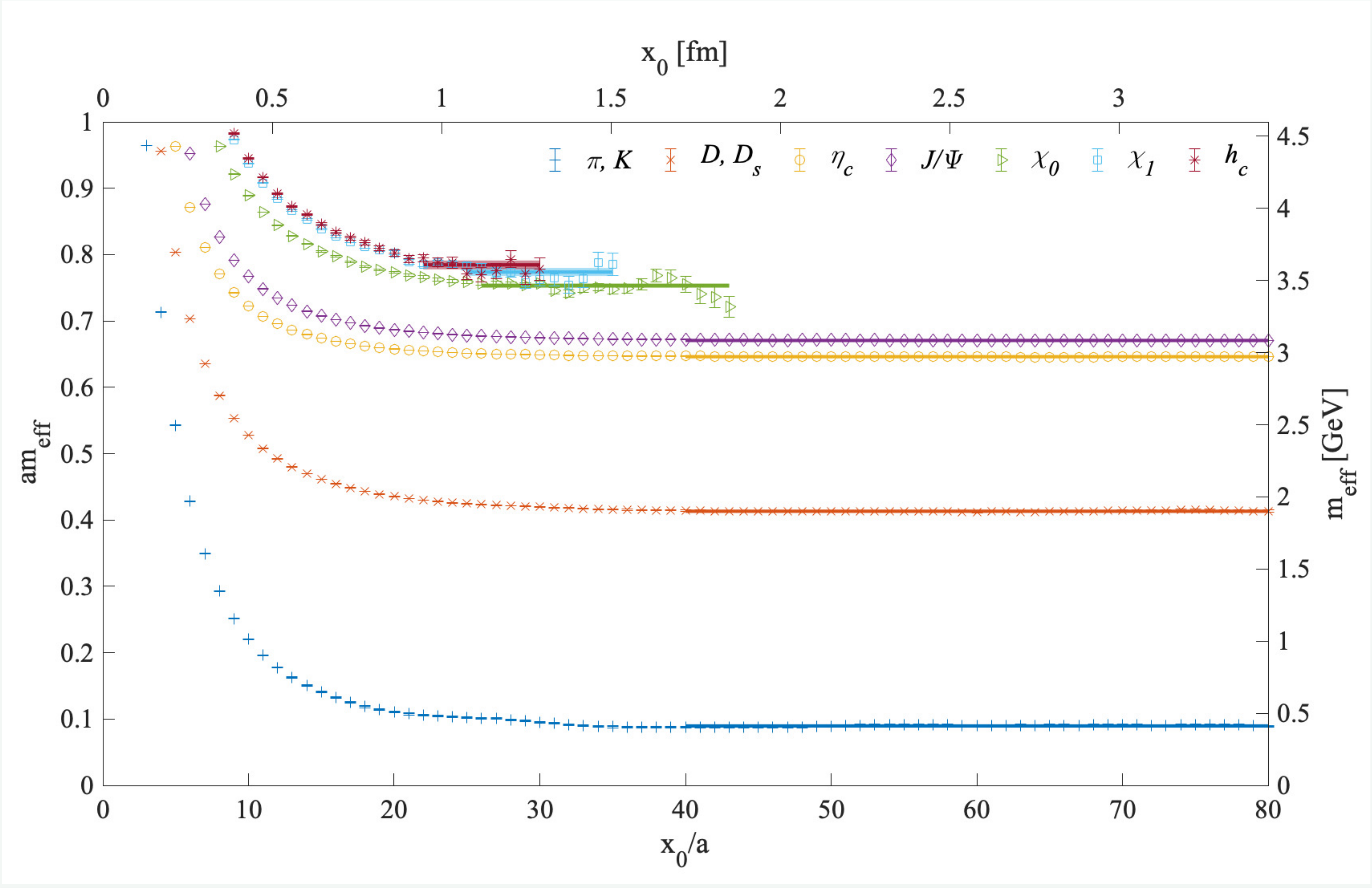
Research Highlights

Simulations with dynamical charm quarks

[Höllwieser et al., arXiv:2002:02866]

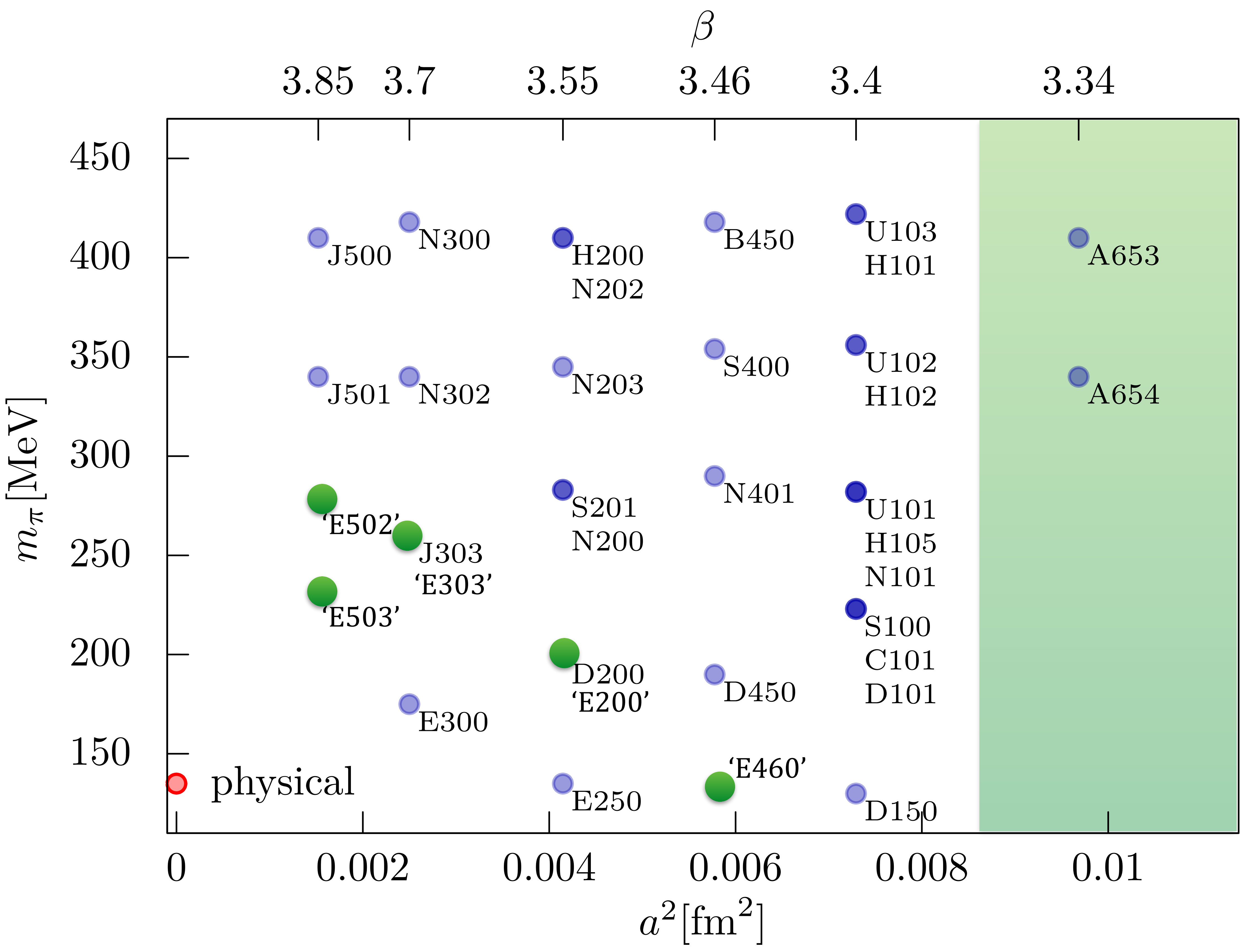
- Heavy quarks: must control lattice artefacts $\longleftrightarrow$ topology freezing
- Pilot study: $N_f = 3 + 1$ flavours of improved Wilson quarks
- Massive renormalisation and improvement scheme: no $\mathrm{O}(am_c)$ cutoff effects
- Simulate very fine lattice spacings $(a \simeq 0.050, 0.045\,\mathrm{fm})$ without topology freezing





Future Perspectives and CPU Requirements

Gauge ensemble generation



$m_u + m_d + m_s \approx \text{const}$

* Populate regime at small lattice spacing and near-physical pion mass
* Add ensembles with larger volumes and/or periodic boundary conditions
* Extend simulations to coarser lattice spacings?
  $\longrightarrow$ modified lattice action *[Francis et al., arXiv:1911.04533]*

$$D = \begin{pmatrix} D_{\rm ee} & D_{\rm eo} \\ D_{\rm oe} & D_{\rm oo} \end{pmatrix},$$

$$D_{\rm ee} + D_{\rm oo} = M_0 \exp\left(\frac{c_{\rm sw}}{M_0}\frac{i}{4}\,\sigma_{\mu\nu}\hat{F}_{\mu\nu}\right)$$

* Add dynamical charm quark?
* Incorporate QED?

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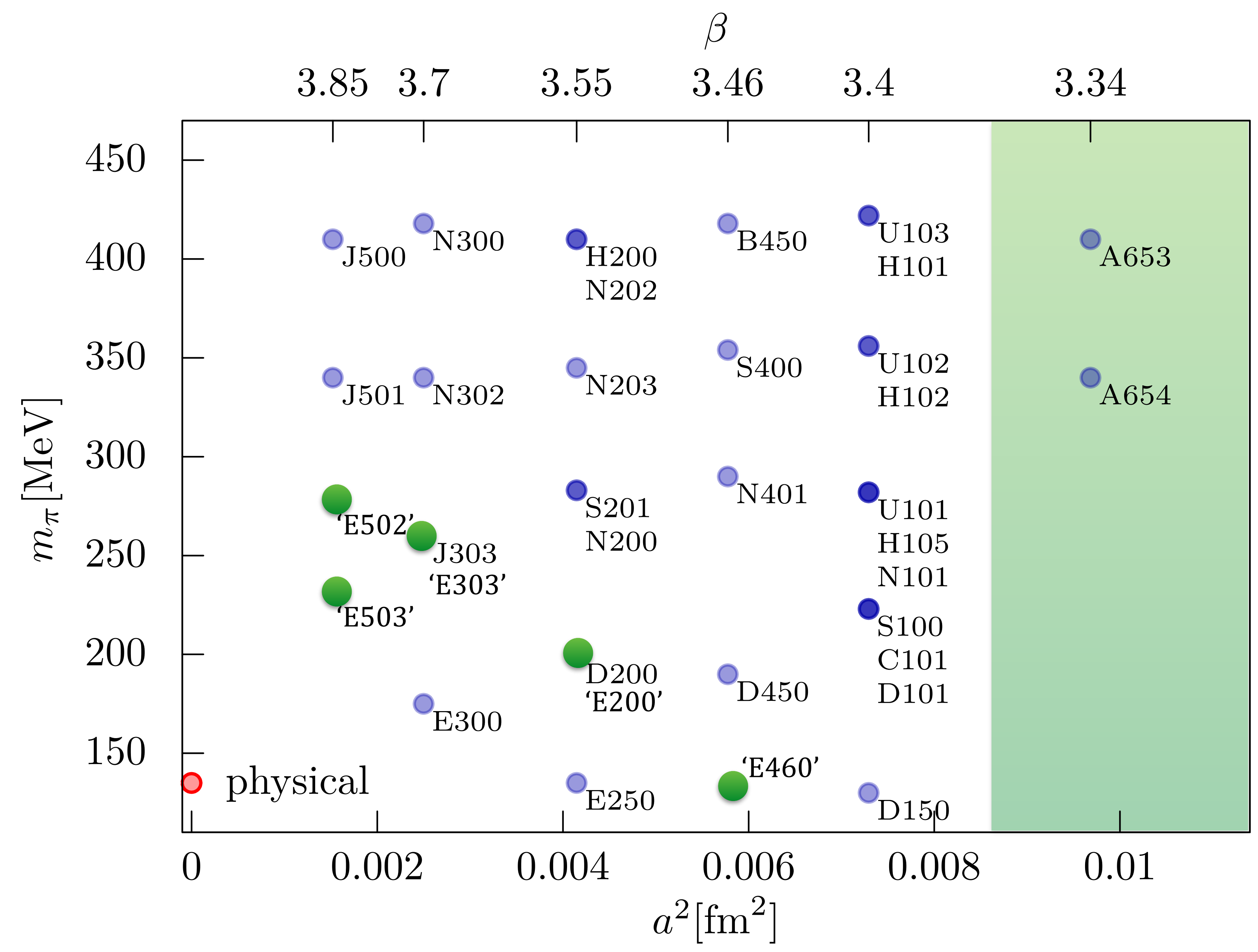

Existing set of $N_f = 2+1$ ensembles:

* Future default lattice size: $96^3 \cdot 192$

Change lattice action:

* Add dynamical charm and/or use exponentiated Clover term

⇒ Generate a new set of ensembles;
concentrate on $m_\pi \approx m_\pi^{\rm phys}, \quad m_\pi L \approx 4-6$

Require factor 5–10 more CPU time in 2020ff

Crucial: must make use of GPU architectures