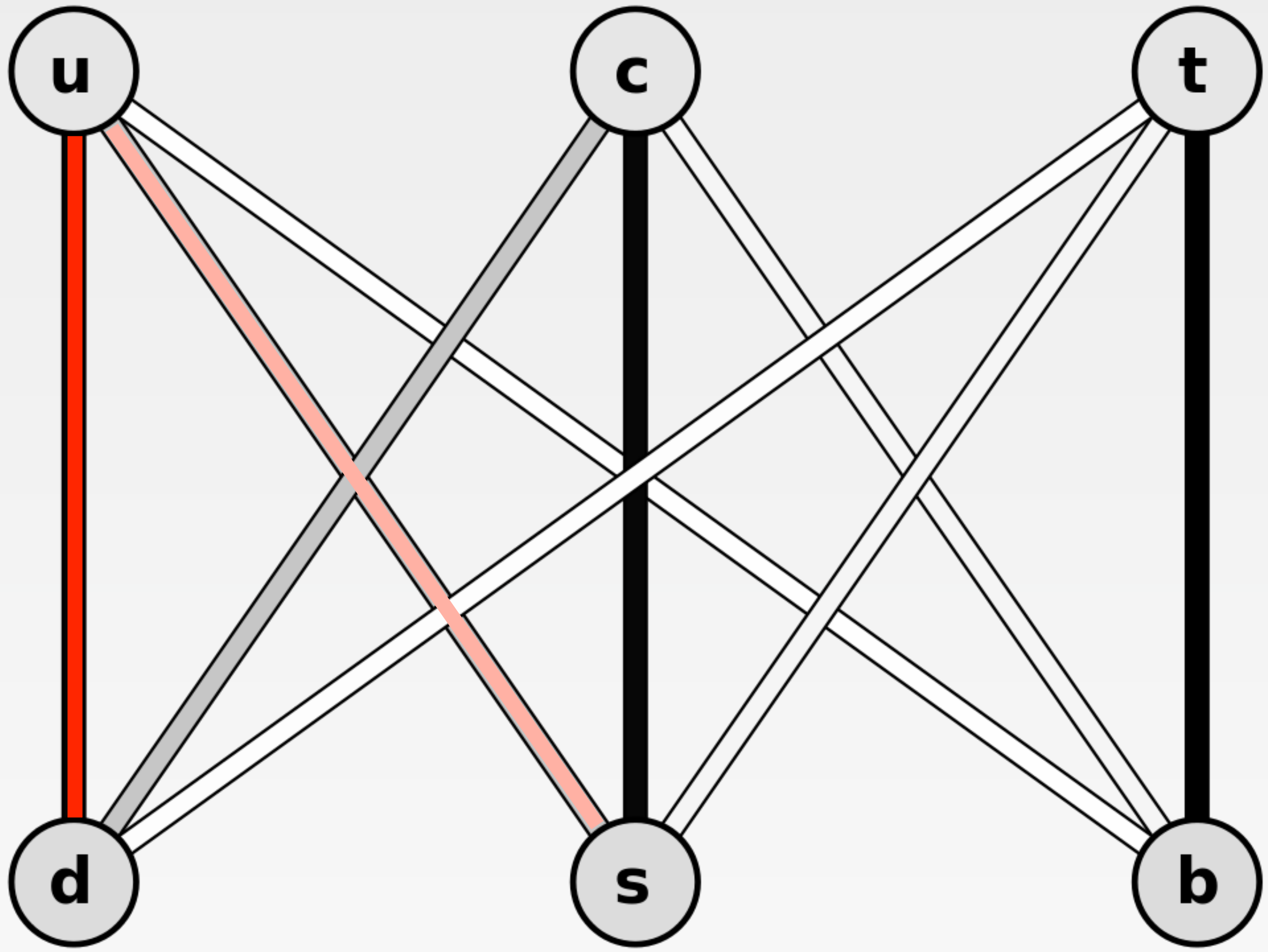


Strange and light flavour physics challenges in Lattice QCD

Antonin Portelli (RBC-UKQCD)

15th of June 2020

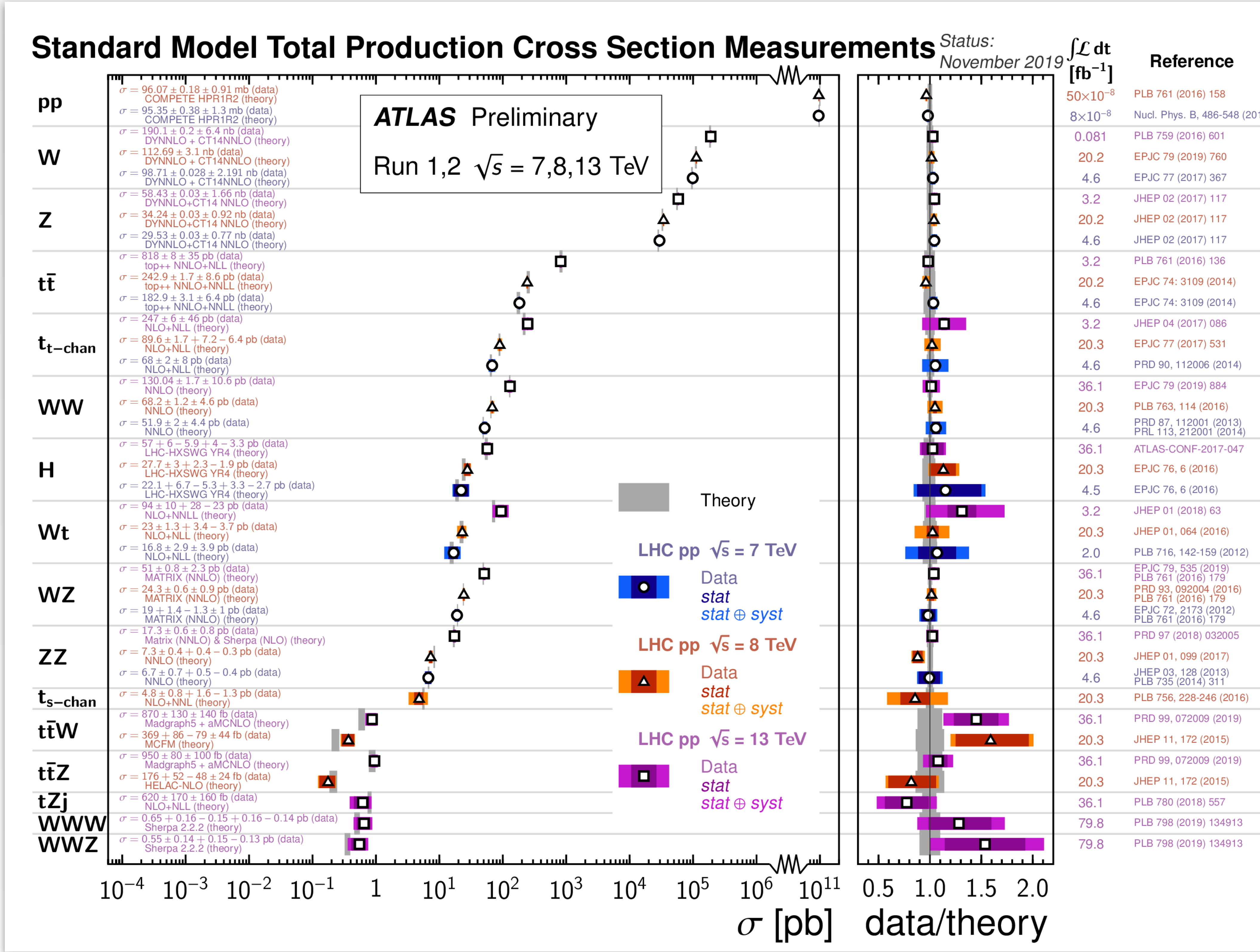
EXALAT Kick-Off Workshop

THE UNIVERSITY of EDINBURGH

- Physics motivations
- Computational challenges
- Software design perspectives

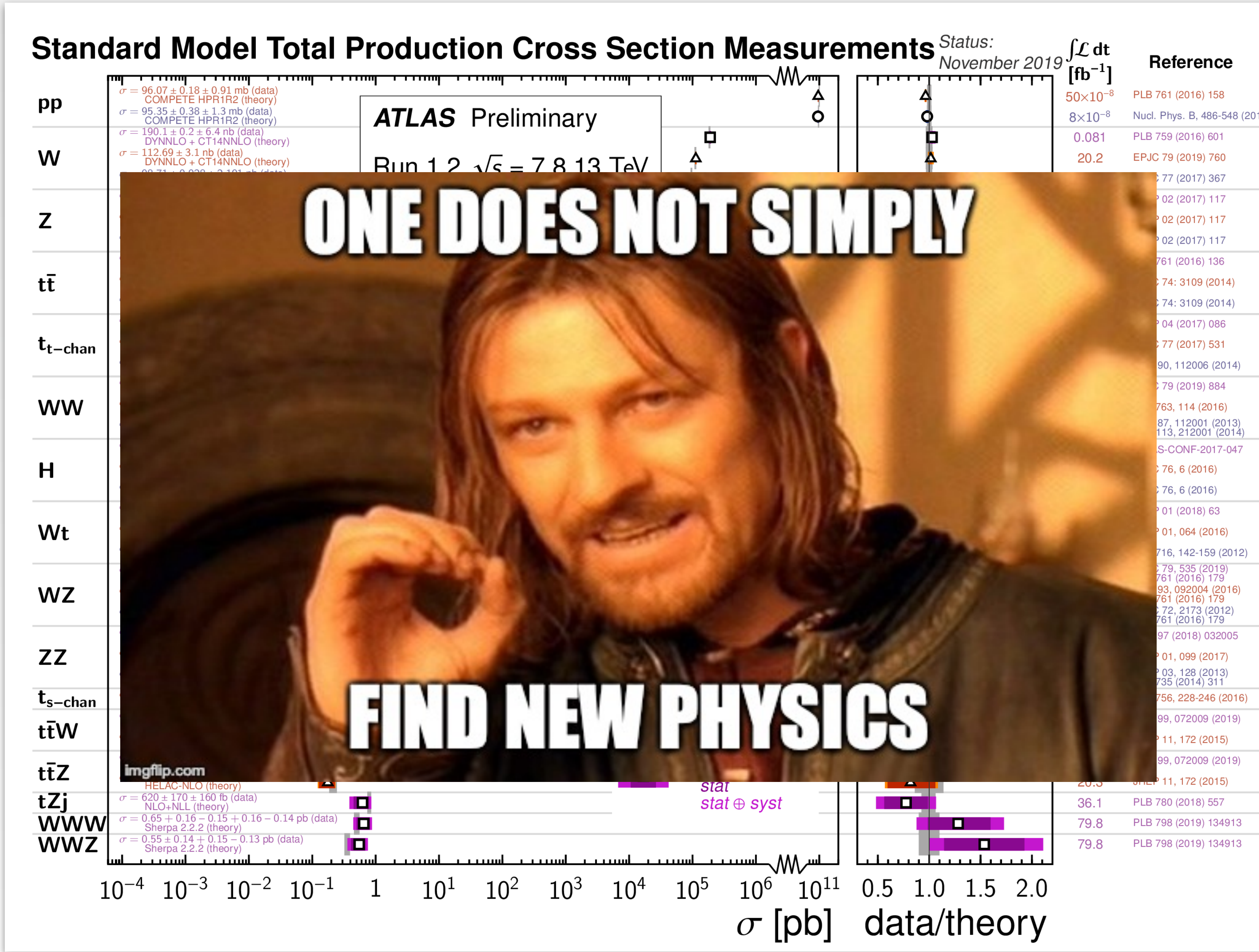
Physics motivations

The Standard Model vs. experiments



[CERN ATL-PHYS-PUB-2019-024]

The Standard Model vs. experiments

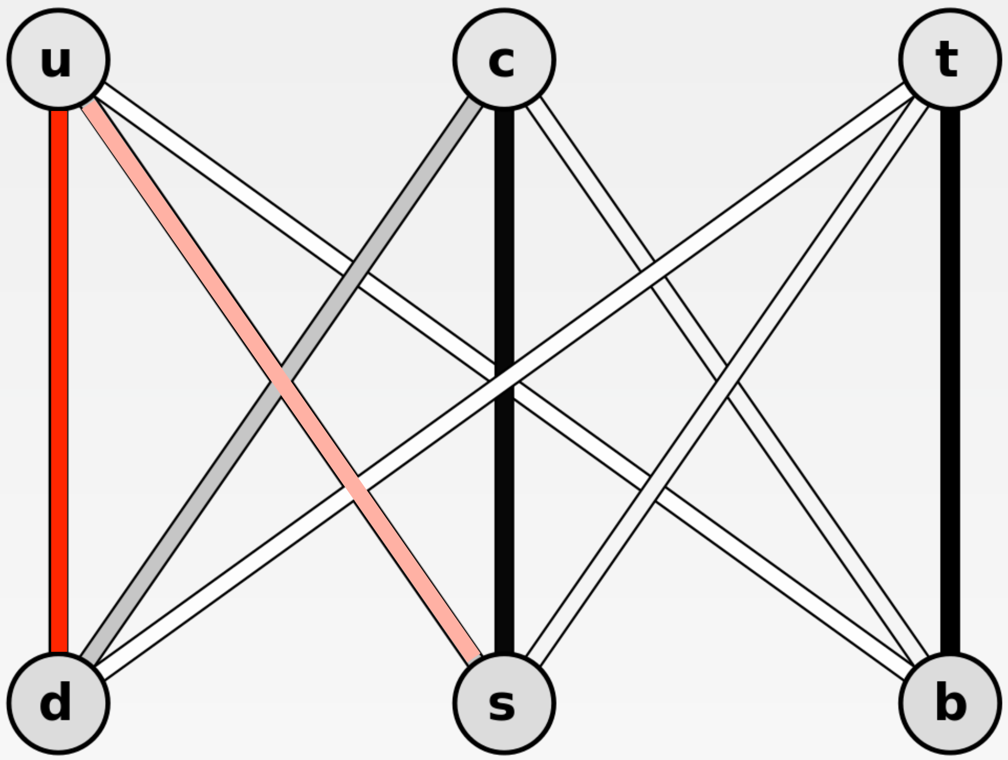


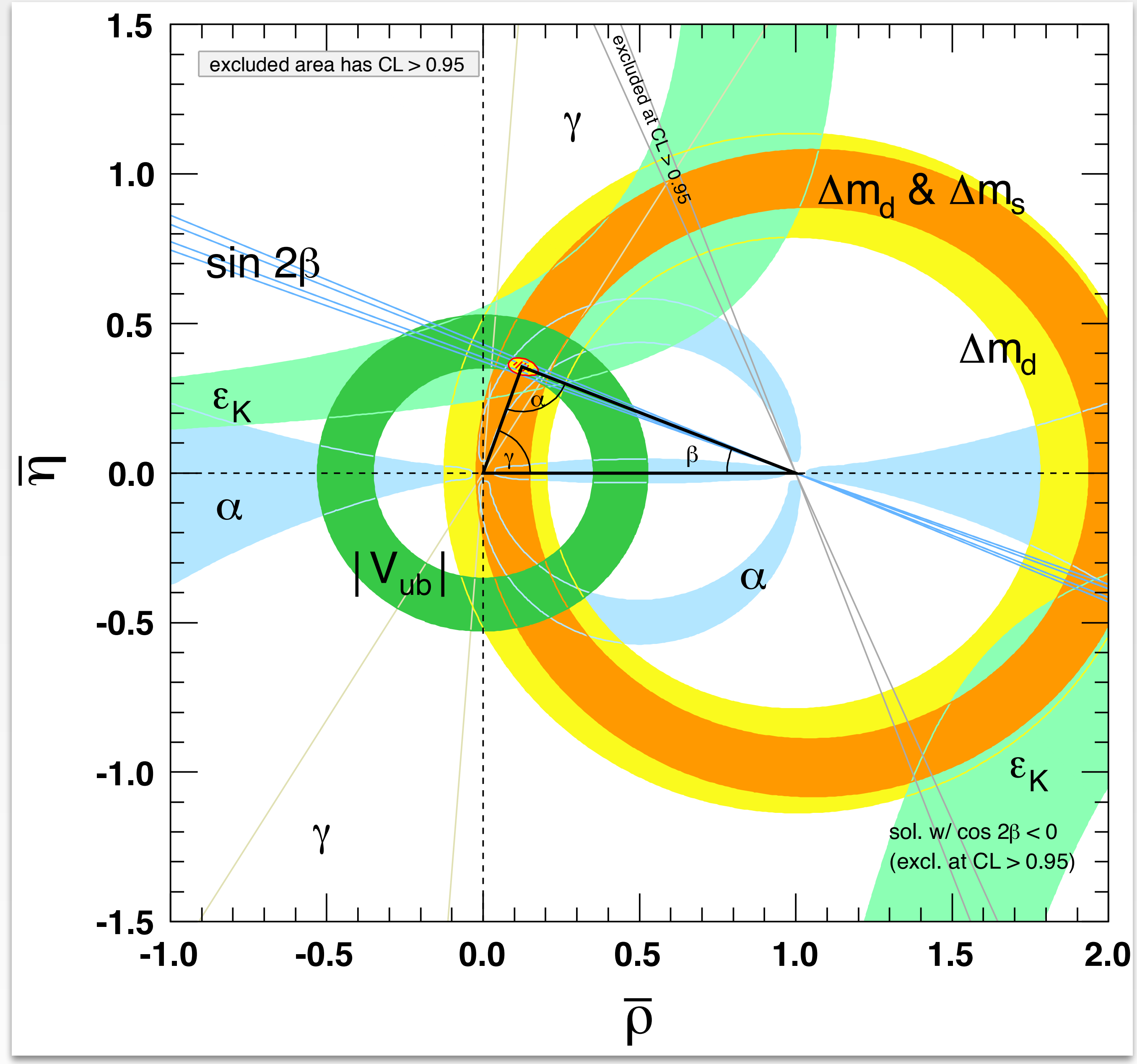
[CERN ATL-PHYS-PUB-2019-024]

Search for new physics

- No "spectacular" new physics in experiments
- Precision physics era:
  it's all about **reliable** and **small** uncertainties
- Looking for anomalies: **indirect** search for new physics
- Flavour structure of the SM is likely dynamically generated by unknown laws of physics.

CKM matrix elements determination





$|V_{ud}| = 0.97370 \pm 0.00014$

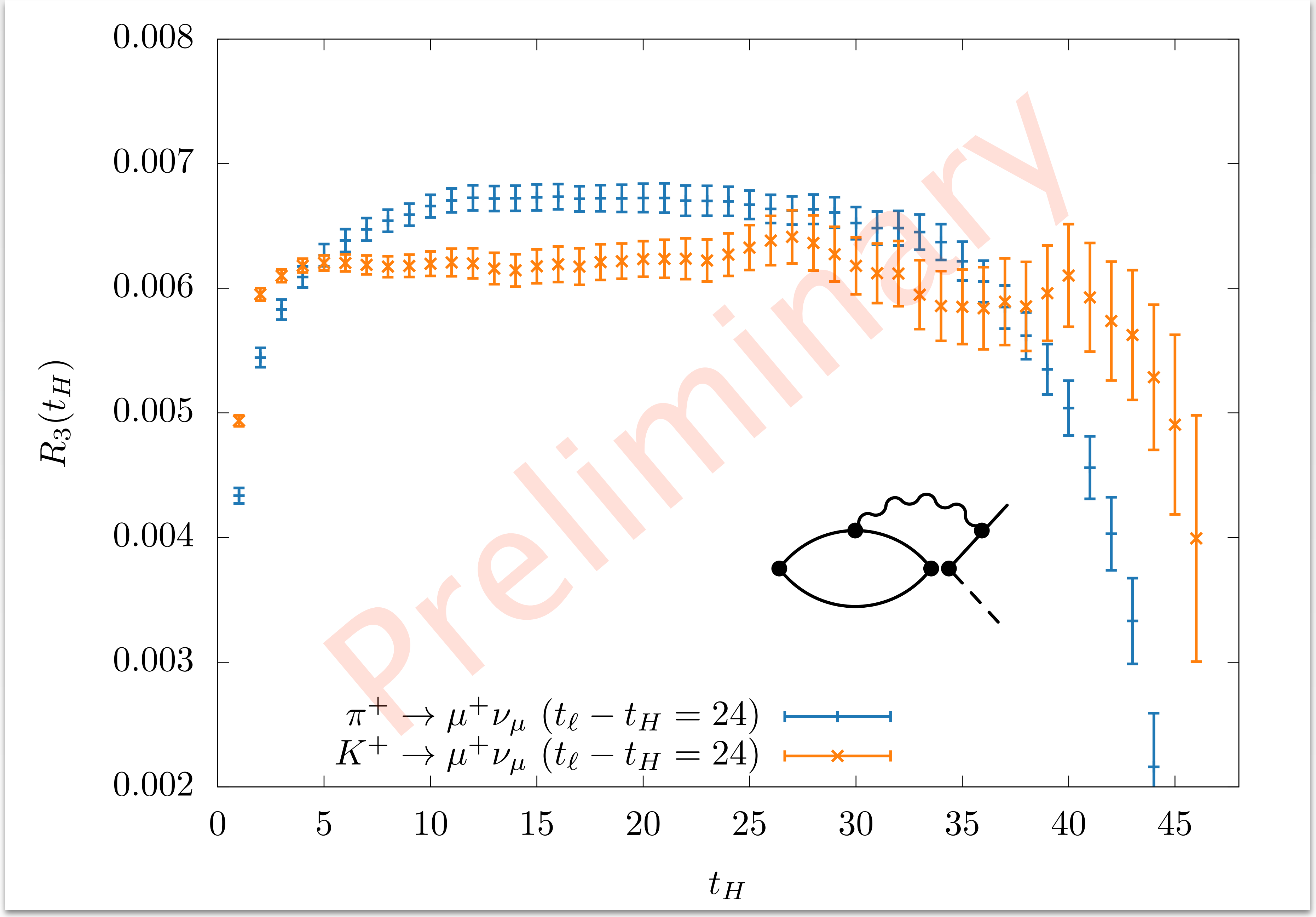
$|V_{us}| = 0.2245 \pm 0.0008$

[PDG 2020]

Light CKM matrix elements

- V_{us} and V_{ud} can be obtained through $K/\pi \to \nu\ell$ $(K_{\ell 2})$ and $K \to \pi\nu\ell$ $(K_{\ell 3})$ decays.
- Uncertainties dominated by hadronic effects.
- Lattice determination beyond 1% precision. **Radiative corrections dominate uncertainty.**

Radiative corrections at the physical point



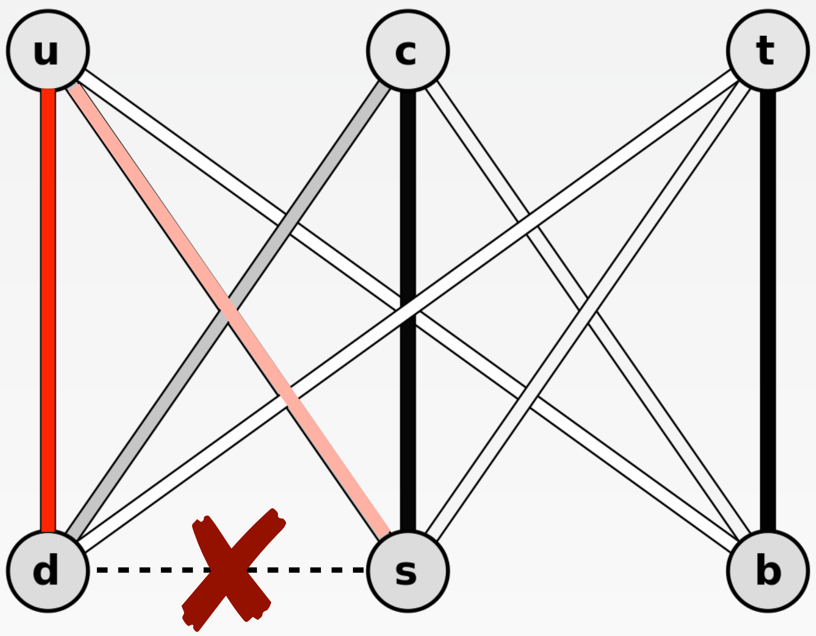
RBC-UKQCD physical point Domain-Wall fermions

$a \simeq 0.12$ fm $\quad N_f = 2+1 \quad 96 \times 48^3$

Light CKM determination roadmap

- Theoretical framework needed for radiative corrections to semi-leptonic decays.
- Semi-leptonic hyperon decays.
(LHCb interest @KAON2019)
- Application of radiative corrections to heavy quark decays.

Rare strange-to-down decays



- Flavour-Changing Neutral Current
- Very suppressed in the SM.
- Experiments:

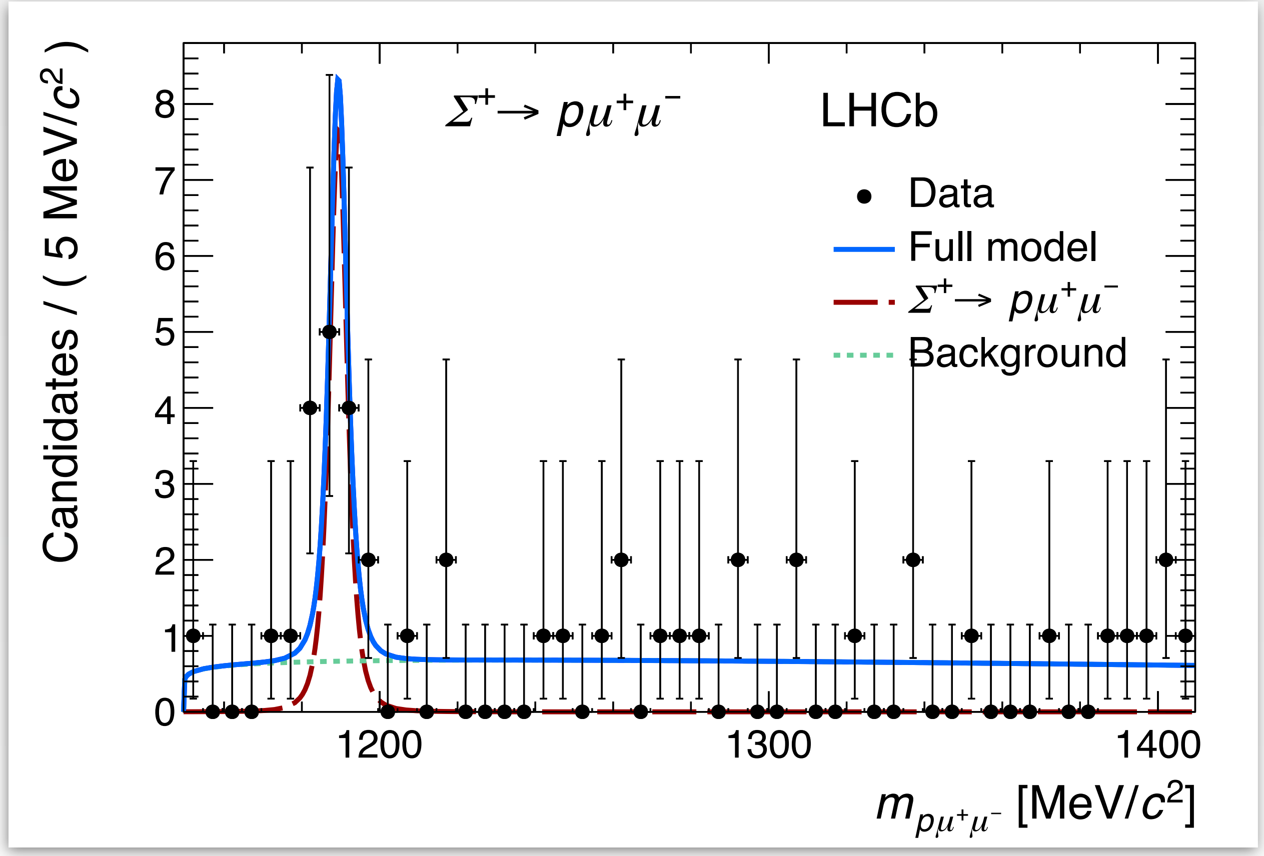
  Rare kaon decays
  NA62, KOTO, LHCb, KLEVER (future)

  Rare hyperon decays
  LHCb
- Important hadronic SM uncertainties

Rare kaon decays

- $K \to \pi\bar{\nu}\nu$ decays: mainly short-distance dominated.
- Main experimental focus.
  Lattice important for precision.
- $K \to \pi\ell^+\ell^-$ decays: long-distance dominated.
- Measurements in progress at NA62 and LHCb.
- **Lattice needed for SM prediction.**
  Important motivation for experiment.

Rare hyperon decays



[LHCb, PRL 120(22), 221803, 2018]

- First LHCb measurement in 2018, more to come.
- SM value poorly know. [He *et al.*, PRD 72(7), 074003, 2005]

Hadronic scattering

- Is that flavour physics? Not directly but highly relevant.
- $\pi\pi$, $K\pi$ scattering to **understand decay products** $K \to \pi\pi,\ D \to \pi\pi,\ B \to K^*\ell^+\ell^-, \ldots$
- $\pi\pi$, $N\pi$ for **intermediate states** in rare decays.
- A lot of development for physical point calculations using distillation. [Peardon *et al.*, PRD 80(5), 054506, 2009]

Computational challenges

Numerical complexity

- Quark propagator $S = D^{-1}\eta$ computed using iterative algorithms.
- Number of iterations grows like condition number

$$\kappa(D) = \left|\frac{\lambda_{\max}}{\lambda_{\min}}\right| = \mathcal{O}\left(\frac{1}{am_u}\right)$$

- Up quark very light: $\kappa(D)$ very large.
- Lattice QCD is one of the worst numerical problem.
- Realistic calculations only possible on large scale supercomputers.

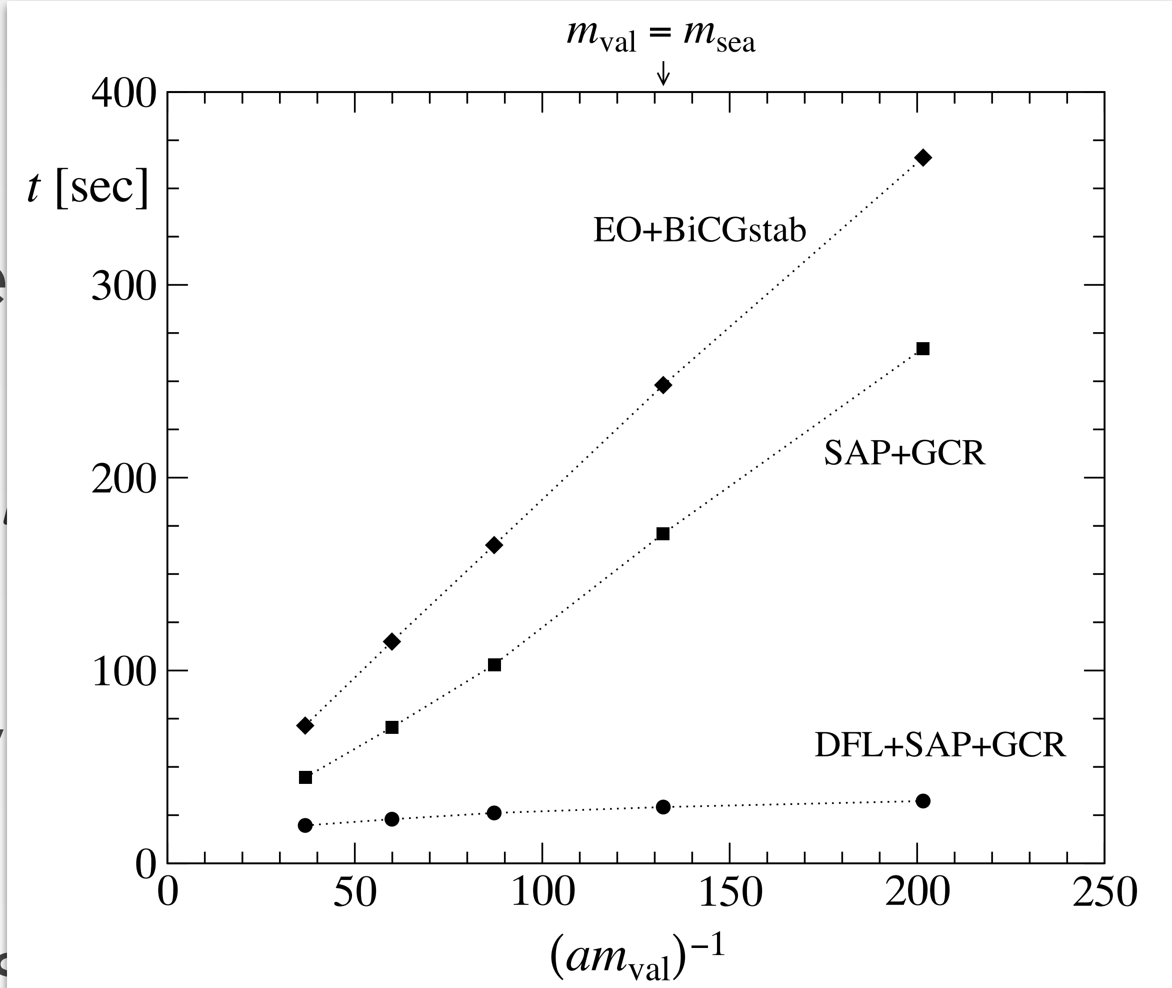
Numerical complexity

- Quark propagator $S = D^{-1}\eta$ computed using iterative algorithms.

- Number of ite umber

- Up quark very

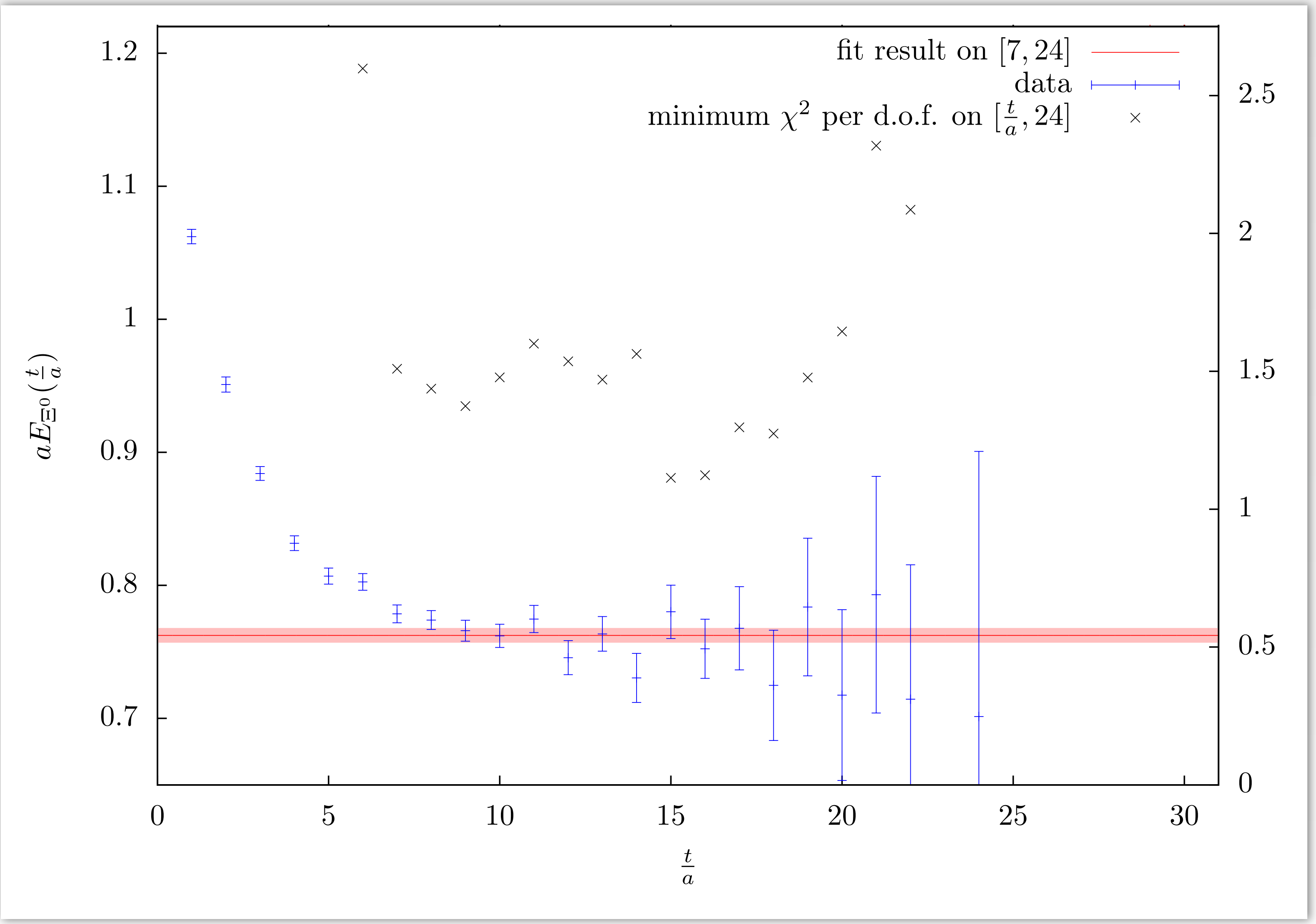
- Lattice QCD is roblem.



[M. Lüscher, arXiv:1002.4232]

- Realistic calculations only possible on large scale supercomputers.

Signal-to-noise ratio



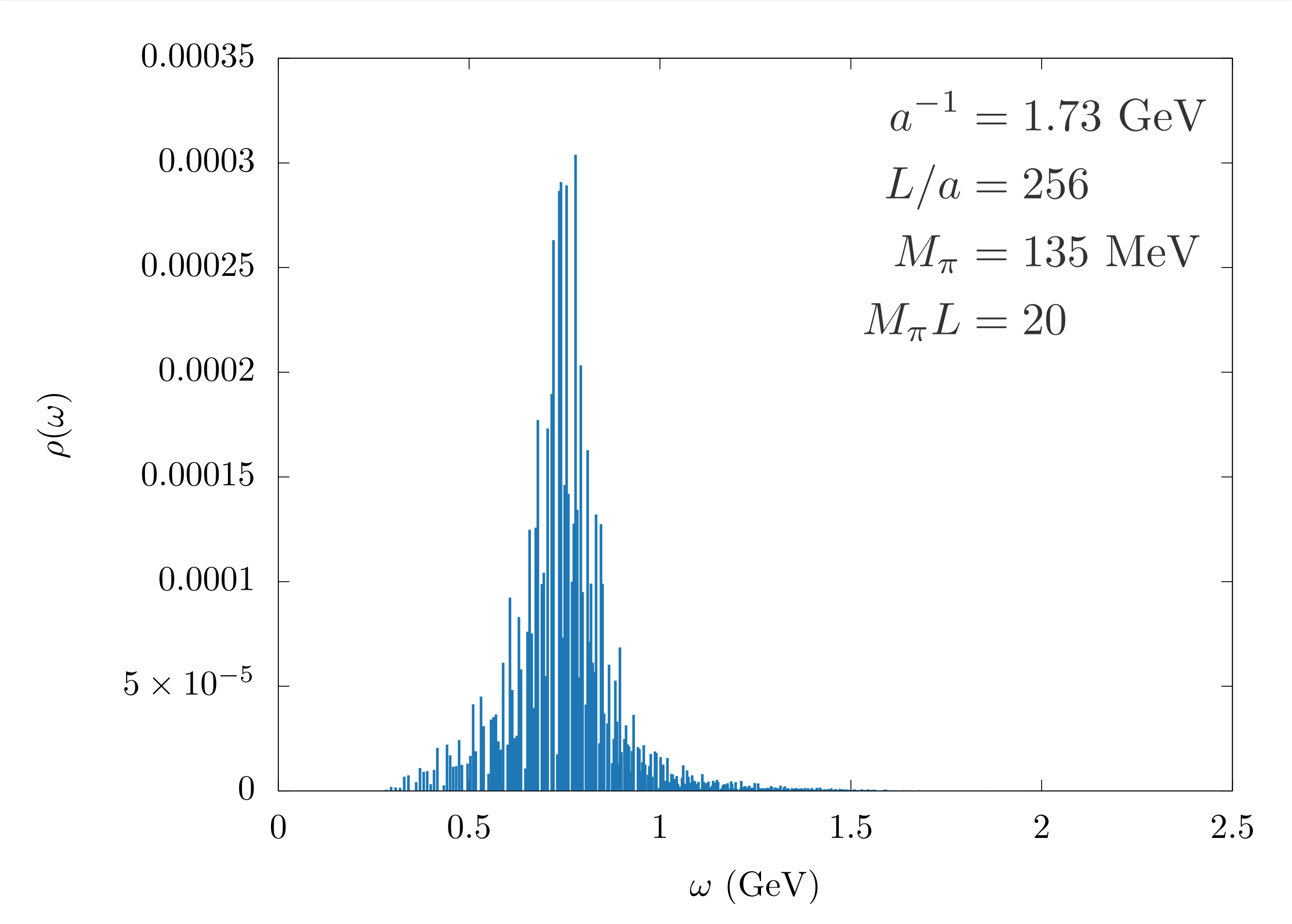
[A.P., PhD thesis]

- Baryons: exponential signal degradation…
- Pushes for new algorithmic developments
(e.g. multi-level algorithms [Cé *et al.*, PRD 93(9), 094507, 2016])

Data footprint

- Increasingly frequent use of eigenvector-based methods.
- Exact deflation using Dirac operator EVs.
- Low-mode averaging using Dirac operator EVs.
- Distillation for scattering using 3D Laplacian EVs.
- Current UKQCD jobs need to load 10 TB of EVs during startup!

New very-large volume paradigms?

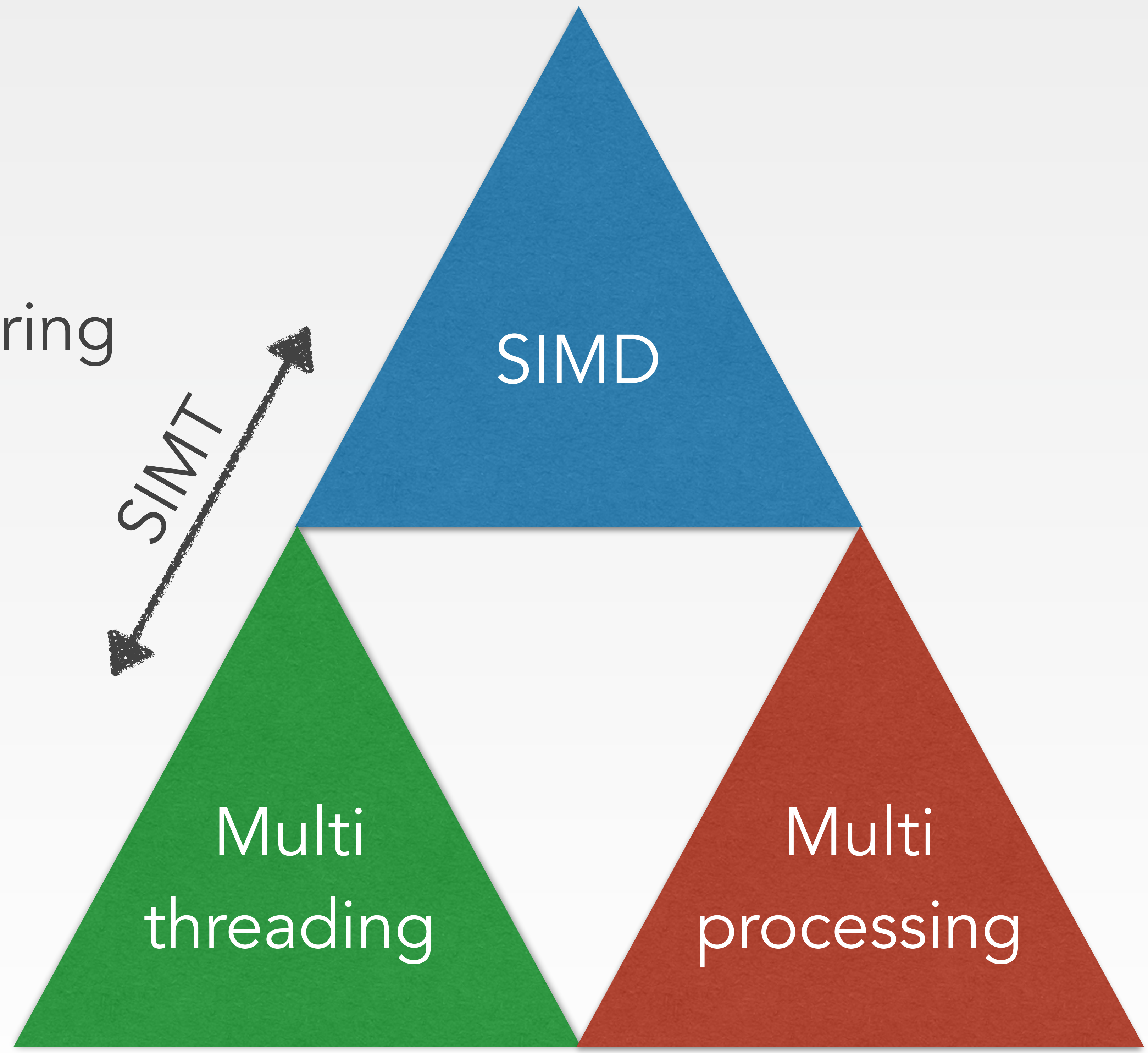


- "**Spectral reconstruction**": understand scattering through spectral densities rather than individual states
  [M.T. Hansen *et al.*, PRD 96(9), 094513, 2016] [M. Hansen *et al.*, PRD 99(9), 094508, 2019]
- Need simulations at **high density of states**.

Software design perspectives

The parallelisation trinity

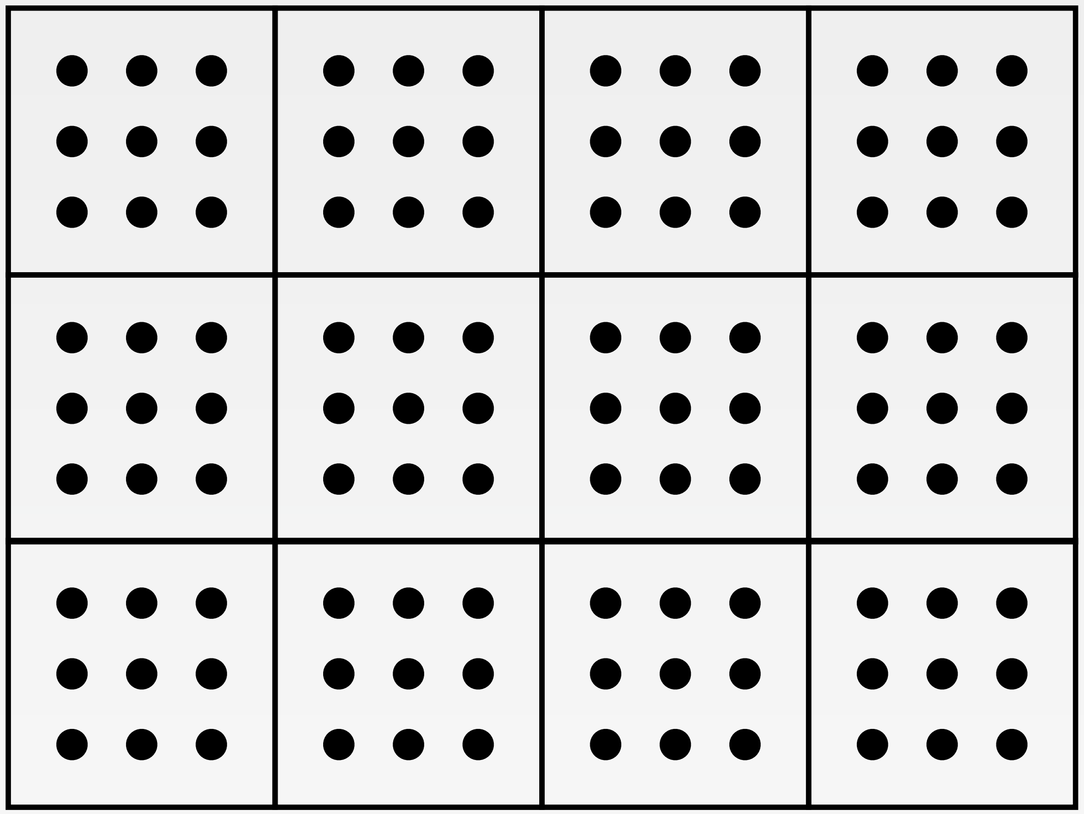
GPUs blurring the lines

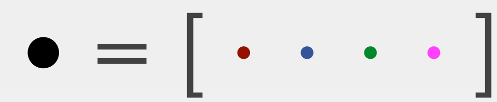


The Grid library

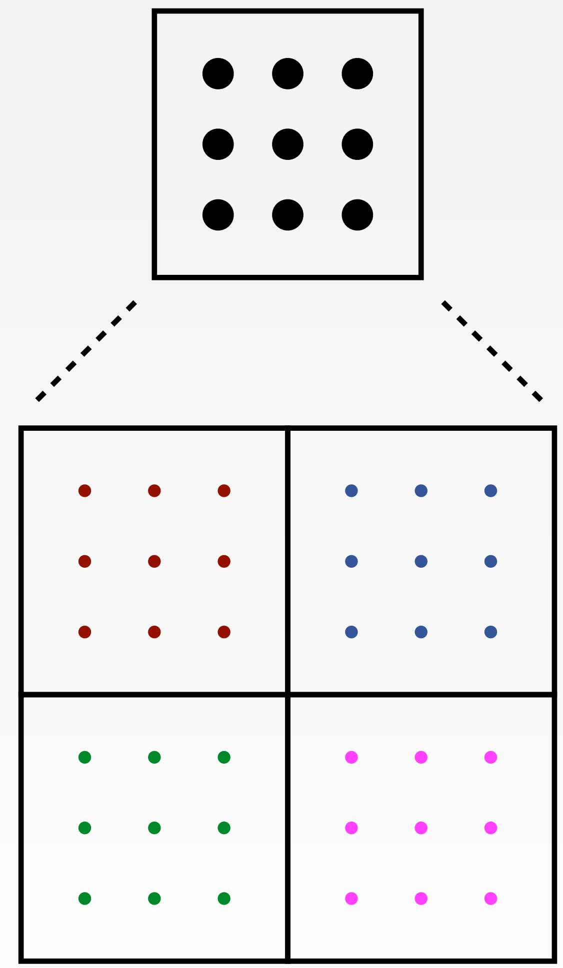
- Free (GPLv2) data parallel C++11 library.
  https://github.com/paboyle/Grid
- Multi-platform, high-level code mostly platform-agnostic.
  SSE, AVX, AVX2, AVX512, QPX, NEONv8, NVIDIA (post-Pascal)
- Implements popular lattice fermion actions
  (Wilson, DWF, Staggered, …)
- Implements many solvers
  (CG (many flavours), multi-grid CG, Lanczos, …)
- Implements full HMC/RHMC interface

Grid lattice layout





SIMD/SIMT vector



Vectorised layout

MPI Cartesian layout

High-efficiency halo exchange

Shared buffer and multi-endpoint comms

More details in

Peter Boyle's talk right after that!

Big data challenges

- Large amounts of **heterogeneous data**.
- Complex & heterogeneous computational workflows.
- **Multi-level workflows**
  (computation, post-processing, data analysis, …)
- Software challenges:
  modular automation, cataloging, fast data access, …

Hadrons workflow management system

- **Dataflow framework** for lattice calculations.
  Entirely built around the **Grid library**.
  https://github.com/aportelli/Hadrons (GPL v2)

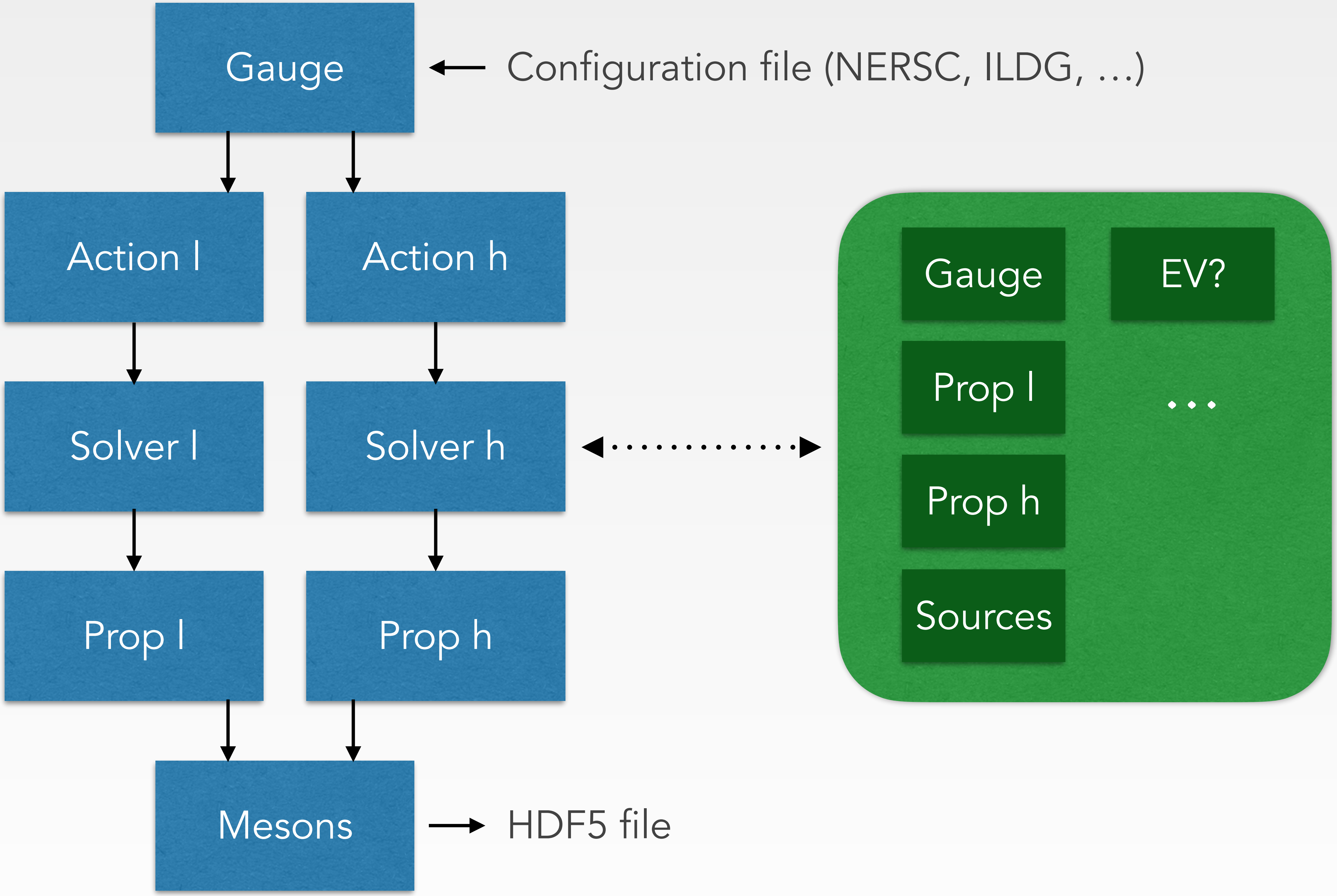
- A lattice computation is represented as a **DAG of elementary steps**, "modules".

- Automatise scheduling the computation with **optimal memory footprint**.

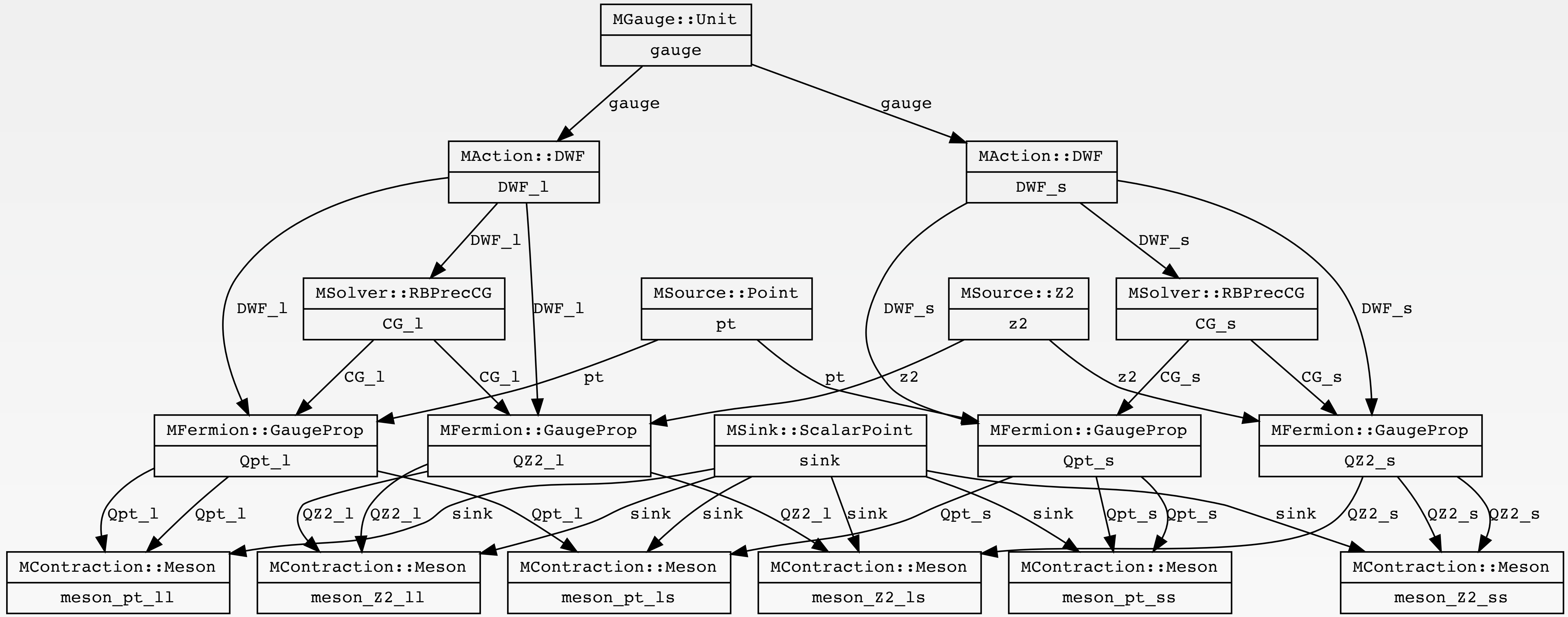
- **Fast I/O** from Grid & HDF5, with checksums and metadata.

- Cataloging of results in **SQLite databases**.

Measurement data flow



Workflow example



Strange & light meson spectrum

(trimmed down version of `Test_hadrons_spectrum`)

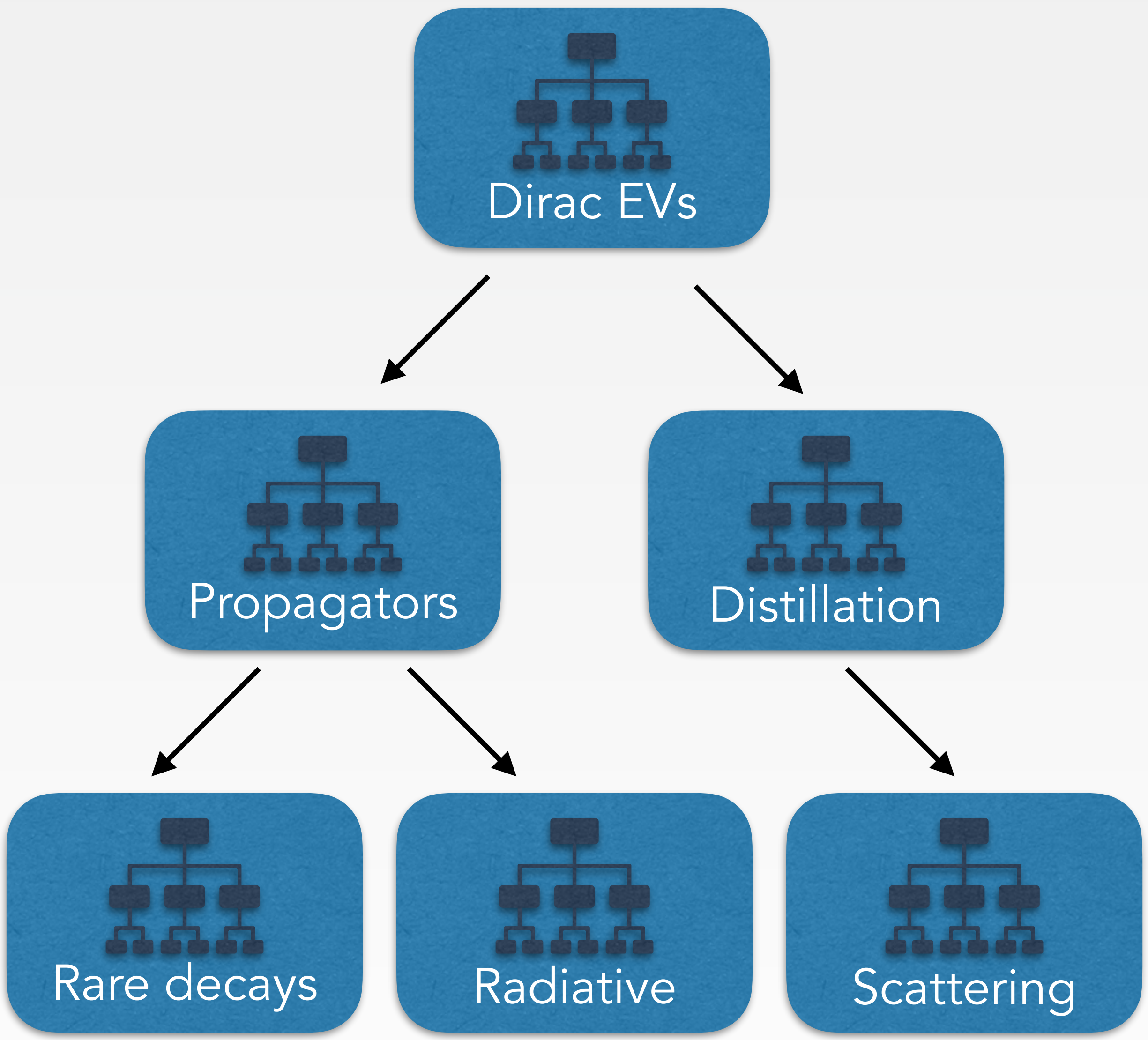
UKQCD production workflow examples

- Rare kaon & hyperon decays.
- Isospin breaking corrections to light leptonic decays.
- Isospin breaking corrections to the hadron spectrum.
- Scattering using distillation.
- Heavy flavour leptonic and semi-leptonic decays.
- Holographic cosmology.

~70% of Tesseract (Edinburgh) ~6% of Cumulus SKL (Cambridge)

Heterogeneous workflows ✓

Future: multi-level workflows



- Higher-level workflow between lattice jobs.
- Currently handled manually.
- More automation needed for future large-scale projects?
- e.g. Pegasus & LIGO https://pegasus.isi.edu

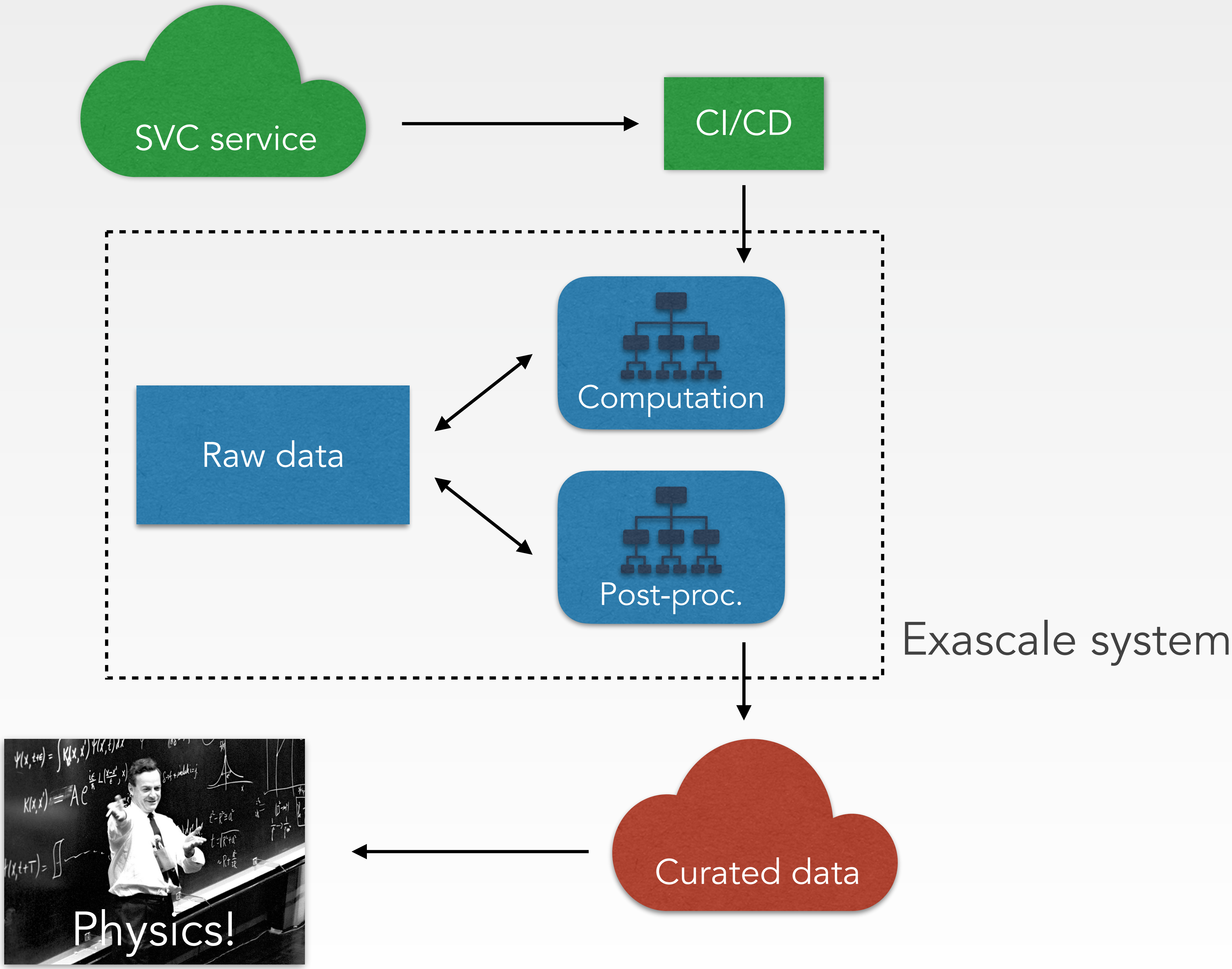
Future: more hierarchical storage

- EV-based methods: frequently need to load large volume of data.
- I/O expensive, needs to be amortised within a job.
- **Even more modularity with faster I/O?**
  NVME technology might be important for lattice?
- Hierarchical storage important to deal with PB of data (e.g. NVME / parallel FS / tape archive)

Future: data curation

- How to share scientific data publicly across an HPC infrastructure?
- How to present large, complex amount of data in an efficiently queryable form?
(*cf.* Hadrons' SQLite support)
- Can we take advantage of decentralised data solutions?
(cloud storage, distributed ledgers, …)

Future: automated workflows

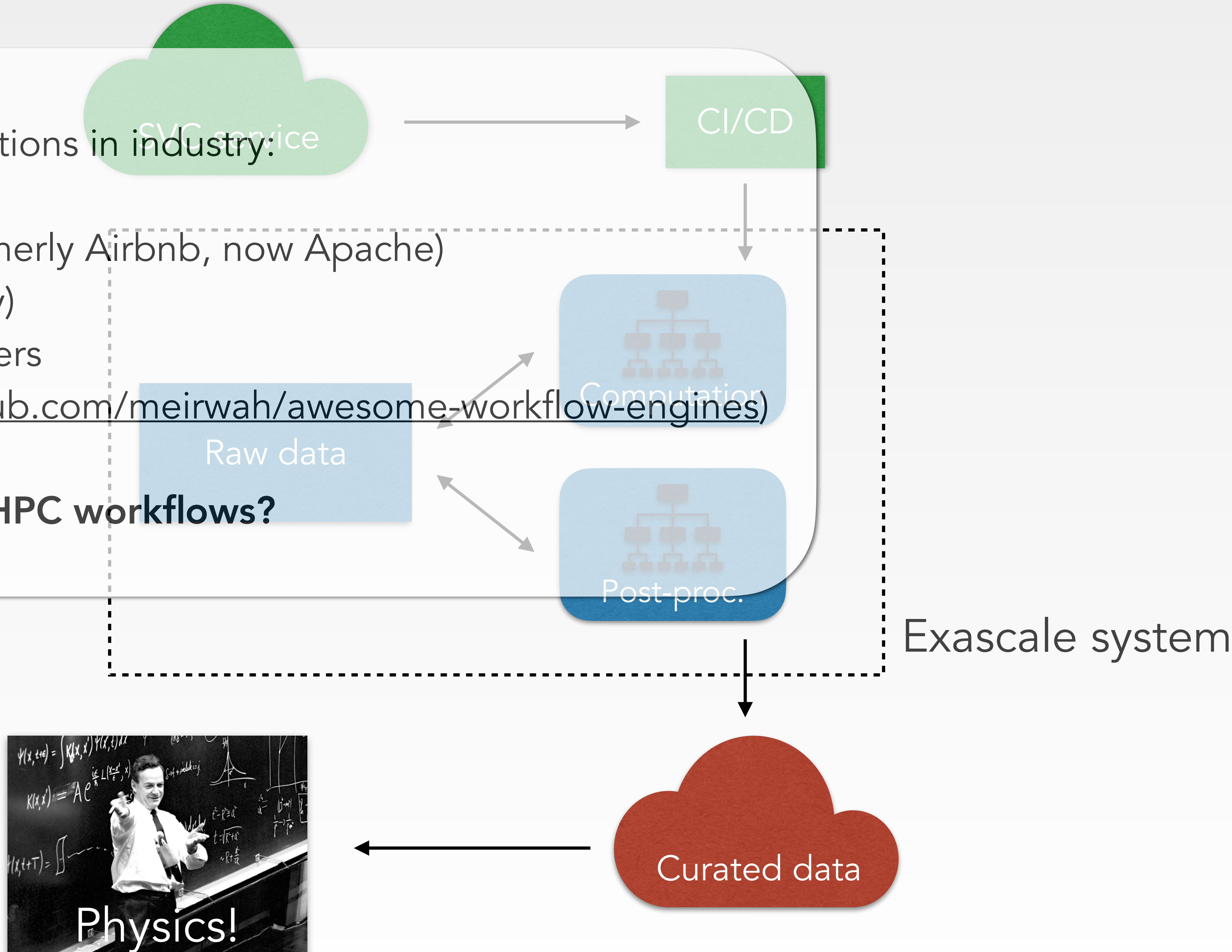


Future: automated workflows

Popular solutions in industry:

AirFlow (formerly Airbnb, now Apache)
Luigi (Spotify)
… many others
(https://github.com/meirwah/awesome-workflow-engines)

Usable for HPC workflows?



Outlook

- Light flavour physics at the core of **current and future international particle physics experiments**.
- The high computational cost of lattice QCD leads to **complex computation methods**.
- These calculations keep **pushing the boundaries** of HPC systems, both for **computational power** and **data storage**.
- Increasingly complex methodologies and large amount of data are a **challenge for automating projects**.

Thank you!

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