FERMILAB-SLIDES-24-0173-T

# Connecting Theory and Experiment through Event Simulation

John Campbell, Walter Giele, Stefan Höche

Fermilab User's Meeting

July 12, 2024

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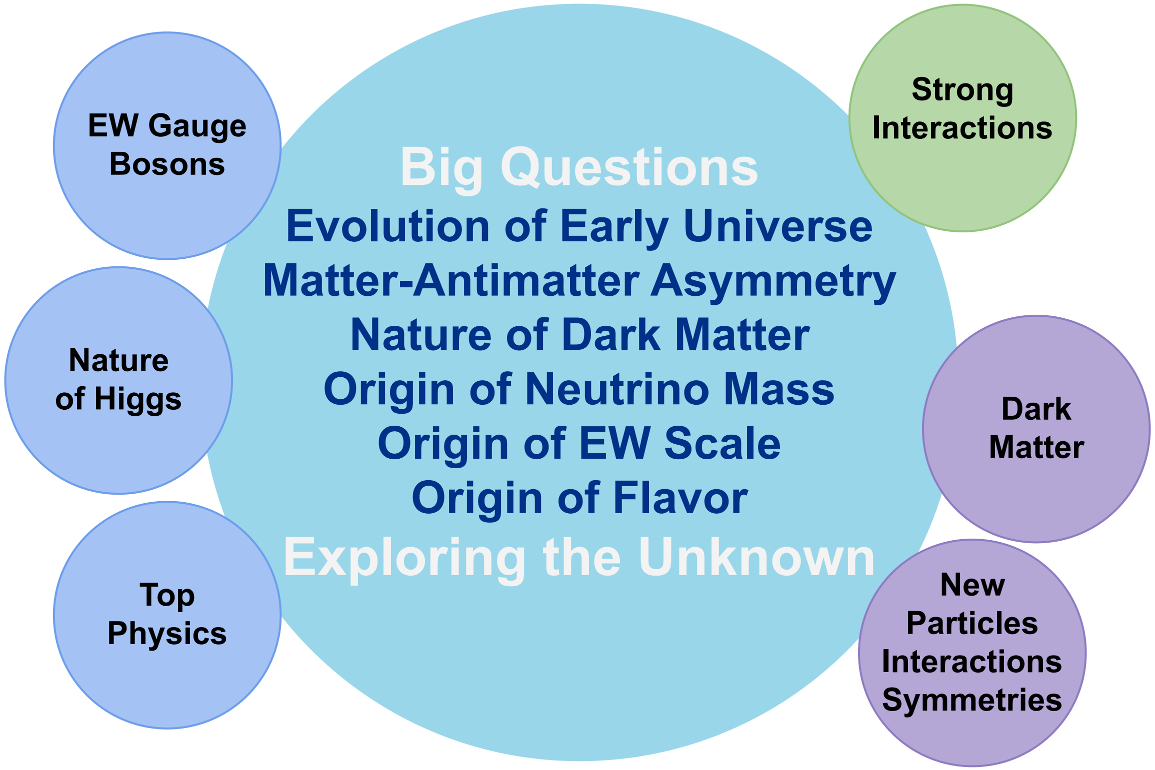
# Physics at the Energy Frontier – Snowmass 2021




- What can we learn about the origin of the EW scale and the EW phase transition from an in-depth study of SM particles at colliders (HL-LHC)?
- What can we learn about the dynamics of strong interactions in different regimes?
- How can we build a complete program of BSM searches which includes both model-specific and model-independent explorations at high scales?

[Narain et al.] arXiv:2211.11084

# Messages from the P5 report

Decipher the Quantum Realm

Elucidate the Mysteries of Neutrinos

Reveal the Secrets of the Higgs Boson

Explore New Paradigms in Physics

Search for Direct Evidence of New Particles

Pursue Quantum Imprints of New Phenomena

Illuminate the Hidden Universe

Determine the Nature of Dark Matter

Understand What Drives Cosmic Evolution

**1. As the highest priority independent of the budget scenarios, complete construction projects and support operations of ongoing experiments and research to enable maximum science.** This includes High-Luminosity LHC, the first phase of Deep Underground Neutrino Experiment (DUNE) and Proton Improvement Plan II, the Rubin Observatory to carry out the Legacy Survey of Space and Time (LSST).

**2. Construct a portfolio of major projects that collectively study nearly all fundamental constituents of our universe and their interactions**, [...]

c. **Offshore Higgs factory, realized in collaboration with international partners**, [...]

[...]

**4. Support a comprehensive effort to develop the resources — theoretical, computational and technological — essential to our 20-year vision for the field**. [...]

[...]

https://www.usparticlephysics.org/

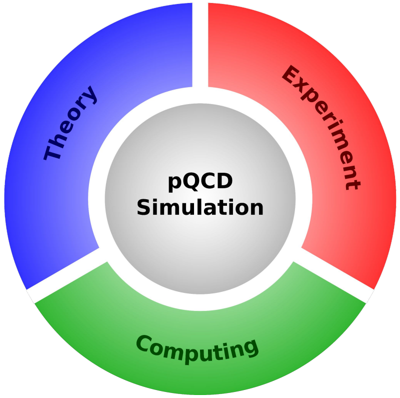
# Perturbative QCD - Connecting Theory & Experiment

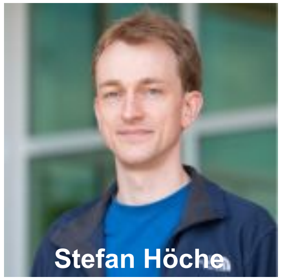
- QCD is a rich theory with different phenomena at different scales
- Experimental precision at LHC unprecedented, theoretical precision must keep up

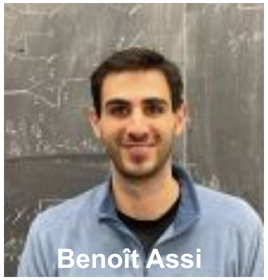
  Any future collider will require even higher precision

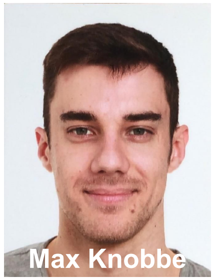
**Fermilab Theory Division provides**

- New techniques for performing state of the art calculations
- Software that is used directly by collider experiments
- Continuous support of these activities & associated codes
- Activities that engage with the experimental community:
  - LHC Higgs Cross Section WG, ATLAS / CMS consulting, …
  - Joint workshops & schools (CTEQ/MCnet, HCPSS, …)
  - Community workshops & reports, e.g. [Campbell et al.] arXiv:2203.11110







# Activities

**Fixed-order perturbative QCD**
MCFM, Pepper

- John Campbell
- Walter Giele
- Stefan Höche
- Joshua Isaacson
- *Benôit Assi*
- *Max Knobbe (starting '24)*

**Semi-analytical Resummation**
MCFM, ResBos

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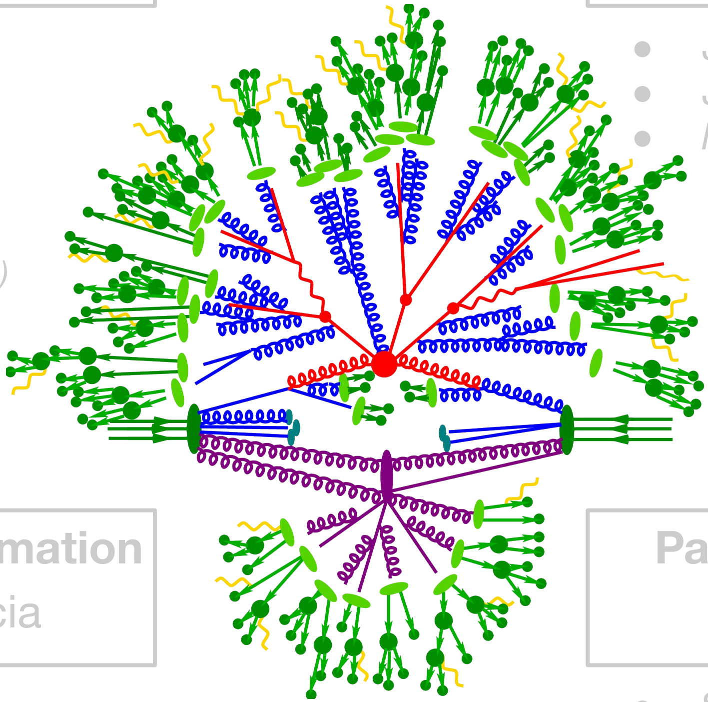

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Sherpa, Alaric, Vincia

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**Particle-level Simulation**
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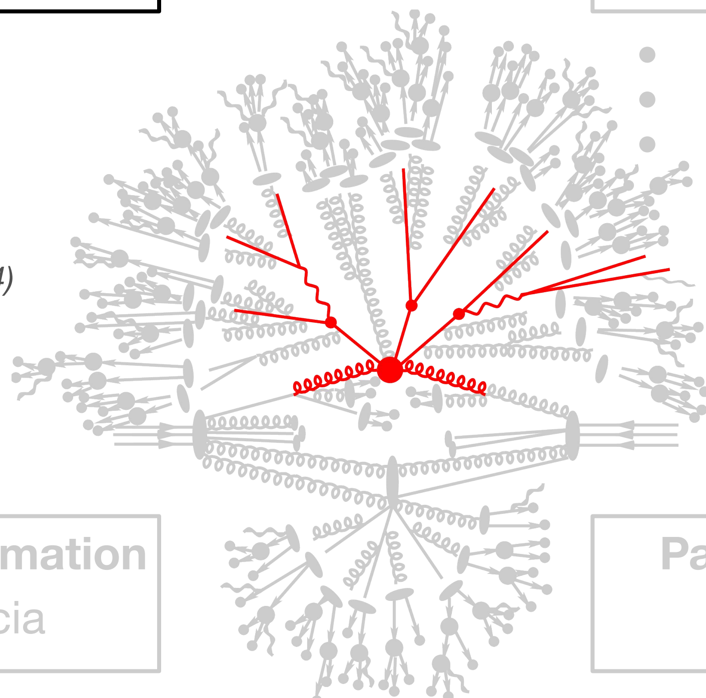

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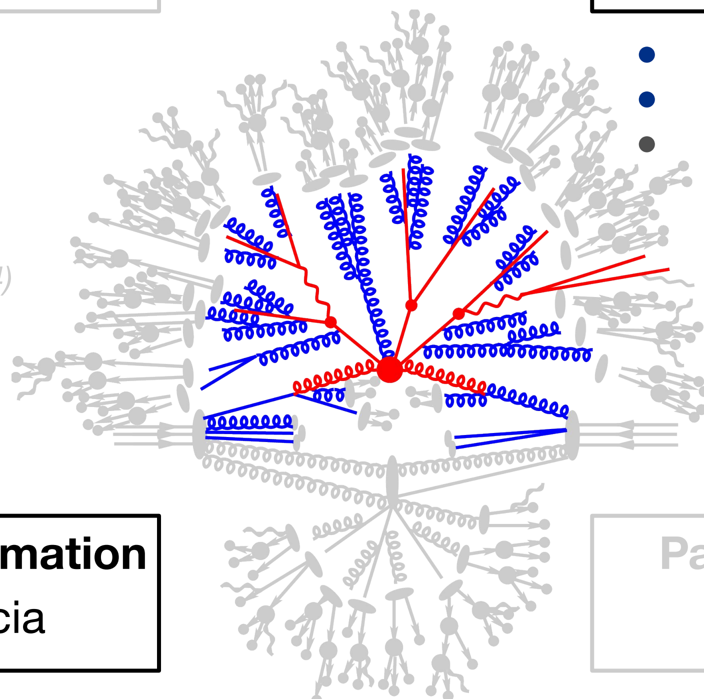

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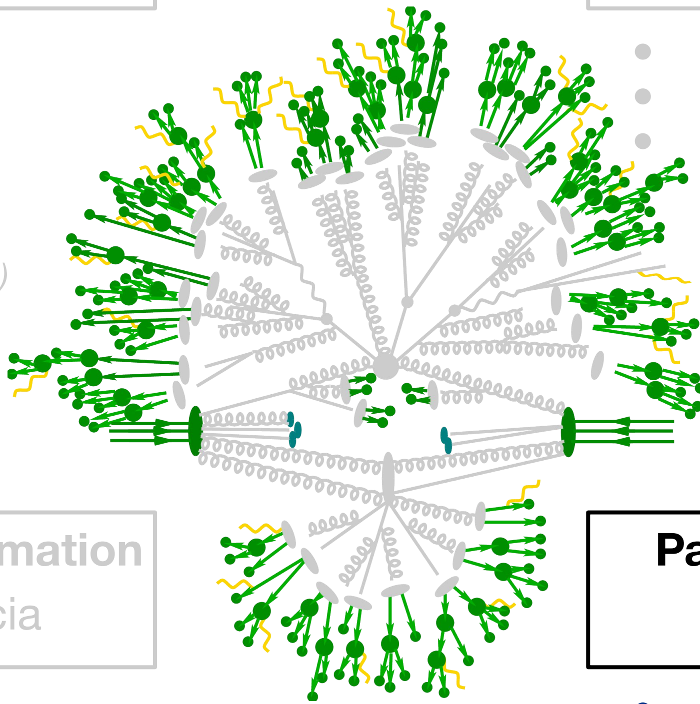

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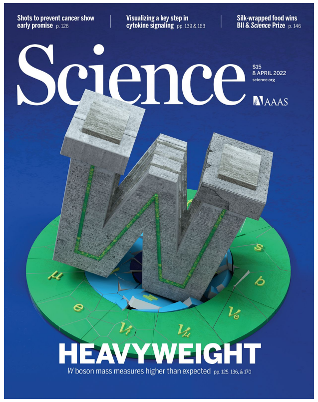
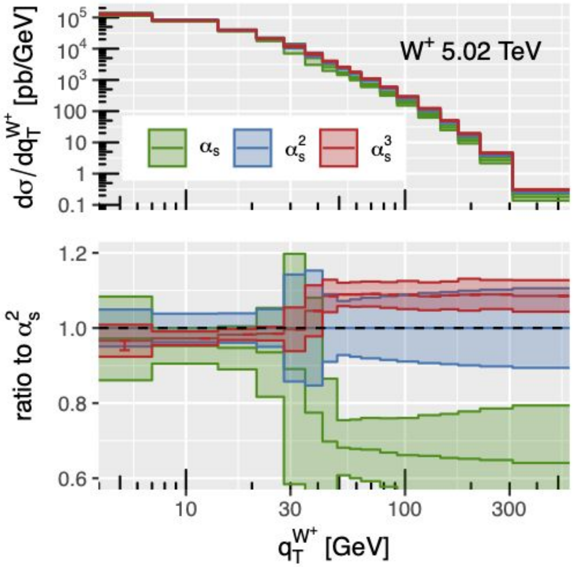
# Precision measurements at colliders

- CDF's measurement of the W-boson mass emphasizes importance of highest precision calculations for extraction of SM parameters at colliders
- Fermilab theory provides two of the most important tools for predictions of the W and Z $p_T$ spectrum:

- ResBos2 – $N^2LO$ fixed order, $N^3LL$ resummed [Isaacson et al.]
- MCFM – $N^3LO$ fixed order, $N^4LL$ resummed [Campbell et al.]

[CDF Collaboration] Science, 376, 6589, 170-176



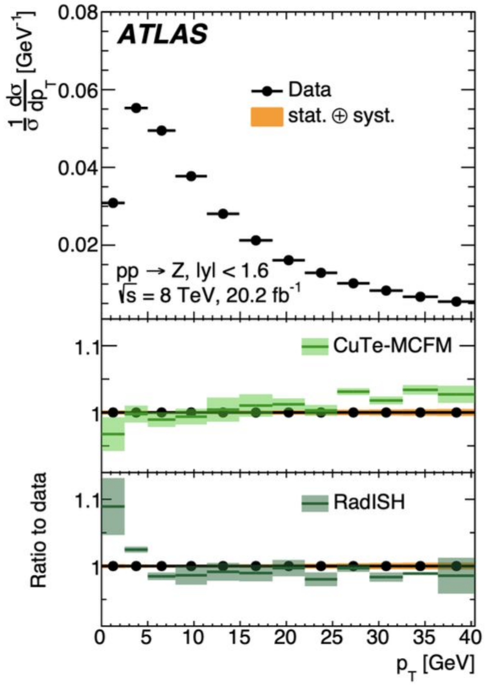

[Campbell, Neumann] arXiv:2308.15382

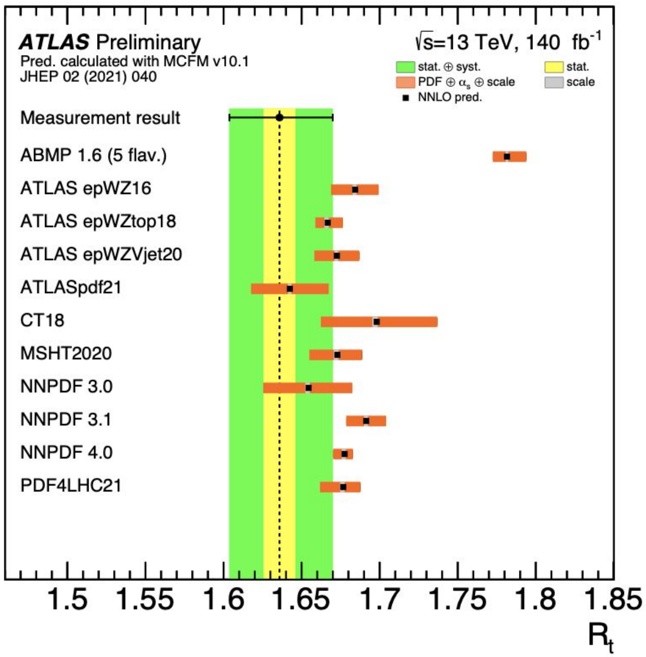
- Control of perturbative uncertainties at an unprecedented level
- Codes made available to ATLAS and CMS for use in ongoing measurements

- **Future $N^3LO+N^4LL$ analysis will examine angular coefficients, input for $m_W$ analysis**
- Also planning a comprehensive study of non-perturbative effects, including use of LQCD constraints in ResBos, MCFM and Sherpa

# State-of-the-art calculations for experiments

[ATLAS Collaboration]
September 2023




[ATLAS Collaboration]
March 2024

- Important to ensure state-of-the-art predictions are available to experiments and can be used by them to provide reliable predictions → public MCFM code
  - For instance, has resulted in input to most precise collider measurement of the strong coupling by ATLAS, reference single-top cross sections in LHC Top WG

- **Plan to extend to other high-interest calculations: gg → Higgs at $N^3LO+N^4LL$**
- Further extensions to NLO electroweak corrections and event shapes at FCC-ee

# Exploring the Unknown – The Higgs Potential

- Higgs self interaction is key to understanding of EW sector
- Measurement will require careful combination of many analyses with full HL-LHC data set
- Heavy flavor channels needed for high statistical significance e.g. via "ABCD" method

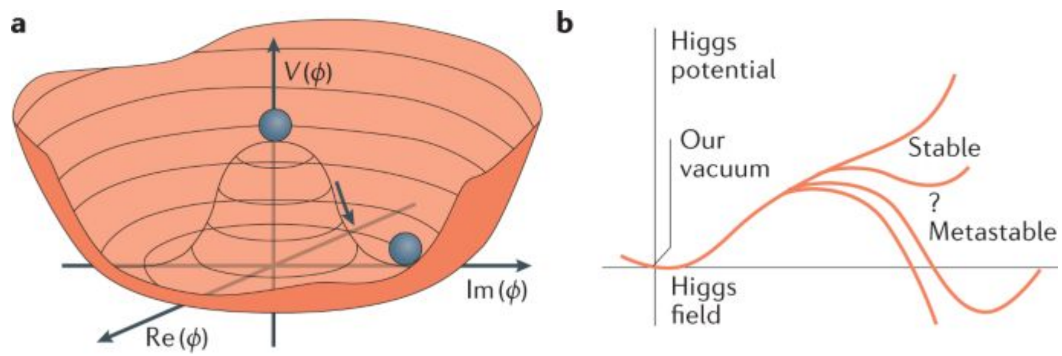
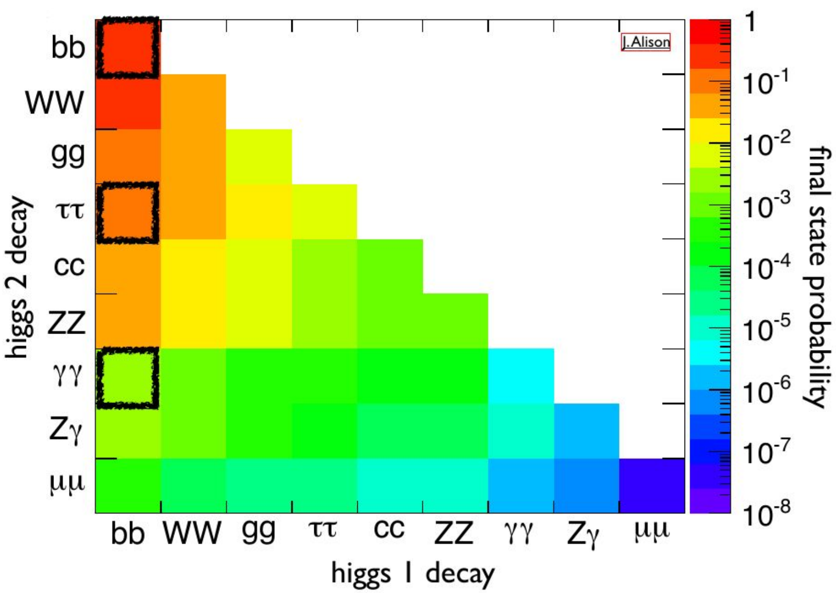



Image Credit: *Nat Rev Phys* **3**, 608–624 (2021)

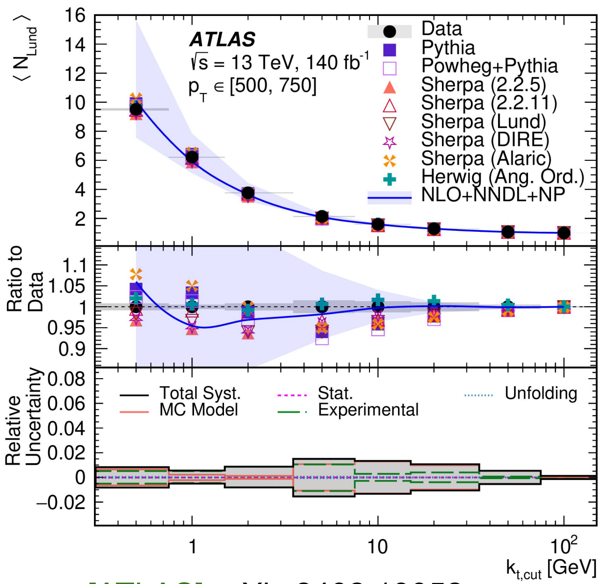



- Predictions for heavy quark production as part of inclusive heavy plus light flavor jets difficult to obtain at high precision
- **Precise extraction of / limit setting on triple Higgs coupling depends crucially on understanding of *all* final states**
- Multiple approaches co-developed at Fermilab & implemented in simulations
  - MCFM [Campbell et al.]
  - Sherpa [SH et al.]

# Parton showers at higher precision

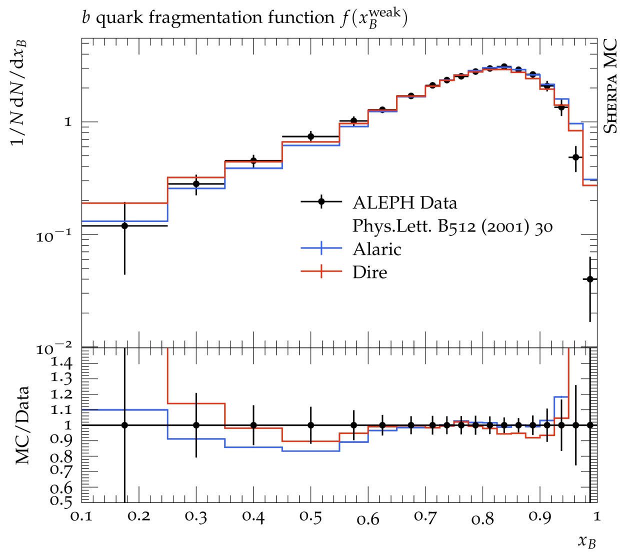
- Parton showers are the core component of collider event generators since PETRA
- Recent analyses revealed drawbacks of dipole-like algorithms as implemented in all major LHC event generators → provably not NLL precise, even in Drell-Yan events
- **Of utmost importance for a potential FCC-ee**

- Fermilab theory develops new algorithm for LHC event generator Sherpa → Alaric
  - Seamless integration with existing multi-jet merging framework
  - Currently working on generic NLO matching




[ATLAS] arXiv:2402.13052

- First ATLAS analysis using Alaric published (↗ also W&C, Aug 16)
- Good description of HQ evolution (relevant for Higgs measurements)
- Extension to NNLL being worked on ↔ NLO corrections to PS



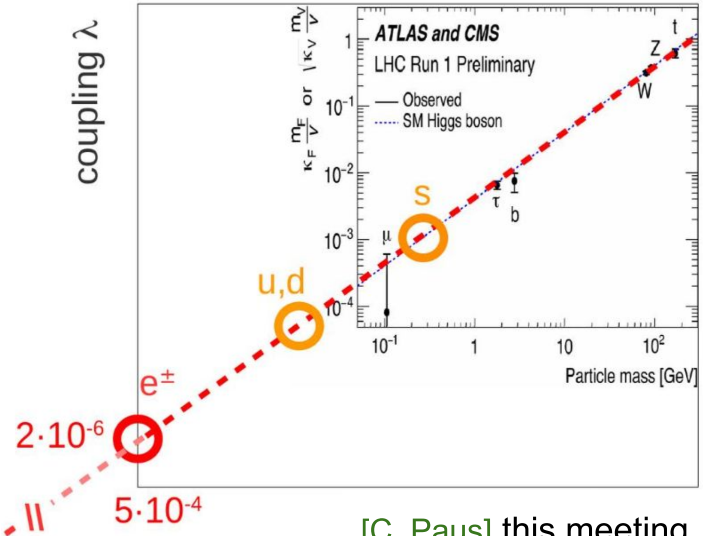

[Herren et al.] arXiv:2208.06057
[Assi, SH] arXiv:2307.00728

# Towards fully differential NNLO-PS matching

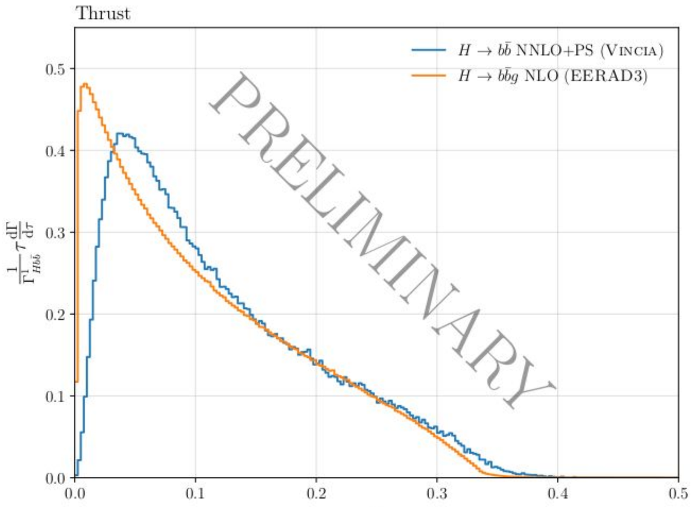
- **Extraction of Higgs Yukawa couplings at FCC-ee will depend on precise modeling of light / heavy flavor jets *at hadron level***
  *(see also Christoph's talk yesterday)*

- Various techniques currently available to match parton showers to NNLO
- Fermilab theory aims at generic, fully differential solution, based on a parton shower that uses the exact fixed-order counterterms (similar to MC@NLO)

- First steps towards solution
  [Campbell et al.] arXiv:2108.07133
  - Formulation of the method
  - Emission generation in Vincia (2→3, 2→4)
  - Test of double-soft / triple-collinear limits




[C. Paus] this meeting




[Preuss] HP2 2022

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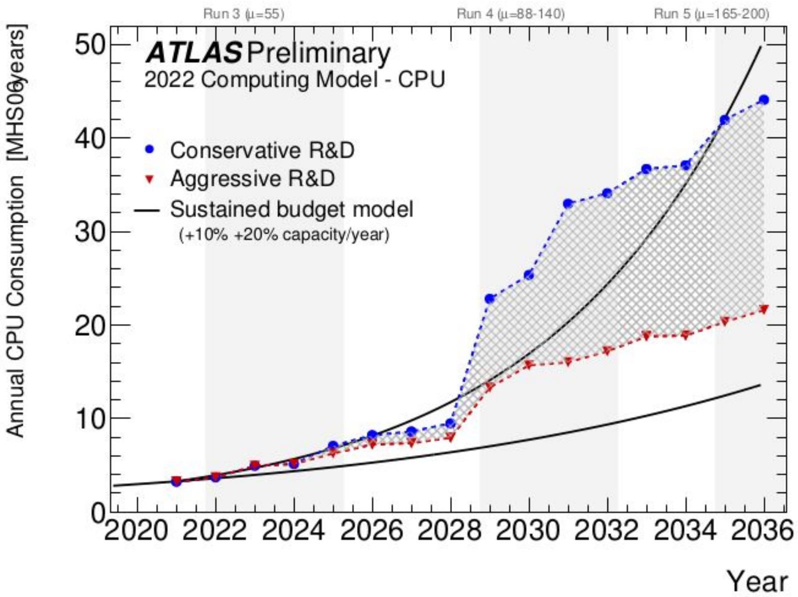
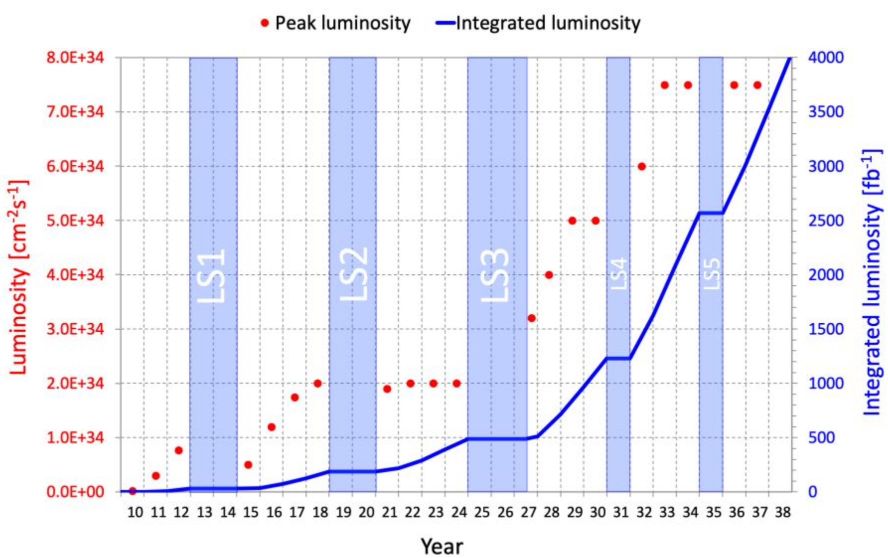
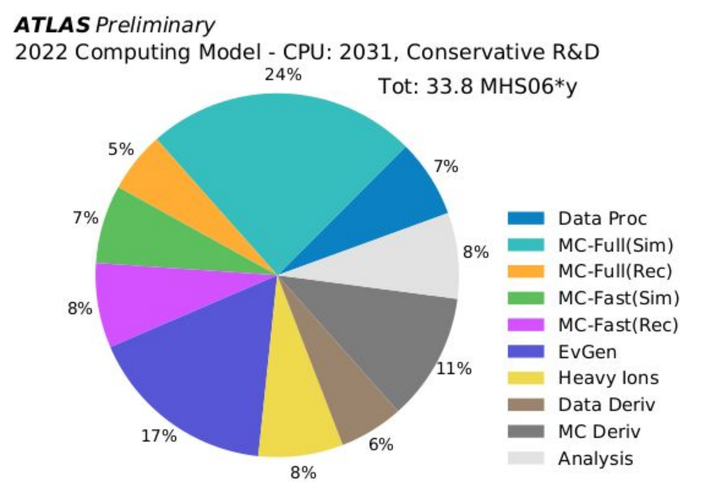
# The future of experimental simulation campaigns

- Projected evolution of LHC computing resources sees cost of event generation on par with detector simulation
- **LHC measurements in danger of being limited by Monte Carlo statistics**
- Even more severe at a potential FCC-ee

- FNAL theory collaborates with ANL MCS and SWIFT-HEP to solve these problems
  [Bothmann et al.] arXiv:2309.13154, arXiv:2209.00843
  https://indico.cern.ch/event/1312061




[ATLAS] CERN-LHCC-2022-005

# Portability of perturbative QCD calculations

- Efficient usage of HPC systems in U.S. and abroad can solve computing bottlenecks

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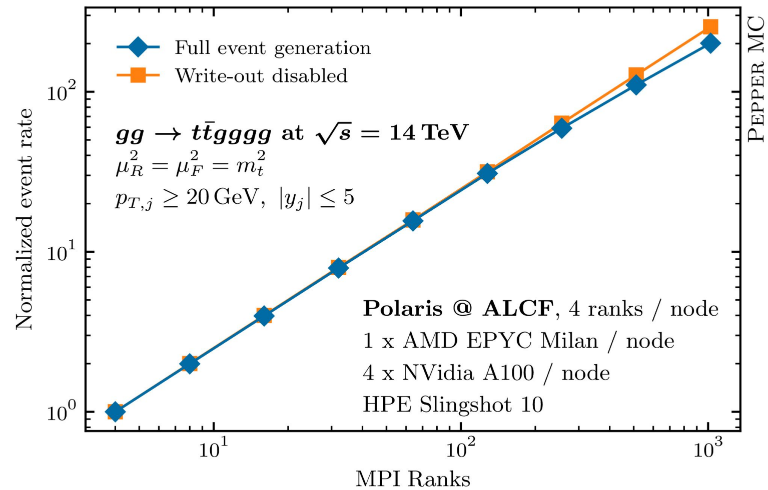
# Portability of perturbative QCD calculations

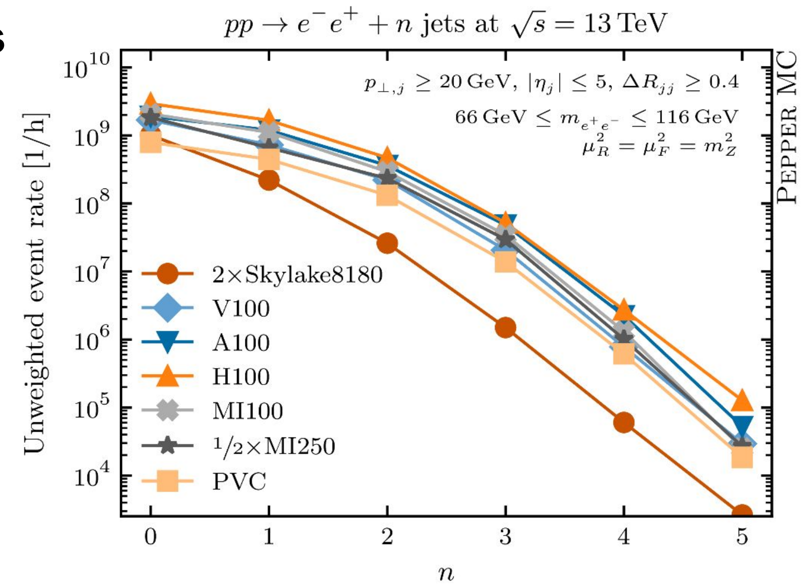
- LHC event simulations face significant challenges in modern computing landscape: many vendors & heterogeneous hardware
- Currently none of the major programs runs on any modern computing platform (at LHC-required production-level quality)

- **Fermilab co-developed first parton-level generator, capable of utilizing all modern hardware with help of DOE-funded Kokkos portability software → Pepper**
- Scalable solution for event production at leading order pQCD, developed in continuing collaboration with ANL MCS

- Pepper is now being extended to include tree-level like components at NLO QCD
- Will provide framework for implementation of next-generation MCFM, to be developed during the next few years

SciDAC Scientific Discovery through Advanced Computing




[Bothmann et al.] arXiv:2311.06198

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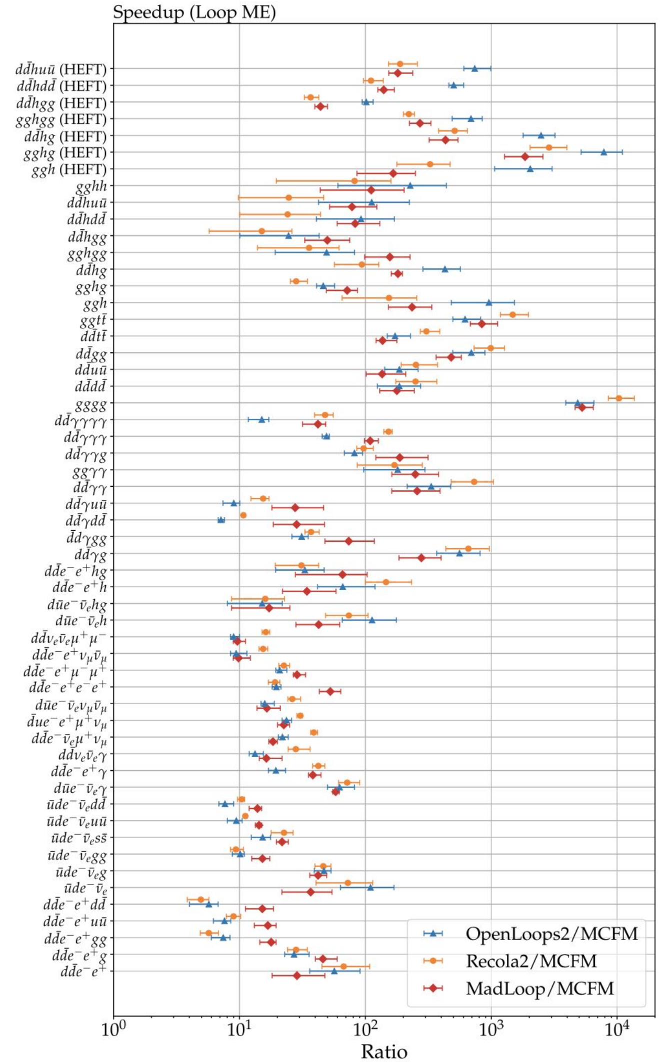
# Efficiency of 1-loop amplitude calculations

- Loop amplitudes must be evaluated in an efficient and stable manner to provide parametric precision
  - Needed for NLO merging & NNLO fixed order
  - Direct translation to research $ savings at the high-luminosity LHC
- Can be realized by using analytic matrix elements rather than off-the-shelf general-purpose tools
  - Cutting edge calculations use methods from algebraic geometry and number theory

- Fermilab theory works on two-pronged approach:
  - Direct analytic calculations for pressing LHC Higgs needs, e.g. Higgs pairs+jets
  - Dedicated implementation of unitarity method to reconstruct compact, one-loop amplitudes using finite-field techniques and twistors

SciDAC
Scientific Discovery through Advanced Computing



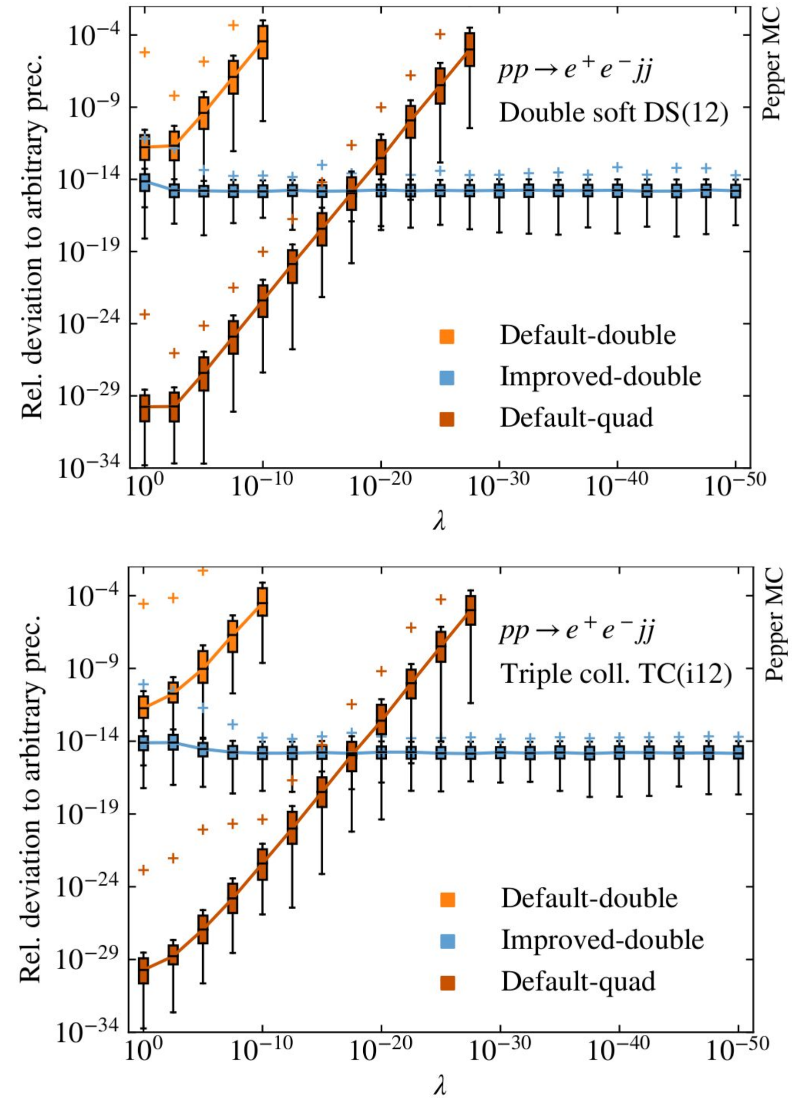

[Campbell et al.] arXiv:2107.04472

# Numerical stability of perturbative calculations

- Perturbative calculations in massless gauge theories develop infrared singularities, due to degenerate asymptotic states (KLN theorem)
- Most numerical calculations depend on phase-space slicing / subtraction methods which evaluate matrix elements in / near critical regions of phase space

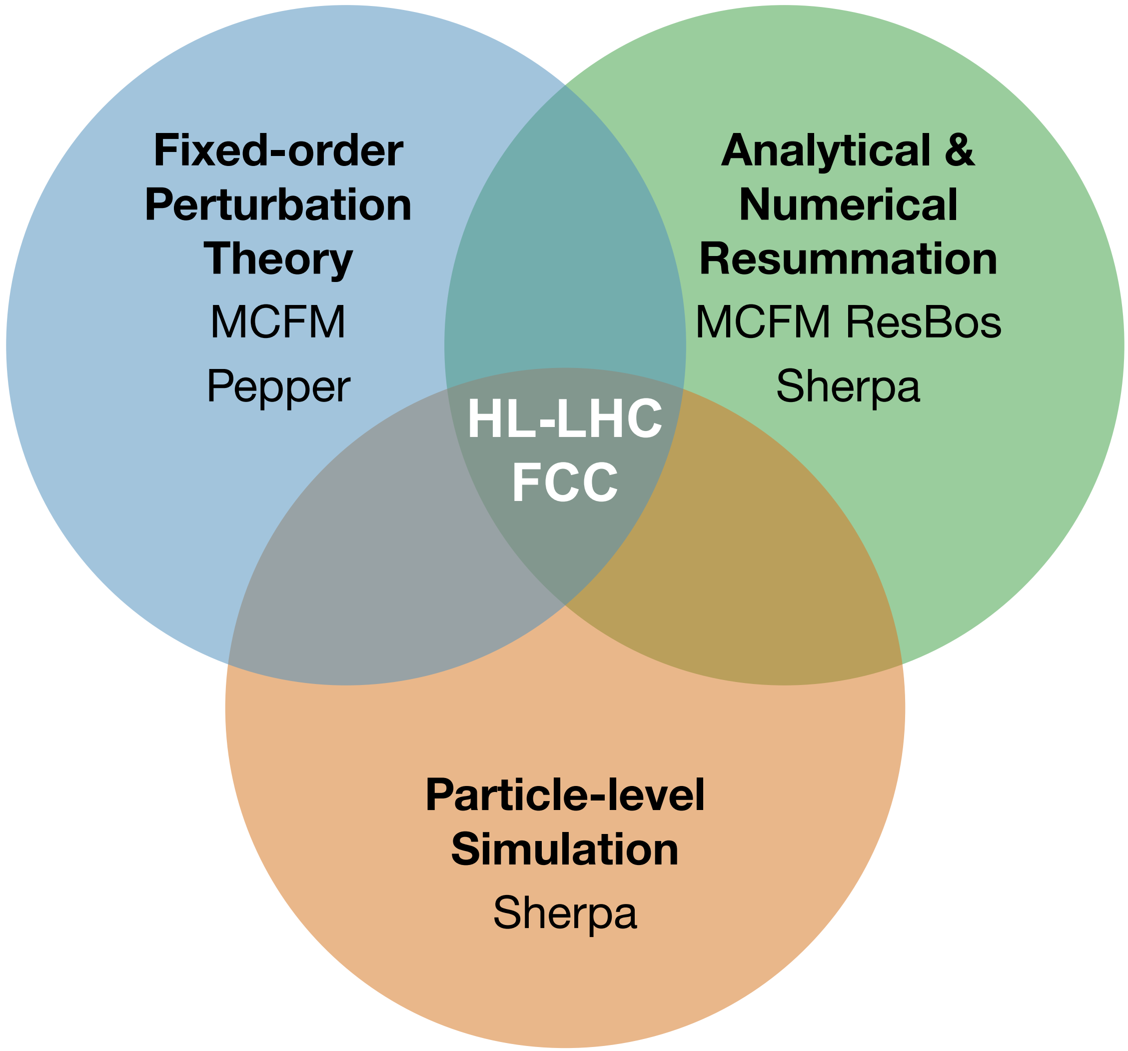
- Fermilab theory provided first systematic understanding of numerically unstable structures, both in Green's functions and in vertices / external wave functions
- **Can now obtain better numerical stability with double precision arithmetic than with previous implementations based on quadruple precision arithmetic**

SciDAC
Scientific Discovery through Advanced Computing




[Campbell et al.] arXiv:2406.07671

# Physics program going forward




All goals aligned with recommendations of P5, see also [Campbell et al.] arXiv:2203.11110

# Summary

- Fermilab theory leads efforts to develop precision probes and tools for the LHC
- Addresses need to keep pace with rapidly shrinking experimental uncertainties
- **Extract maximum return on LHC investment, as well as prepare for FCC-ee**

- **Broad application across the program: Higgs, DM, BSM, future colliders**
- New and exciting synergies with other efforts, e.g. MCs for neutrino physics

- This research direction benefits greatly from the laboratory setting
  - Not widely supported in U.S. university groups
  - Utilizing a wealth of local expertise and resources (theory, experiment, computing) both at Fermilab & ANL (ALCF)
- Enhances local experimental hub (theory resource)

- **Future work will build on existing strengths and recent progress, targeting better theoretical tools from a holistic perspective, exploiting the synergies between individual research programs**
- Growing interest / involvement in FCC-ee, EIC and beyond