Optimising the Computational Footprint in Precision Particle Physics

Example of: Integrating sustainability goals in HEP computing-related research grant applications.

Problem: grant funding extremely competitive, with low success rates.
Main driver = maximal scientific ambition, not minimal resource usage.

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Some Background

Home = Australia (Melbourne)

Until recently, air travel seemed the sole climate impact of our professional activities that we could do something about.

PYTHIA = widely used HEP simulation (MC event generator)

State of the art for high-p_T physics studies = **"multi-leg merging"**

For the experts: @ **LO** (MLM, CKKW-L, UMEPS) or **NLO** (NL^3, UNLOPS, FxFx).

CPU requirements grow factorially with process complexity.

Paradigm: pay the price, to do the calculations. (No alternative?)

During 2019, we were deciding what to focus on in an upcoming grant proposal.

That summer, Australia experienced relentless, devastating bush fires (the "black summer"); prompted us to look for *any* connection between the actual research we do, and climate impact.

Optimisation = doing the same thing quicker, with less resources

Unrealistic to get research grant to do **only** that?

But realistic to include as **one** goal among several?

Change of Paradigm (at least for us): Efficient algorithms = goal in itself

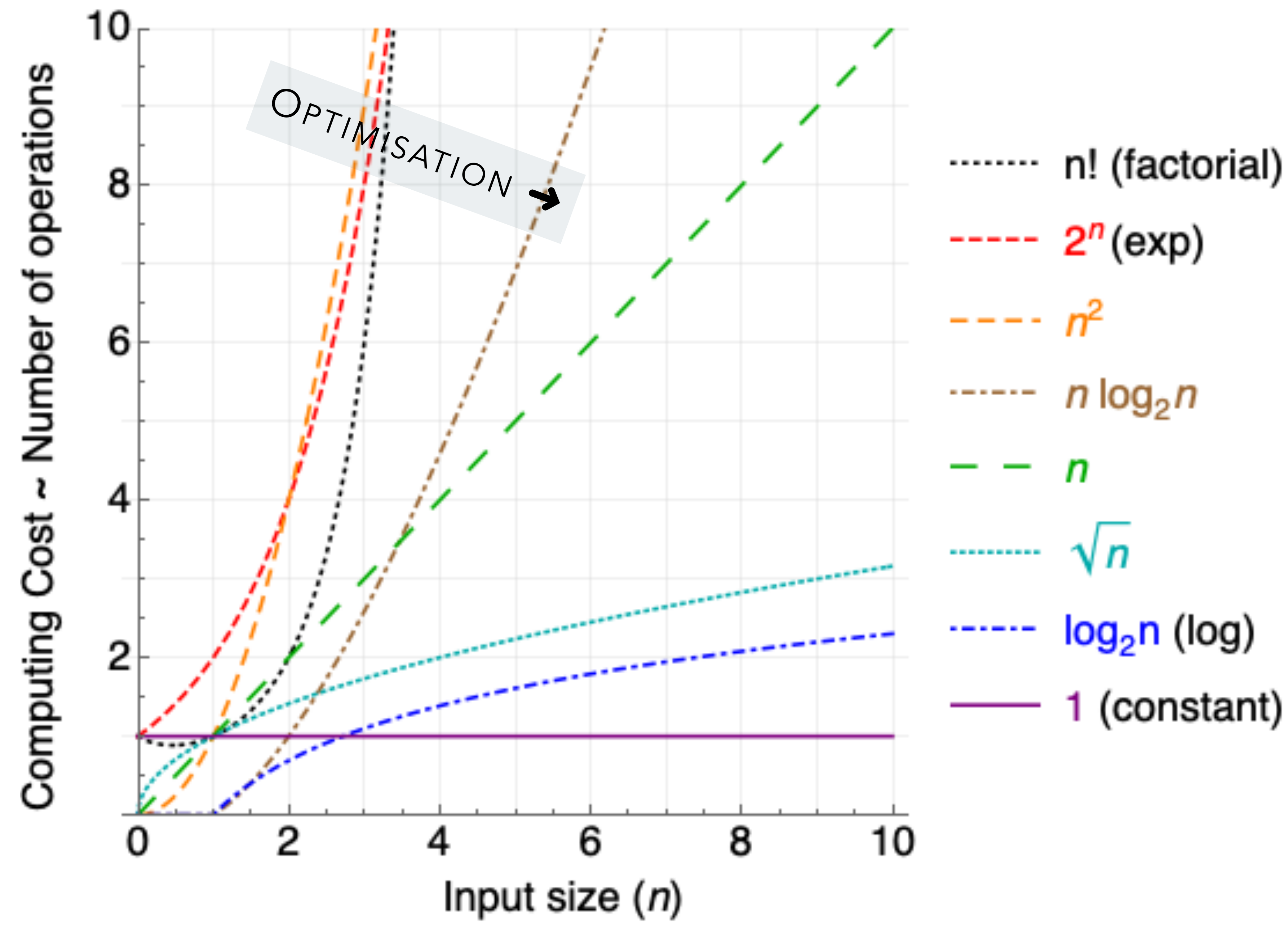
Not just as point of pride, or to enable "big" studies, but to reduce impact.

Had idea to reduce factorial growth of merging algorithms to polynomial or better

Old proof of concept arXiv:1109.3608 promising but mathematically challenging.

Decided to frame the grant proposal around that.

+ pursue new developments pushing the state-of-the-art in that context.



Learning Curve

(Apologies for the hyperbole; these are grant summaries; note also there is always some randomness in grant successes/failures)

DP21: What did not work (they did not buy it; grant not awarded)

Putting footprint & optimisation **first**:

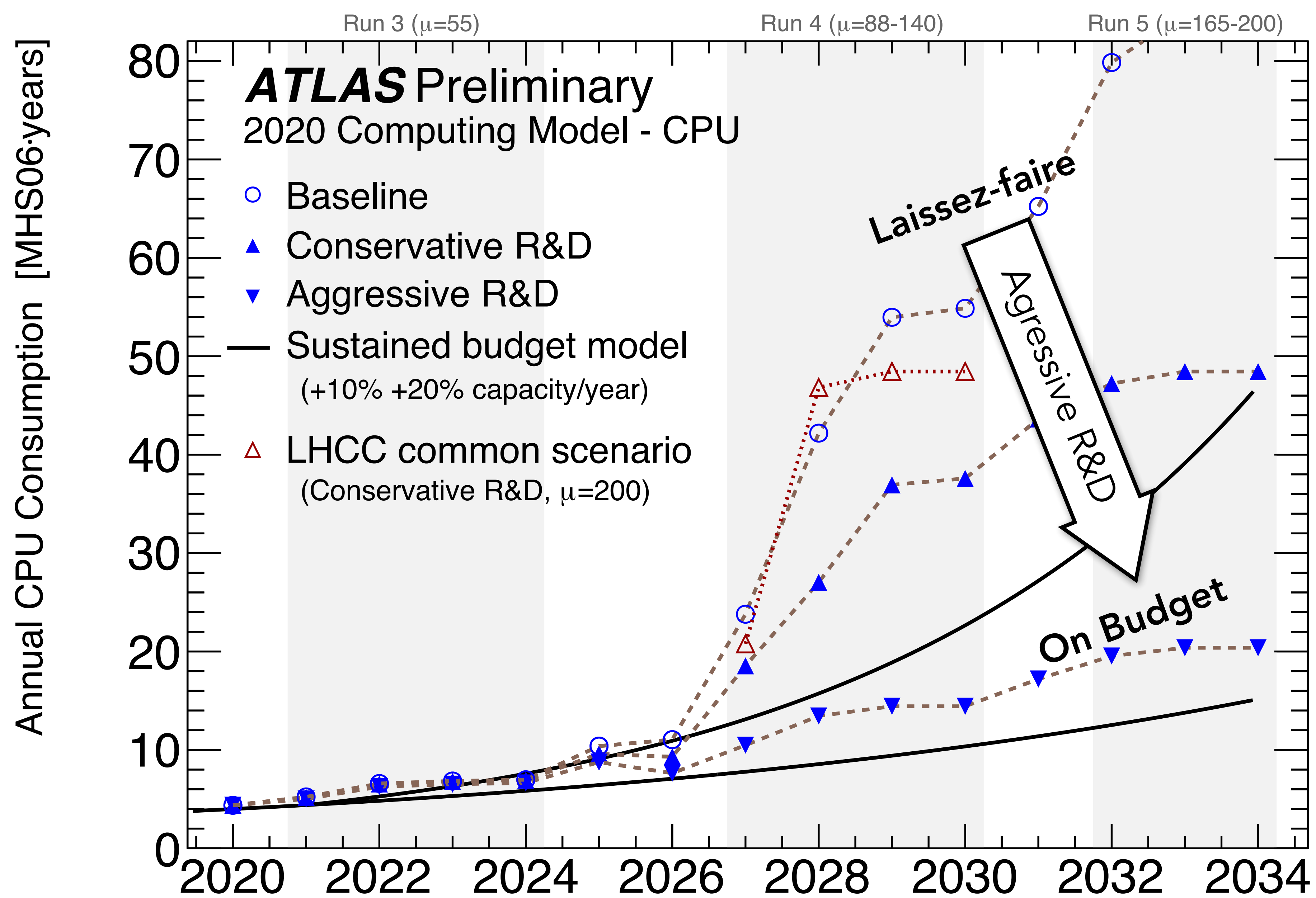
In a future of increasingly ambitious targets for limiting global energy consumption, scientific disciplines that rely heavily on large-scale computing will need to identify new ways of maximising the scientific output that can be achieved with the lowest possible resource usage, without compromising on scientific goals. This project aims to vastly reduce the computational footprint of some of the most advanced and resource-intensive calculations in particle physics, while retaining and even improving their accuracy. Such so-called merged matrix-element / parton-shower calculations represent the global state of the art and are used extensively in the field, but current approaches are limited by very high computational resource requirements.

DP22: What did work (➜ post doc position at Monash opening soon!)

Putting **scientific ambition first** (but retaining computational footprint as explicit aspect):

This project aims to deliver a breakthrough technique in theoretical-computational particle physics, with significant potential for high-precision applications. The project targets some of the most advanced and resource-intensive calculations in particle physics, which are widely used but currently limited by extremely high computational resource requirements. This project expects to develop a novel approach that will vastly reduce the computational complexity while at the same time improving their accuracy relative to the current global state of the art. Expected outcomes include the new methodology itself as well as a full-fledged and open-access simulation code based on it, which should be highly efficient.

Projected computing needs of the LHC experiments have been flagged as requiring aggressive R&D developments to meet requirements



CERN-LHCC-2020-015 unpublished preprint
(until recently impossible to refer to in ARC applications)

Keeping up with LHC will require increasingly precise calculations, for increasingly complex event types.

Any current bottlenecks are likely to become increasingly important.

Goes hand in hand with minimising footprint.

Obviously, many individual elements — but furnishes another argument to use.

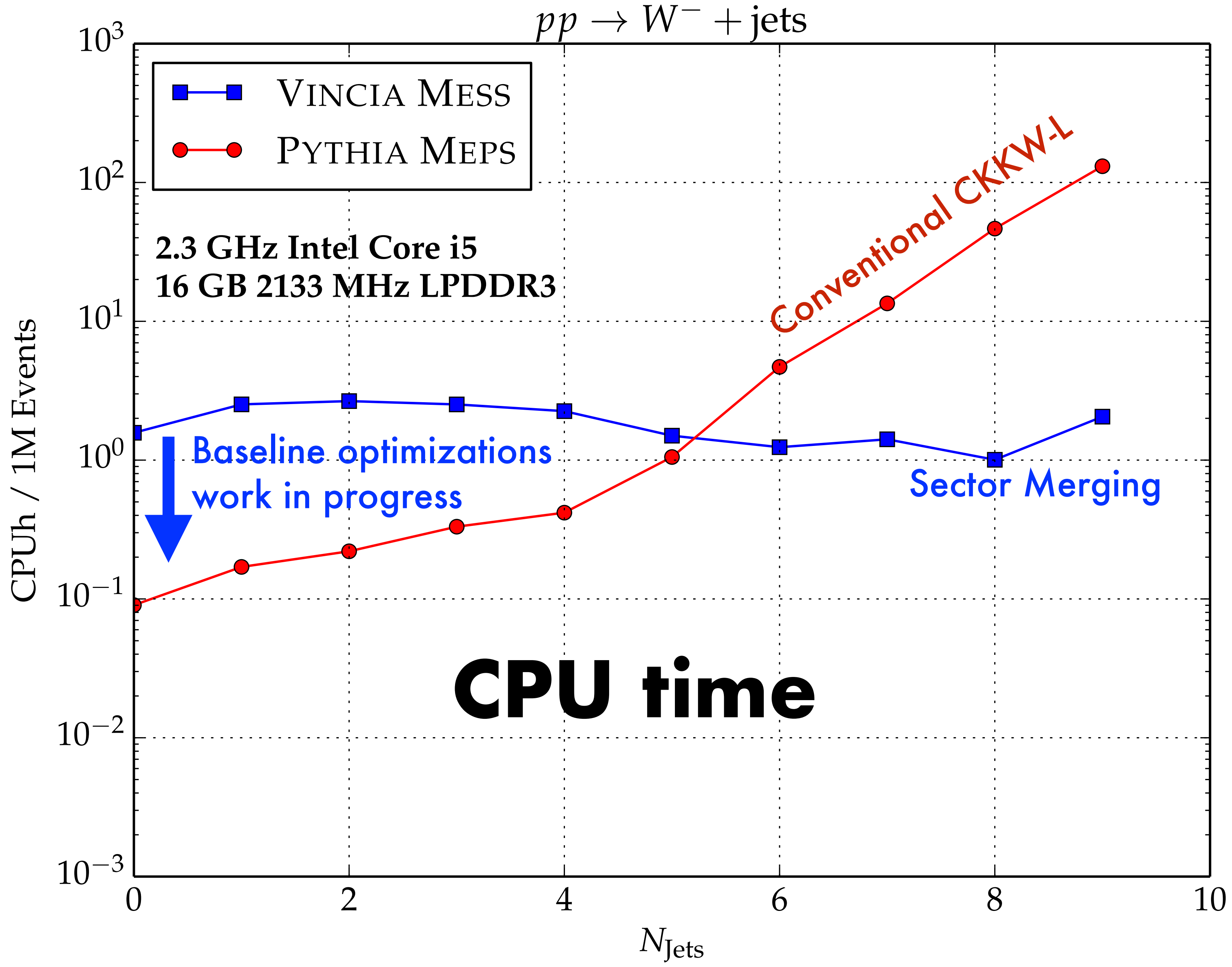
(+ algorithmic techniques and "best practices" communicated to students)

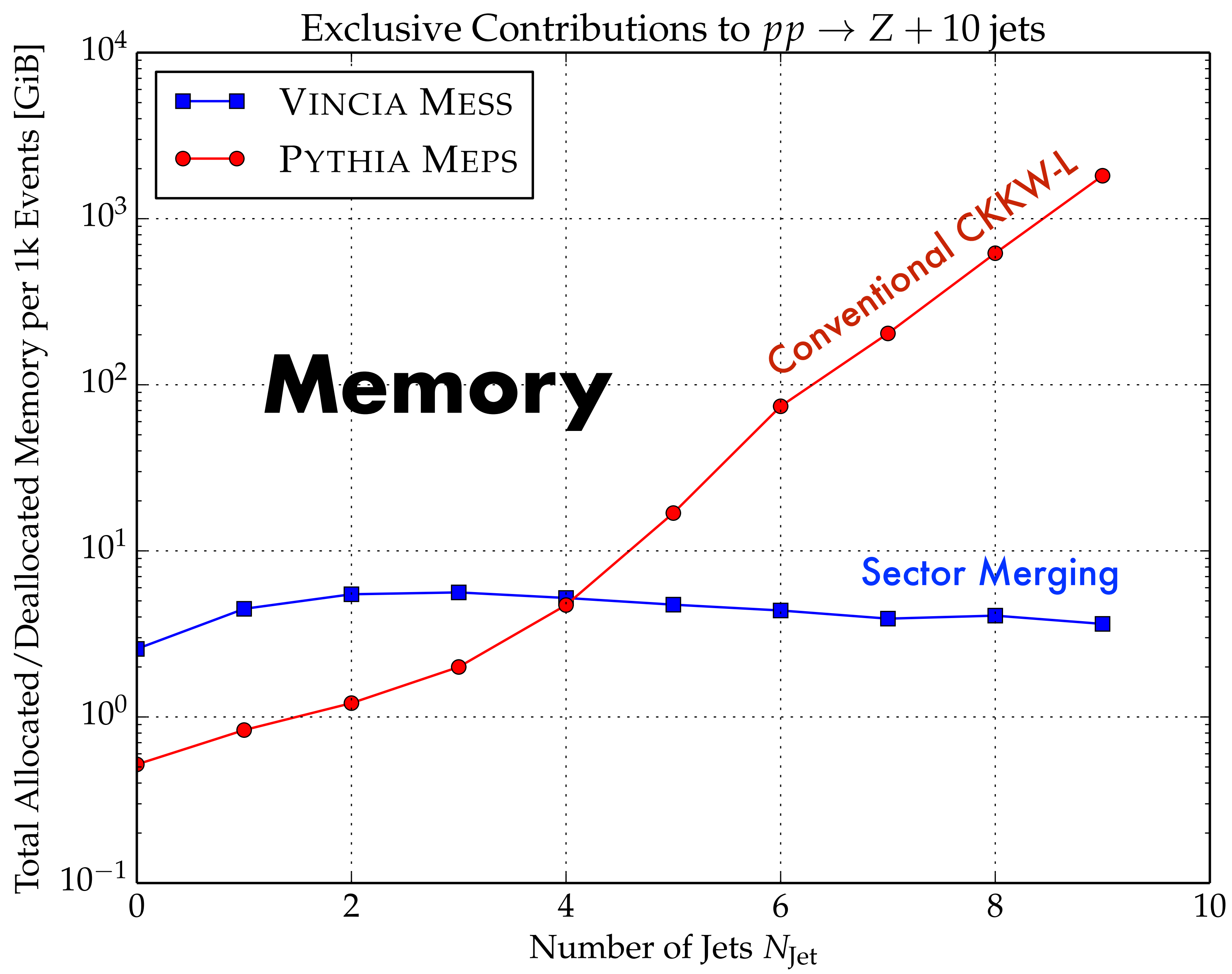
➜ Optimisation skills and ways of thinking transferred to industry

Preliminary Results: Tree-Level Merging

Sectorized CKKW-L Merging in Pythia 8.306 (for Vincia Showers Only)

Brooks & Preuss, "Efficient multi-jet merging with the VINCIA sector shower", arXiv:2008.09468





Extensions now pursued:

Sectorized matching at **NNLO** (proof of concept in arXiv:2108.07133)

+ Sectorized **multi-leg merging at NLO**, iterated matrix-element corrections, …

(Also note recent interesting work by Danziger et al., arXiv:2109.11964 and by Bothmann et al., arXiv:2209.00843)