Unbinned Unfolding with OmniFold

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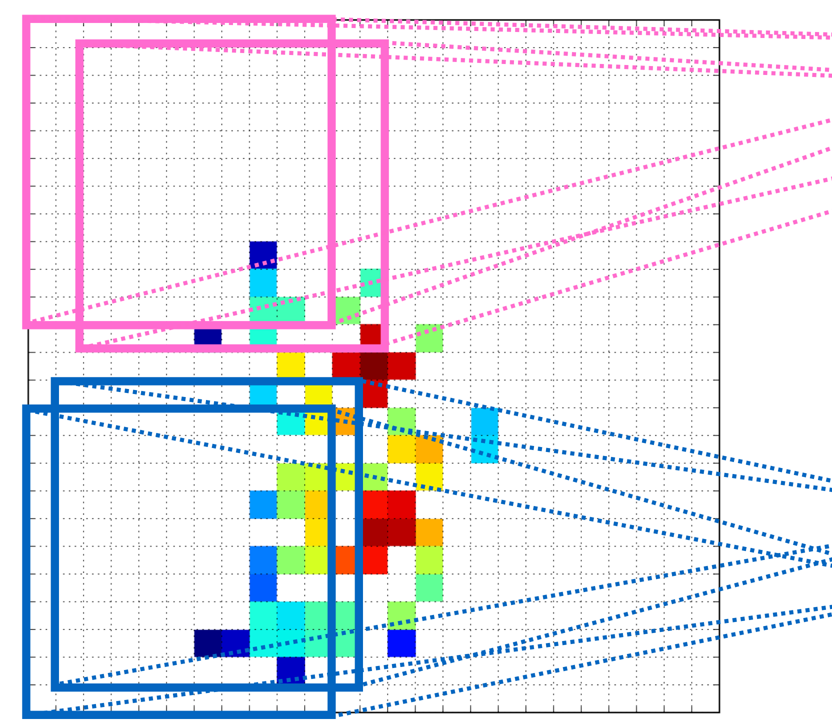

BERKELEY LAB

BIDS
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Scaling ML Meeting
May 2024

Unfolding

Deconvolution (“unfolding”):

correcting for detector effects

Unfolding

Deconvolution ("unfolding"):
correcting for detector effects

Key aspect of all cross section measurements, across particle/nuclear/astro physics (!)

Unfolding

Proton-Proton

Nucleus-Nucleus

Neutrino-Nucleus

Electron-Proton

Cosmic Rays

Electron-Positron

Particle/Nuclear/Astro Physics Experiments

Deconvolution ("unfolding"): correcting for detector effects

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Deconvolution ("unfolding"):
correcting for detector effects

Key aspect of **all** cross section measurements, across particle/nuclear/astro physics (!)

Why "unfold" instead of "fold"?

Unfolding is ill-posed, BUT only way to compare different experiments and to compare with non fully exclusive predictions. Data also survive much longer.

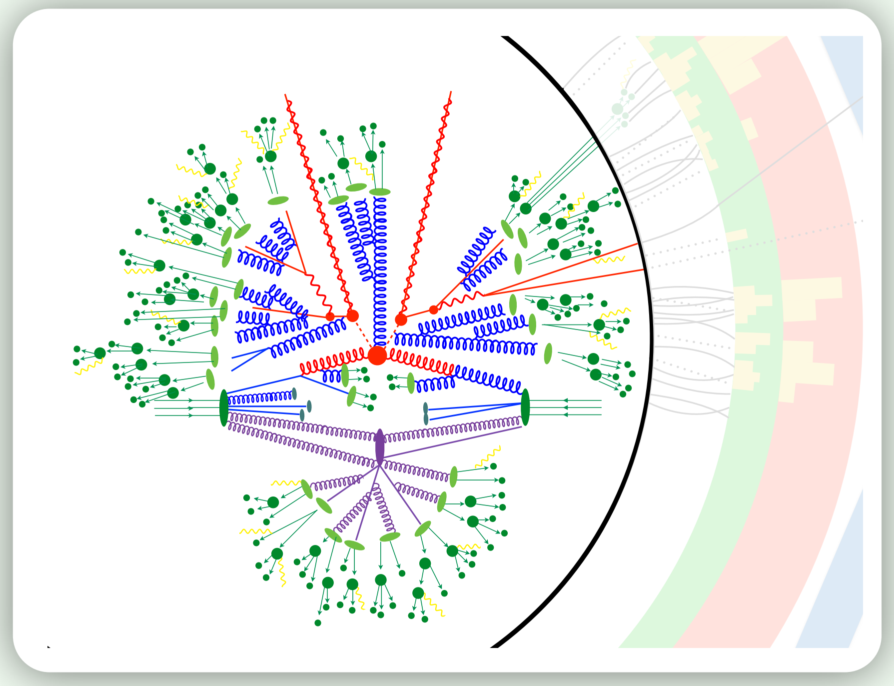
The Unfolding Challenge

2203.16722

The Unfolding Challenge

Particle Level

Want this



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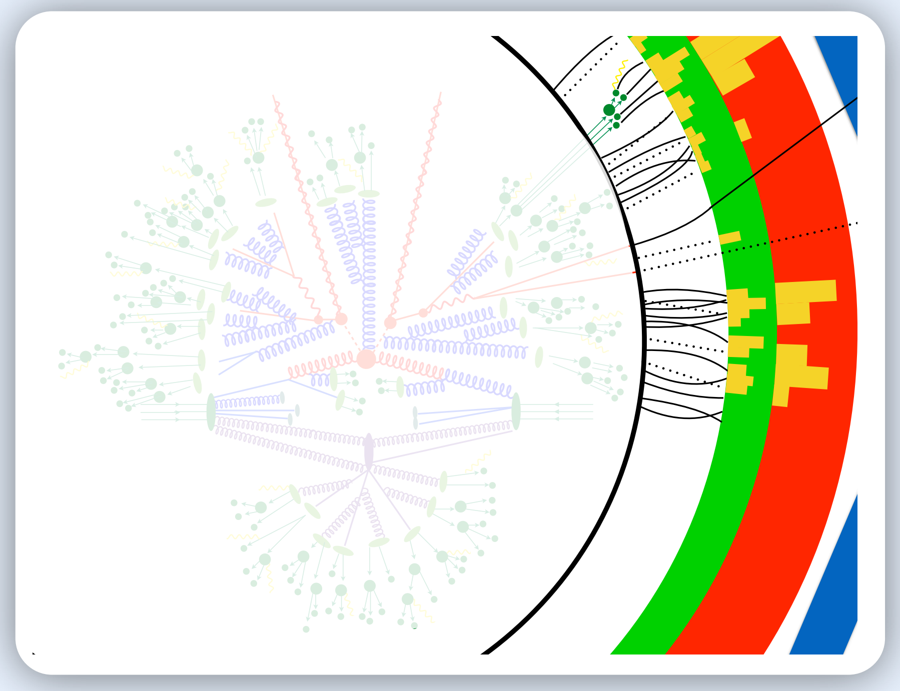
Detector Level

The Unfolding Challenge

Particle Level

Measure this



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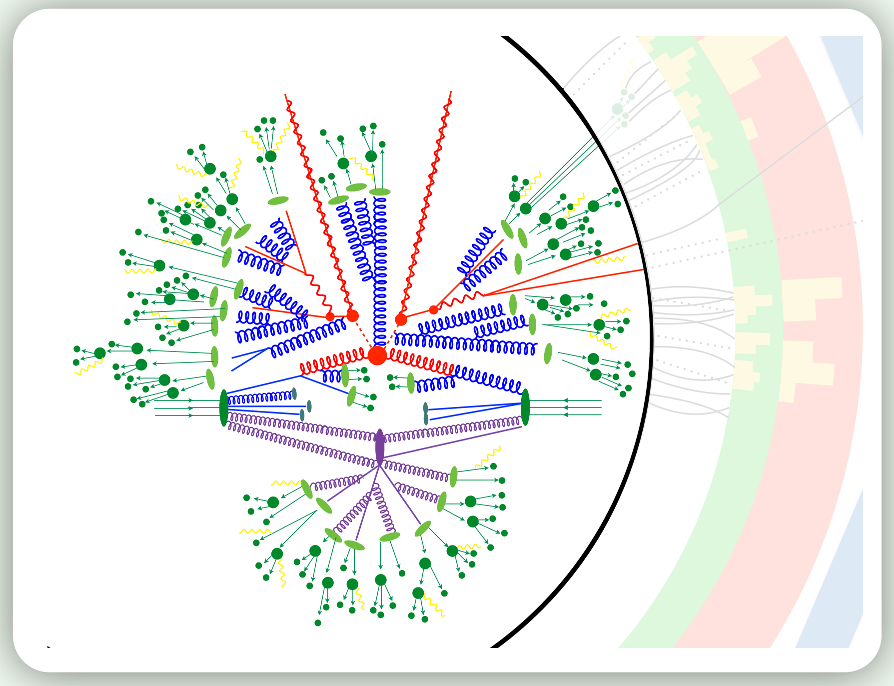

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Detector Level

The Unfolding Challenge

Particle Level

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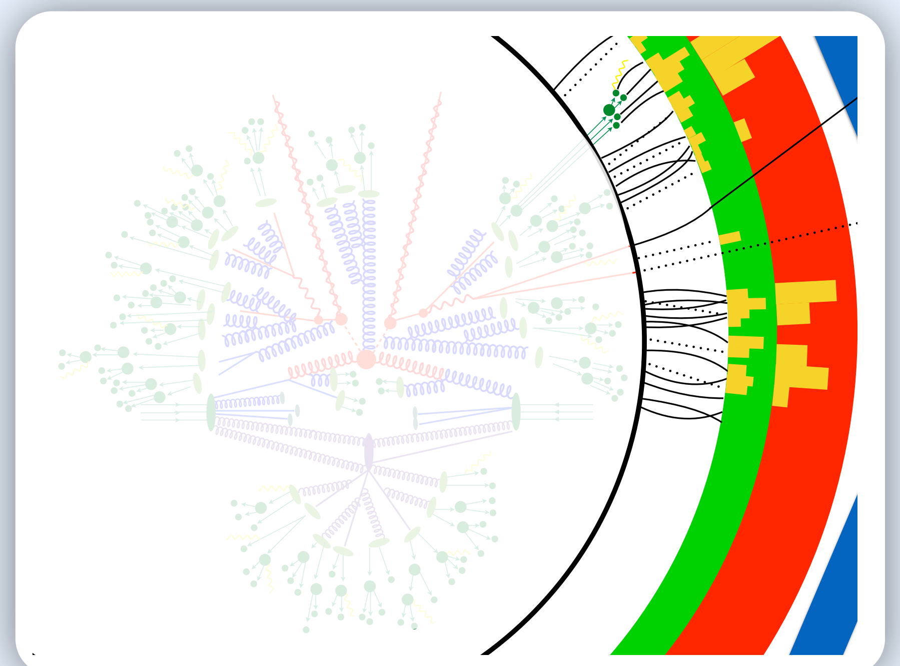
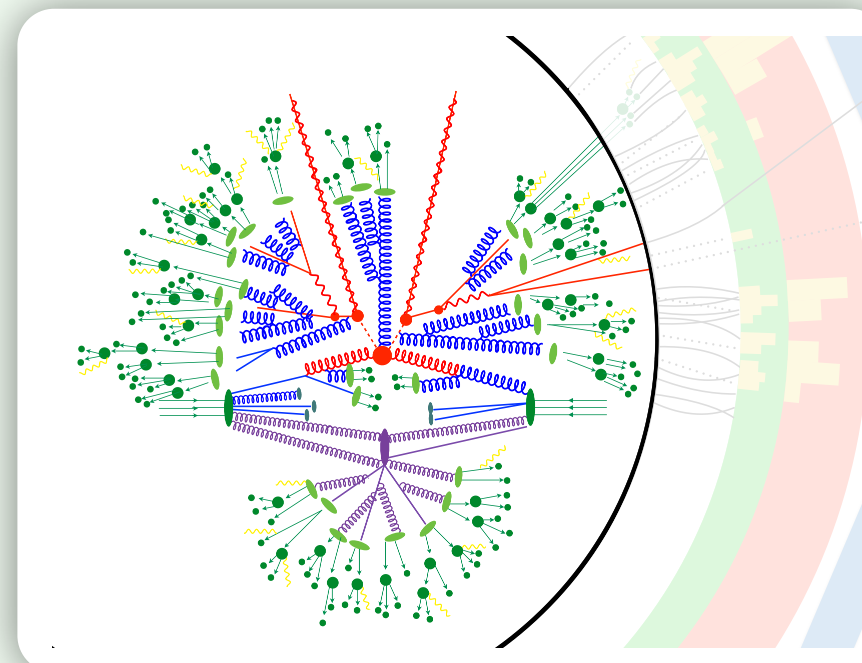
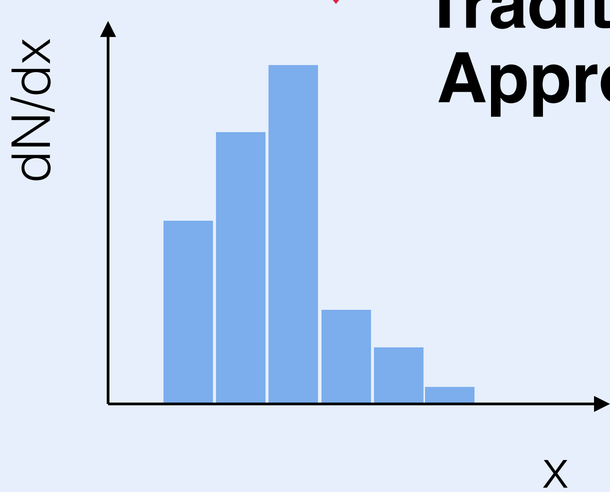


Want this

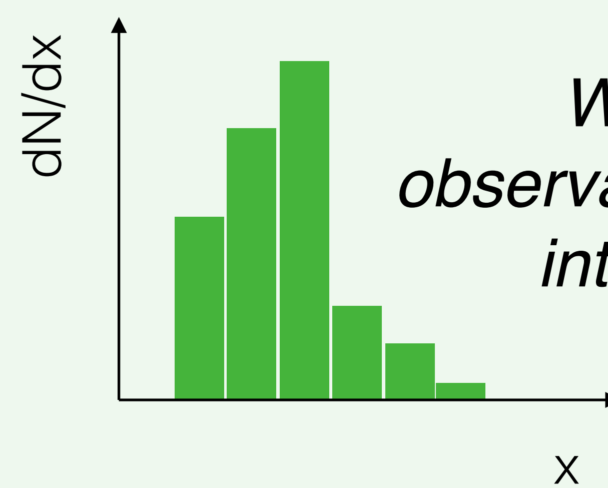


Traditional Approach



$$\hat{T} \approx R^{-1}M$$

Target observable



We pick O(1) observables & discretize into O(10) bins

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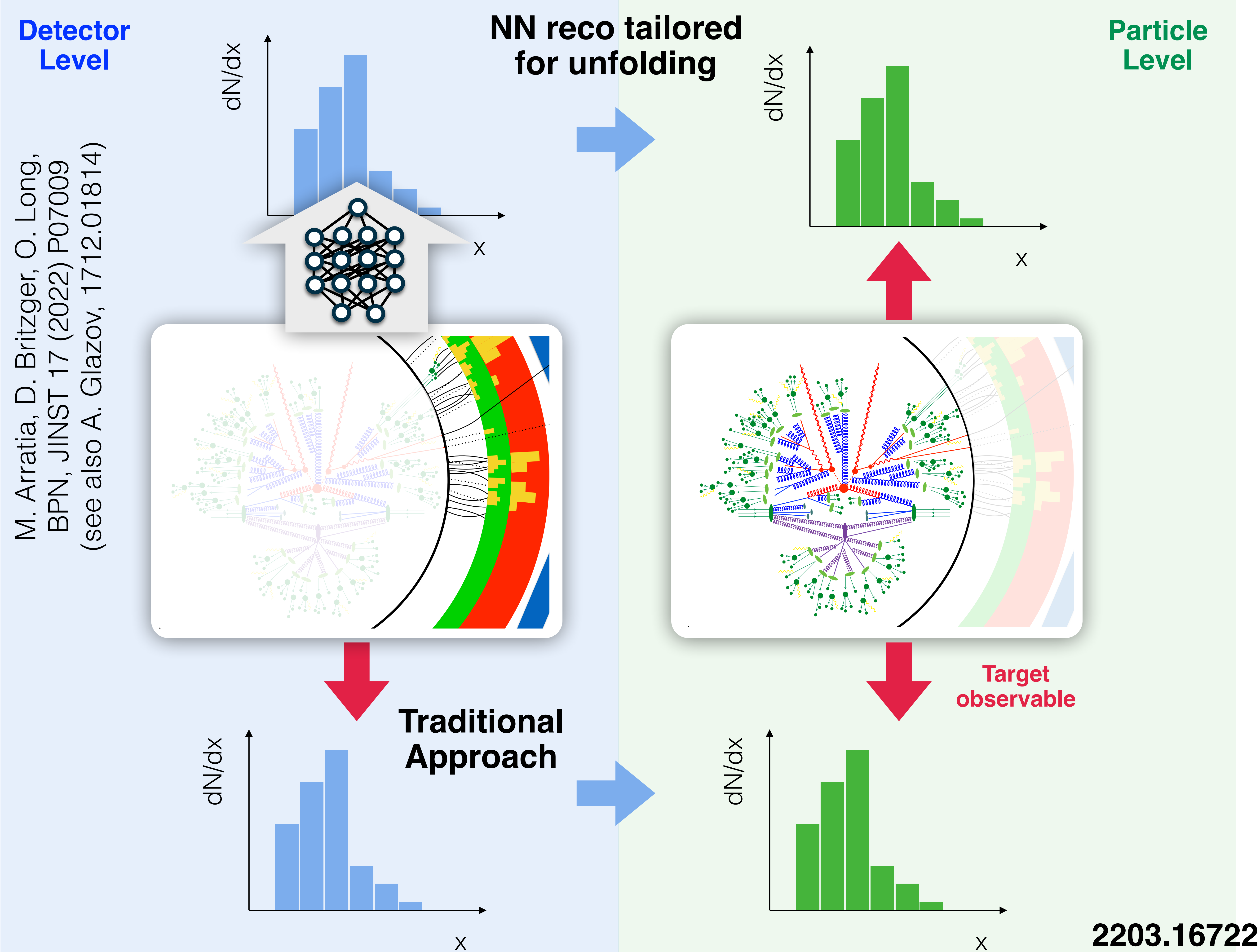
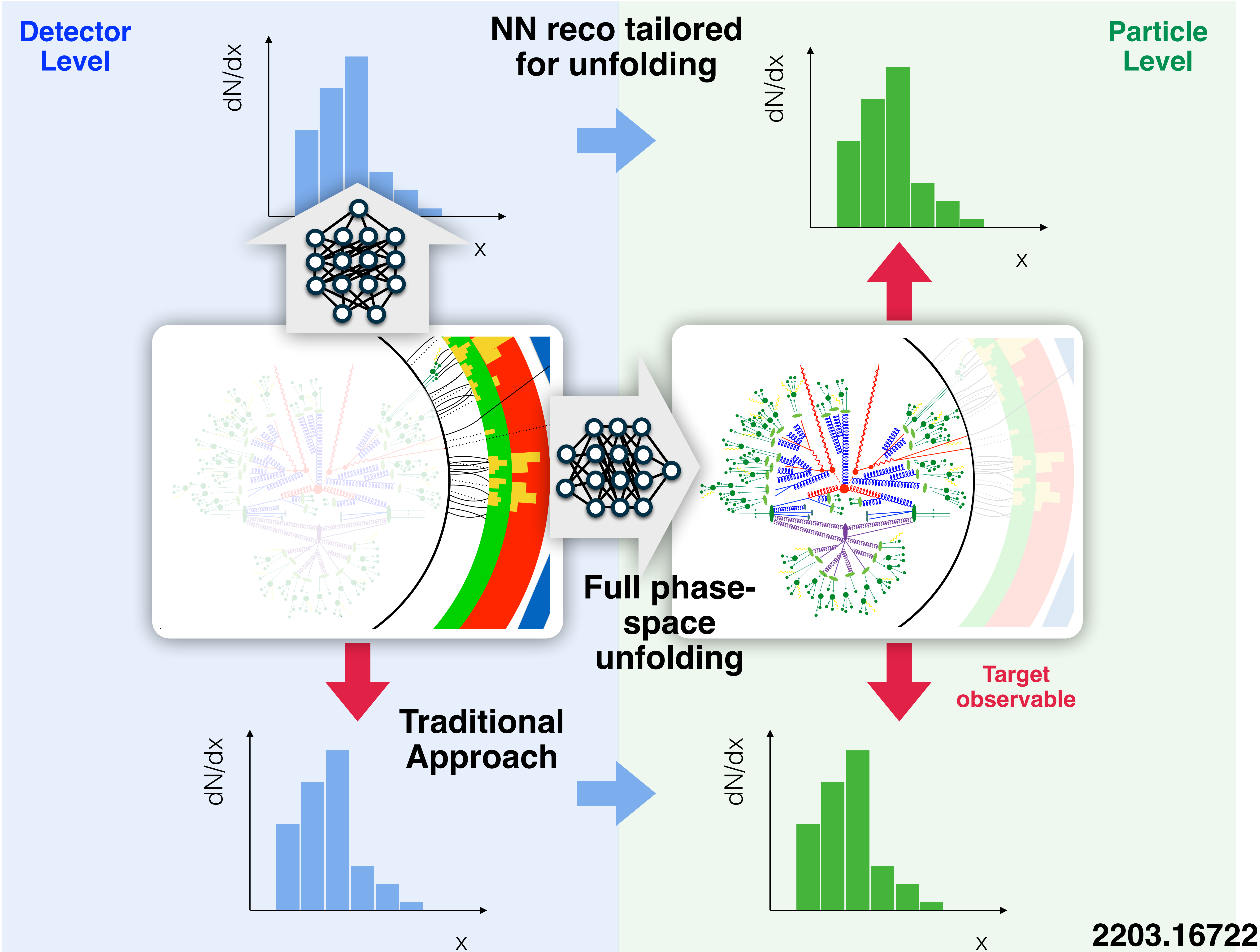

Detector Level
NN reco tailored for unfolding
Particle Level
M. Arratia, D. Britzger, O. Long, BPN, JINST 17 (2022) P07009
(see also A. Glazov, 1712.01814)
dN/dx
x
dN/dx
x
Target observable
Traditional Approach
dN/dx
x
dN/dx
x
2203.16722


Detector Level
NN reco tailored for unfolding
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Full phase-space unfolding
Traditional Approach
Target observable
dN/dx
x
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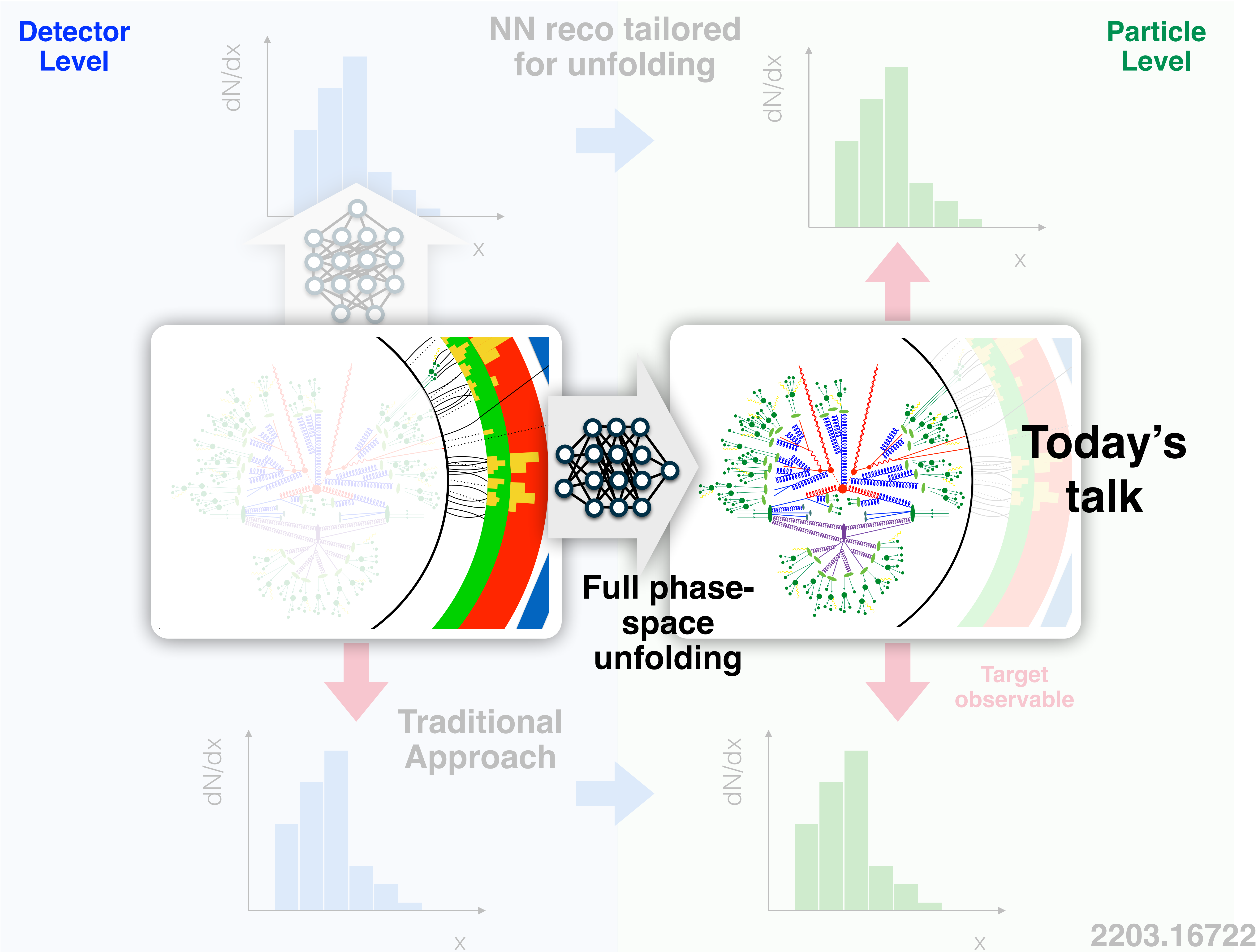
2203.16722


Detector Level
NN reco tailored for unfolding
Particle Level
dN/dx
x
dN/dx
x
Today's talk
Full phase-space unfolding
Target observable
Traditional Approach
dN/dx
x
dN/dx
x
2203.16722

Why unbinned (+high-dimensional)?

For a community white paper, see JINST 17 (2022) P01024, 2109.13243

Why unbinned (+high-dimensional)?

Inference-Aware Binning

Optimal binning depends on downstream task. Not possible with current setup.

What about moments?
(see also K. Desai, BPN, J. Thaler, [paper])

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Derivative Measurements

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Derivative Measurements

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Higher Dimensions

Some phenomena can't be probed in a few dimensions.

What about observables that are not per-event?

For a community white paper, see JINST 17 (2022) P01024, 2109.13243

Landscape of Methods

Classifier-Based Methods

Learn (unfolded) data
likelihood ratio w.r.t. simulation

For references, see JINST 17 (2022) P01024, 2109.13243 (and papers that cite it!)

Landscape of Methods

Classifier-Based Methods

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Density-Based Methods

Learn (unfolded) data probably density implicitly or explicitly.

For references, see JINST 17 (2022) P01024, 2109.13243 (and papers that cite it!)

Landscape of Methods

Classifier-Based Methods

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I'll focus here today because:

Learn a small correction (start close to the right answer)

&

~prior independent (if maximum likelihood)

Density-Based Methods

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Density-Based Methods

Learn (unfolded) data probably density implicitly or explicitly.

I won't talk about these at all, but there has been a lot of work with GANs, VAEs, NFs, Diffusion…

GANs: K. Datta, D. Kar, D. Roy, 1806.00433; M. Bellagente, A. Butter, G. Kasieczka, T. Plehn, R. Winterhalder, SciPost Phys. 8 (2020) 070, …

VAEs: J. Howard, S. Mandt, D. Whiteson, Y. Yang, Sci. Rep. 12 (2022) 7567, …

NFs: M. Bellagente et al., SciPost Phys. 9 (2020) 074; M. Vandegar, M. Kagan, A. Wehenkel, G. Louppe, PMLR 11 (2021) 2107; M. Backes, A. Butter, M. Dunford, B. Malaescu, 2212.08674, …

Diffusion: A. Shmakov et al., 2305.10399; S. Diefenbachar, G. Liu, V. Mikuni, B. Nachman, W. Nie, 2308.12351

For references, see JINST 17 (2022) P01024, 2109.13243 (and papers that cite it!)

Landscape of Methods

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I'll focus here today because:

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&

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My focus will be on a method called **OmniFold**.

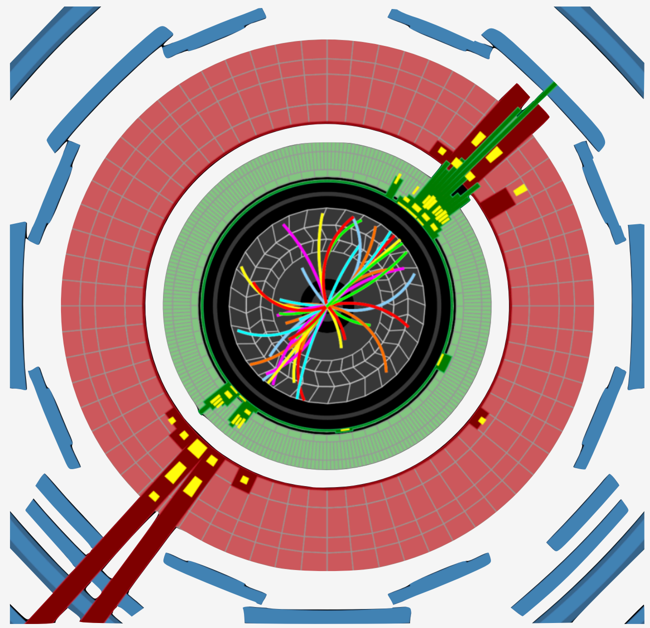
For references, see JINST 17 (2022) P01024, 2109.13243 (and papers that cite it!)

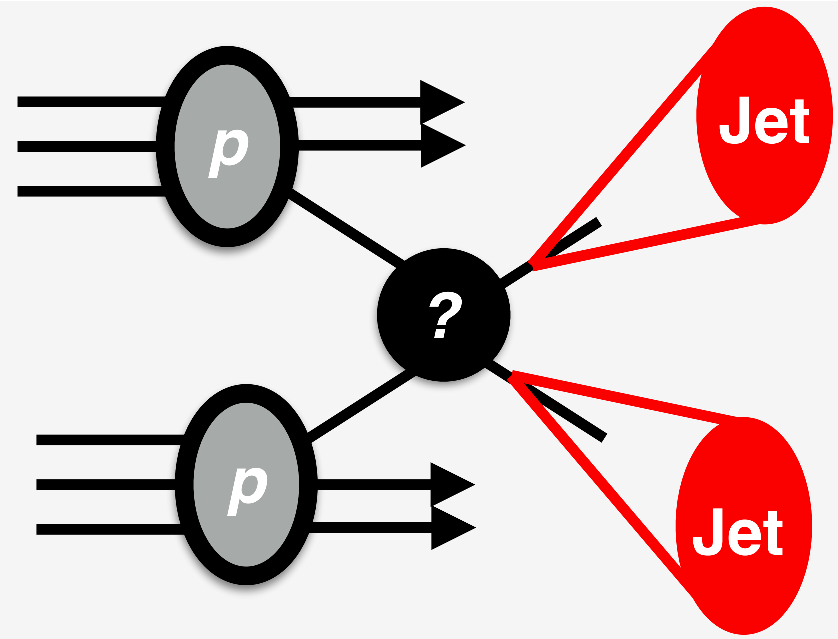
A brief introduction to OmniFold

Detector-level

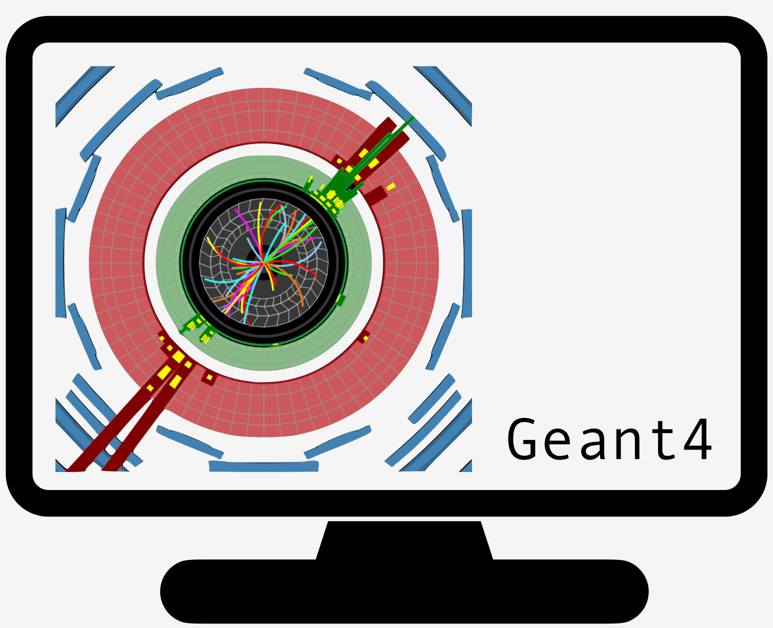
Particle-level

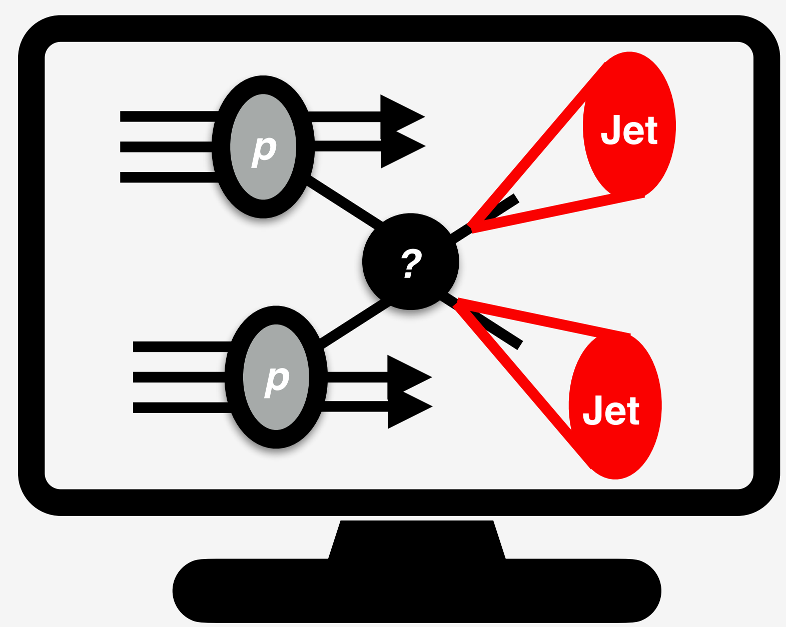
Nature



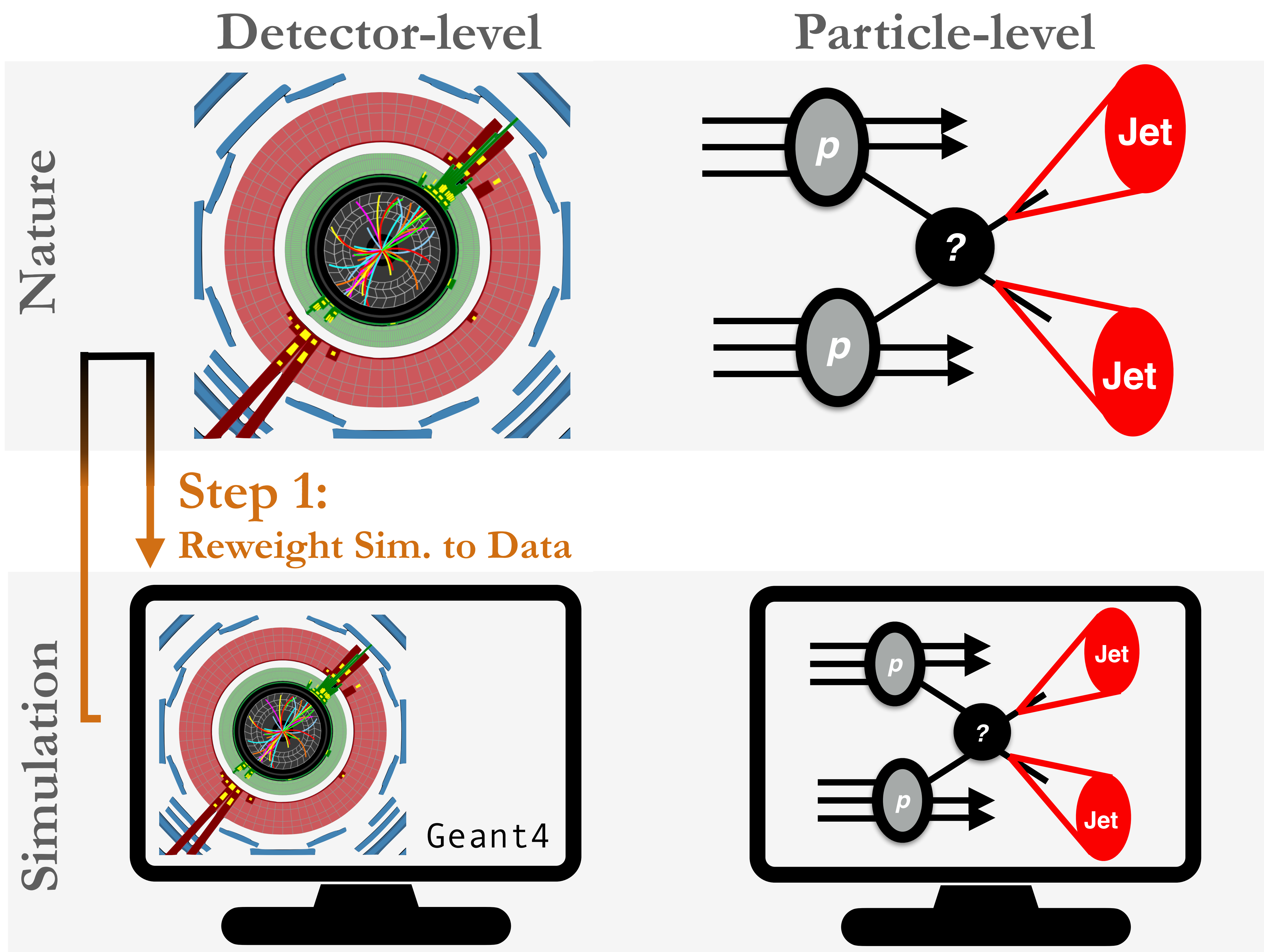


Simulation





A brief introduction to OmniFold



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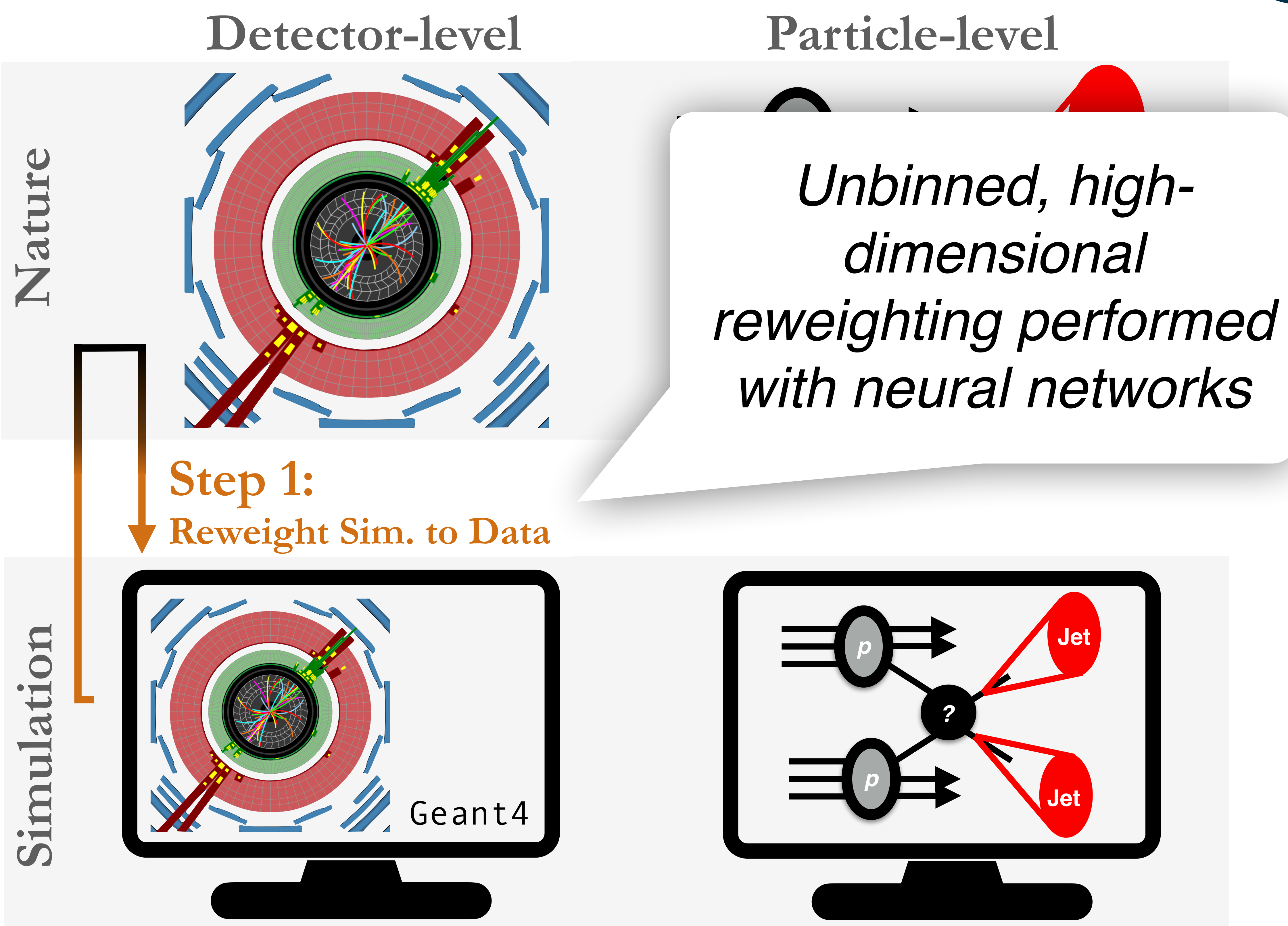

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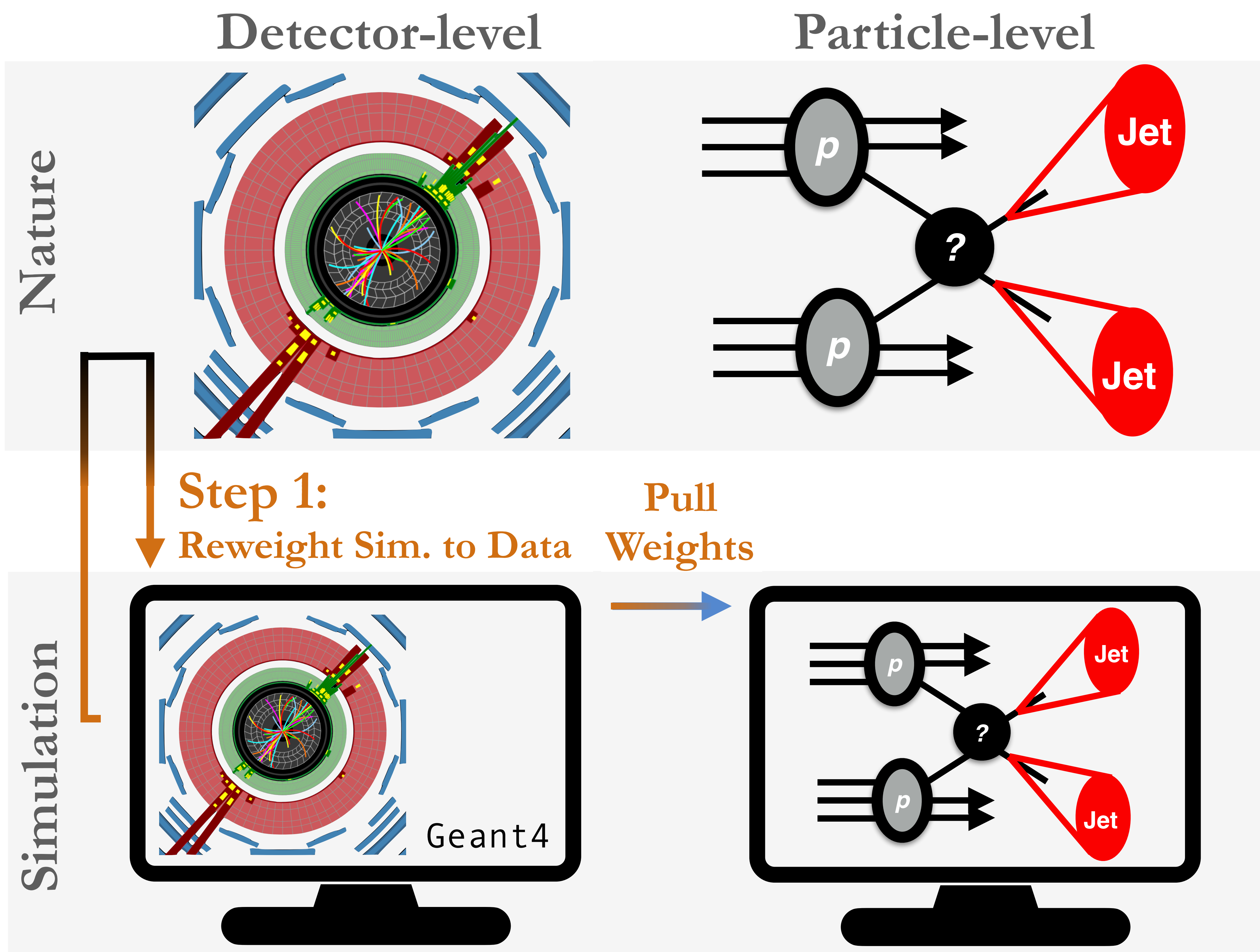

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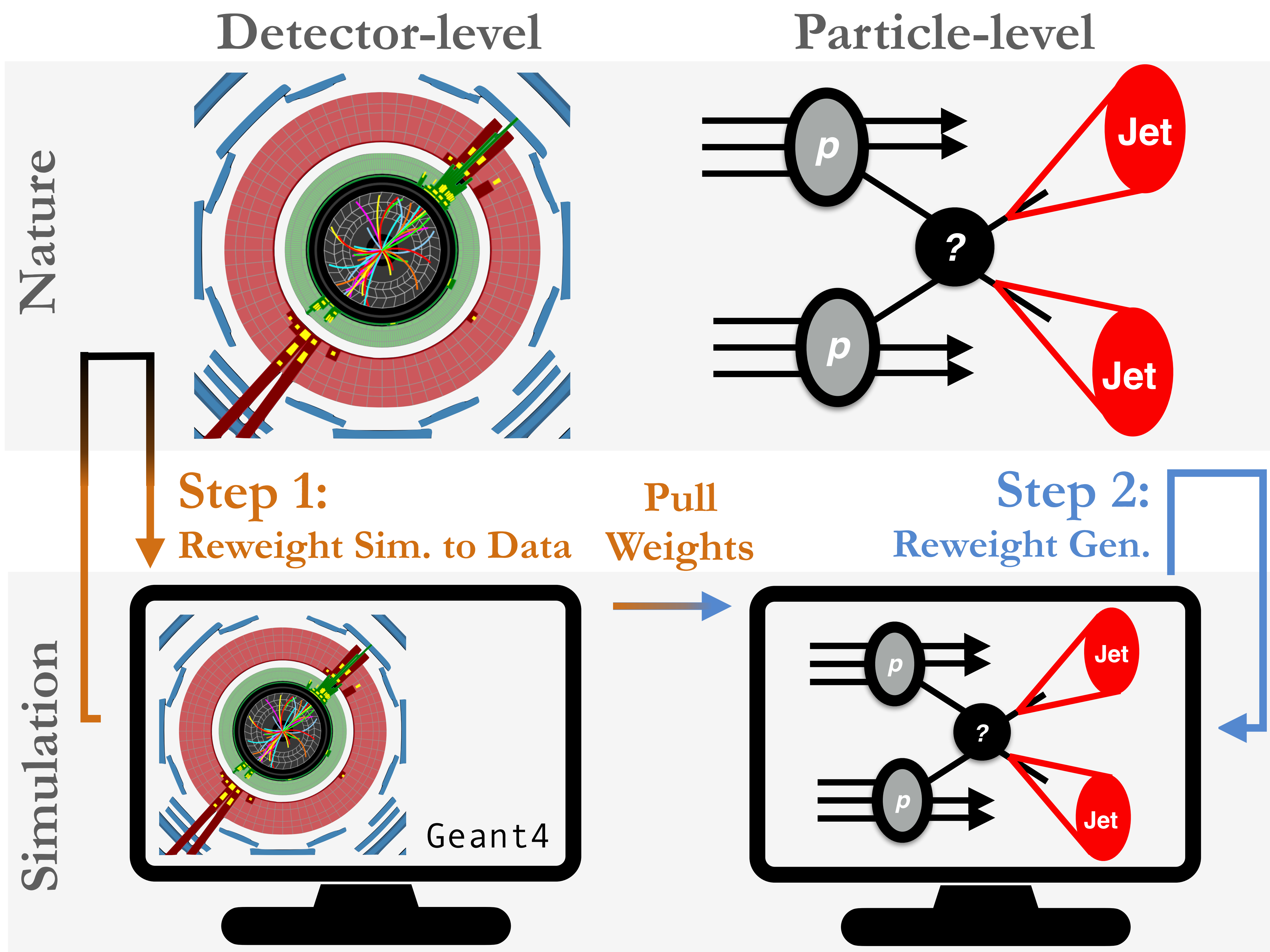

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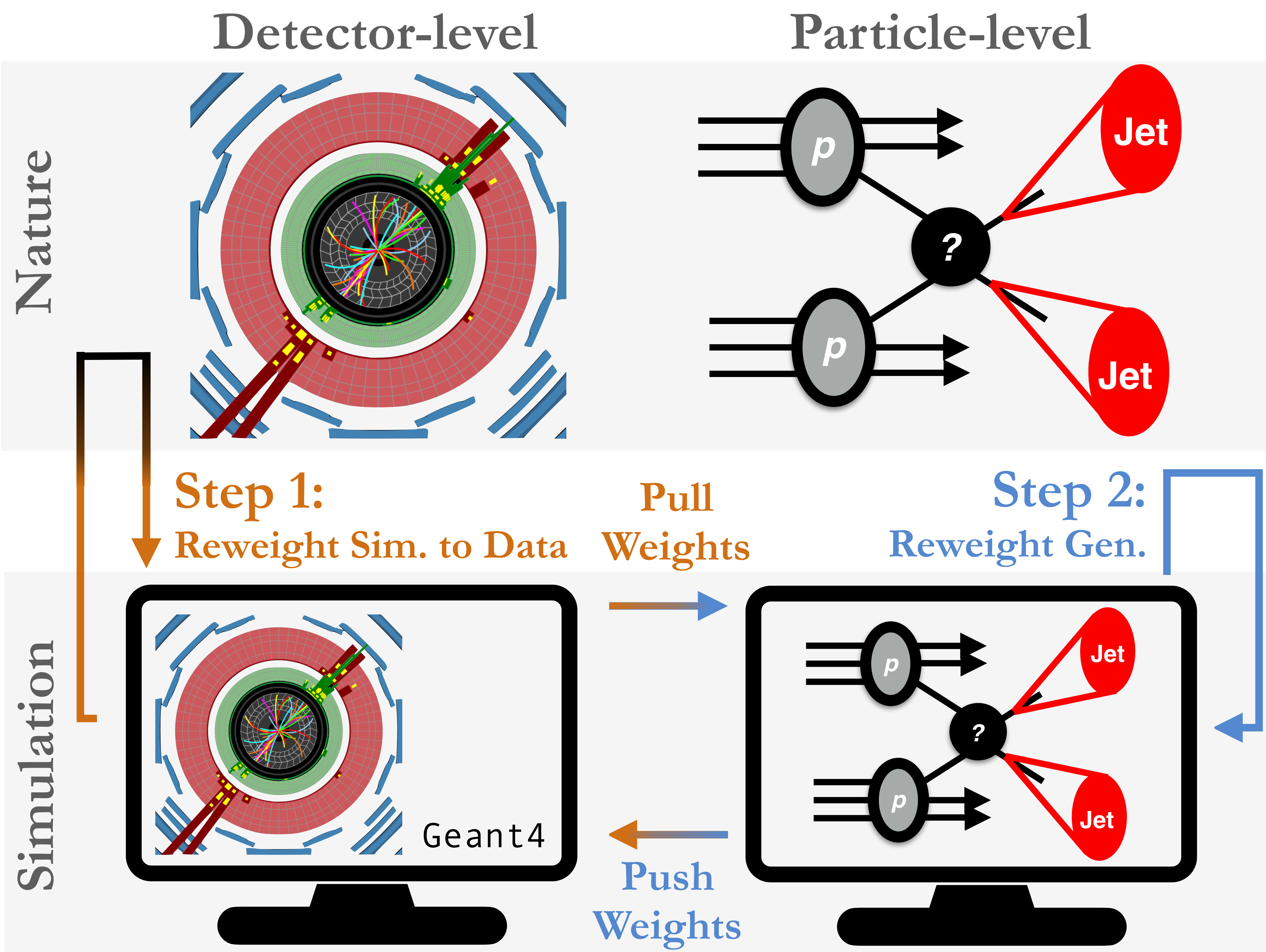

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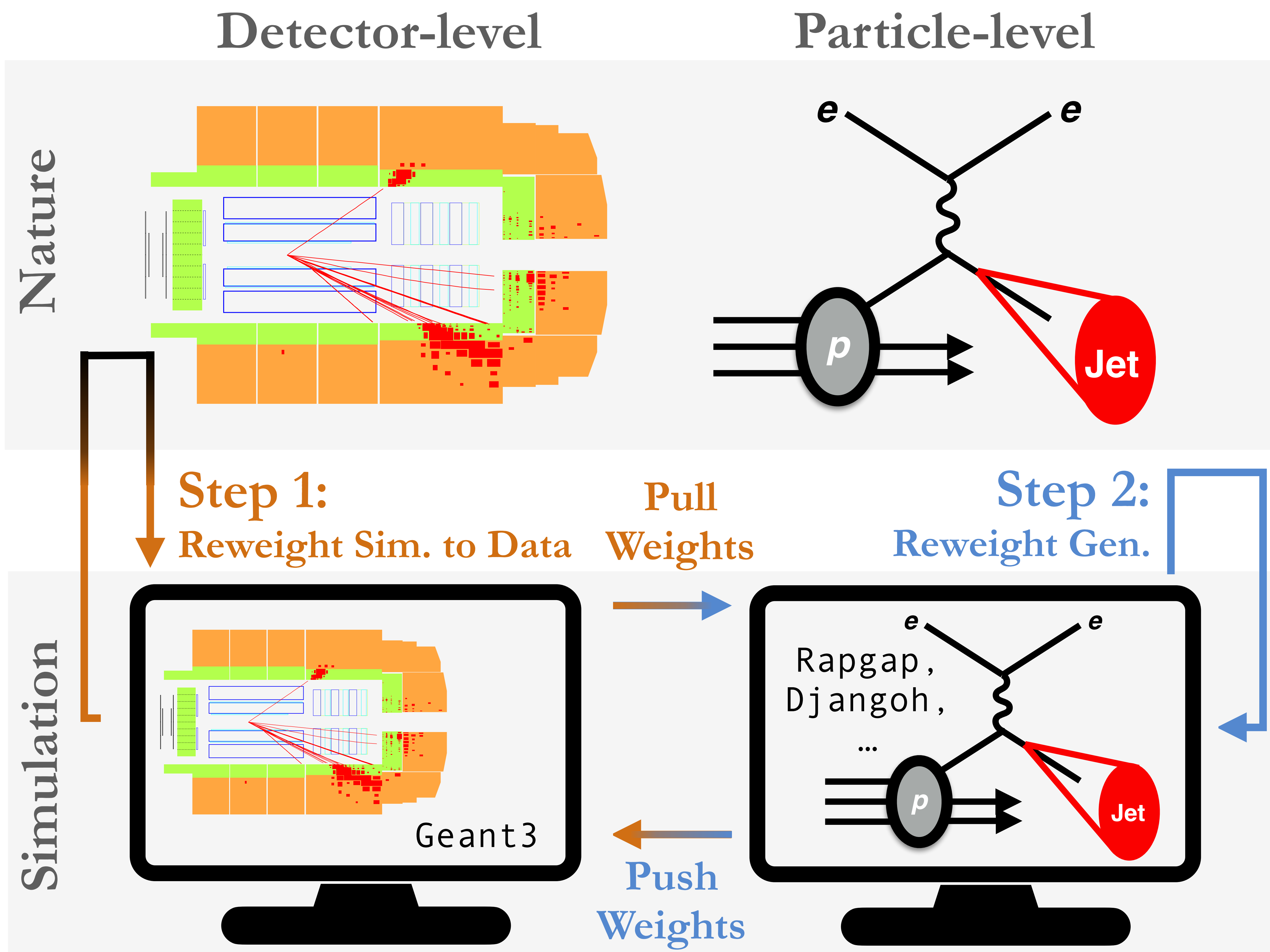

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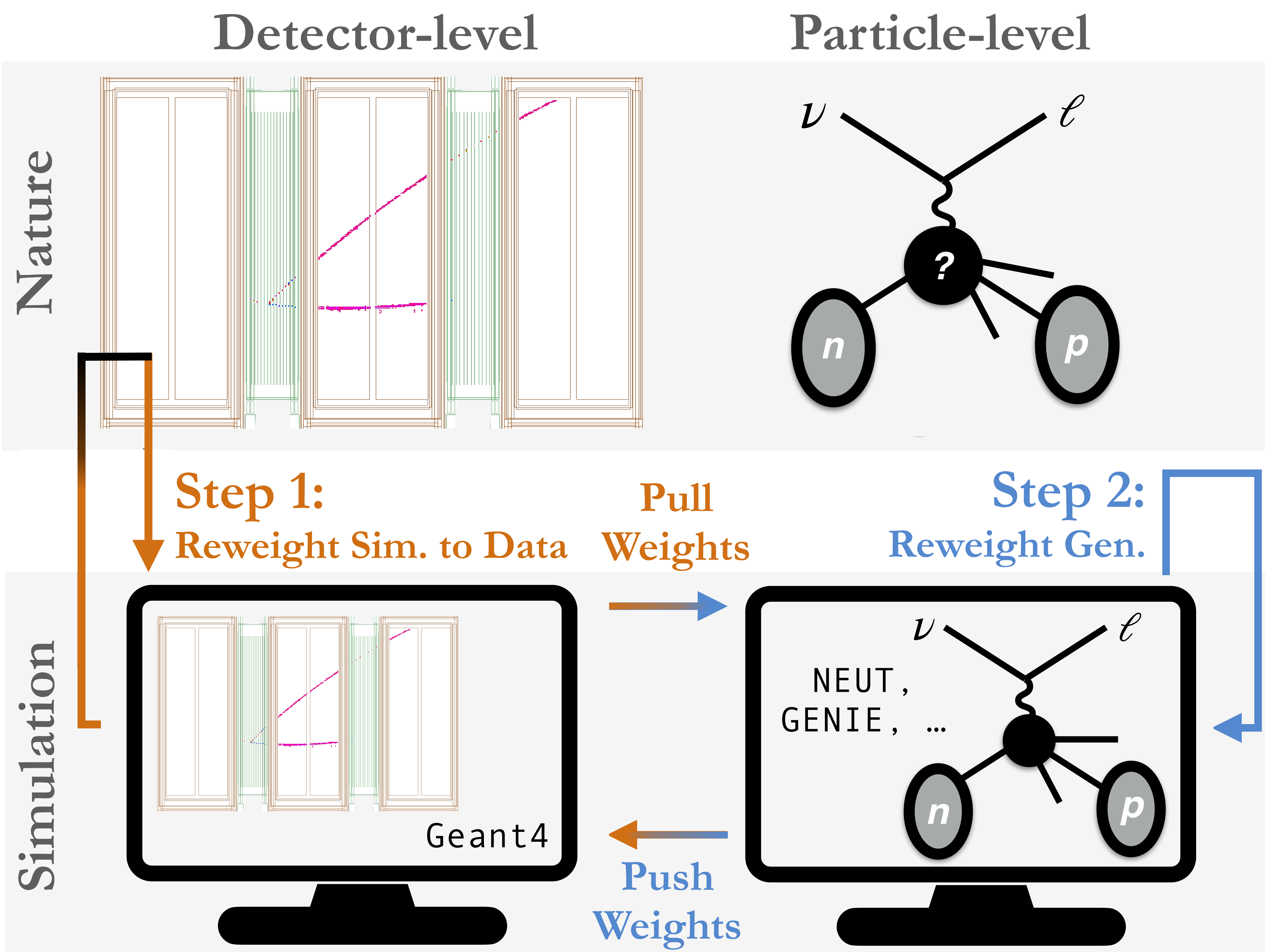
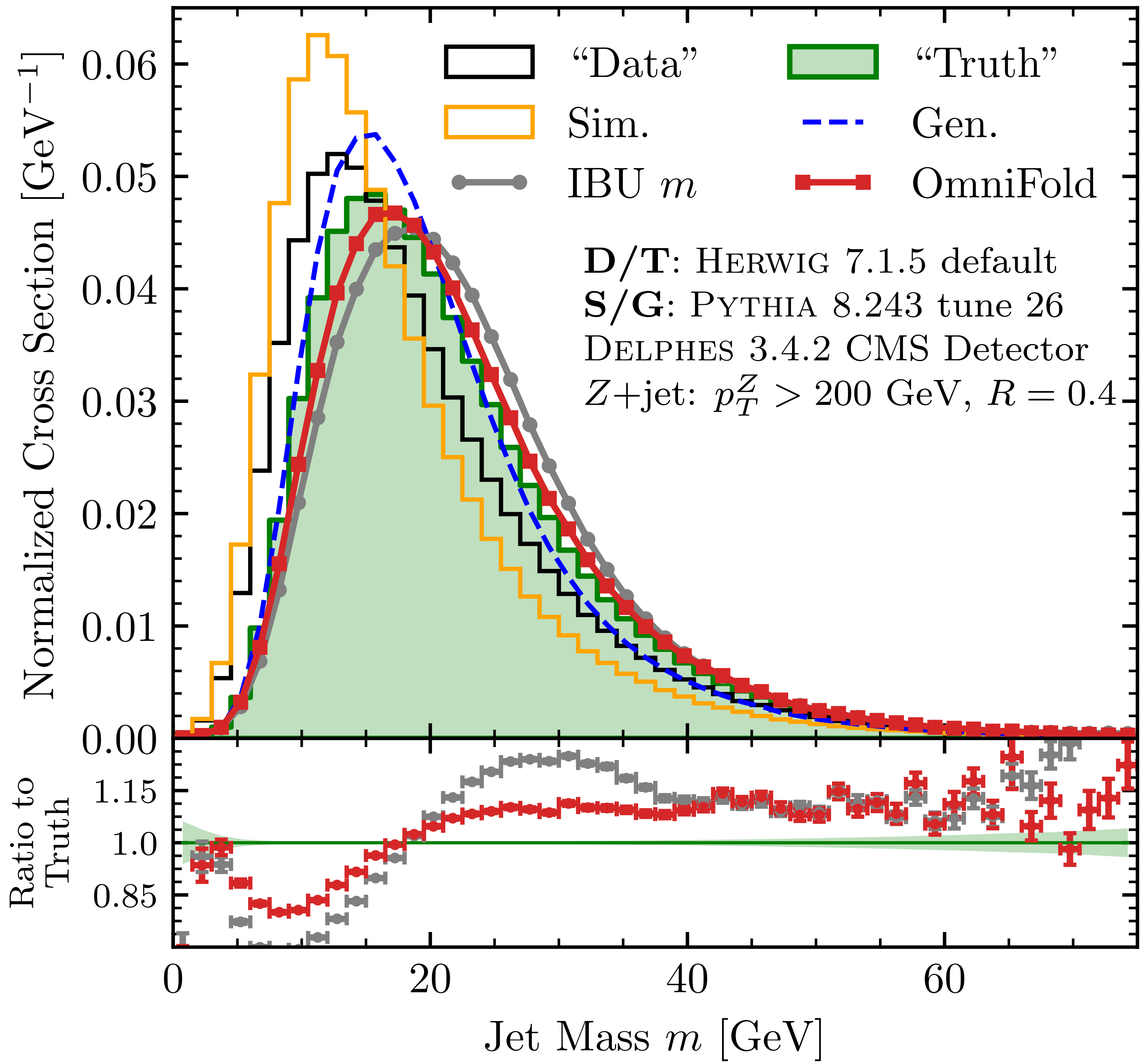
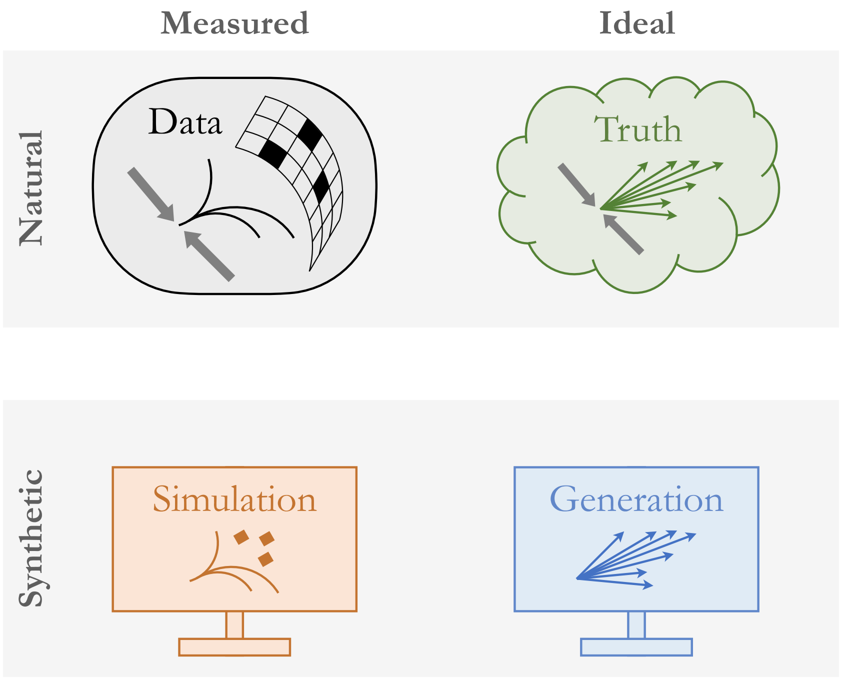


Full phase-space unfolding

A. Andreassen, P. Komiske, E. Metodiev, BPN, J. Thaler, PRL 124 (2020) 182001





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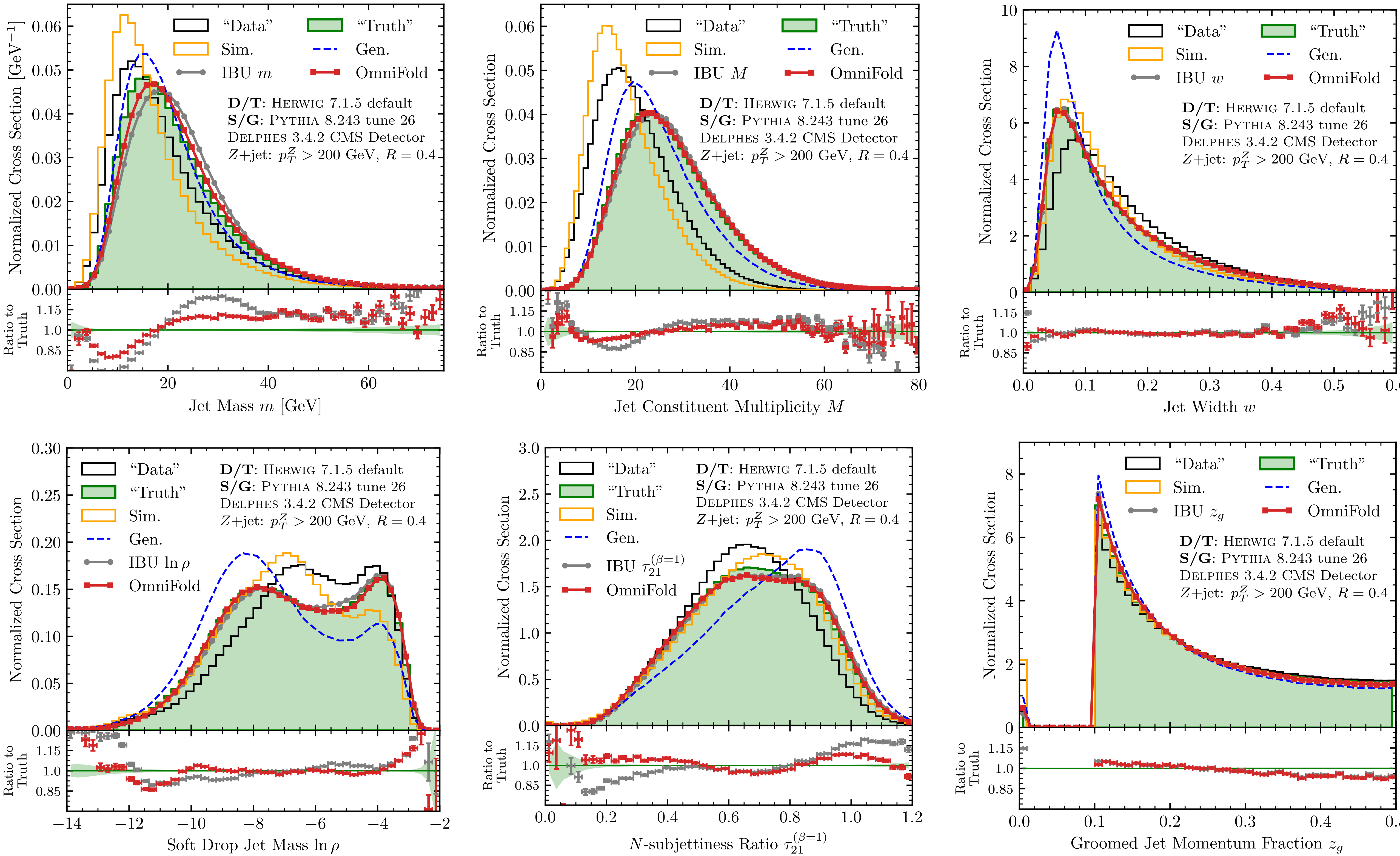


Full phase-space unfolding

We see excellent closure for the full phase space!

OmniFold is:

- *Unbinned*
- *Maximum likelihood**
- *Improves the resolution from correlations with detector response*

**when binned, OmniFold converges to Lucy-Richardson (aka Iterative Bayesian Unfolding)*

*In fact, OmniFold can also work on low-level inputs (e.g. energy flow particles). In that case, you can construct observables **after** the measurement.*

→Physics details in Miguel's talk

Some technical details

Please ask if you are interested, but briefly, OmniFold…

- Can accommodate backgrounds (unbinned) via neural positive reweighing
- Can accommodate acceptance effects
- Has a number of choices for how to update weights and/or keep track of acceptance effects

https://github.com/hep-lbdl/OmniFold

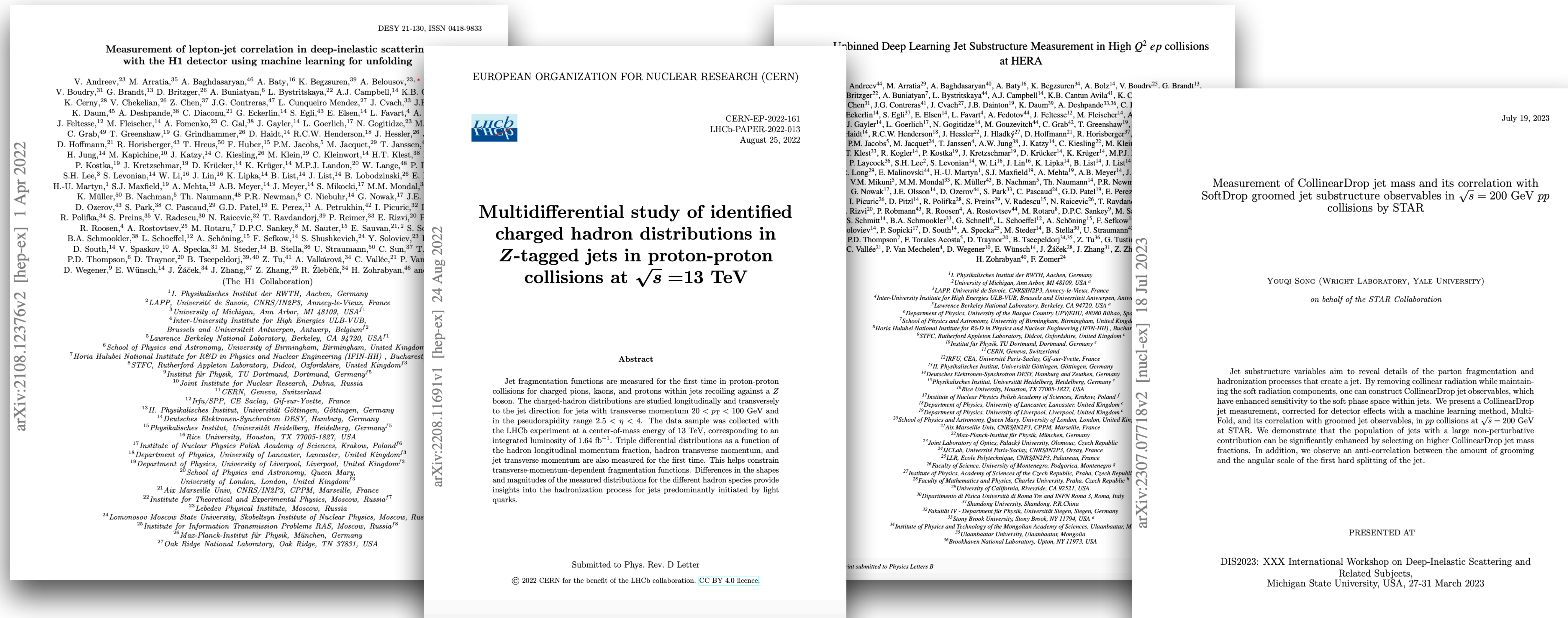
See A. Andreassen et al., ICLR SimDL for details [https://simdl.github.io/files/12.pdf]

First Results

I'll now spend a ~1 minute flashing the first unbinned measurement results

There is no time to give the physics content justice, so I'll be brief, but please let me know if you have any questions!

Results from H1, LHCb, STAR, …



+CMS open data study

Future + challenges

So far, OmniFold seems to work as designed!
Exciting to see where this will take us.

There are still some challenges we need to overcome:

- OmniFold is computationally expensive (need to train many networks, especially with ensembling to reach precision)
- How to publish an unbinned result? (all results so far are presented as binned) - see 2109.13243. Breaks HEPData!
- Modeling/closure uncertainties in high dimensions (not a new problem, but perhaps more acute)
- What about profiling? See 2302.05390 for a partial solution.

ATLAS Analysis

ATLAS Paper Draft
STDM-2020-17

Supporting internal notes

Support note: https://cds.cern.ch/record/2758374

A simultaneous unbinned differential cross section measurement of twenty-four Z+jets kinematic observables with the ATLAS detector

Z boson events at the Large Hadron Collider can be selected with high purity and are sensitive to a diverse range of QCD phenomena. As a result, these events are often used to probe the nature of the strong force, improve Monte Carlo event generators, and search for deviations from Standard Model predictions. All previous measurements of Z boson production characterize the event properties using a small number of observables and present the results as differential cross sections in predetermined bins. In this analysis, a machine learning method called OmniFold is used to produce a simultaneous measurement of twenty-four Z+jets observables using $139\ \text{fb}^{-1}$ of proton-proton collisions at $\sqrt{s} = 13$ TeV collected with the ATLAS detector. Unlike any previous fiducial differential cross-section measurement, this result is presented unbinned as a dataset of particle-level events, allowing for flexible re-use in a variety of contexts and for new observables to be constructed from the twenty-four measured observables.

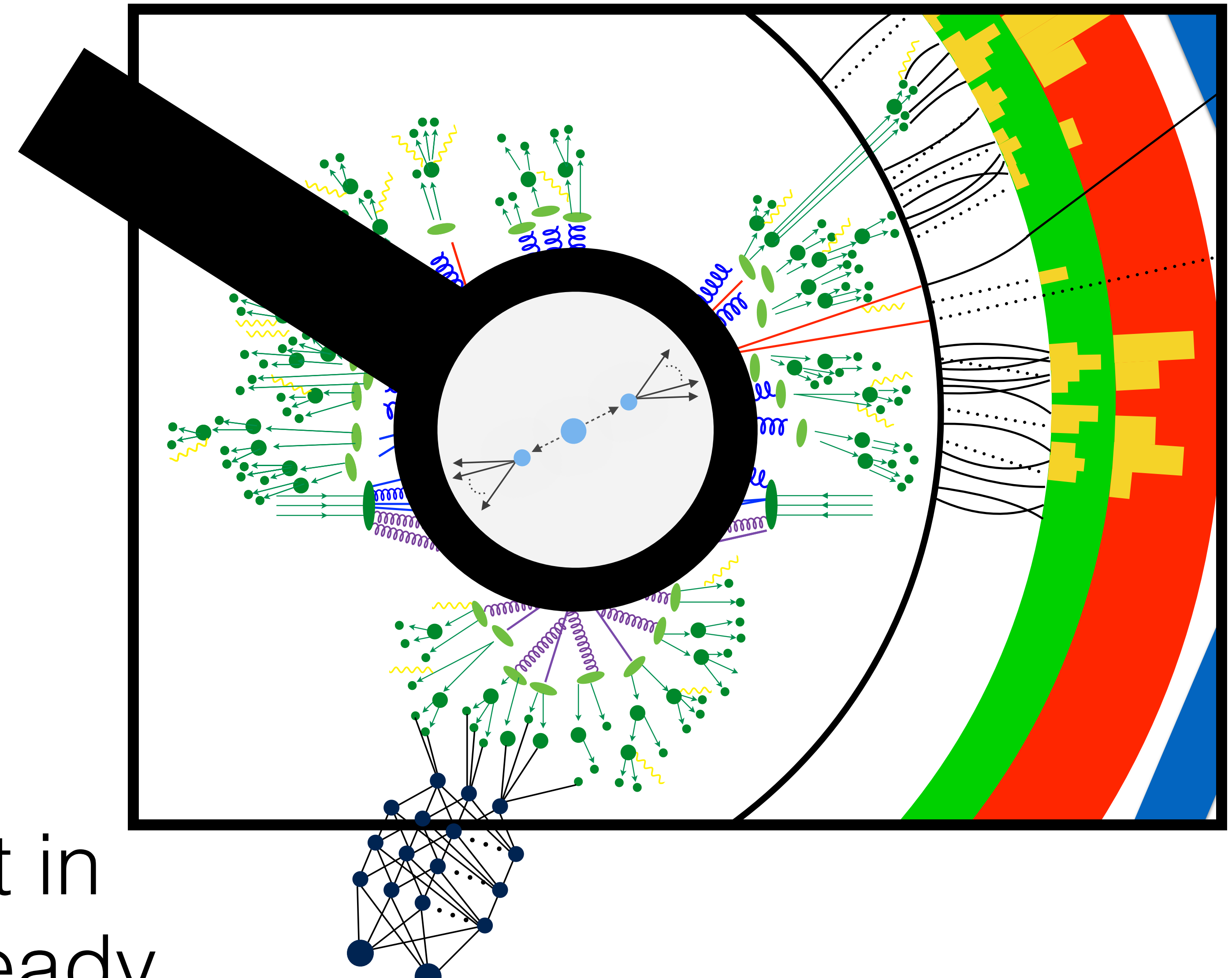
Document created on May 29, 2024 using ATLAS LaTeX Version 15.3.0.

+Jupyter Notebooks
+Data

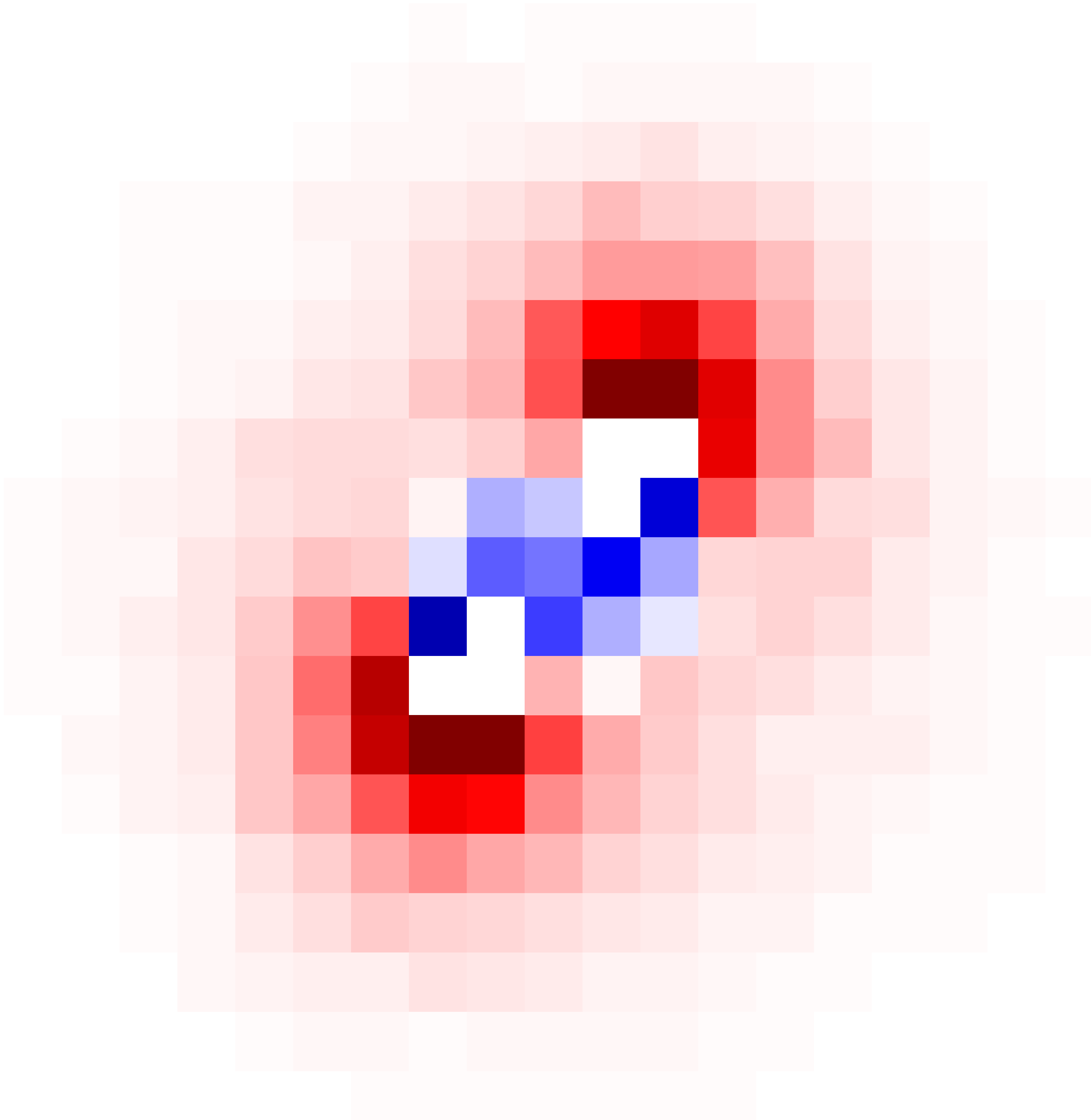
Conclusions and Outlook

A **new measurement paradigm** is possible, enabled by ML-based unfolding methods

We can analyze our data **holistically** and **future-proof** it using unbinned techniques



More R&D is required, but in parallel, these tools are already starting to **deliver science results**!



Fin.