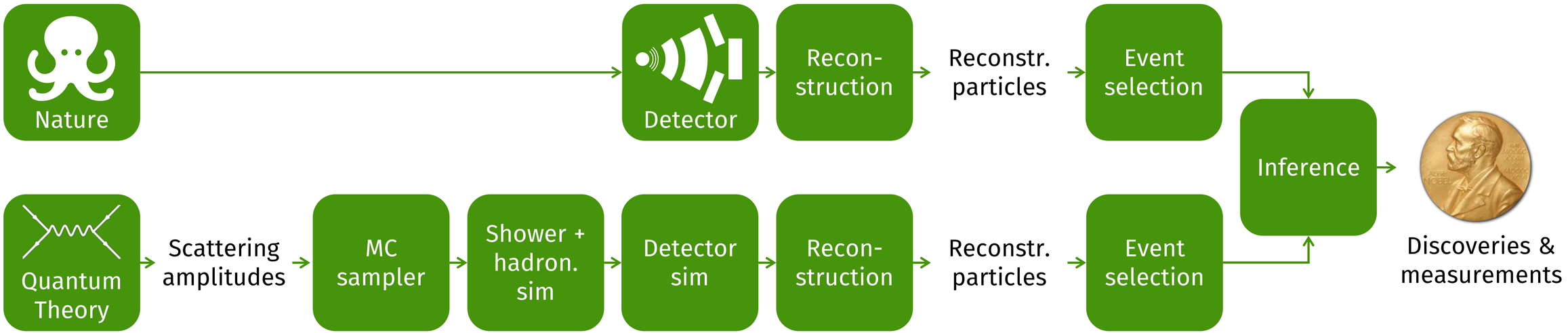
L-GATr

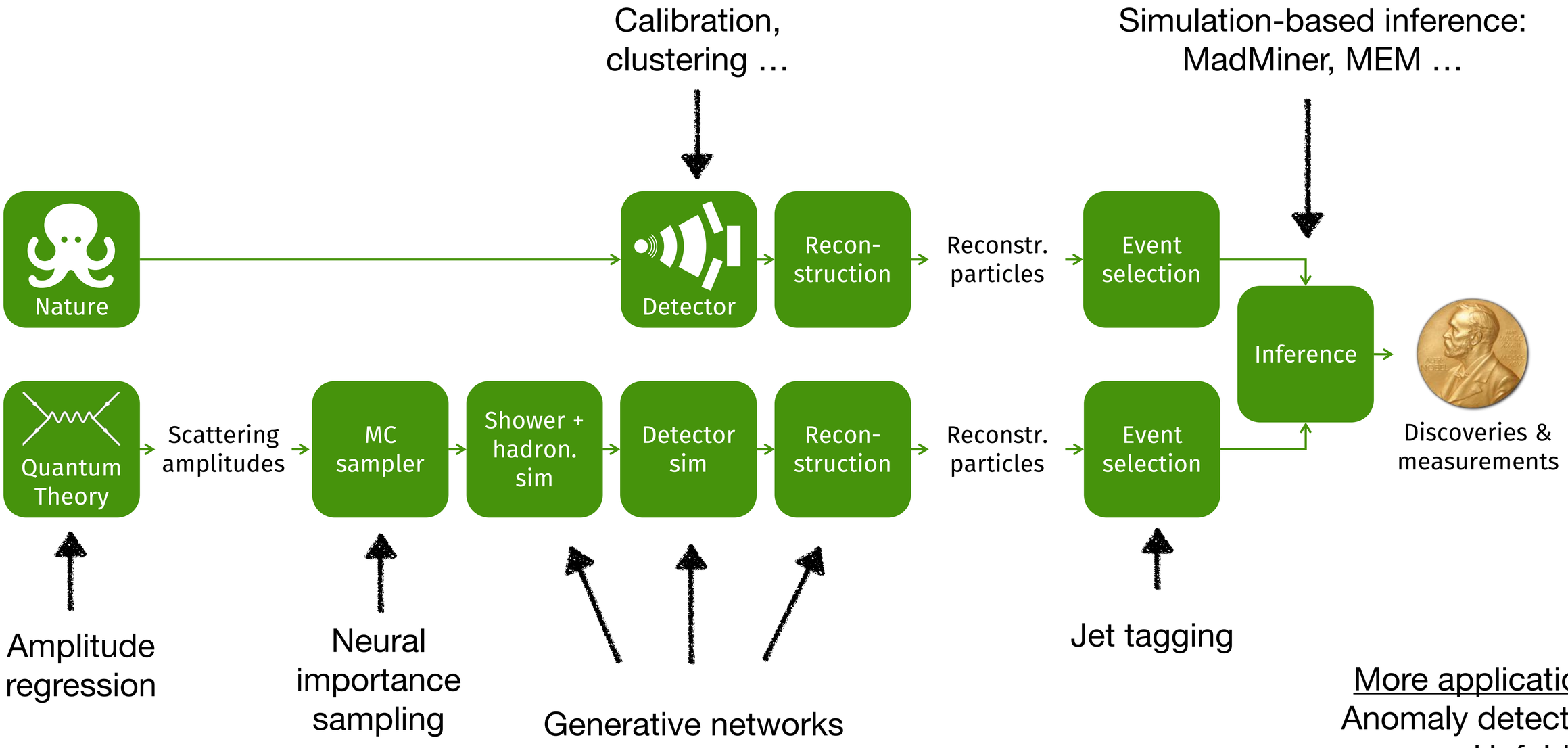
Jet Tagging with Lorentz-Equivariant Geometric Algebra Transformers

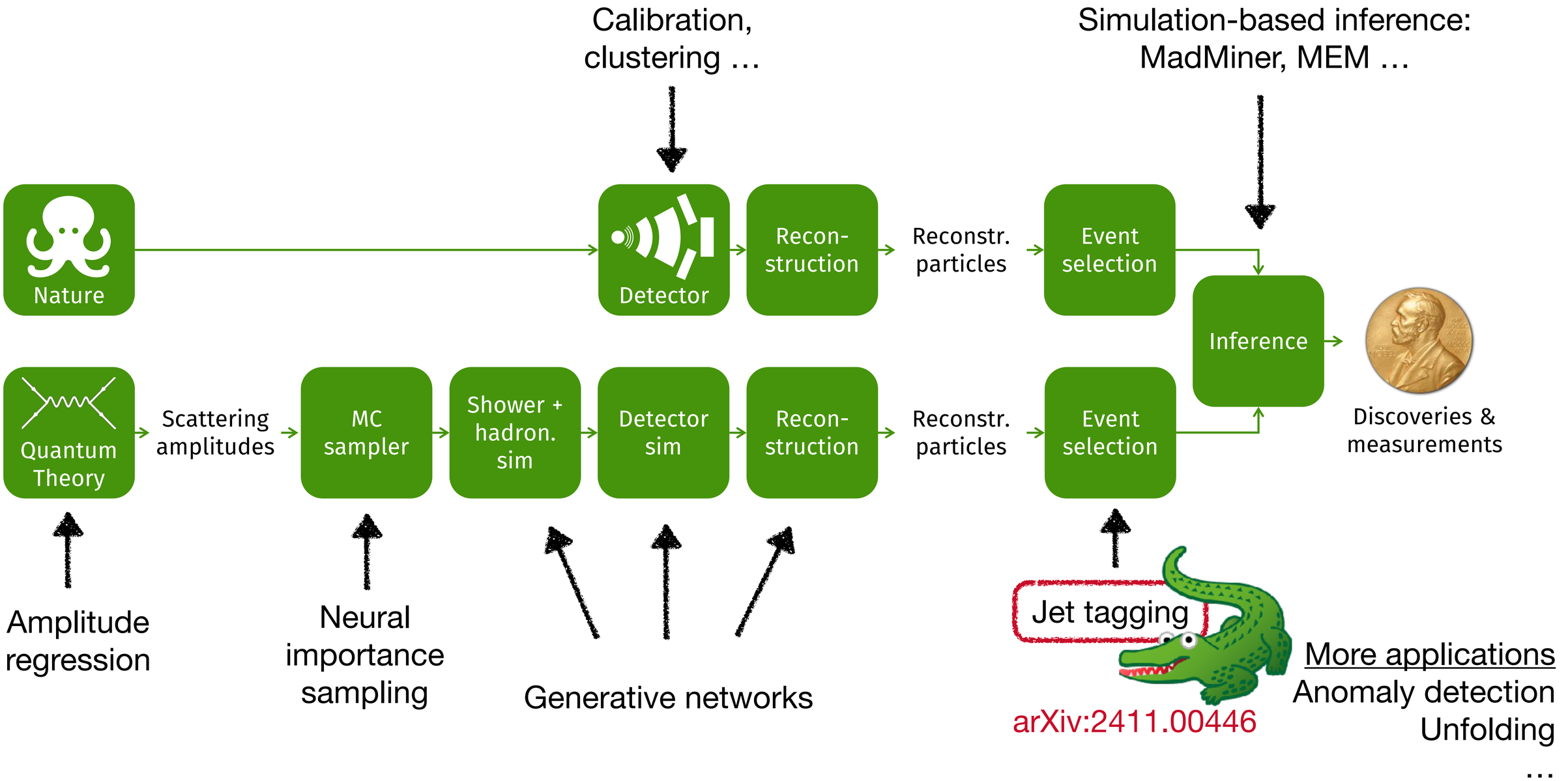
Johann Brehmer, Víctor Bresó,
Pim de Haan, Tilman Plehn, Huilin Qu,
Jonas Spinner, Jesse Thaler

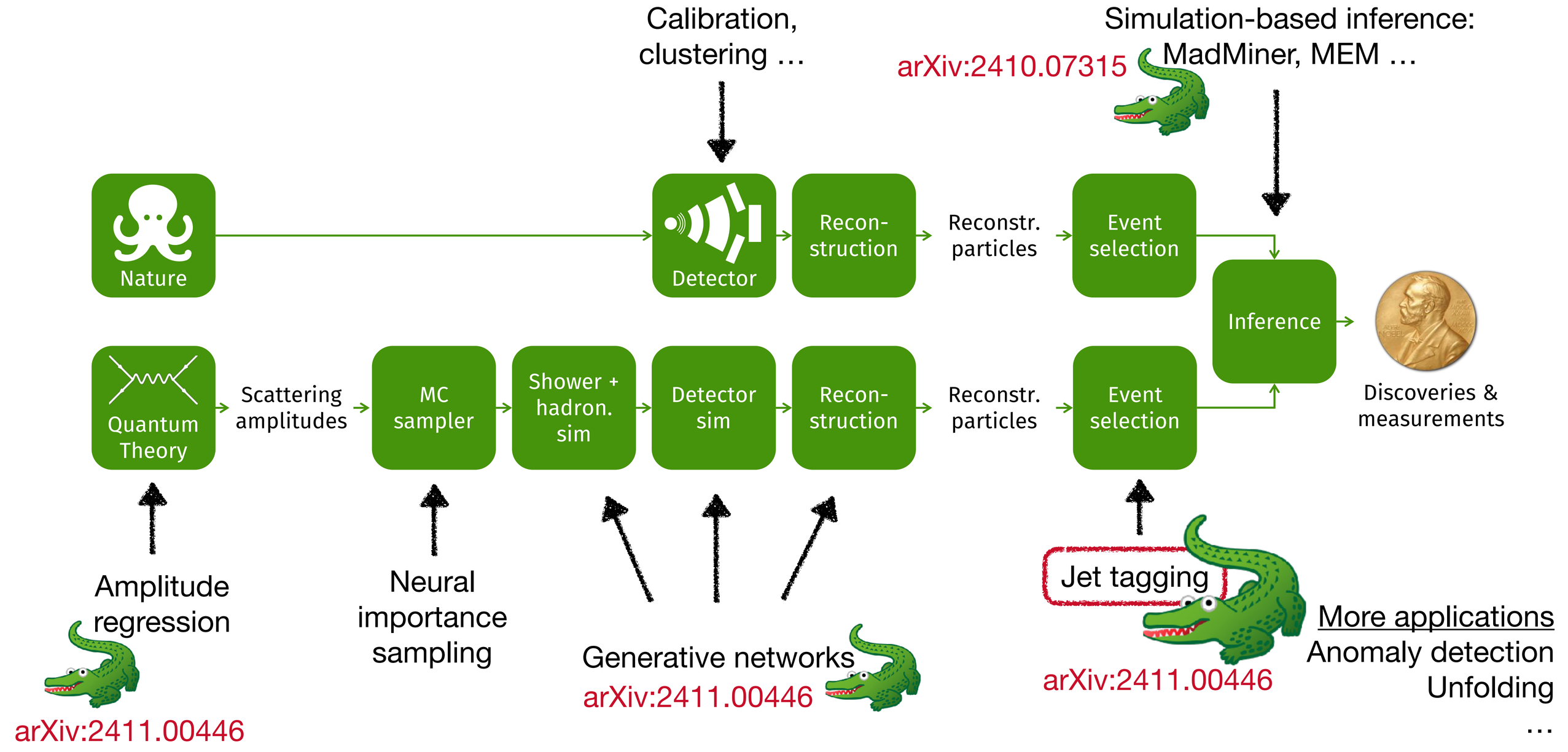
arXiv:2405.14806, arXiv:2411.00446

UNIVERSITÄT
HEIDELBERG
ZUKUNFT
SEIT 1386


Nature
Detector
Recon-
struction
Reconstr.
particles
Event
selection
Inference
Discoveries &
measurements
Quantum
Theory
Scattering
amplitudes
MC
sampler
Shower +
hadron.
sim
Detector
sim
Recon-
struction
Reconstr.
particles
Event
selection


Calibration, clustering …
Simulation-based inference: MadMiner, MEM …
Nature
Detector
Recon-struction
Reconstr. particles
Event selection
Inference
Discoveries & measurements
Quantum Theory
Scattering amplitudes
MC sampler
Shower + hadron. sim
Detector sim
Recon-struction
Reconstr. particles
Event selection
Amplitude regression
Neural importance sampling
Generative networks
Jet tagging
More applications
Anomaly detection
Unfolding
…


Calibration,
clustering …
Simulation-based inference:
MadMiner, MEM …
Nature
Detector
Recon-
struction
Reconstr.
particles
Event
selection
Inference
Discoveries &
measurements
Quantum
Theory
Scattering
amplitudes
MC
sampler
Shower +
hadron.
sim
Detector
sim
Recon-
struction
Reconstr.
particles
Event
selection
Amplitude
regression
Neural
importance
sampling
Generative networks
Jet tagging
arXiv:2411.00446
More applications
Anomaly detection
Unfolding
…


Calibration, clustering …
Simulation-based inference: MadMiner, MEM …
arXiv:2410.07315
Nature
Detector
Recon-struction
Reconstr. particles
Event selection
Inference
Discoveries & measurements
Quantum Theory
Scattering amplitudes
MC sampler
Shower + hadron. sim
Detector sim
Recon-struction
Reconstr. particles
Event selection
Amplitude regression
Neural importance sampling
Generative networks
arXiv:2411.00446
Jet tagging
arXiv:2411.00446
More applications
Anomaly detection
Unfolding
…
arXiv:2411.00446

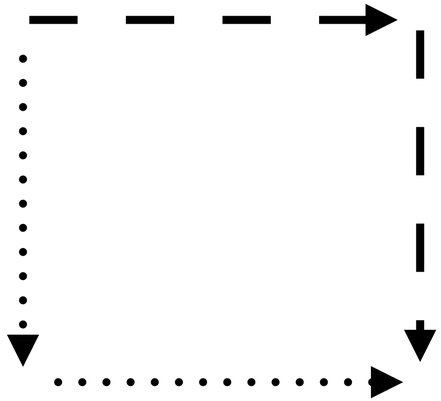
Lorentz-Equivariant
Geometric **A**lgebra
Transformer

=

$$\begin{pmatrix} 1 \\ \gamma^\mu \\ \sigma^{\mu\nu} \\ \gamma^\mu\gamma_5 \\ \gamma_5 \end{pmatrix}$$

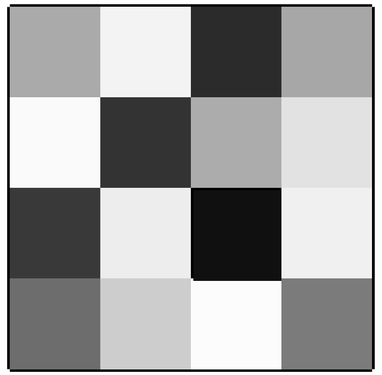
Geometric algebra
representations

+



Lorentz-Equivariant
layers

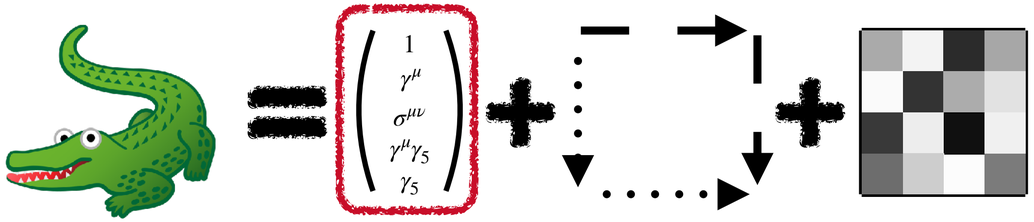
+



Transformer
architecture

GATr was originally
developed for E(3)
arXiv:2305.18415

L-GATr

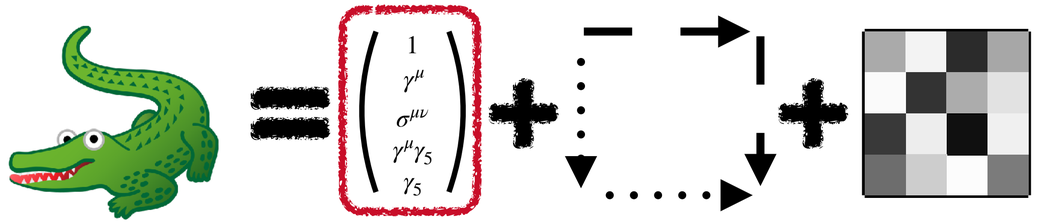


Geometric algebra = Clifford algebra

Geometric algebra = Vector space + geometric product $xy = \frac{\{x, y\}}{2} + \frac{[x, y]}{2}$

- Symmetric part $\{x, y\}$: scalar/inner product
- Antisymmetric part $[x, y]$: outer product (yields higher-order objects)

L-GATr



Geometric algebra = Clifford algebra

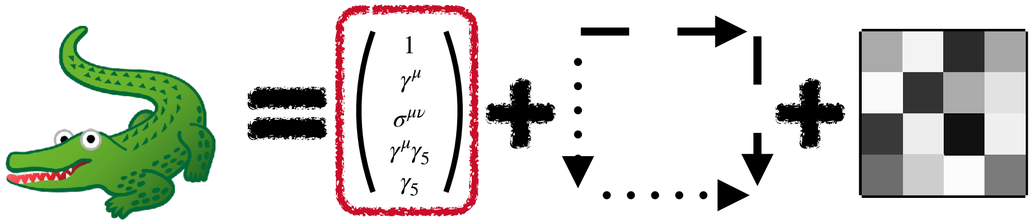
Geometric algebra = Vector space + geometric product $xy = \frac{\{x, y\}}{2} + \frac{[x, y]}{2}$

- Symmetric part $\{x, y\}$: scalar/inner product
- Antisymmetric part $[x, y]$: outer product (yields higher-order objects)

Spacetime geometric algebra: Geometric algebra over vector space $\mathbb{R}^4$ with Minkowski metric $g = \mathrm{diag}(1, -1, -1, -1)$

- Basis elements γ^μ are orthonormal: $\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$
- Dirac algebra is the same up to $\mathbb{R} \to \mathbb{C}$

L-GATr



Building multivectors

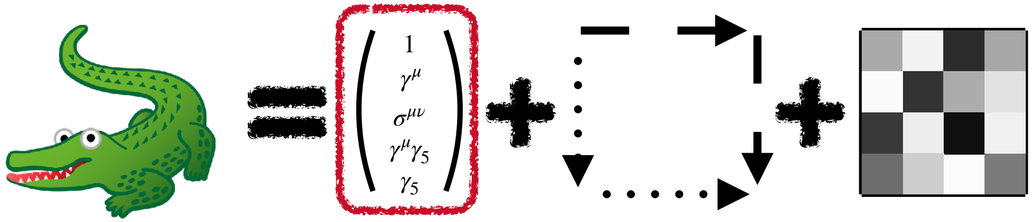
- Scalar and vectors $1,\ \gamma^\mu$ (1+4 objects)
- Product of two vectors: $\gamma^\mu\gamma^\nu = \frac{\{\gamma^\mu,\gamma^\nu\}}{2} + \frac{[\gamma^\mu,\gamma^\nu]}{2} = g^{\mu\nu} + \sigma^{\mu\nu}$ (6 new objects)
- Axial vector: $\epsilon_{\mu\nu\rho\sigma}\gamma^\nu\gamma^\rho\gamma^\sigma \propto \gamma_\mu\gamma^5$ (4 new objects)
- Pseudoscalar: $\gamma^5 = \gamma^0\gamma^1\gamma^2\gamma^3 = \frac{1}{4!}\epsilon_{\mu\nu\rho\sigma}\gamma^\mu\gamma^\nu\gamma^\rho\gamma^\sigma$ (1 new object)

Multivector: $x = x^S 1 + x^V_\mu\gamma^\mu + x^B_{\mu\nu}\sigma^{\mu\nu} + x^A_\mu\gamma^\mu\gamma^5 + x^P\gamma^5$ with $(x^S, x^V_\mu, x^B_{\mu\nu}, x^A_\mu, x^P) \in \mathbb{R}^{16}$

Particle: $x^V = (E, p_x, p_y, p_z), \quad x^S = \text{PID}$

L-GATr

Geometric algebra representations



$$x^S \in \mathbb{R}$$

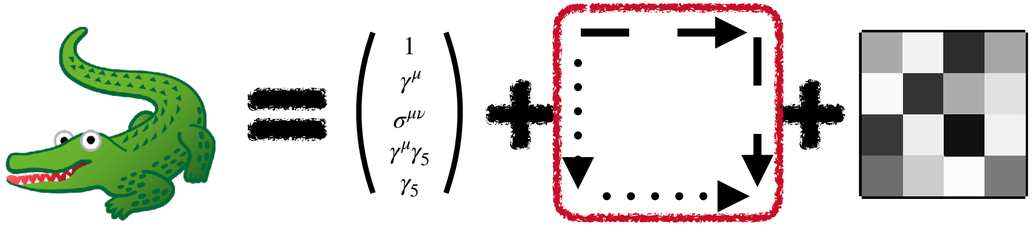
$$\begin{pmatrix} x^S \\ x^V_\mu \\ x^B_{\mu\nu} \\ x^A_\mu \\ x^P \end{pmatrix} \in \mathbb{R}^{16}$$

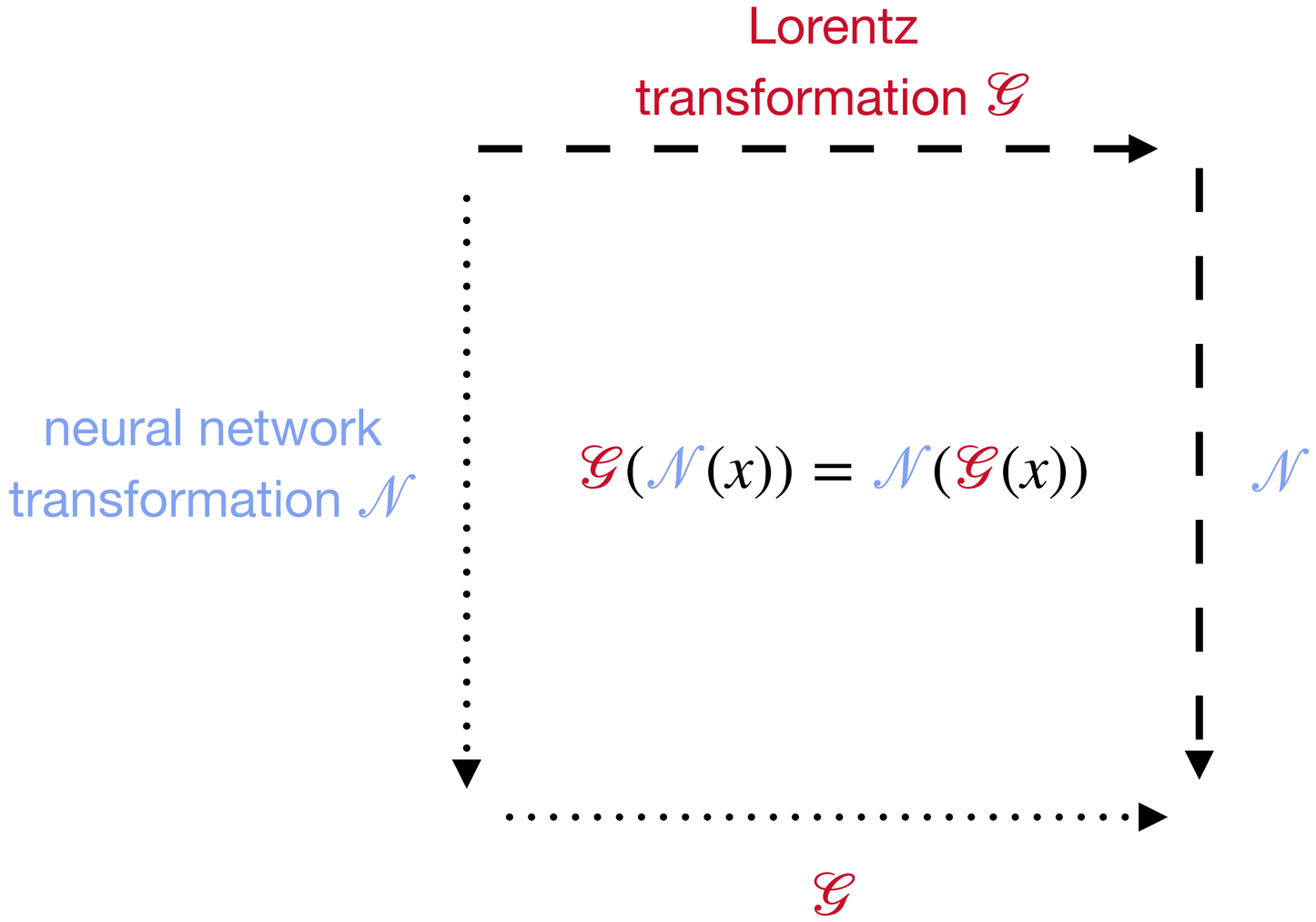
scalar channels

multivector channels

L-GATr

Lorentz Equivariance

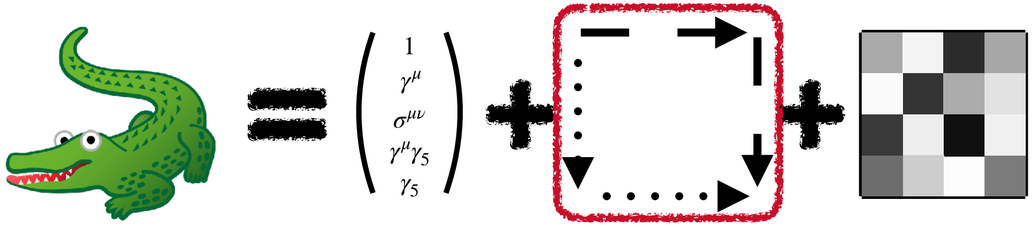




Equivariance = Covariance

L-GATr

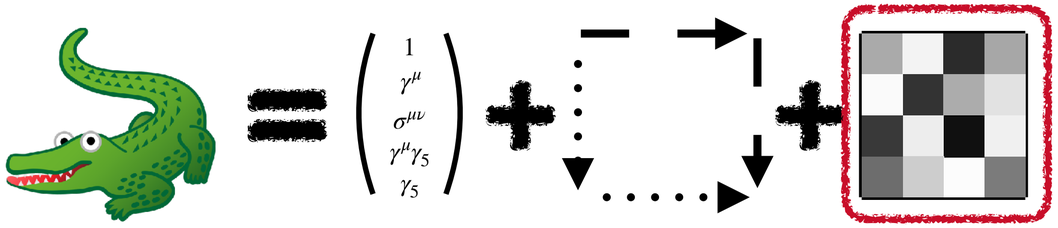
GATr-ing all transformer layers

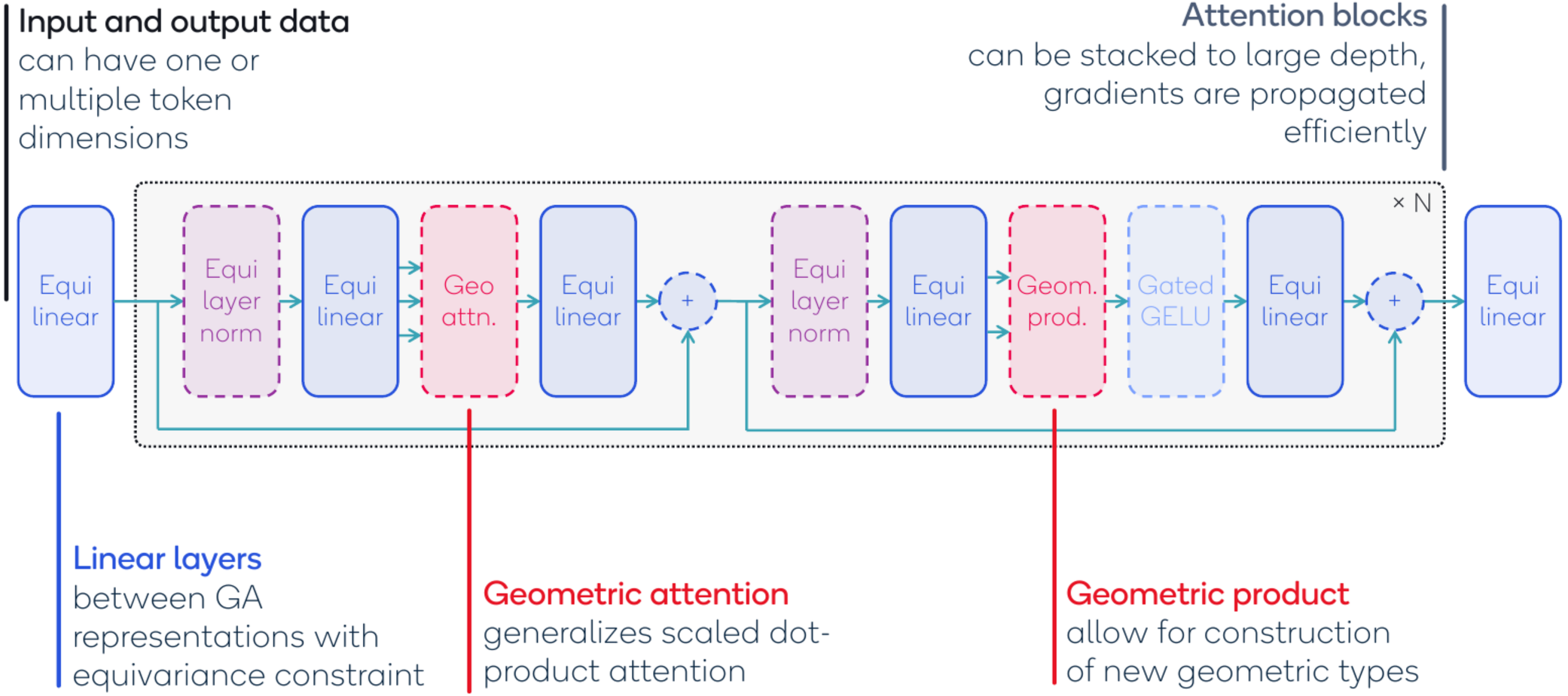


Layer type	Transformer	L-GATr
Linear(x)	$vx + w$	$\sum_{k=0}^{4} v_k \langle x \rangle_k \left(+ \sum_{k=0}^{4} w_k \gamma^5 \langle x \rangle_k \right)$
Attention$(q, k, v)_{ic}$	$\sum_{j=1}^{n_t} \mathrm{Softmax}_j \left(\sum_{c'=1}^{n_c} \frac{q_{ic'} k_{jc'}}{\sqrt{n_c}} \right) v_{jc}$	$\sum_{j=1}^{n_t} \mathrm{Softmax}_j \left(\sum_{c'=1}^{n_c} \frac{\langle q_{ic'}, k_{jc'} \rangle}{\sqrt{16 n_c}} \right) v_{jc}$
LayerNorm(x)	$x \left[\frac{1}{n_c} \sum_{c=1}^{n_c} x_c^2 + \epsilon \right]^{-1/2}$	$\mathbf{x} \left[\frac{1}{n_c} \sum_{c=1}^{n_c} \sum_{k=0}^{4} \left\lvert \left\langle \langle x_c \rangle_k, \langle x_c \rangle_k \right\rangle \right\rvert + \epsilon \right]^{-1/2}$
Activation(x)	GELU(x)	GELU$(\langle x \rangle_0) x$
GP(x, y)	—	xy

L-GATr

Full architecture

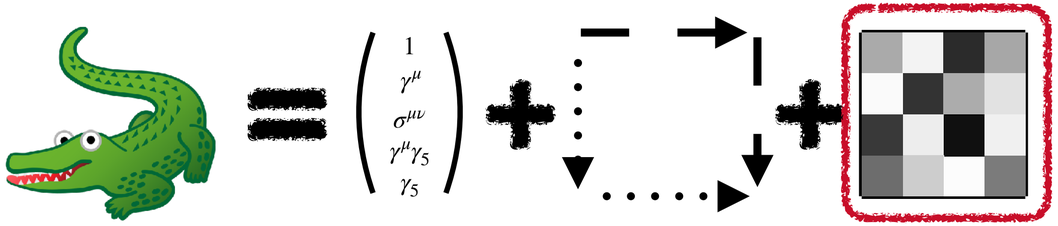


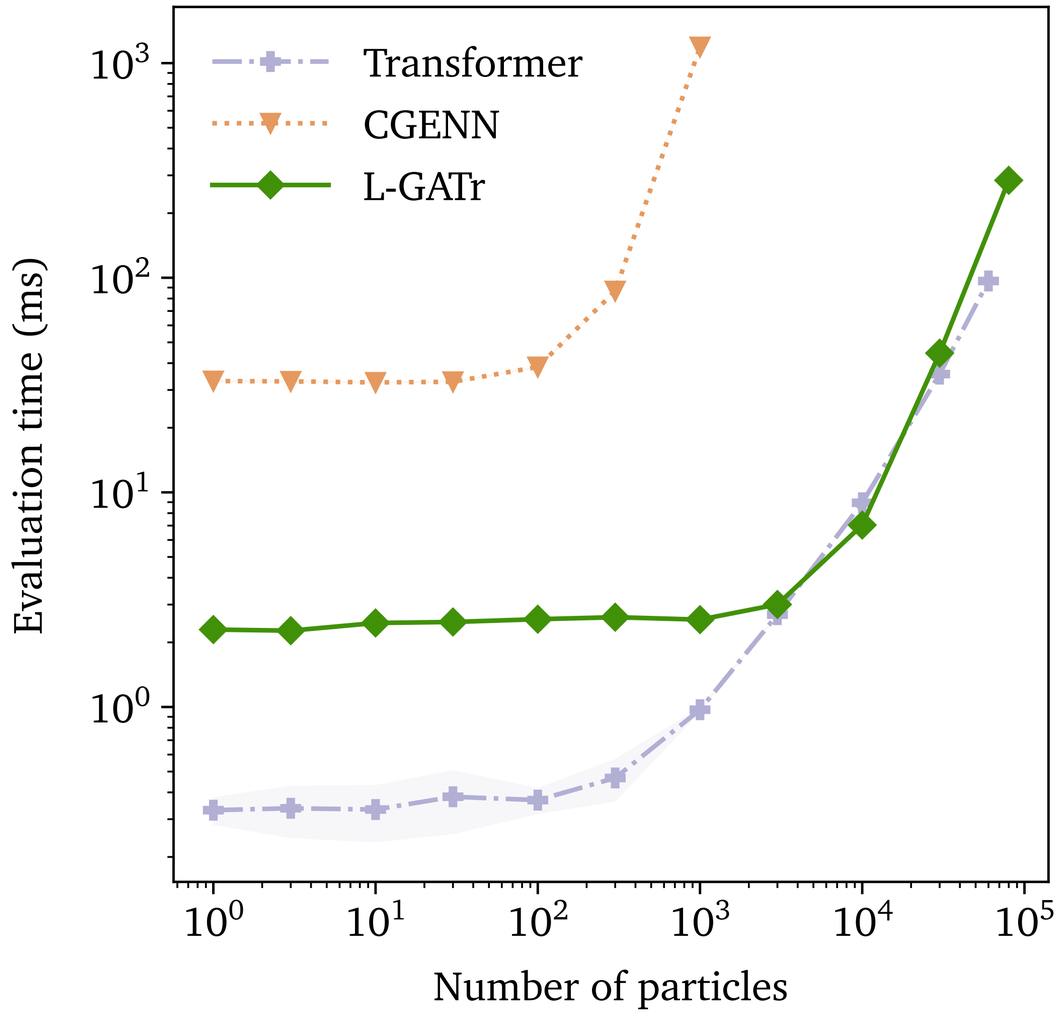


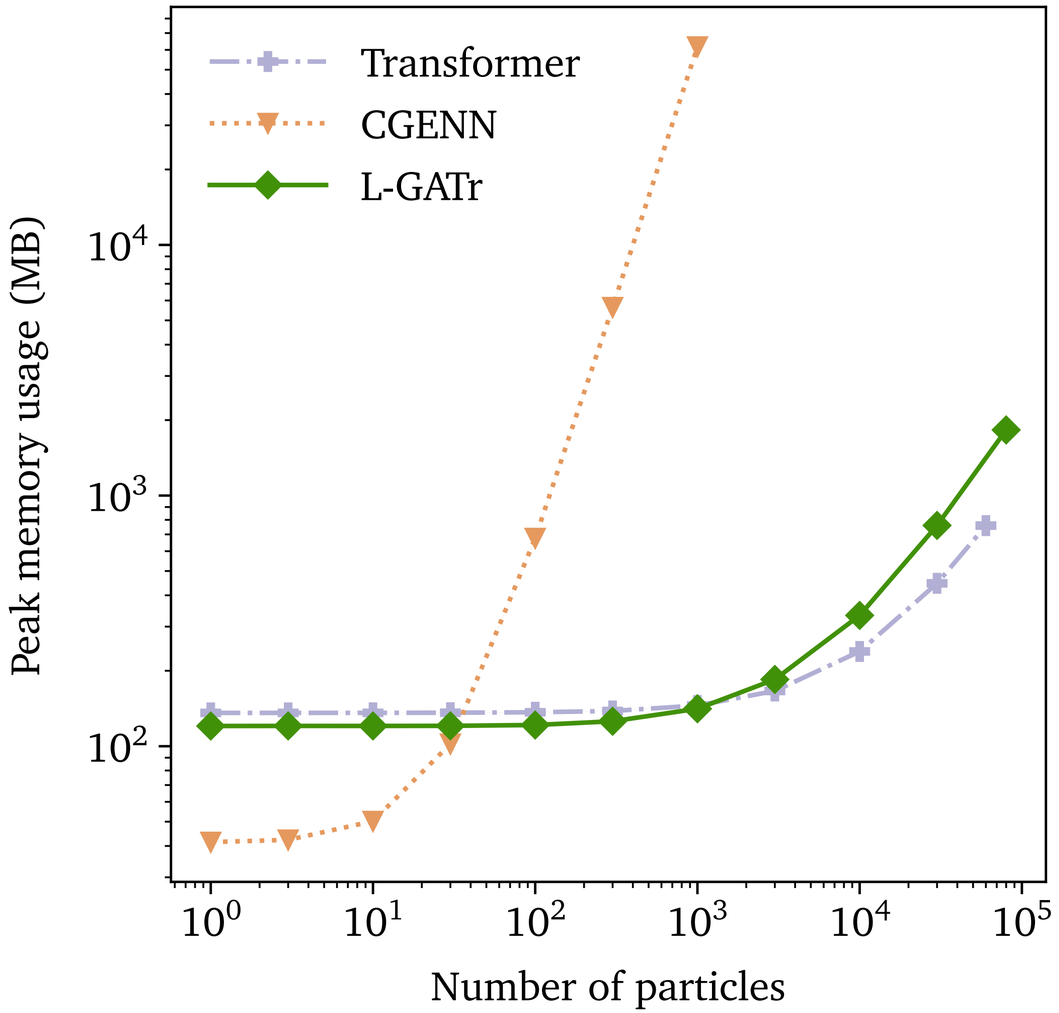
Credits to Johann Brehmer

L-GATr

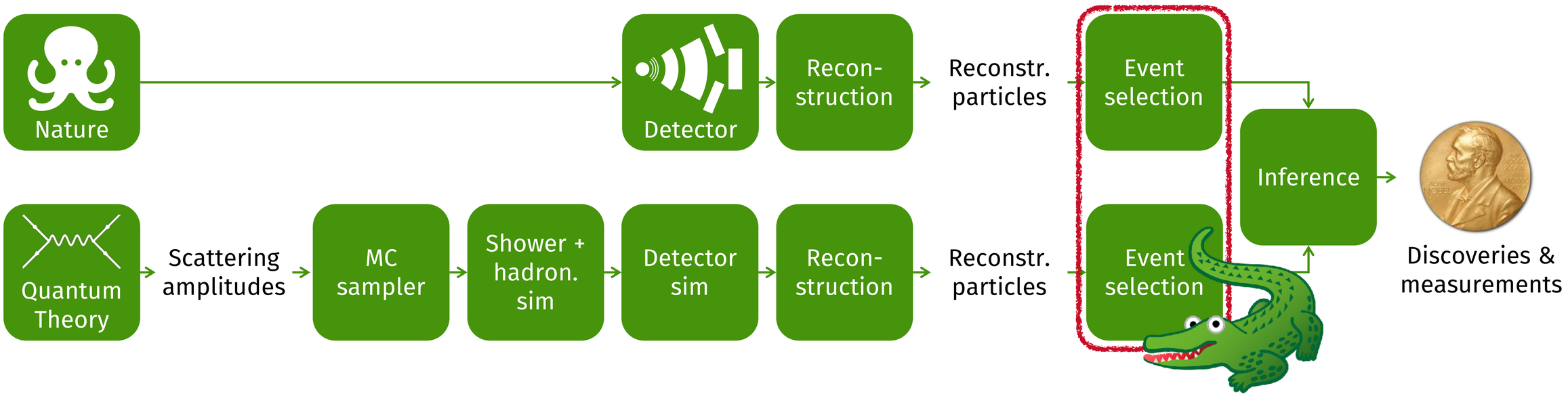
Processing thousands of particles







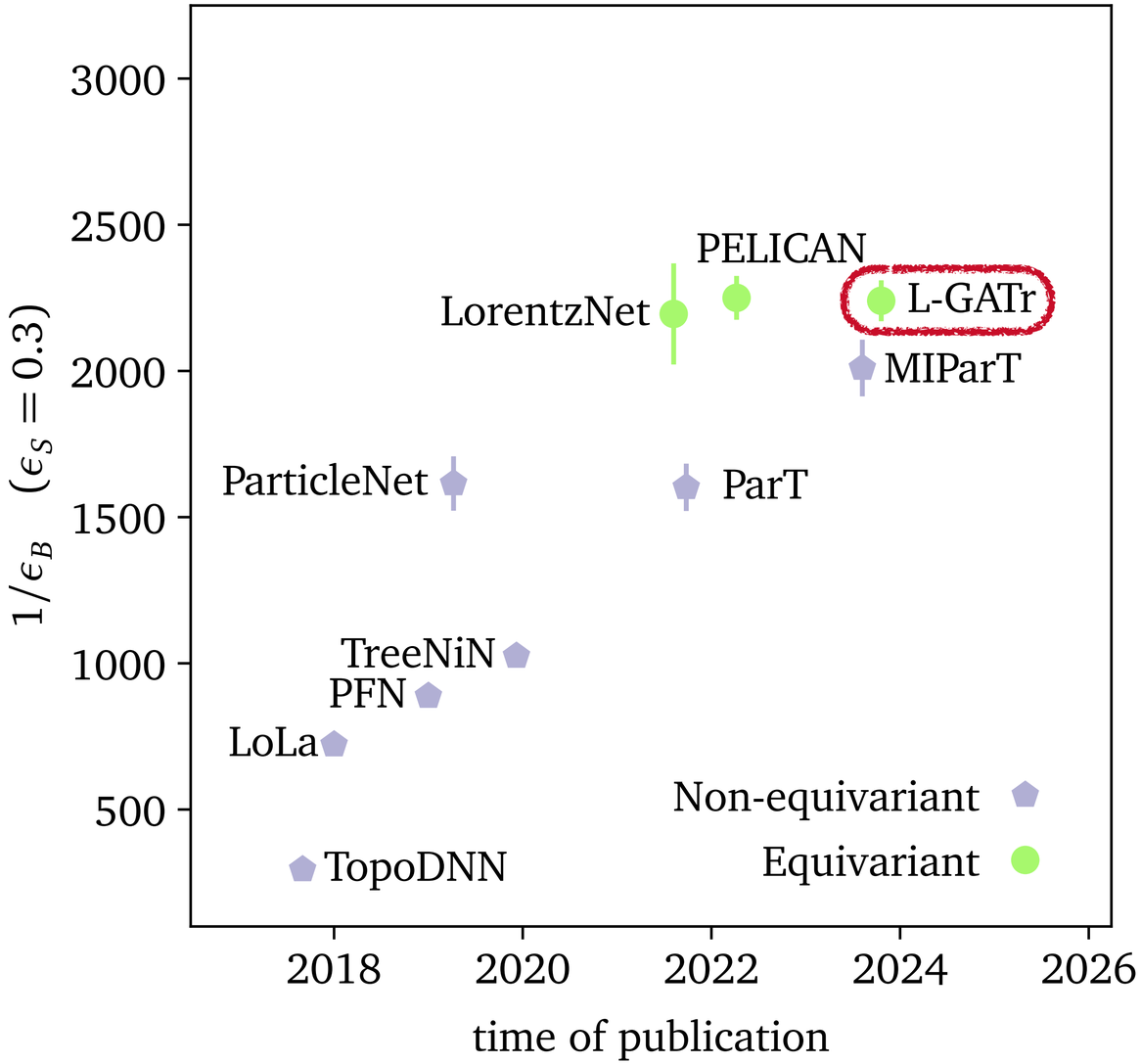
Jet Tagging with L-GATr



Jet Tagging with L-GATr

The history of top tagging

All top-performing taggers
use Lorentz symmetry



Jet Tagging with L-GATr

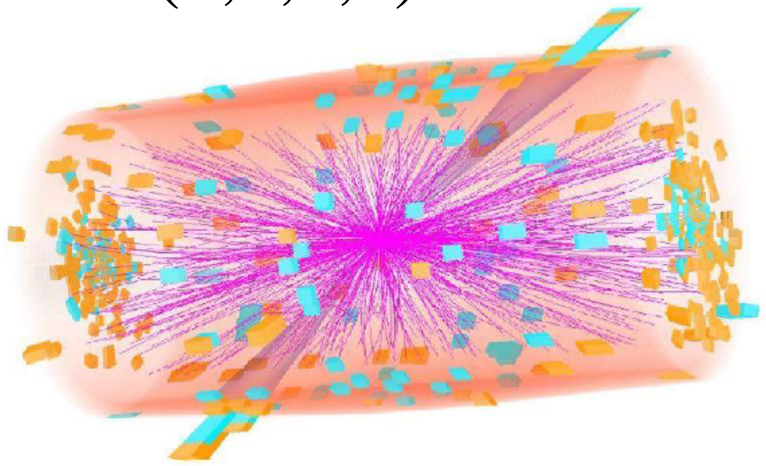
Symmetry breaking with multivectors

The jet tagging score is not Lorentz-invariant

- Beam direction breaks invariance under rotations around the x- and y-axis
- Detector breaks boost invariance

Add reference multivectors as extra particles to break Lorentz symmetry

- Beam reference multivector: $x^V = (0,0,0, \pm 1)$ or $x^B_{12} = 1$
- Time reference multivector: $x^V = (1,0,0,0)$



All Lorentz-invariant taggers use symmetry-breaking inputs

Jet Tagging with L-GATr

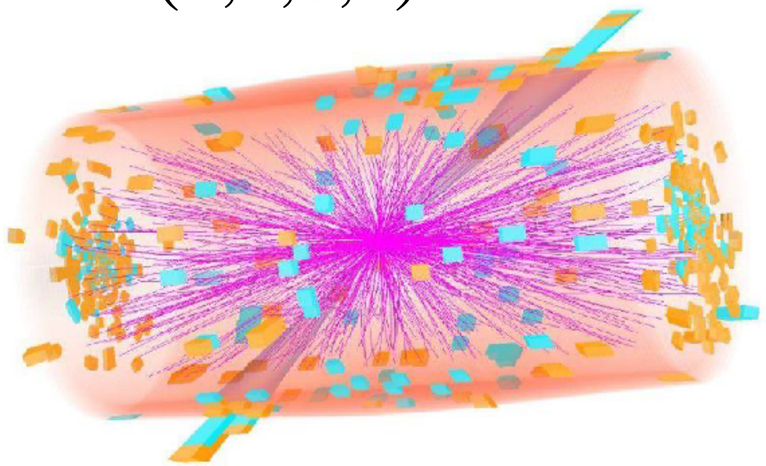
Symmetry breaking with multivectors

Beam	Time	Embedding	AUC	$1/\epsilon_B$ ($\epsilon_S = 0.3$)
–	–	Token	0.9844	1422
$x_3^V = \pm 1$	–	Token	0.9850	1905
–	$x_0^V = 1$	Token	0.9865	1923
$x_{12}^B = x_{13}^B = x_{23}^B = 1$	$x_0^V = 1$	Token	0.9863	2009
$x_{12}^B = 1$	$x_0^V = 1$	Channel	0.9865	2060
$x_0^V = 1, x_3^V = \pm 1$	$x_0^V = 1$	Token	0.9869	2114
$x_3^V = \pm 1$	$x_0^V = 1$	Token	0.9869	2152
$x_{12}^B = 1$	$x_0^V = 1$	Token	0.9870	2240

Several choices give
essentially the same performance

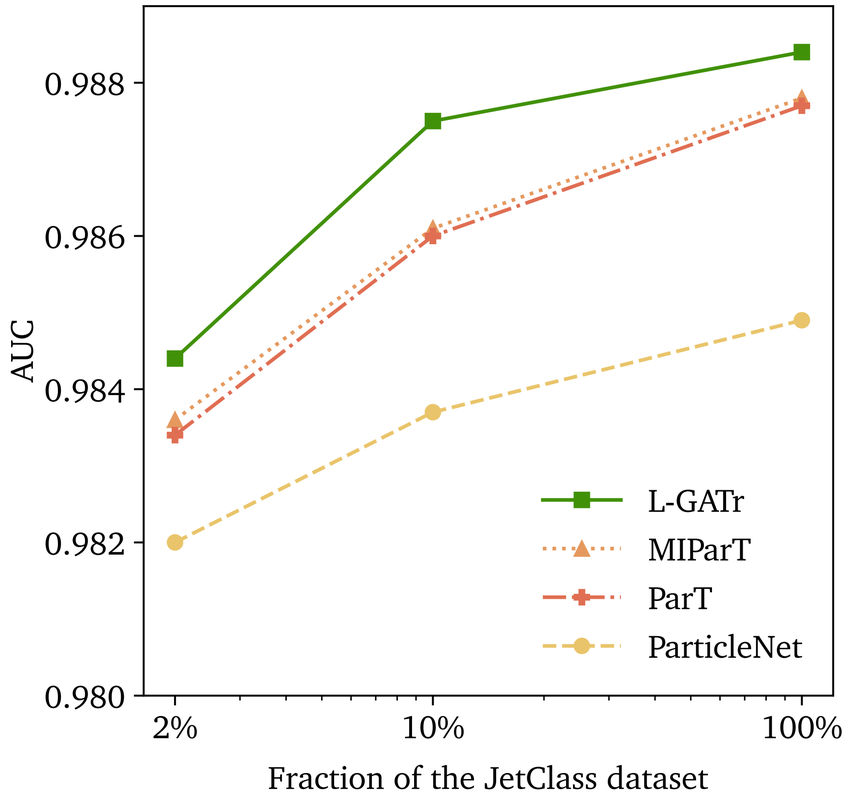
Add reference multivectors as extra particles to break Lorentz symmetry

- Beam reference multivector:
  $x^V = (0,0,0, \pm 1)$ or $x_{12}^B = 1$
- Time reference multivector:
  $x^V = (1,0,0,0)$



Jet Tagging with L-GATr

Training on 100M jets

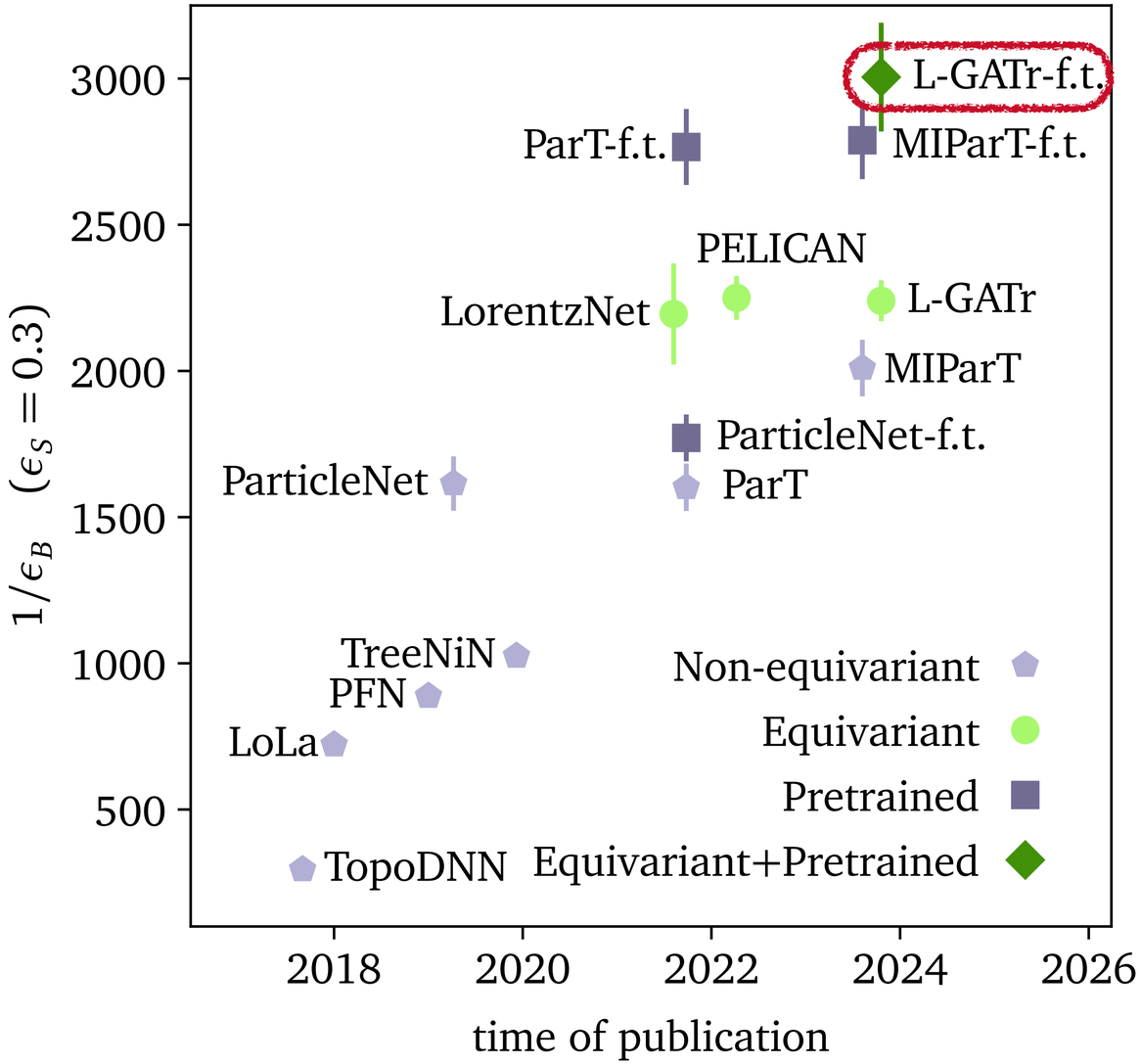


Transformers significantly outperform graph networks

	All classes		$H \to b\bar{b}$	$H \to c\bar{c}$	$H \to gg$	$H \to 4q$	$H \to l\nu q\bar{q}'$	$t \to bq\bar{q}'$	$t \to bl\nu$	$W \to q\bar{q}'$	$Z \to q\bar{q}$
	Accuracy	AUC	$\text{Rej}_{50\%}$	$\text{Rej}_{50\%}$	$\text{Rej}_{50\%}$	$\text{Rej}_{50\%}$	$\text{Rej}_{99\%}$	$\text{Rej}_{50\%}$	$\text{Rej}_{99.5\%}$	$\text{Rej}_{50\%}$	$\text{Rej}_{50\%}$
ParticleNet [58]	0.844	0.9849	7634	2475	104	954	3339	10526	11173	347	283
ParT [59]	0.861	0.9877	10638	4149	123	1864	5479	32787	15873	543	402
MIParT [60]	0.861	0.9878	10753	4202	123	1927	5450	31250	16807	542	402
L-GATr	0.865	0.9884	12195	4819	128	2304	5764	37736	19231	580	427

Jet Tagging with L-GATr

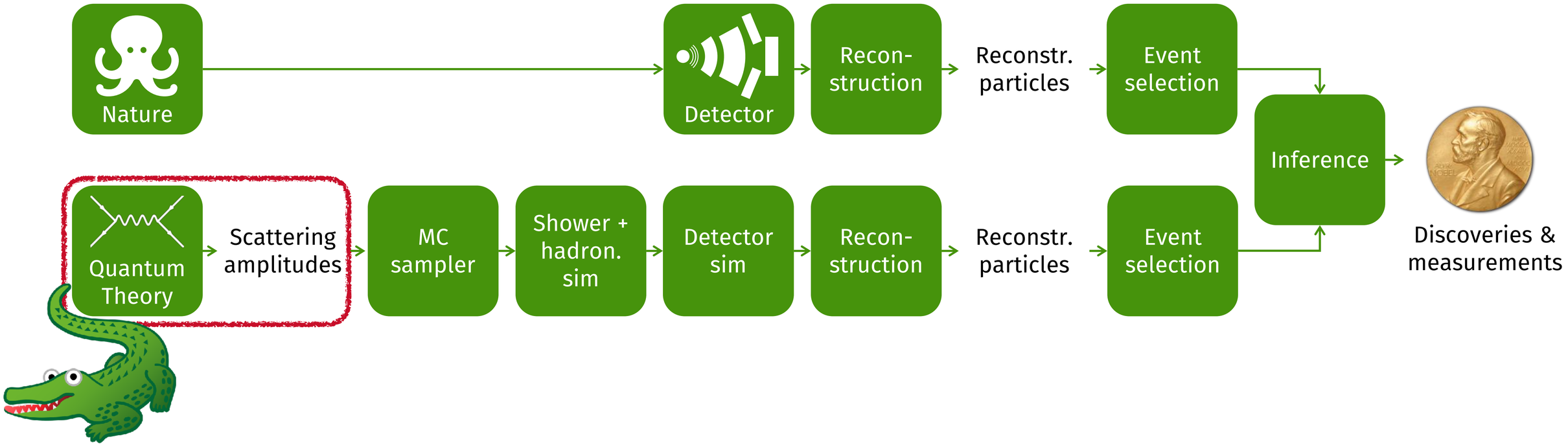
Transfer learning for top tagging



L-GATr combines benefits from pretraining and Lorentz equivariance

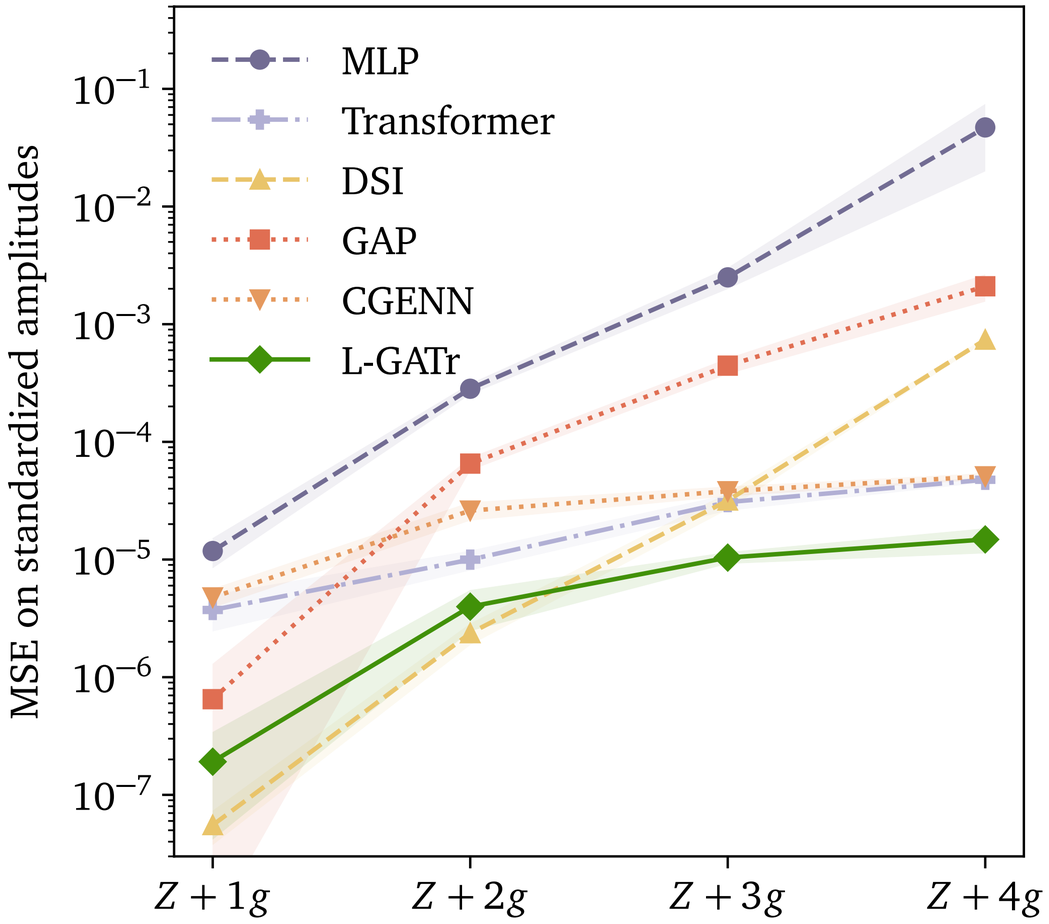
L-GATr beyond jet tagging

QFT amplitude regression



L-GATr beyond jet tagging

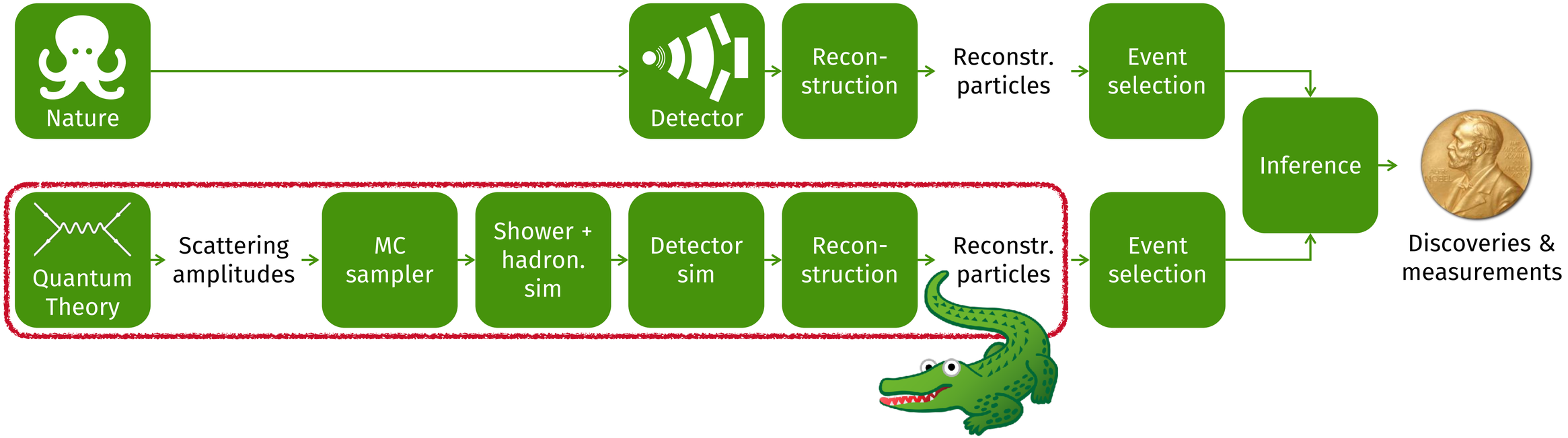
QFT amplitude regression



The combination Lorentz-equivariance + permutation-equivariant Transformer scales best to high multiplicity

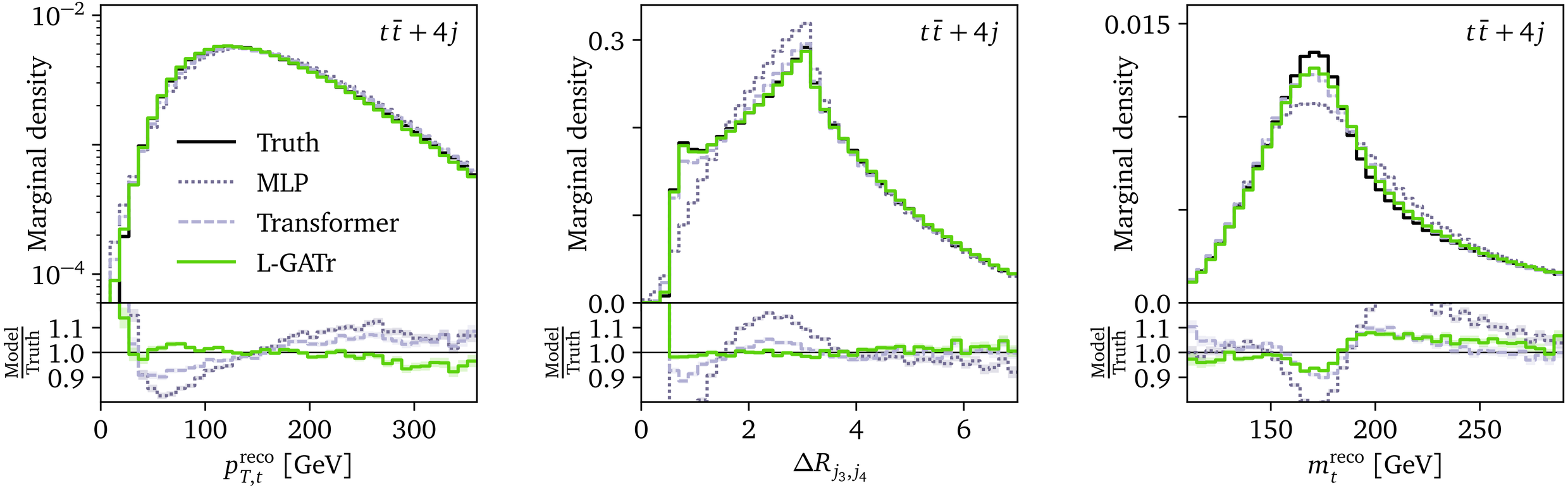
L-GATr beyond jet tagging

LHC event generation



L-GATr beyond jet tagging

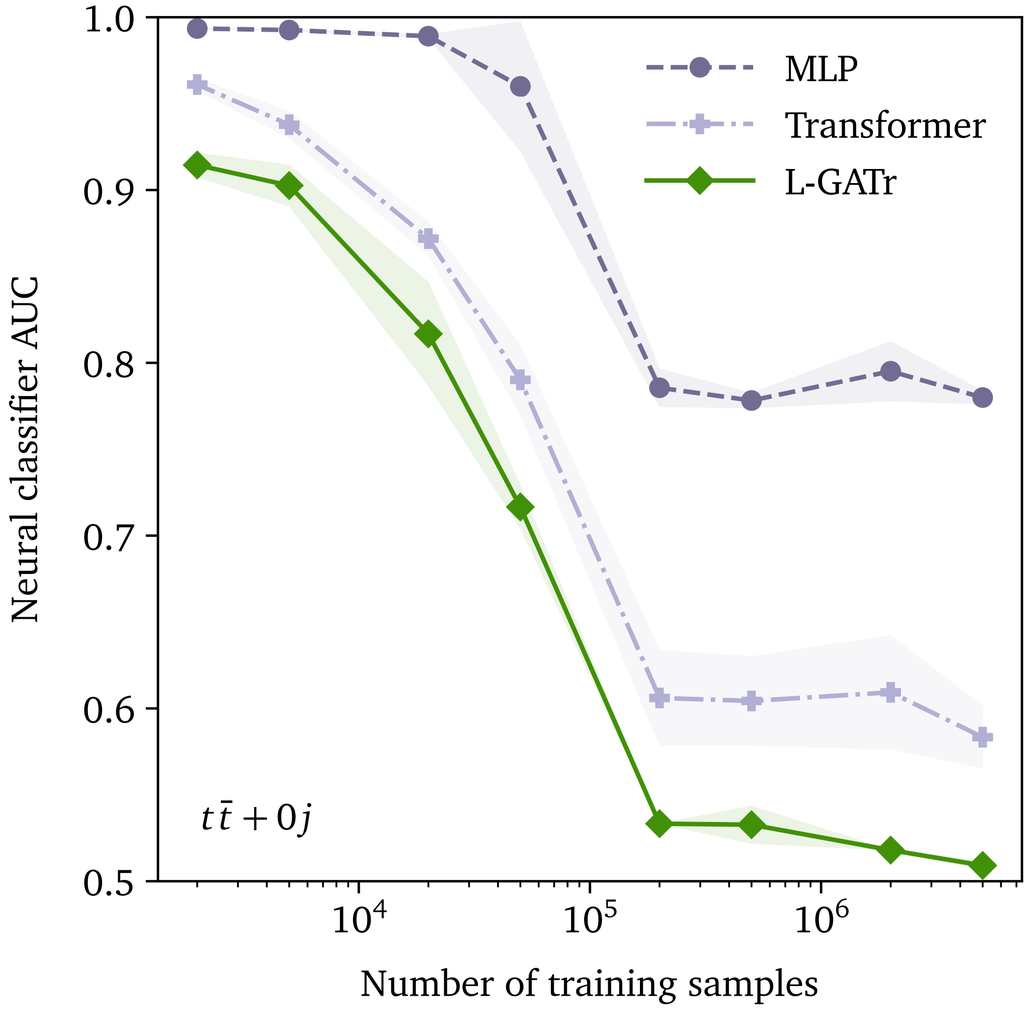
LHC event generation



Equivariance helps,
especially for angular correlations

L-GATr beyond jet tagging

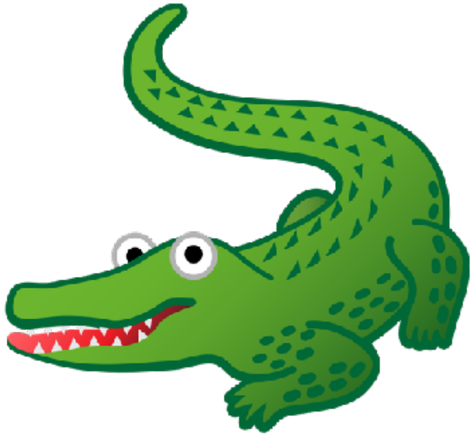
LHC event generation



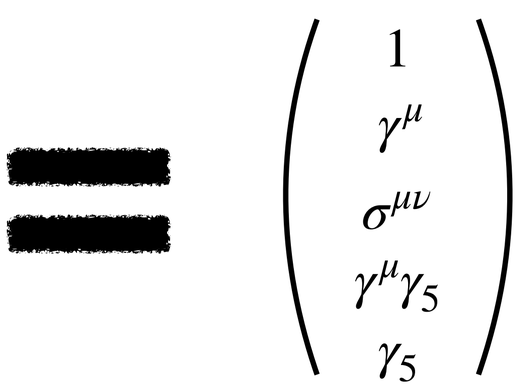
L-GATr generates samples that a classifier can barely distinguish from the ground truth

Messages

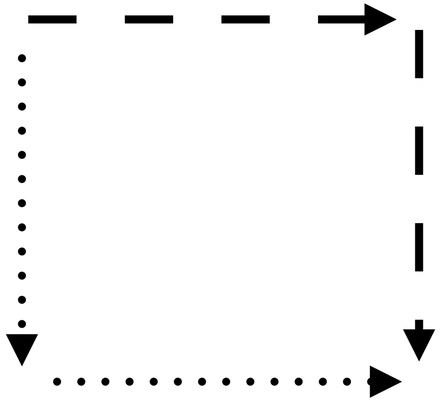
- L-GATr is a multi-purpose architecture for LHC physics
- In jet tagging, L-GATr combines the benefits from equivariance + pretraining
- Including symmetry-breaking inputs is essential



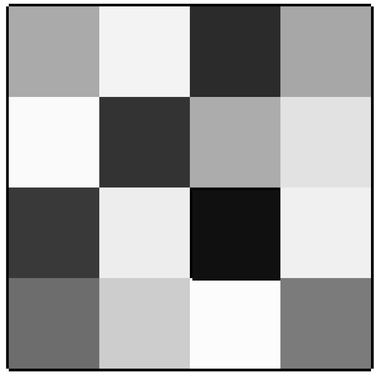
Lorentz-Equivariant
Geometric **A**lgebra
Transformer



Geometric algebra
representations



Lorentz-Equivariant
layers



Transformer
architecture

L-GATr is easy to use

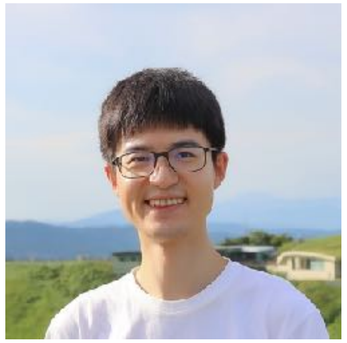
```python
from gatr import GATr, SelfAttentionConfig, MLPConfig
from gatr.interface import embed_vector, extract_scalar, embed_spurions
import torch


class ExampleWrapper(torch.nn.Module):
    """Example wrapper around a L-GATr model.

    Parameters
    ----------
    num_blocks : int
        Number of transformer blocks
    hidden_mv_channels : int
        Number of hidden multivector channels
    hidden_s_channels : int
        Number of hidden scalar channels
    """

    def __init__(self, blocks=6, hidden_mv_channels=16, hidden_s_channels=32):
        super().__init__()
        self.gatr = GATr(
            in_mv_channels=3,
            out_mv_channels=1,
            hidden_mv_channels=hidden_mv_channels,
            in_s_channels=None,
            out_s_channels=None,
            hidden_s_channels=hidden_s_channels,
            num_blocks=num_blocks,
            attention=SelfAttentionConfig(),  # Use default parameters for attention
            mlp=MLPConfig(),  # Use default parameters for MLP
        )
```

```python
def forward(self, fourmomenta):
    """Forward pass.

    Parameters
    ----------
    fourmomenta : torch.Tensor with shape (batchsize, num_points, 4)
        fourmomentum point cloud input data

    Returns
    -------
    outputs : torch.Tensor with shape (batchsize, 1)
        Model prediction: a single scalar for the whole point cloud.
    """
    batchsize, num_points, _ = fourmomenta.shape

    # Embed fourmomentum point cloud inputs in GA
    multivectors = embed_vector(fourmomenta).unsqueeze(-2)  # (batchsize, num_points, 1, 1

    # Append spurions for symmetry breaking (optional)
    spurions = embed_spurions(beam_reference="xyplane", add_time_reference=True, device=fo
    spurions = spurions[None, None, ...].repeat(batchsize, num_points, 1, 1)  # (batchsize
    multivectors = torch.cat((multivectors, spurions), dim=-2)  # (batchsize, num_points,

    # Pass data through GATr
    multivector_outputs, _ = self.gatr(multivectors, scalars=None)  # (batchsize, num_poin

    # Extract scalar outputs
    outputs = extract_scalar(multivector)  # (batchsize, num_points, 1)

    # Mean aggregation to extract a single scalar for the whole point cloud
    score = outputs.mean(dim=1)

    return score
```


Victor Bresó


Pim de Haan


Tilman Plehn


Huilin Qu


Jesse Thaler


Johann Brehmer

Lorentz-Equivariant Geometric Algebra Transformer for High-Energy Physics

Jonas Spinner*, Victor Breso*, Pim de Haan, Tilman Plehn, Jesse Thaler, Johann Brehmer
NeurIPS 2024, arXiv:2405.14806

CS paper

A Lorentz-Equivariant Transformer for all of the LHC

Johann Brehmer, Víctor Bresó, Pim de Haan, Tilman Plehn, Huilin Qu, Jonas Spinner, Jesse Thaler
arXiv:2411.00446

HEP paper

L-GATr code

For what will **you** use L-GATr?

Bonus material

Network	Accuracy	AUC	$1/\epsilon_B$ ($\epsilon_S = 0.5$)	$1/\epsilon_B$ ($\epsilon_S = 0.3$)
TopoDNN [54]	0.916	0.972	–	295 ± 5
LoLa [9]	0.929	0.980	–	722 ± 17
N-subjettiness [55]	0.929	0.981	–	867 ± 15
PFN [56]	0.932	0.9819	247 ± 3	888 ± 17
TreeNiN [57]	0.933	0.982	–	1025 ± 11
ParticleNet [58]	0.940	0.9858	397 ± 7	1615 ± 93
ParT [59]	0.940	0.9858	413 ± 16	1602 ± 81
MIParT [60]	0.942	0.9868	505 ± 8	2010 ± 97
LorentzNet* [10]	0.942	0.9868	498 ± 18	2195 ± 173
CGENN* [14]	0.942	0.9869	500	2172
PELICAN* [42]	0.9426 ± 0.0002	0.9870 ± 0.0001	–	2250 ± 75
L-GATr* [35]	0.9423 ± 0.0002	0.9870 ± 0.0001	540 ± 20	2240 ± 70
ParticleNet-f.t. [60]	0.942	0.9866	487 ± 9	1771 ± 80
ParT-f.t. [60]	0.944	0.9877	691 ± 15	2766 ± 130
MIParT-f.t. [60]	0.944	0.9878	640 ± 10	2789 ± 133
L-GATr-f.t.* (new)	0.9442 ± 0.0002	0.98792 ± 0.00004	661 ± 24	3005 ± 186

Event generation

Conditional Flow Matching

Continuous normalising flow (CNF)
connect a simple base density
to a complex target density
through a neural differential equation

$$\frac{d}{dt}x = v_t(x)$$

Continuous normalising flows
arXiv:1806.07366

Conditional flow matching (CFM)
is a simple way to train CNFs
by comparing the learned velocity $v_t(x)$
to a conditional target velocity $u_t(x \,|\, x_1)$

$$\mathscr{L} = \left\langle (v_t(x) - u_t(x \,|\, x_1))^2 \right\rangle$$

Conditional flow matching
arXiv:2210.02747

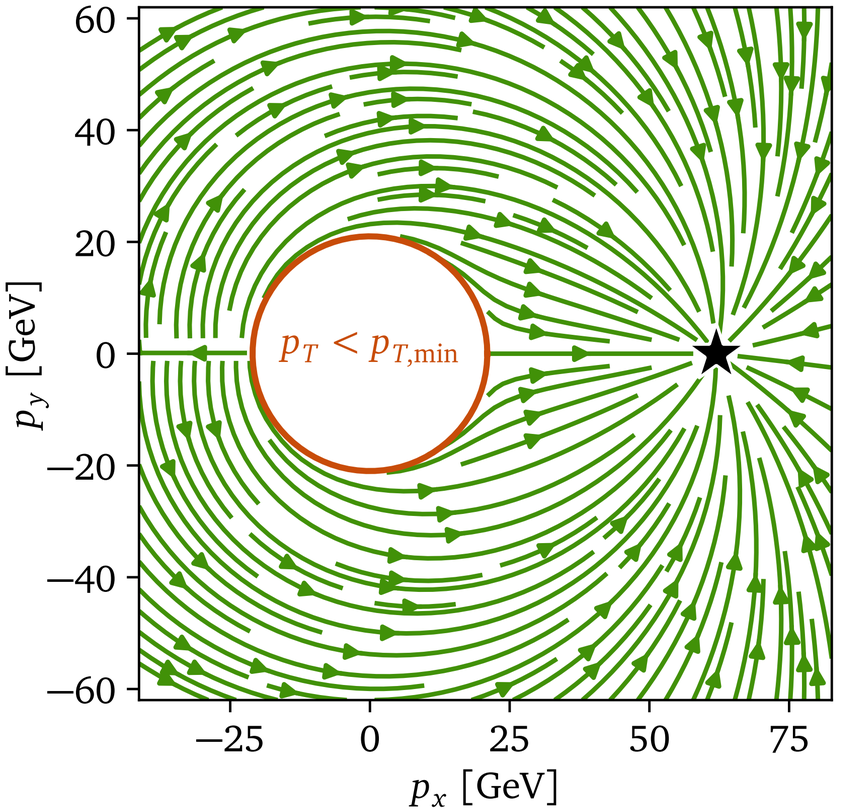
How to pick the target velocity $u_t(x \,|\, x_1)$?

Event generation

Physics-inspired target trajectories

Straight trajectories in ‘modified jet momenta’ x:

$$p = \begin{pmatrix} E \\ p_x \\ p_y \\ p_z \end{pmatrix} \quad \rightarrow \quad f^{-1}(p) = x = \begin{pmatrix} x_p \\ x_m \\ x_\eta \\ x_\phi \end{pmatrix} \equiv \begin{pmatrix} \log(p_T - p_{T,\text{min}}) \\ \log m^2 \\ \eta \\ \phi \end{pmatrix}$$

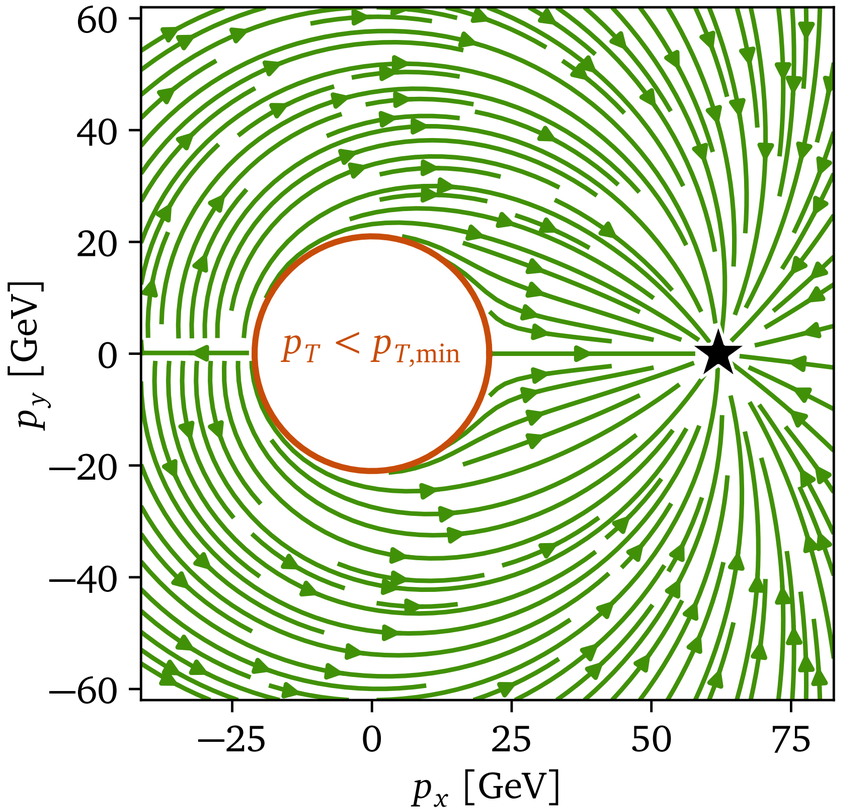


Event generation

Physics-inspired target trajectories

Straight trajectories in ‘modified jet momenta’ x:

$$p = \begin{pmatrix} E \\ p_x \\ p_y \\ p_z \end{pmatrix} \quad \rightarrow \quad f^{-1}(p) = x = \begin{pmatrix} x_p \\ x_m \\ x_\eta \\ x_\phi \end{pmatrix} \equiv \begin{pmatrix} \log(p_T - p_{T,\text{min}}) \\ \log m^2 \\ \eta \\ \phi \end{pmatrix}$$



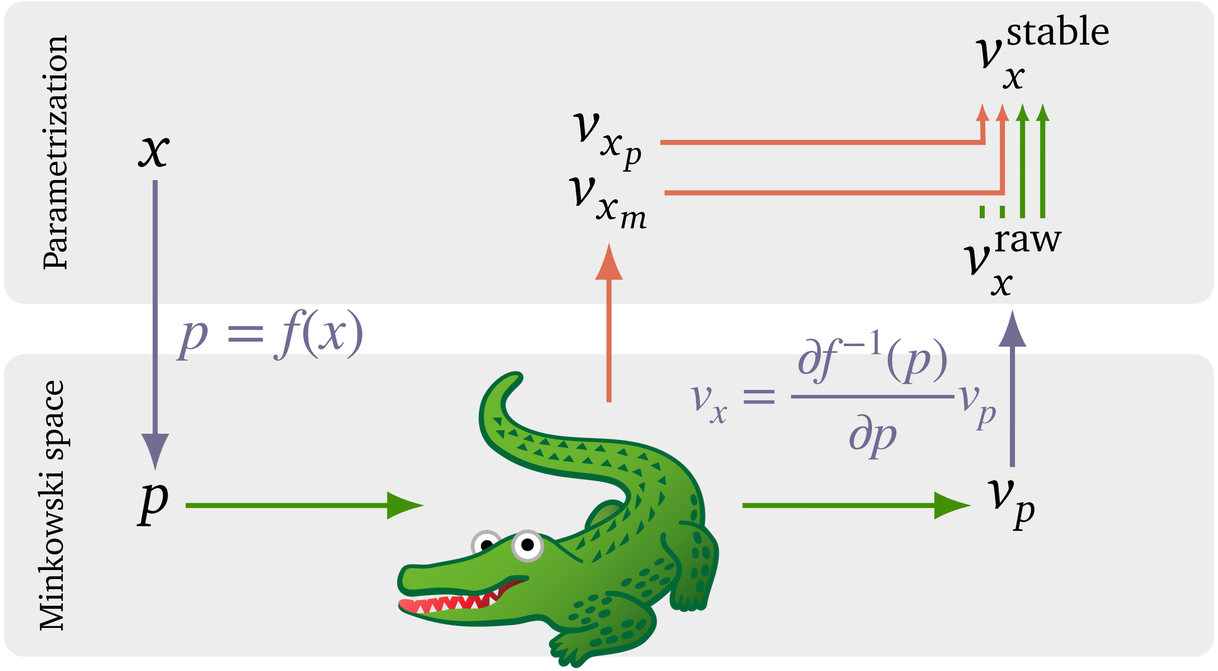
Data	Architecture	Base distribution	Periodic	Neg. log-likelihood	AUC
p	L-GATr	rejection sampling	✓	-30.80 ± 0.17	0.945 ± 0.004
x	MLP	rejection sampling	✓	-32.13 ± 0.05	0.780 ± 0.003
x	L-GATr	rejection sampling	✗	-32.57 ± 0.05	0.530 ± 0.017
x	L-GATr	no rejection sampling	✓	-32.58 ± 0.04	0.523 ± 0.014
(default) x	L-GATr	rejection sampling	✓	-32.65 ± 0.04	0.515 ± 0.009

Event generation

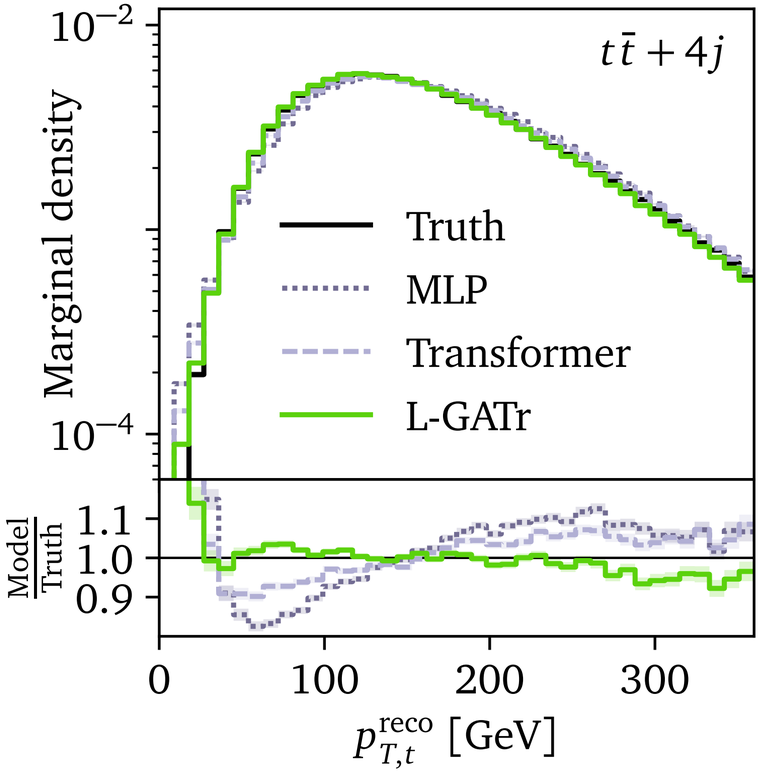
How to extract the CFM velocity field $v_x(x)$?

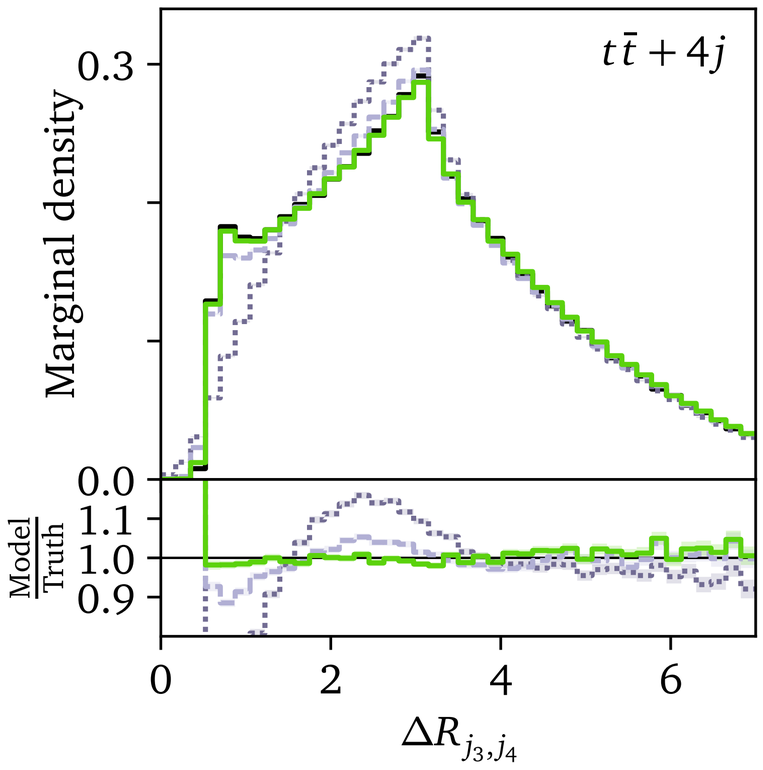
Extend standard CFM workflow
with L-GATr:

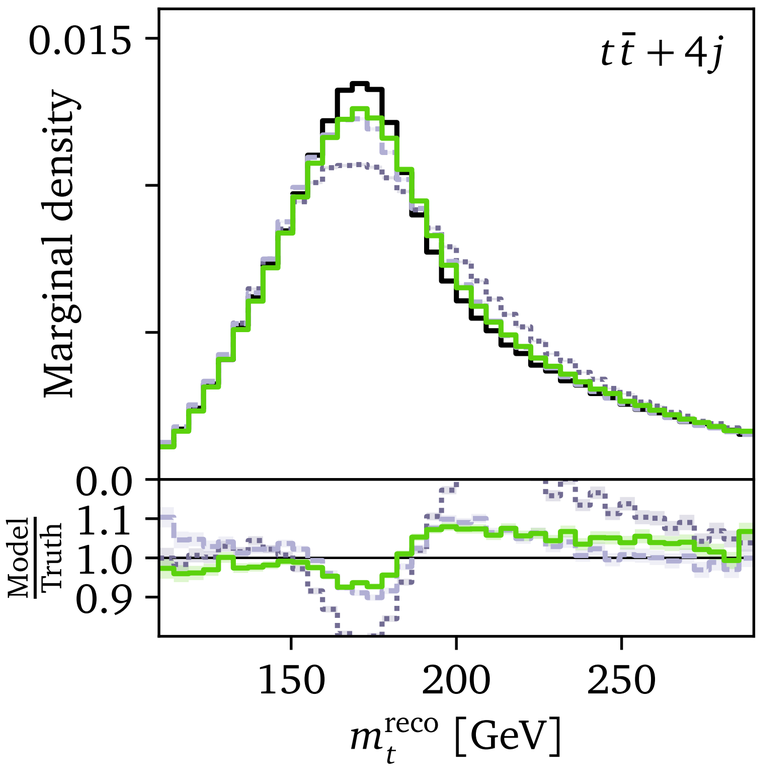
- Transformations $f(x)$
  between Minkowski space p
  and the parametrization x
- Equivariant operations
  using multivectors
- Symmetry-breaking operations
  using scalars
  (required for numerical stability)



Event generation

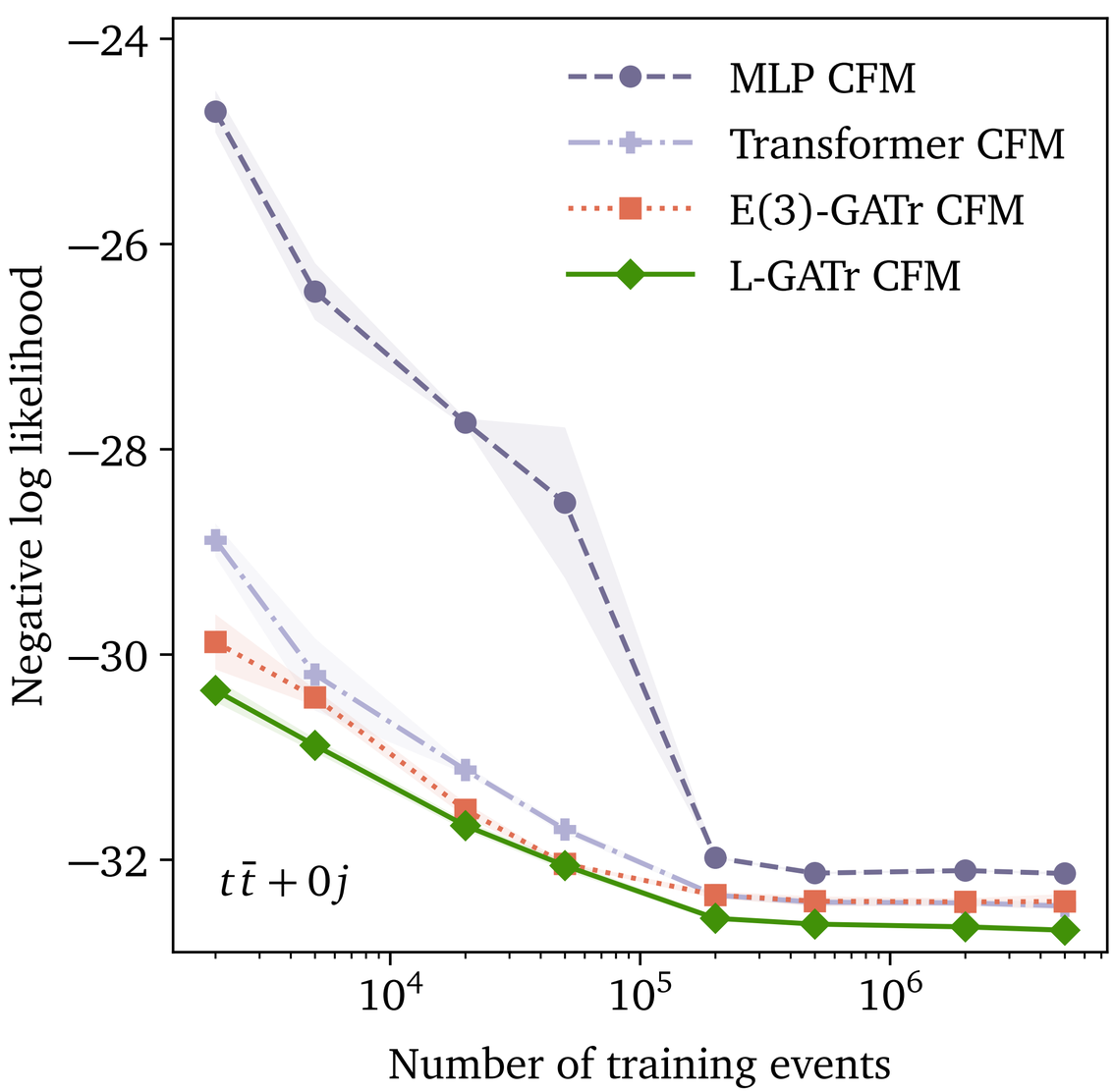


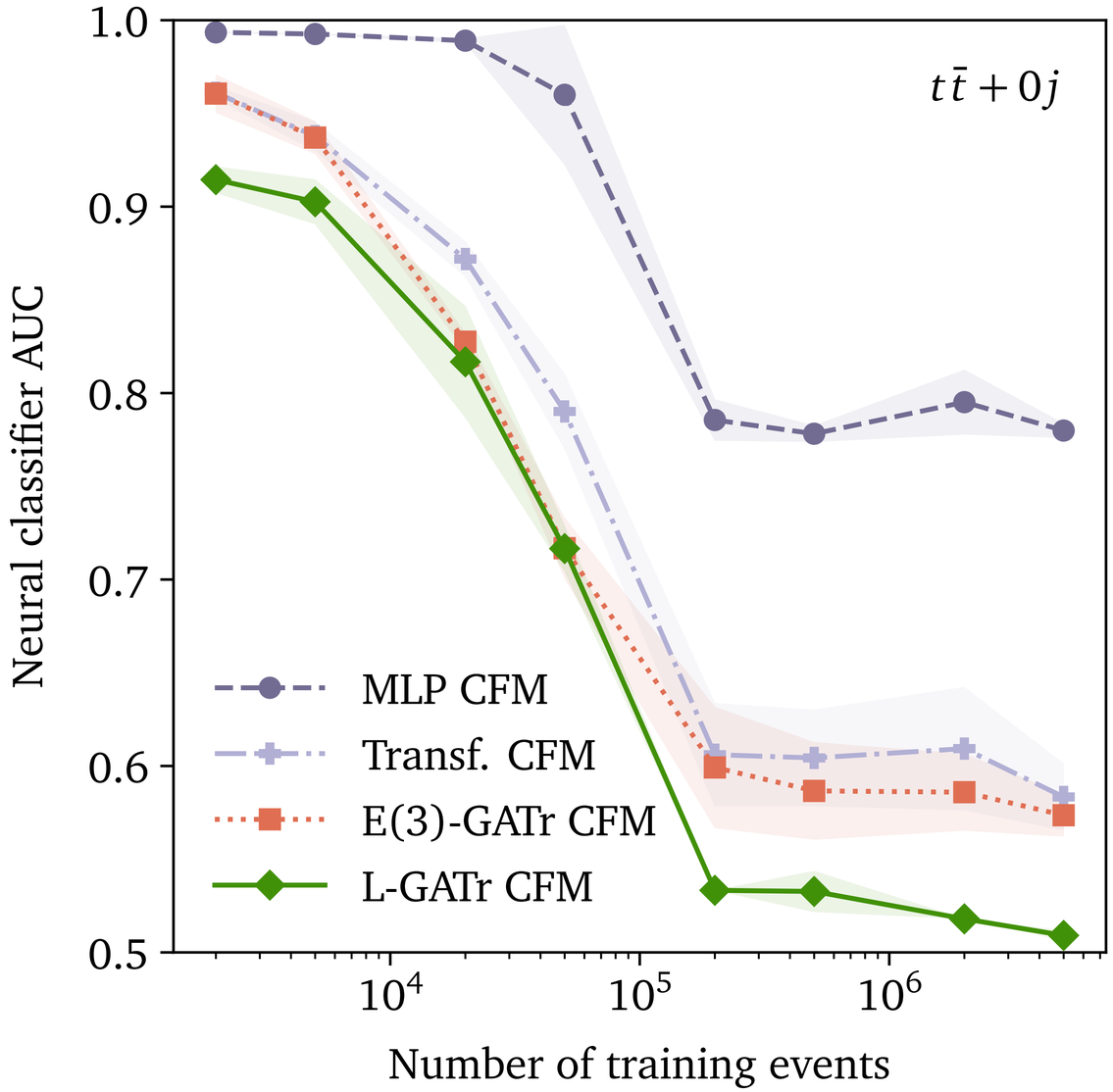




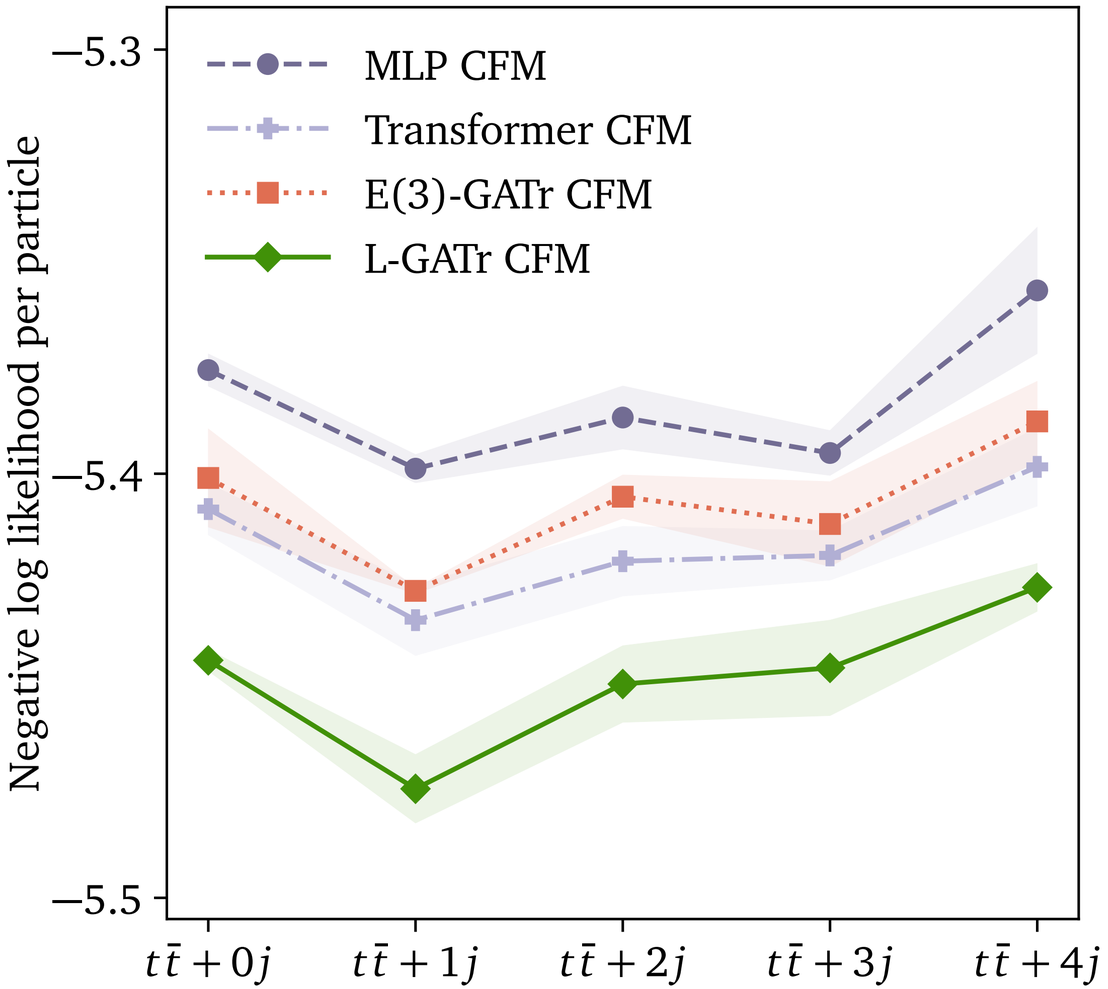
Equivariance helps,
especially for angular correlations

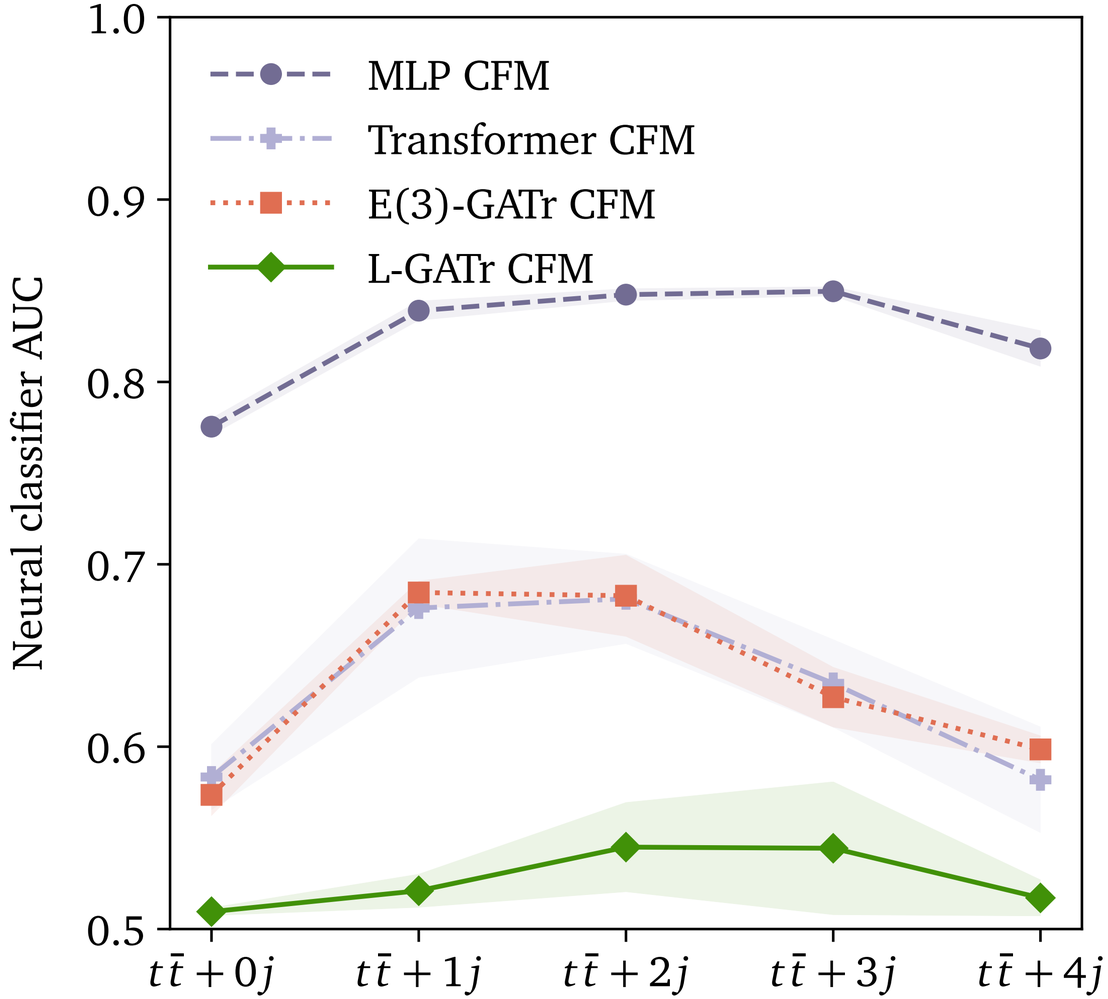
Event generation



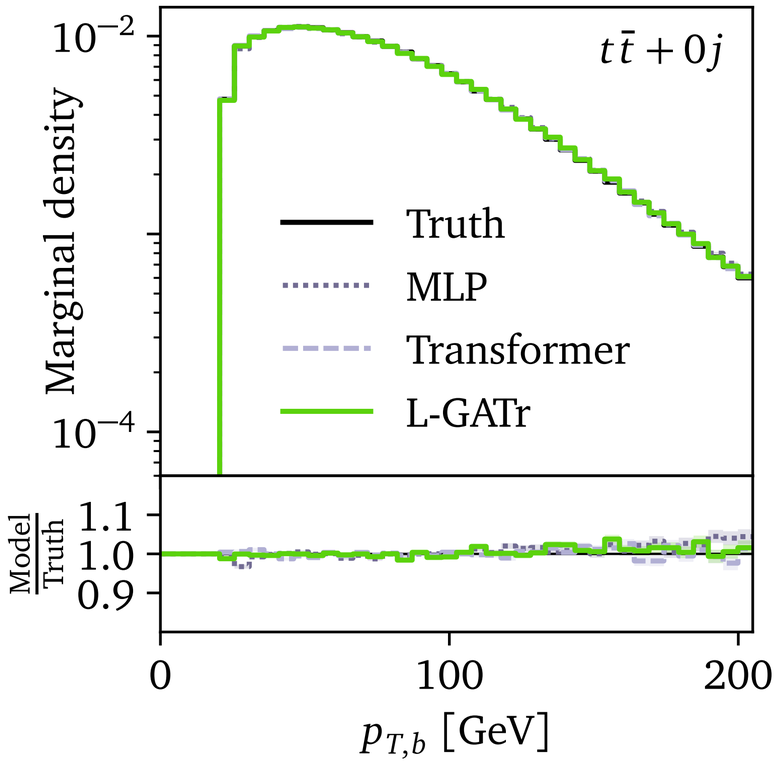


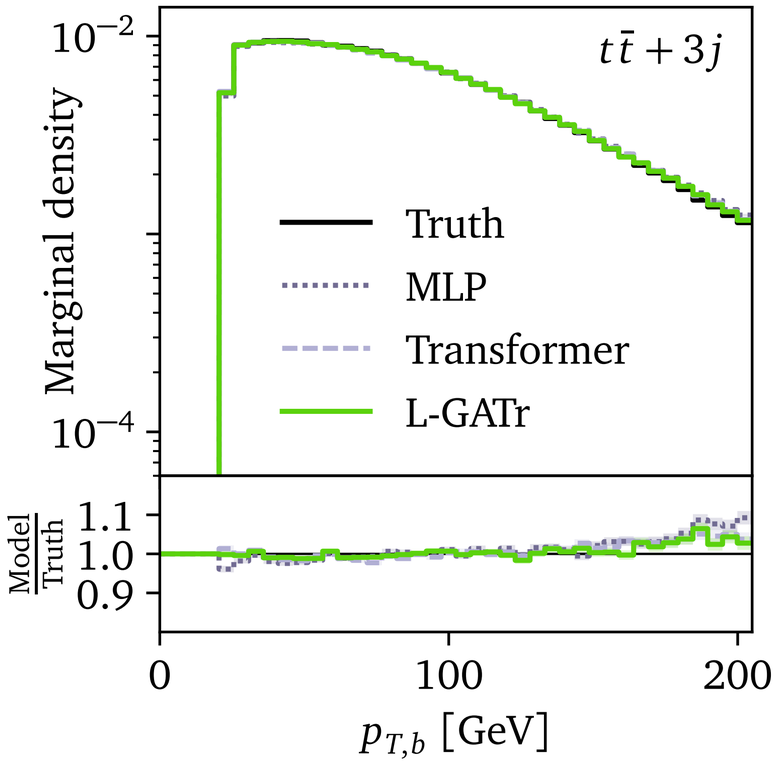
Event generation

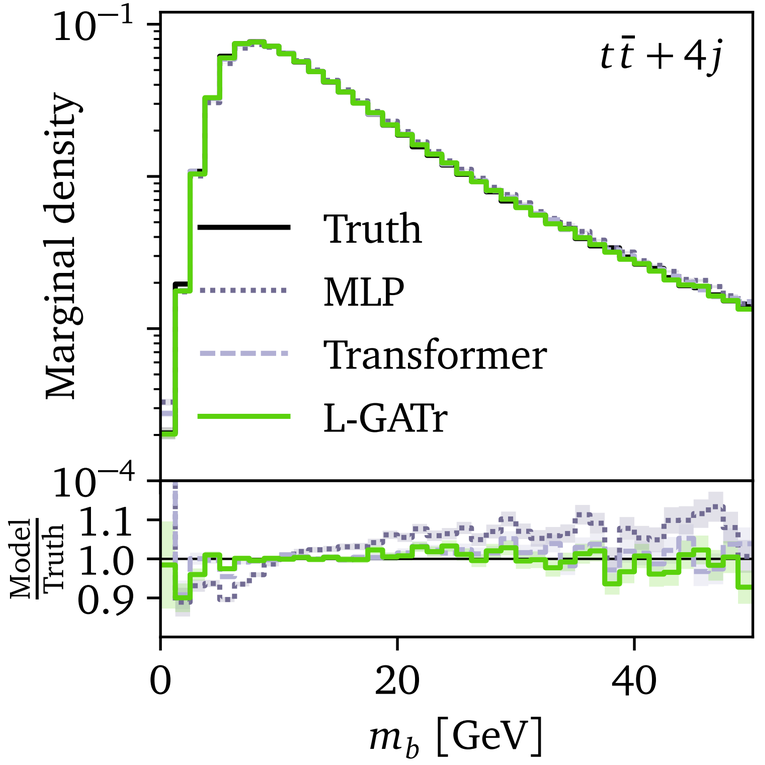




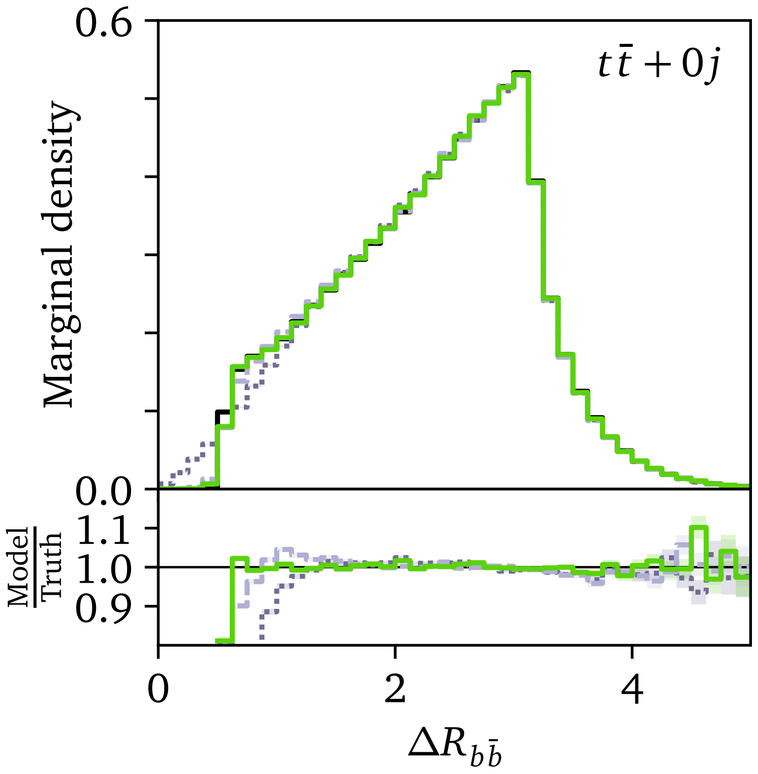
Event generation

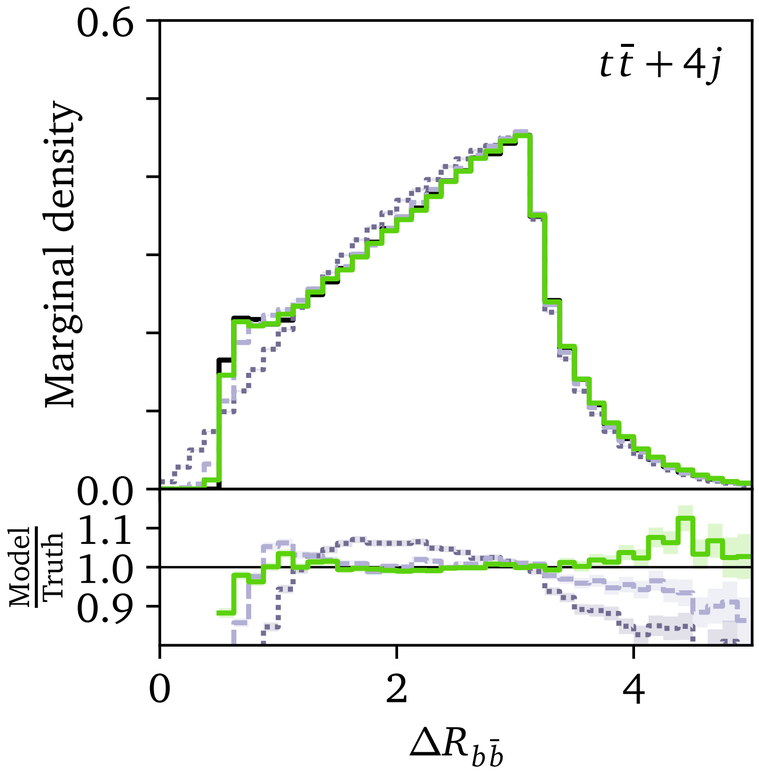


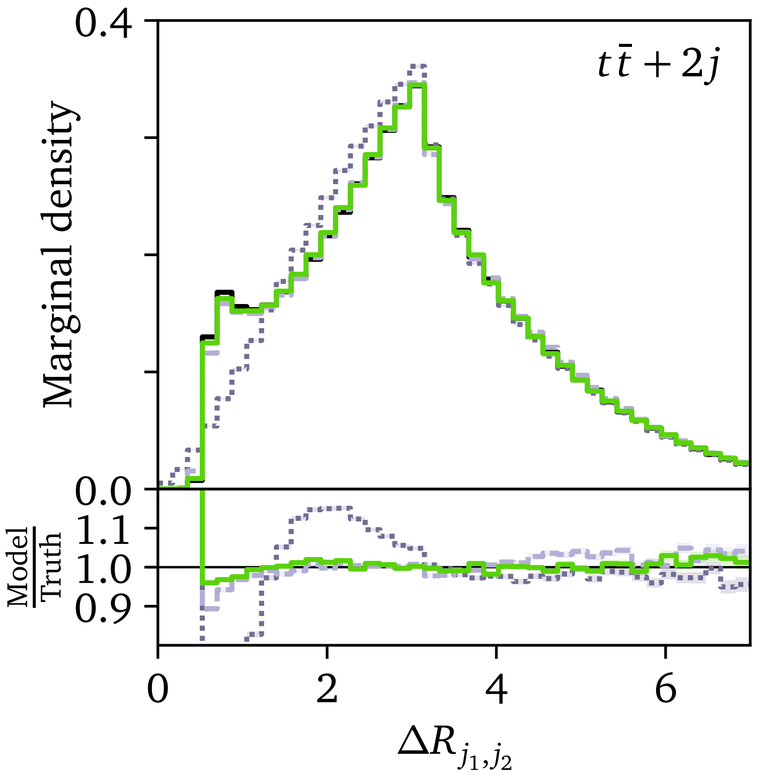




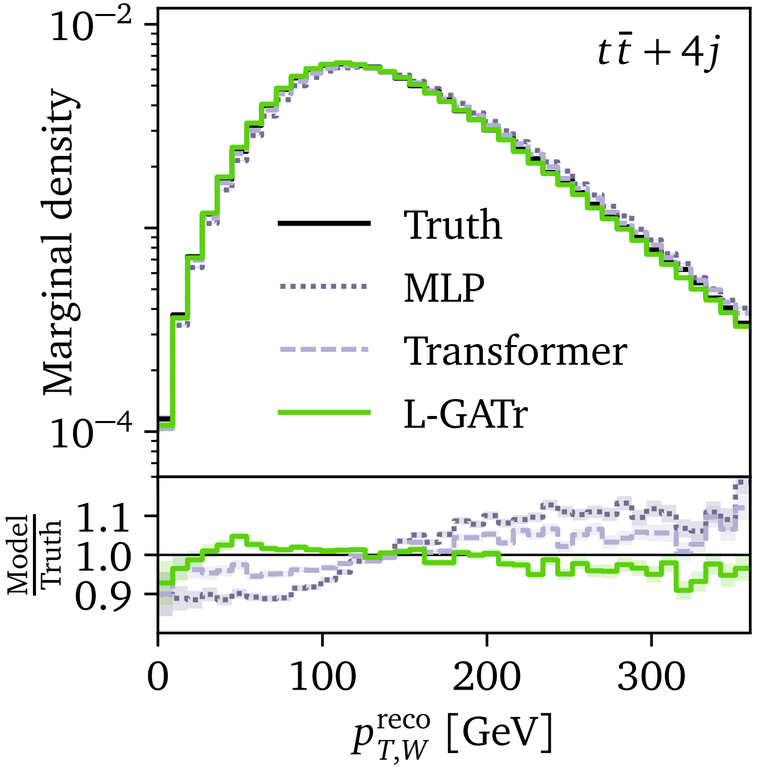
Event generation

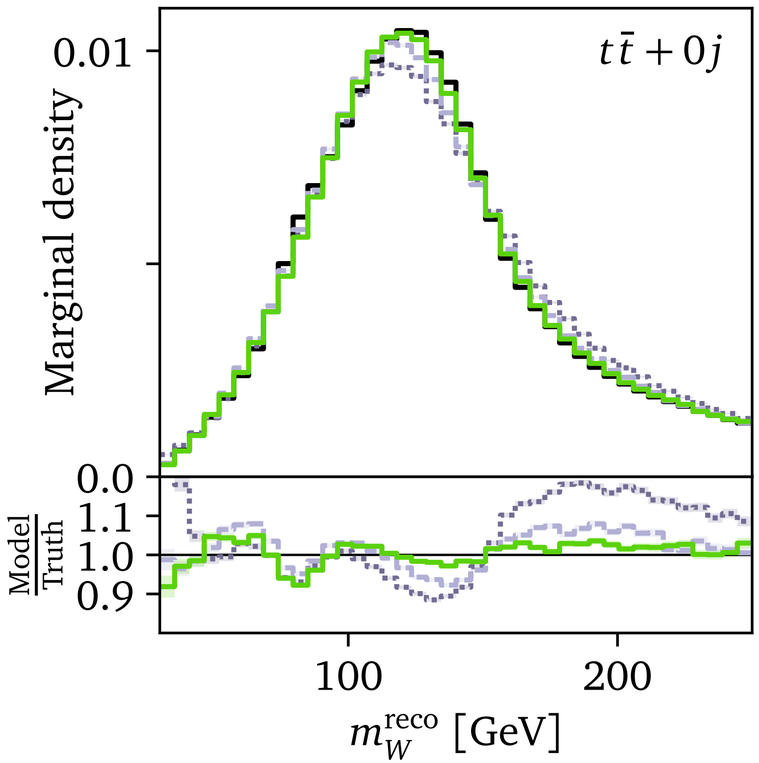


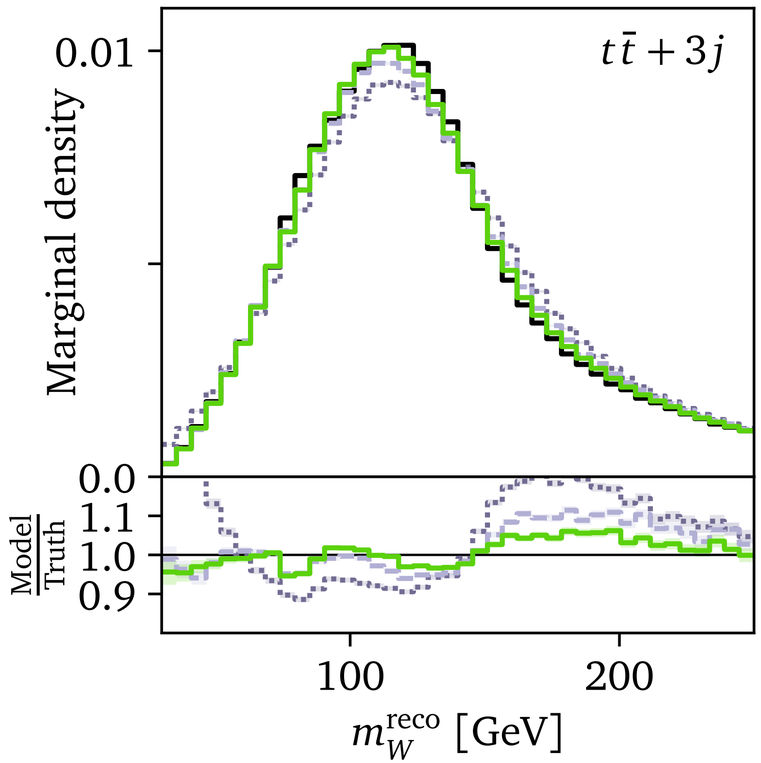




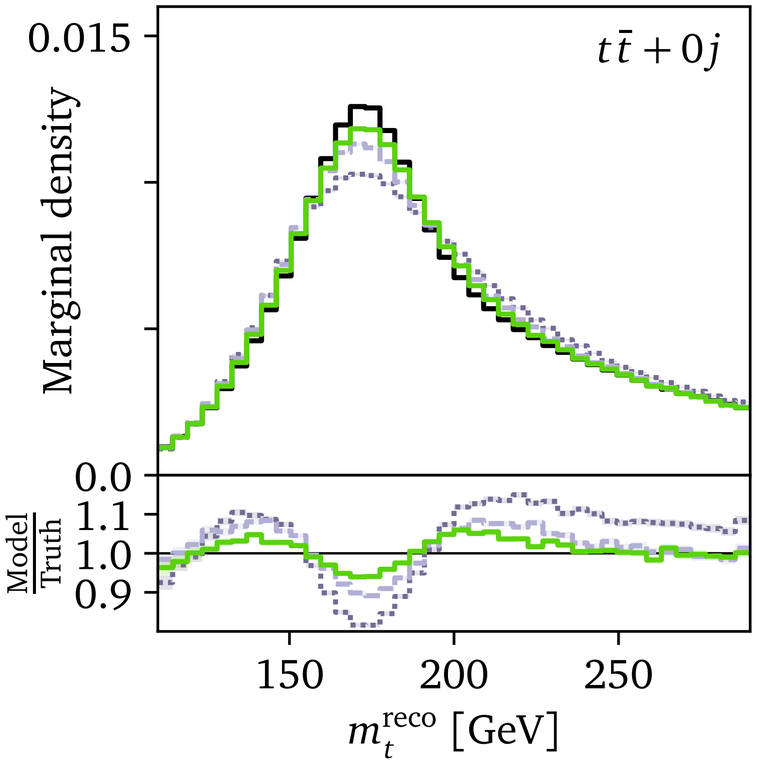
Event generation

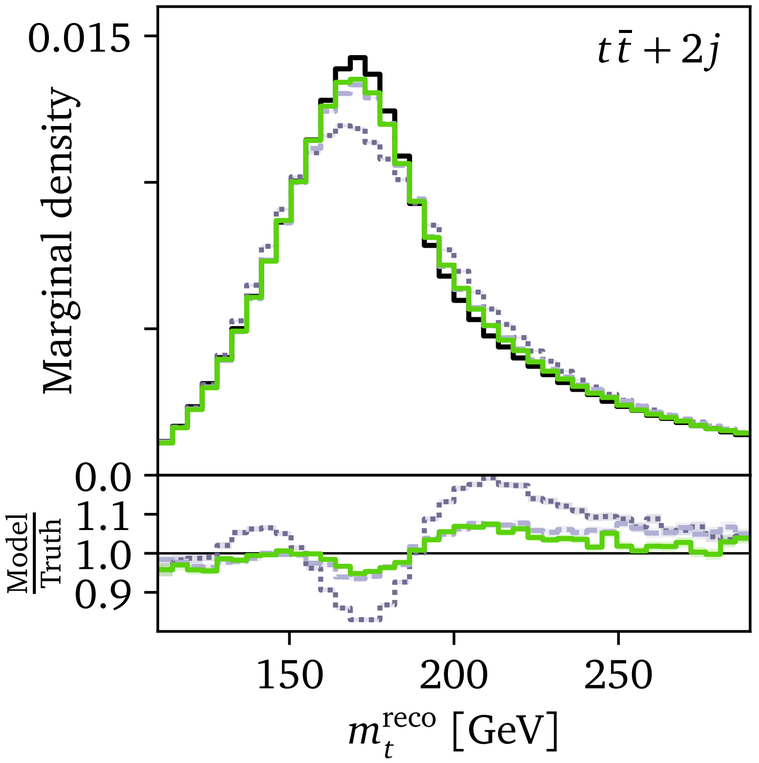


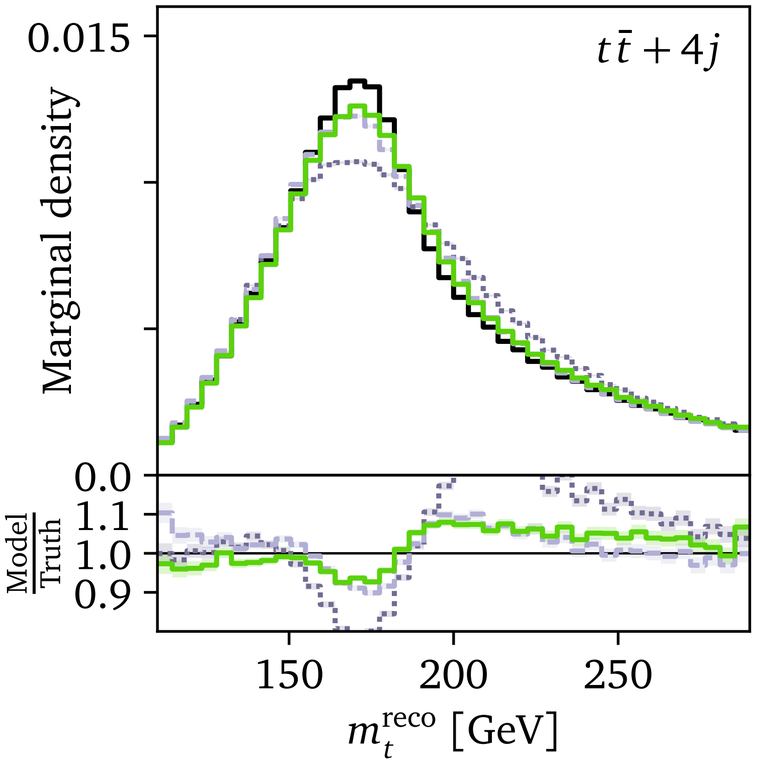




Event generation

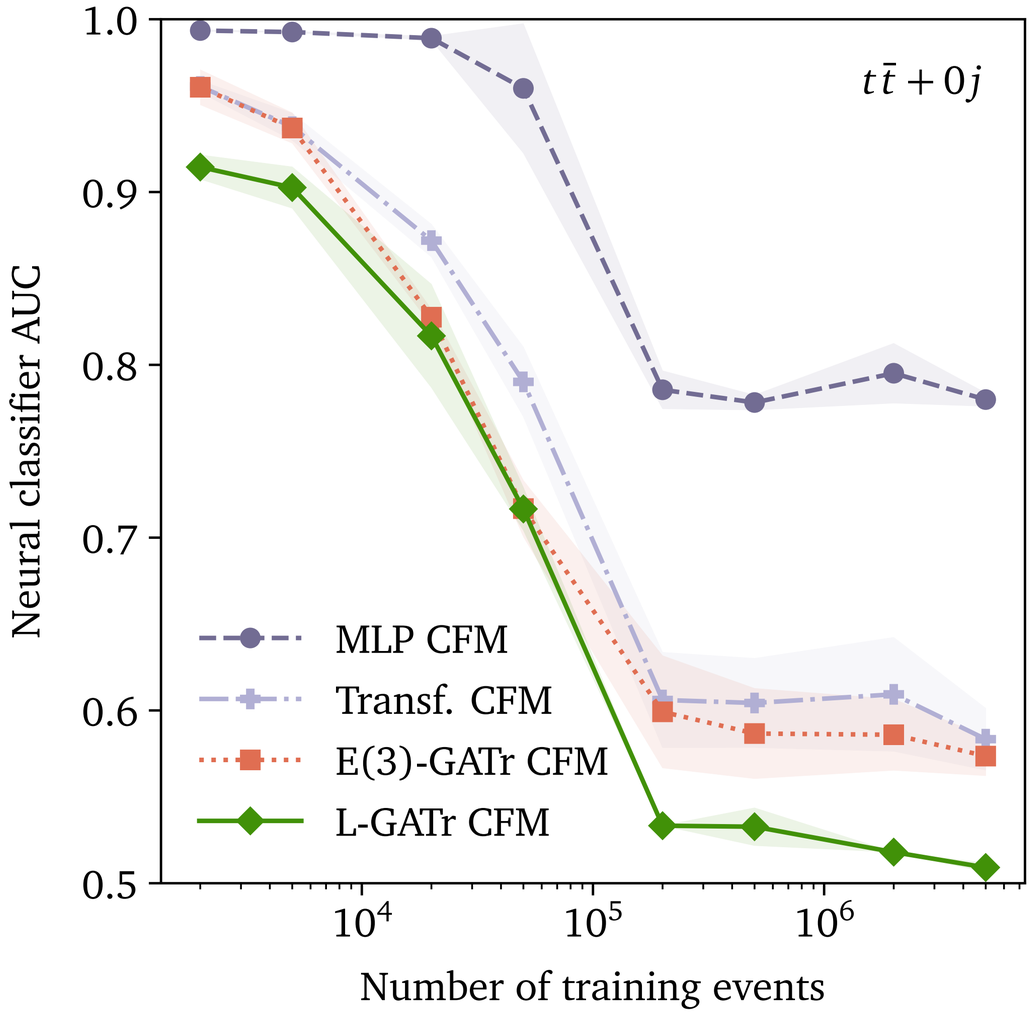






Event generation

Boost equivariance lets L-GATr shine



L-GATr and E(3)-GATr are both not boost equivariant:

- E(3)-GATr: No boost equivariance at all
- L-GATr: Boost equivariance broken by reference multivectors

Equivariant networks
with full symmetry breaking
outperform non-equivariant networks