SuperCalo

Calorimeter shower super-resolution

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ML4Jets, Hamburg

RUTGERS
UNIVERSITY | NEW BRUNSWICK

[2308.11700] **IP**, J. Raine, D. Shih

Fast Calorimeter Simulation

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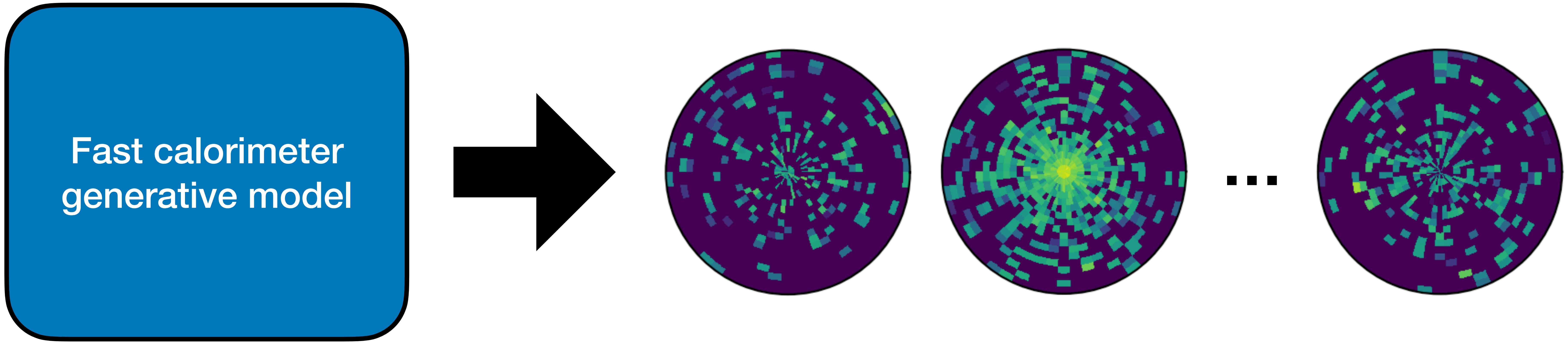

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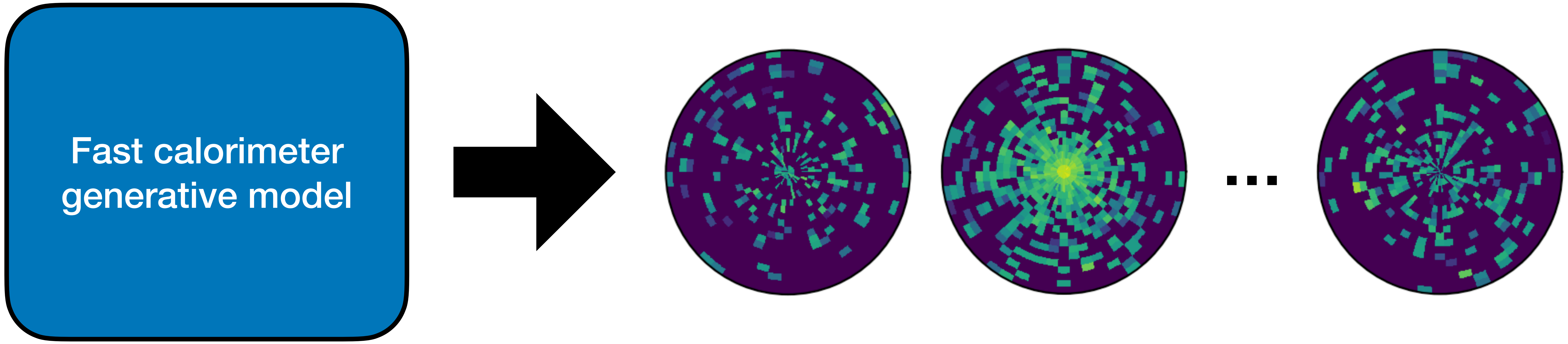

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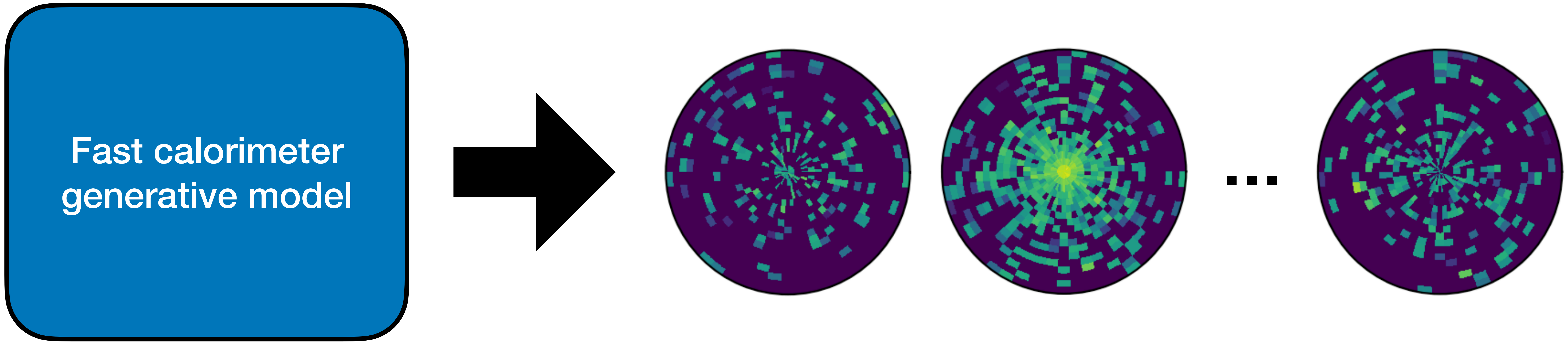

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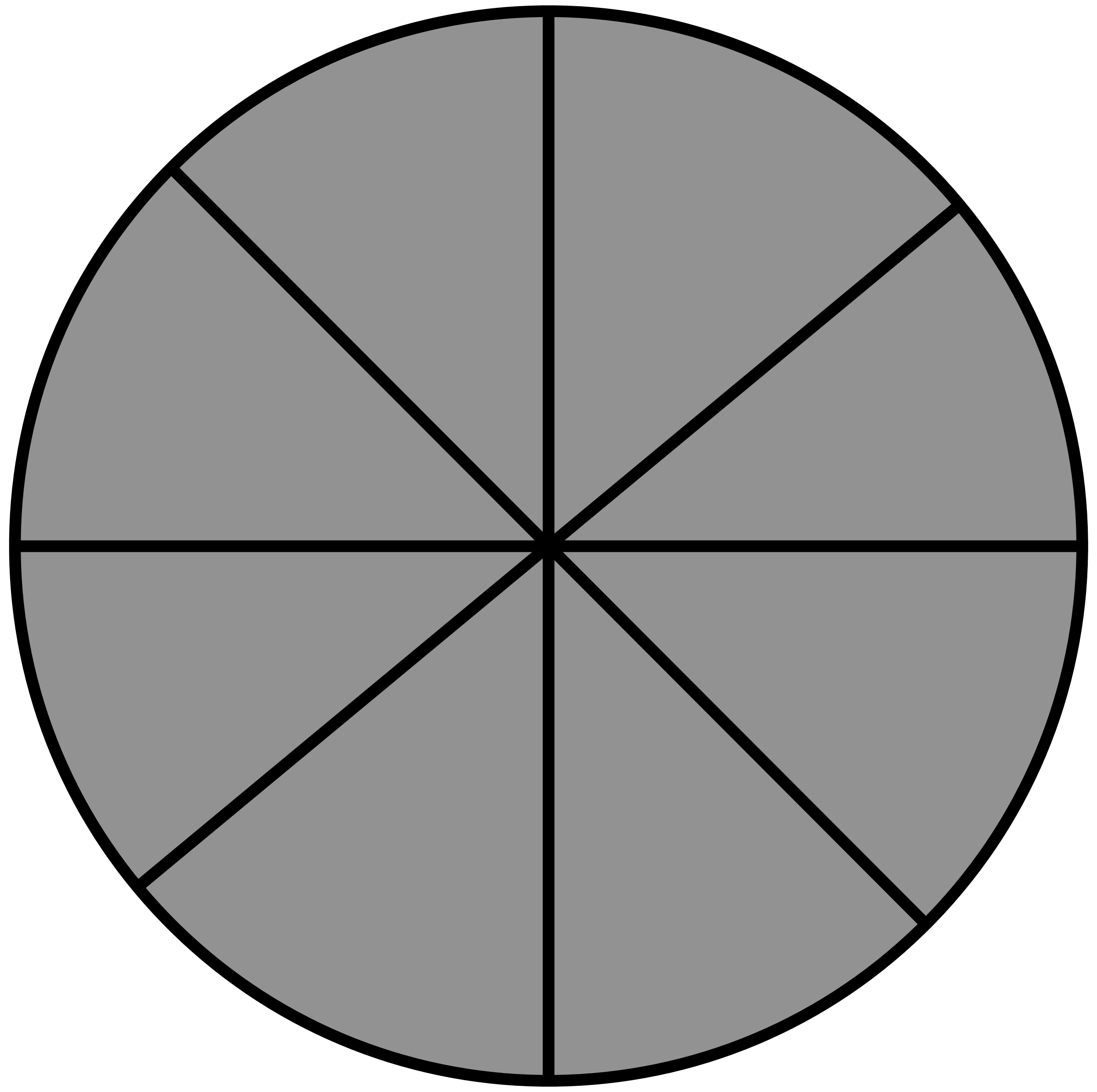
- **Enter SuperCalo!**

Main idea!



Low-resolution

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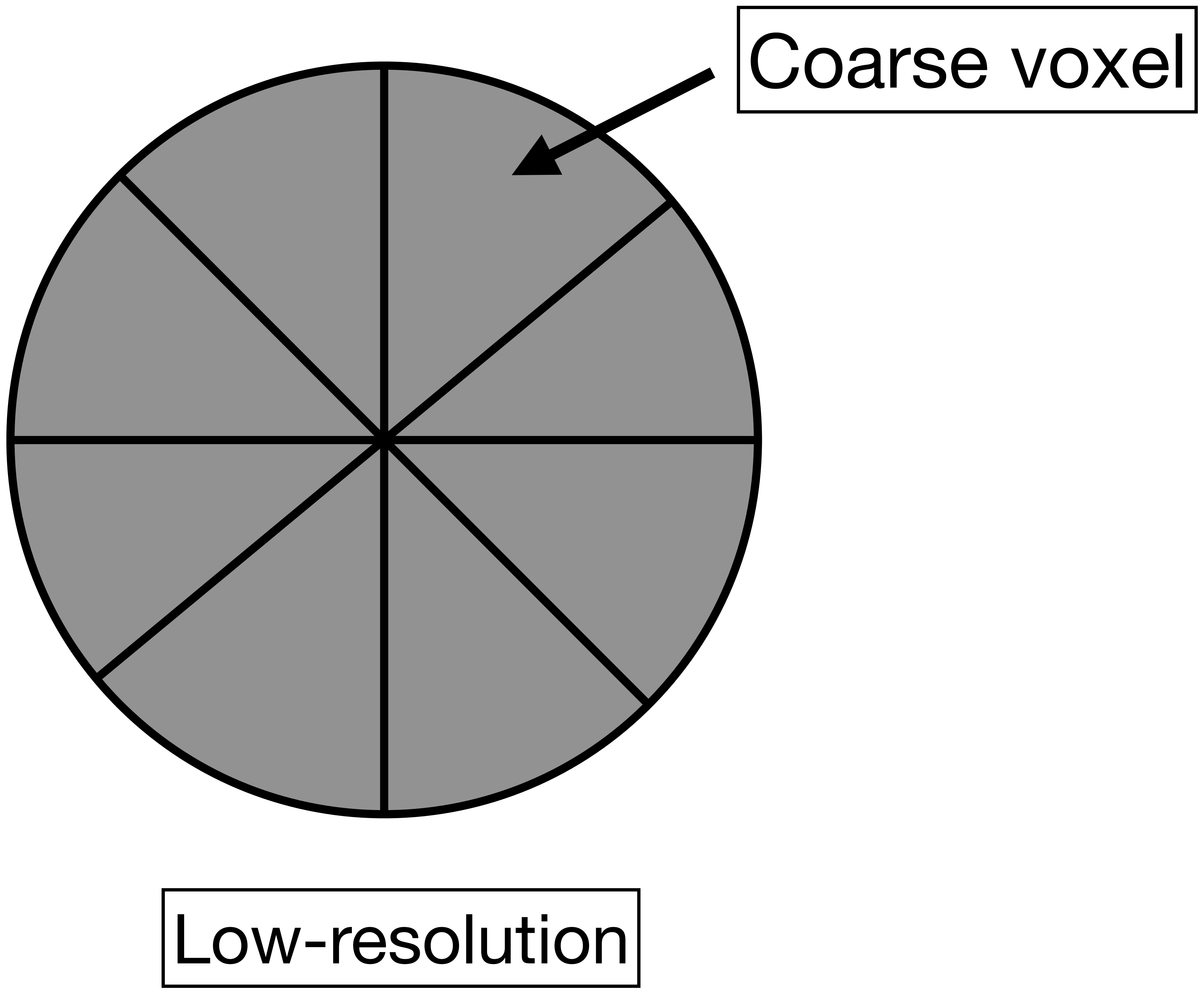

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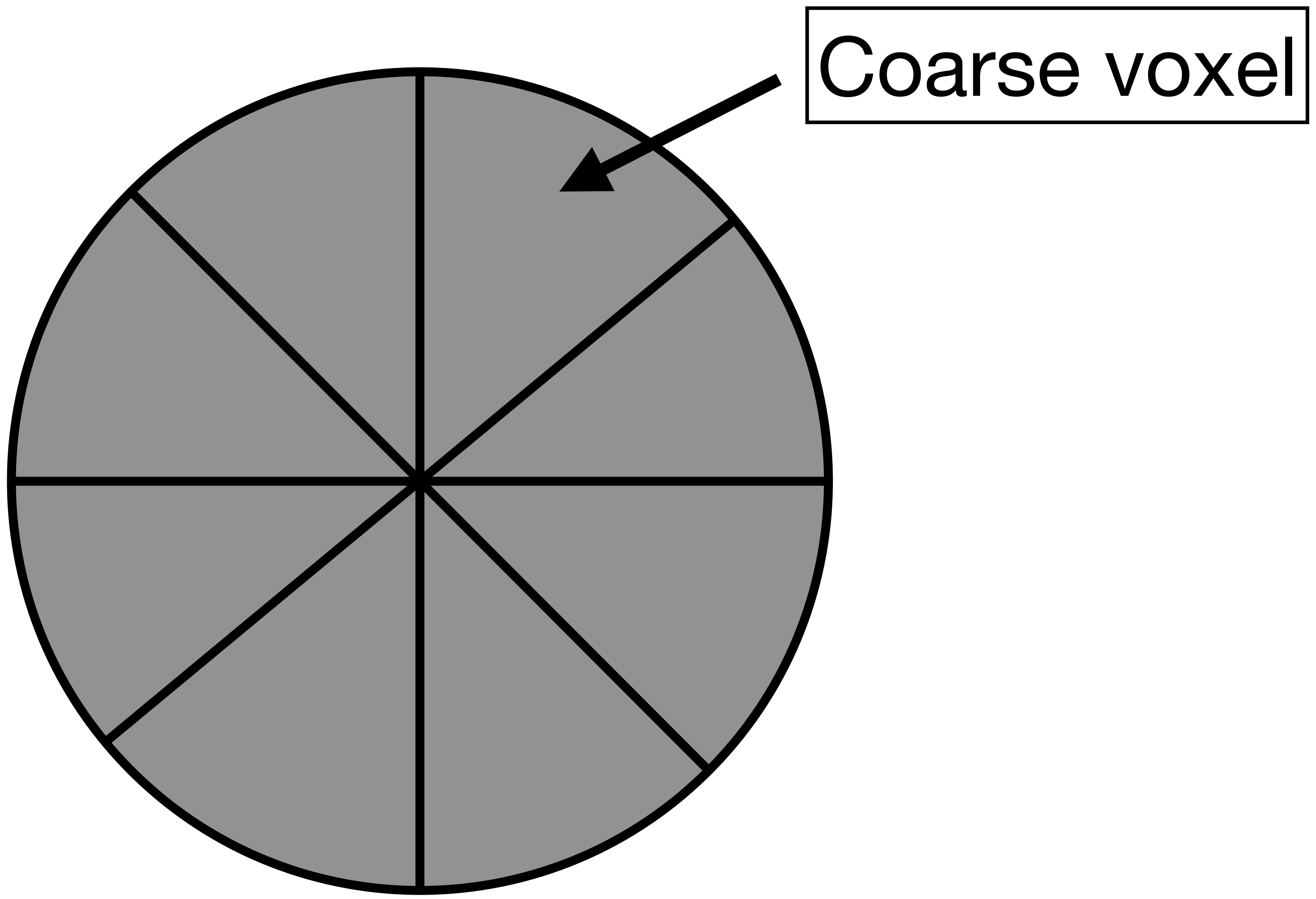

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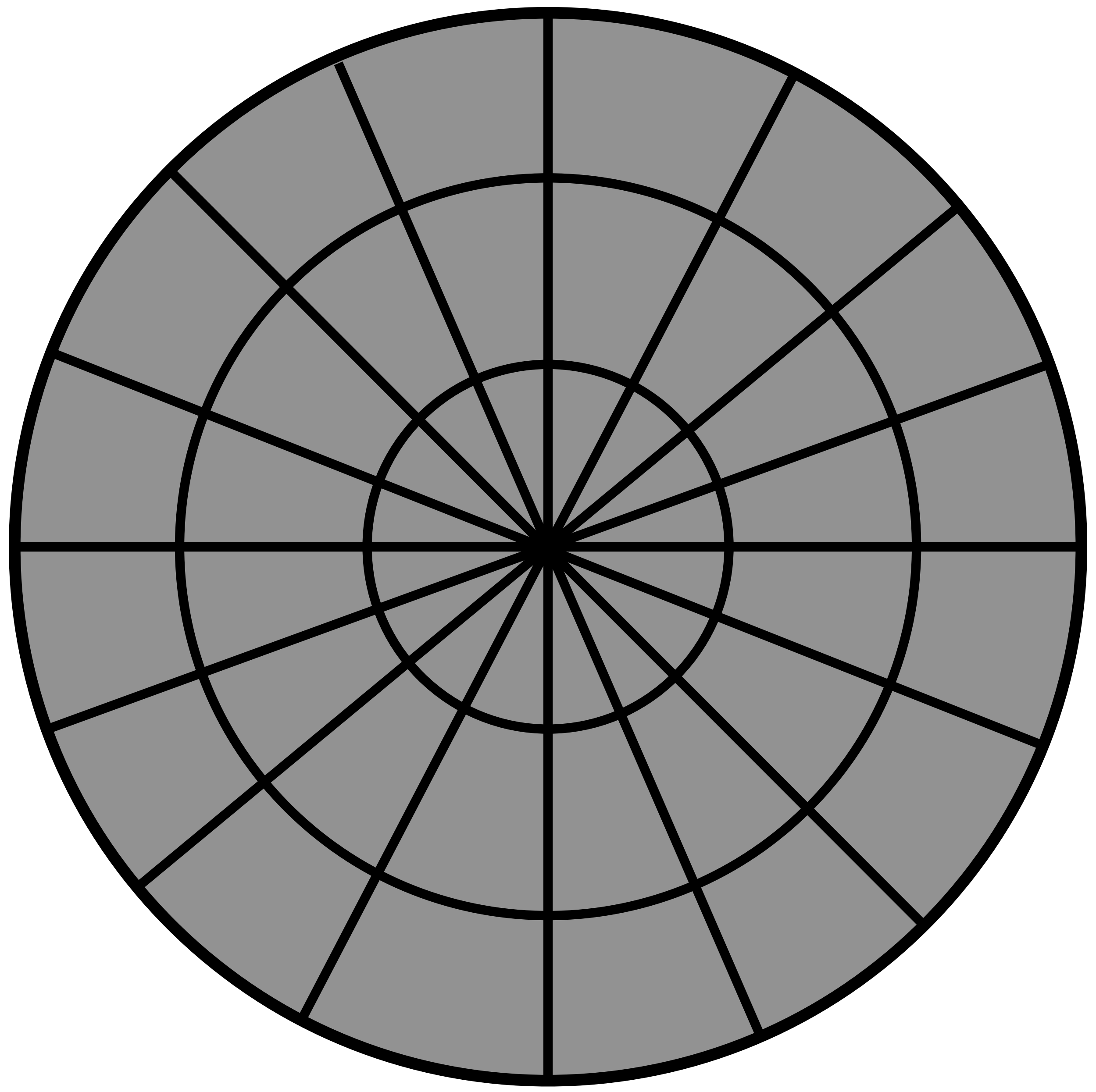

High-resolution

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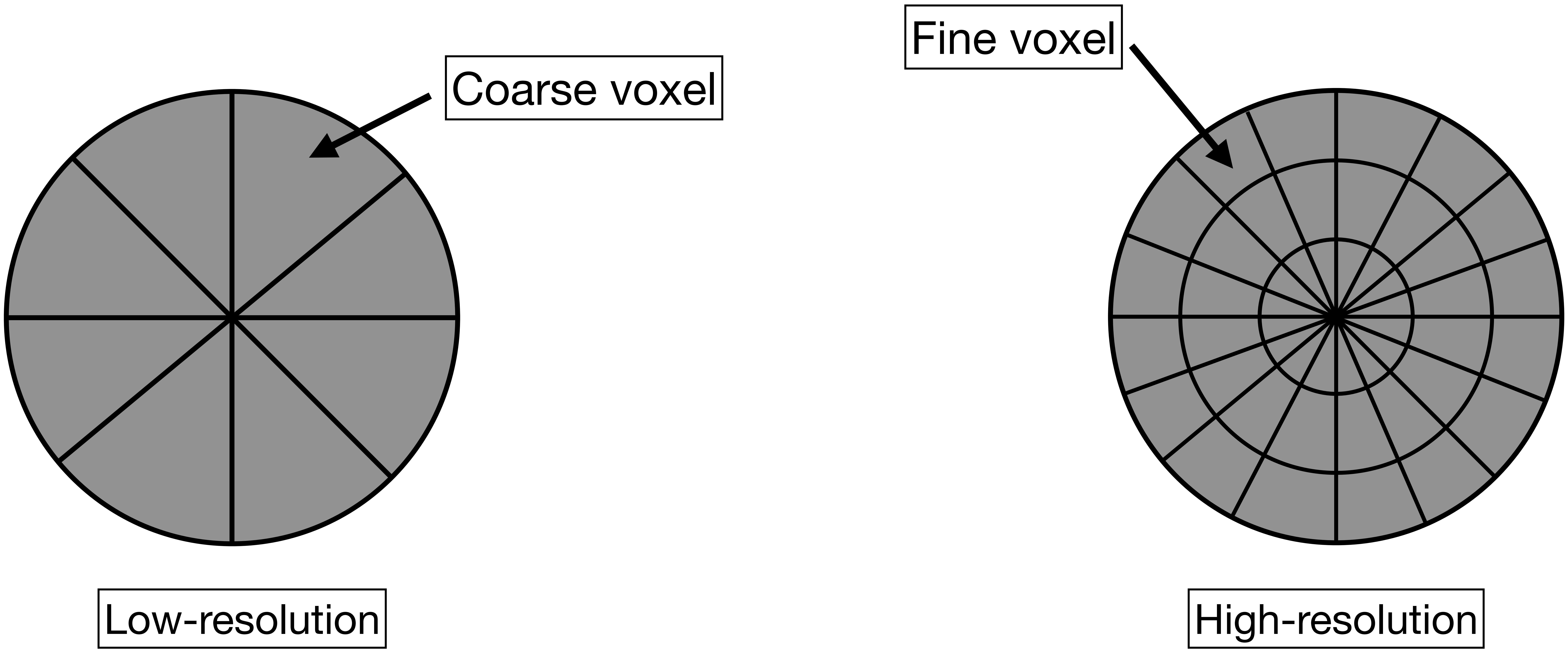

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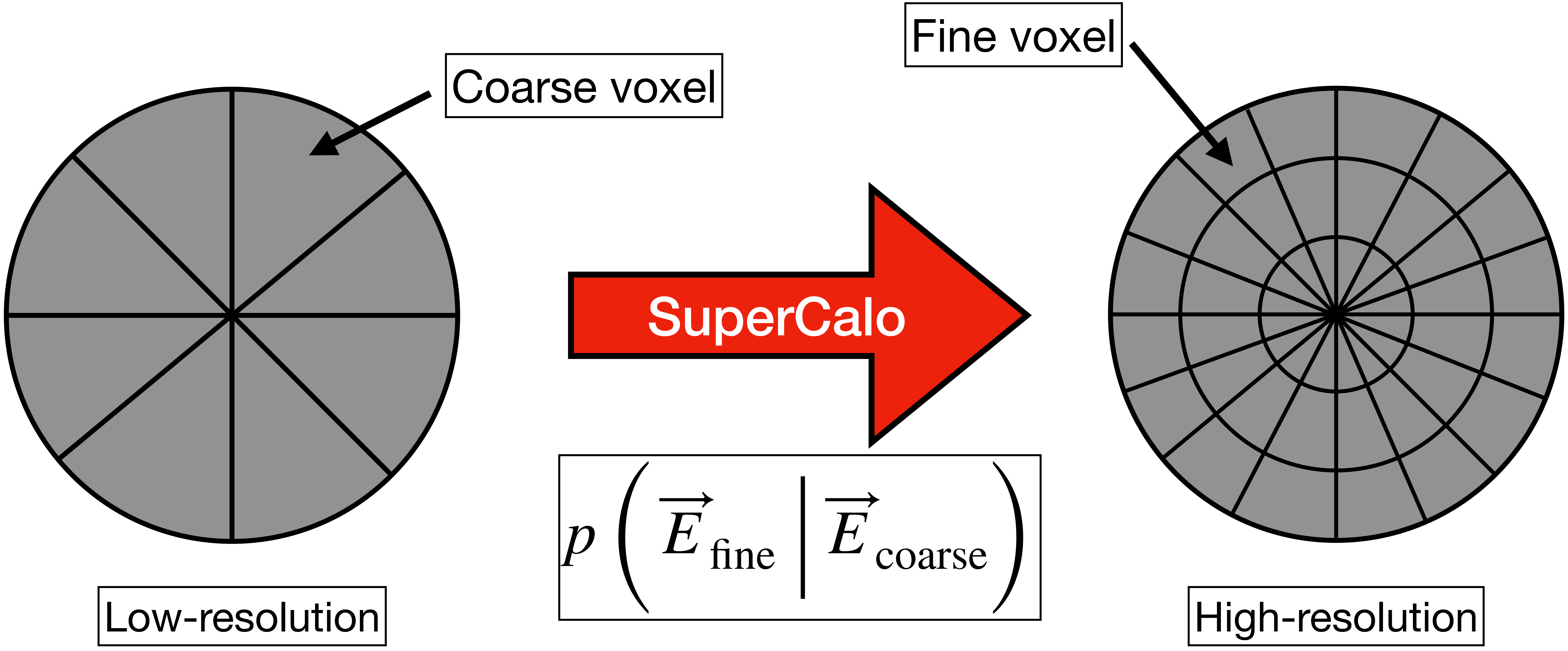

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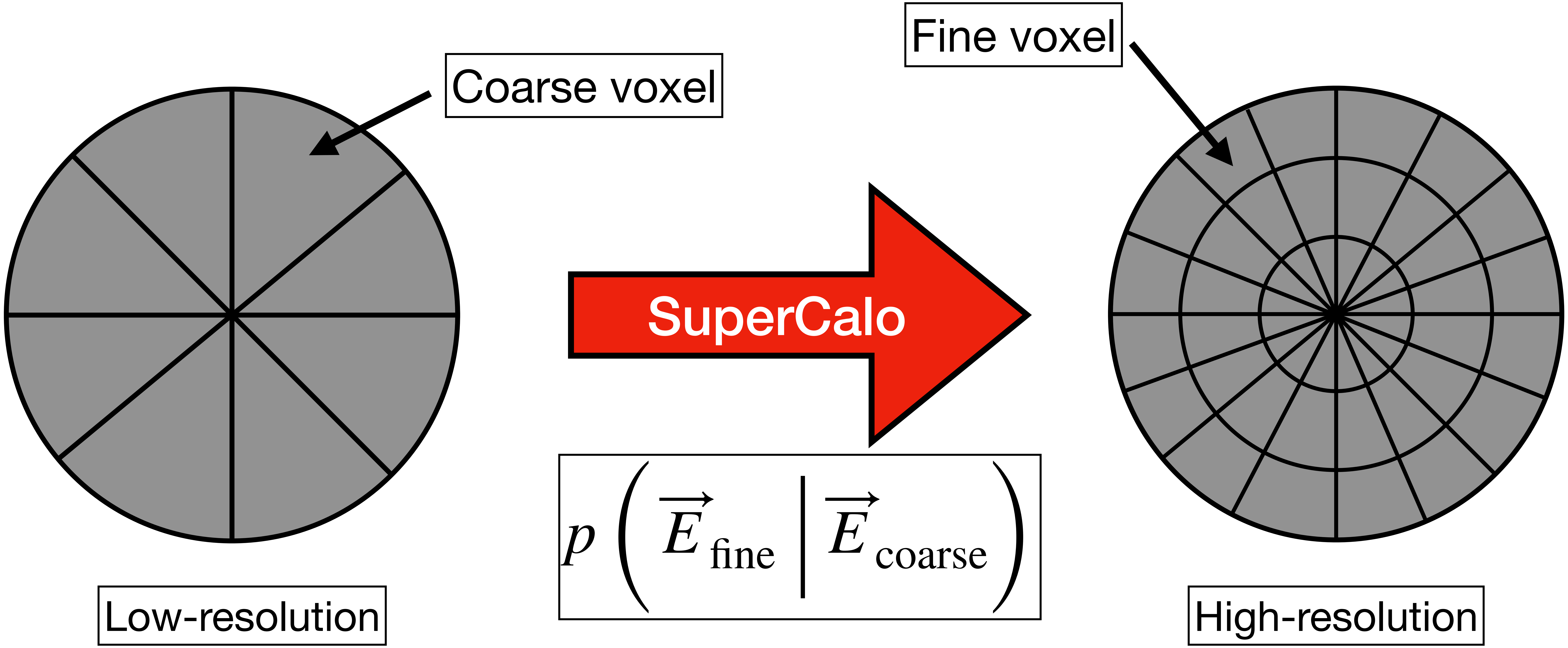

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Ansatz: $$p\left(\vec{E}_{\text{fine}} \,\middle|\, \vec{E}_{\text{coarse}}\right) = \prod_{i=1}^{N_{\text{coarse}}} q\left(\vec{e}_{\text{fine},i} \,\middle|\, E_{\text{coarse},i} \;, \ldots\right)$$

- Coarse voxel index i

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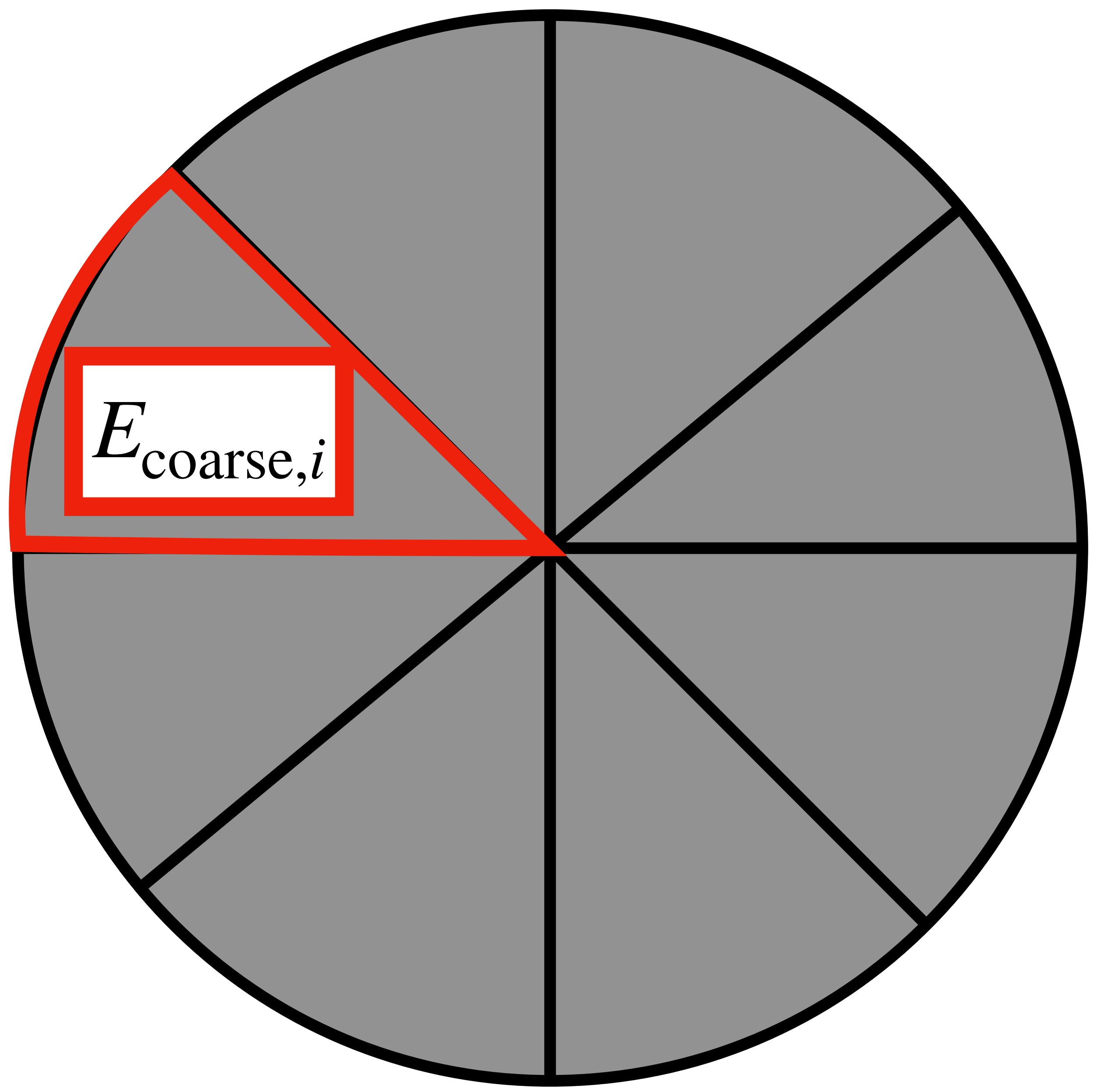

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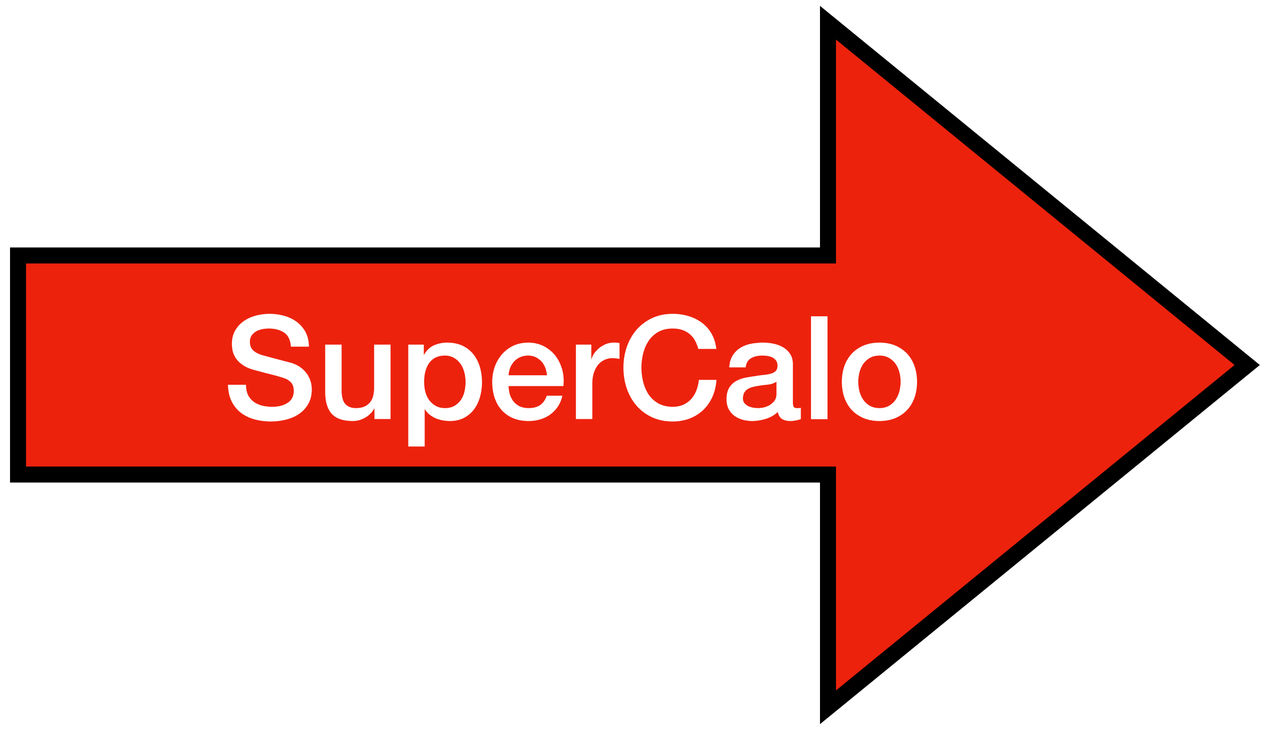

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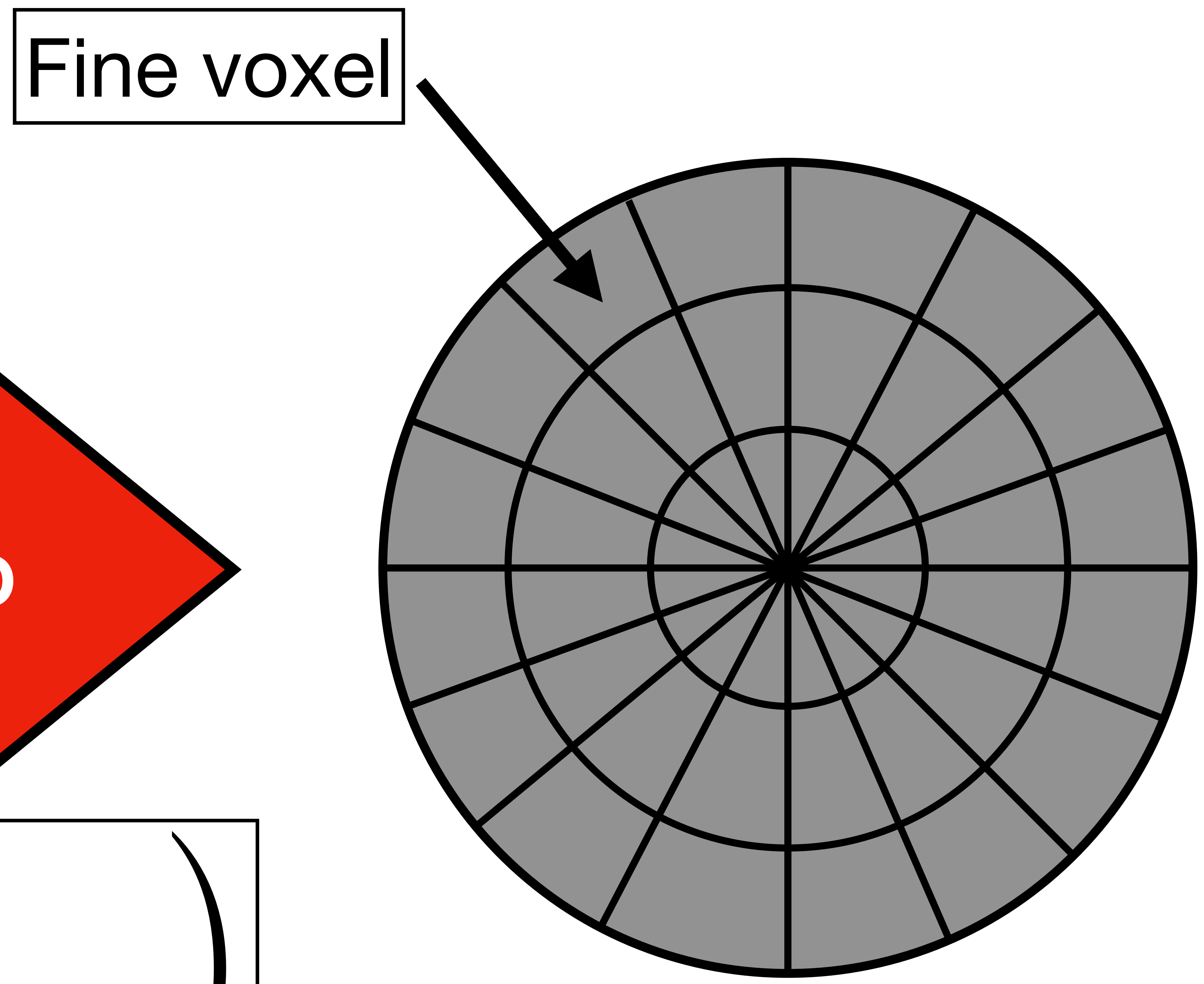

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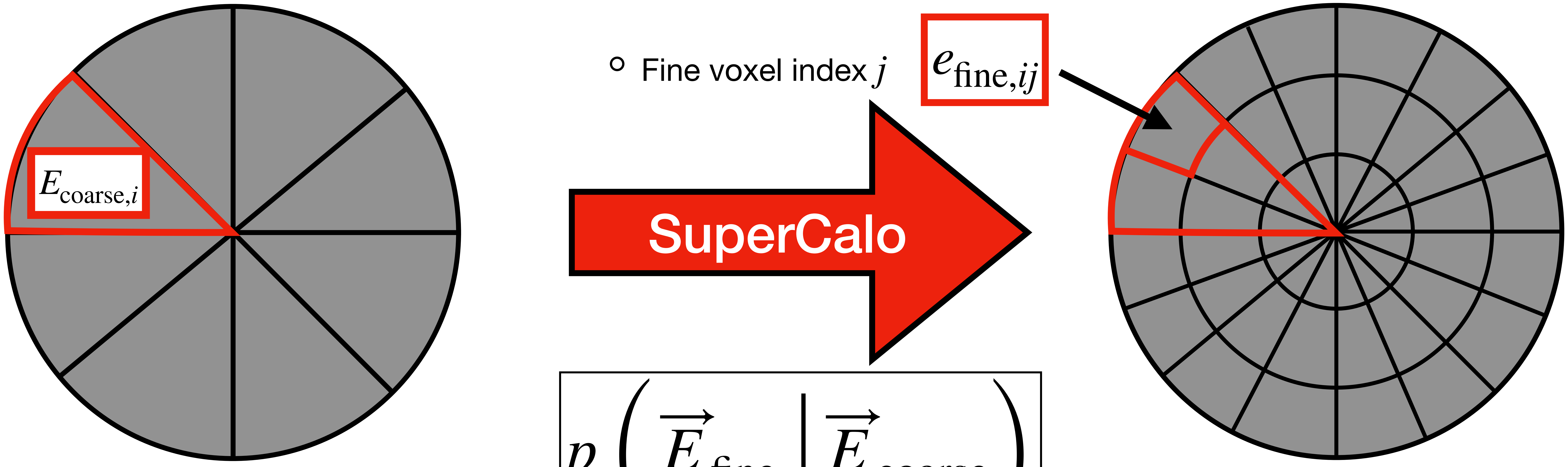

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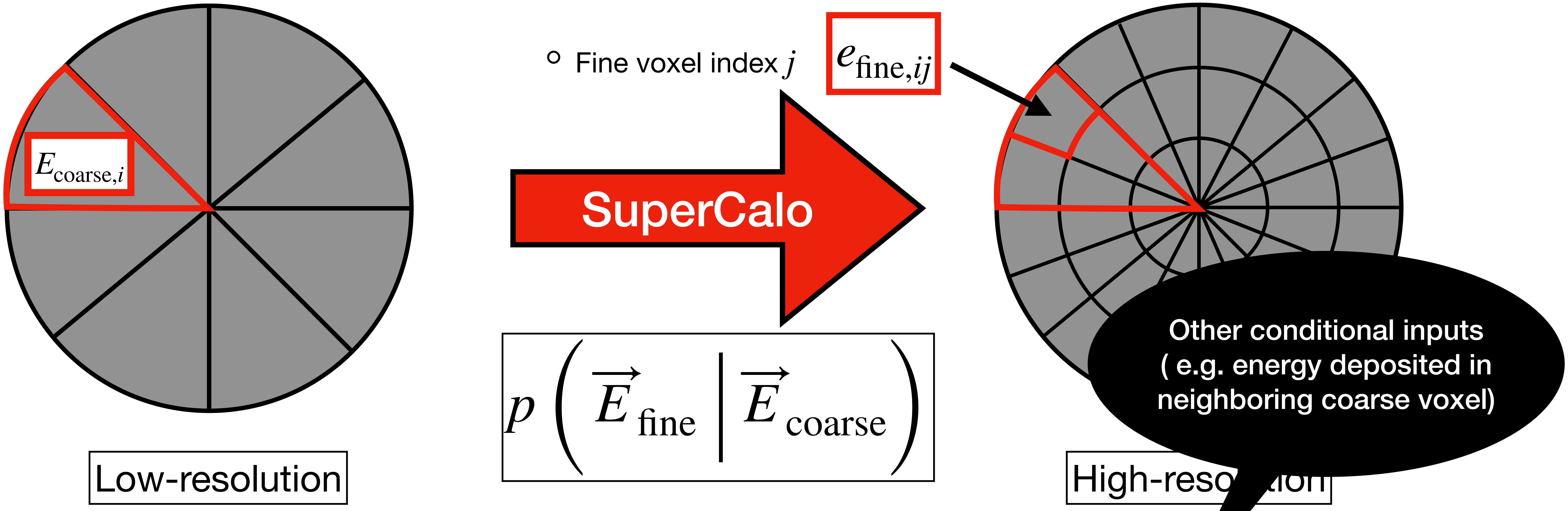

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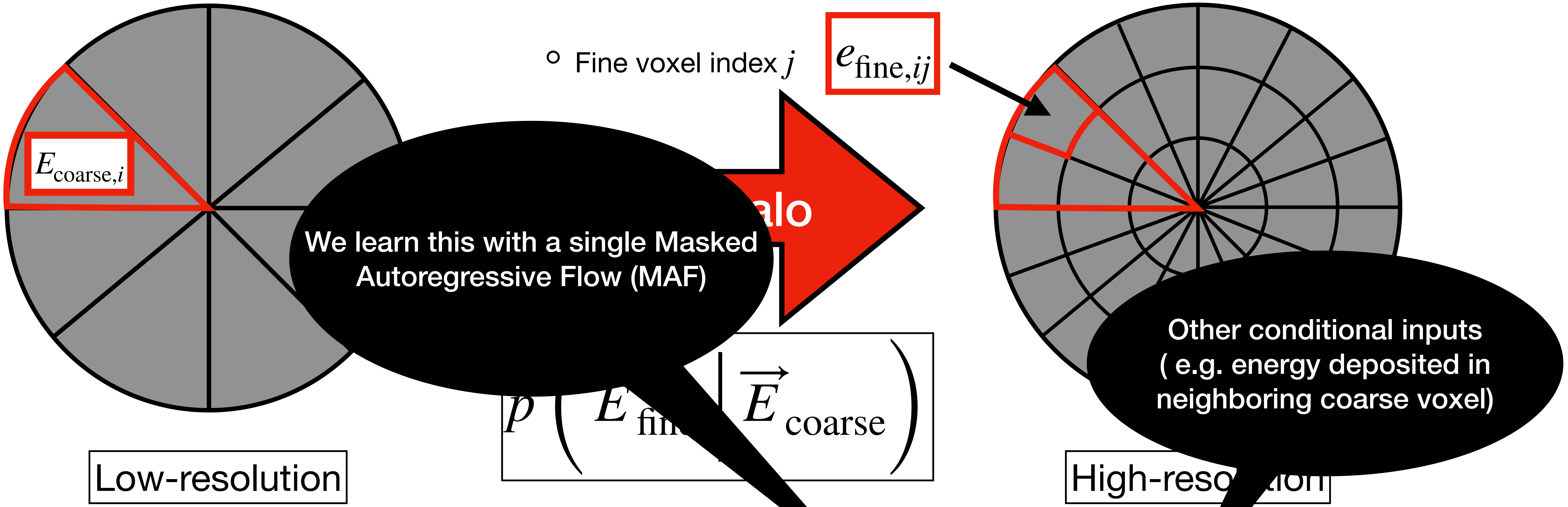

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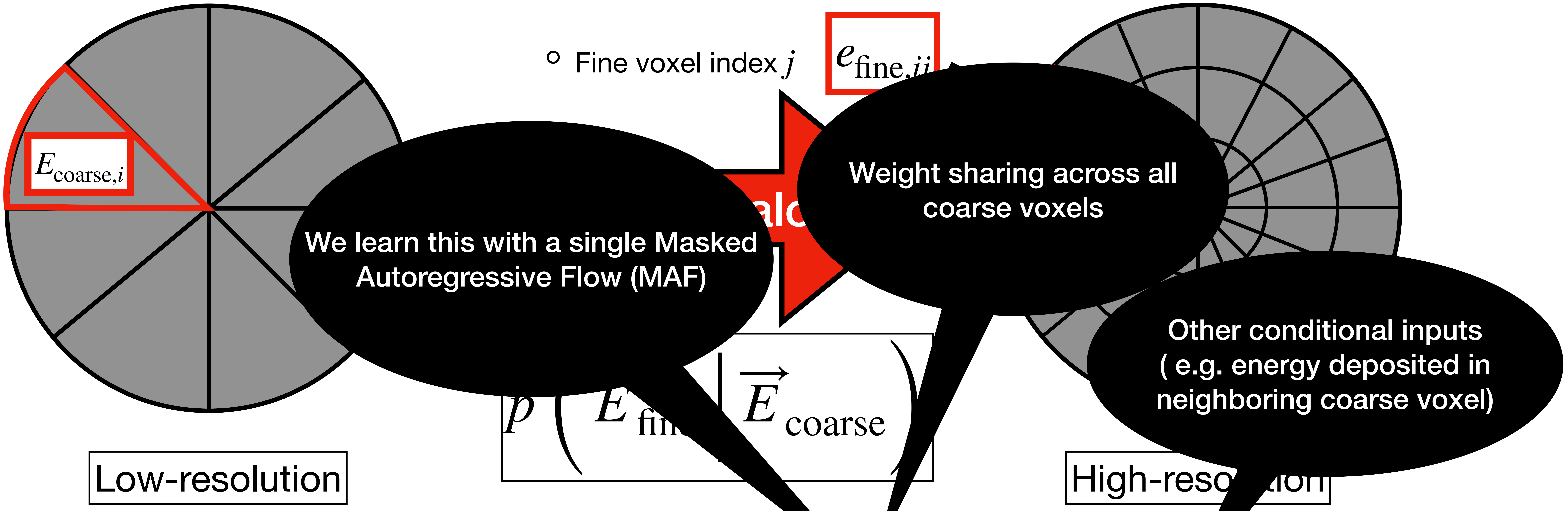

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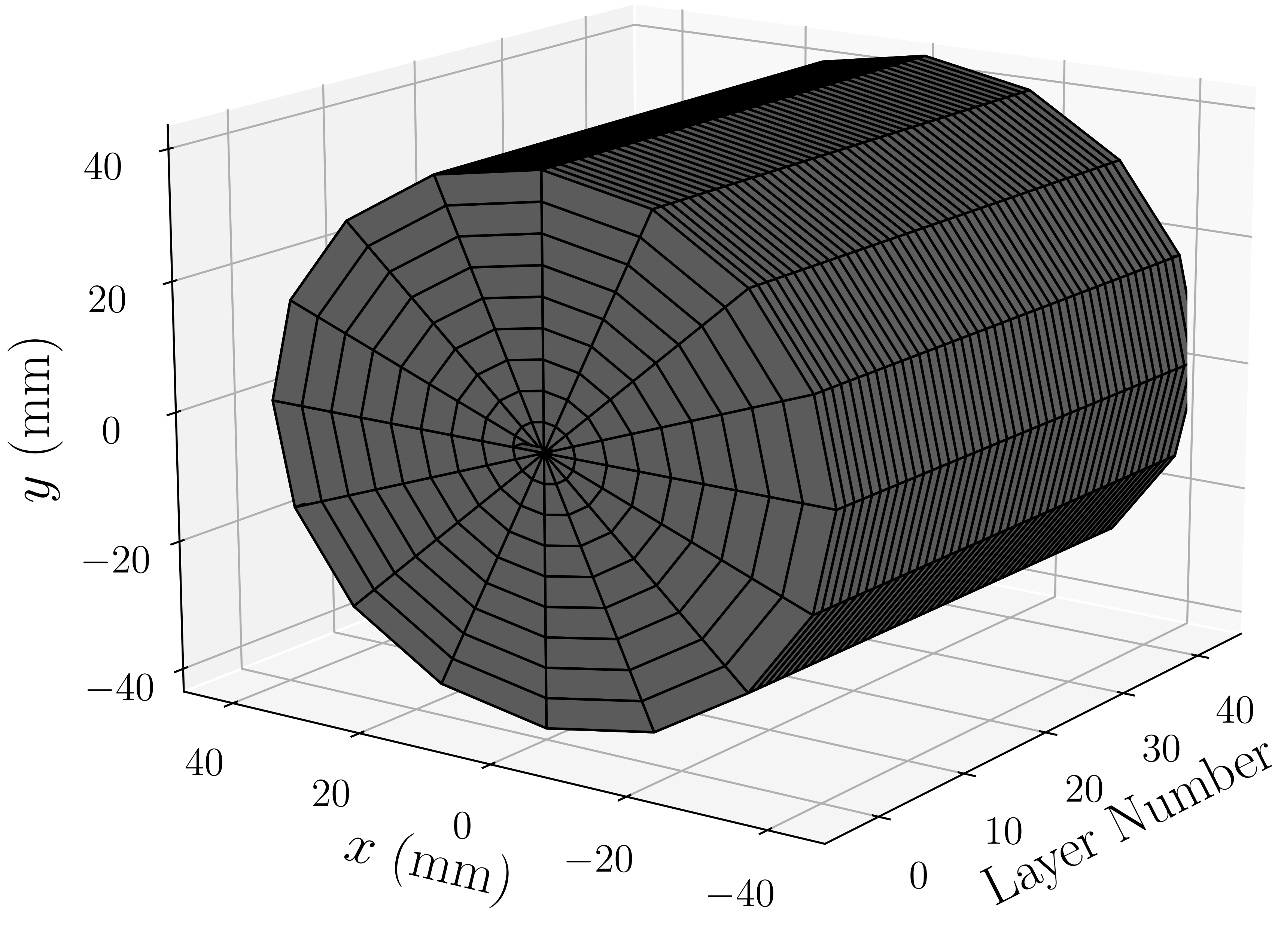
Dataset



- Dataset 2 of CaloChallenge

  M.F. Giannelli, G. Kasieczka, C. Krause, B. Nachman, D. Salamani, D. Shih, A. Zaborowska
  https://doi.org/10.5281/zenodo.6366271

- Idealized calorimeter with concentric cylinders of absorber (W) and active material (Si)

Geometry:

- **45** layers (z)
- **16** angular (α) bins
- **9** radial (r) bins

} **6480** voxels

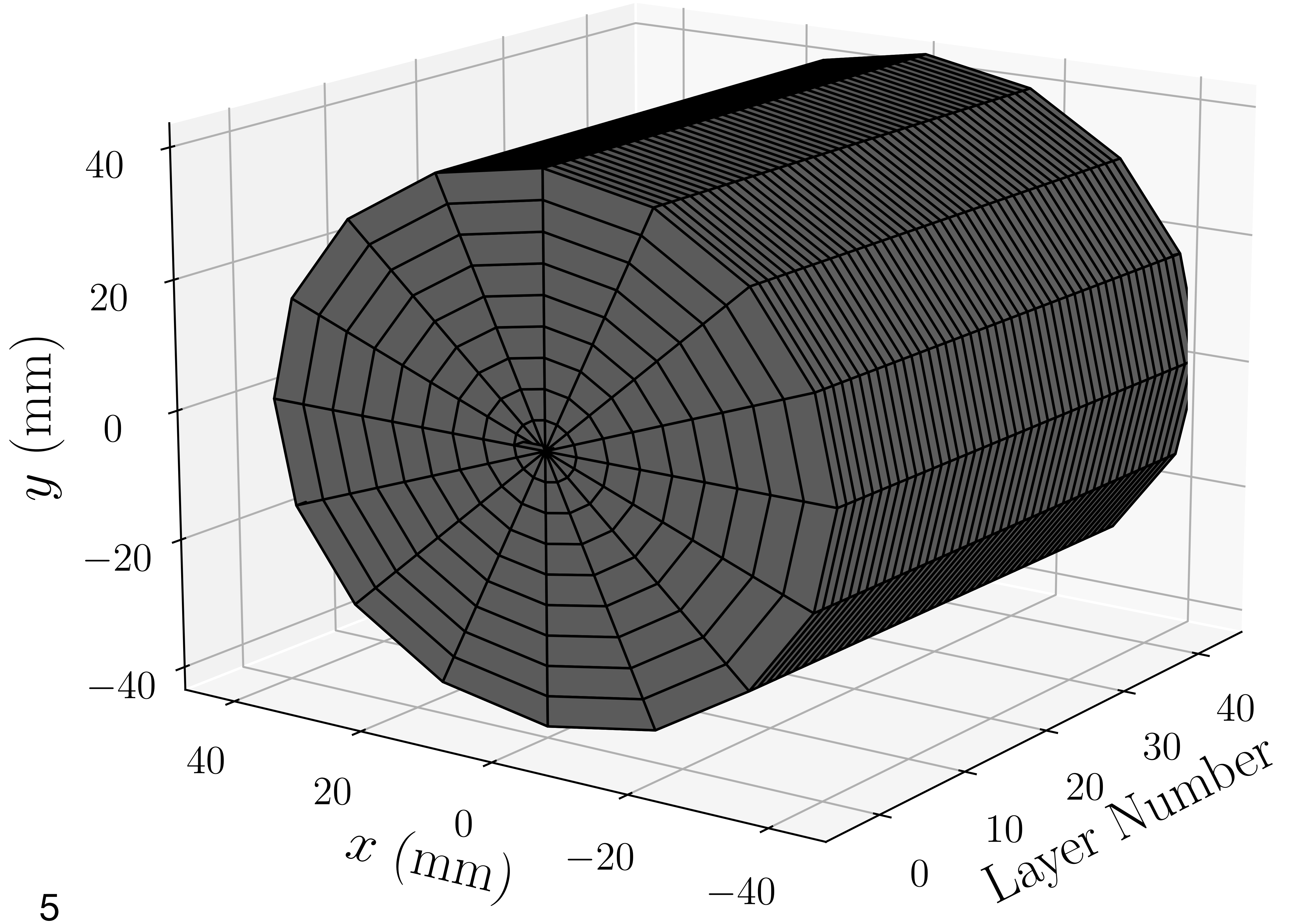
Format:

Total **100k** e^- showers

- Incident energy (1-dim) ~ [1 GeV, 1 TeV]
- Fine voxel energies (6480-dim)

Coarse voxelization

- **Many possible choices** with no obvious best choice!



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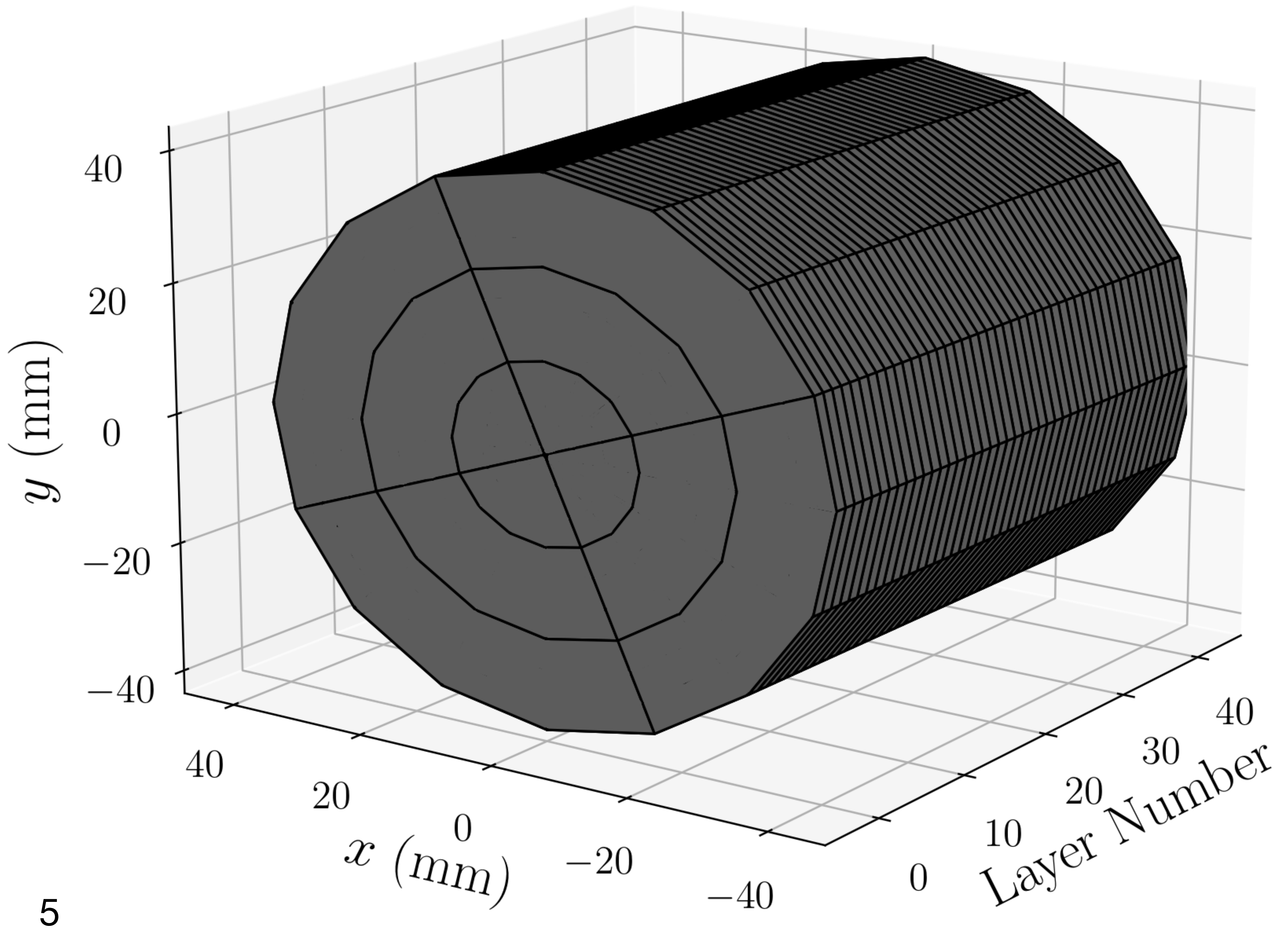

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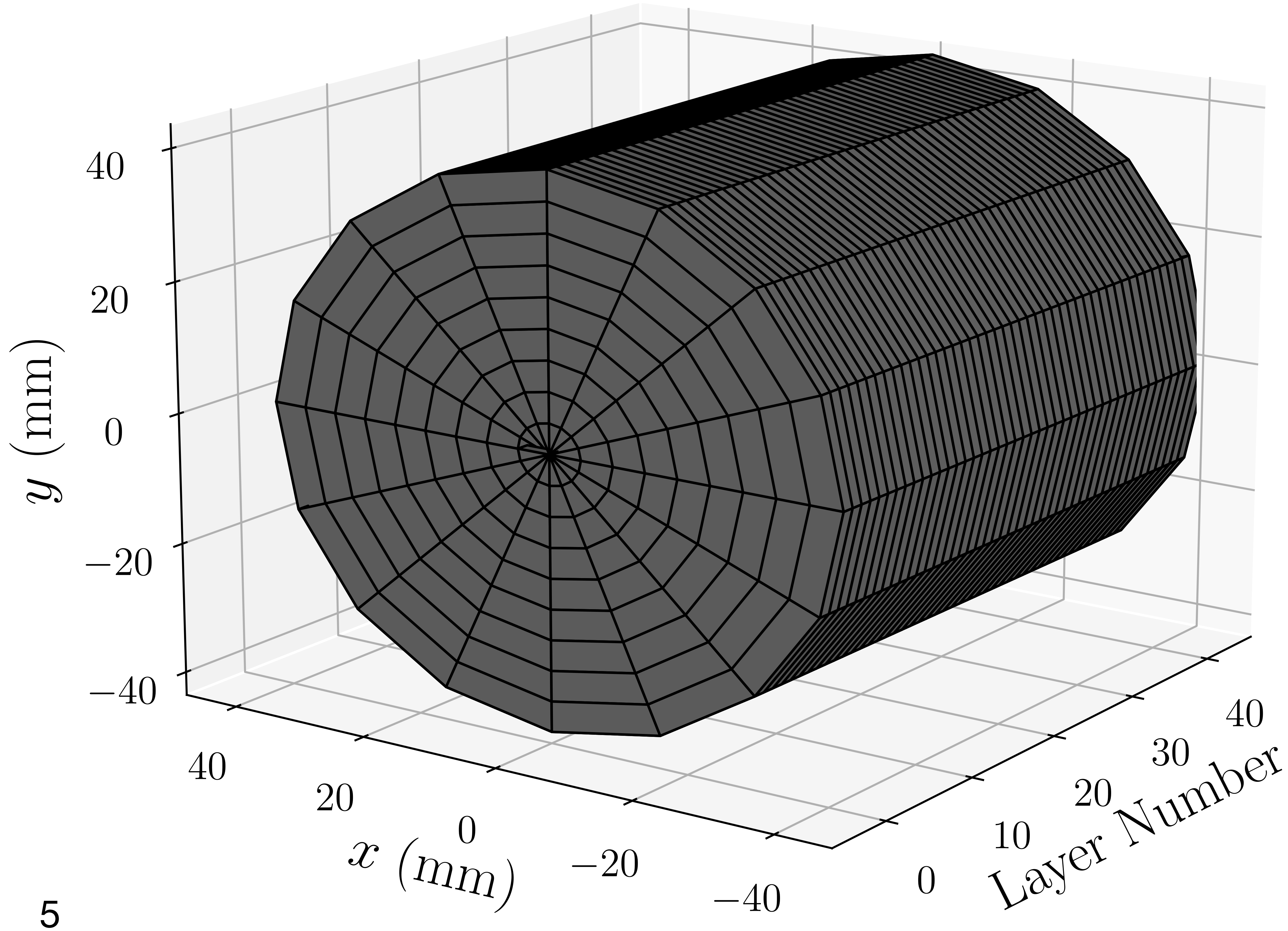


Coarse voxelization

- **Many possible choices** with no obvious best choice!

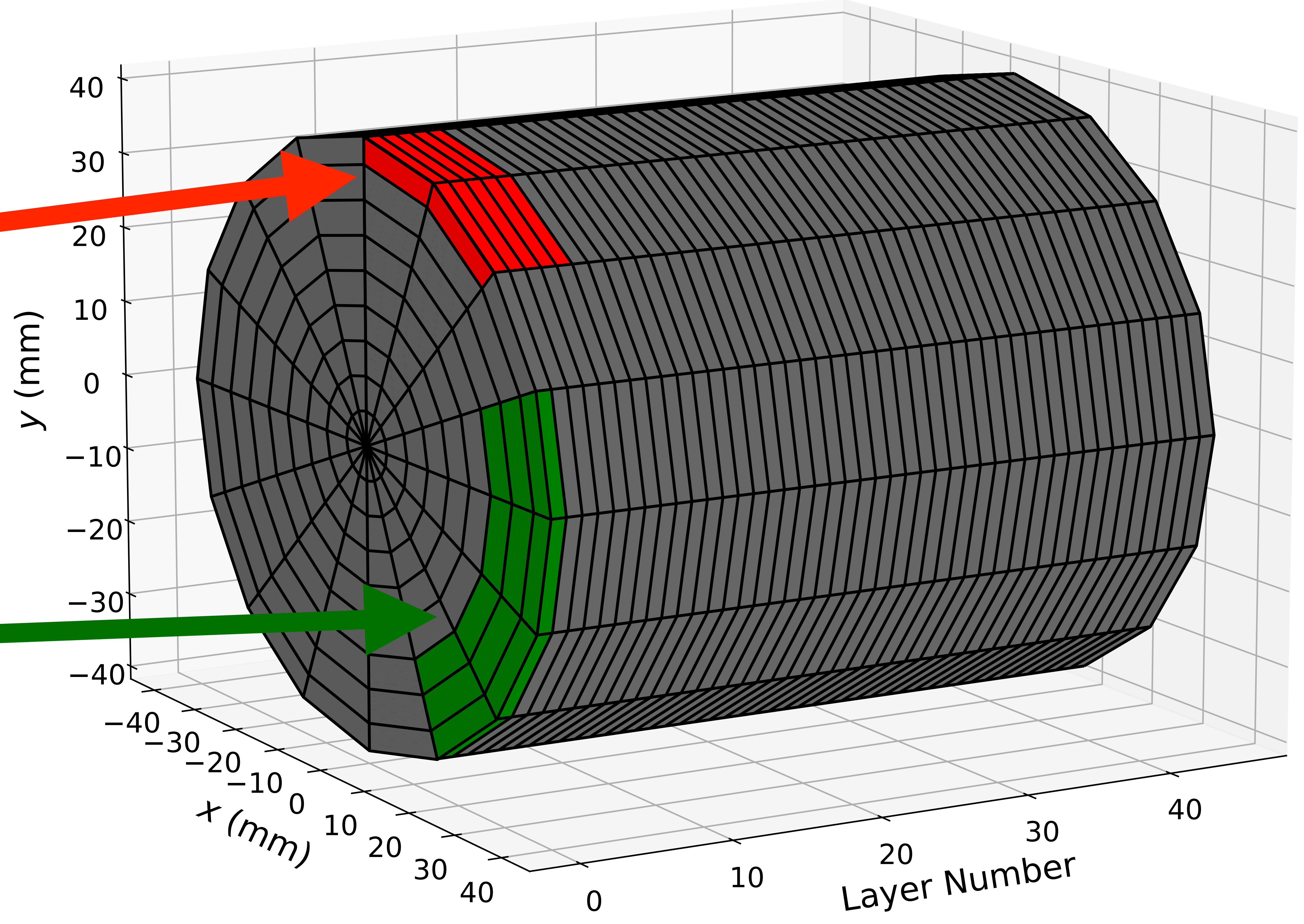
- Experimented with **two** choices:

Choice A (red) :

1 coarse voxel = 1 r × 2 α × 5 z

Choice B (green) :

1 coarse voxel = 3 r × 4 α × 1 z



Comparing coarse voxelization choices

Choice B (only group in r and α) fails to capture inter-layer correlations!

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Compute ρ

$$\rho \equiv \frac{\vec{e}^{\,(n)}_{\text{fine}} \cdot \vec{e}^{\,(n+1)}_{\text{fine}}}{\left|\vec{e}^{\,(n)}_{\text{fine}}\right| \left|\vec{e}^{\,(n+1)}_{\text{fine}}\right|}$$

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Dot product of fine voxels contained in adjacent layers*

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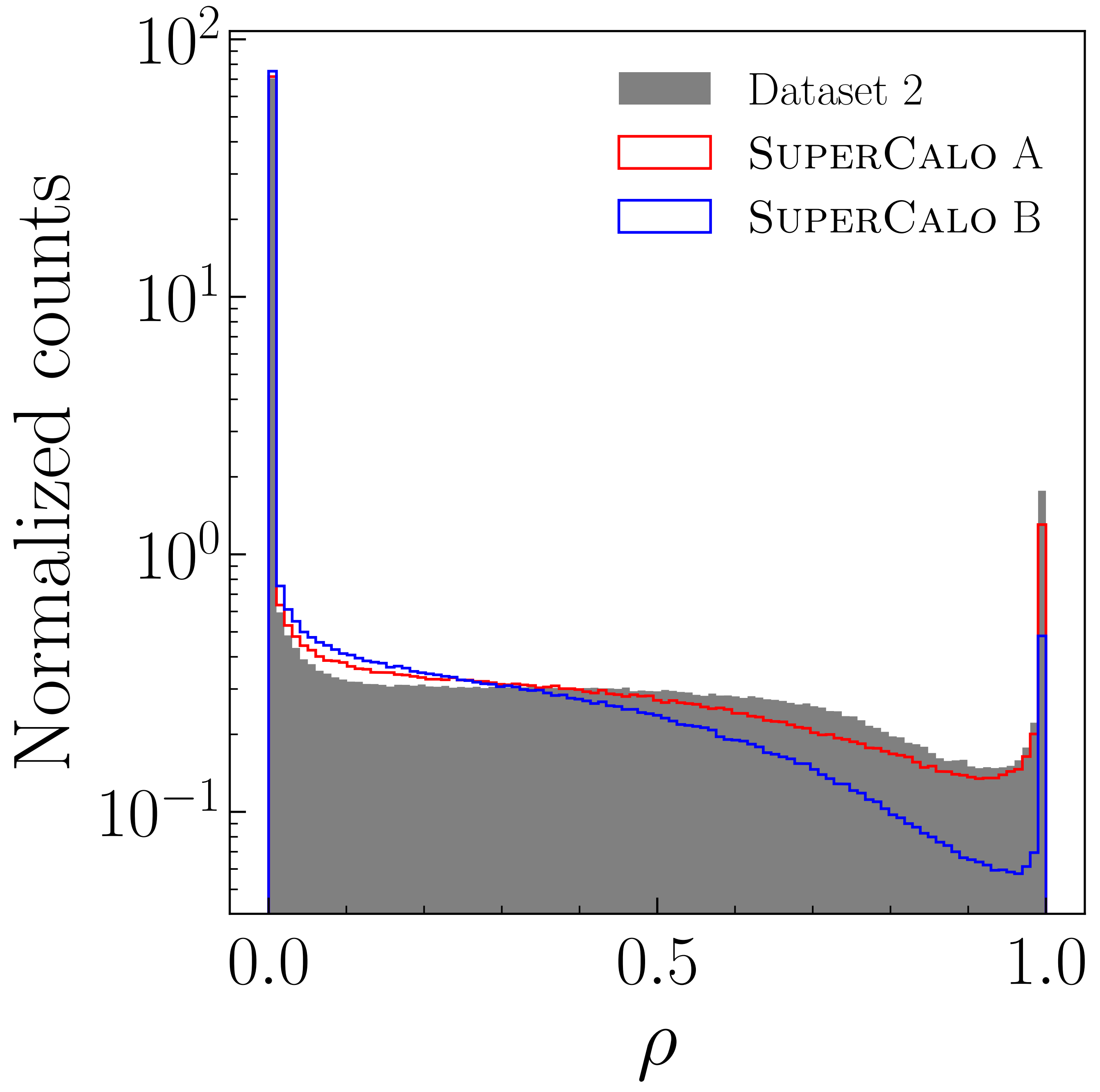

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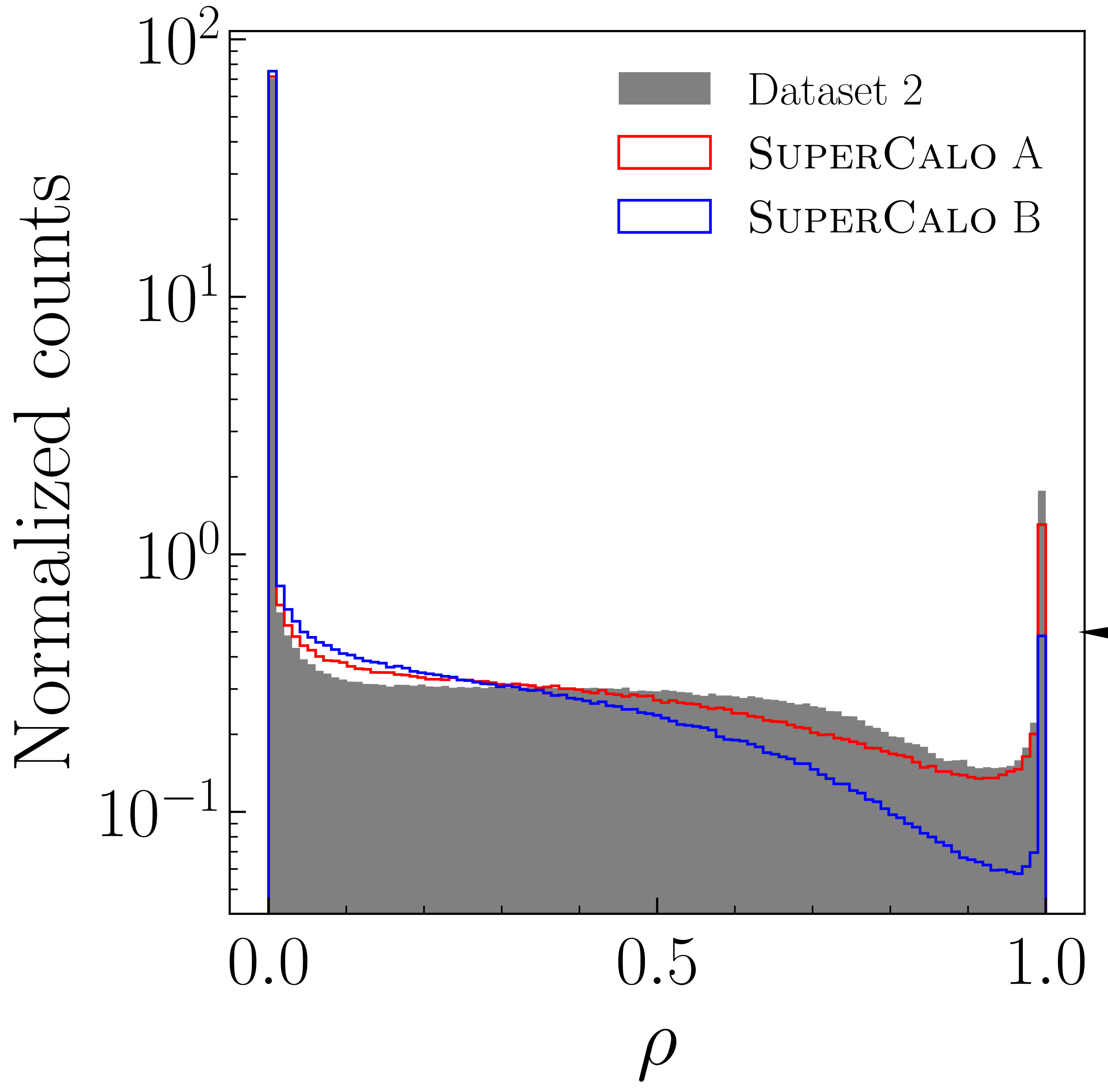

Stick with Choice A for rest of talk!

Full chain

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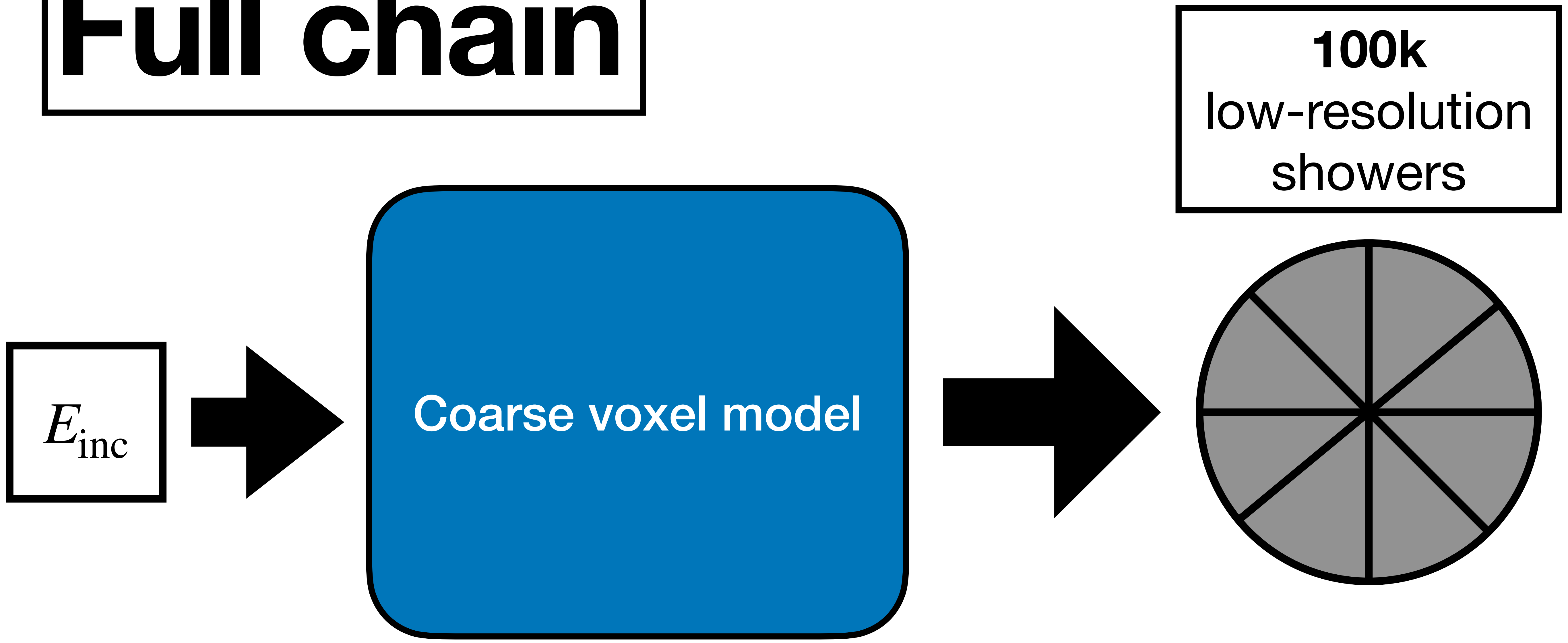

100k
low-resolution
showers
E_{inc}
Coarse voxel model

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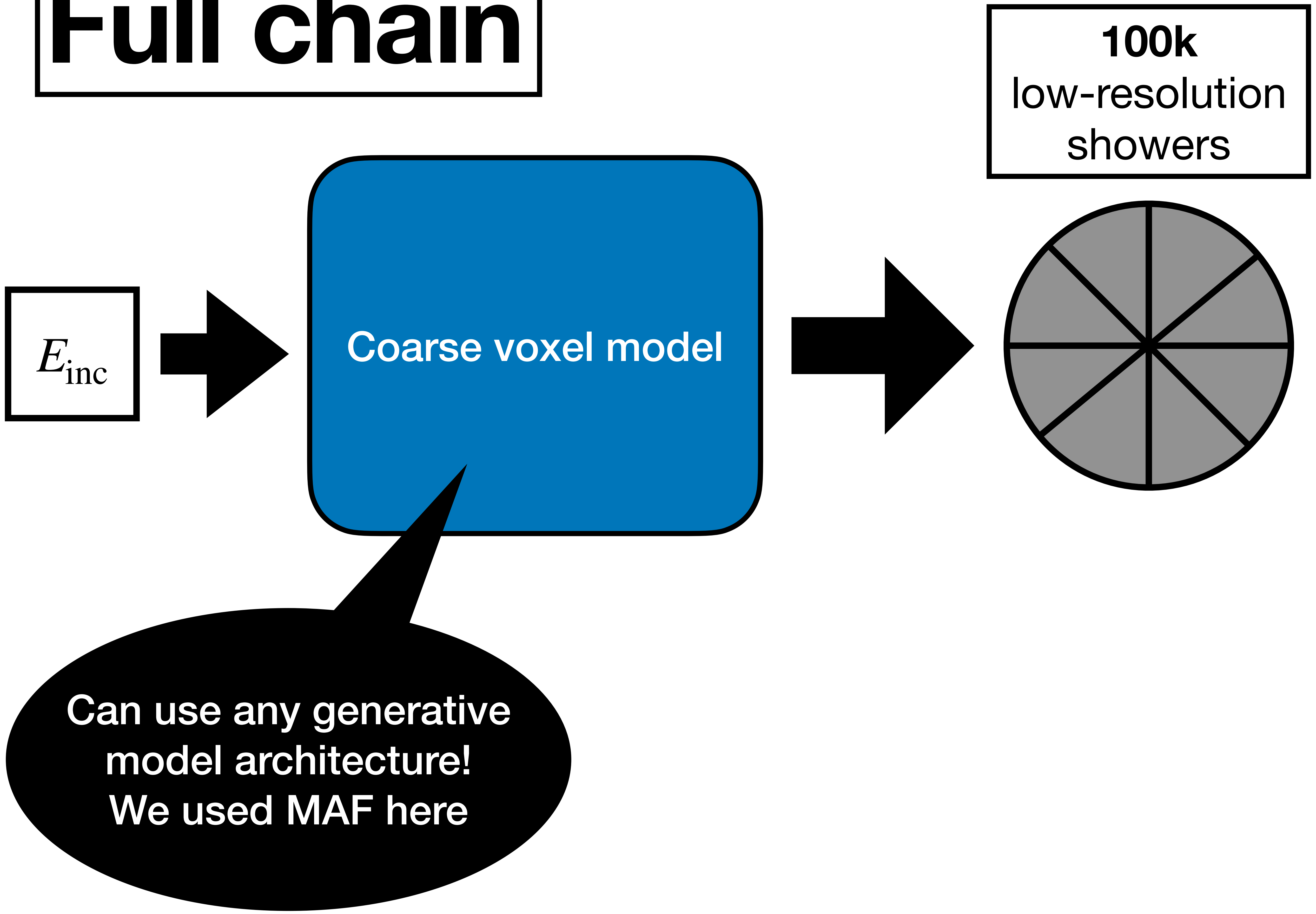
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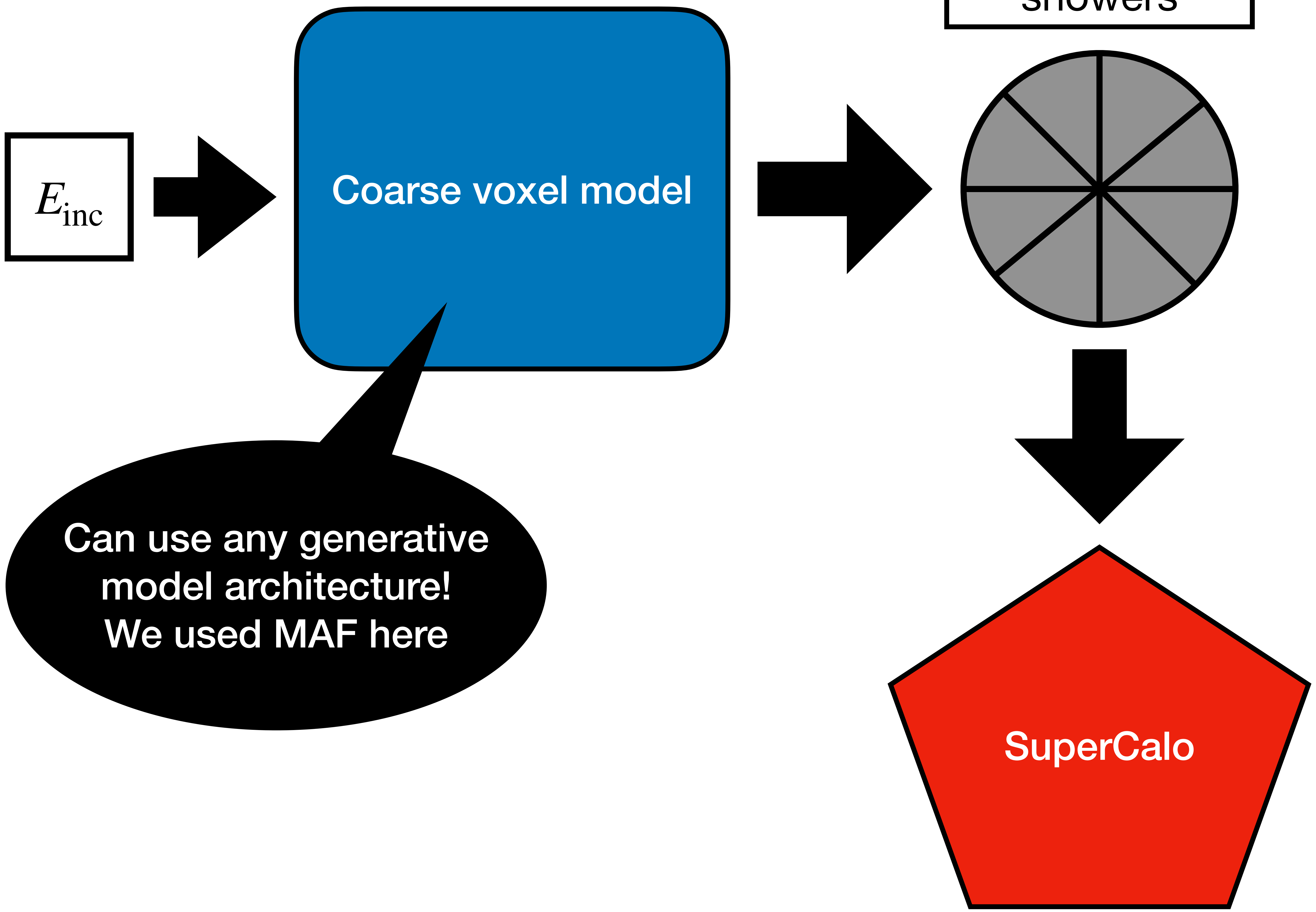
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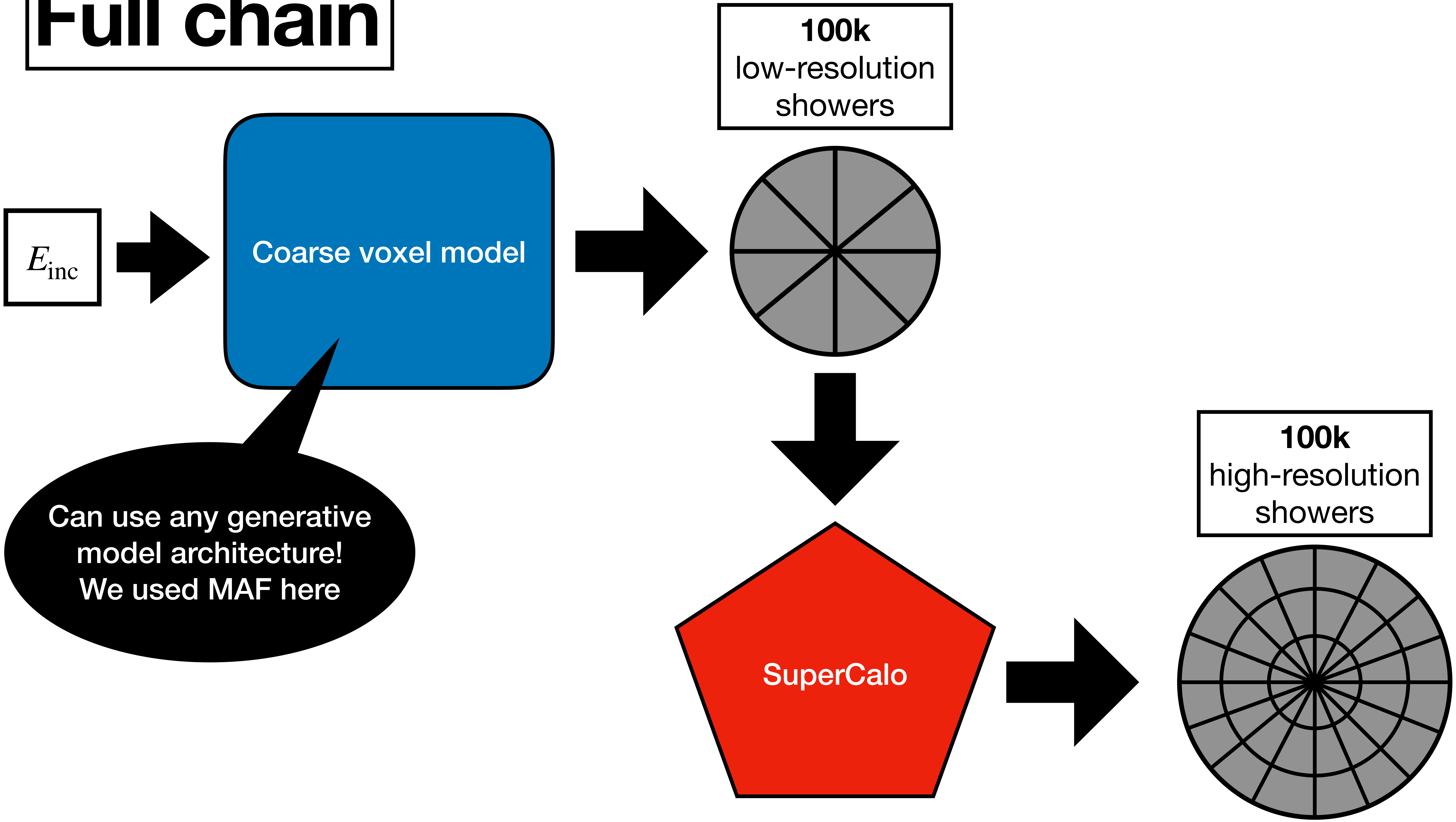

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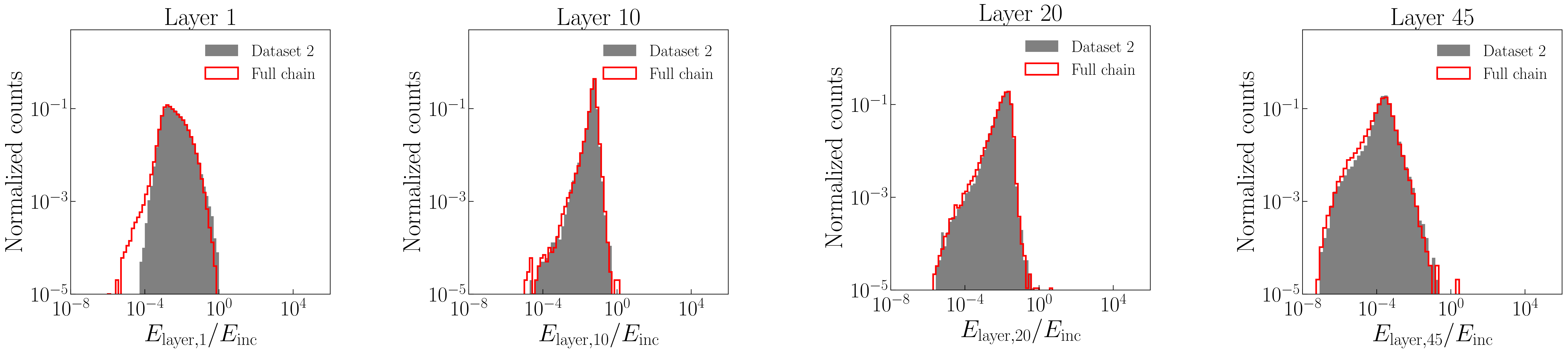
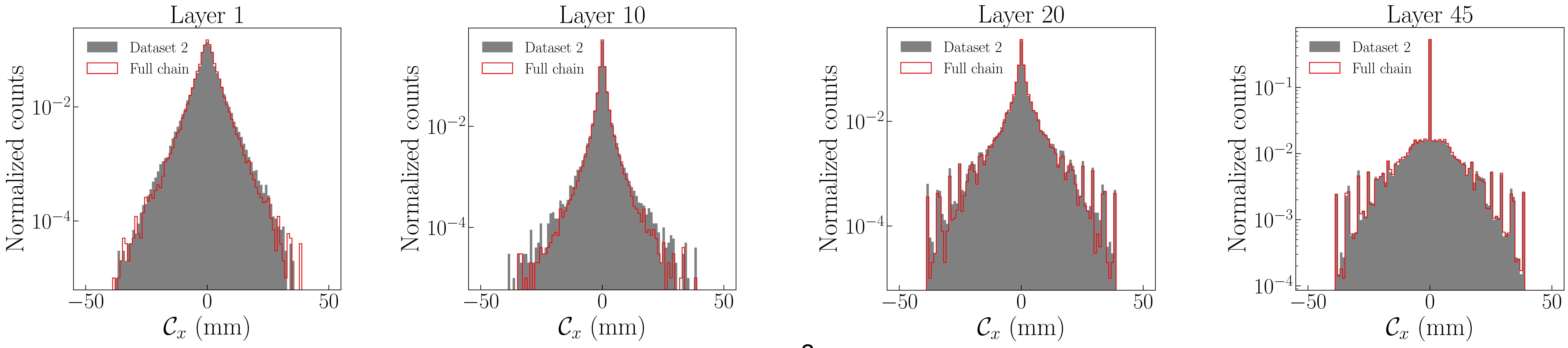
SuperCalo
100k high-resolution showers

Histograms of HLFs

Total deposited energy per layer



Shower shape (center of energy)



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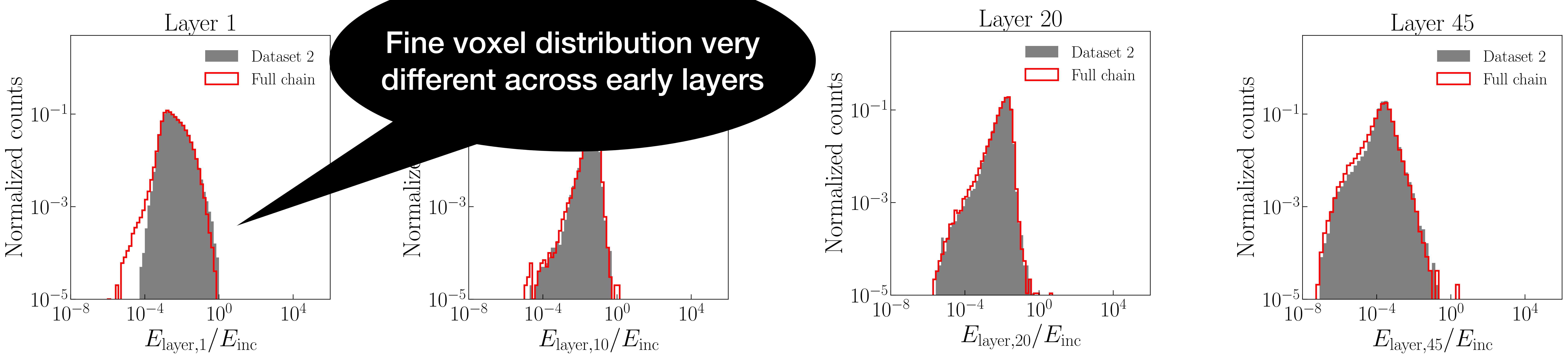

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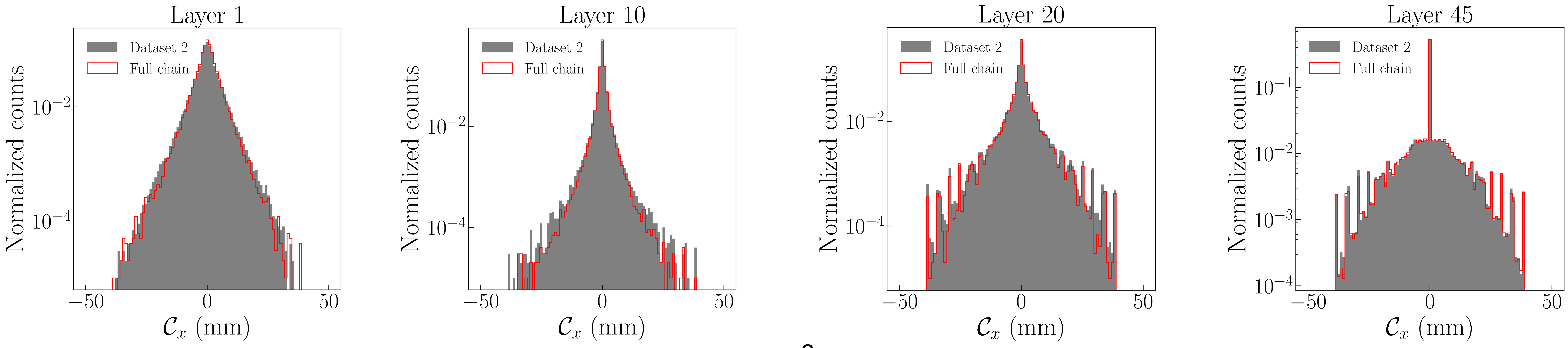

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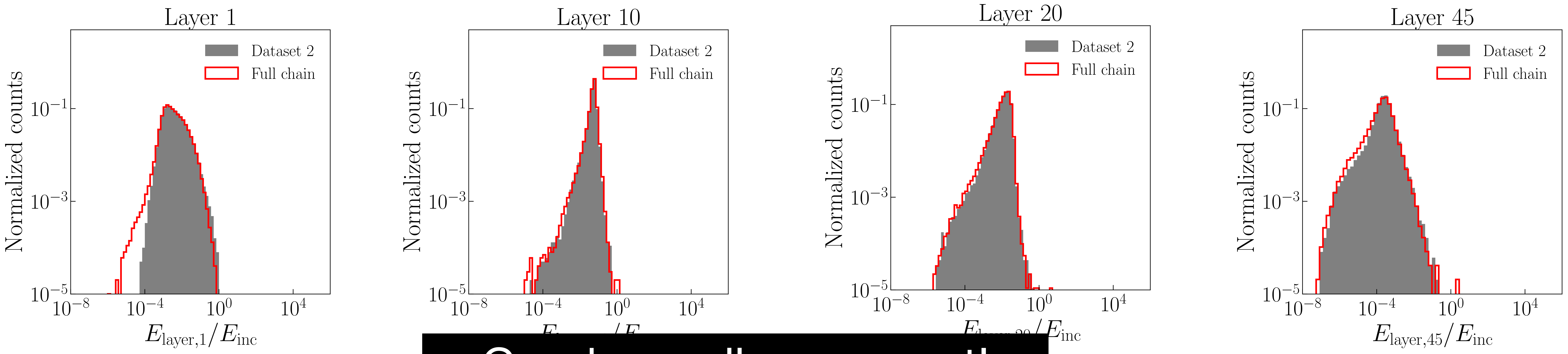
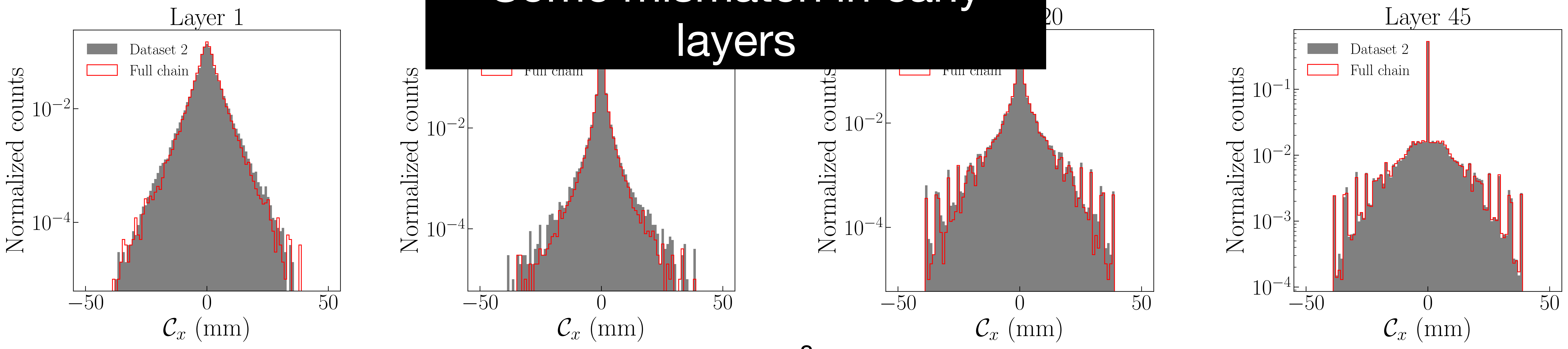


Good overall agreement!
Some mismatch in early layers



Classifier test

- According to Neyman-Pearson lemma, we have $p_{\text{GEANT4}}(x) = p_{\text{generated}}(x)$ if optimal classifier cannot distinguish between two datasets
- Trained binary classifier directly on low-level (voxels) and high-level features of SuperCalo and Geant4 samples.

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	low-level features		high-level features	
Model	AUC	JSD	AUC	JSD
Full chain	**0.726(19)**	**0.117(19)**	**0.715(3)**	**0.110(4)**
iCaloFlow	0.797(5)	0.210(7)	0.798(3)	0.214(5)

iCaloFlow [2305.11934]: M. Buckley, C. Krause, **IP**, D. Shih

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All AUC and JSD < 1
$\Longrightarrow$High-fidelity samples

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Better performance compared to another MAF-based model

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How much variation do we get from upsampling?

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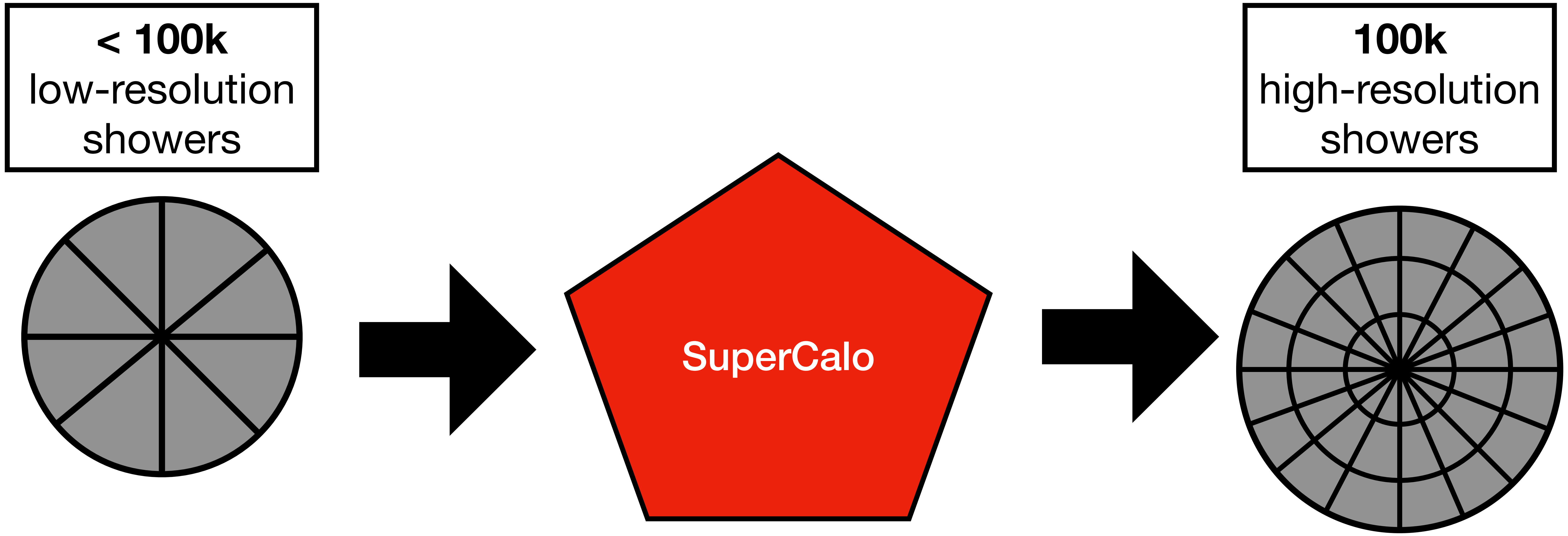

Variation study

How much variation do we get from upsampling?

Number of coarse showers	low-level features		high-level features	
	AUC	JSD	AUC	JSD
2×10^4	0.762(3)	0.160(4)	0.724(2)	0.119(3)
1×10^4	0.795(4)	0.208(6)	0.738(4)	0.135(5)
5×10^3	0.852(4)	0.310(6)	0.759(3)	0.162(3)
2×10^3	0.938(2)	0.556(7)	0.818(3)	0.255(6)
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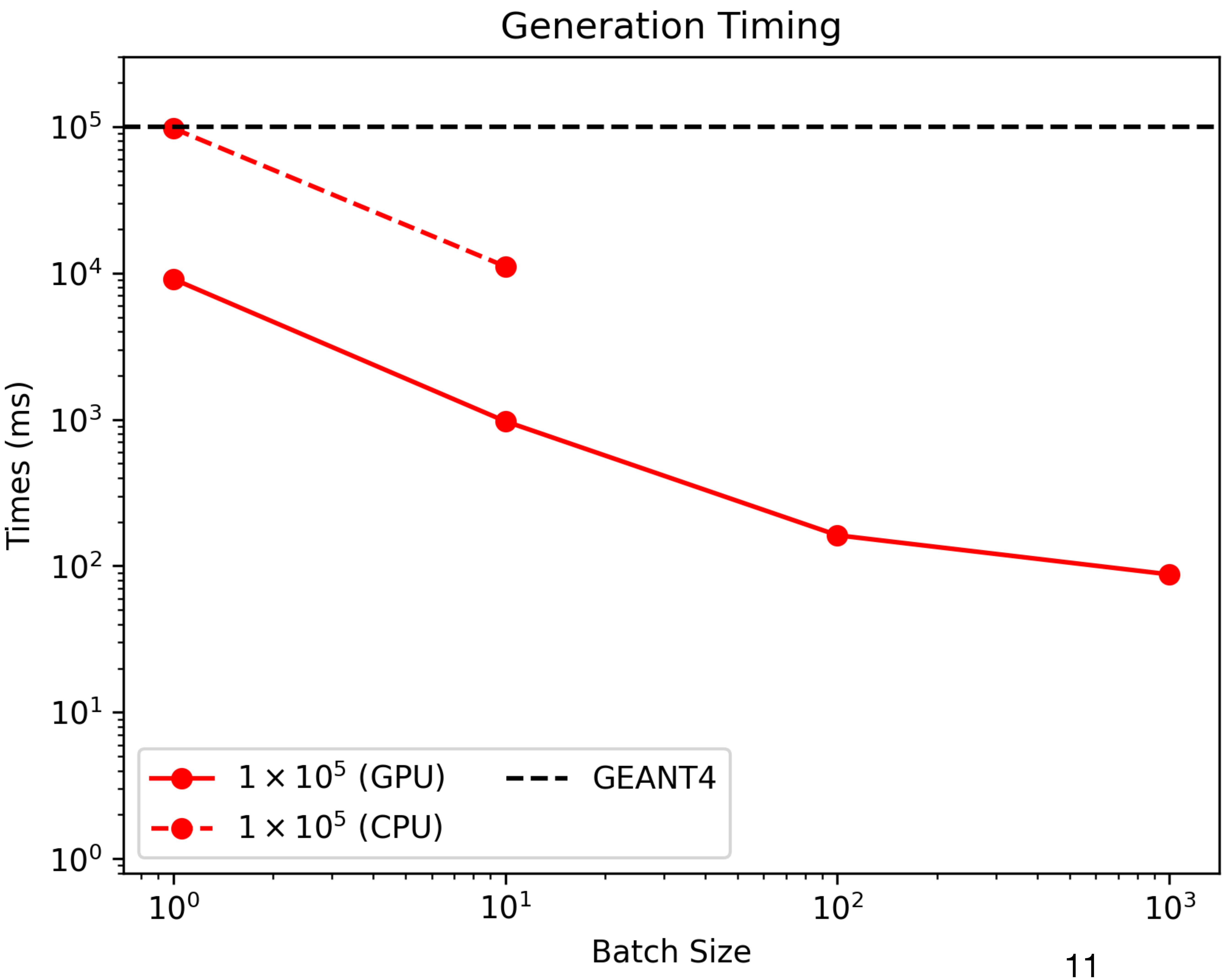
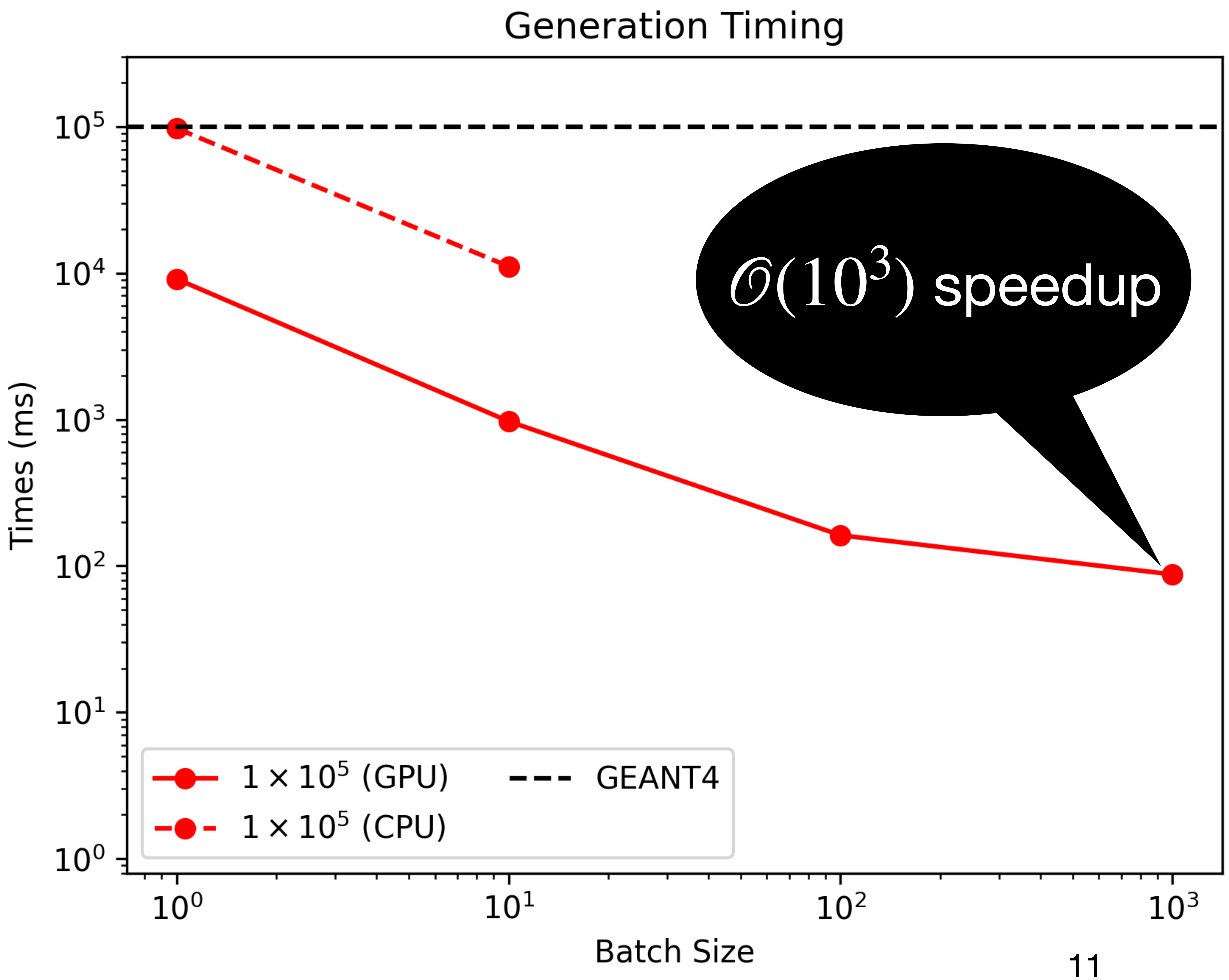
Classifier only fully catches on when we start from 1000 coarse showers!

Timing


Generation Timing
Times (ms)
Batch Size
10^0
10^1
10^2
10^3
10^4
10^5
1×10^5 (GPU)
1×10^5 (CPU)
GEANT4

Timing



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GEANT4
$\mathcal{O}(10^3)$ speedup

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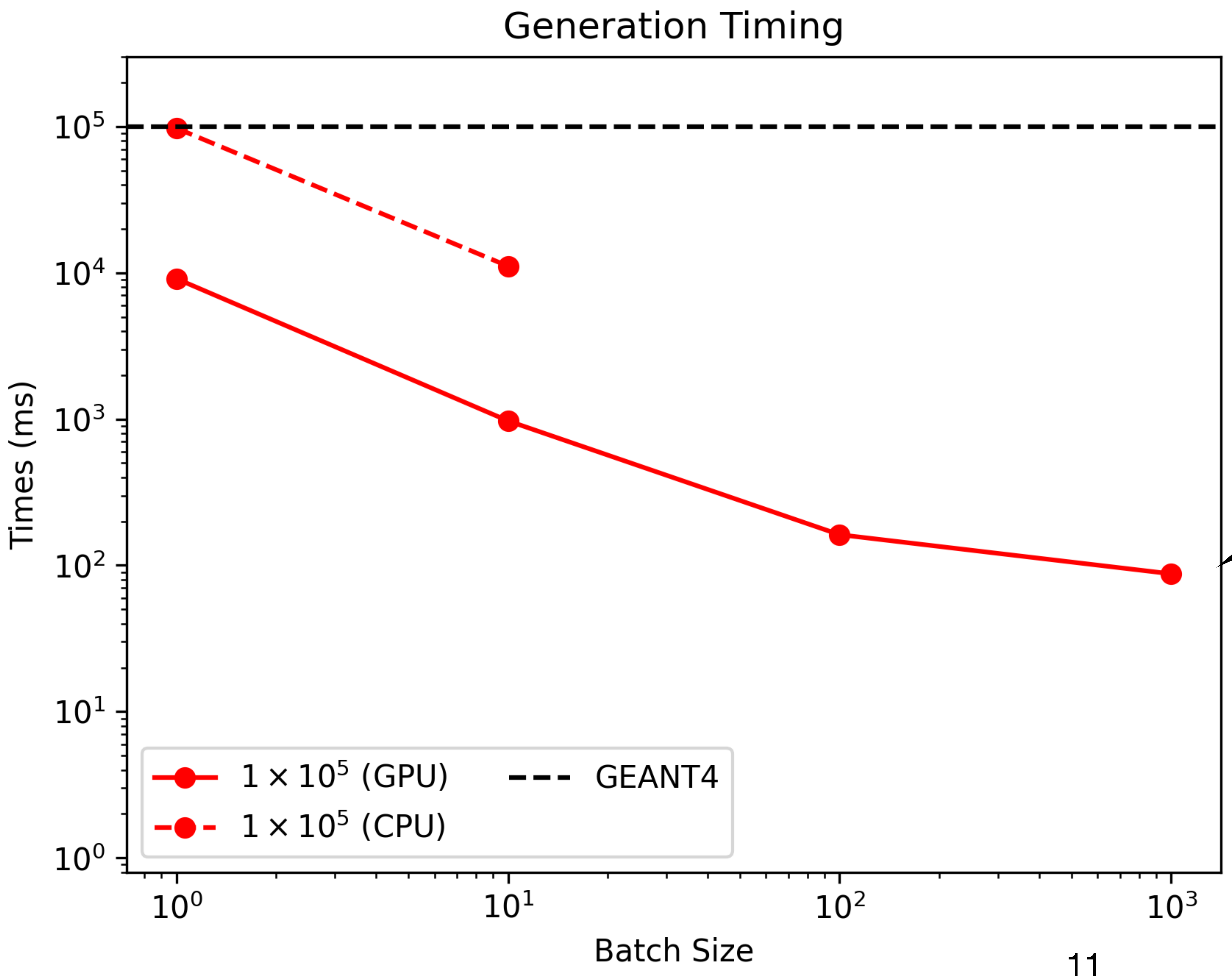

Factor of ~1.9 speedup compared to iCaloFlow MAF

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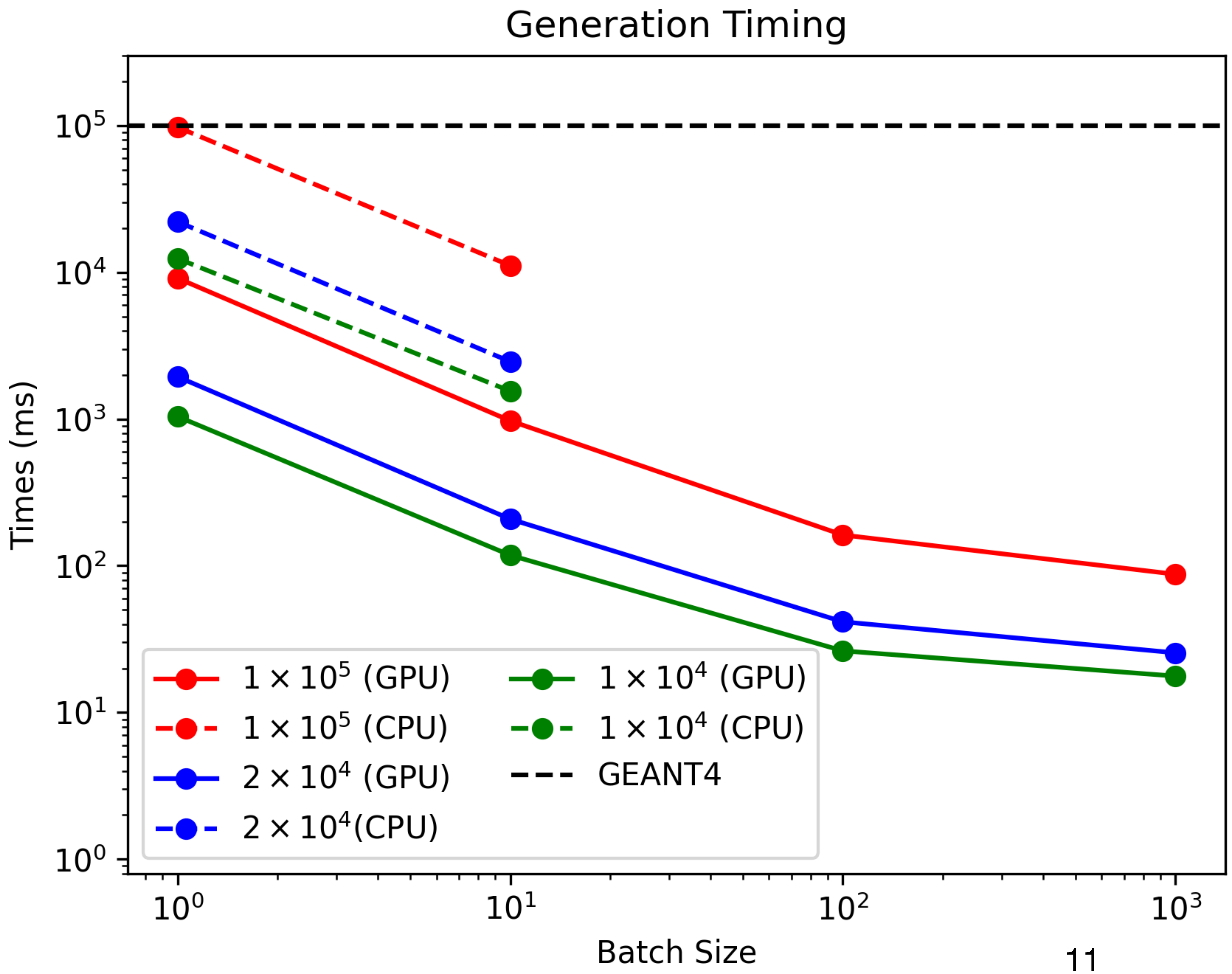


Additional speedup by resampling low-res

Conclusions and Outlook

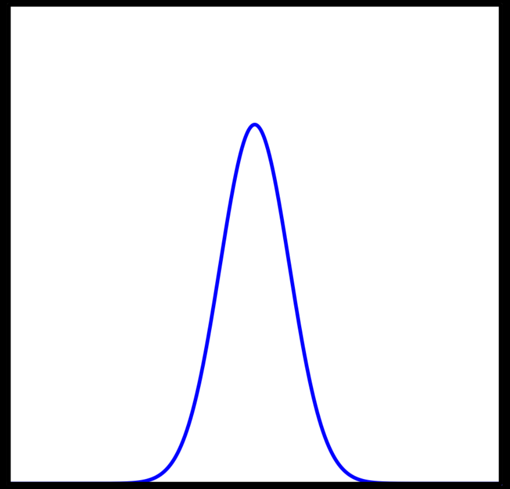
- Generate high-dim showers by **upsampling coarse showers** with SuperCalo
- Achieved $\mathcal{O}(10^3)$ **speedup** vs GEANT4 and **~1.9 speedup** vs approach with similar architecture
- SuperCalo generates high-dim showers with **substantial variation**
- SuperCalo approach can be **generalized to any** generative model architecture

Thank you!

Backup

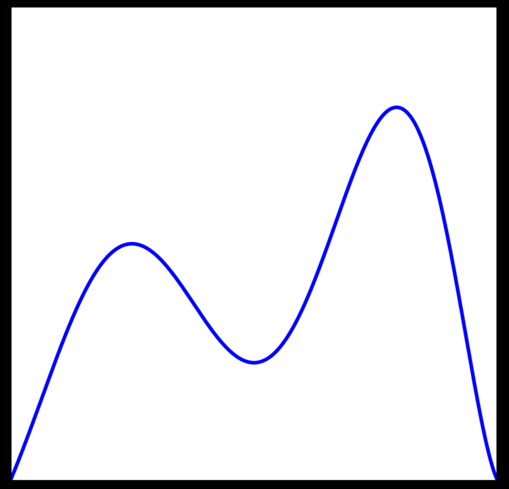
Normalizing Flows

Latent space
with simple base distribution
z ~ Z



Bijective transformation f

Data space
with more complex distribution
x ~ X



$$p(x) = \pi(f(x)) \left| \det \frac{\partial f(x)}{\partial x} \right|$$

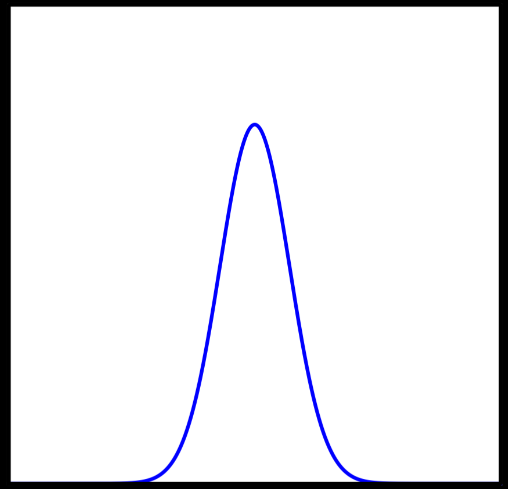
where $f(x) = z$

Density estimation, $p(x)$

Sample generation

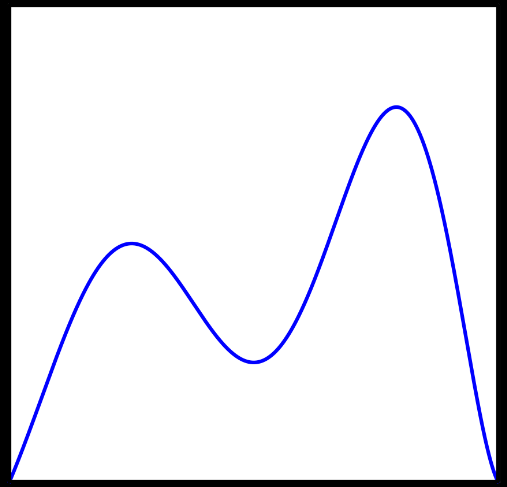
Normalizing Flows

Latent space
with simple base distribution
z ~ Z



Bijective transformation f

Data space
with more complex distribution
x ~ X



$$p(x) = \pi(f(x)) \left| \det \frac{\partial f(x)}{\partial x} \right|$$

where $f(x) = z$

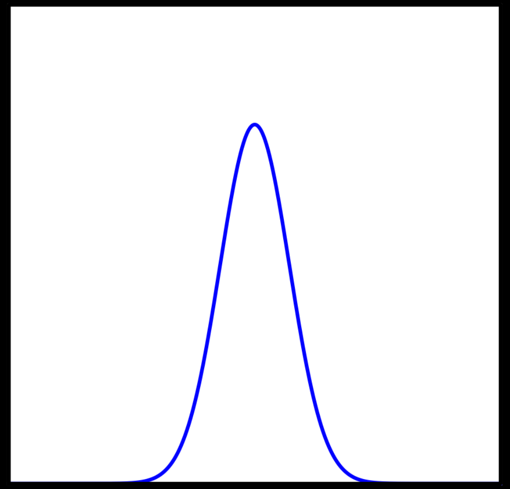
Needs to be tractable!

Density estimation, $p(x)$

Sample generation

Normalizing Flows

Latent space
with simple base distribution
z ~ Z



Bijective transformation f

$$p(x) = \pi(f(x)) \left| \det \frac{\partial f(x)}{\partial x} \right|$$

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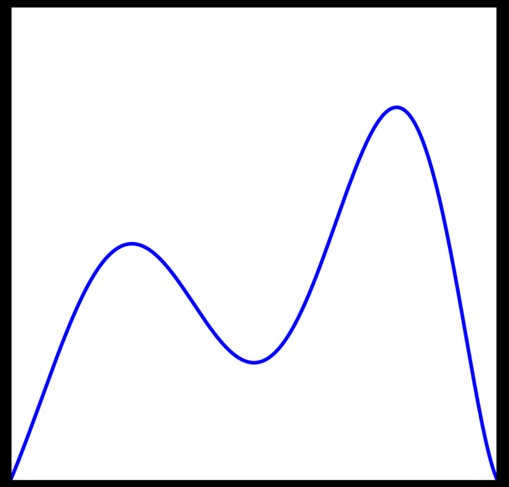
Data space
with more complex distribution
x ~ X



Density estimation, $p(x)$

Sample generation

Conditional inputs

1. Incident energy of the incoming particle, E_{inc}
2. Deposited energy in coarse voxel i, $E_{\text{coarse},i}$
3. Fine layer energies of layers spanned by coarse voxel i
4. Deposited energy in neighboring coarse voxels in α, r and z directions
5. One-hot encoded coarse layer number
6. One-hot encoded coarse radial bin

Architecture and training

- **MAF-RQS** flows for all models
- Noise added to voxels during training
  - Uniform random of noise **[0, 1] keV**
- LR schedule: **OneCycle LR**

Model	dim of base distribution	number of MADE blocks	layer sizes: input	layer sizes: hidden	layer sizes: output	number of RQS bins	RQS tail bound
Flow-1	45	8	256	1×256	1035	8	14
Flow-2	648	8	648	1×648	14904	8	6
SuperCalo A	10	8	128	2×128	230	8	14
SuperCalo B	12	8	128	2×128	276	8	14

Pre-processing

- Flow-1
  - **Log**-transformed E_{inc} (E_{inc} normalized by constant) $E_{\mathrm{inc}} \to \log_{10} \frac{E_{\mathrm{inc}}}{10^{4.5}\ \mathrm{MeV}} \in [-1.5, 1.5].$
  - **Logit**-transformed $E_{\mathrm{layer},i}$ ($E_{\mathrm{layer},i}$ normalized by constant) $E_{\mathrm{layer},i} \to x_i \equiv (E_{\mathrm{layer},i} + \mathrm{rand}[0, 5\ \mathrm{keV}])/65\ \mathrm{GeV}$

$$y_i = \log \frac{u_i}{1-u_i}, \quad u_i \equiv \alpha + (1-2\alpha)x_i,$$

- Flow-2
  - **Log**-transformed $E_{\mathrm{coarse},i}$ ($E_{\mathrm{coarse},i}$ normalized by constant) $E_{\mathrm{coarse},i} \to \log_{10}\left((E_{\mathrm{coarse},i} + \mathrm{rand}[0, 5\ \mathrm{keV}])/E_{\mathrm{coarse,max}}\right)+6$
  - **Log**-transformed $E^{(\mathrm{coarse})}_{\mathrm{layer},i}$ $E^{(\mathrm{coarse})}_{\mathrm{layer},i} \to \frac{1}{4} \log_{10}\left(E^{(\mathrm{coarse})}_{\mathrm{layer},i}\right)$

Pre-processing

- SuperCalo
  - **Logit**-transformed $E_{\mathrm{coarse},i}$ ($E_{\mathrm{coarse},i}$ normalized by constant)

$$E_{\mathrm{coarse},i} \to \tilde{x}_i \equiv (E_{\mathrm{coarse},i} + \mathrm{rand}[0, 1\ \mathrm{keV}])/E_{\mathrm{coarse,max}}$$

$$\tilde{y}_i = \log \frac{\tilde{u}_i}{1-\tilde{u}_i}, \quad \tilde{u}_i \equiv \alpha + (1-2\alpha)\tilde{x}_i$$

  - **Logit**-transformed e_{ij} (e_{ij} normalized by $E_{\mathrm{coarse},i}$)

$$e_{\mathrm{fine},ij} \to \hat{x}_{ij} \equiv (e_{\mathrm{fine},ij} + \mathrm{rand}[0, 0.1\ \mathrm{keV}])/E_{\mathrm{coarse,i}}$$

$$\hat{y}_{ij} = \log \frac{\hat{u}_{ij}}{1-\hat{u}_{ij}}, \quad \hat{u}_{ij} \equiv \alpha + (1-2\alpha)\hat{x}_{ij}$$