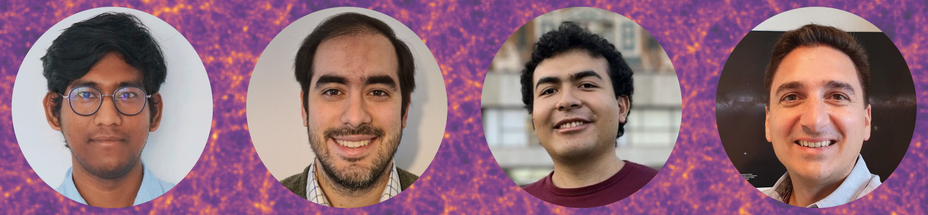
Application of Machine Learning to the Identification of Dark Matter Haloes

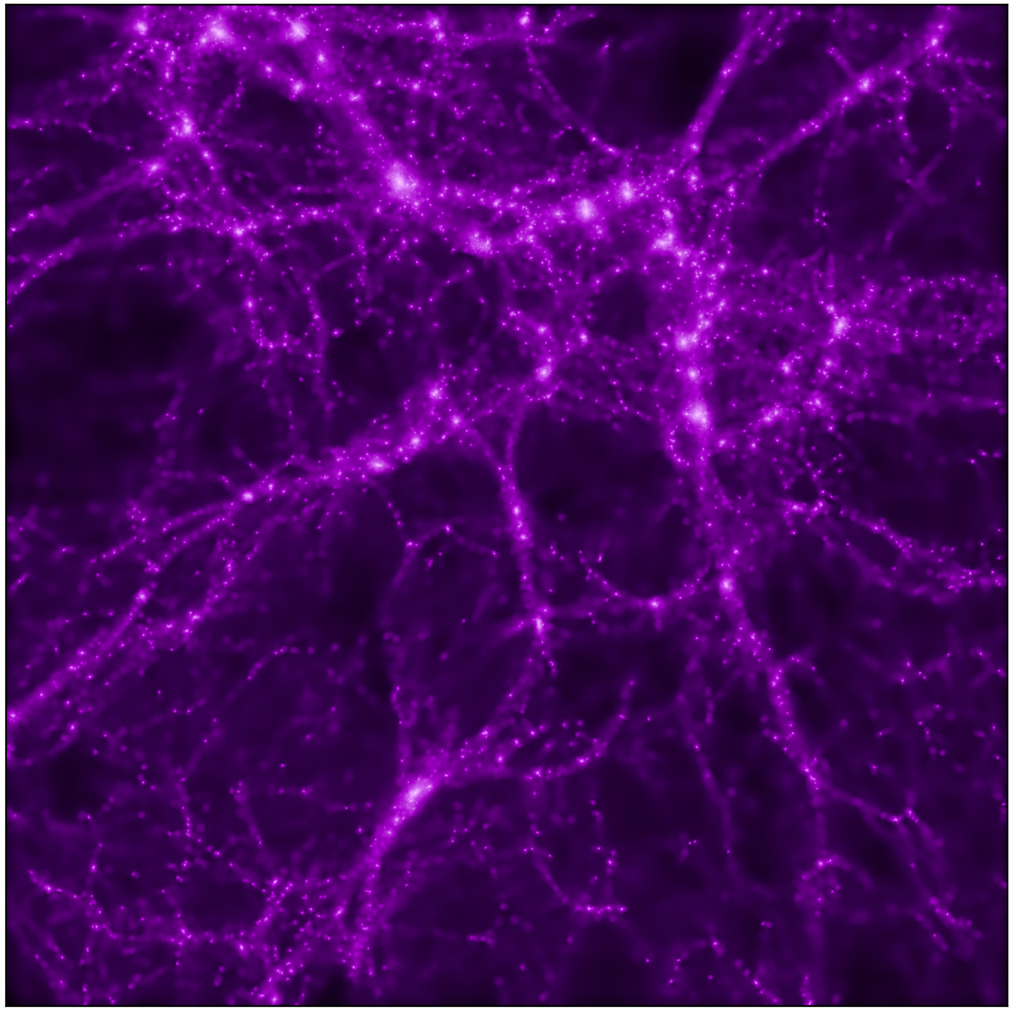
Soumadeep Maiti

Carlos Correa, Alejandro Pérez Fernández, Ariel Sánchez
MPE, OPINAS



Quantum Universe Attract.Workshop, 2025

N-body simulations



Credits: Carlos Correa & Andrea Fiorilli

- As time progresses (redshift z decreases), structures collapse, and the **cosmic web** becomes more defined
- Theoretical frameworks are difficult to model at highly **non-linear scales**
- Theoretical approach: simulation-based inference (**SBI**)

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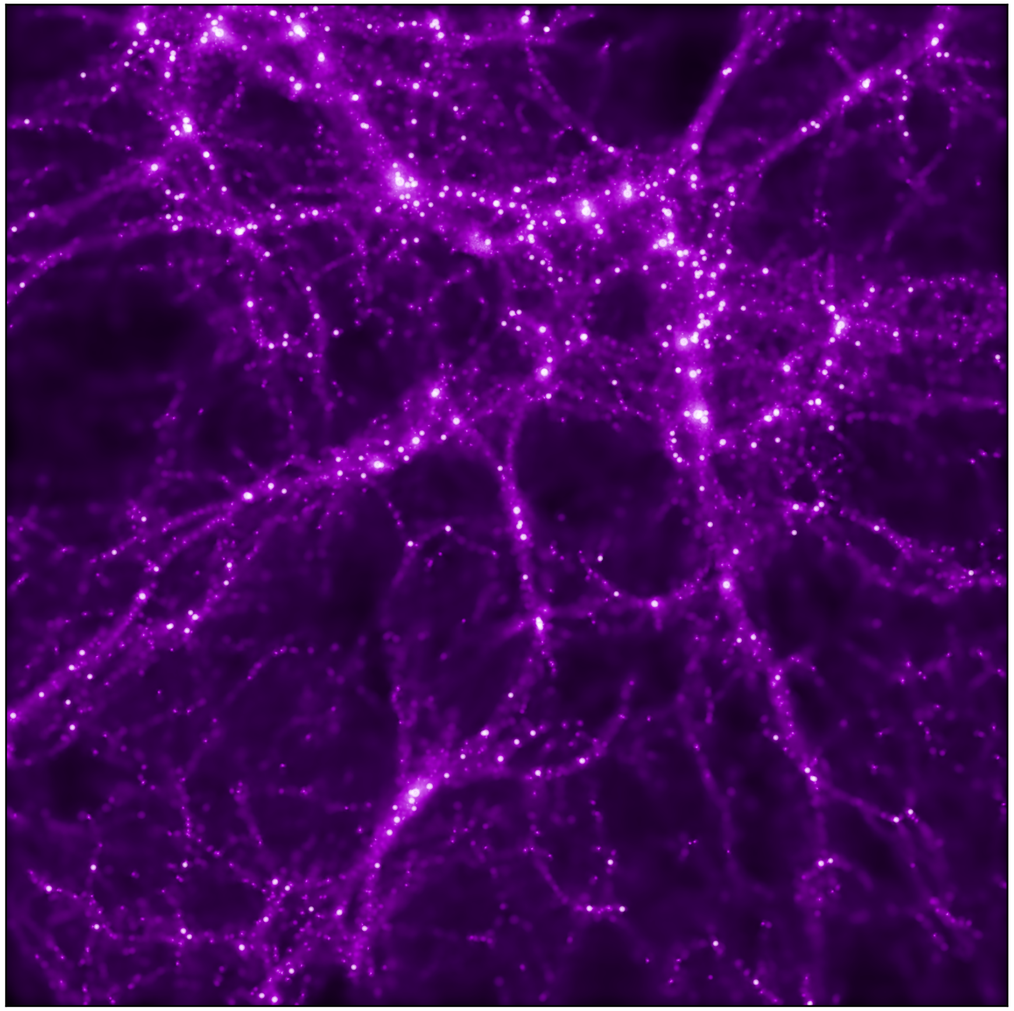

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- Theoretical frameworks are difficult to model at highly **non-linear scales**
- Theoretical approach: simulation-based inference (**SBI**)
- **Dark matter haloes** appears at the highest peaks in the full density field

Why do we need a faster halo identification method?

- Current Halo Finders: **FOF** (Friends-of-Friends, Davis et al. 1985), **ROCKSTAR**(Robust Overdensity Calculation using K-Space Topologically Adaptive Refinement, Behroozi et al. 2013), etc.
- Increasing demand for **fast** and **mass** production of halo catalogue without sacrificing accuracy
- Halo identification in bigger simulations are computationally expensive

Halo Finders

↓

Time

↓

Machine Learning Algorithm

←

Particle Classifier (CNN)

+

Clustering Algorithm (FoF)

←

Dark Matter Haloes

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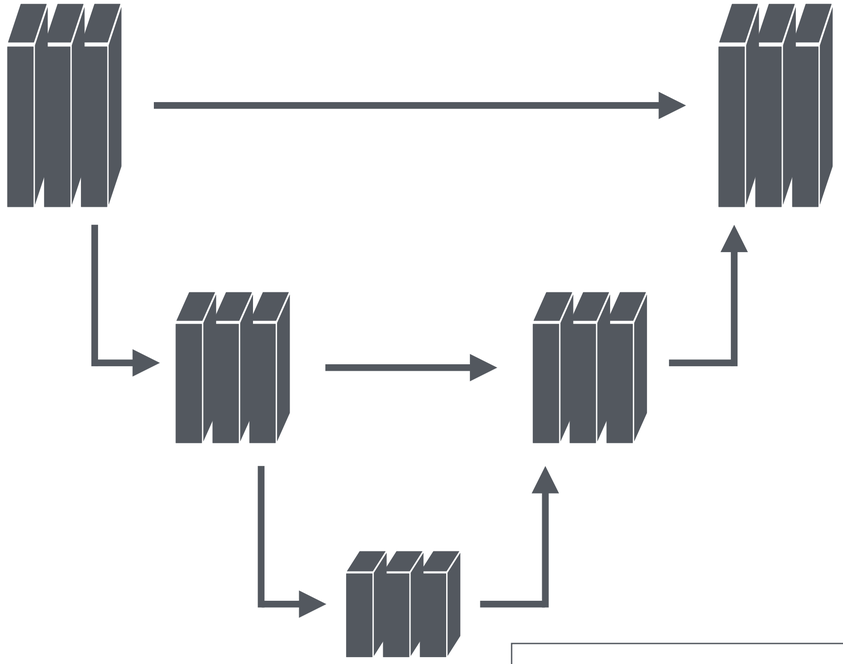
Convolutional Neural Networks

An example: Image segmentation (V-Net)

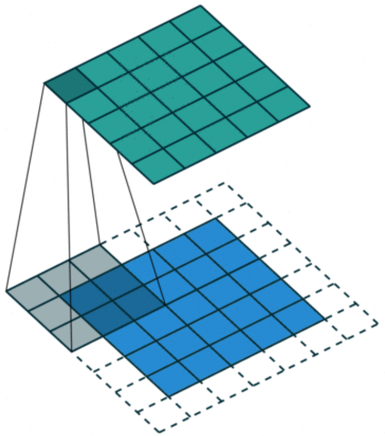
Input channels:
RGB



Output channels:
#classes

Target: true mask

Loss: cross entropy



concatenation

downsampling

upsampling

- State-of-the-art architecture
- Applications: Medical imaging, video surveillance, pedestrian detection, …

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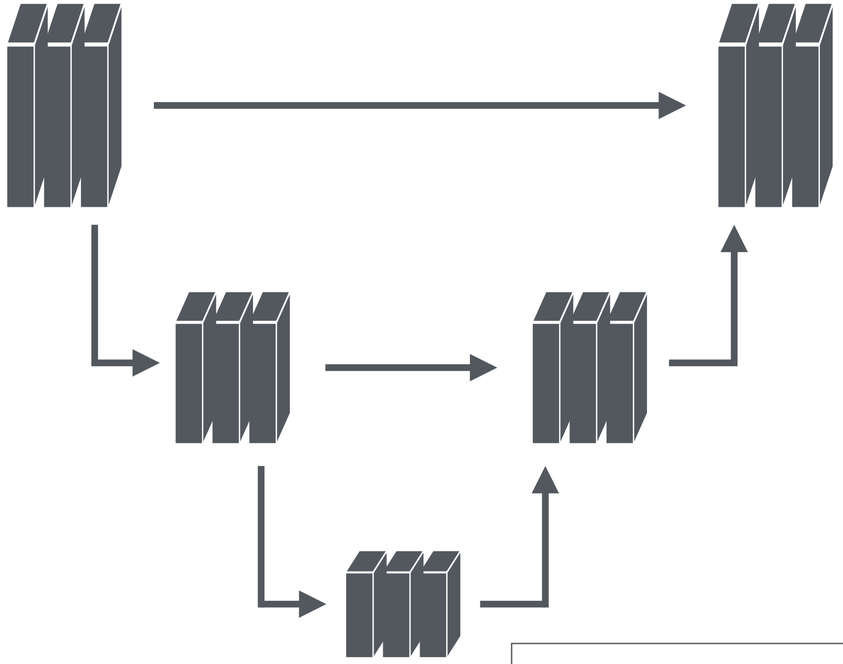

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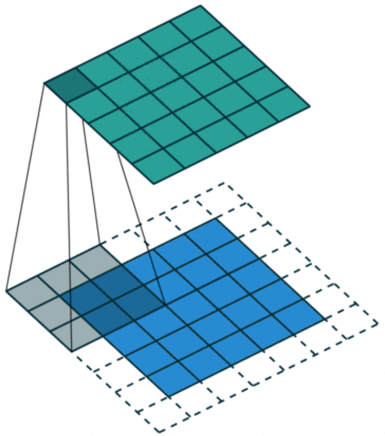

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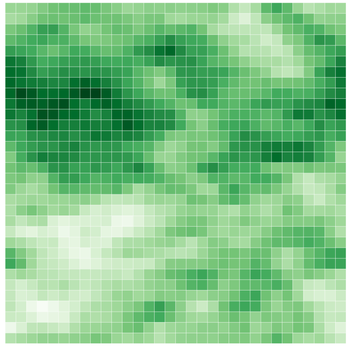
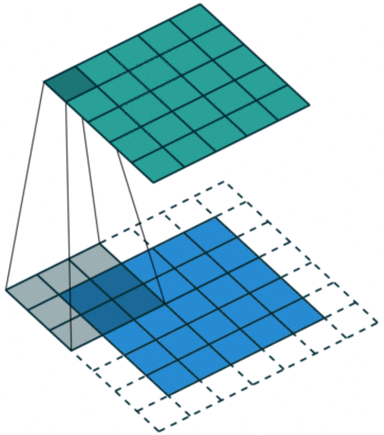
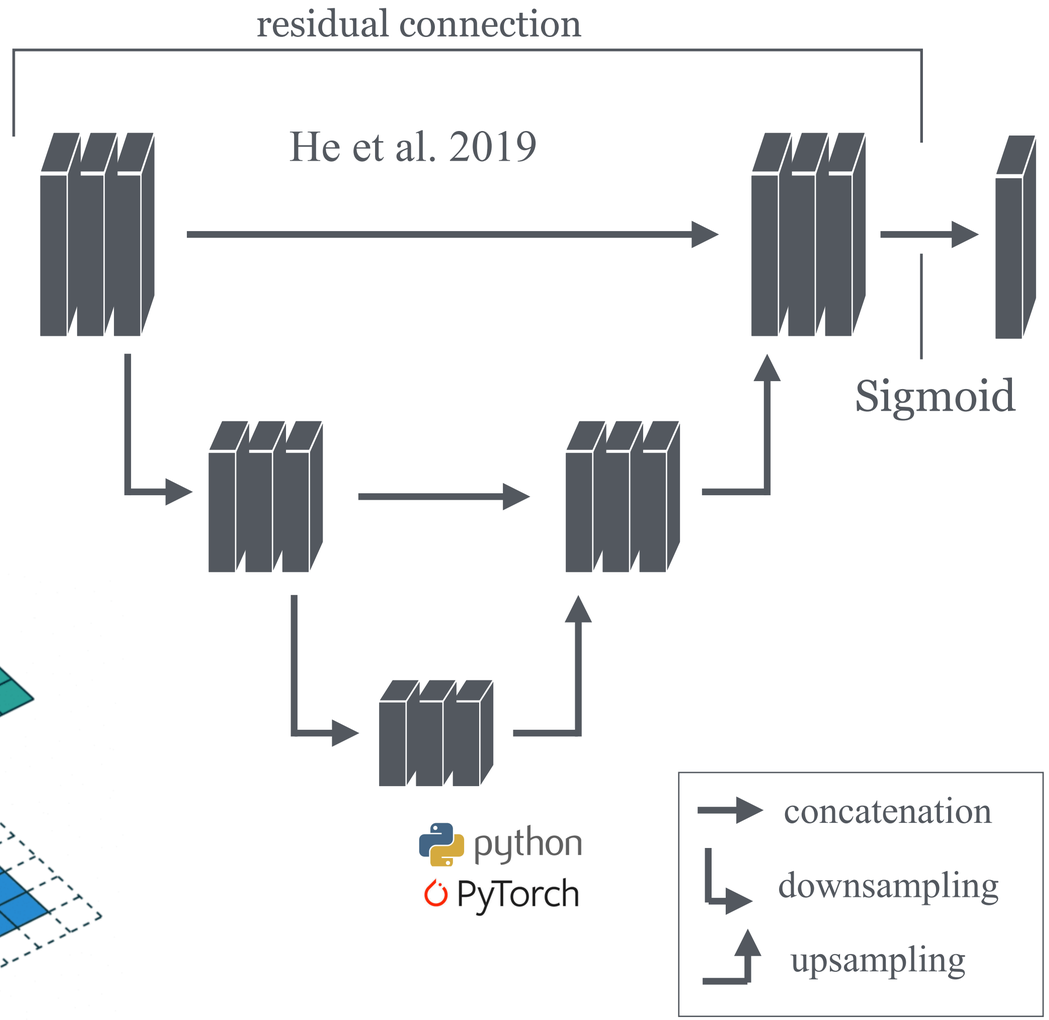
Learning the Dark Matter Particles



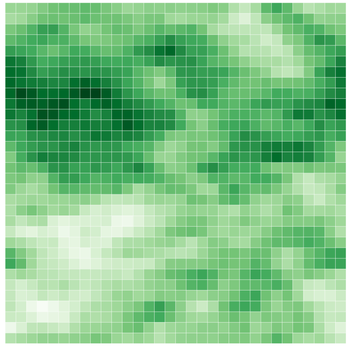
Input channels:
ψ_i, $\mathbf{v}_i$



2D convolution



Learning the Dark Matter Particles



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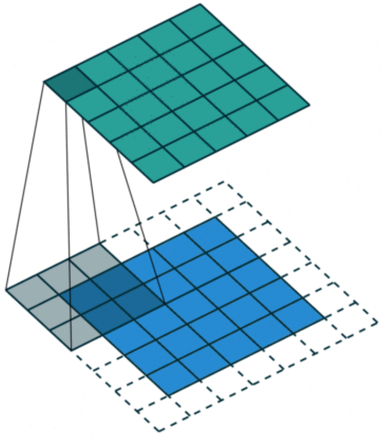

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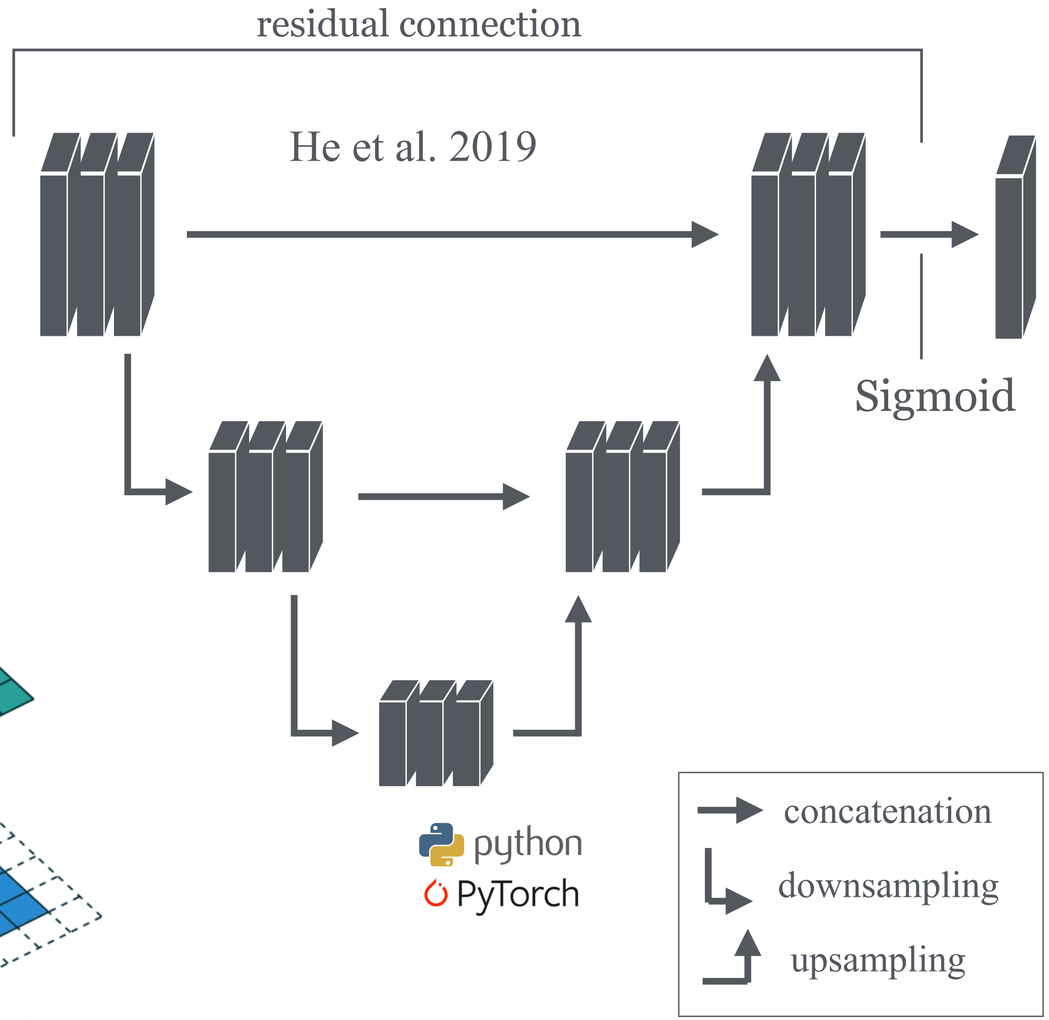

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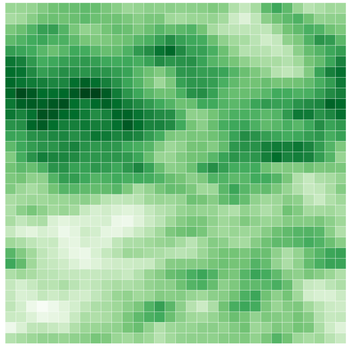

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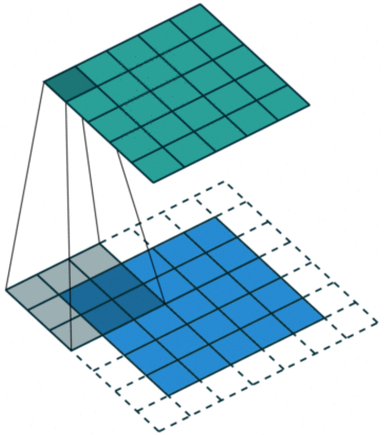

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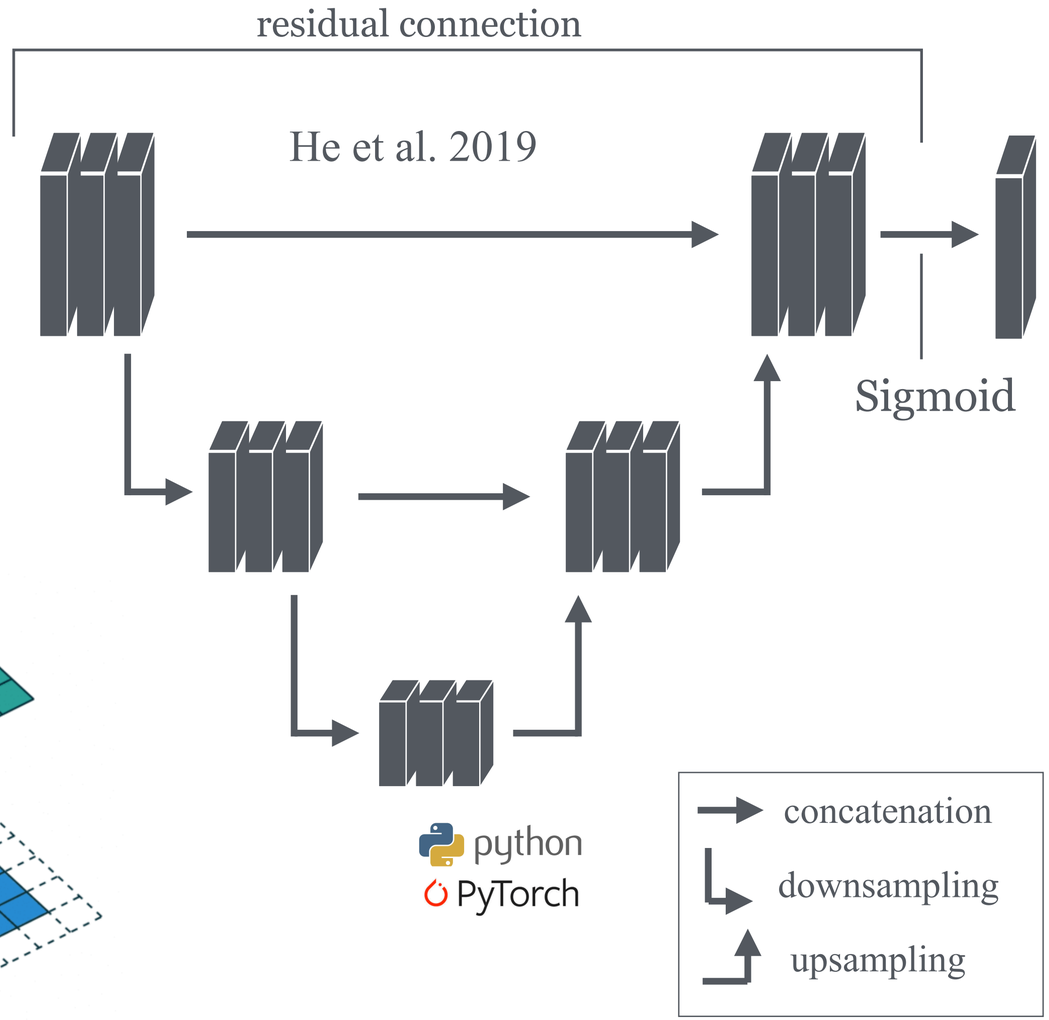
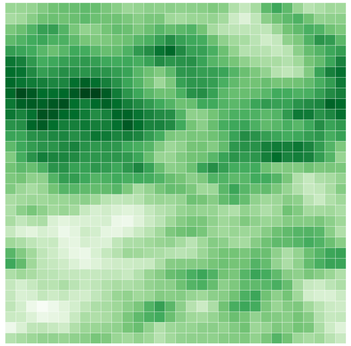


0	0	0	0	0	0	0	0	0	1
1	0	1	0	0	1	0	0	0	1
0	0	0	0	1	0	1	0	0	1
0	0	0	1	0	0	0	1	1	0
1	0	0	0	0	0	1	1	1	0
0	0	1	0	1	0	0	0	0	0
0	0	0	0	0	0	0	0	0	1
0	1	0	0	0	1	0	0	0	1
1	0	0	1	0	0	0	1	0	0
0	1	0	0	0	0	0	0	0	0

Output channels:
1, 0

Learning the Dark Matter Particles



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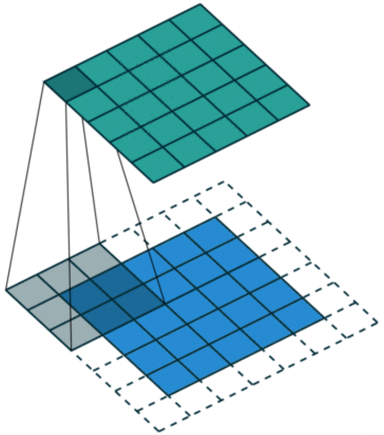

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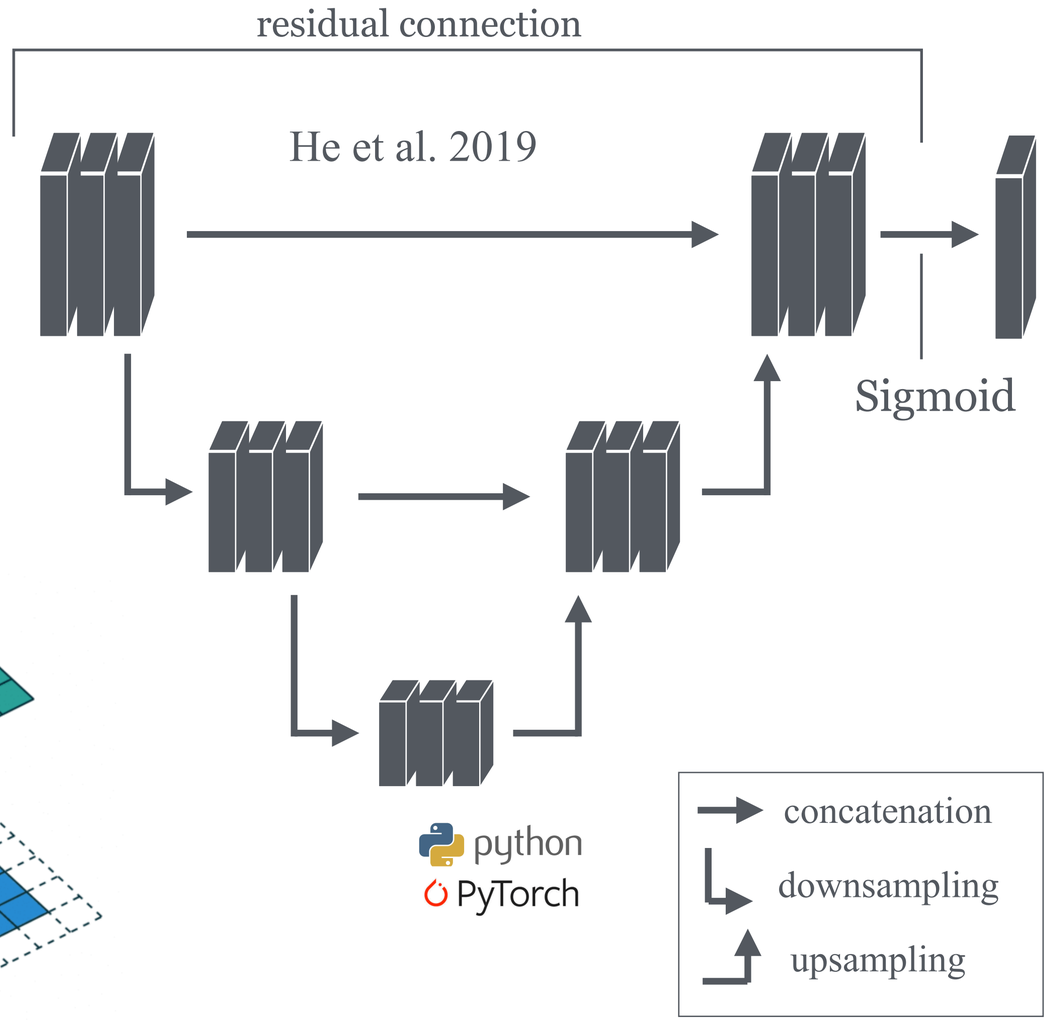

0	0	0	0	0	0	0	0	0	1
1	0	1	0	0	1	0	0	0	1
0	0	0	0	1	0	1	0	0	1
0	0	0	1	0	0	0	1	1	0
1	0	0	0	0	0	1	1	1	0
0	0	1	0	1	0	0	0	0	0
0	0	0	0	0	0	0	0	0	1
0	1	0	0	0	1	0	0	0	1
1	0	0	1	0	0	0	1	0	0
0	1	0	0	0	0	0	0	0	0

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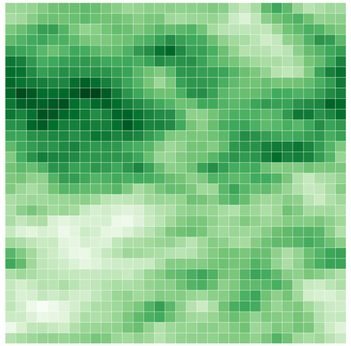
1, 0

0	0	1	0	0	0	0	0	0	0
1	0	1	0	1	1	0	0	0	1
0	0	0	0	1	0	0	0	0	1
0	0	0	1	0	0	0	1	1	0
1	0	0	0	0	0	1	1	1	0
0	0	1	0	1	0	0	0	0	0
0	0	0	0	0	0	0	0	0	1
0	1	0	0	0	1	0	0	0	1
1	0	0	1	0	0	0	1	0	0
0	1	0	0	0	0	0	0	0	0

Target: Rockstar Catalogue

Learning the Dark Matter Particles



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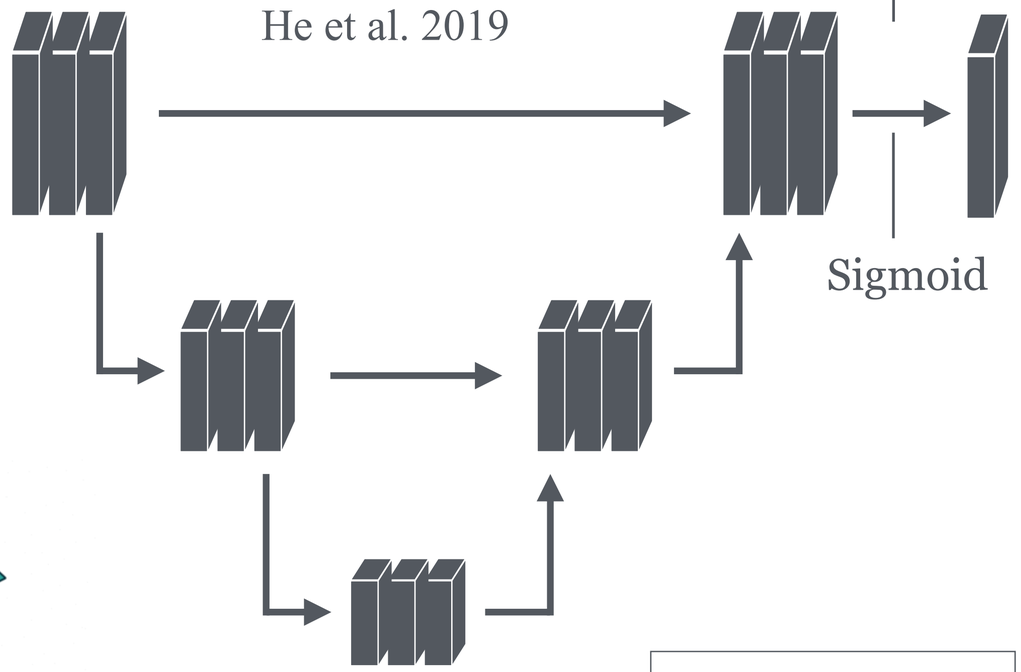
residual connection

He et al. 2019



Sigmoid

python
PyTorch

concatenation
downsampling
upsampling

0	0	0	0	0	0	0	0	0	1
1	0	1	0	0	1	0	0	0	1
0	0	0	0	1	0	1	0	0	1
0	0	0	1	0	0	0	1	1	0
1	0	0	0	0	0	1	1	1	0
0	0	1	0	1	0	0	0	0	0
0	0	0	0	0	0	0	0	0	1
0	1	0	0	0	1	0	0	0	1
1	0	0	1	0	0	0	1	0	0
0	1	0	0	0	0	0	0	0	0

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0	0	0	0	1	0	0	0	0	1
0	0	0	1	0	0	0	1	1	0
1	0	0	0	0	0	1	1	1	0
0	0	1	0	1	0	0	0	0	0
0	0	0	0	0	0	0	0	0	1
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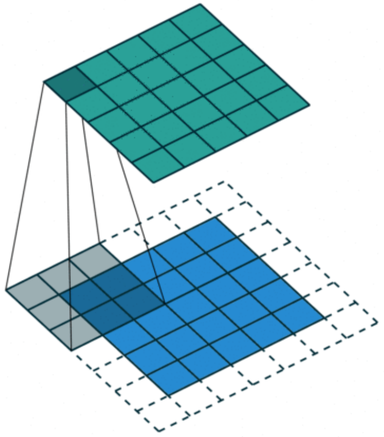
1	0	0	1	0	0	0	1	0	0
0	1	0	0	0	0	0	0	0	0

Target: Rockstar Catalogue

Loss: Binary Cross Entropy



2D convolution

Building Dataset

- Cosmology: Planck cosmology
- Simulation: **Set ref** using Gadget4 (Springel et al. 2021)
- Apply **Rockstar** on the Snapshots
- Label DM particles $(\mathbf{1}, \mathbf{0})$ based on the Halo Catalogue
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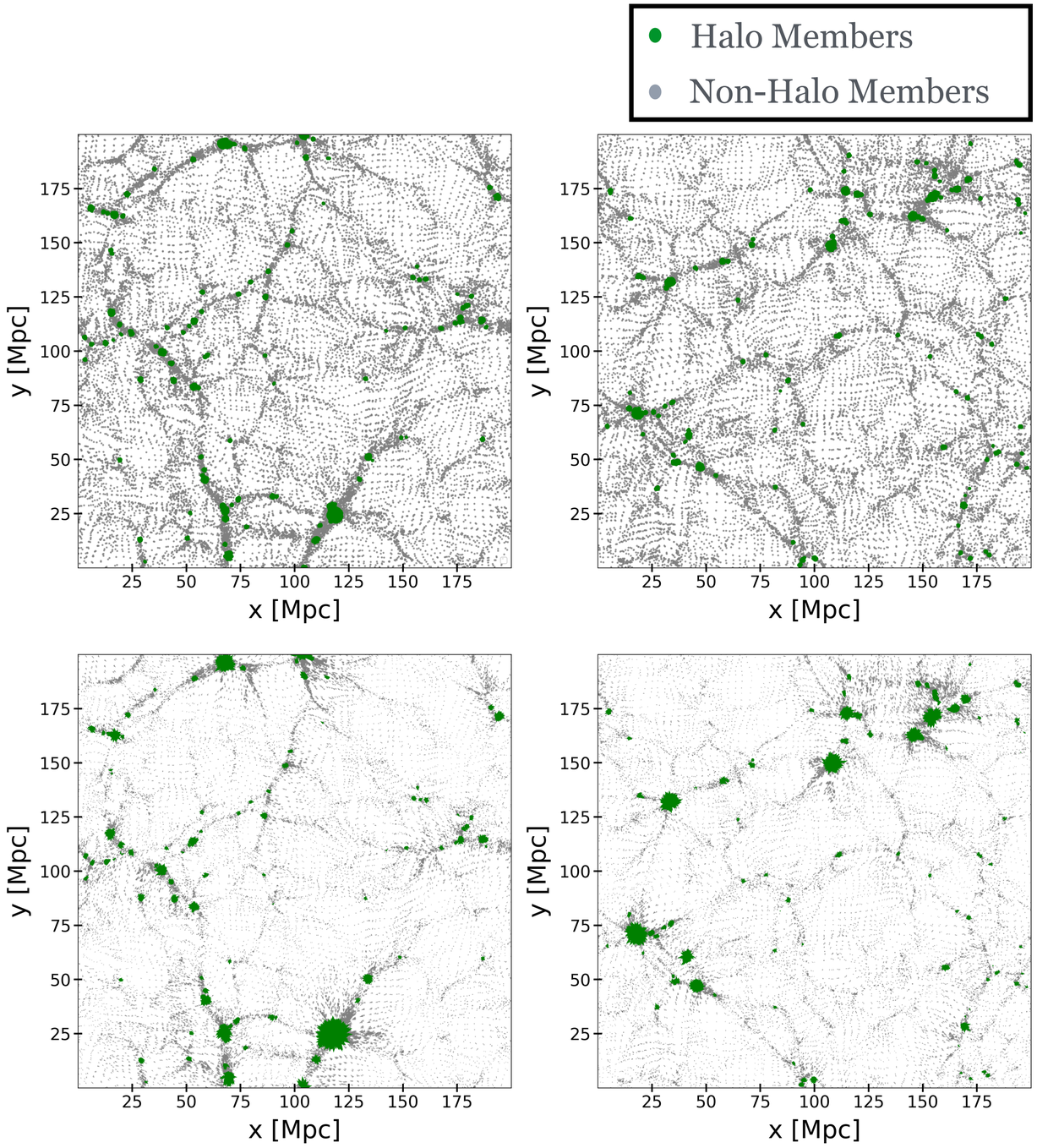

$L200 - N128^3$

CNNs' Performance

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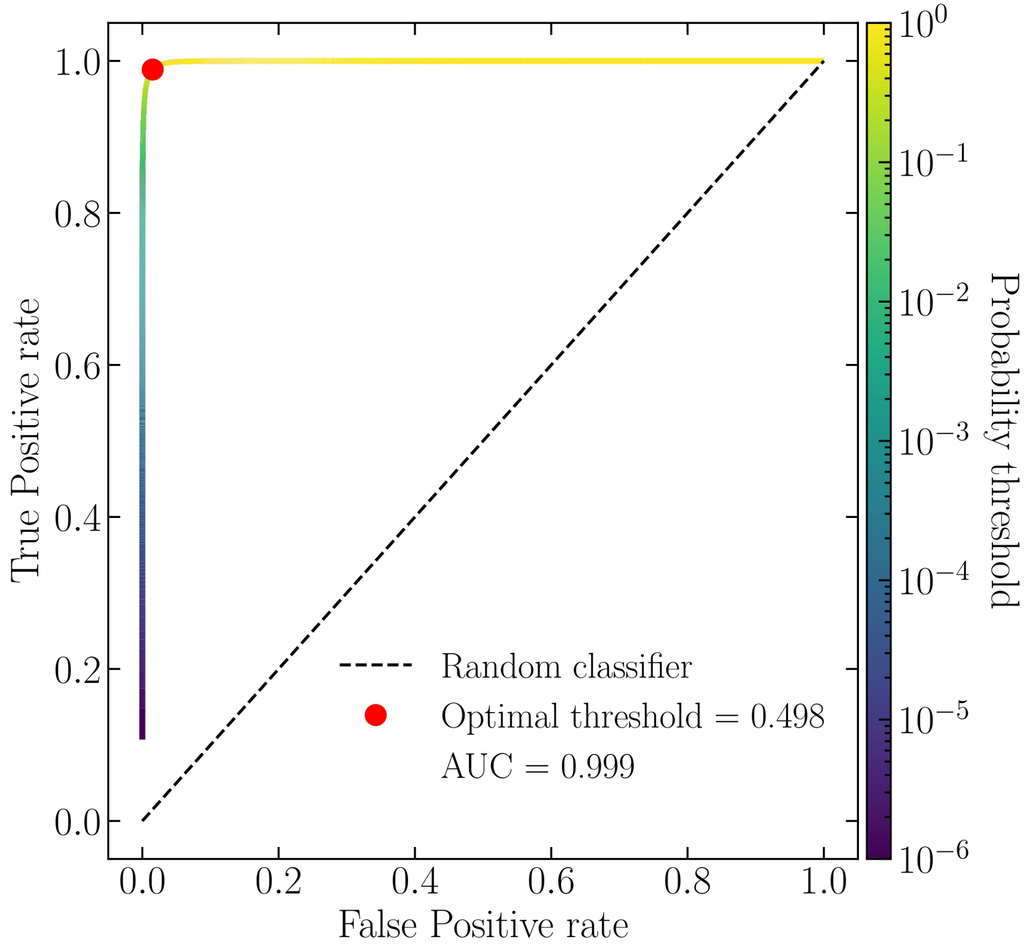
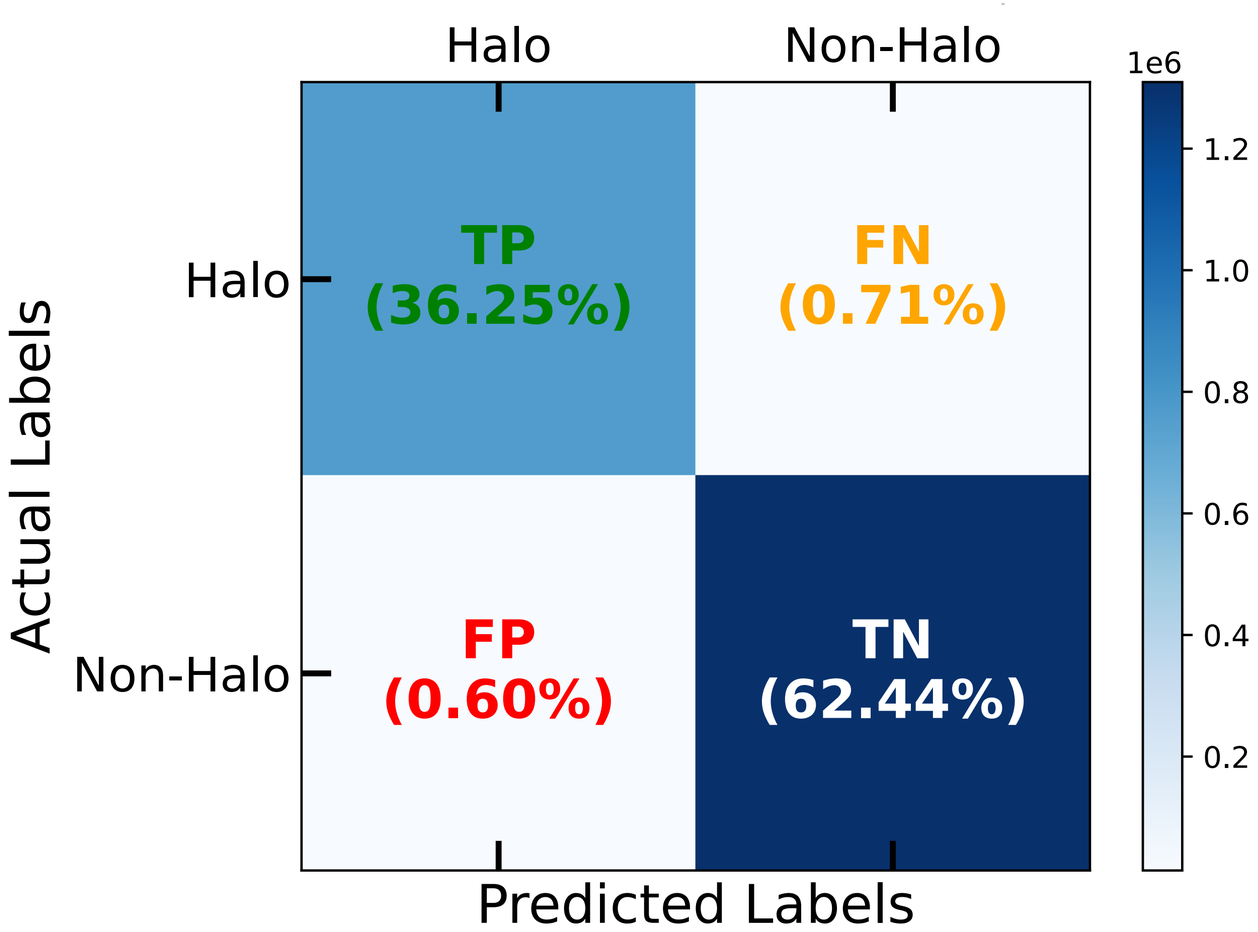


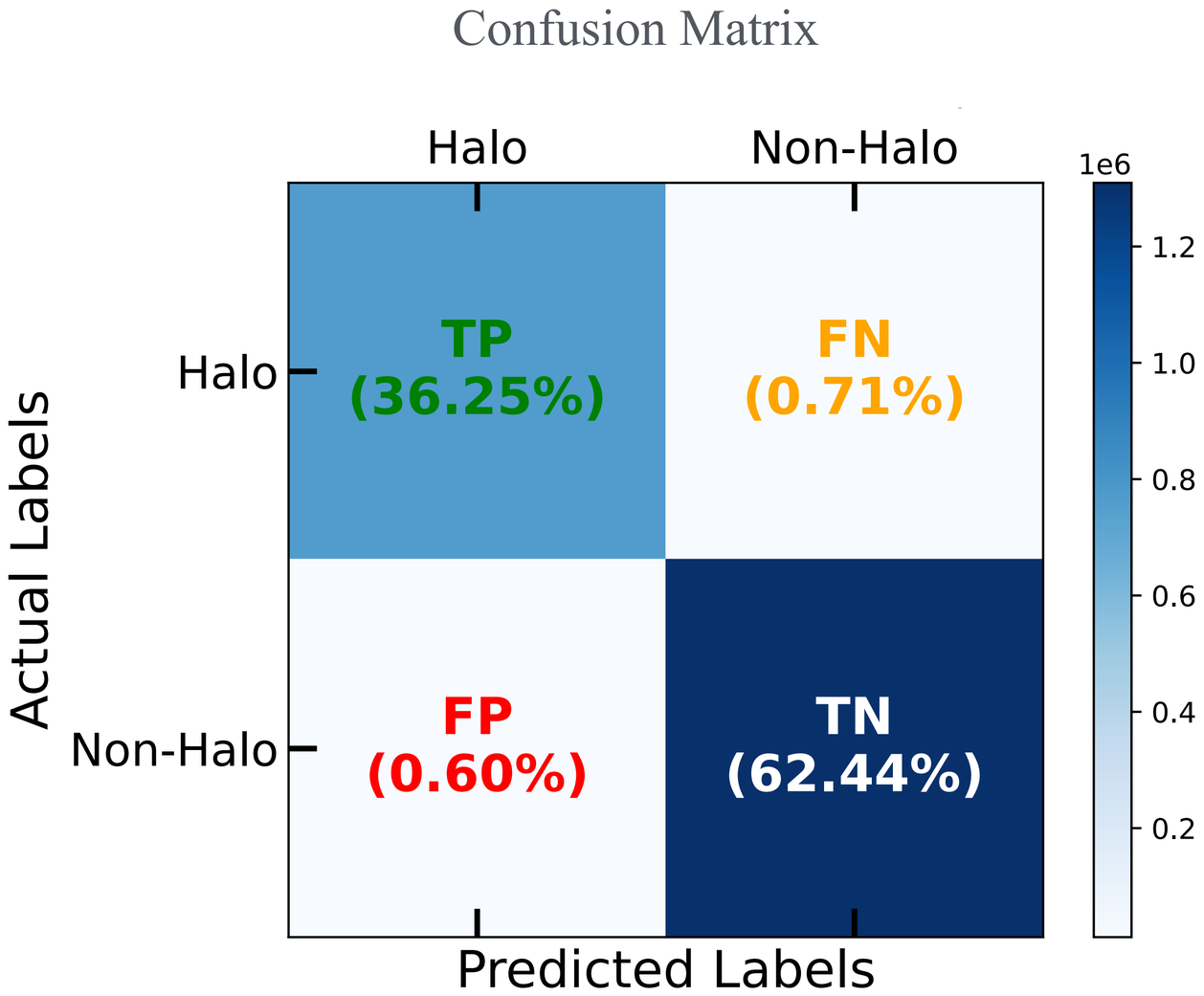
CNNs' Performance

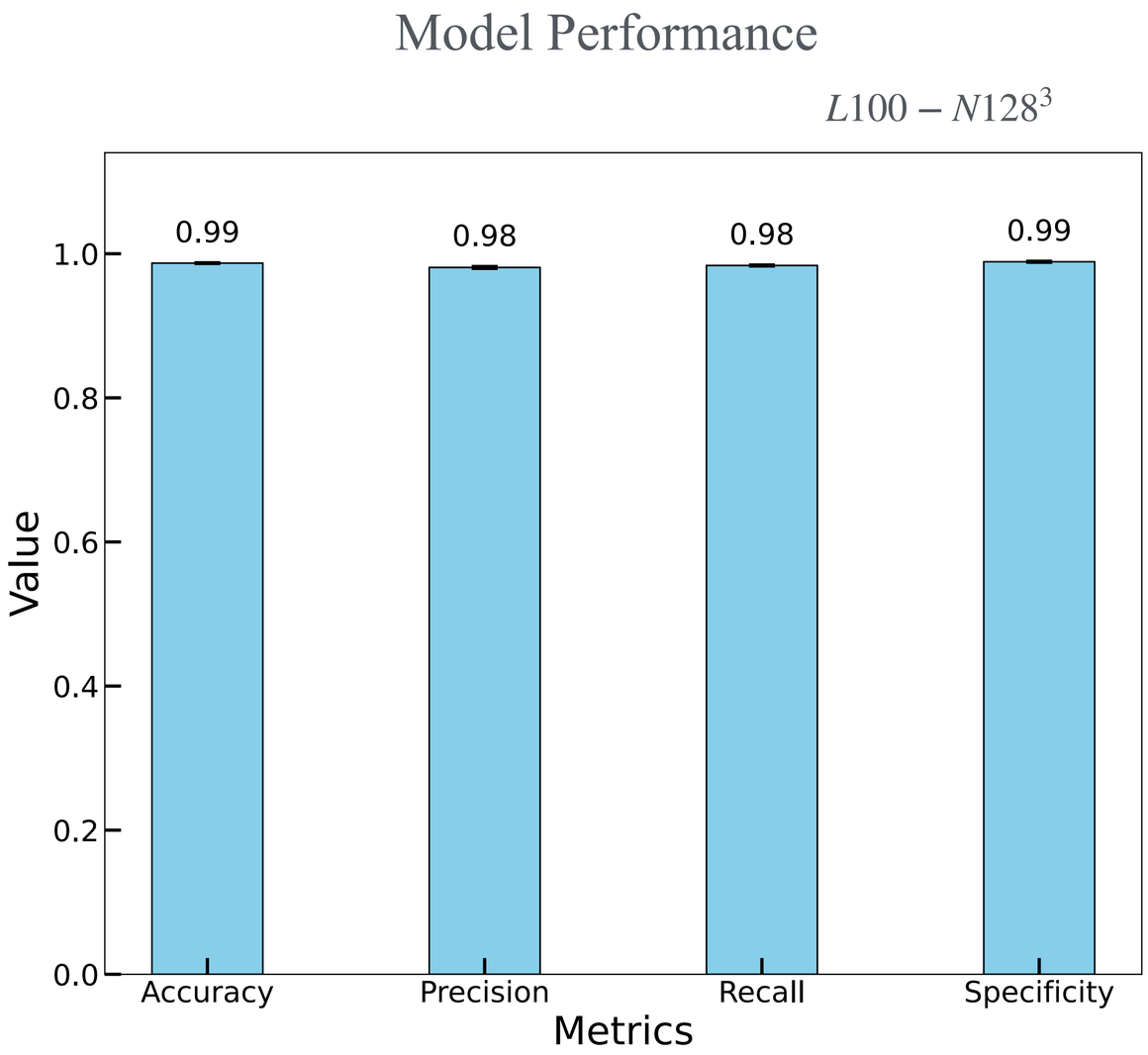
Confusion Matrix



- Correctly Classified: **98.69%**
- Misclassified: **1.31%**

CNNs' Performance





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Trained Models

ROCKSTAR

Mass / Resolution	M_{200b}	M_{vir}
$L200 - N64^3$	✓	✓
$L400 - N128^3$	✓	✓
$L200 - N128^3$	✓	✓
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Resolution Increase

Trained Model on RAVEN GPUs (MPCDF)

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ROCKSTAR

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Trained Model on RAVEN GPUs (MPCDF)

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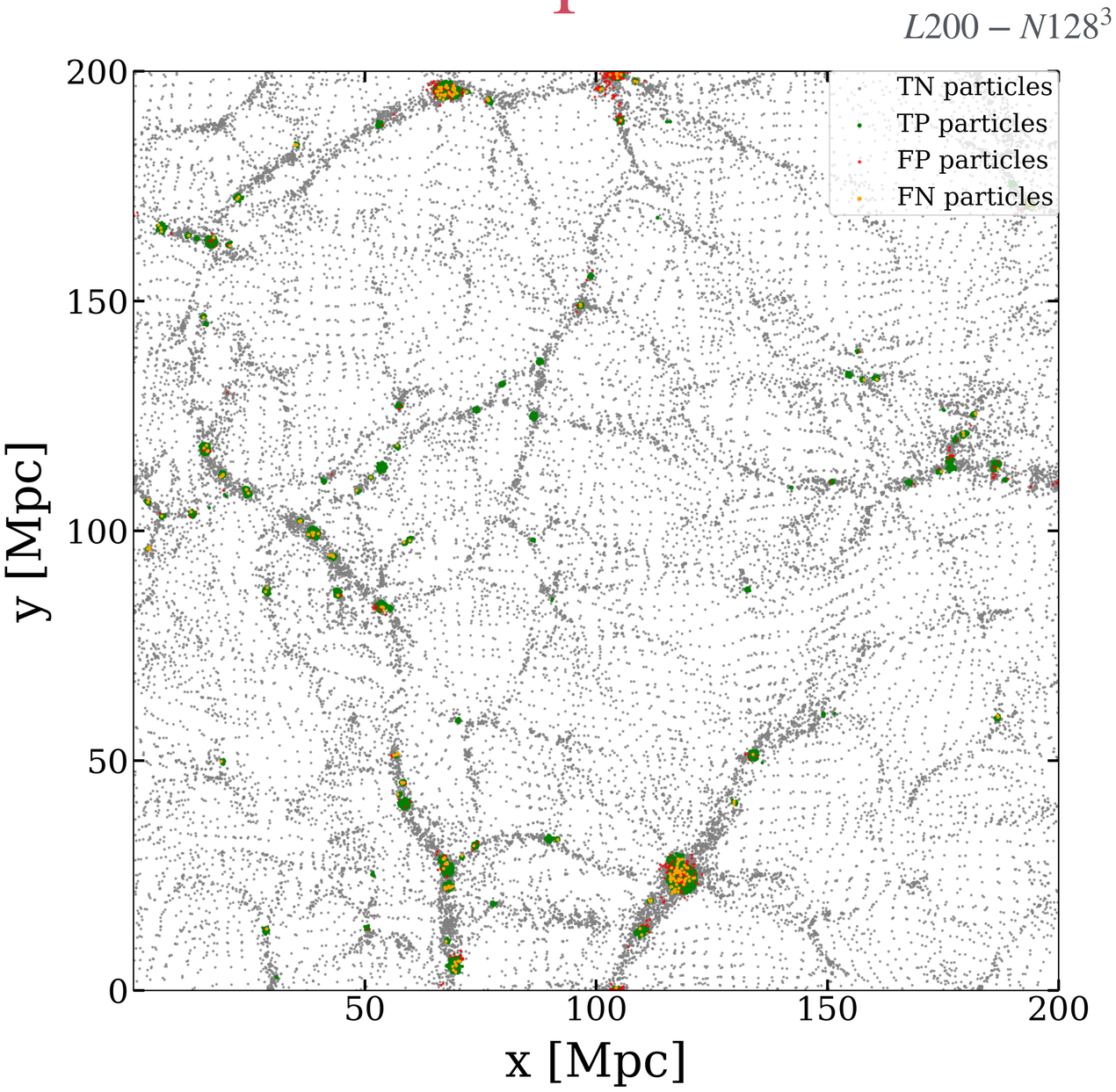

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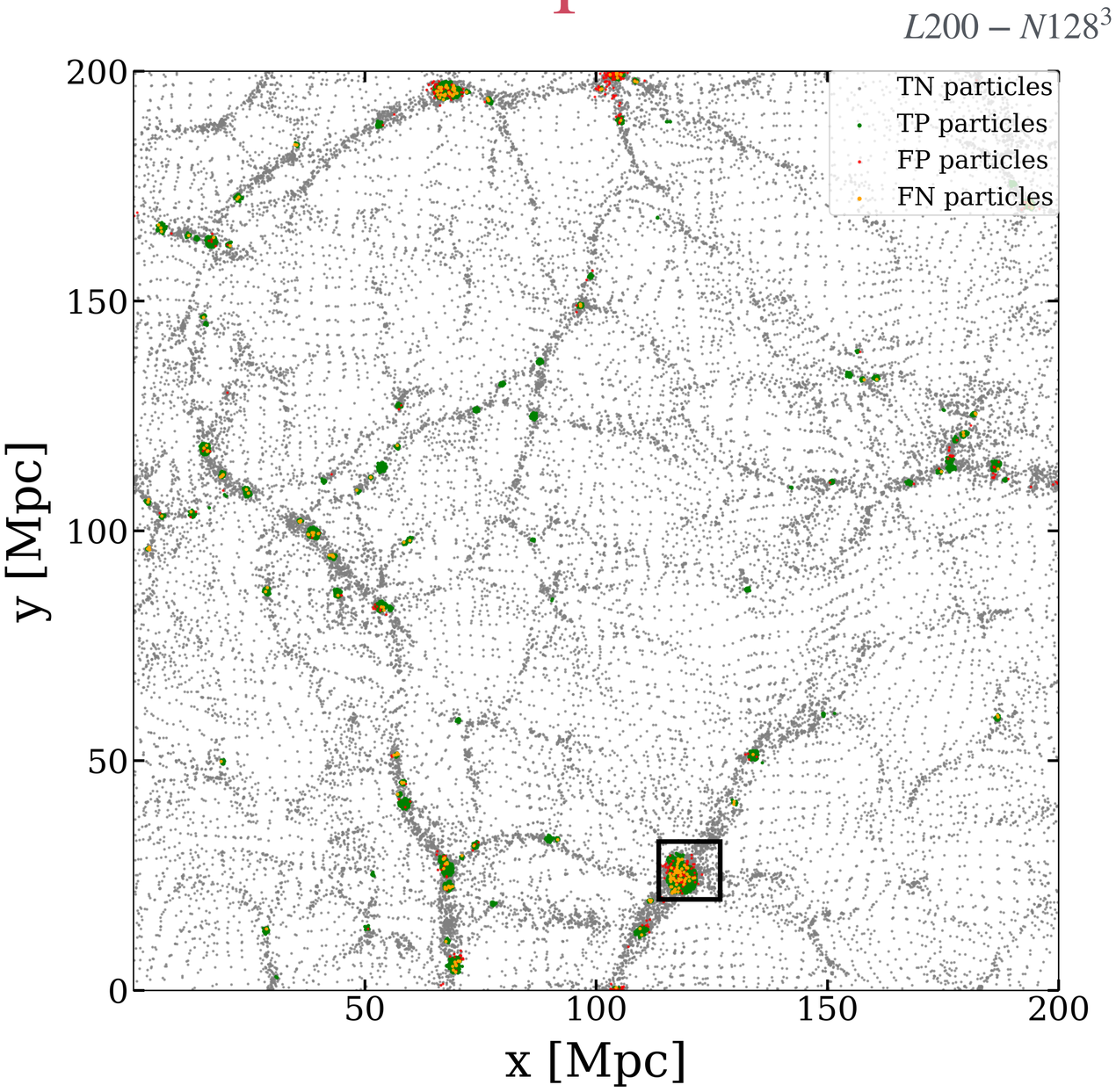

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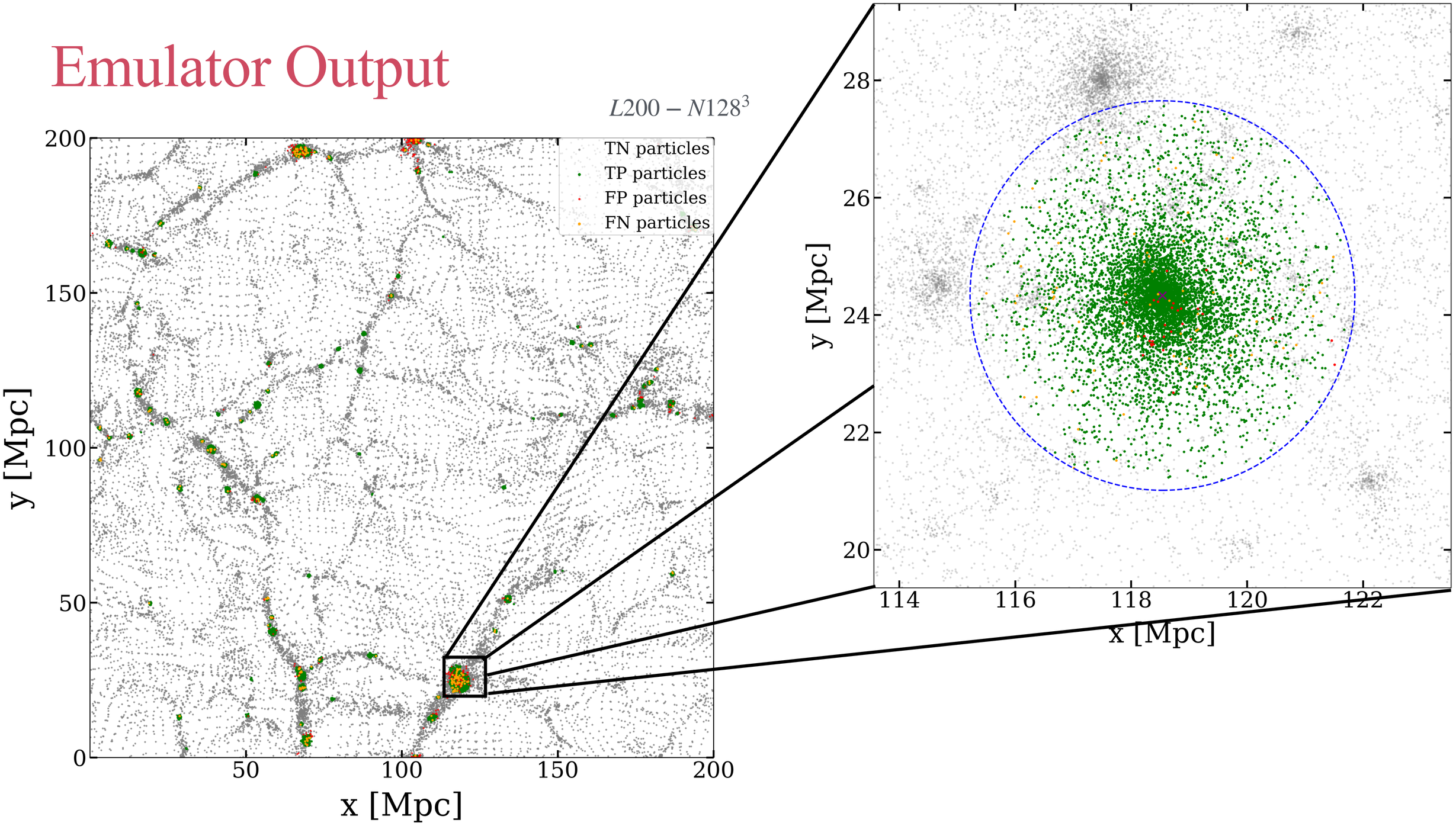

Recovering Centres of Emulator Output

- Applied FoF on Emulator Identified Positive (TP+FP) Particles
- One-to-one correspondence of Rockstar and FoF Centers.

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$L200 - N128^3$

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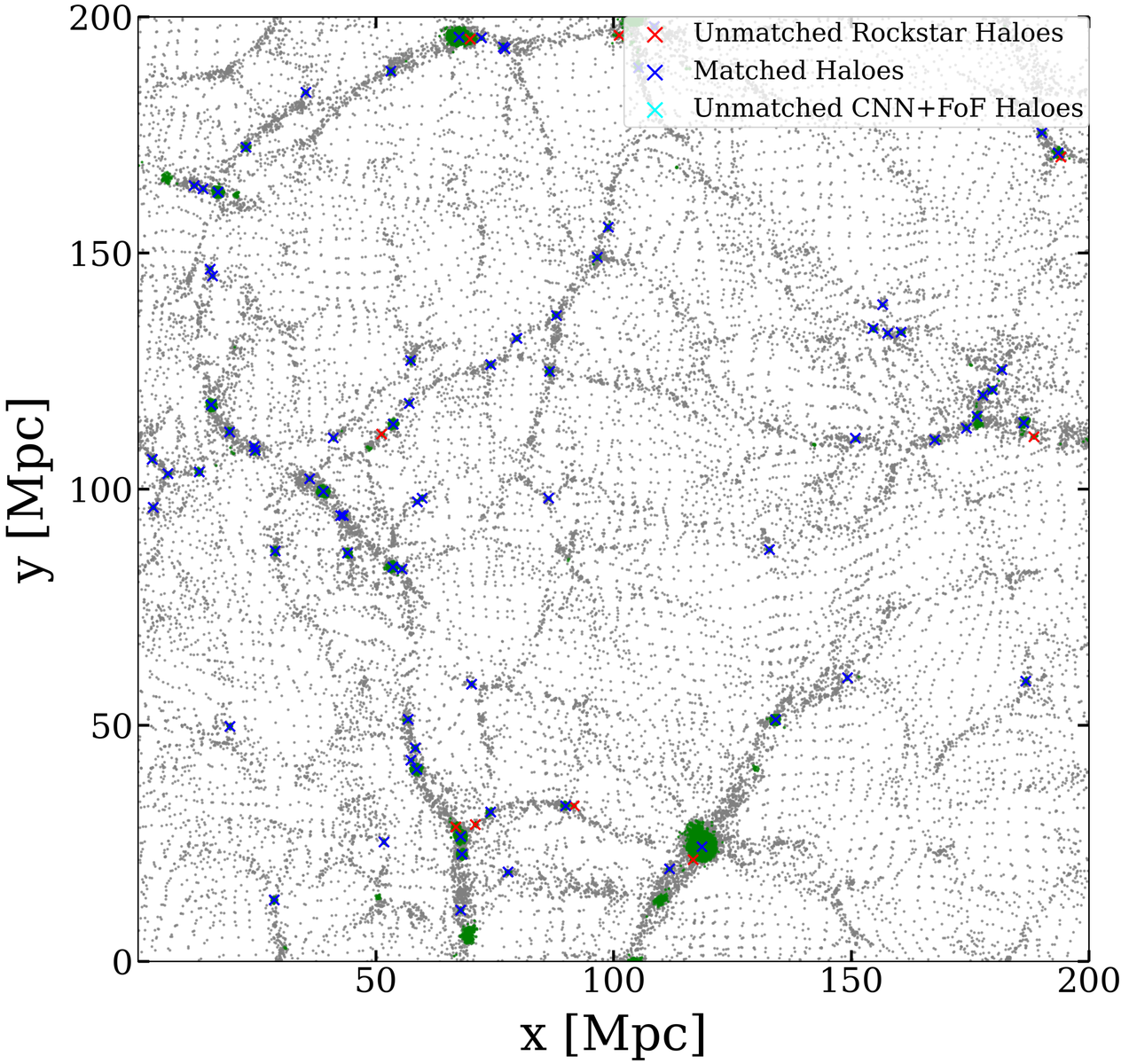

Halo Matchings

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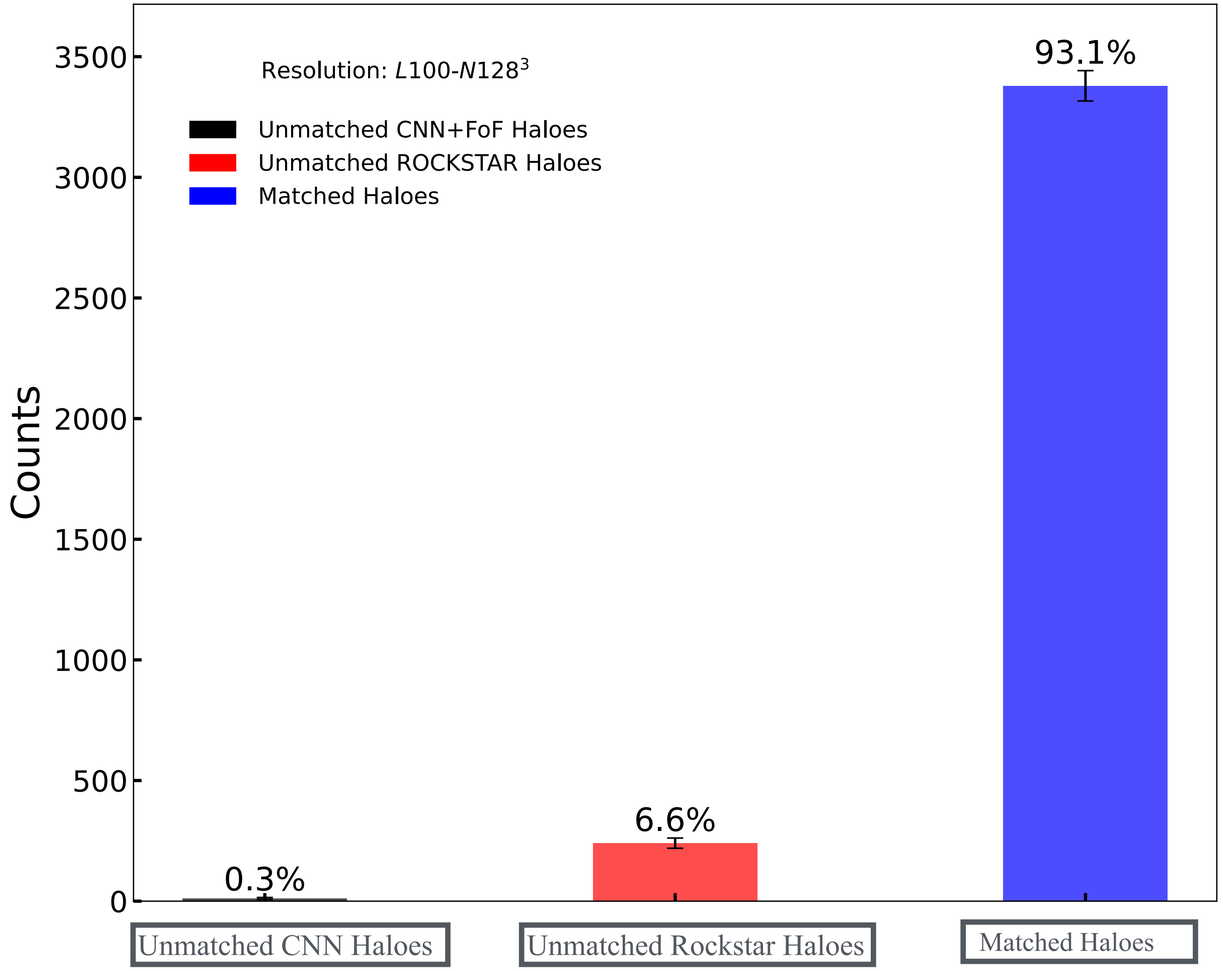

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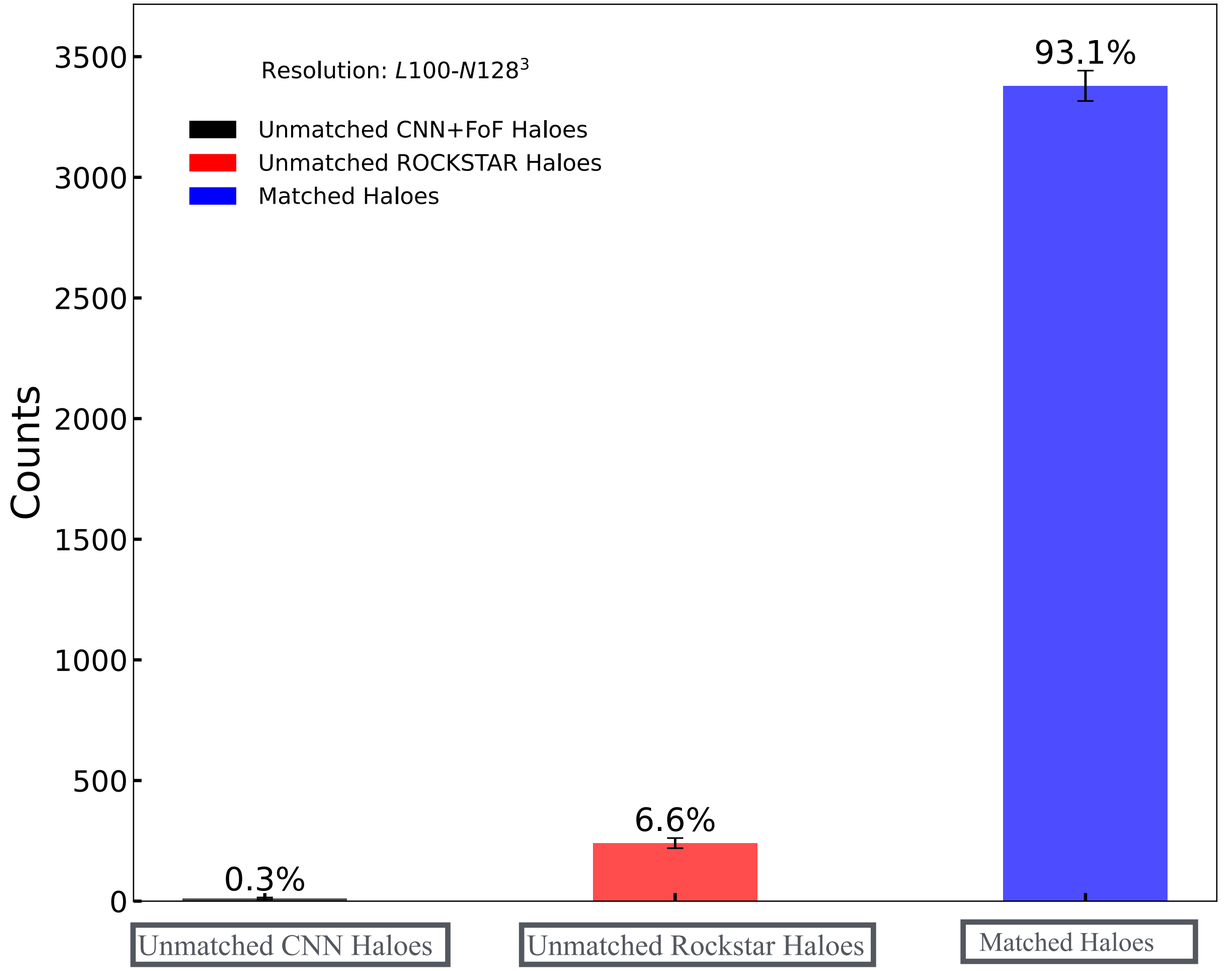
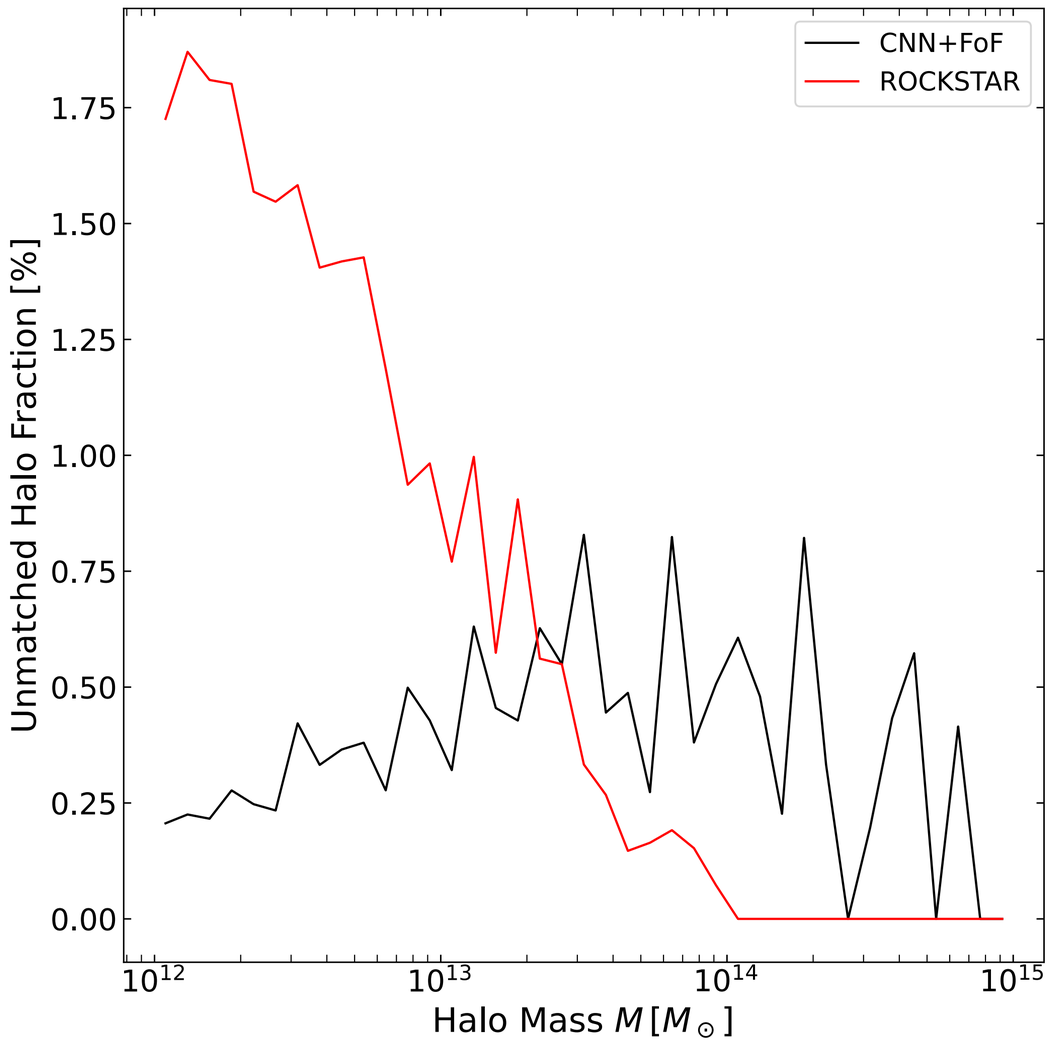
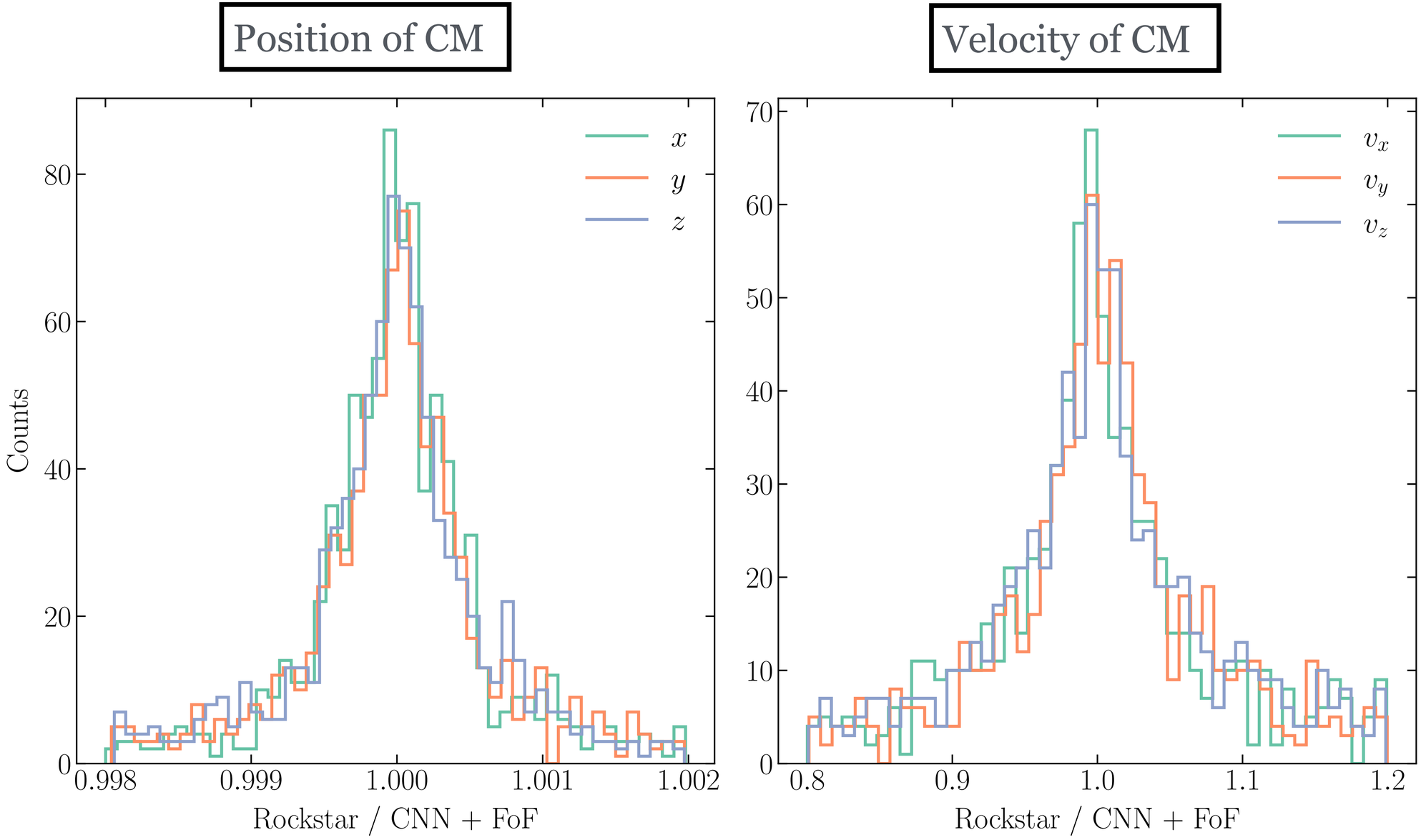




Position and Velocity Recovery



Clustering Statistics

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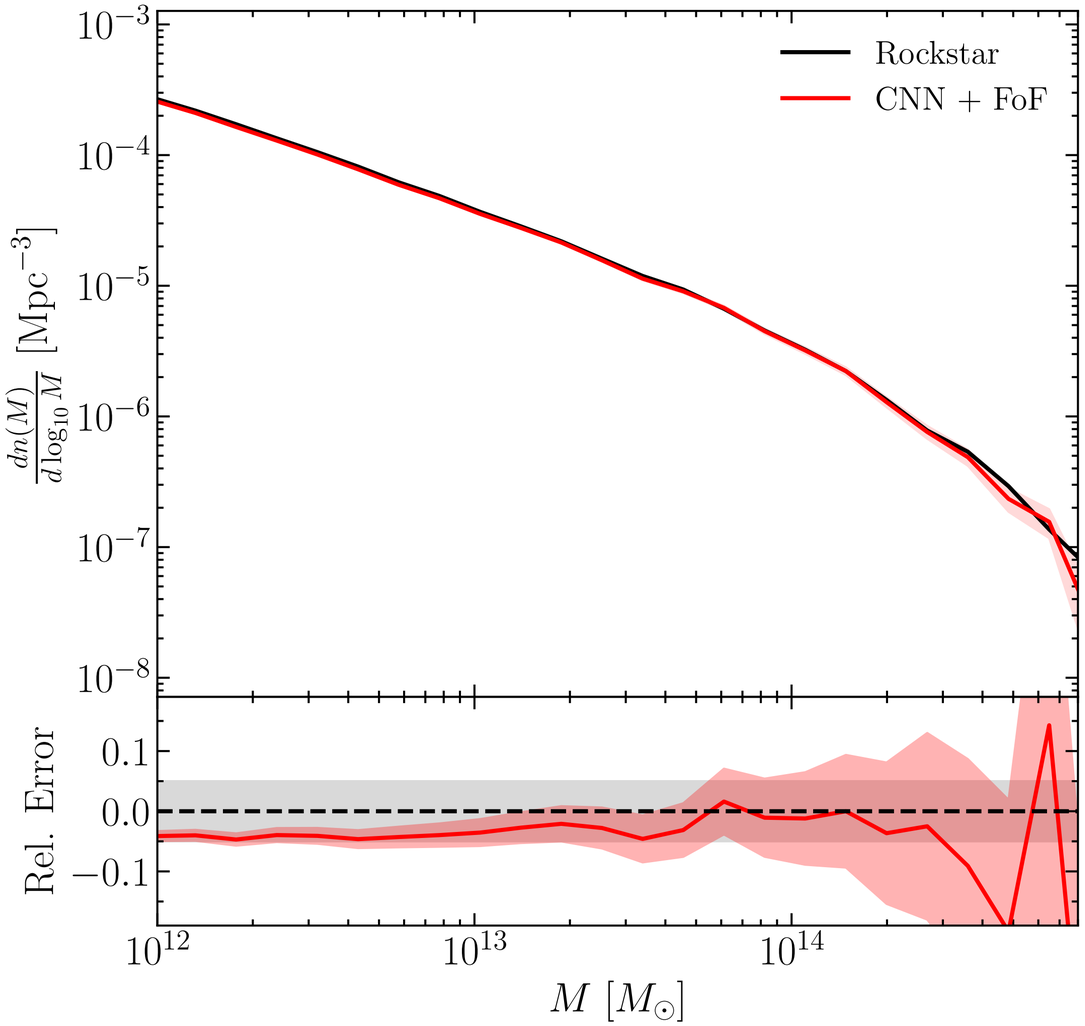
Halo Mass Function



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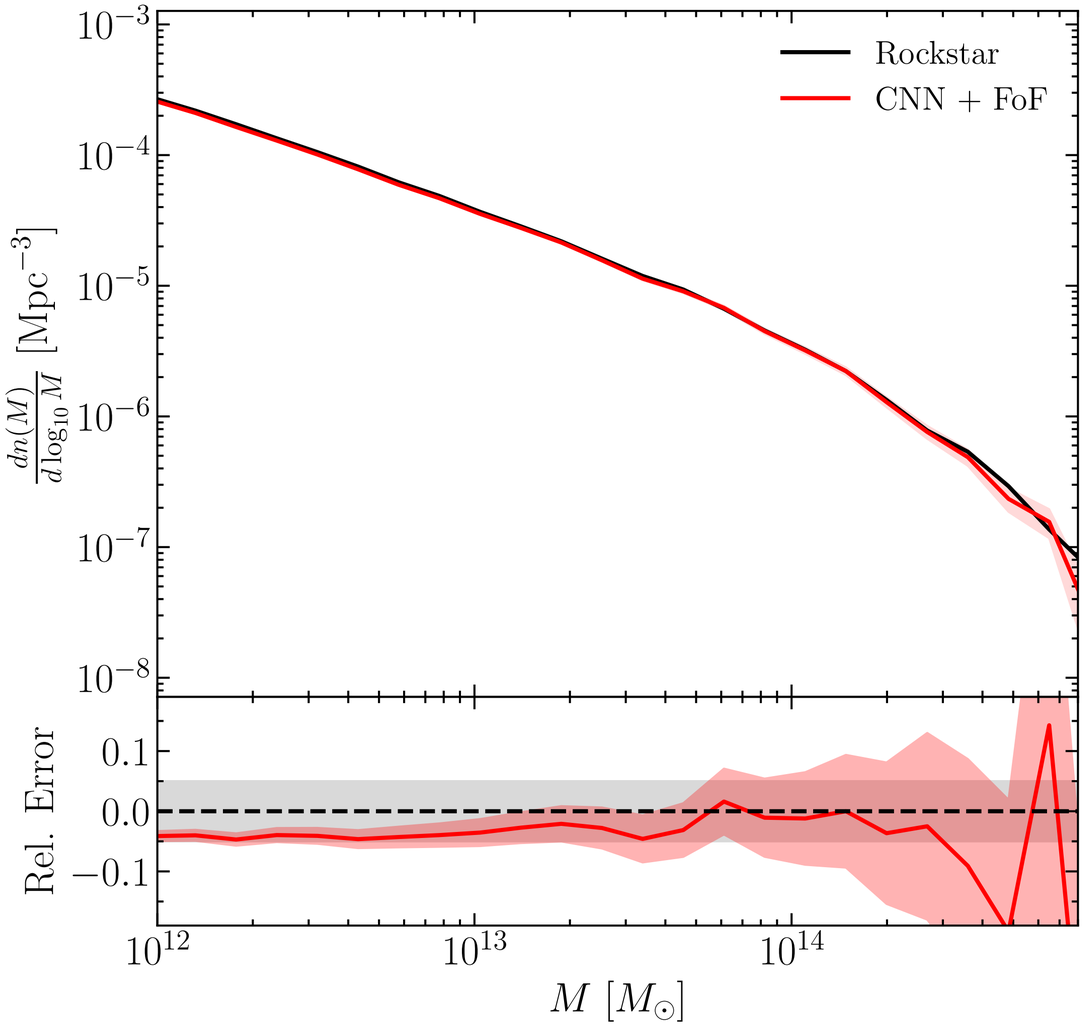
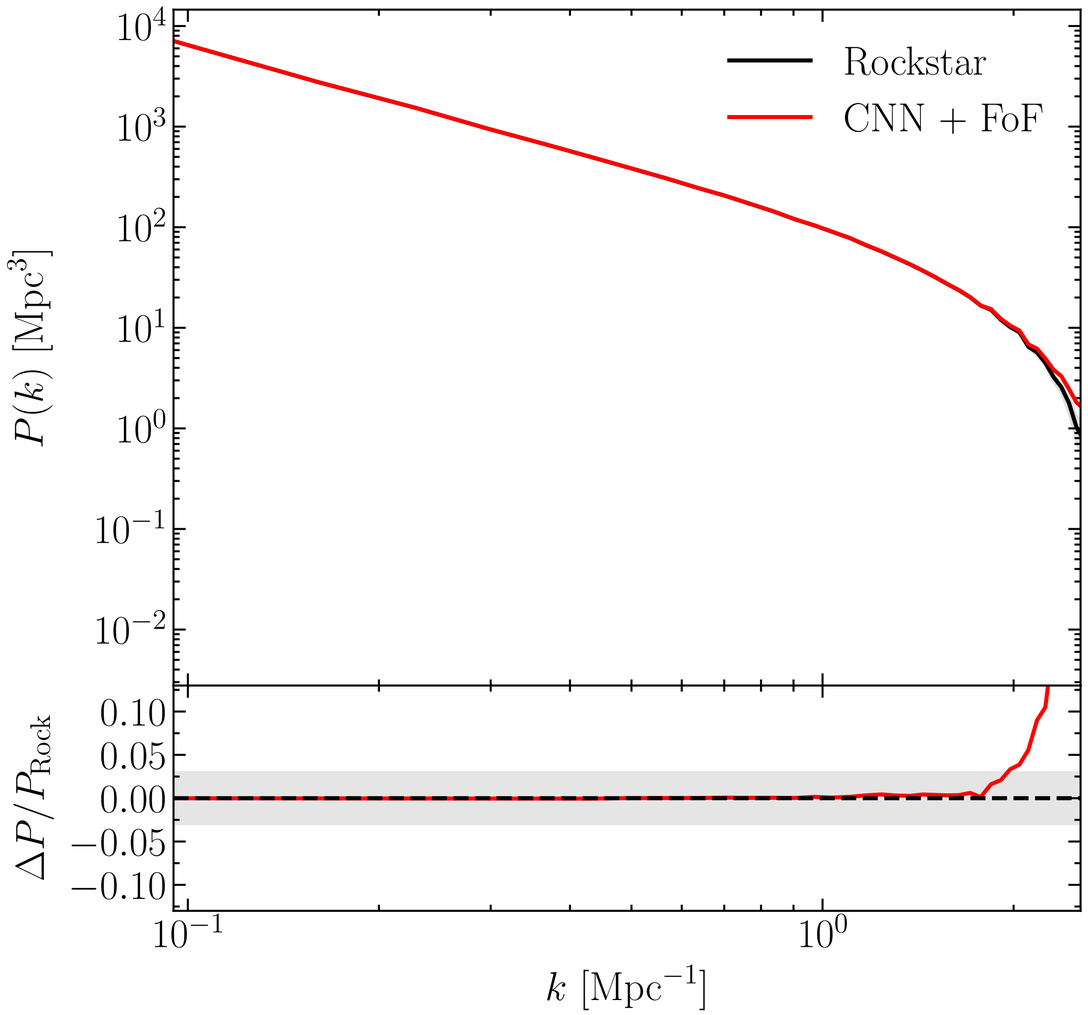
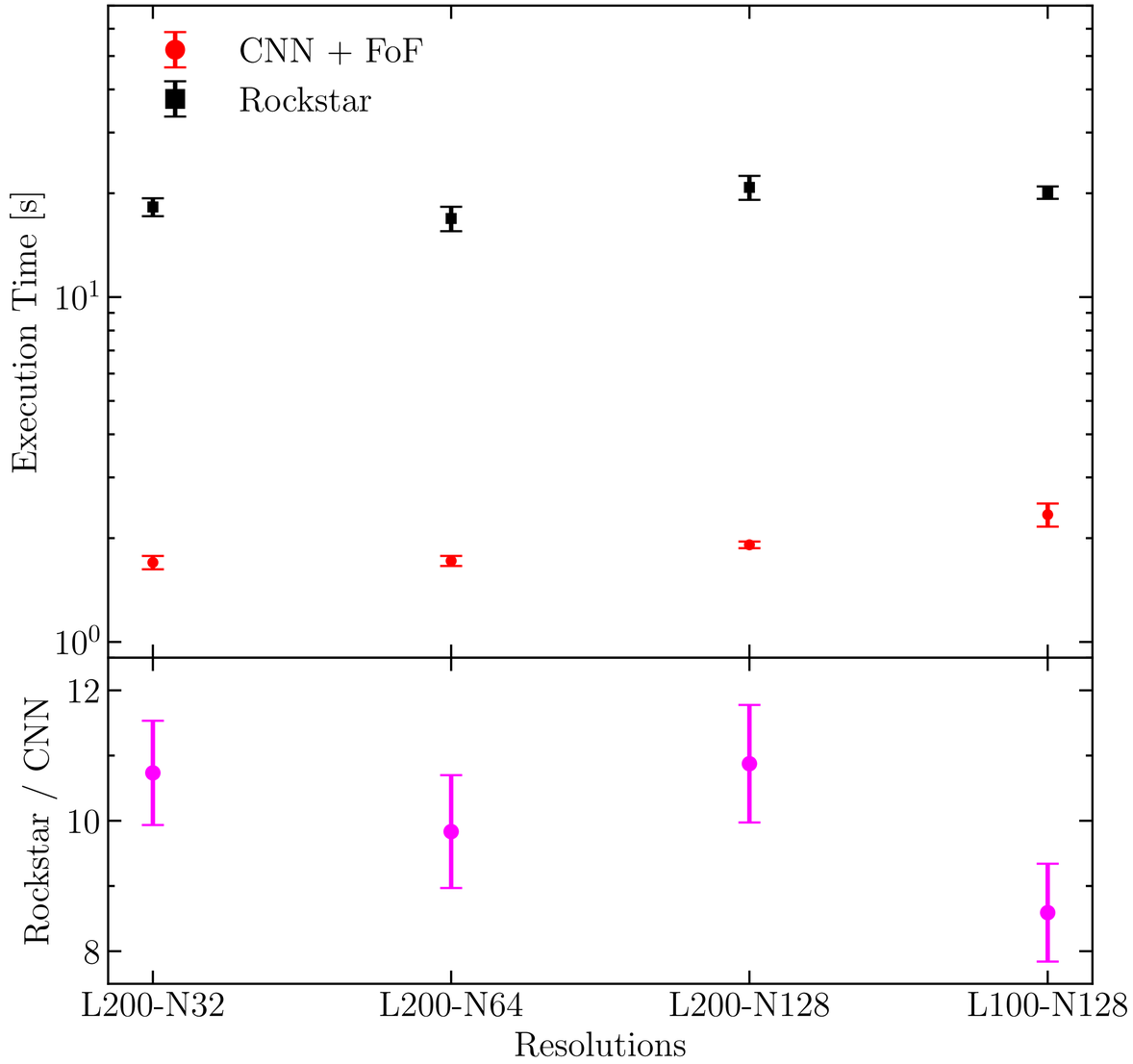


Power Spectrum



Runtime Comparison



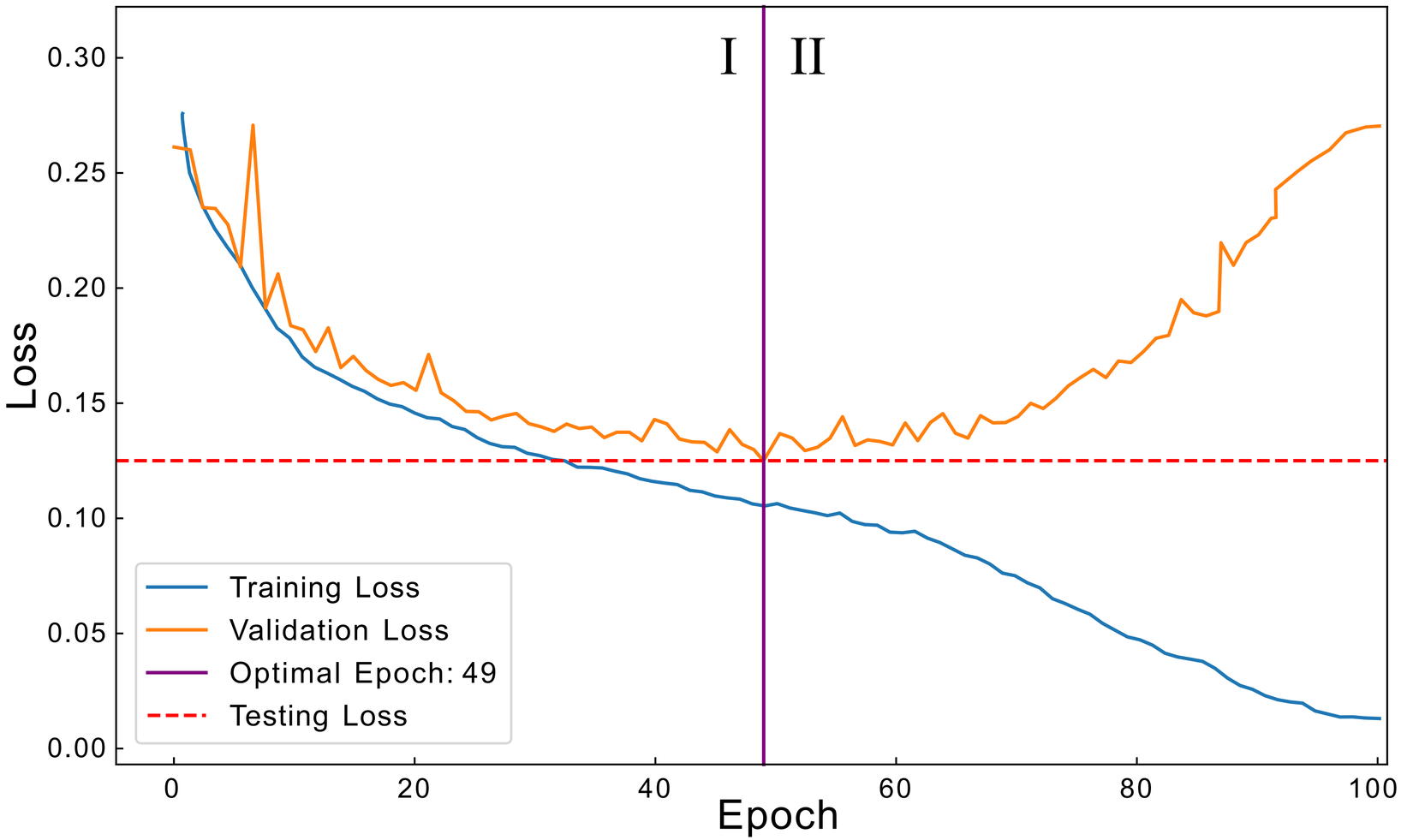
Conclusions

Final Remarks and Future work

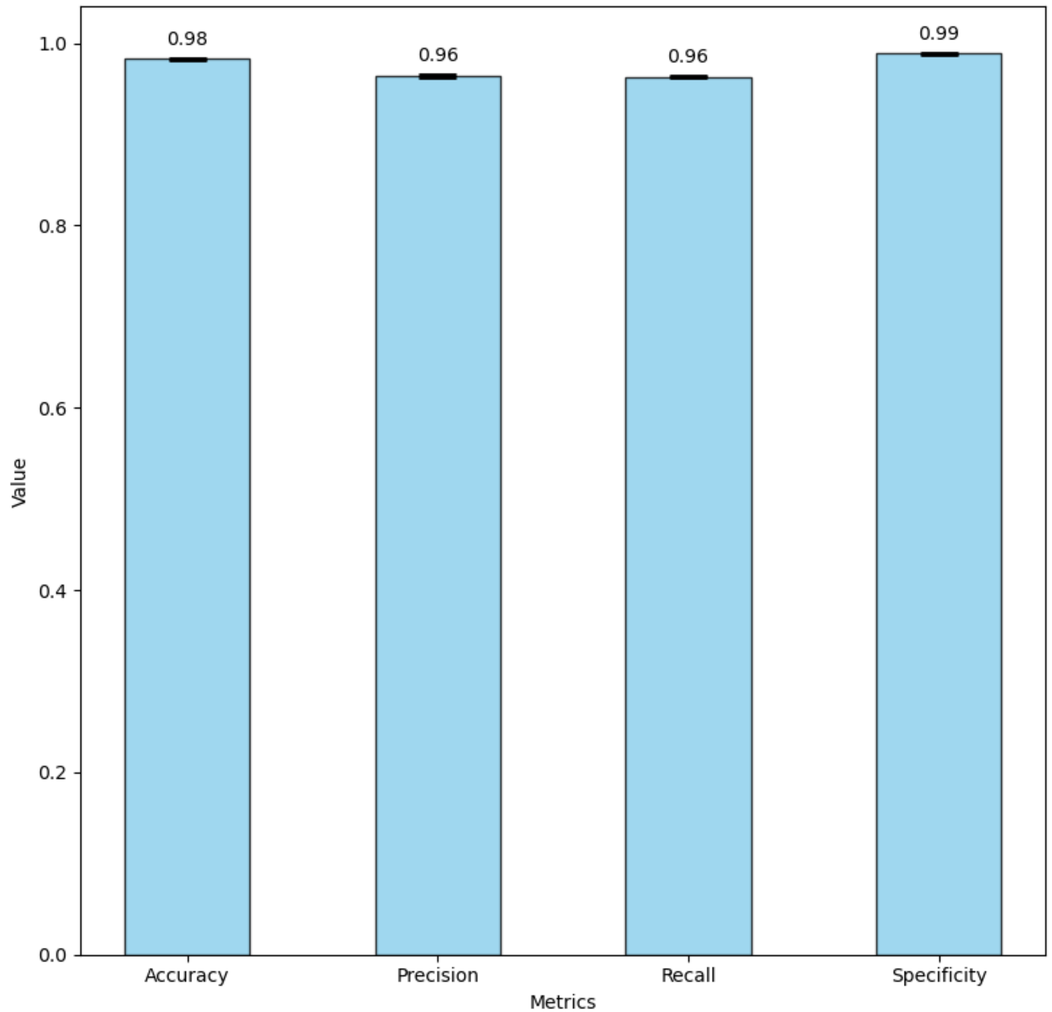
- **Massive** and **Fast** production of **halo catalogues** for cosmological analyses
- Halo Finder based on ML 2 steps: **classification** of particles with a CNN and **clustering algorithm** (FoF) to get the centers
- Our models:
  - **Resolutions**: $L200 - N128^3$, $L100 - N128^3$, etc.
  - **Mass definitions**: M_{200b}, M_{vir}
- **Classification step** works at **particle level** and it is cost-effective. Metrics show a very good performance (99% in accuracy)
- **Centre recovery step** is also working very well, as the matching analysis shows
- However it is still a bottleneck because of using FoF (work in progress $\longrightarrow$ extension of the CNN to also do this task)
- Apply our method to **bigger box** sizes. With the model of $L100 - N128^3$ we can work on $L1500 - N2048^3$ (work in progress)
- Cosmological analysis (work in progress)


Thank You

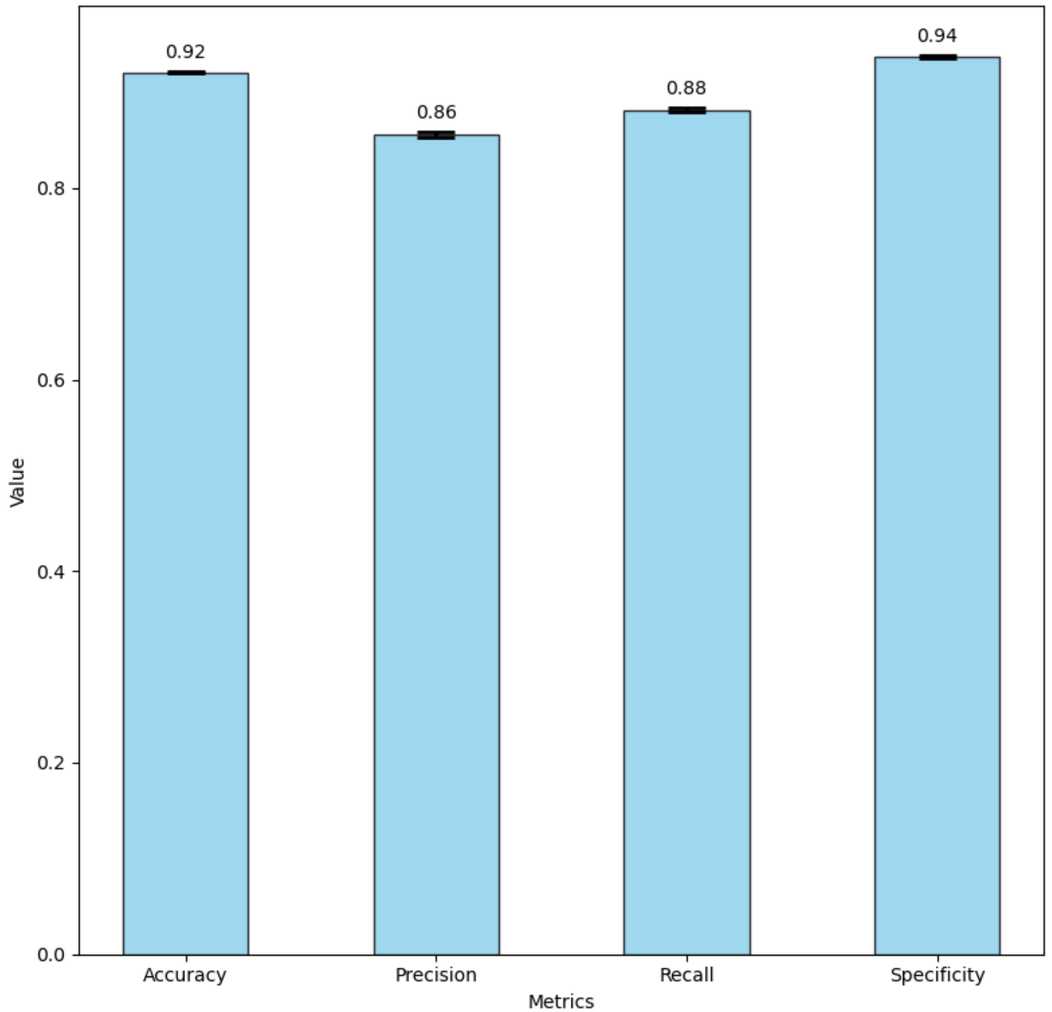
Backup

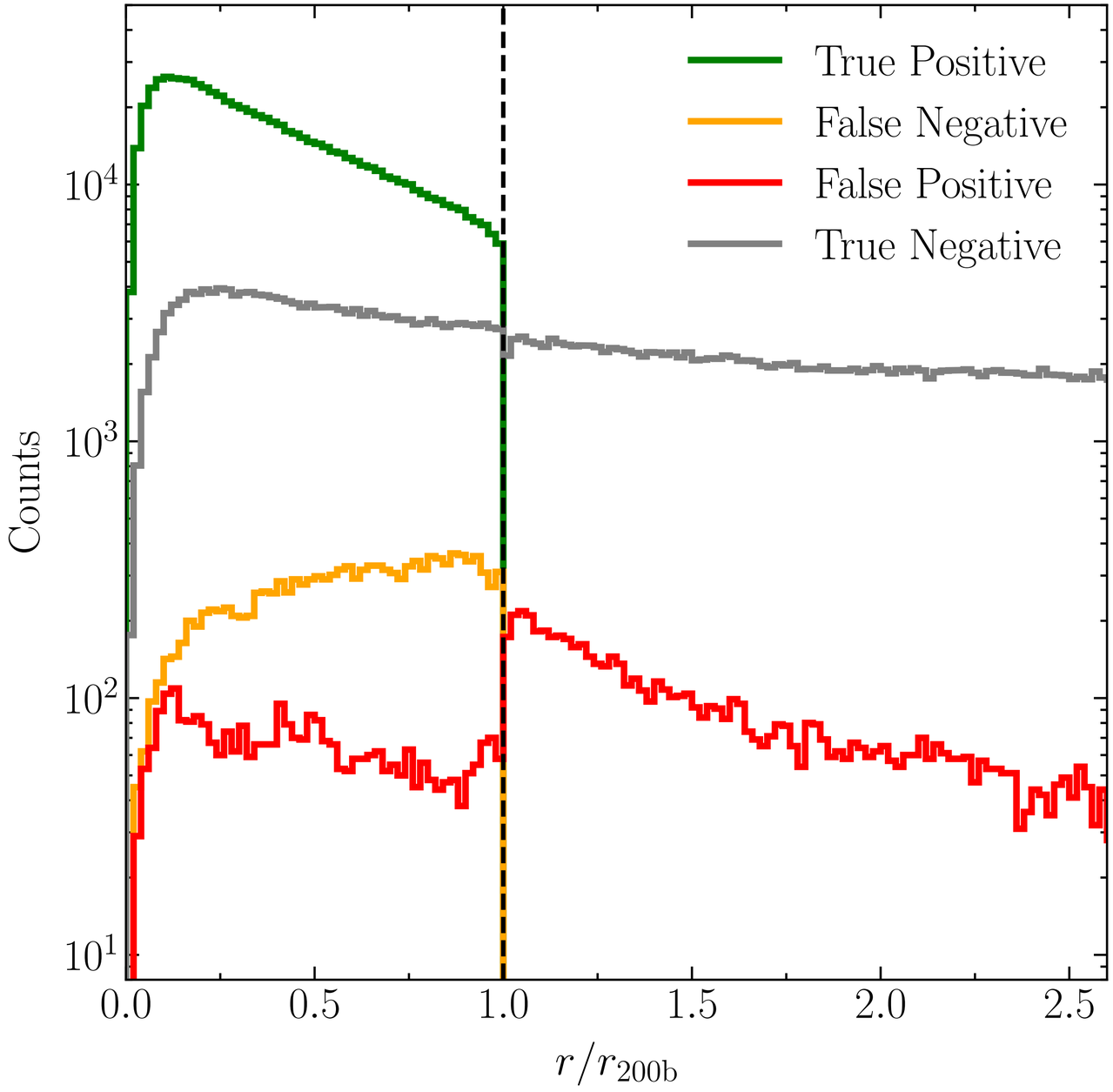

I
II
0.30
0.25
0.20
0.15
0.10
0.05
0.00
Loss
0
20
40
60
80
100
Epoch
Training Loss
Validation Loss
Optimal Epoch: 49
Testing Loss

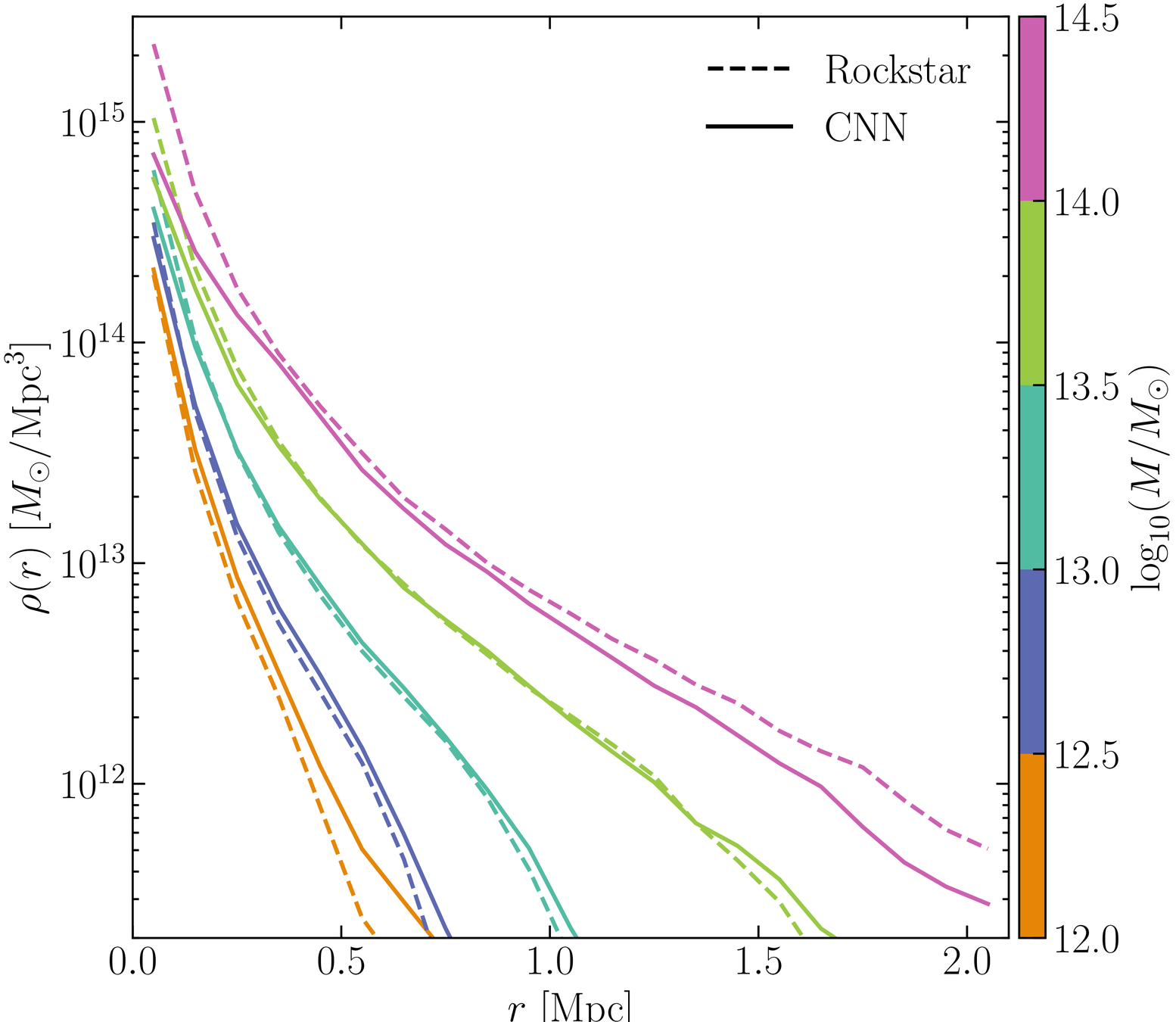
$\mathbf{M_{vir}}$



$\mathbf{M_{FoF}}$




True Positive
False Negative
False Positive
True Negative
Counts
10^4
10^3
10^2
10^1
0.0
0.5
1.0
1.5
2.0
2.5
r/r_{200b}


Rockstar
CNN
10^{15}
10^{14}
10^{13}
10^{12}
$\rho(r)$ $[M_\odot/\mathrm{Mpc}^3]$
0.0
0.5
1.0
1.5
2.0
r [Mpc]
14.5
14.0
13.5
13.0
12.5
12.0
$\log_{10}(M/M_\odot)$