Super-resolution simulations

Speaker: Yueying Ni

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Simeon Bird (UCR), & Yu Feng (UCB)

Outline

- **Motivation**
- **Methodology / Design of the Task**
- **Validation / Tests**
- **Future Prospect**

Publication:

Li et al. PNAS May11, 2021 118 (19) [arXiv:2010.06608]

Ni et al. MNRAS.507.1021N [arXiv:2105.01016]

Repository:

https://github.com/eelregit/map2map

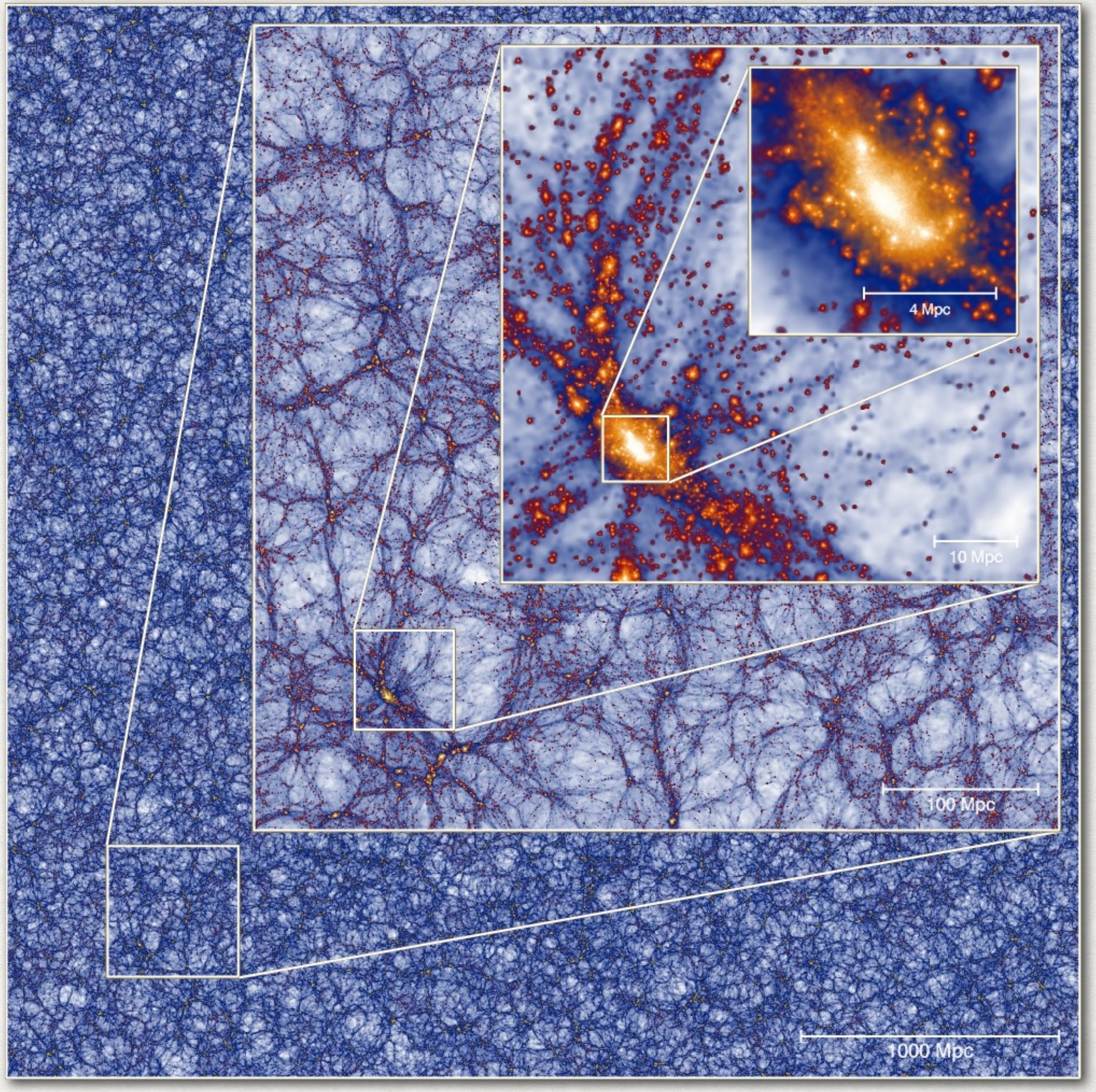
Trained model:

https://github.com/yueyingn/SRS-map2map

Why super resolution (SR)

Cosmological simulations are expensive

- Large dynamic range with nonlinear evolution
- Time complexity $\sim \mathcal{O}$ (num_particles $\times$ time_steps)
- Multi-scale physical process in hydrodynamic simulations of galaxy formation



Millennium-XXL (N-body simulation)

Large dynamic range & multi-scale physical process

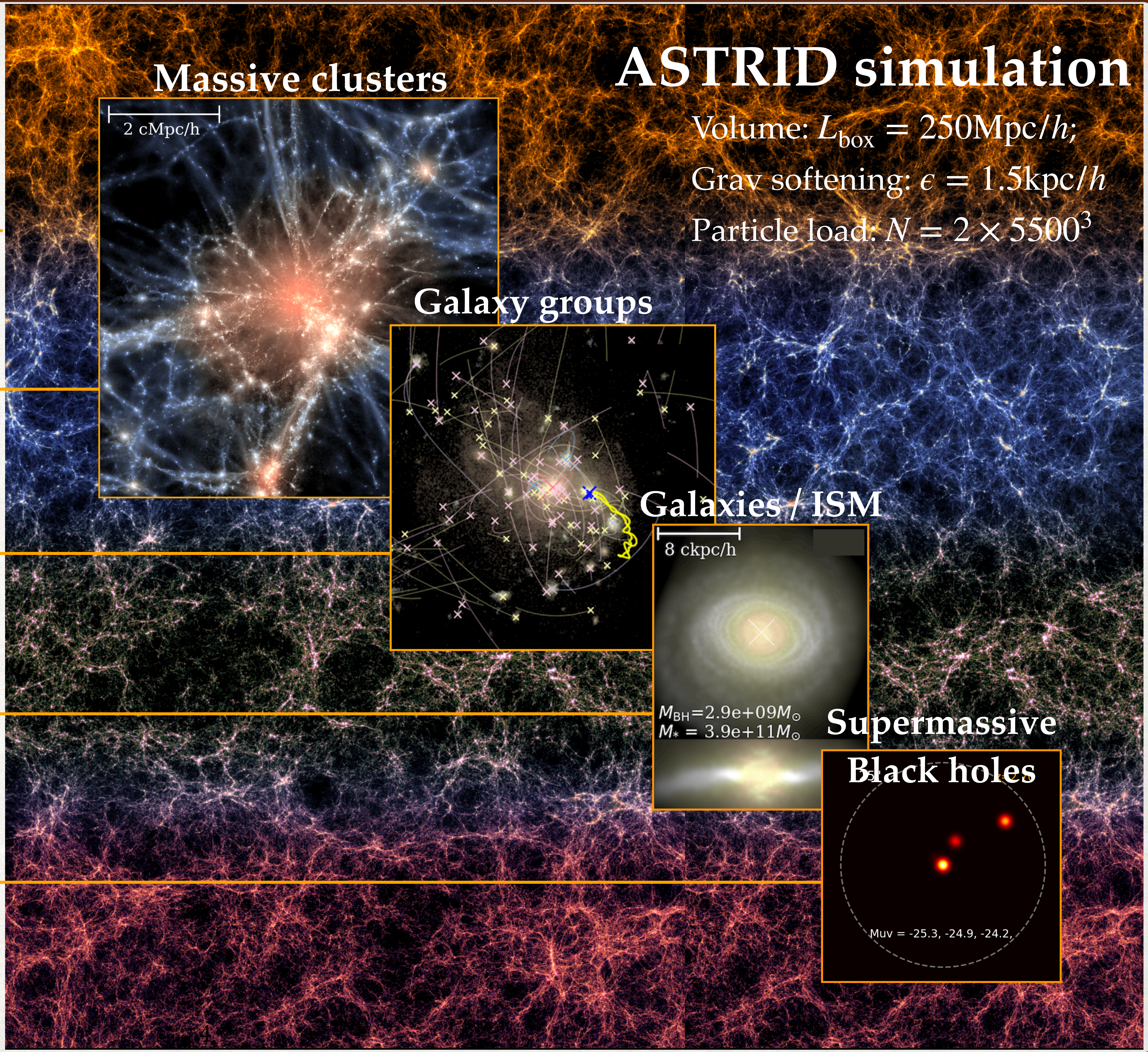
Cosmic Web: >100 Mpc

Massive clusters: ~10 Mpc

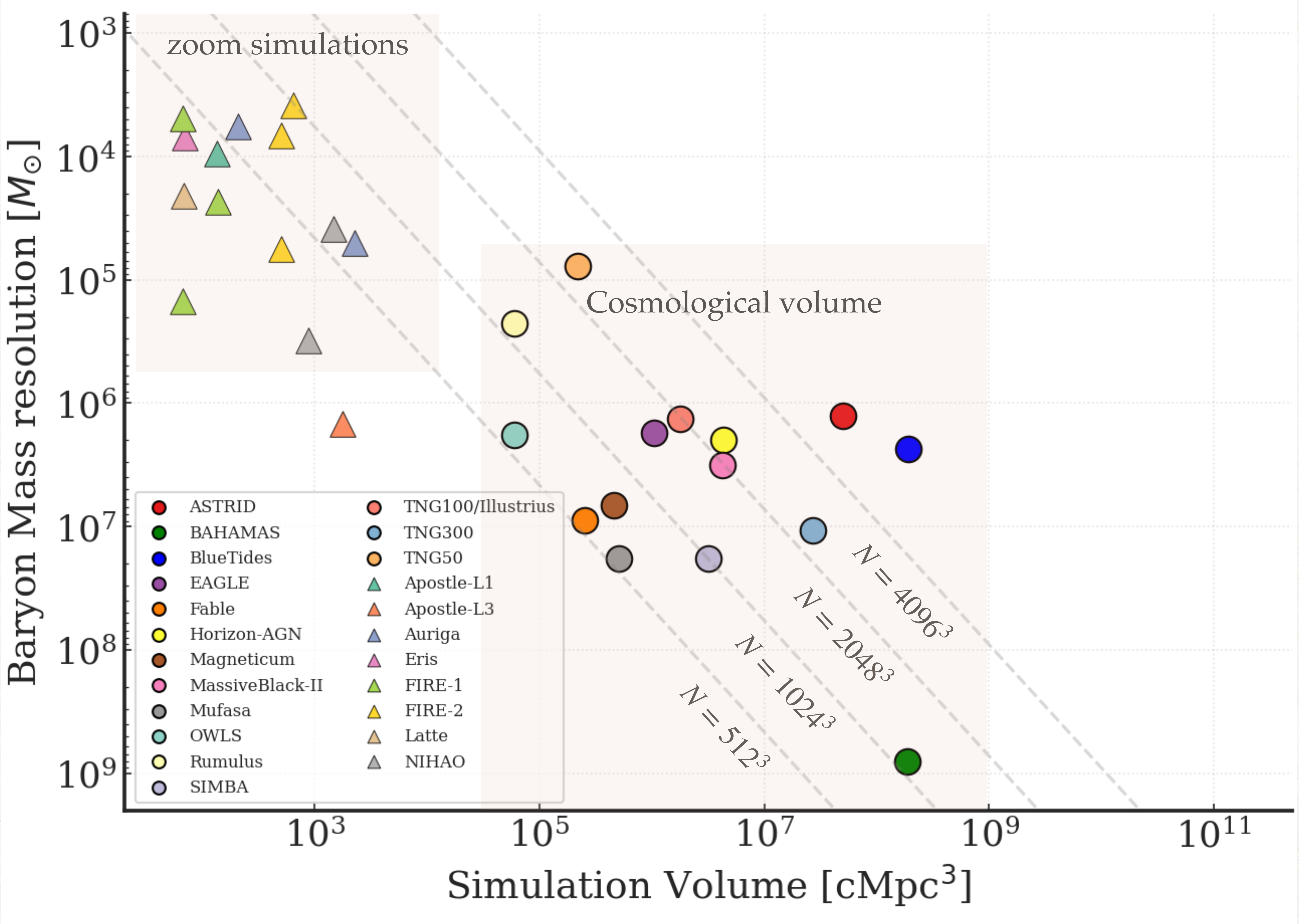
Groups of galaxies: ~1 Mpc

Galaxies/ISM: ~10 kpc

SMBH/AGN: 1 ~ 10 kpc



We want to push cosmological simulations to larger volume and higher resolution



(Plot adapted from Nelson et al 2019)

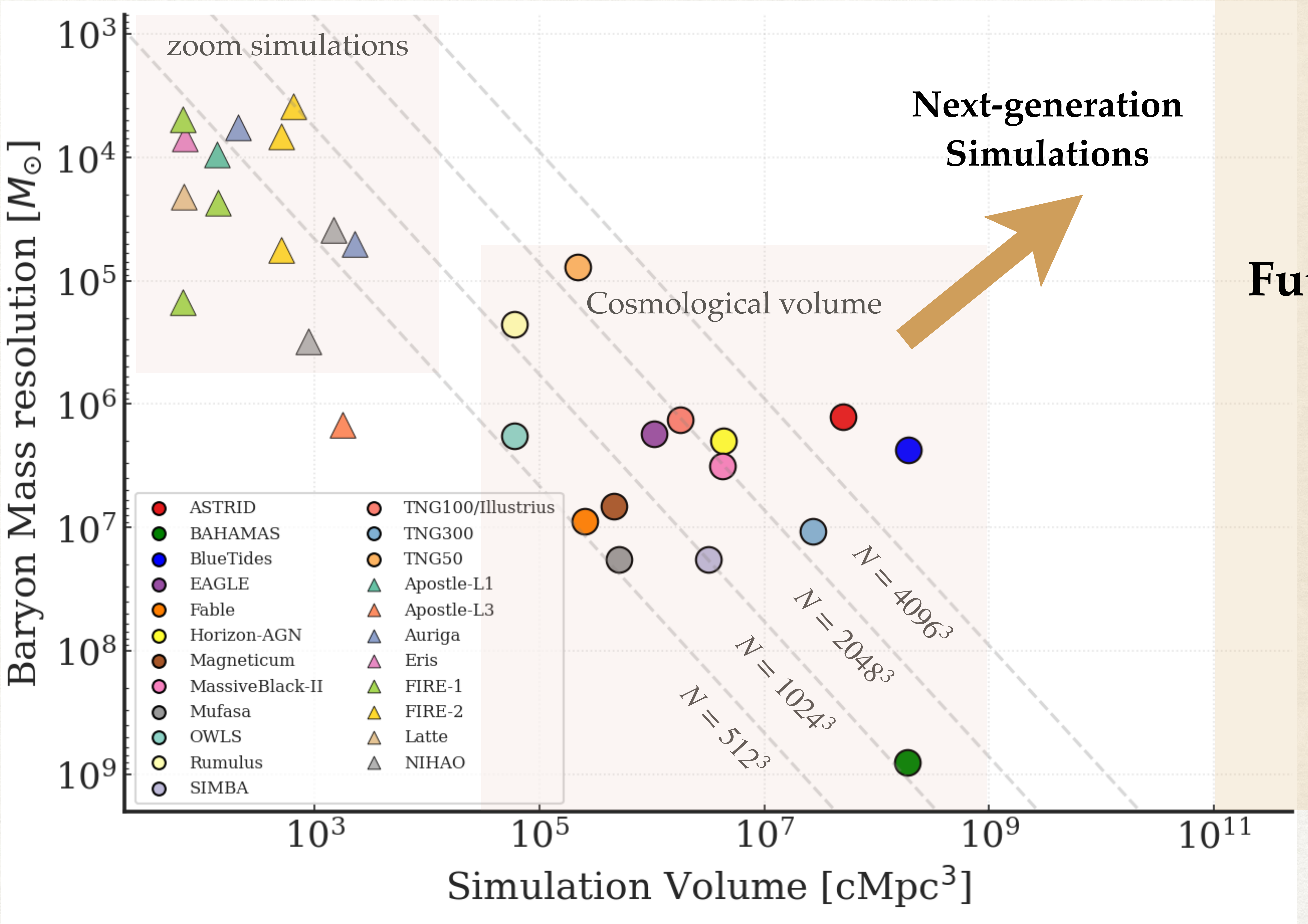
Larger volume:

- better statistics
- long-short mode coupling

Higher resolution

- better resolve the internal structure of halo
- model the physical process of galaxy formation

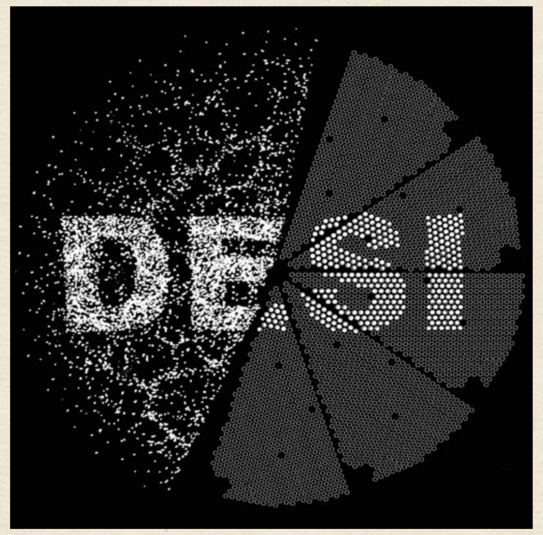
We want to push cosmological simulations to larger volume and higher resolution



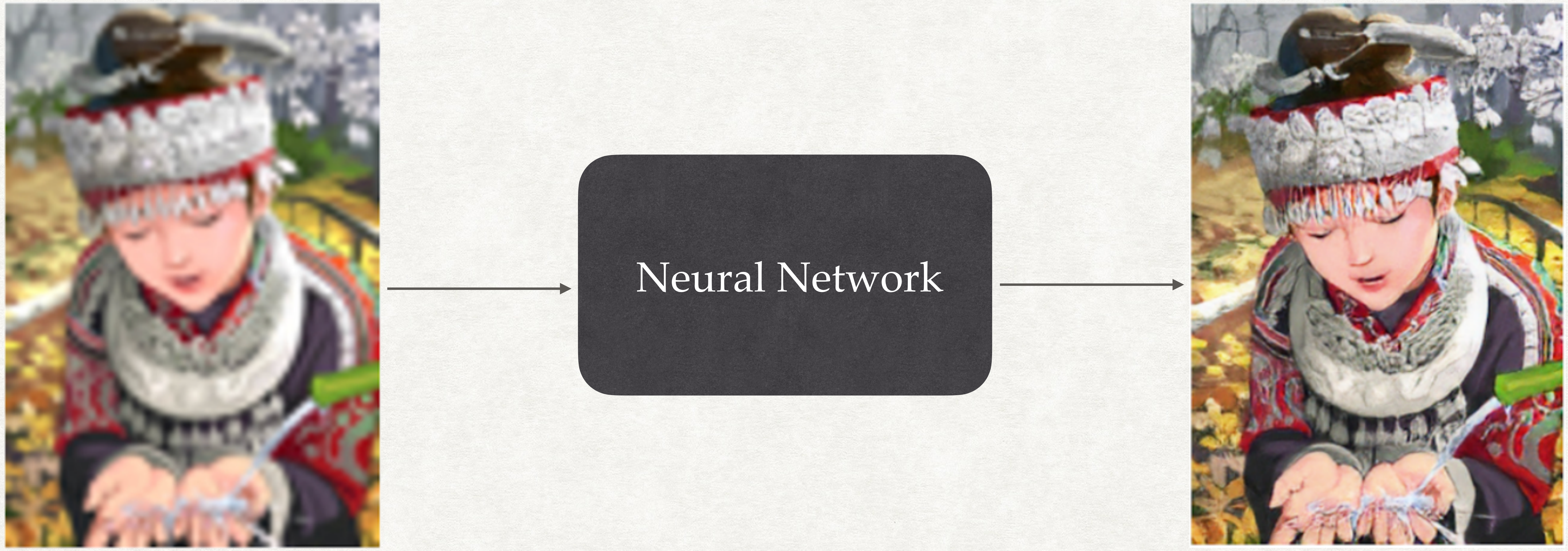
(Plot adapted from Nelson et al 2019)

Future large sky surveys

$> 10^{14}\mathrm{cMpc}^3$



What is SR — Deep learning image super resolution



What is SR — Deep learning image super resolution

HR LR SR

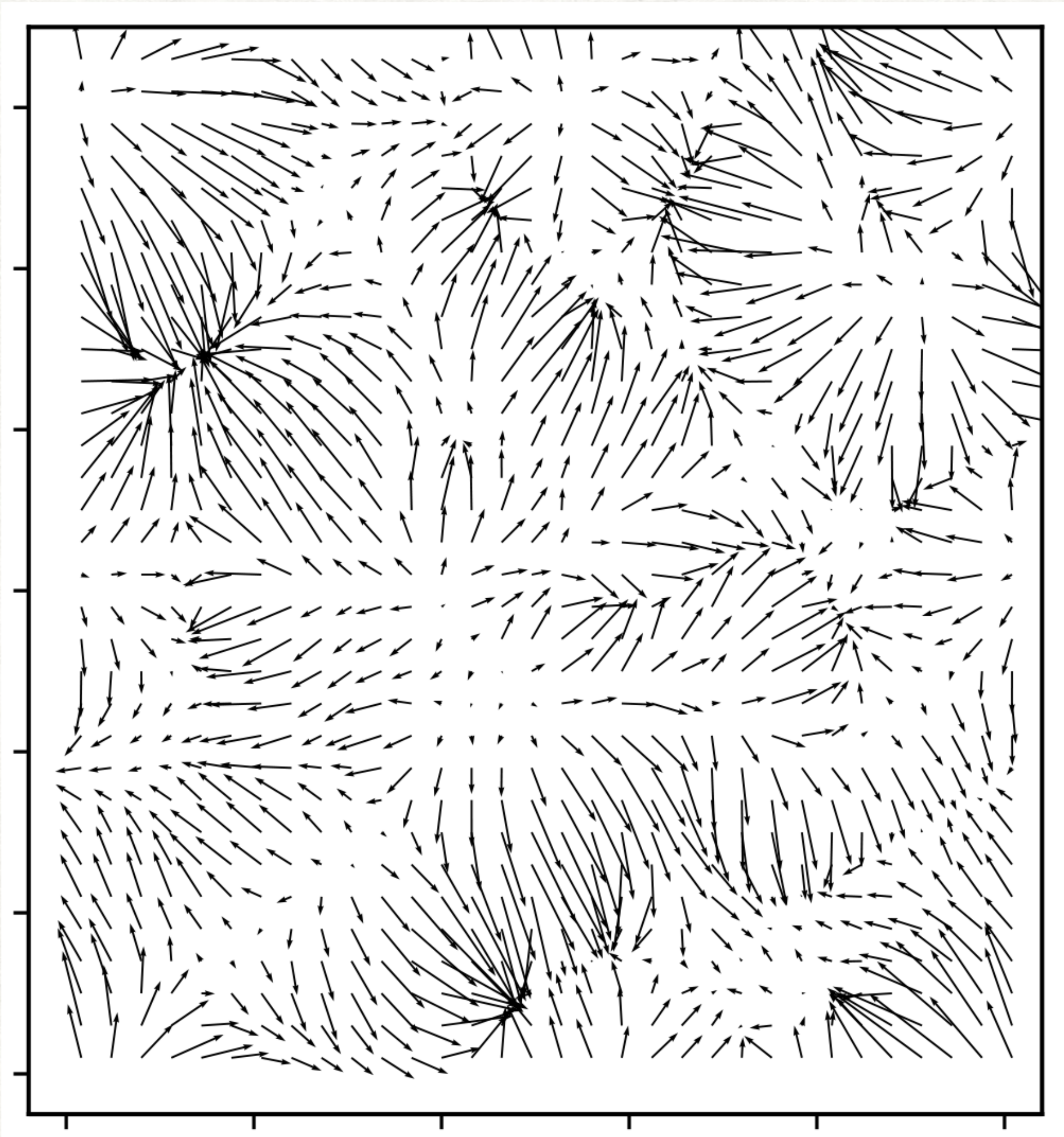
[1808.03344] Deep Learning for Single Image Super-Resolution: A Brief Review
[1902.06068] Deep Learning for Image Super-resolution: A Survey

SR simulation: train a deep learning model to generate small-scale features from low-resolution (LR) simulations

LR —> SR: full phase-space distribution with 512x more tracer particles
(therefore we enhance the mass resolution by 512 times)

How to SR an N-body simulation I : Format the N-body simulation

x

a xy-slice  y

Particle displacement

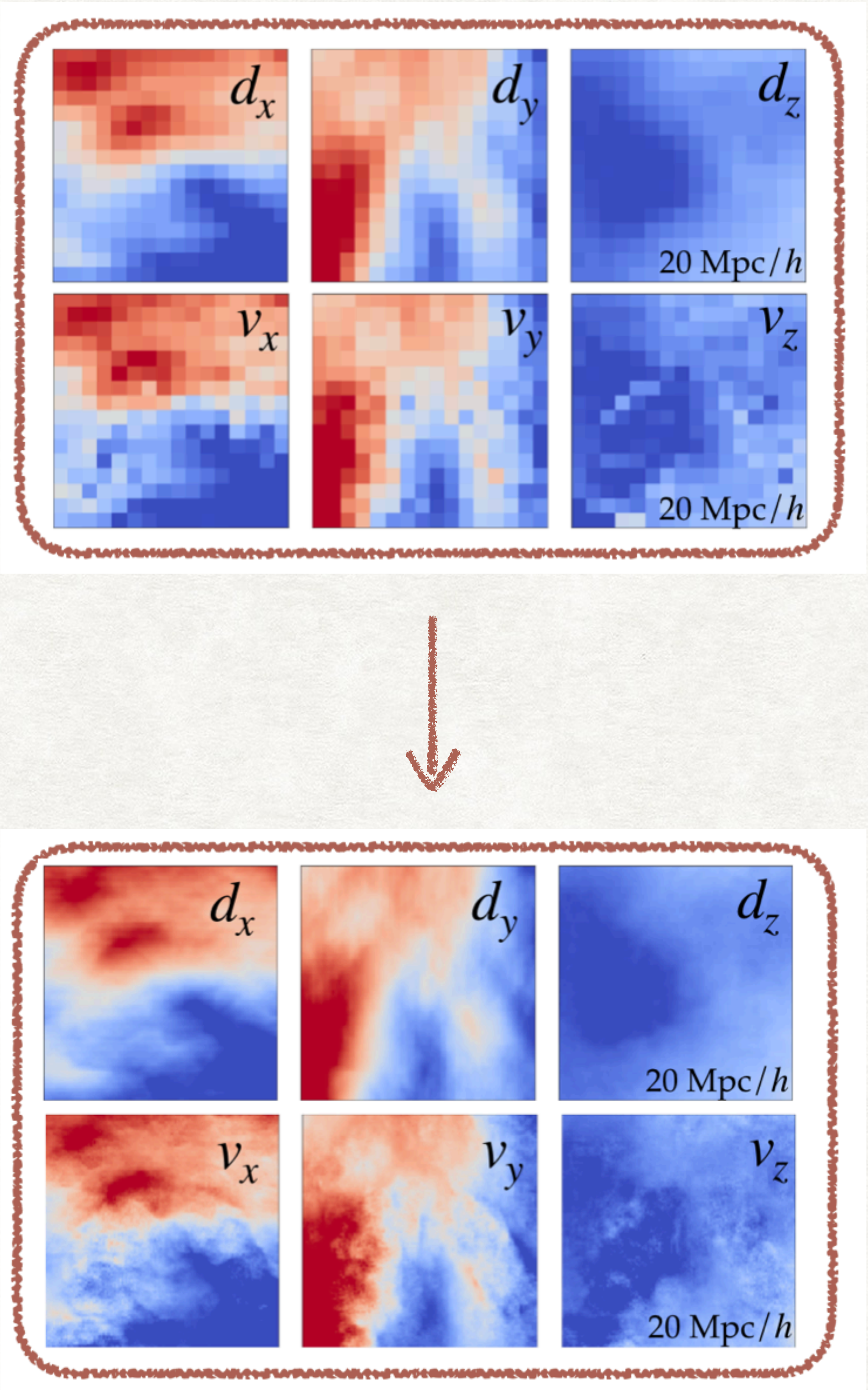
$$\boxed{\mathbf{d}_i} = \boxed{\mathbf{x}_i} - \boxed{\mathbf{q}_i} \quad (i = 1, \ldots. N)$$

Final Position   Initial (Cartesian) grid

3D images with **6 channels** $\{d_x \, d_y \, d_z \, v_x \, v_y \, v_z\}$

LR

HR



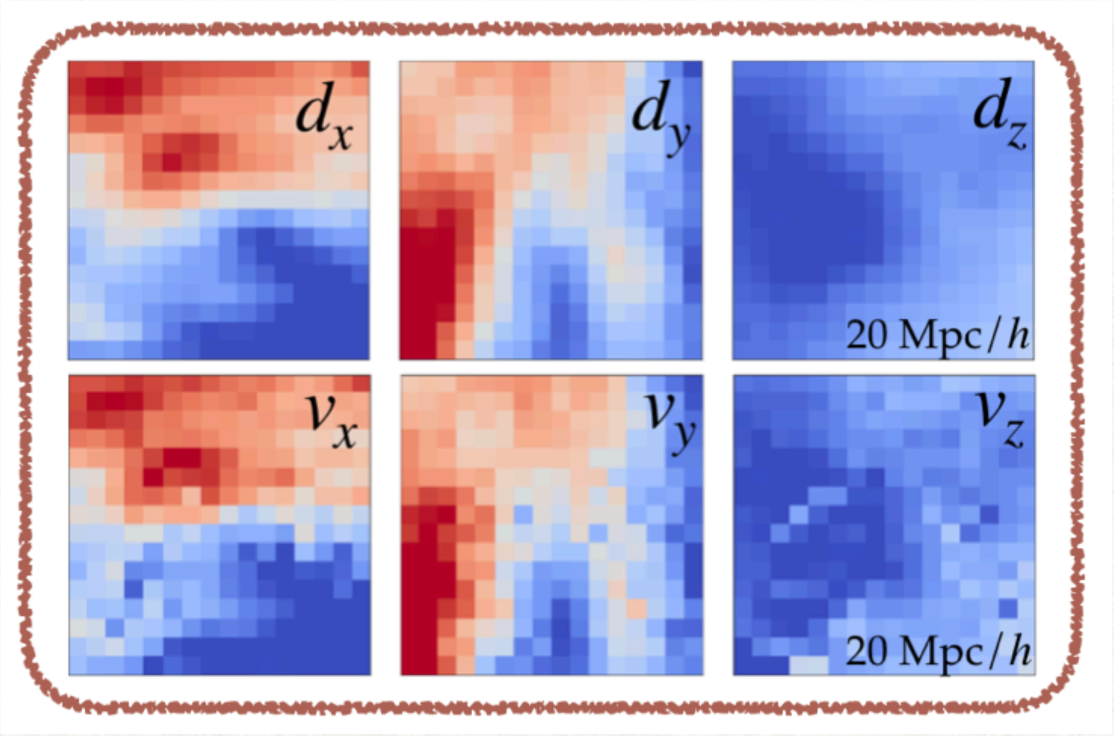
How to SR an N-body simulation I : Format the N-body simulation

3D images with **6 channels** $\{d_x\, d_y\, d_z\, v_x\, v_y\, v_z\}$

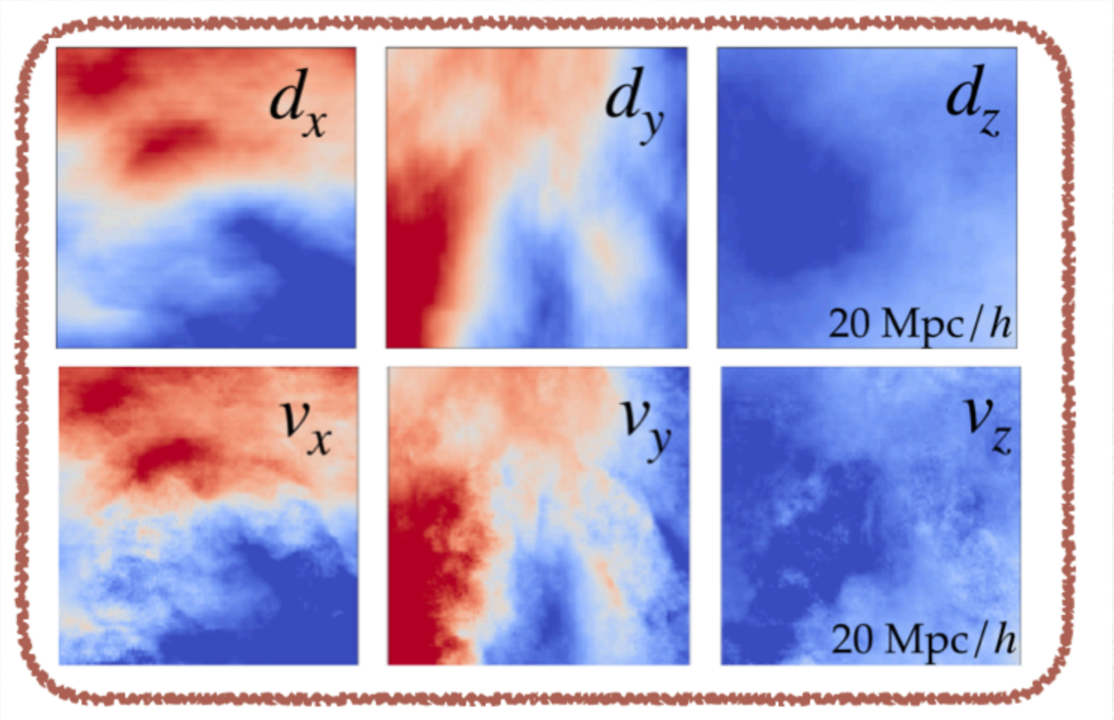
Advantages of ***Lagrangian description***:

- ***conserves mass*** by construction
- Better describes the field with ***large dynamic range*** (resolve to smaller scales for high density region)
- SR results can be ***formatted as simulations*** with distinguishable tracer particles will their 6D phase space distribution

LR



HR



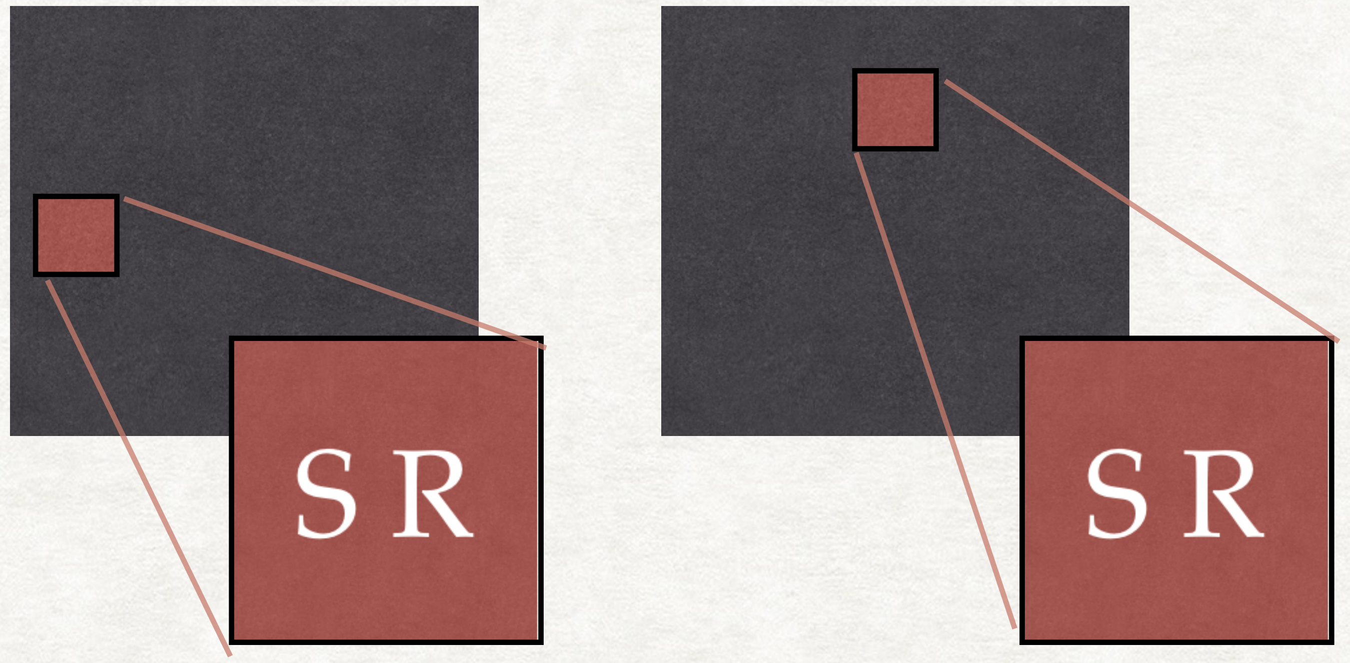
How to SR an N-body simulation II : Symmetry

Mass conservation

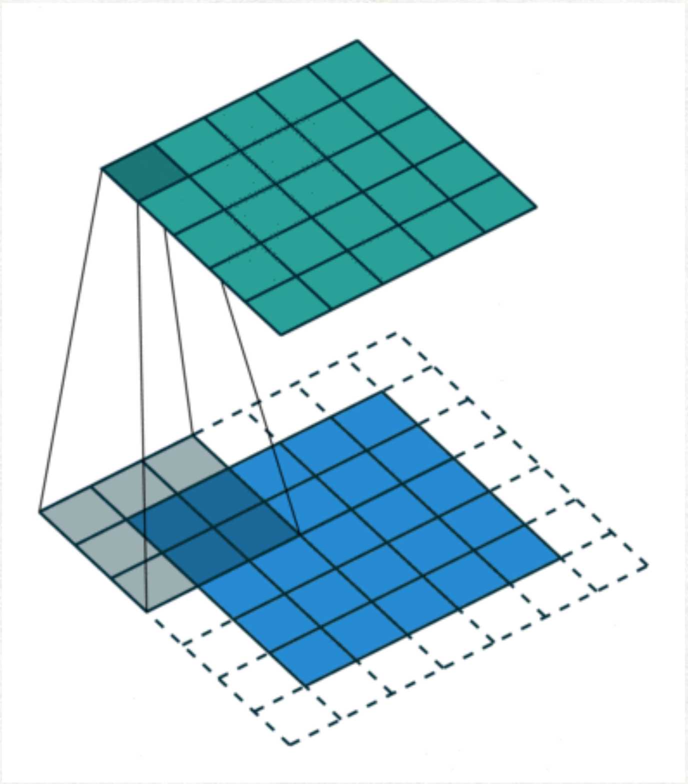
- Mass naturally conserved in Lagrangian prescription

Translational symmetry

- CNN feature by construction
- periodic padding (on the LR input)

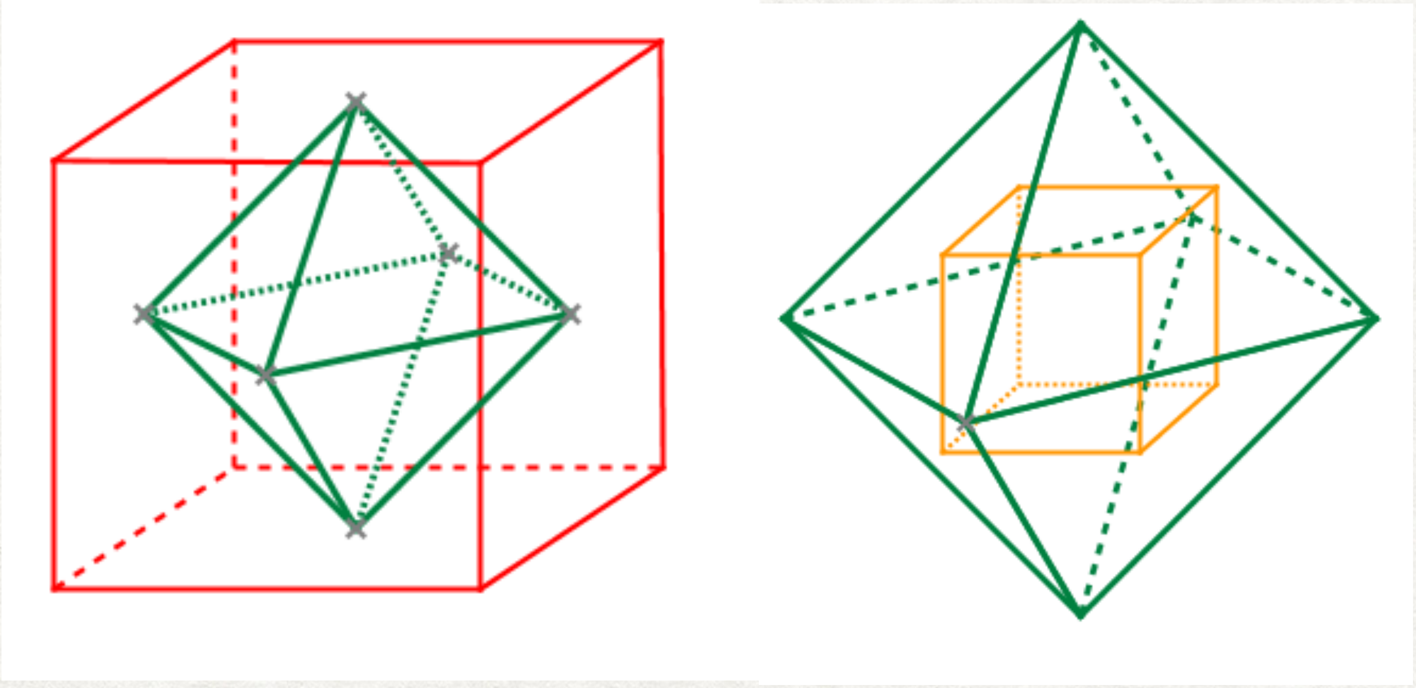


Convolution neural net

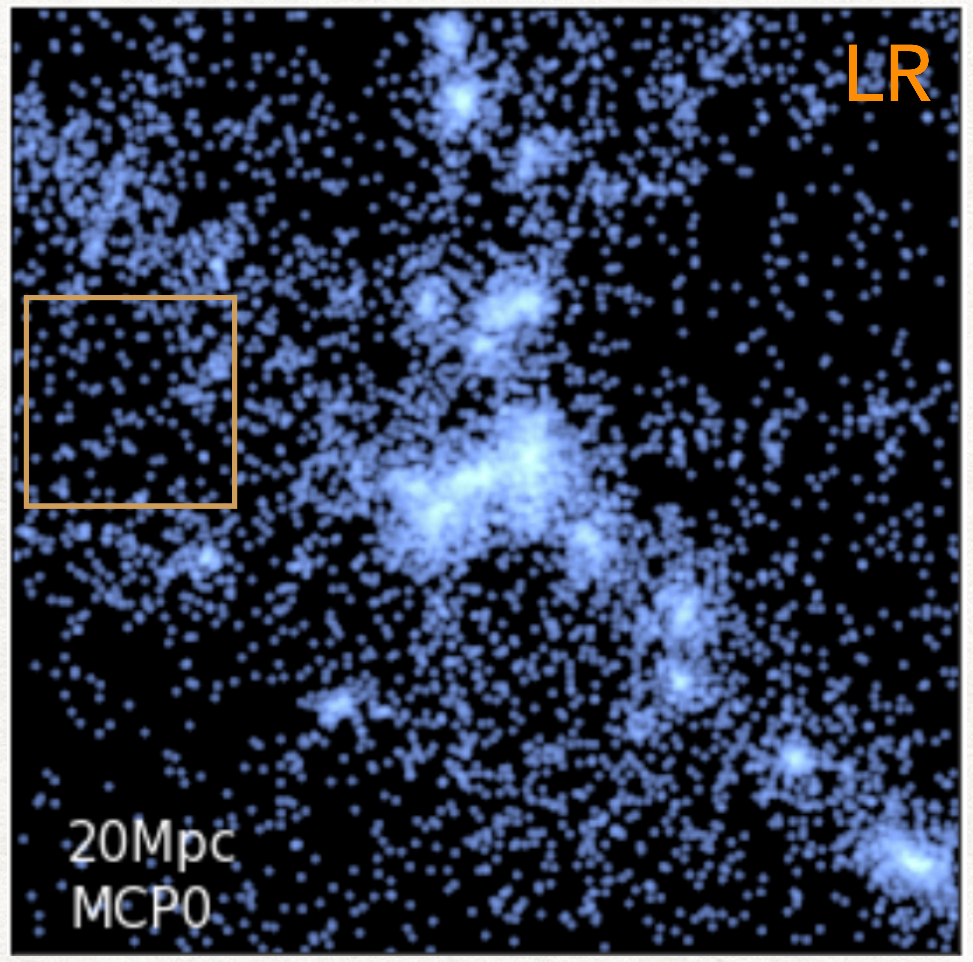


Rotational symmetry

- Data augmentation with 48 operations from the O_h point group
- Brute-force approach to teach a model to be symmetry awareness

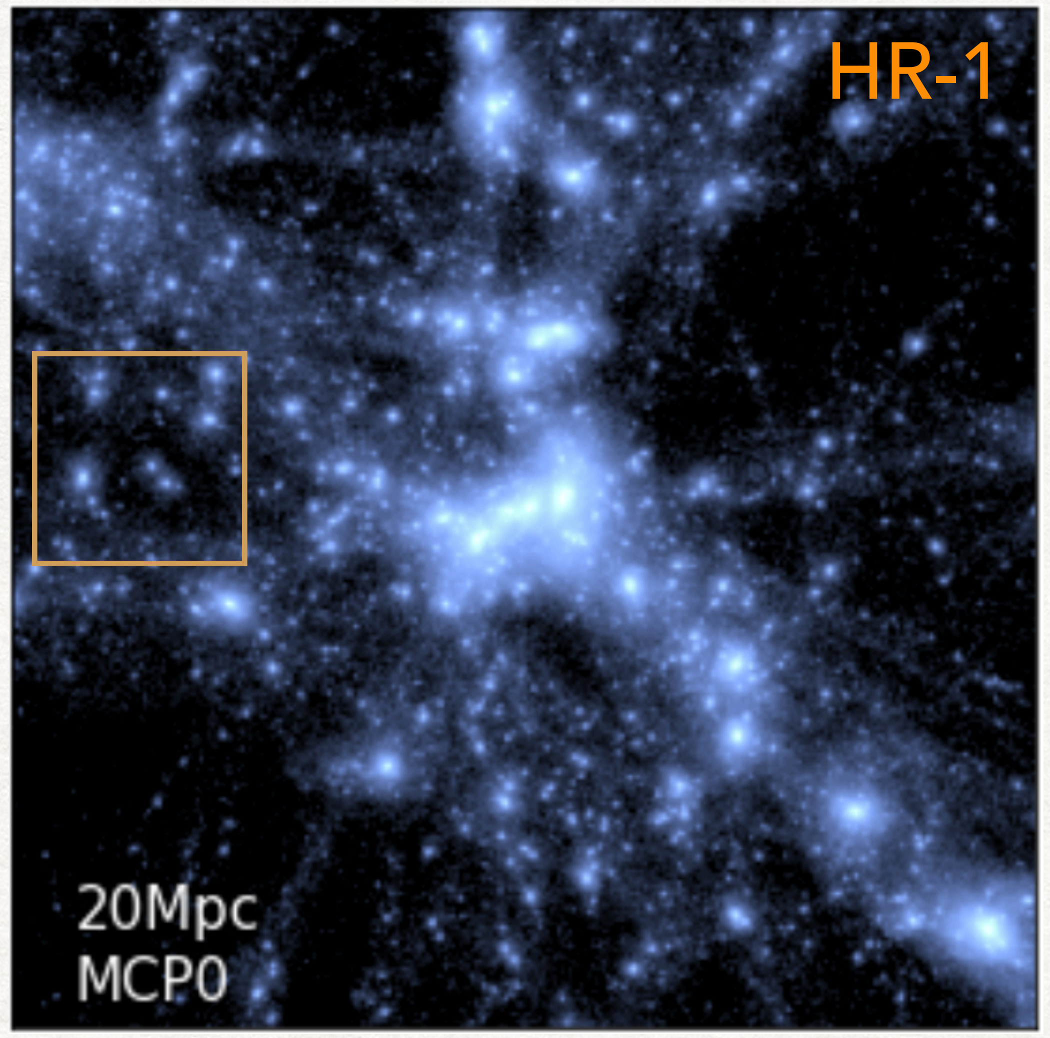


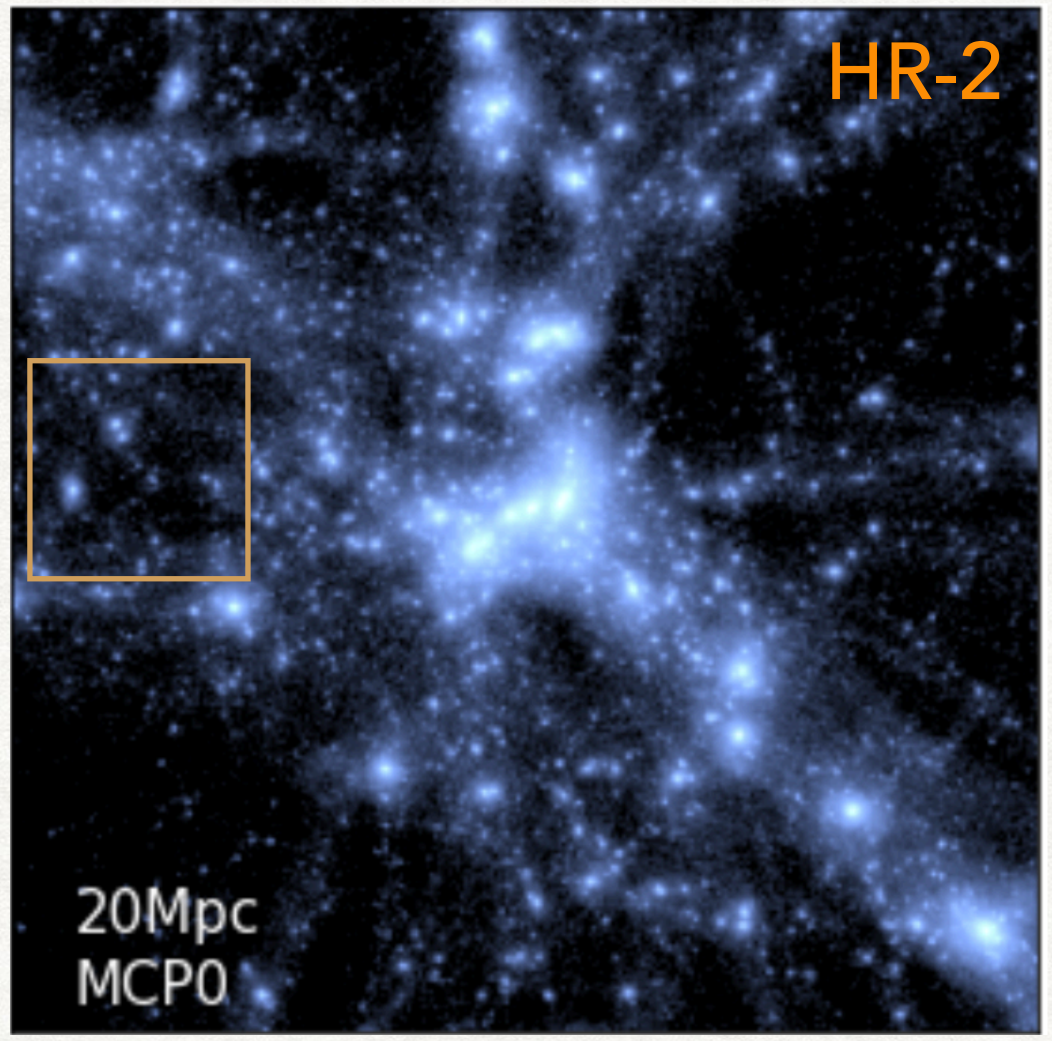
How to SR an N-body simulation III : Stochasticity

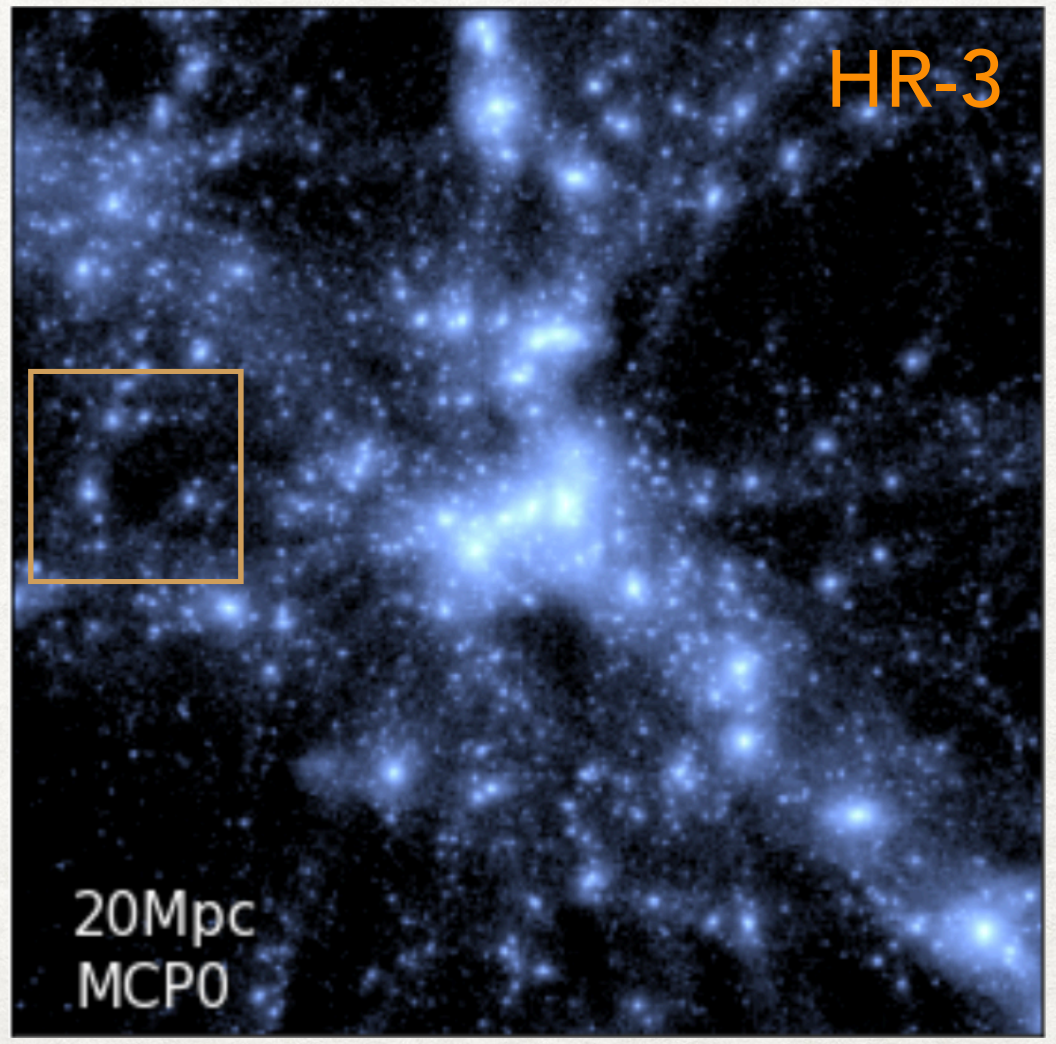


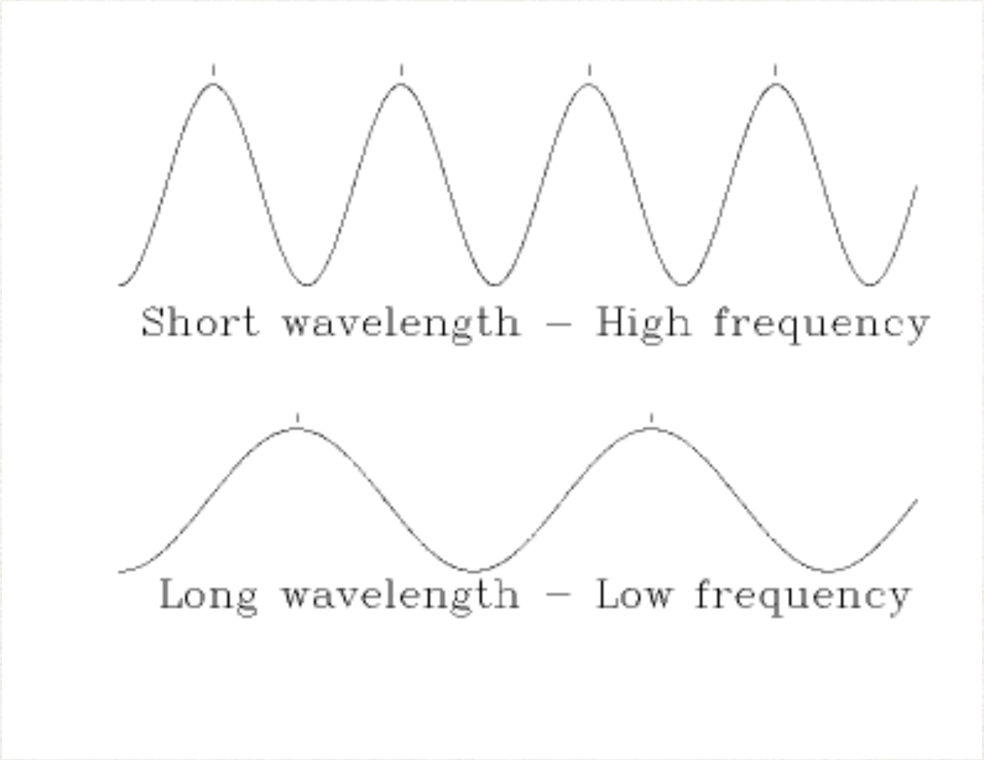
LR —> HR

one-to-many task









Only in HR Initial Conditions

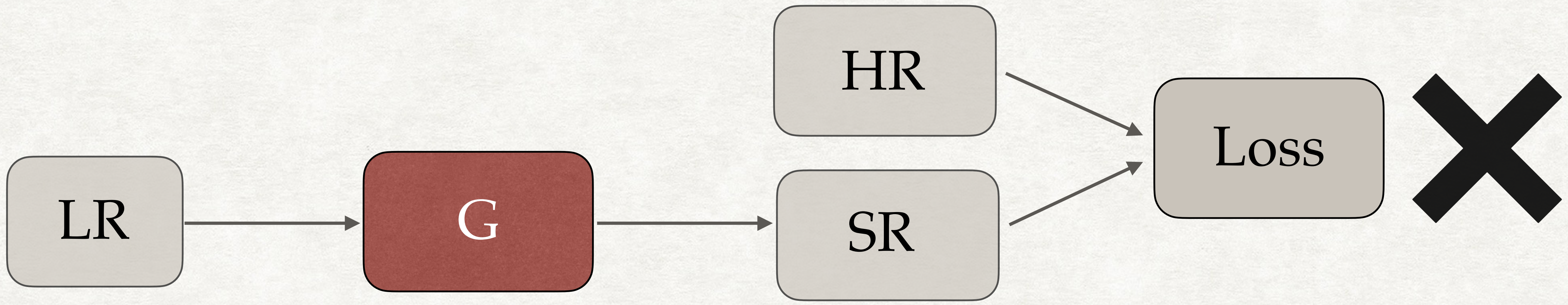
LR Initial Conditions

How to SR an N-body simulation III : Stochasticity

Stochasticity consequence 1: need for better loss function

- Simple loss functions aim to minimize the pixel-wise (rather than statistical) difference between SR and HR

Supervised learning?

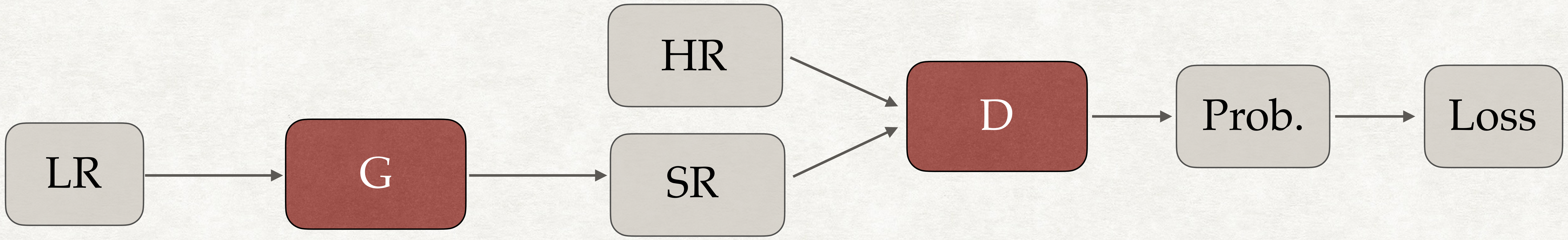


How to SR an N-body simulation III : Stochasticity

Stochasticity consequence 1: need for better loss function

- Use generative adversarial network (**GAN**) that adds another (discriminator) network to evaluate SR output.
- Train generator (G) and discriminator (D) alternatively in a game

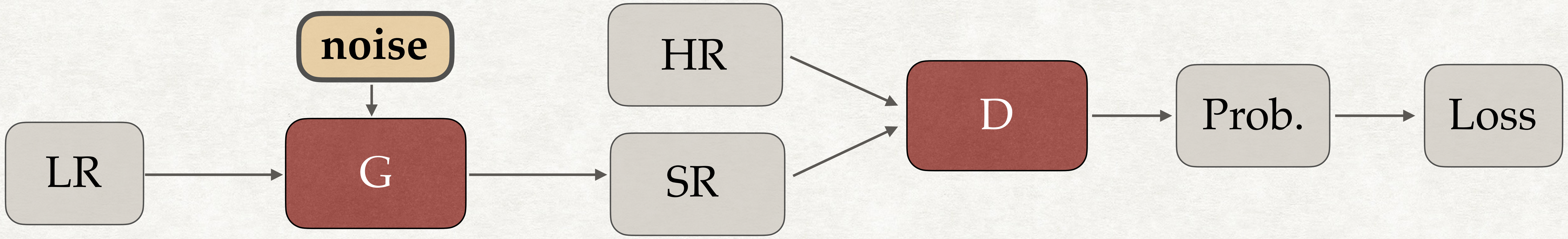
    Update G to fool D, and update D to distinguish SR from HR



How to SR an N-body simulation III : Stochasticity

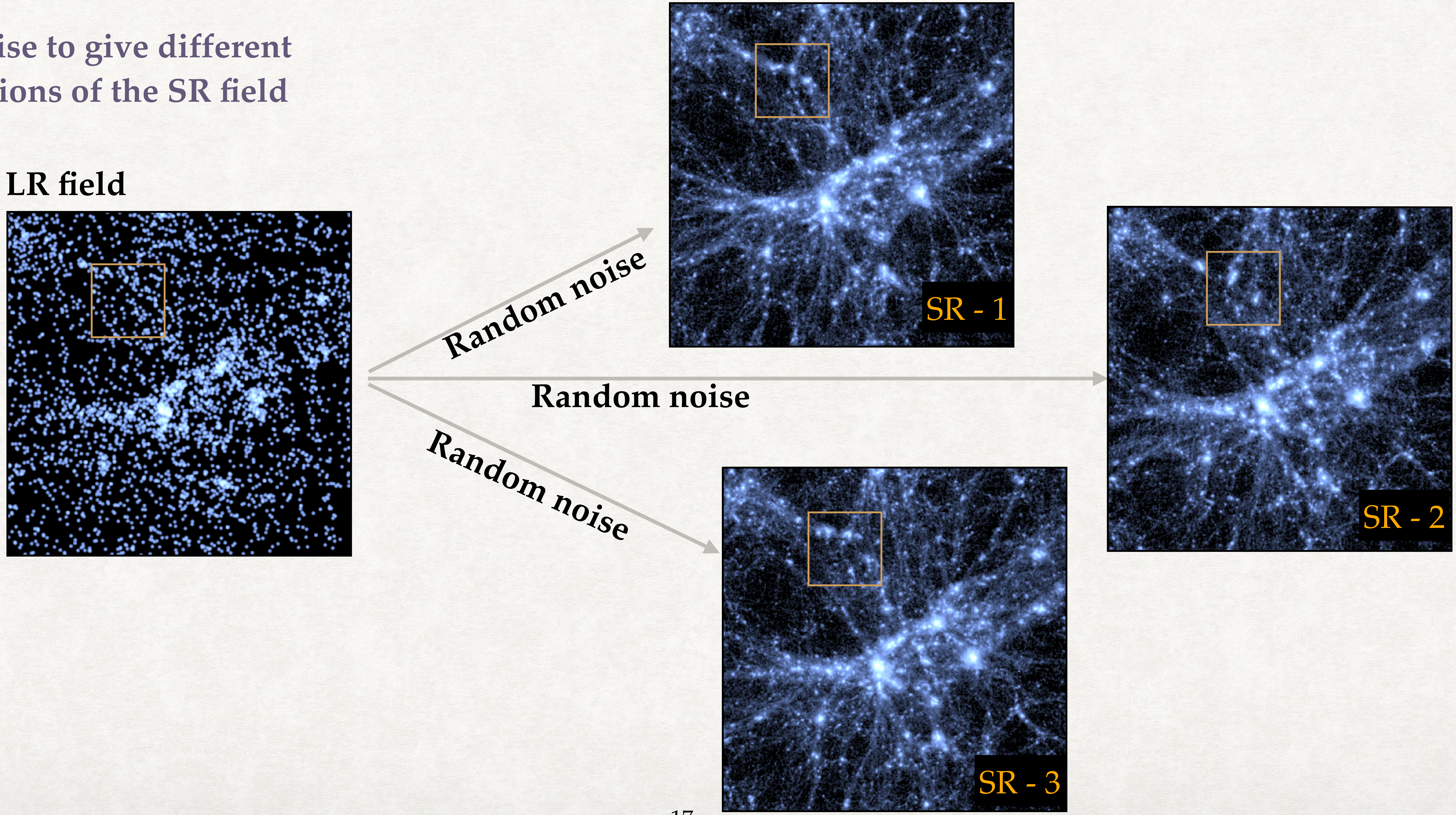
Stochasticity consequence 2: need for randomness

- Add noises throughout our (generator) neural network
- SR realizations are different among themselves (and with HR samples)



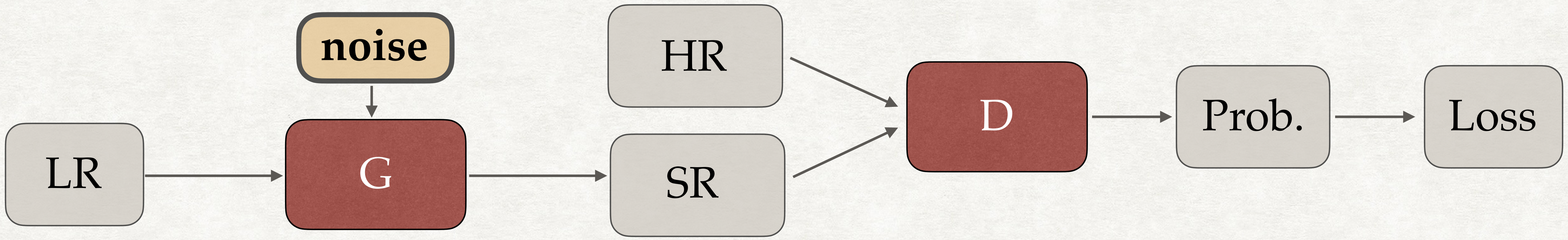
How to SR an N-body simulation III : Stochasticity

Add noise to give different realizations of the SR field



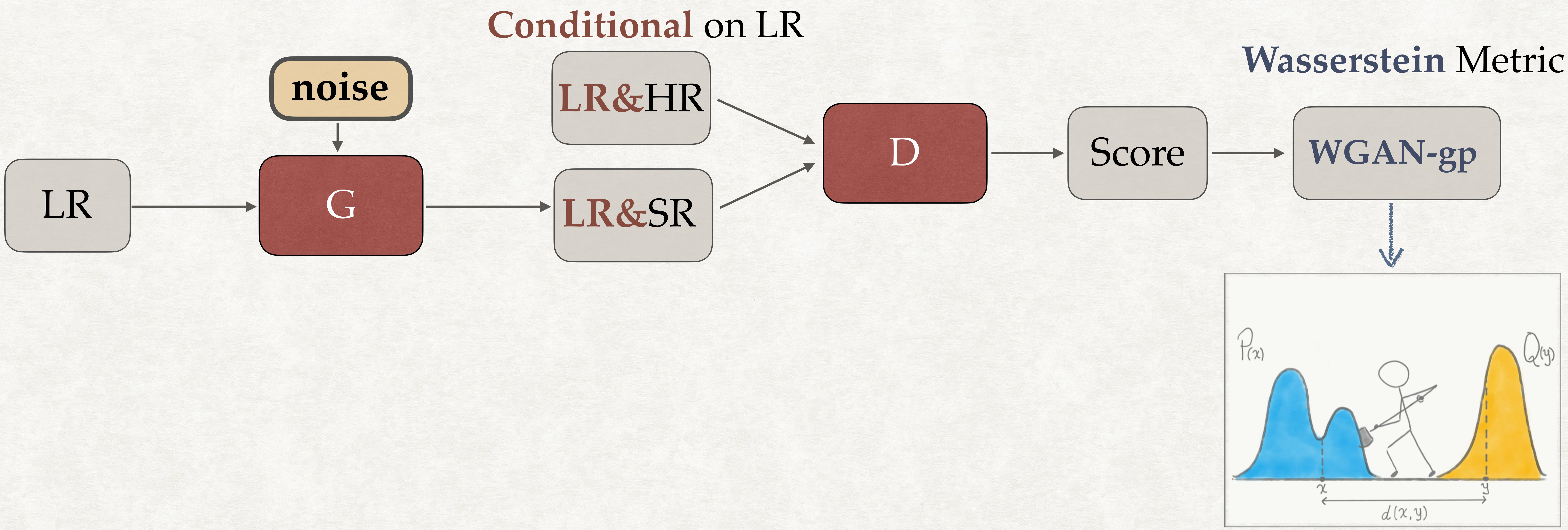
How to train SR model : GAN

- Generative model: learn the a probability distribution of data

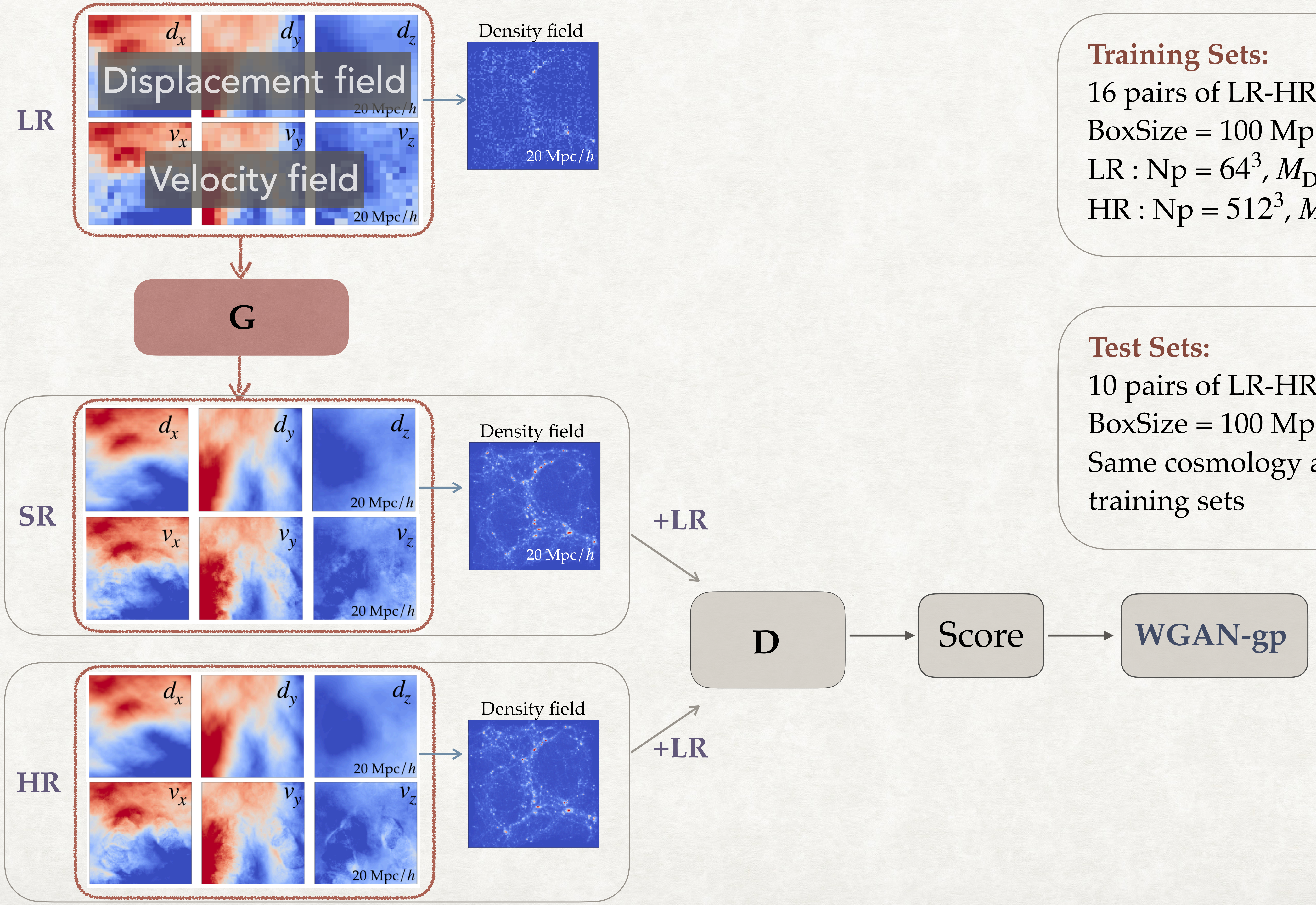


How to train SR model : cGAN & WGAN

- cGAN: help G to generate SR samples with right long- and short-wavelength mode coupling
- Wasserstein metric: better quantify the distance between generated field distribution and authentic distribution



How to train SR model : training procedure

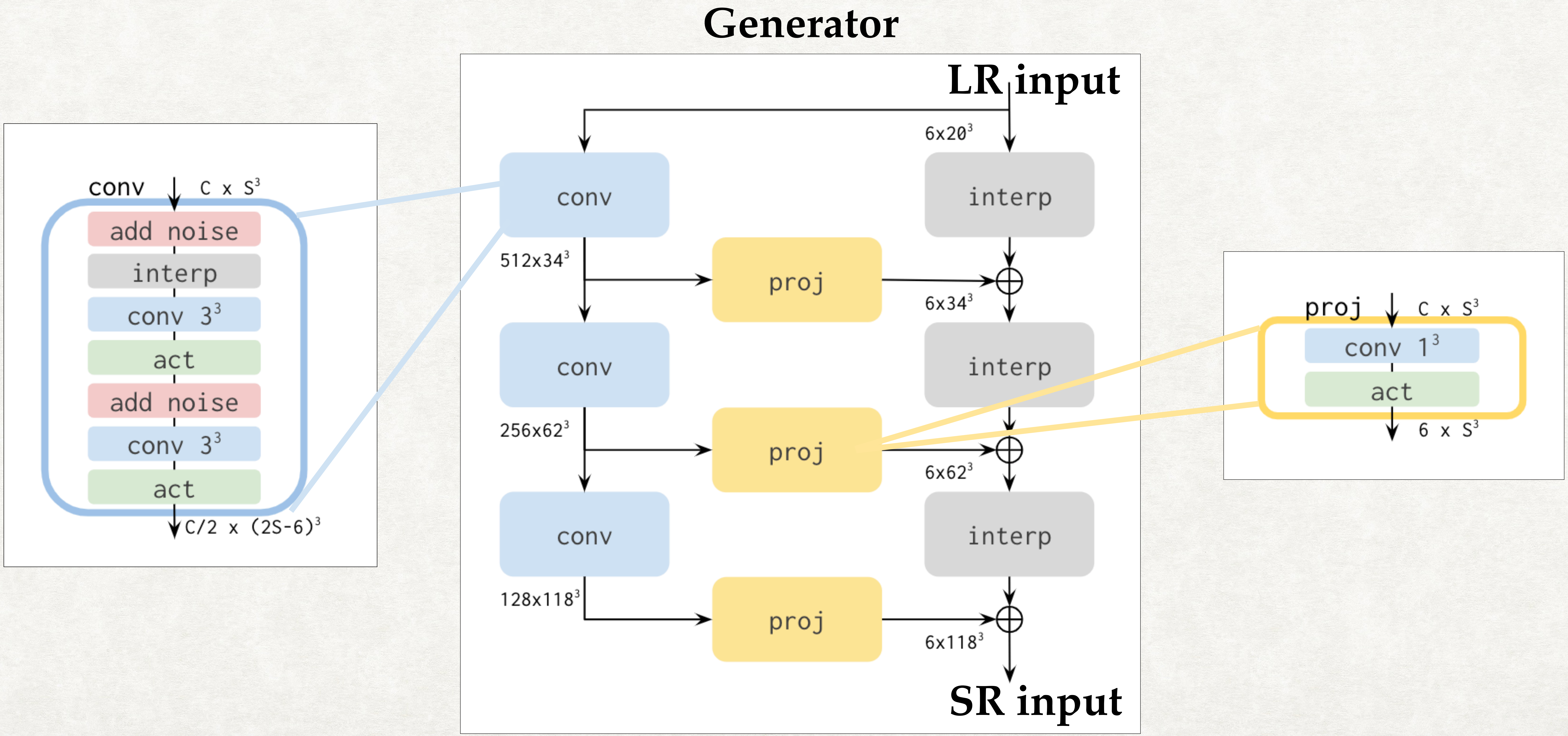


Training Sets:
16 pairs of LR-HR simulations
BoxSize = 100 Mpc/h
LR : Np = 64^3, $M_{\rm DM} = 3 \times 10^{11} M_\odot$
HR : Np = 512^3, $M_{\rm DM} = 5.8 \times 10^{8} M_\odot$

Test Sets:
10 pairs of LR-HR simulations
BoxSize = 100 Mpc/h
Same cosmology and resolution as the training sets

Model Architecture: Generator

Based on styleGAN2



Model Architecture: Generator

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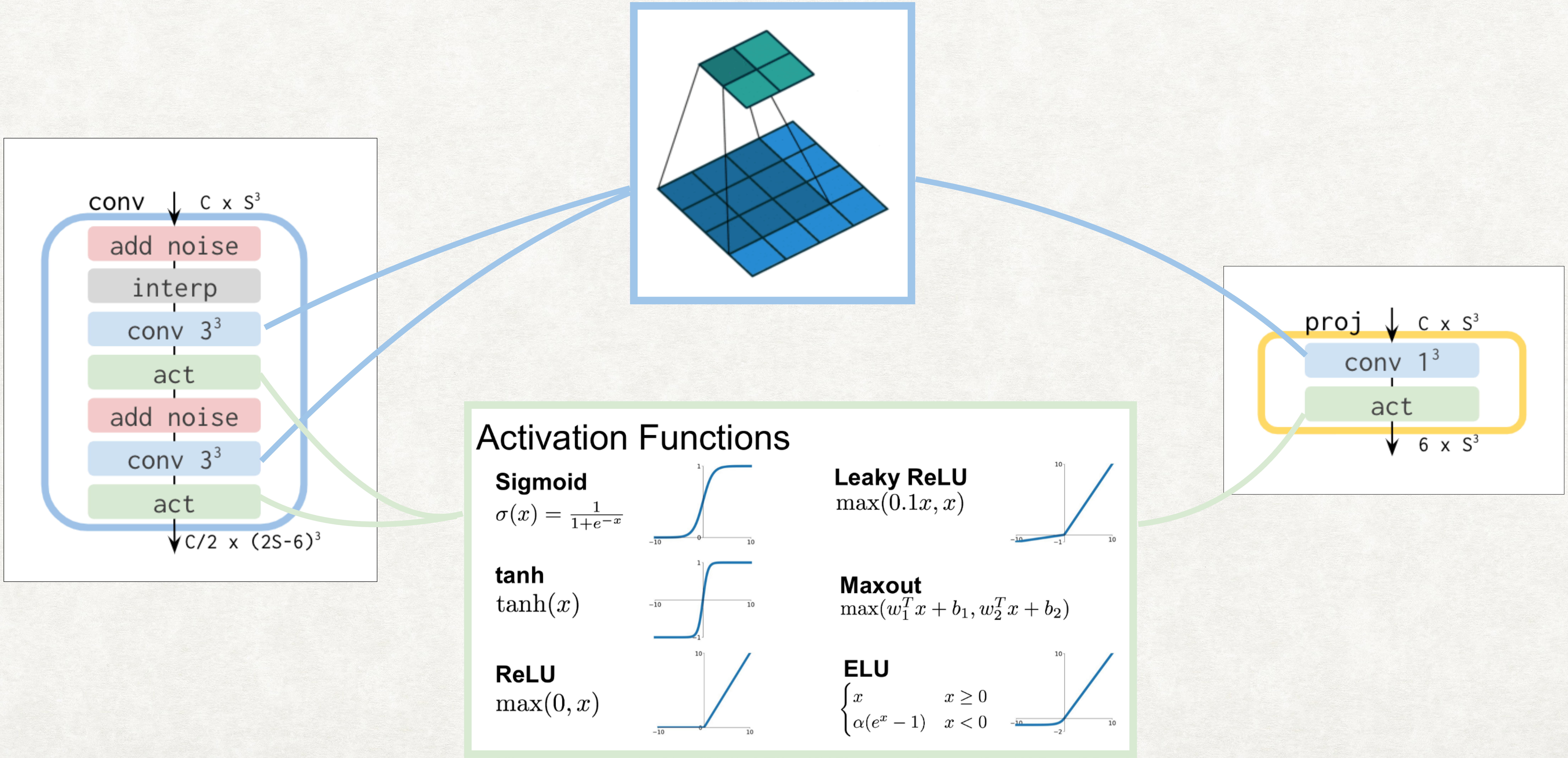
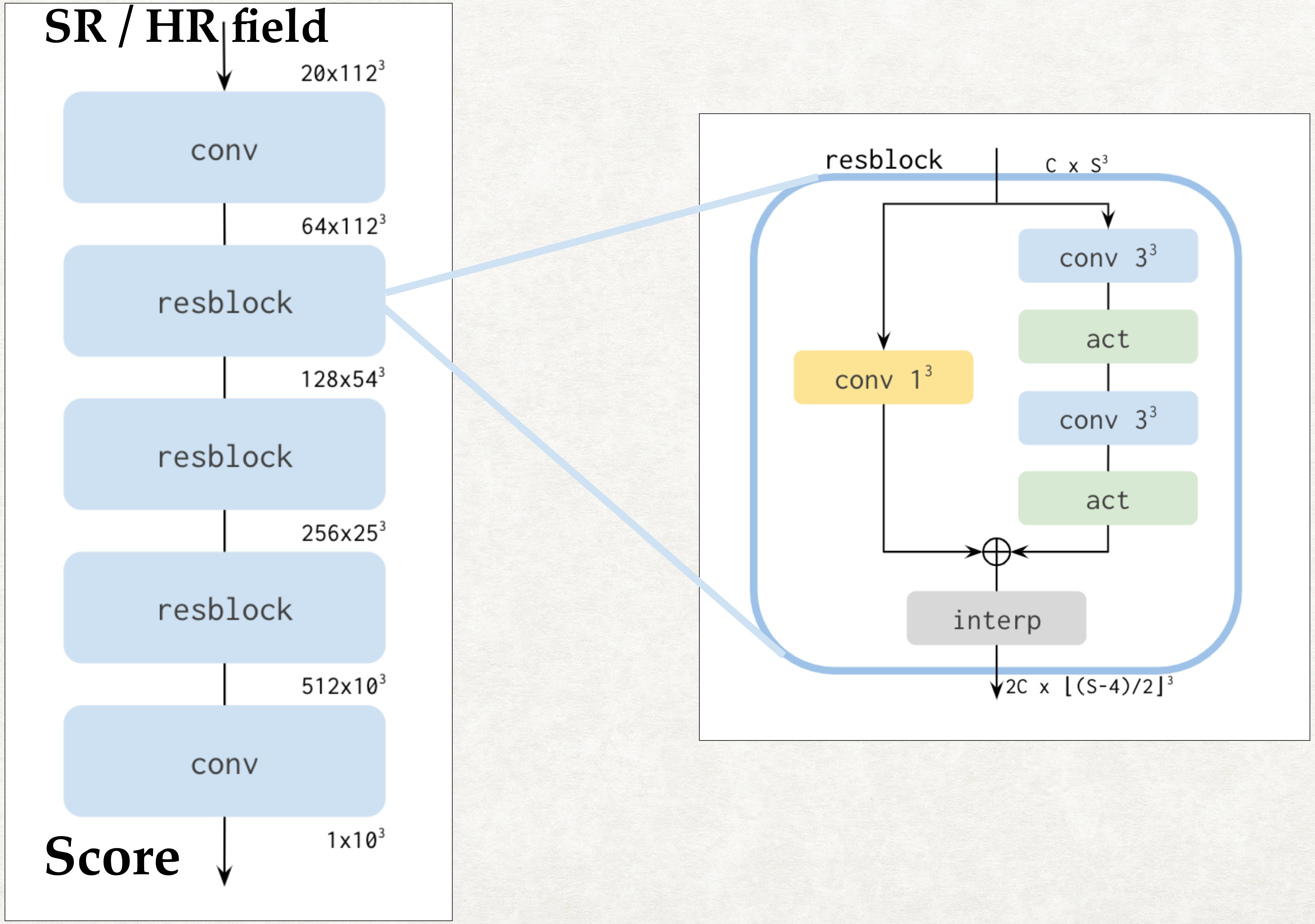
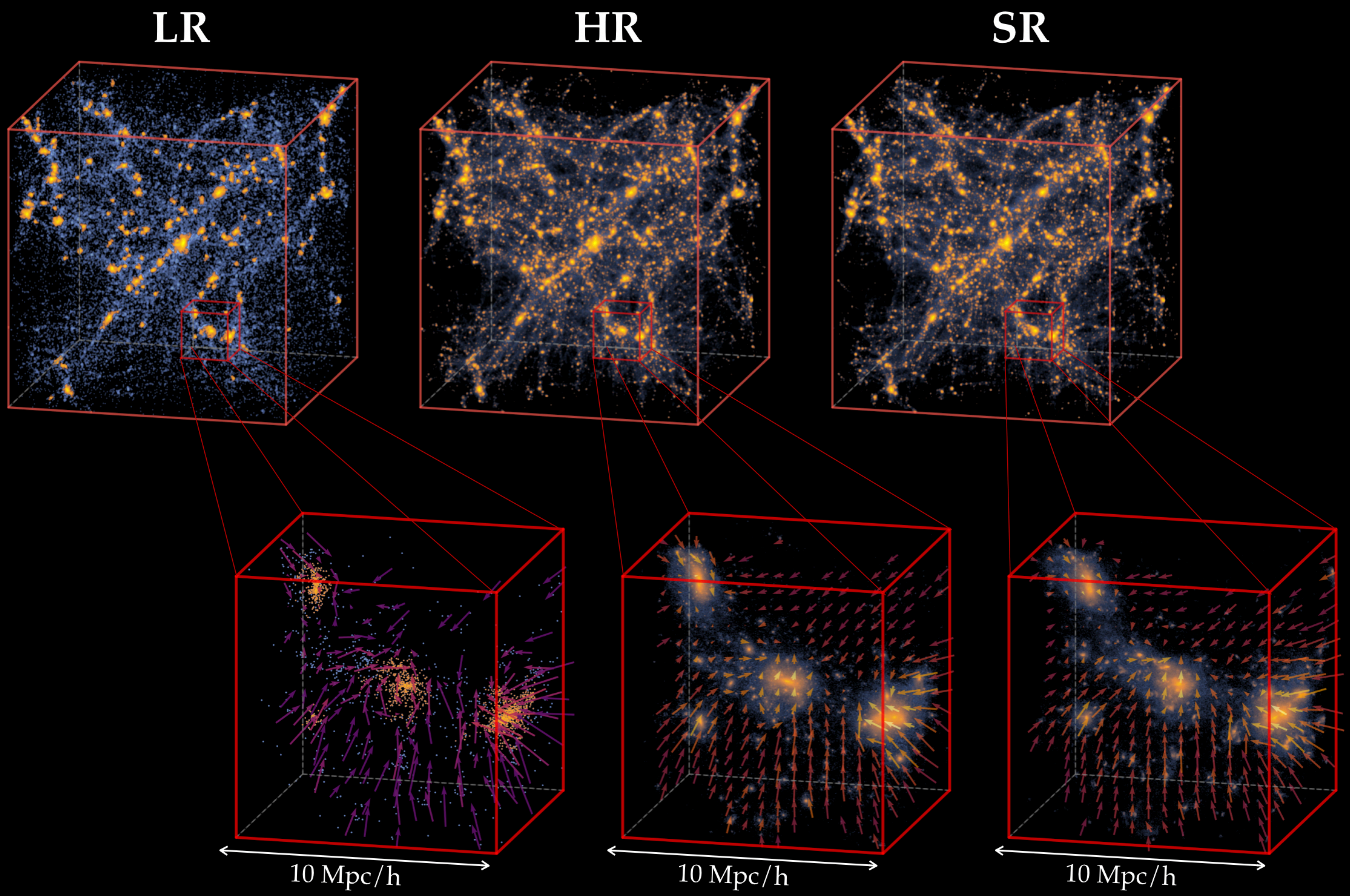


Model Architecture: Discriminator

ResNet



Validation of the SR fields



Validation Metrics

Full field statistics :

- Matter power spectrum (two point statistics)
- Bispectrum (three point statistics)
- Redshift space 2D power spectrum (velocity)

Halo catalog statistics:

- Abundance of halos and subhalos
- Mean occupation distribution of subhalos
- 2-point correlation function
- Redshift-space correlation
- Pairwise velocity distribution

Test Sets:
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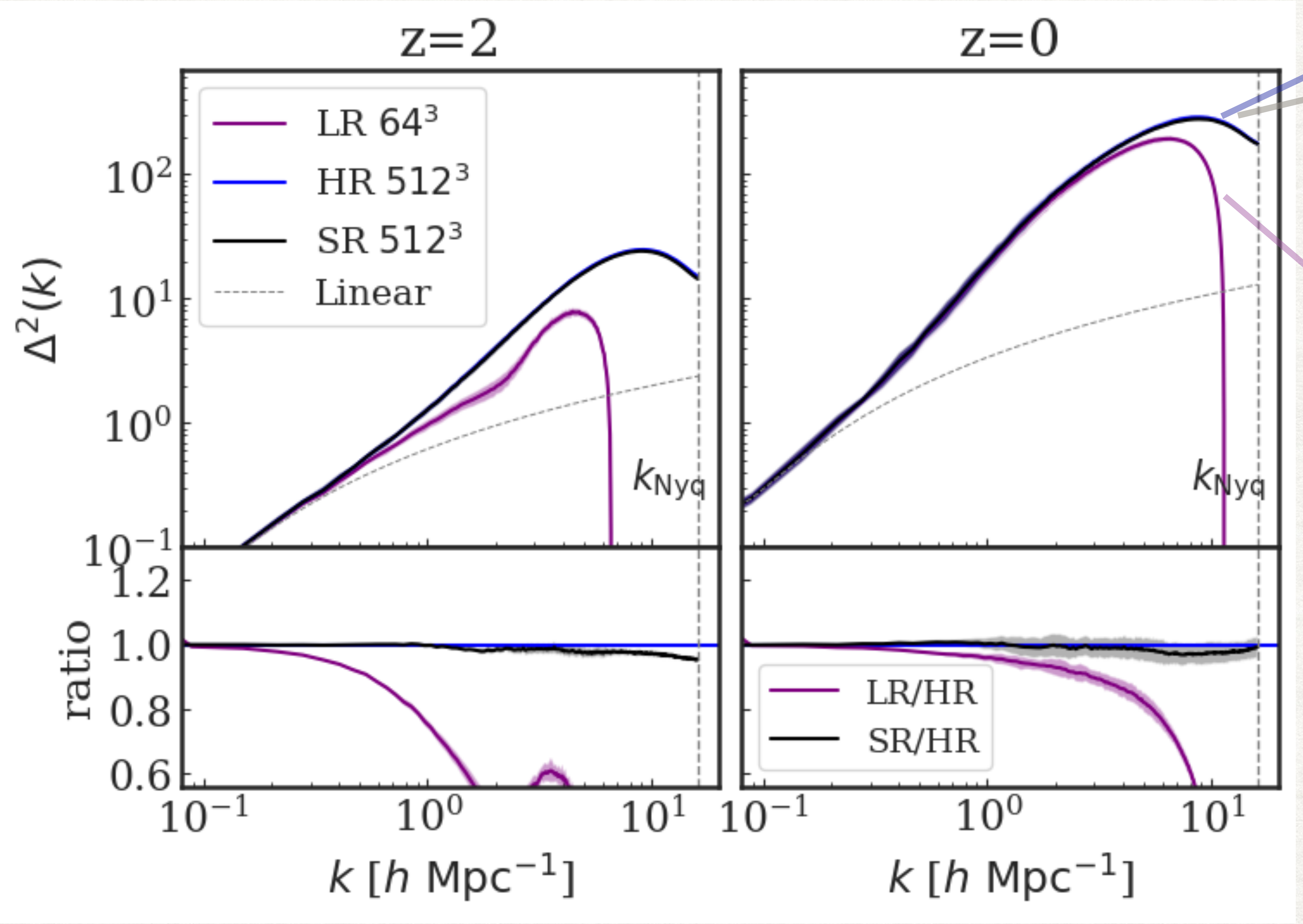
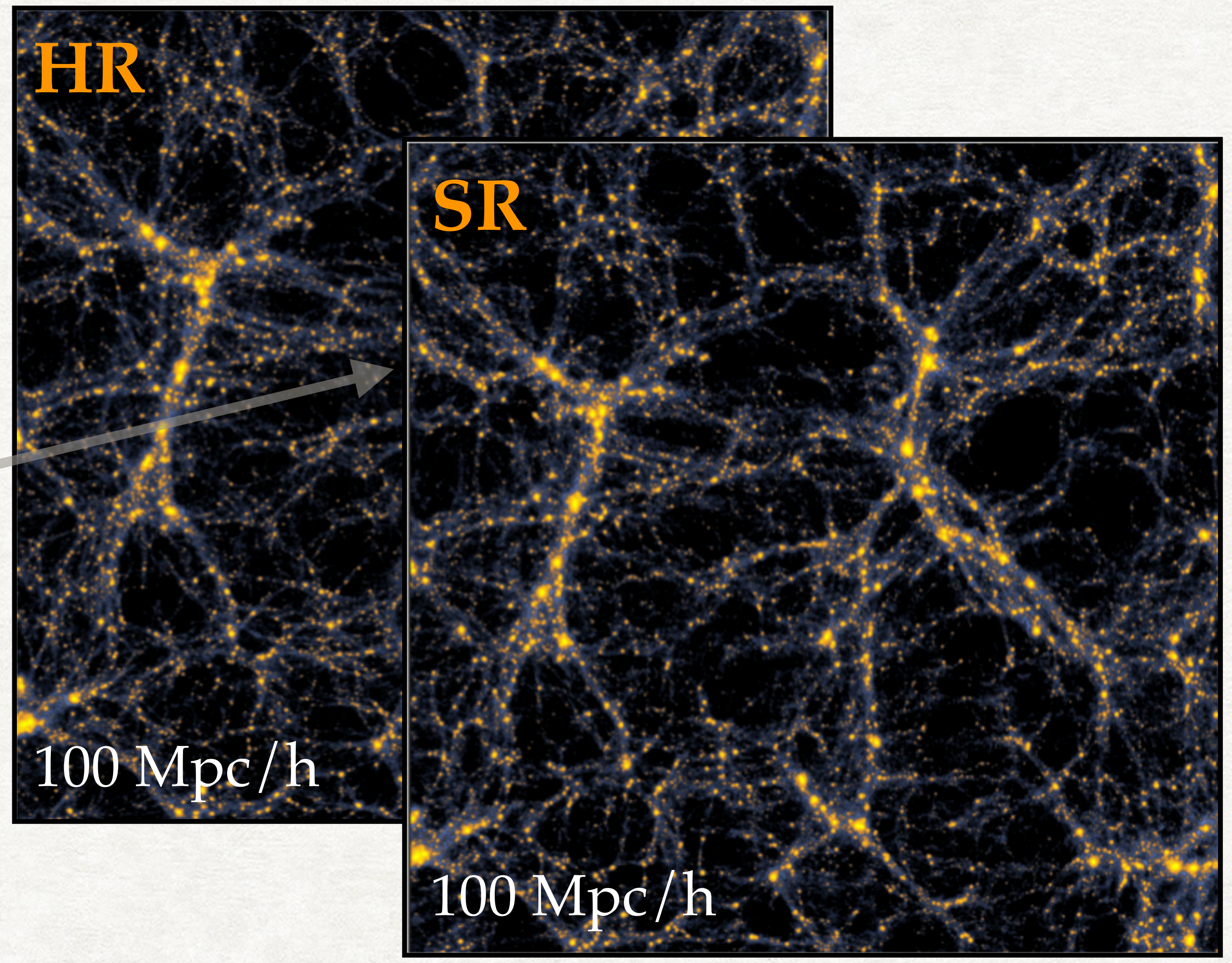
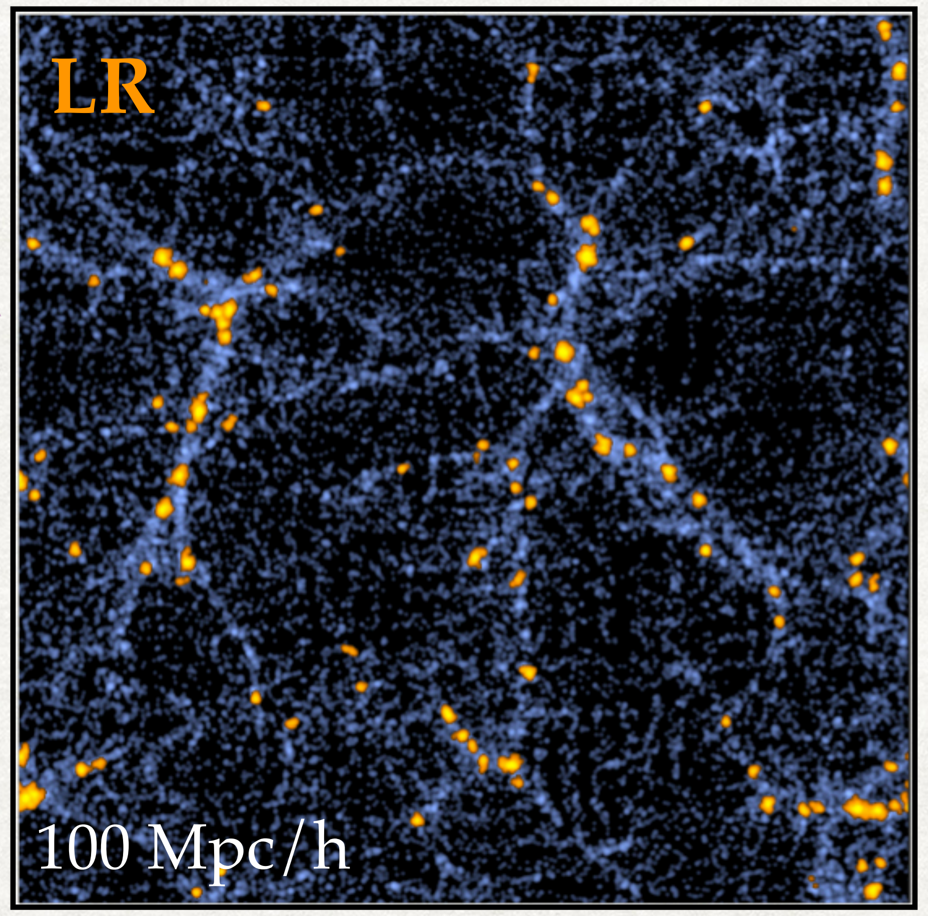
Full field statistics: Matter power spectrum

Dimensionless power $\Delta^2(k) \equiv k^3 P(k)/2\pi^2$

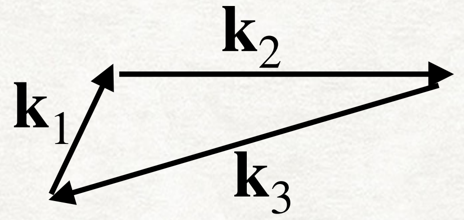






Full field statistics: Bispectra

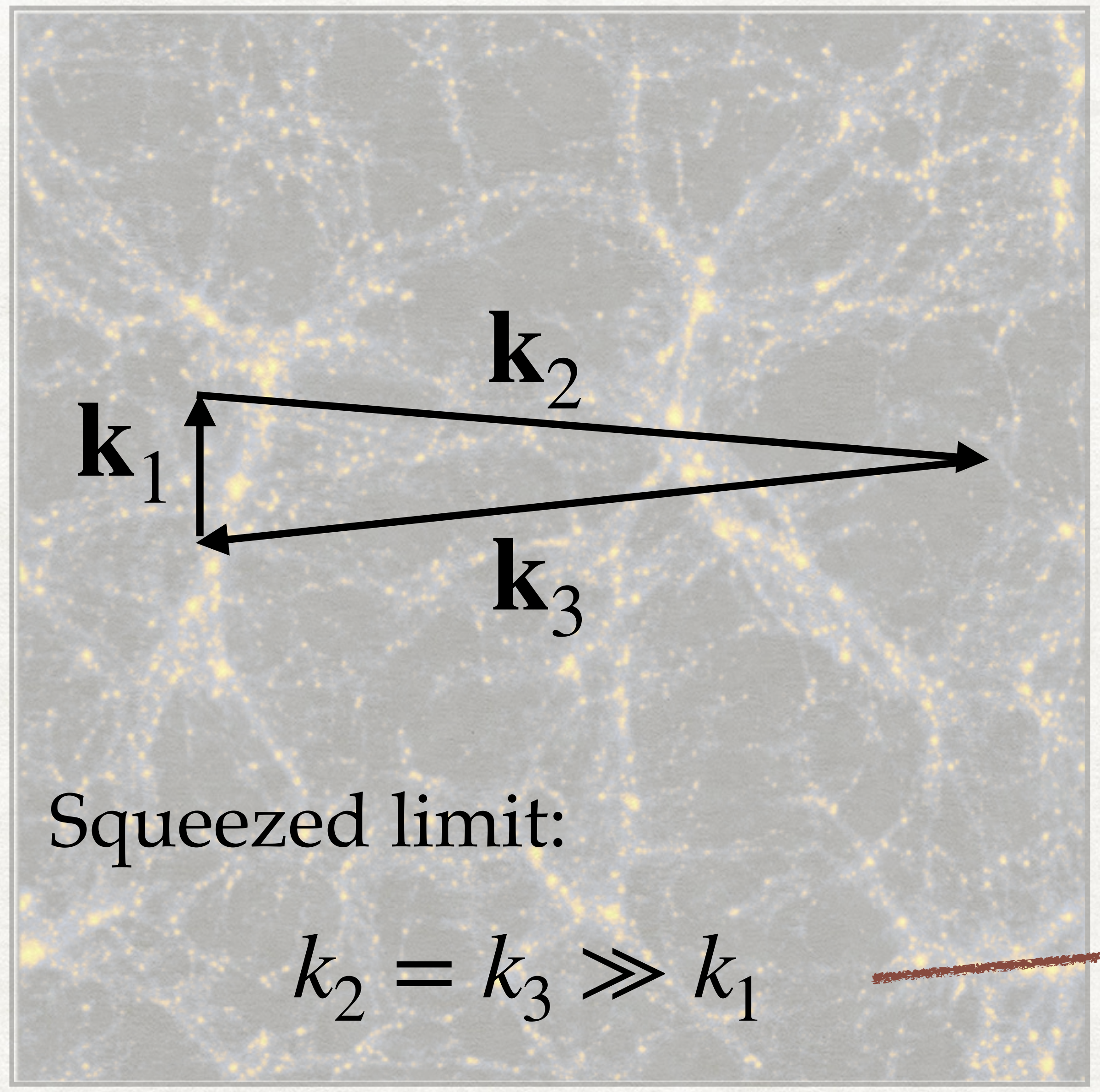
Primary diagnostic for **non-Gaussianity**
Defined for closed triangles (statistical homogeneity and isotropy)

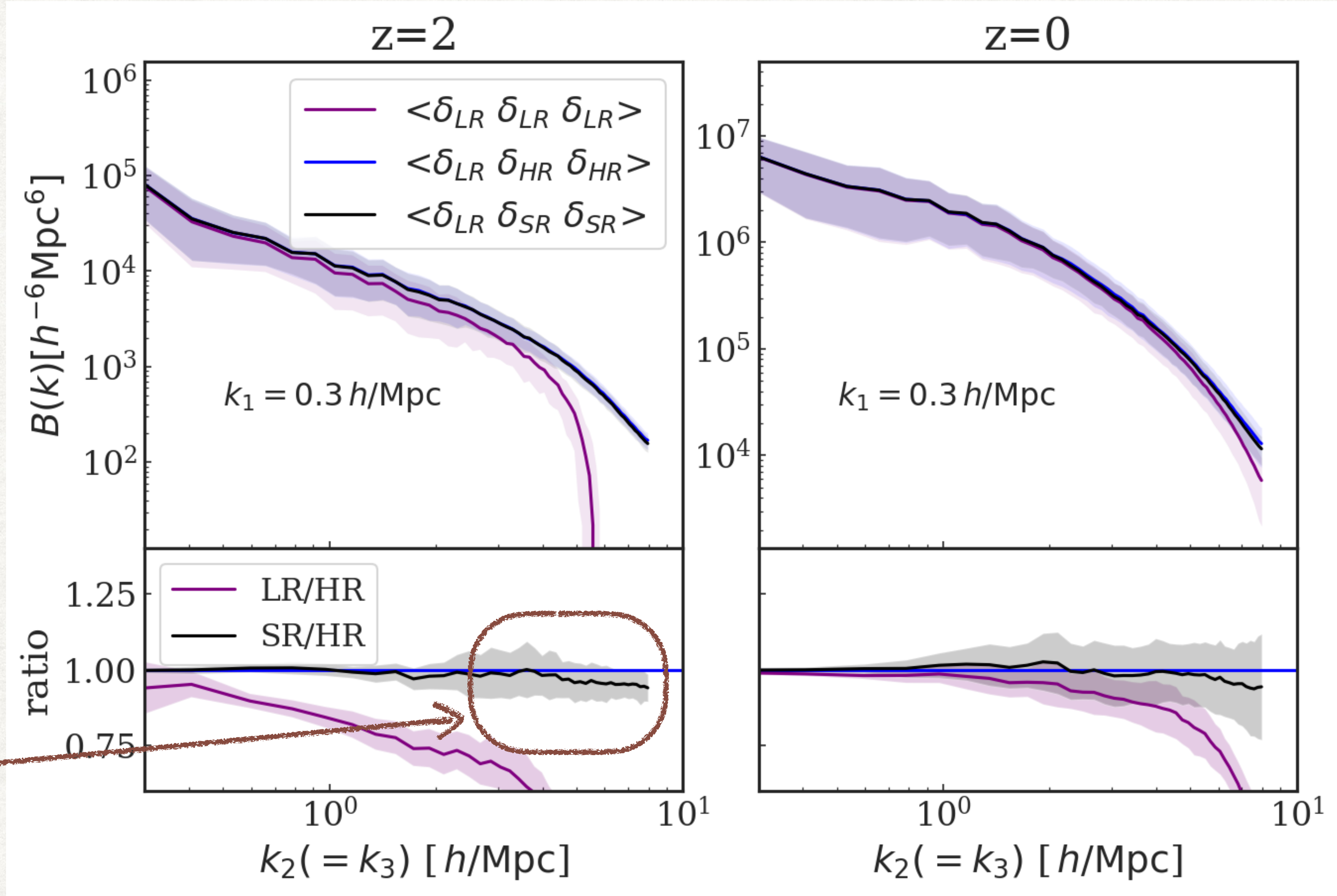


$$(2\pi)^3 B\left(\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{k}_3\right) \delta_{\mathrm{D}}\left(\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3\right)=\left\langle\delta\left(\boldsymbol{k}_1\right) \delta\left(\boldsymbol{k}_2\right) \delta\left(\boldsymbol{k}_3\right)\right\rangle$$

Isosceles triangles

$k_2 = k_3$





Full field statistics: Redshift-space distortion

The peculiar velocity makes the redshift-space clustering anisotropic

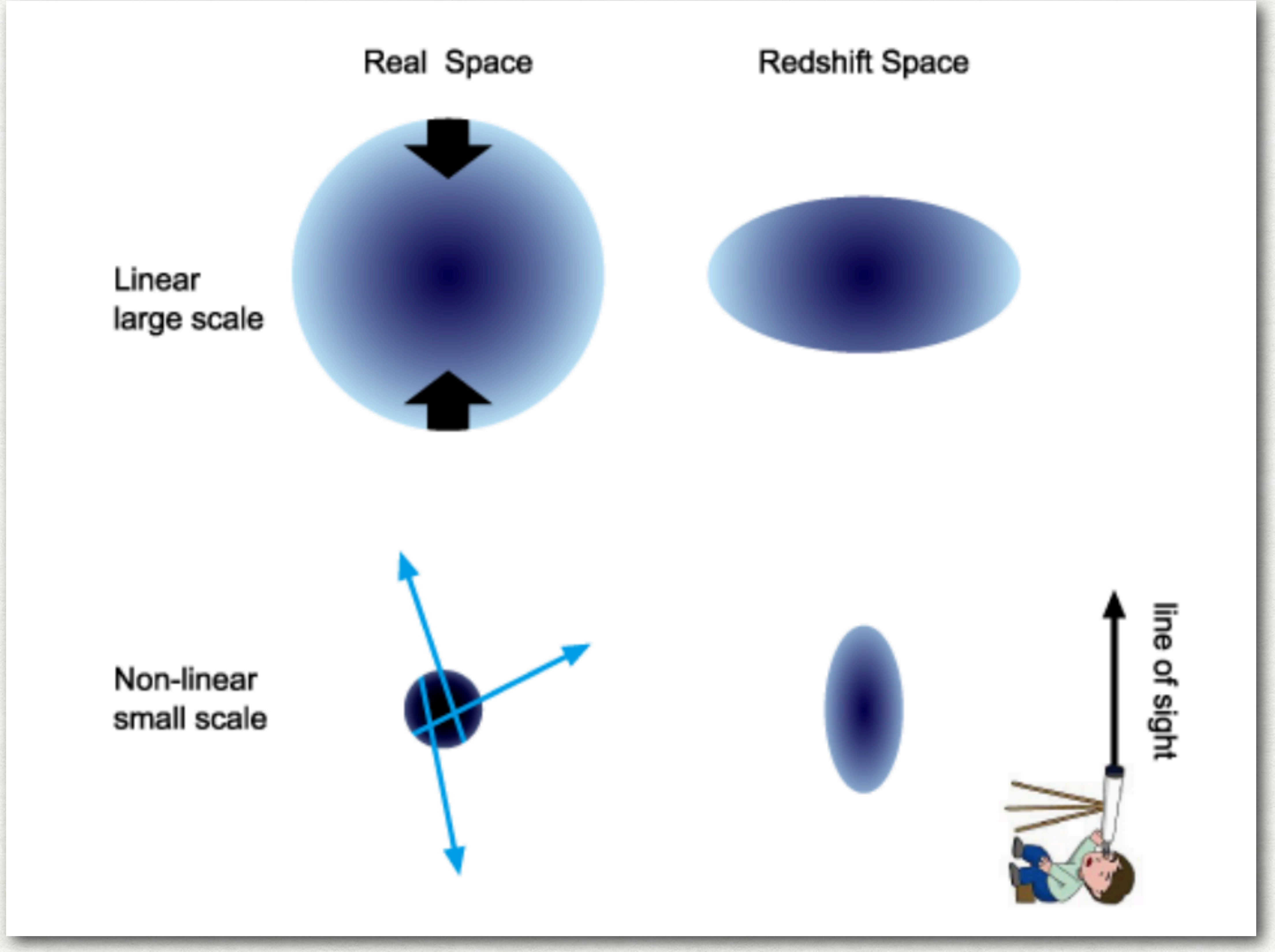


Image from: Shun Saito
RSD lecture note

real-space coordinate

peculiar velocity along the line of sight

$$\boxed{\mathbf{s} = \mathbf{x} + \frac{v_z}{aH(a)}\hat{z}}$$

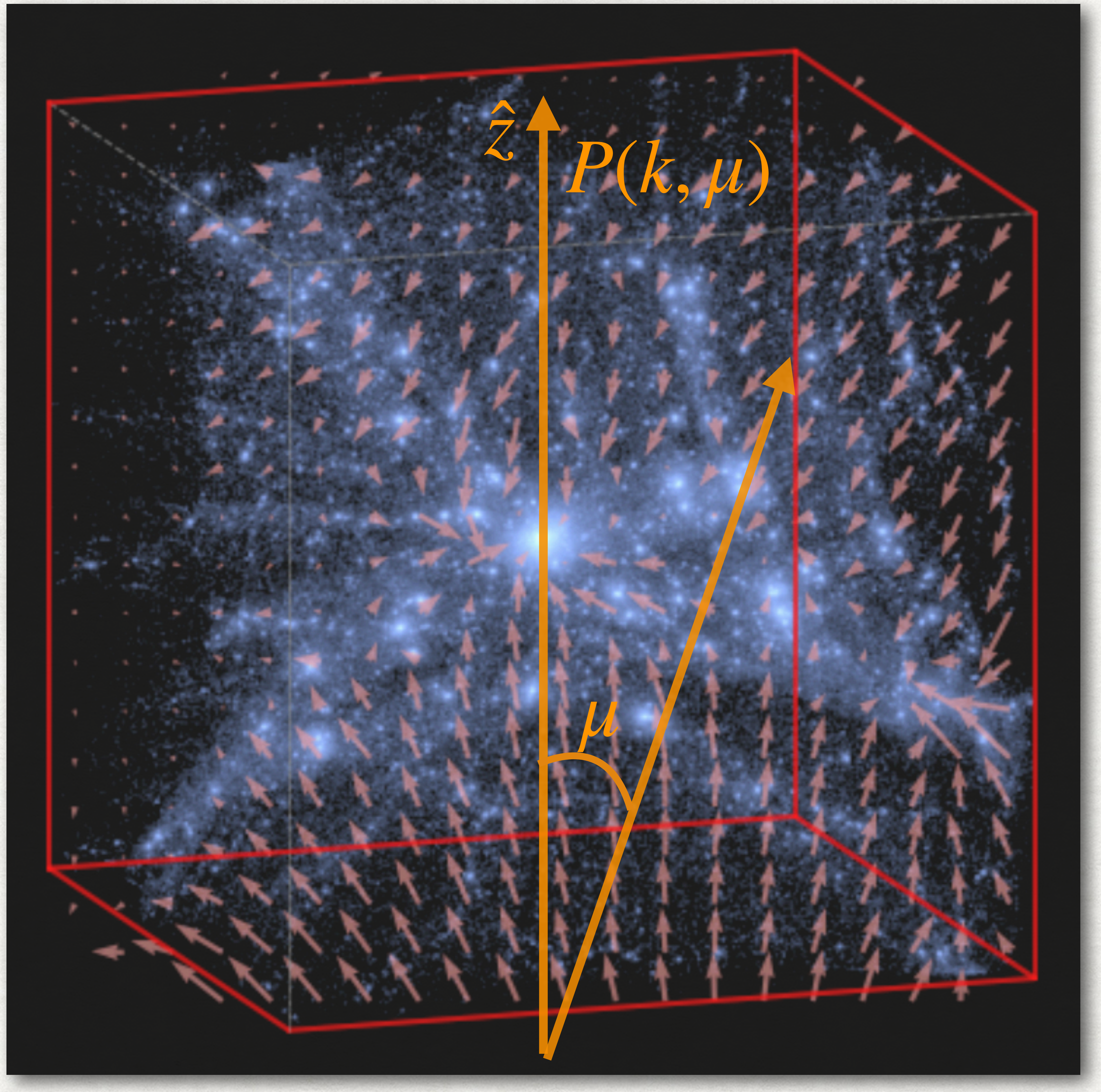
redshift-space coordinate

The line of sight direction

a: scale factor
$H(a)$: Hubble expansion rate

Full field statistics: Redshift-space distortion

The peculiar velocity makes the redshift-space clustering anisotropic —> 2D power spectrum $P(k, \mu)$



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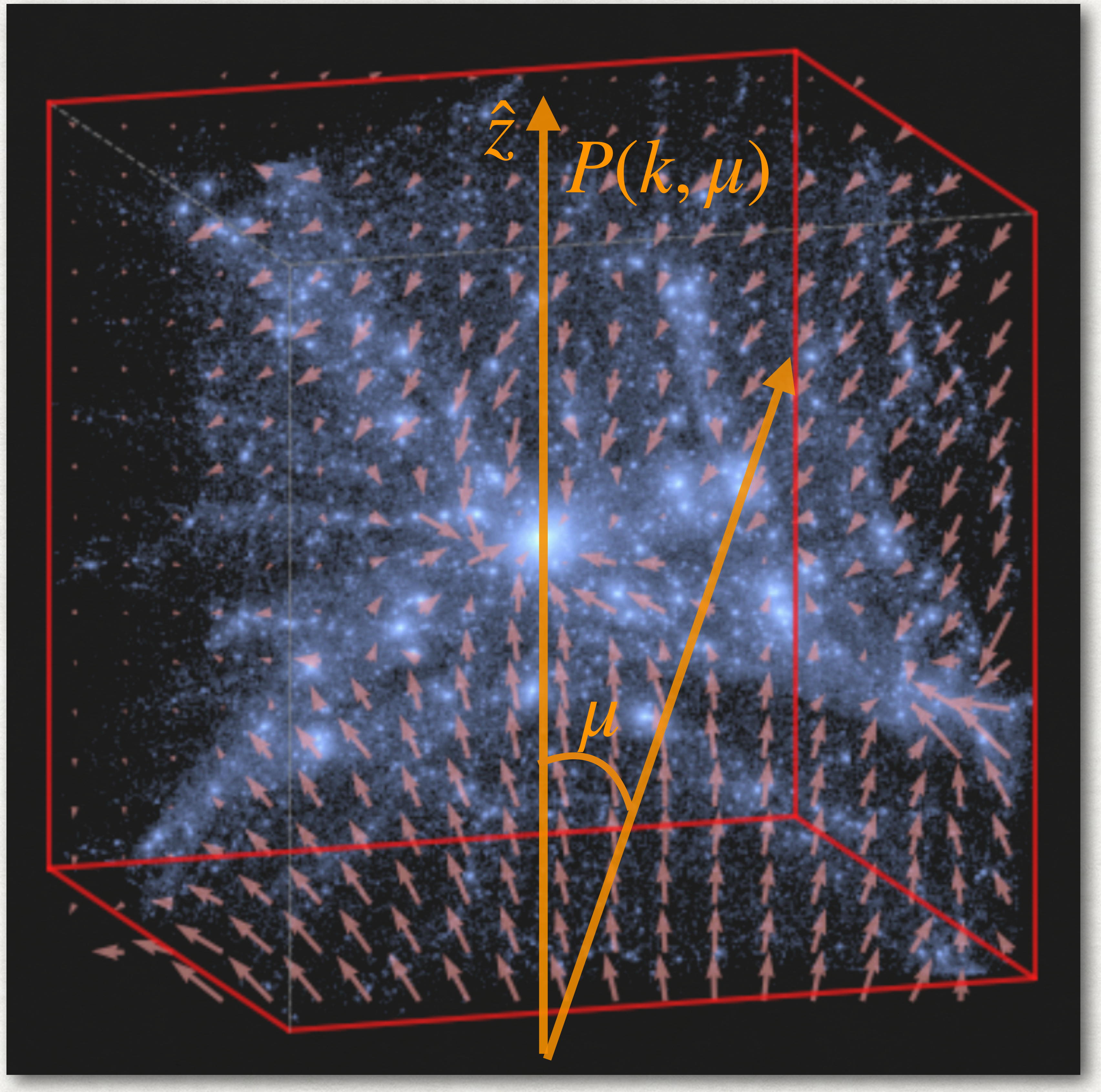

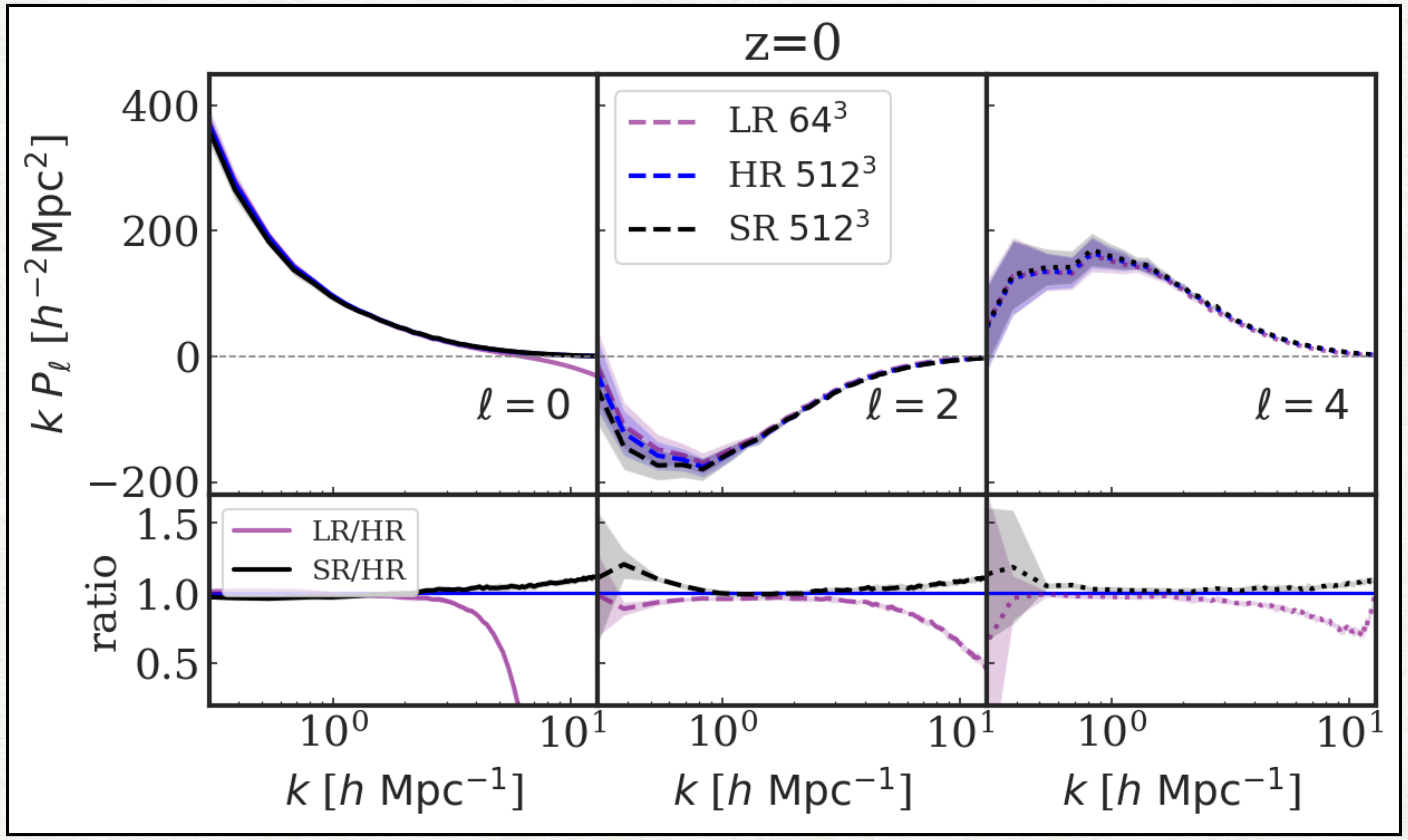

$$P_\ell(k) = (2\ell + 1) \int_0^1 d\mu P(k, \mu) \mathscr{L}_\ell(\mu)$$

Validation Metrics

Full field statistics :
- Matter power spectrum (two point statistics)
- Bispectrum (three point statistics)
- Redshift space 2D power spectrum (velocity)

Test Sets:
10 pairs of LR-HR simulations
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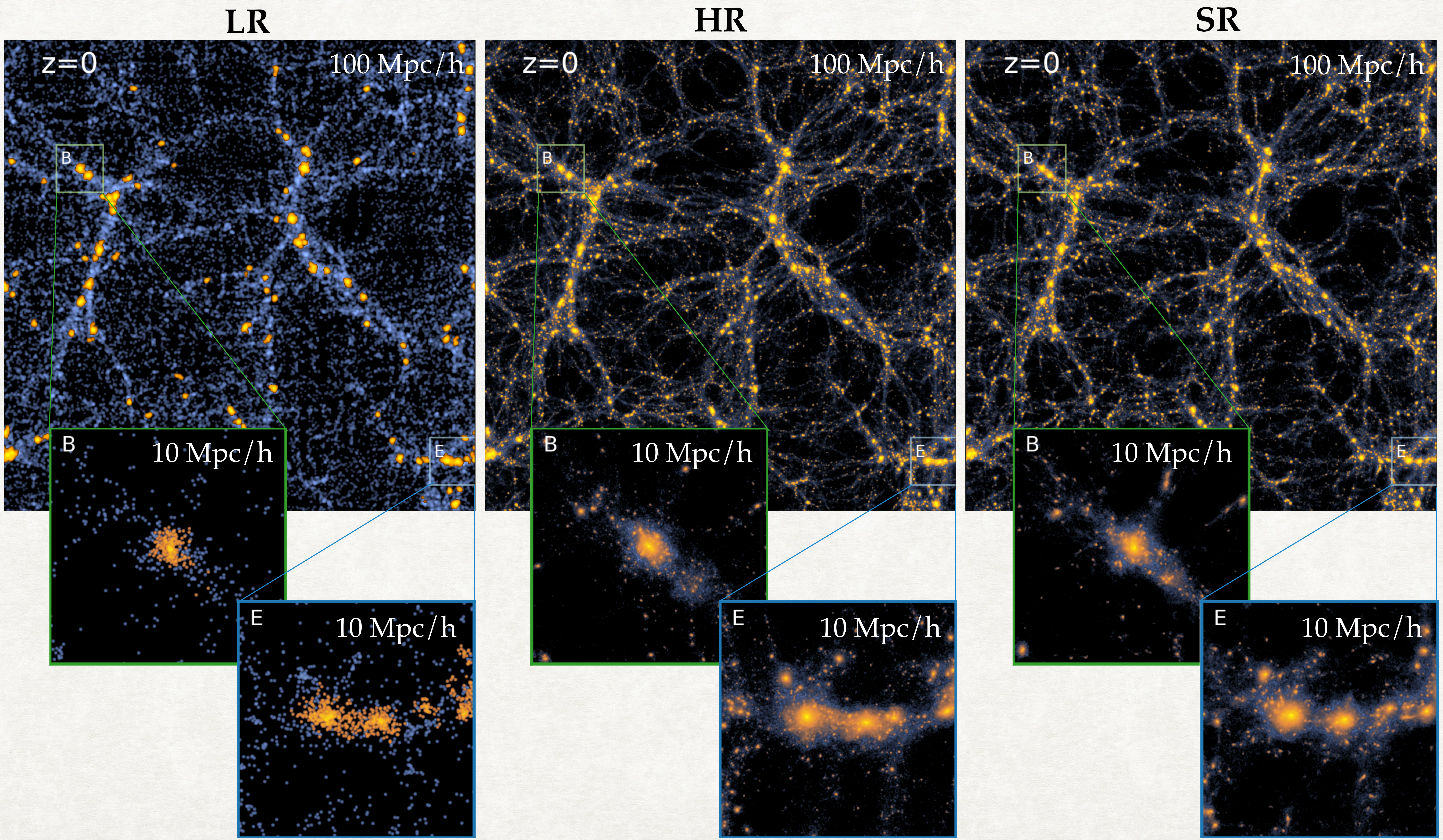
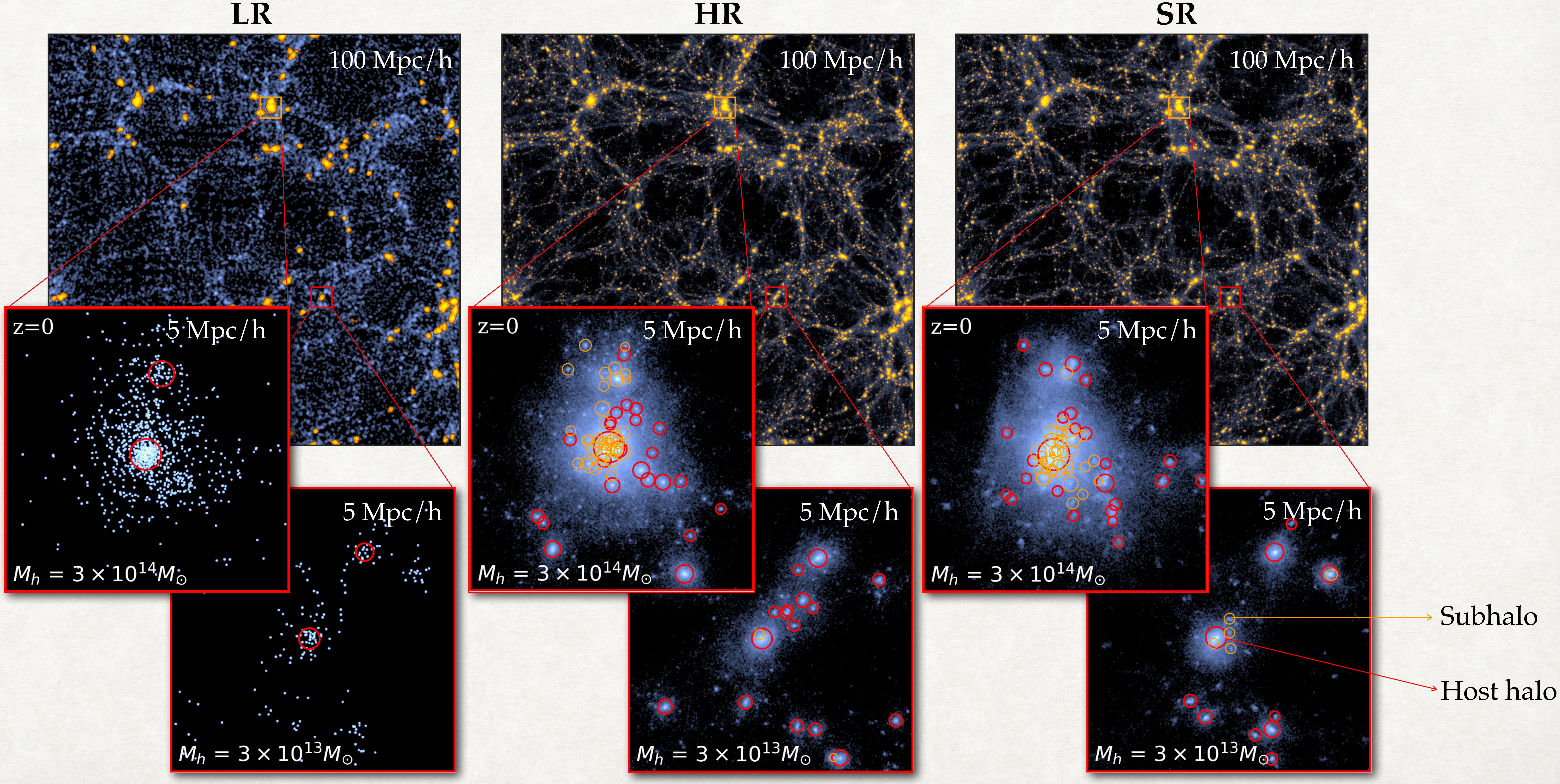
Same cosmology and resolution as the training sets

Halo catalog statistics:
- Abundance of halos and subhalos
- Mean occupation distribution of subhalos
- 2-point correlation function
- Redshift-space correlation
- Pairwise velocity distribution

Halo catalogs : halos

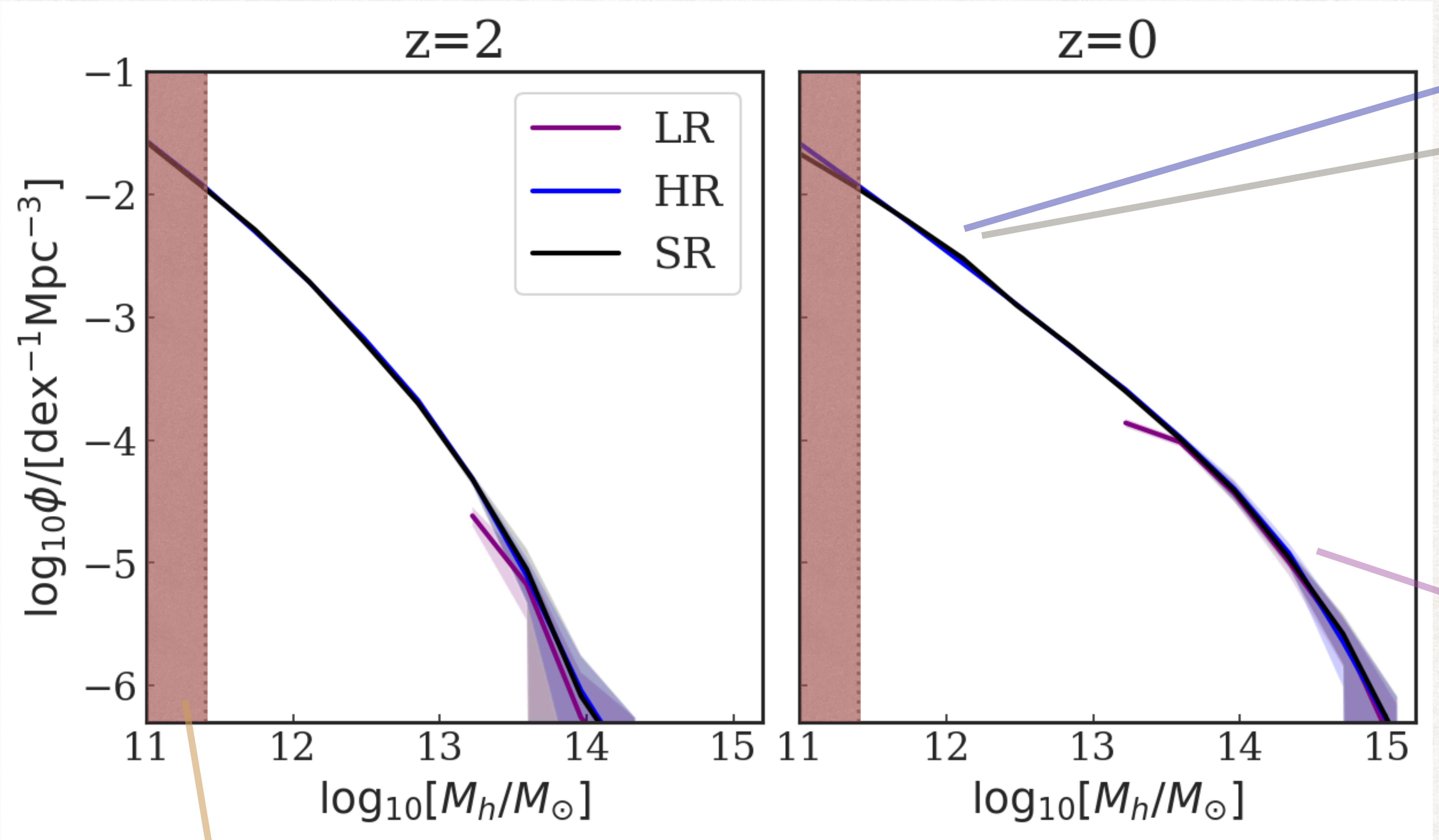


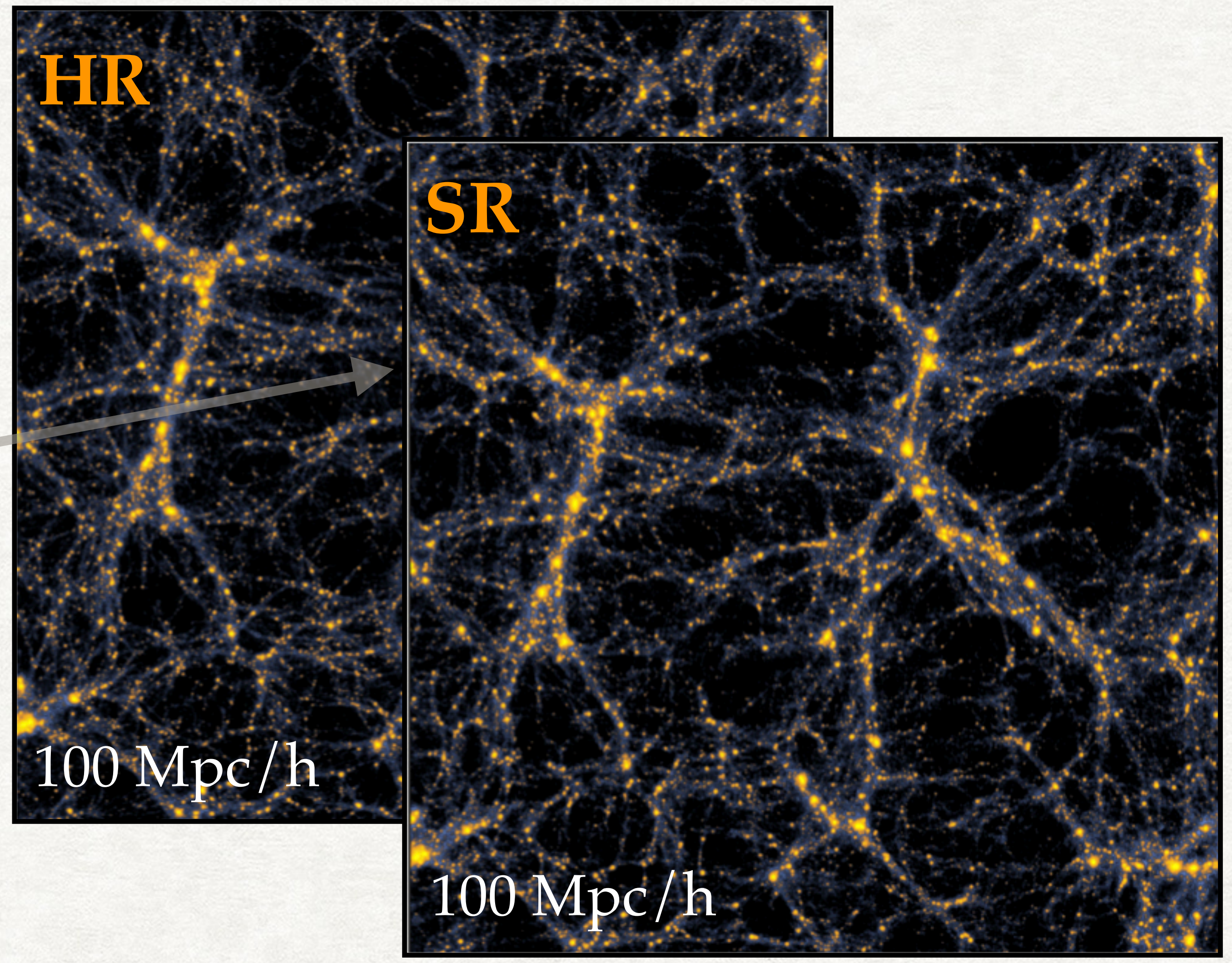
Halo catalogs : subhalos

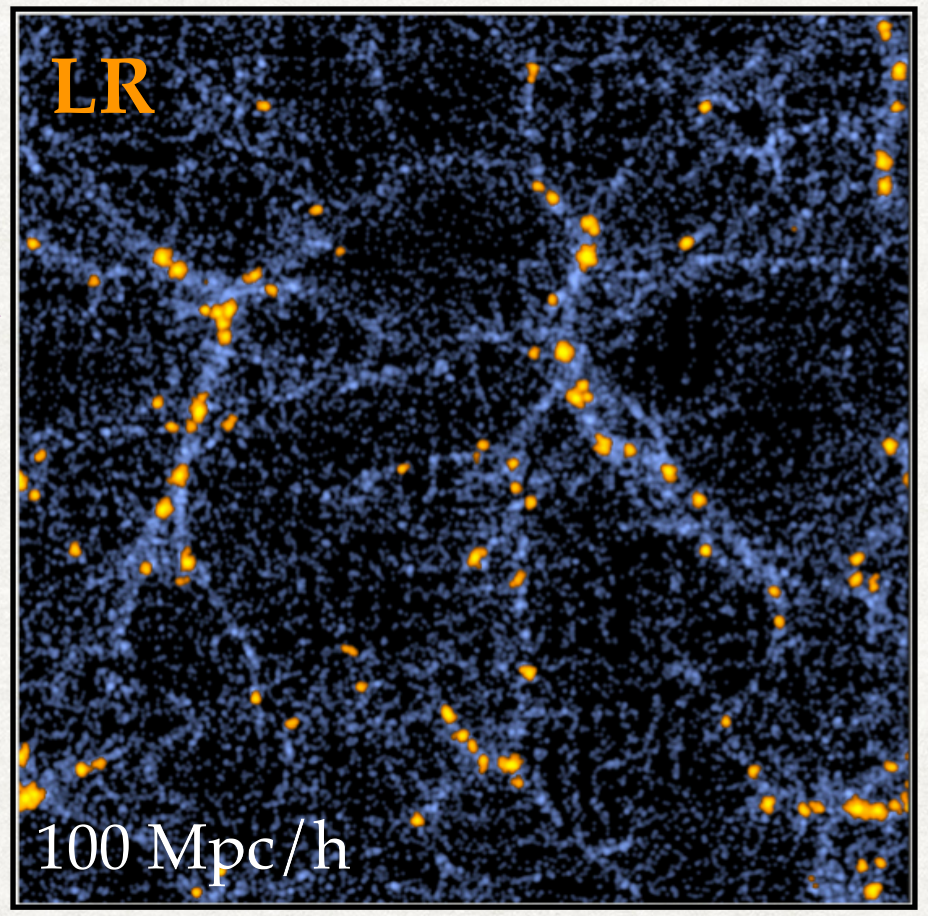


Halo catalog statistics : halo abundance

Abundance of **host halos**



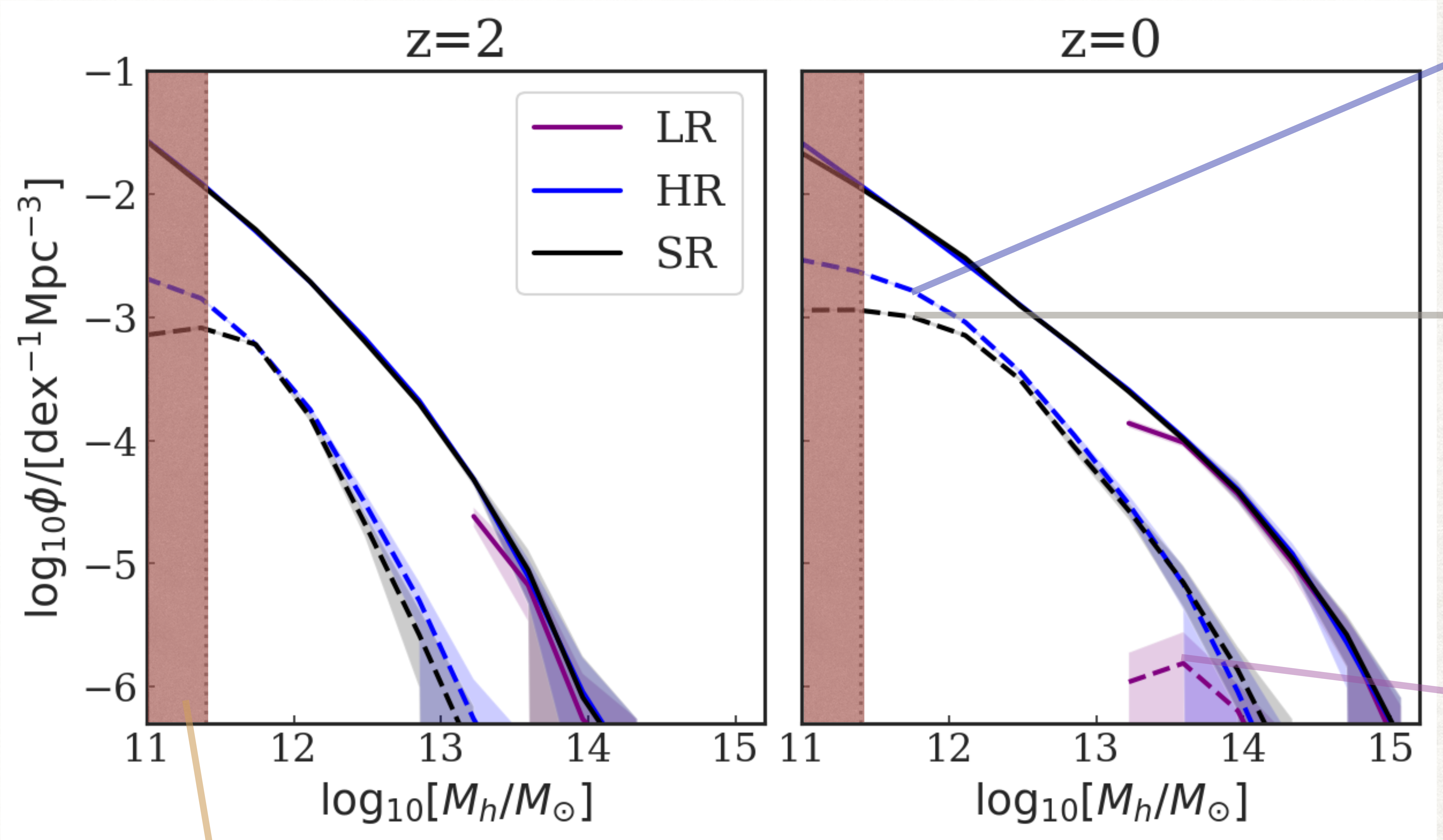


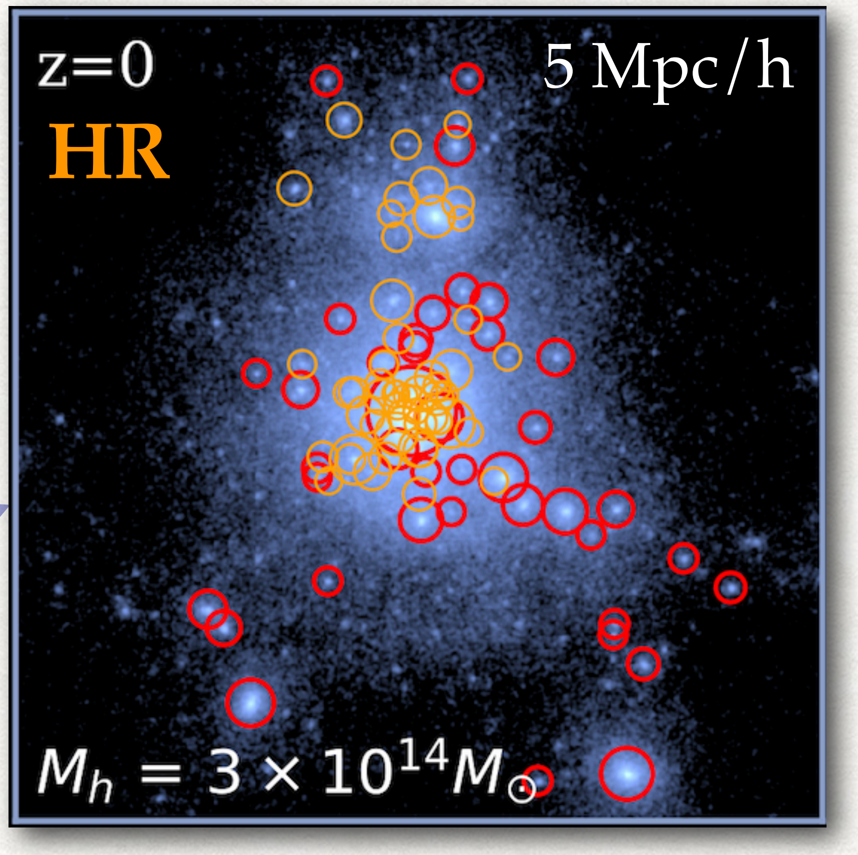


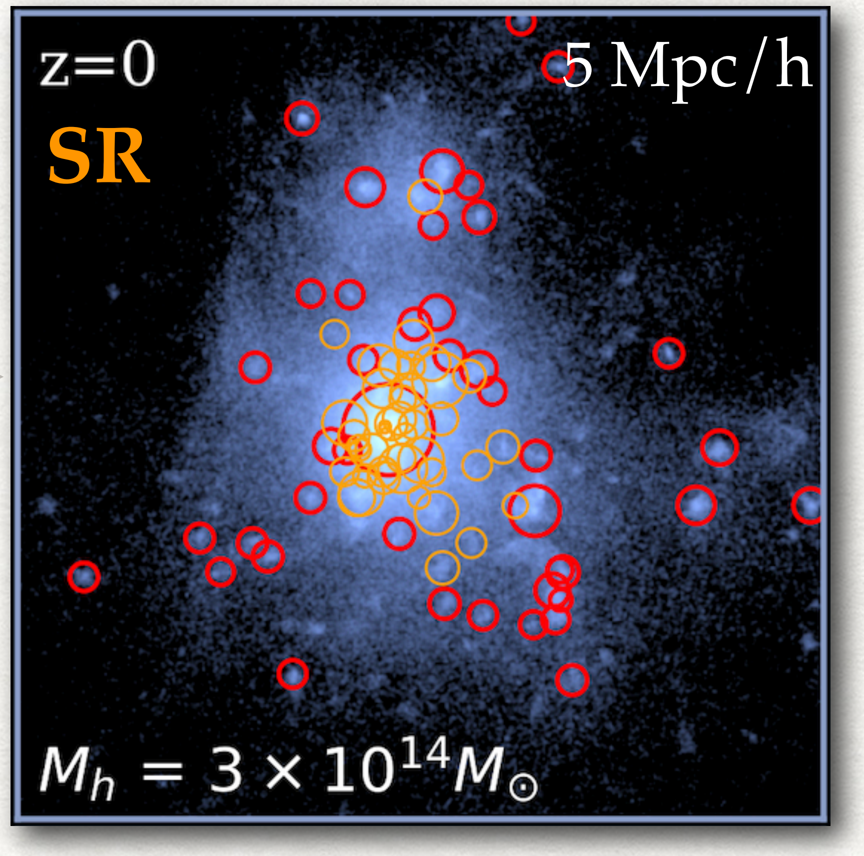
Resolution limit: 300 particles

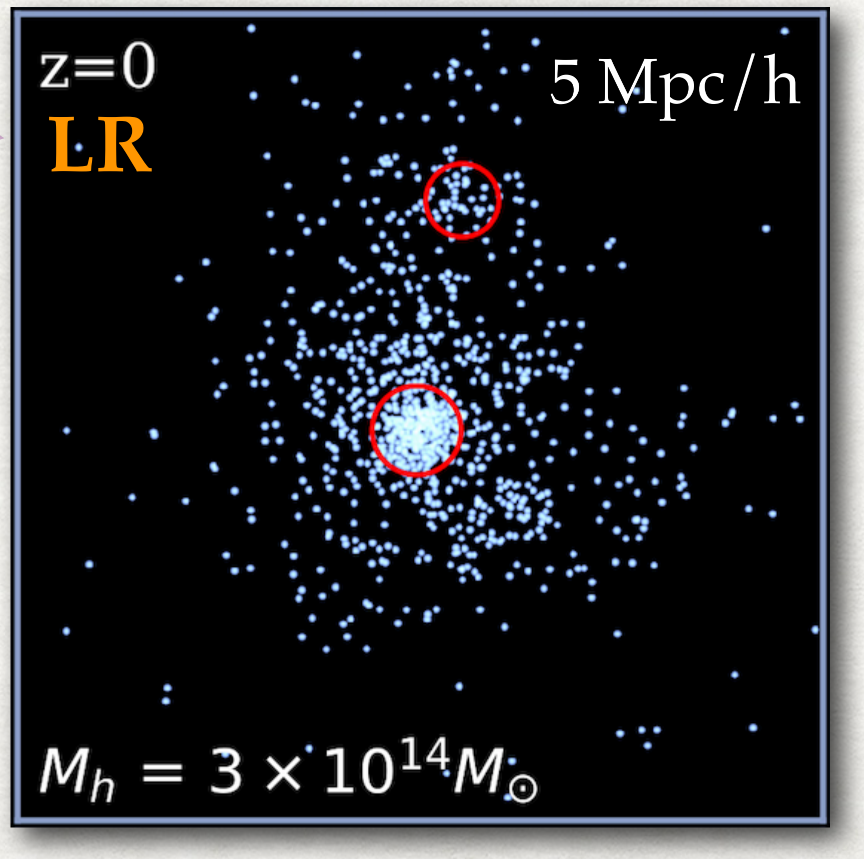
Halo catalog statistics : subhalo abundance

Abundance of **subhalos**





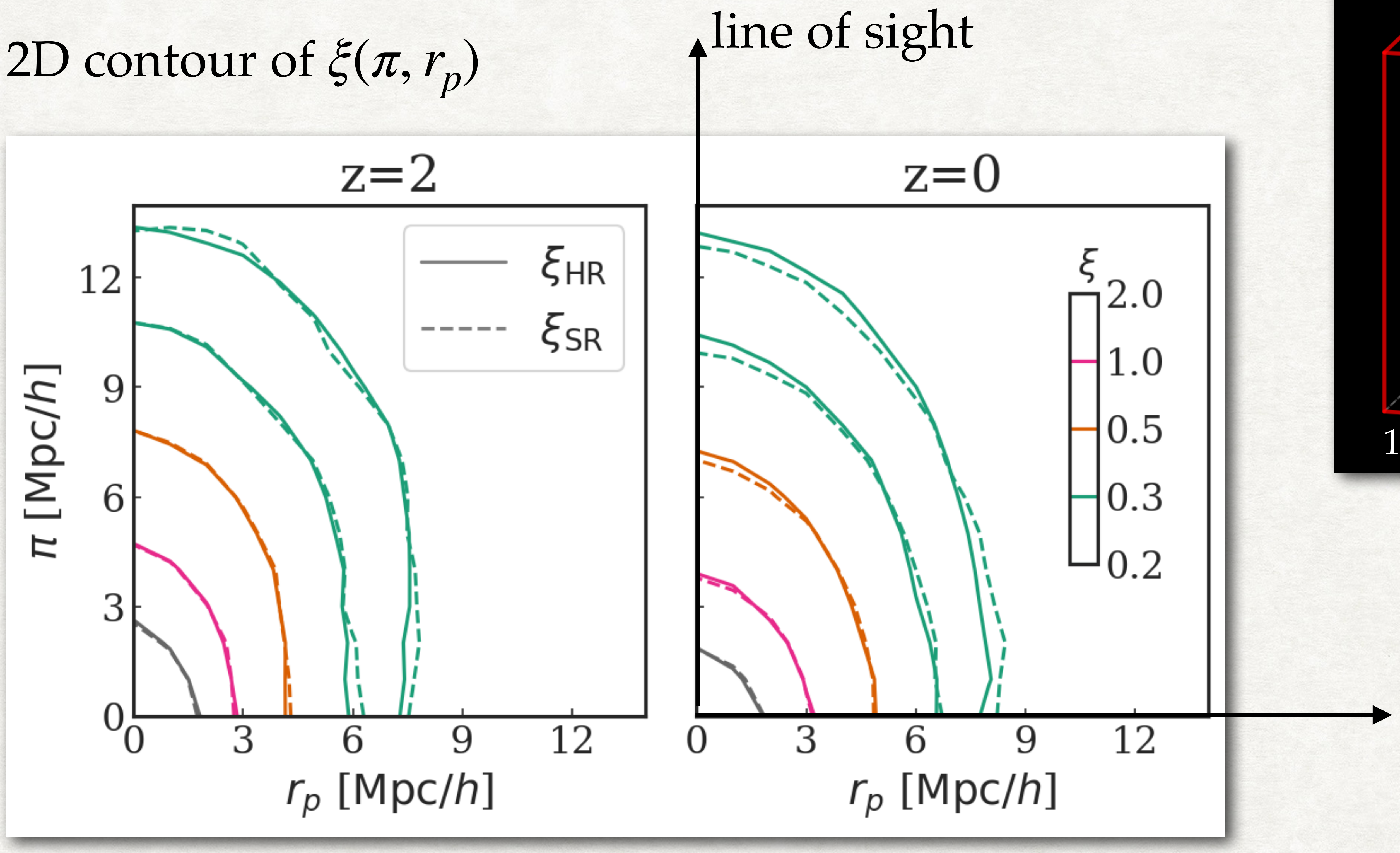


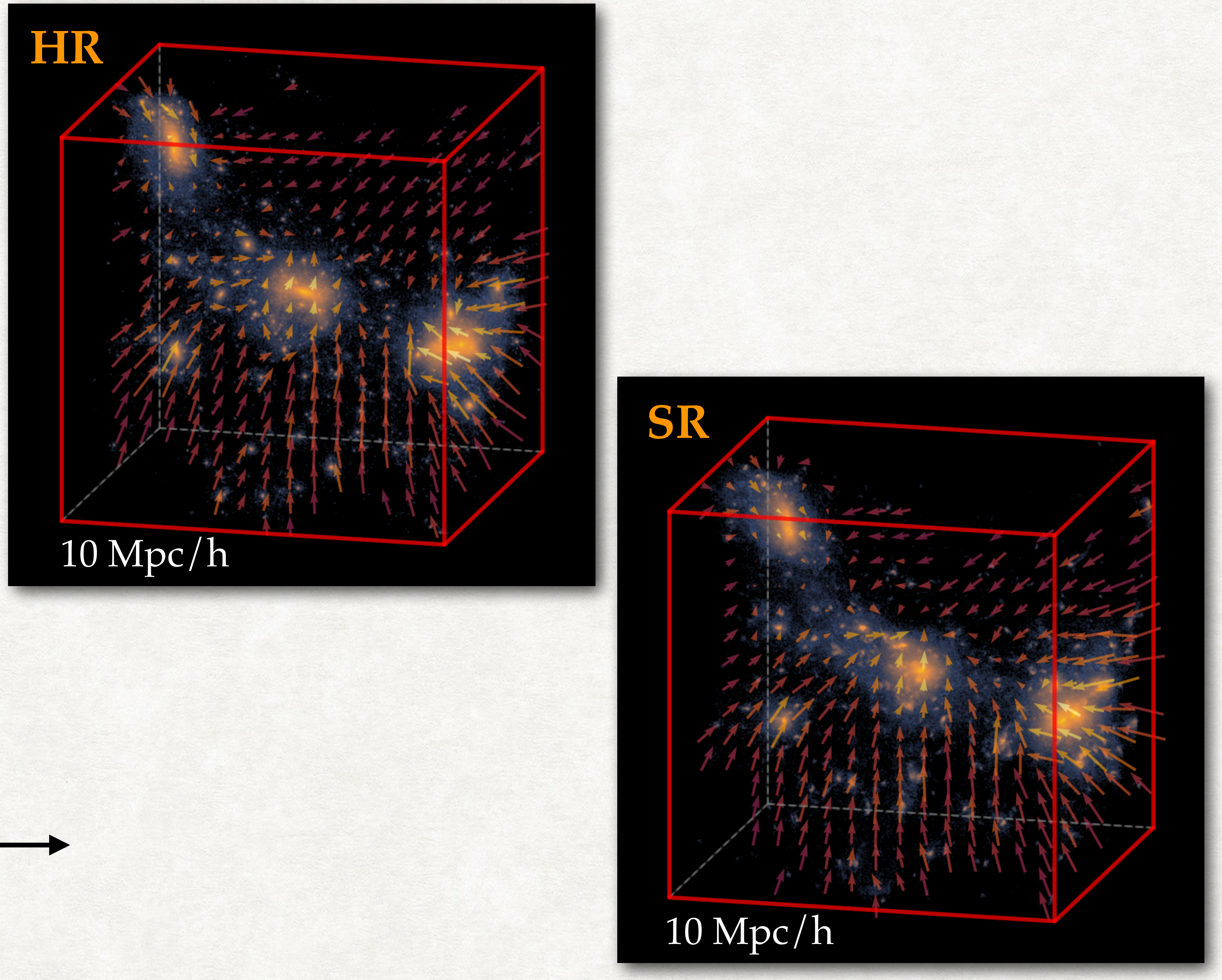


Resolution limit: 300 particles

Halo catalog statistics : redshift-space correlation

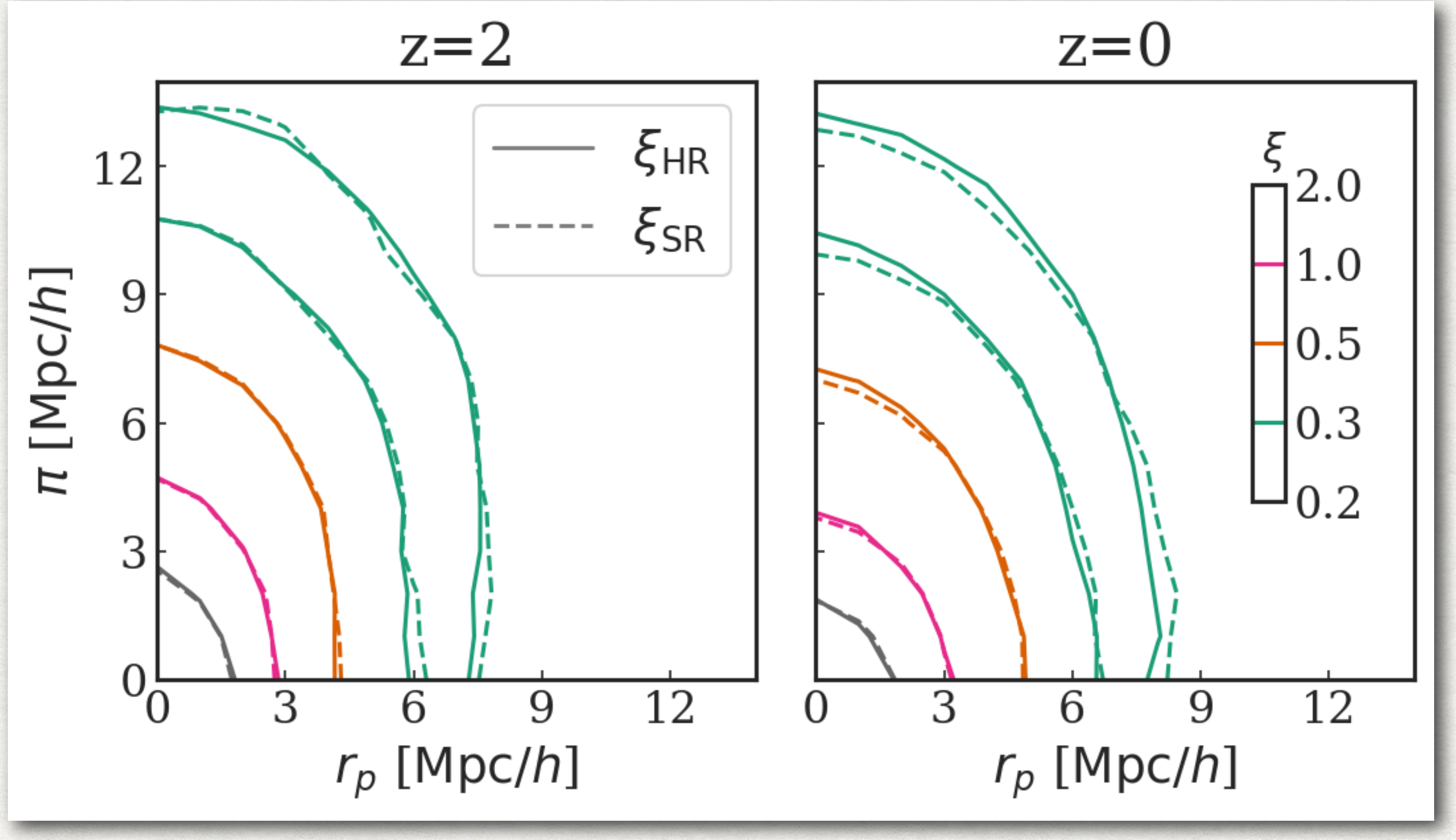
2D contour of $\xi(\pi, r_p)$



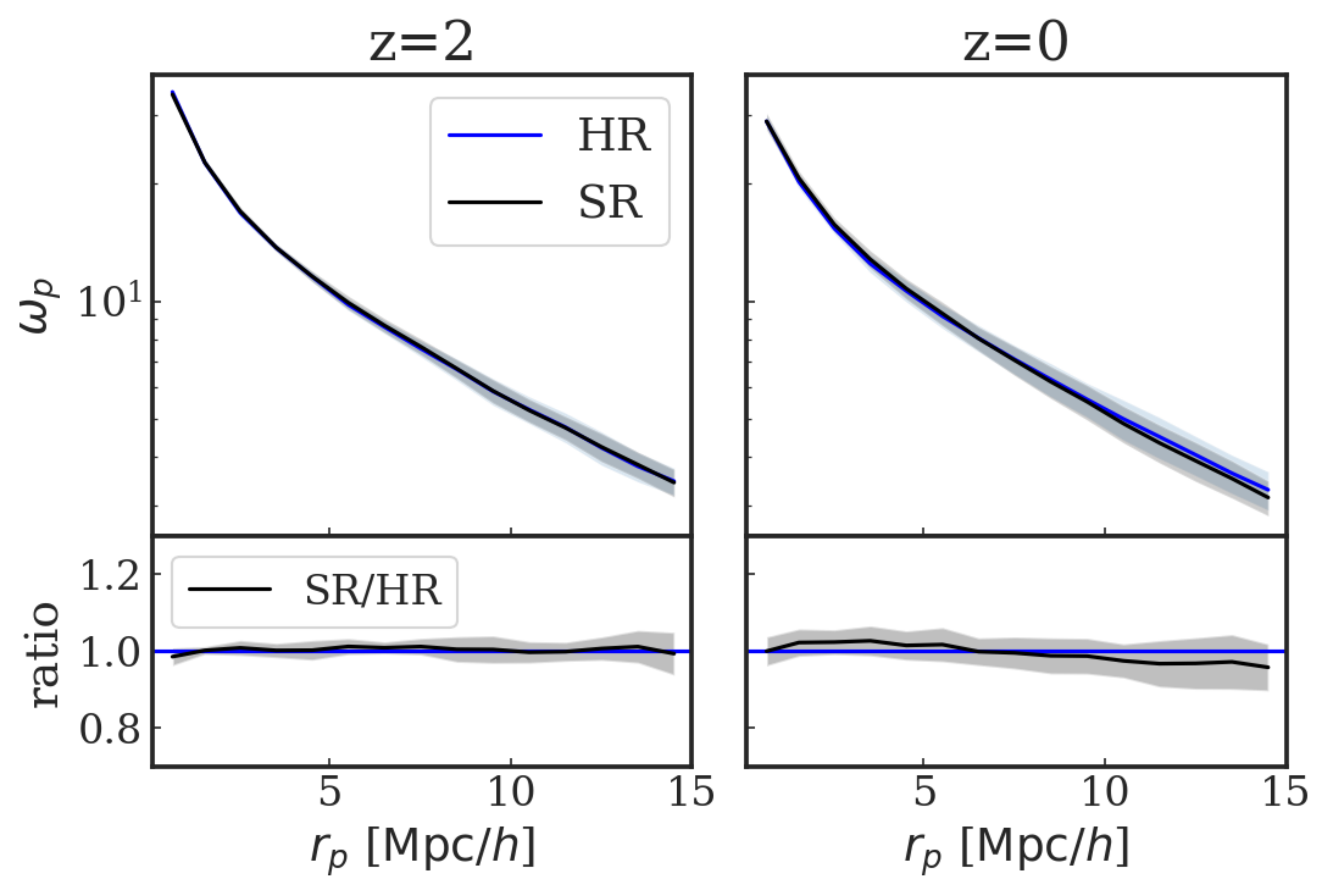


Halo catalog statistics : redshift-space correlation

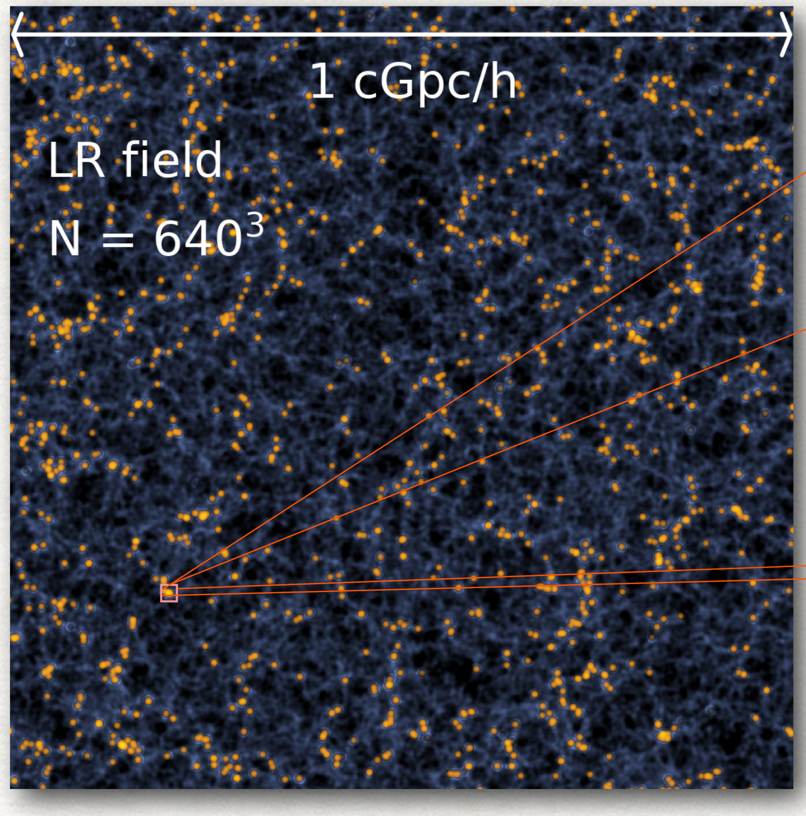
2D contour of $\xi(\pi, r_p)$

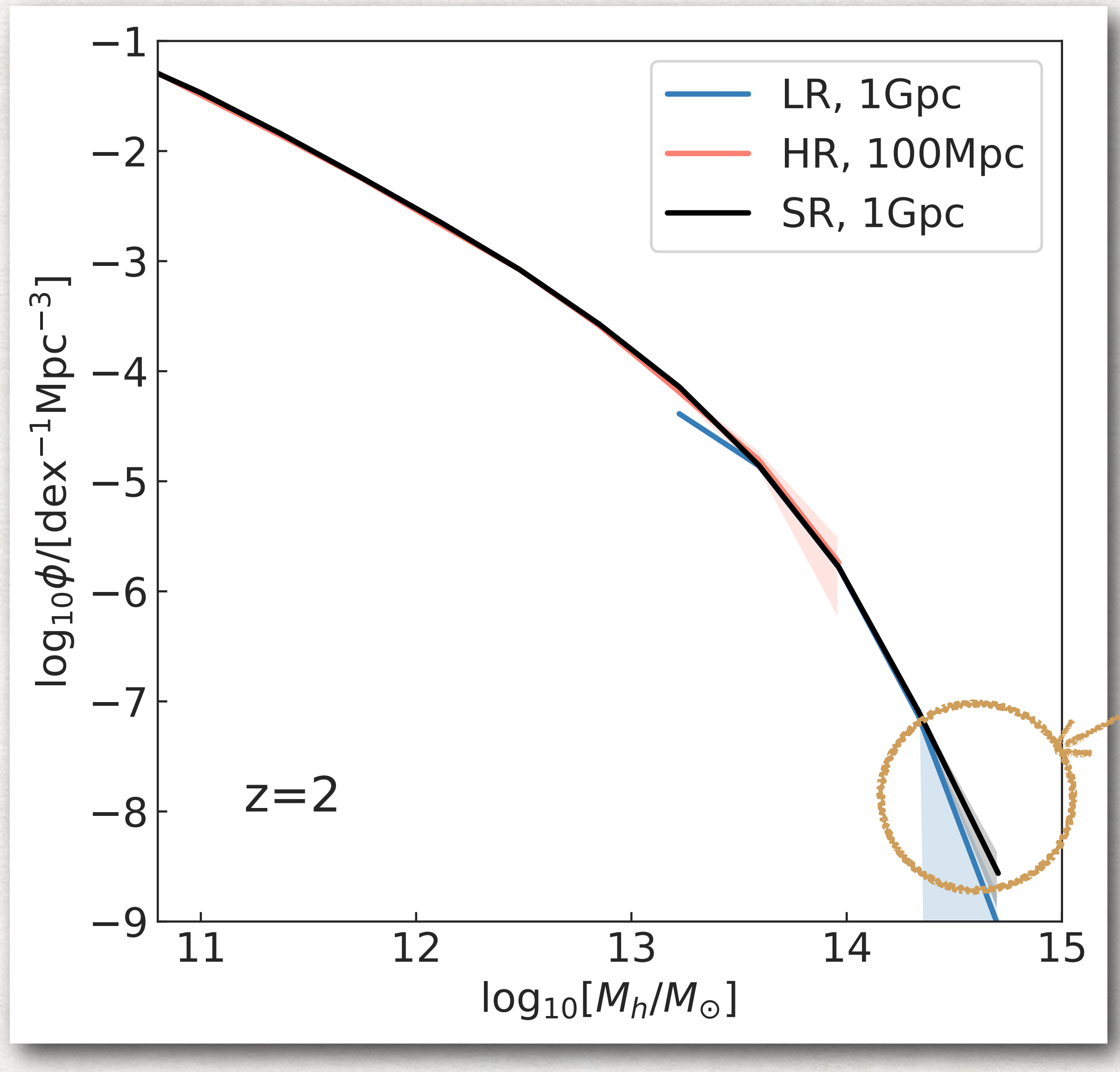


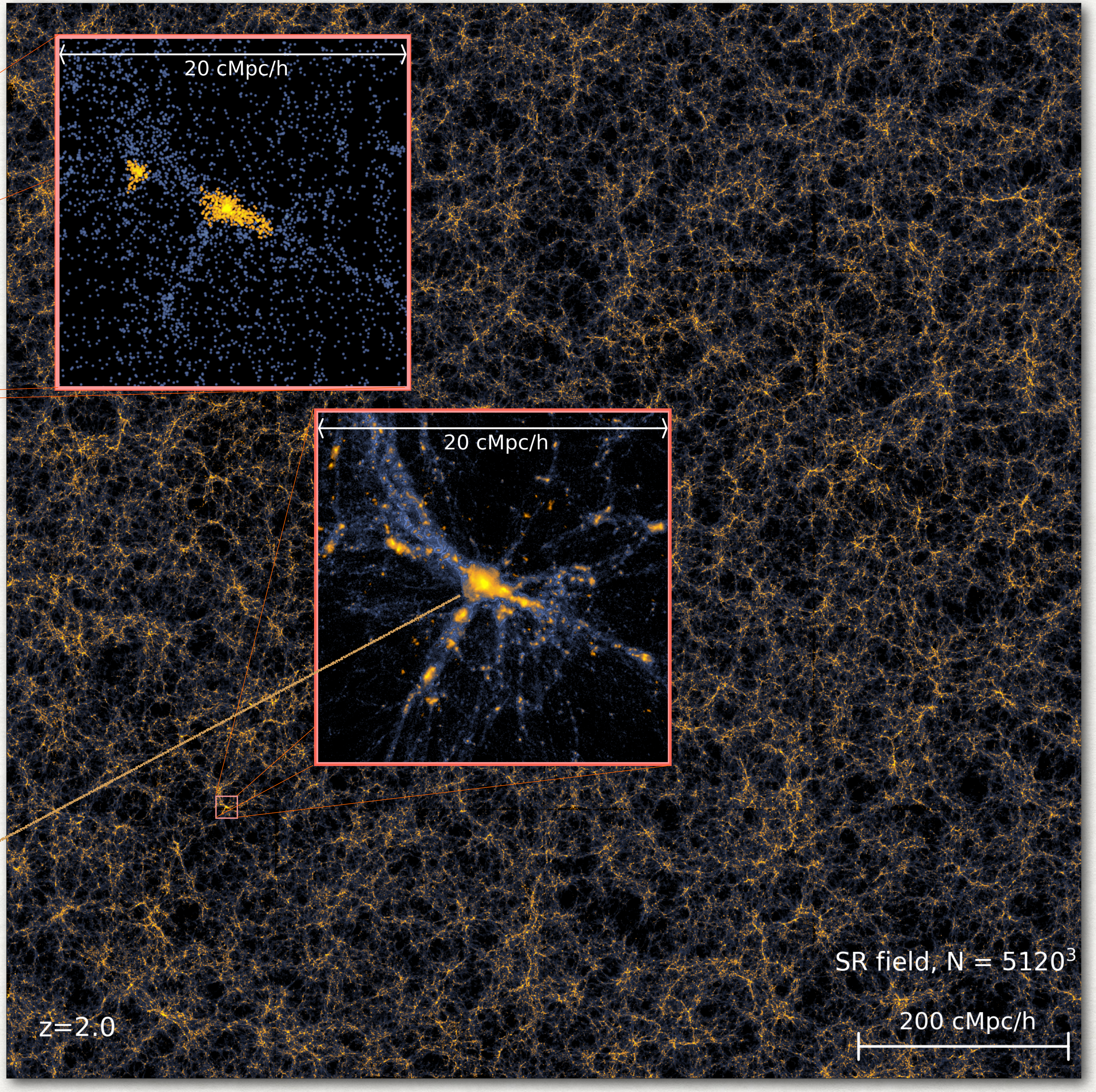
$$\omega_p(r_p) = 2\int_0^\infty d\pi \xi(r_p, \pi)$$



Apply to 1 Gpc/h volume







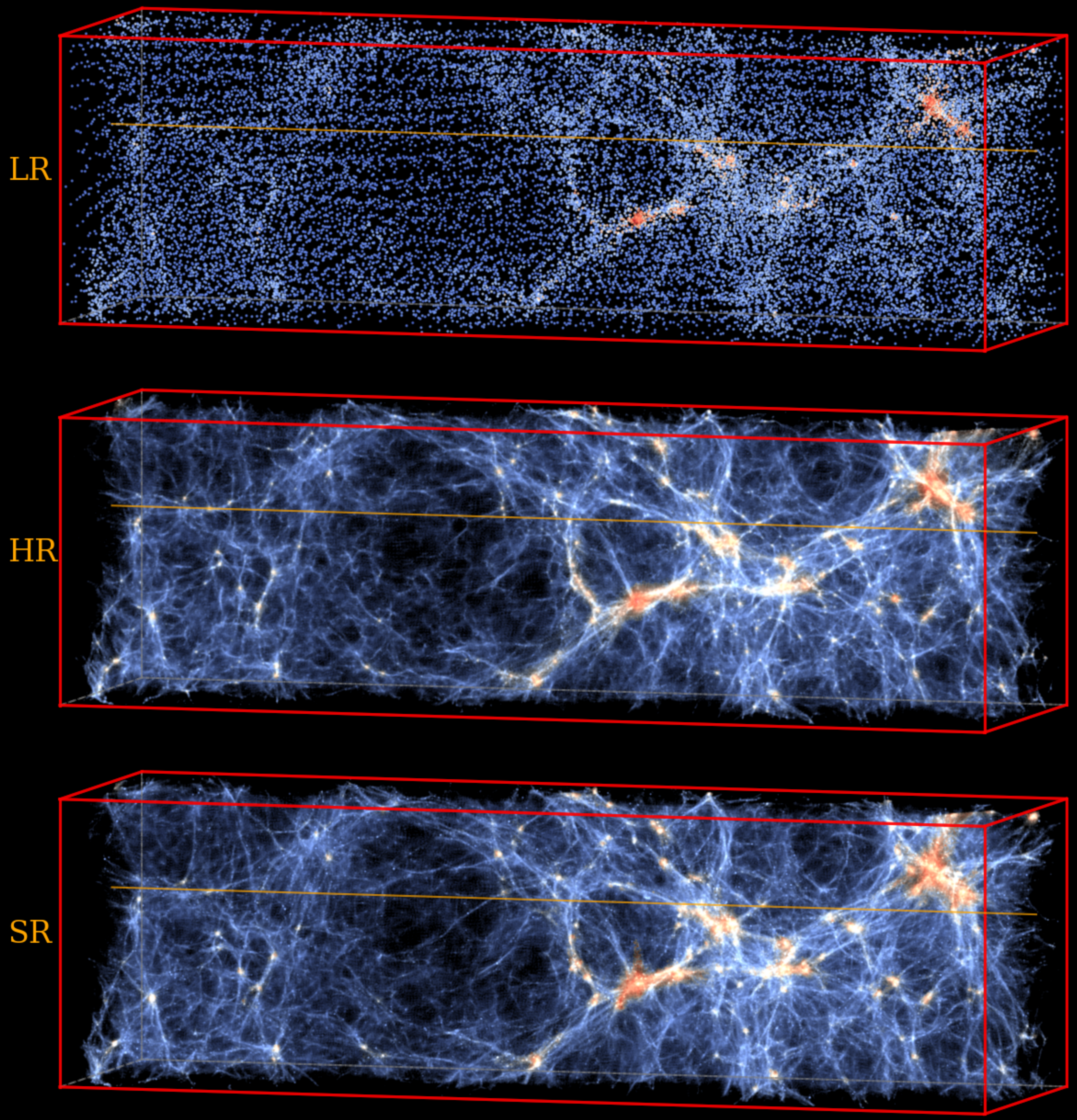
costs ~ 16 hours
with a single GPU

SR for hydro simulations
(Preliminary)

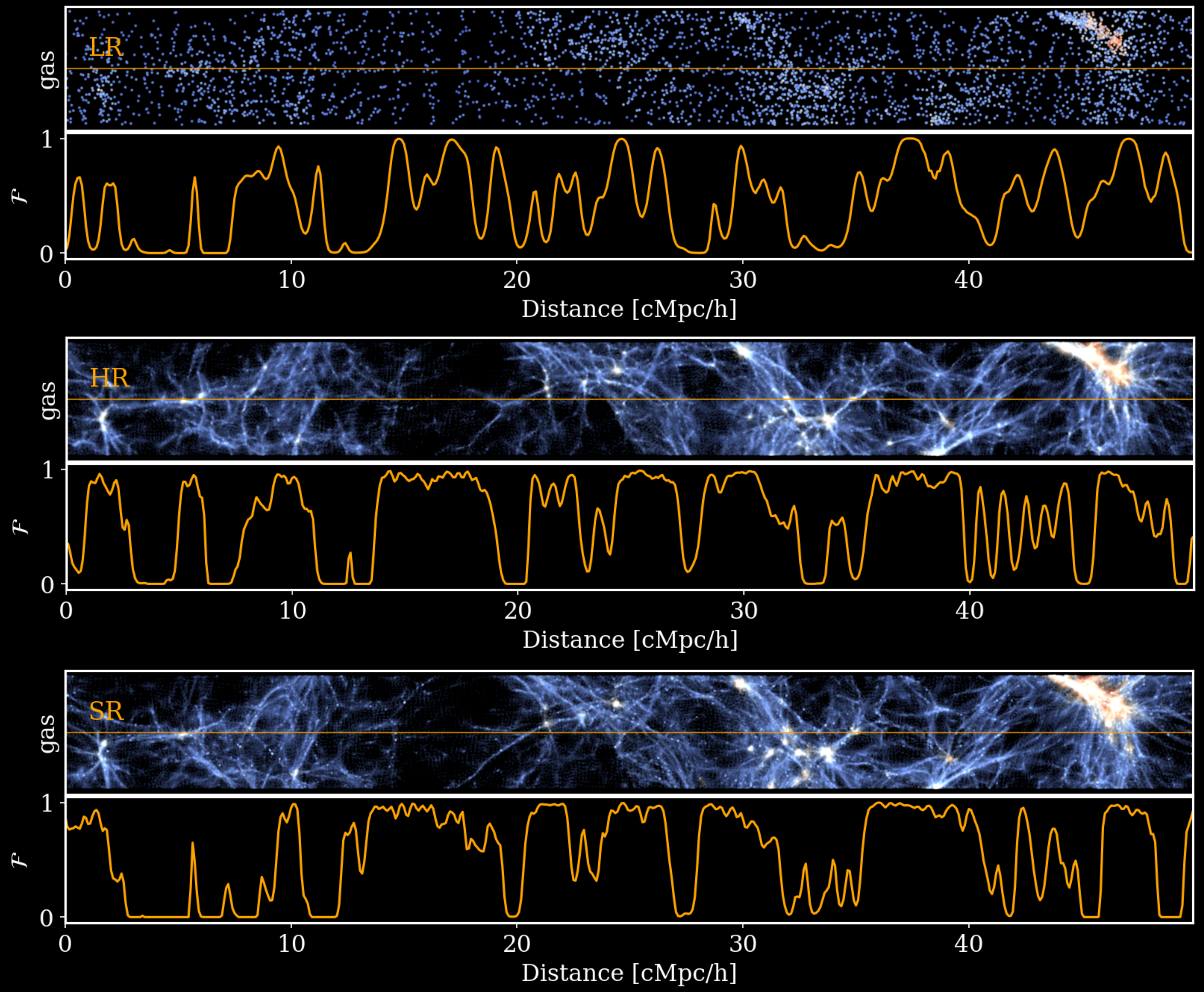
Test by observables ——
Lya spectra

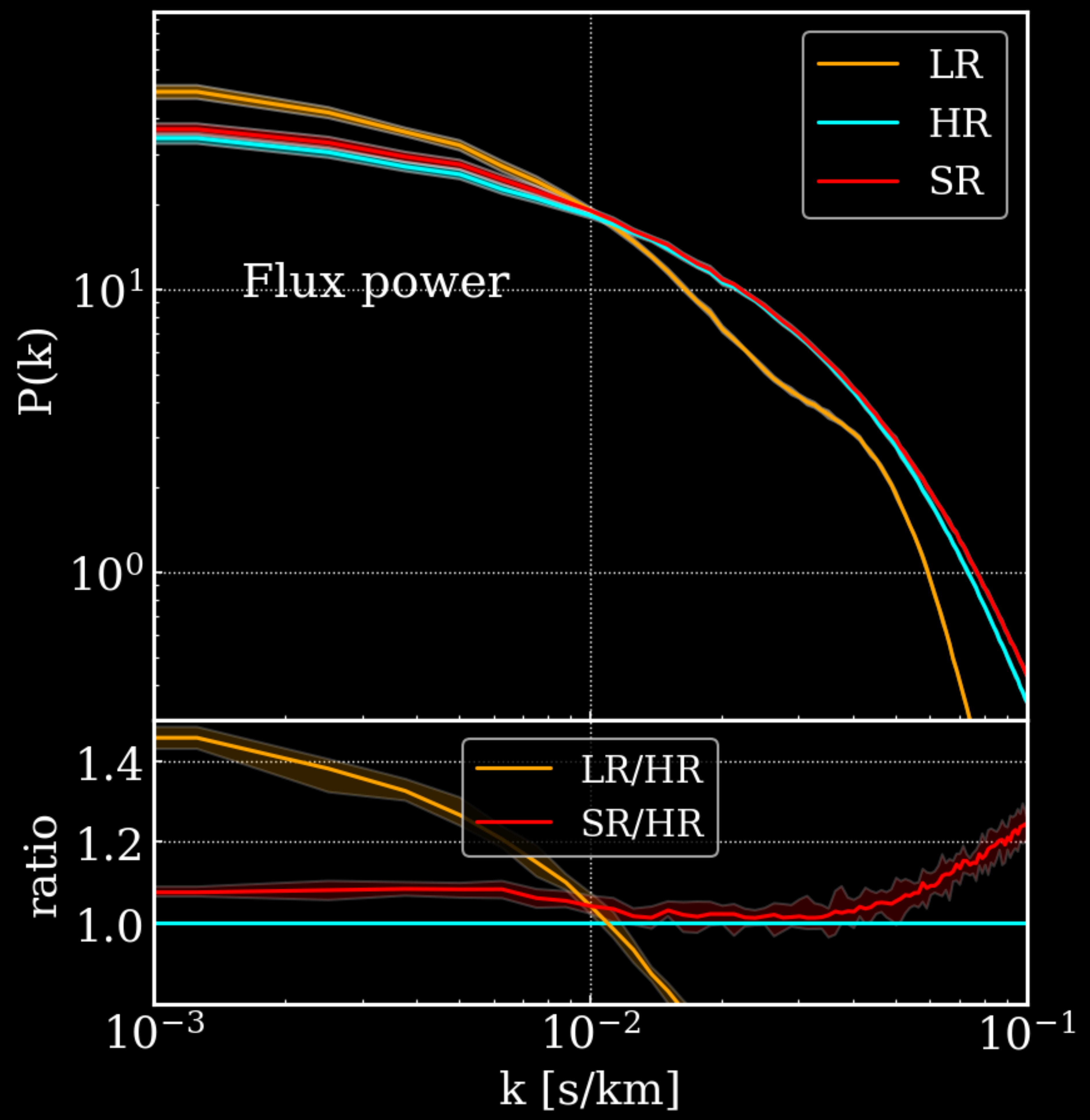
density
&
temperature
&
peculiar velocity

of IGM gas



SR for hydro simulations (Preliminary)





Summary

- SR model: generate the full 6D phase space N-body simulation output with 512 higher mass resolution
- The generated SR fields give statistically good agreement with the authentic HR fields
- Show potential to apply the SR model to large cosmic volume and generate mock catalogs

Challenges and future directions

- Improve the performance on small scales / subhalos
- Accommodate for different cosmology and include the redshift dependency
- Development for hydrodynamic simulation