

# Effects of the initial conditions on cosmological $N$ -body simulations

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# Outline

- 1 Cosmological  $N$ -body simulations
- 2 Effects of the initial conditions
- 3 Applications: galaxy interactions in the Horizon run 4 cosmological simulation
- 4 Summary & Perspectives

# Outline

## ① Cosmological $N$ -body simulations

- Structure formation
- Gravity: the  $N$ -body problem

## ② Effects of the initial conditions

## ③ Applications: galaxy interactions in the Horizon run 4 cosmological simulation

## ④ Summary & Perspectives

# Structure formation

- Main driver of structure formation: gravity
- The linear regime is well understood, and can be described analytically. The overdensity  $\delta \ll 1$  obeys

$$\ddot{\delta} + 2\frac{\dot{a}}{a}\dot{\delta} - 4\pi G\bar{\rho}\delta = 0, \quad (1)$$

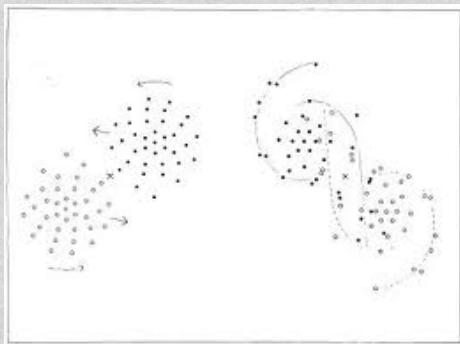
where  $a(t)$  is the *expansion factor*.

- However, When  $\delta \lesssim 1$ , this approximation is not valid anymore: structure formation is a highly non-linear process
- Gas physics is also highly non-linear, and dominant at small scales
- *Cosmological simulations are necessary to understand the detailed physics of structure formation*

# Cosmological simulation

## History

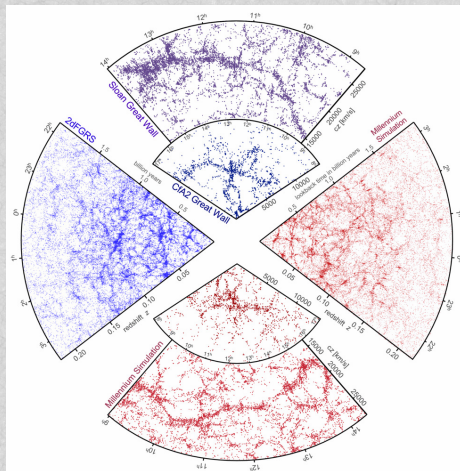
- First  $N$ -body simulation: Holmberg (1941)
  - Gravity and electromagnetism are  $1/r^2$  laws
  - Simulated 2 galaxies with 37 light-bulbs
  - Gravitational force  $\propto$  light received by the light bulb
- First “real” simulation: Von Hoerner (1960, 1963): motions of stars in clusters (16 and 235 stars)
- First cosmological simulations: Miyoshi & Kiahara (1975): 200 particles
- Horizon run 3 (Kim et al 2011):  $7210^3$  particles,  $10 h^{-1}\text{Gpc}$



Holmberg (1941)

# Cosmological simulations

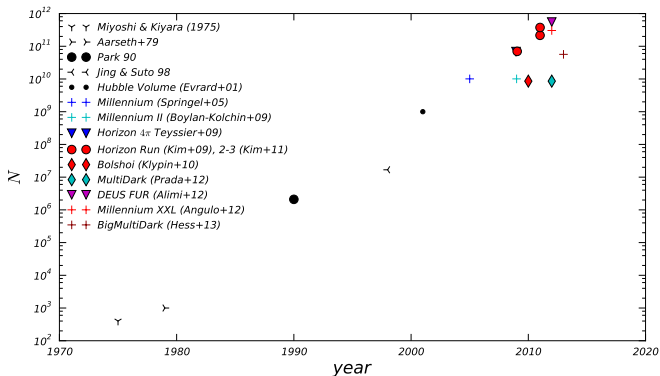
- Remarkably successful in simulating the large-scale structures of the Universe
- Topology of the large-scale structures: Voids, walls, filaments, clusters
- At galactic scales, there are still some unsolved problems



Credit: V. Springel

# Cosmological simulations

## Large simulations



- Exponential growth
- Need for parallel computation ( $\approx 1000$  cores)

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# Gravity

<sup>a</sup>Not in the *elementary* particle sense! Mass of a particle typically  $10^{6-8} h^{-1} M_{\odot}$  in cosmological simulations



# Gravity

- Gravity is the main driver of structure formation
- It has an infinite range ( $\phi(r) \propto 1/r$ )
- The cosmological density field is discretised in  $N$  particles<sup>a</sup> of mass  $m$
- Need for good statistics and low cosmic variance: large box
- Need for good mass and length resolution to accurately describe the small scales: (very) large  $N$

<sup>a</sup>Not in the *elementary* particle sense! Mass of a particle typically  $10^{6-8} h^{-1} M_{\odot}$  in cosmological simulations



# Gravity

## Direct force computation

- Consider a distribution of  $N$  point particles of mass  $m$
- A particle  $i$  will feel the gravitational force

$$\mathbf{F}_i = -G \sum_{j \neq i} \frac{m_j m_i}{r_{ij}^2} \mathbf{u}_{ij} \quad (2)$$

- Direct computation:  $N(N-1)/2 = \mathcal{O}(N^2)$
- Prohibitive for large  $N$  (Now (2013):  $N \simeq 10^{11-12}$ )
- Need for smarter techniques
- Or dedicated hardware (GRAvity piPE, GRAPE, Makino & Funato 1993)

# Gravity

## Particle mesh (PM) (1)

Hockney et al. (1974); Efstathiou & Eastwood (1981)

Idea:

$$\nabla^2 \Phi = 4\pi G \rho \Leftrightarrow \Phi(\mathbf{x}) = \mathcal{G} * \rho(\mathbf{x}), \quad (3)$$

where  $\mathcal{G}(\mathbf{r}) = -G/|\mathbf{r}|$  is the Green function of the Laplacian operator.

In Fourier space: just a multiplication

$$\hat{\Phi}(\mathbf{k}) = \hat{\mathcal{G}}(\mathbf{k}) \hat{\rho}(\mathbf{k}). \quad (4)$$

Fast Fourier transform (FFT):  $\mathcal{O}(N \log N)$ , inverse FFT = FFT.

# Gravity

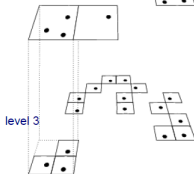
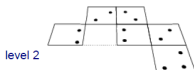
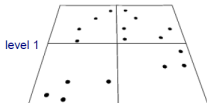
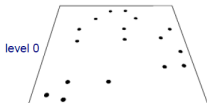
## Particle mesh (PM) (2)

- Compute the density on the grid from the particles distribution
  - Nearest grid point (NGP): the particle belongs to 1 cell. Piecewise constant.
  - Clouds-in-cell (CIC): particle split into 8 cells. Continuous
  - Triangular shaped cloud (TSC): particle split into 27 cells. Continuous derivative
- Fourier transform the density: get the potential
- Differentiate the potential to get the force: finite differences
- Interpolate the force back to particle (same interpolation scheme as (1))

# Gravity

## Tree code

Oct-tree in two dimensions



## Tree algorithms

**Idea:** Use hierarchical multipole expansion to account for distant particle groups

$$\Phi(\mathbf{r}) = -G \sum_i \frac{m_i}{|\mathbf{r} - \mathbf{x}_i|}$$

We expand:

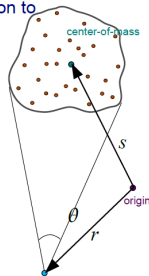
$$\frac{1}{|\mathbf{r} - \mathbf{x}_i|} = \frac{1}{|(\mathbf{r} - \mathbf{s}) - (\mathbf{x}_i - \mathbf{s})|}$$

for  $|\mathbf{x}_i - \mathbf{s}| \ll |\mathbf{r} - \mathbf{s}| \quad \mathbf{y} \equiv \mathbf{r} - \mathbf{s}$

and obtain:

$$\frac{1}{|\mathbf{y} + \mathbf{s} - \mathbf{x}_i|} = \frac{1}{|\mathbf{y}|} - \frac{\mathbf{y} \cdot (\mathbf{s} - \mathbf{x}_i)}{|\mathbf{y}|^3} + \frac{1}{2} \frac{\mathbf{y}^T [3(\mathbf{s} - \mathbf{x}_i)(\mathbf{s} - \mathbf{x}_i)^T - \mathbf{I}(\mathbf{s} - \mathbf{x}_i)^2] \mathbf{y}}{|\mathbf{y}|^5} + \dots$$

the dipole term  
vanishes when  
summed over all  
particles in the  
group



Credits: V. Springel

# Gravity

## Hybrid methods

- PM: Quick and efficient, intrinsically periodic (FFT)
  - But the resolution is given by the number of grid cells
  - Very expensive for high-resolution
  - Force anisotropies at the cell level
- Tree code: efficient at small distances
- TreePM: combine PM for large-scale forces, and tree for small-scales (Gadget-2,3, GOTPM, ...)
- $P^3M$ : long-range forces computed with PM, short-range with PP
- Adaptive  $P^3M$  ( $AP^3M$ ):  $P^3M$  refined in clustered regions
- Adaptive mesh refinement (AMR): PM, refined when needed (ART Kravtsov et al 1997; RAMSES, Teyssier 2002; Enzo, O'Shea et al 2004)

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# Cosmological simulations at 1% precision

- Era of precision cosmology: CMB, SN lightcurves, redshift surveys, ...
- Large upcoming & ongoing surveys (SDSS, (Big)BOSS, LSST, Euclid, DES, ...): precision of  $\approx 1\%$
- Need for massive companion simulations with a 1% level precision
- Can we trust  $N$ -body simulations? To what extent?
  - How sensitive to the initial conditions are the statistics at a given redshift?

# Generating the Initial conditions

- Generate the initial particle positions and velocities
  - Apply a displacement to a pre-initial configuration (preIC)
  - The displacement depends on the cosmology and the starting redshift
- Initial redshift?
- Pre-initial configuration: glass versus grid
- Order of Lagrangian perturbation theory (LPT)?
  - 1LPT or 2LPT? (i.e. Scoccimarro 1998, Crocce et al. 2006)

# Generating the Initial Conditions

- Initial redshift (Knebe et al 2005, Heitmann et al 2008, Reed et al 2013)
  - Too high  $z_i$ : small displacement, not accurate (numerical noise)
  - Too low  $z_i$ : linear regime not valid anymore (shell crossing)
  - Optimum  $z_i$  depends on the mean particle separation
- PrelCs: Glass versus grid
  - Grid: regular mesh, easy but have preferred directions ( $x, y, z$ )
  - Glass (White 1996): isotropic, but need  $\approx 200$  timesteps to reach the equilibrium, and noise on small scales
    - Start with random positions
    - evolve with negative  $G$
    - reach a state of equilibrium (“glass”)

# Lagrangian perturbation theory

Mapping the Lagrangian (initial) positions  $\mathbf{q}$  into Eulerian (after displacement) positions  $\mathbf{x}$

$$\mathbf{x}(\mathbf{q}, z) = \mathbf{q} + \Psi(\mathbf{q}, z),$$

$$\mathbf{v}(\mathbf{q}, z) = \dot{\Psi}(\mathbf{q}, z)$$

$\Psi$ : Displacement field.

- LPT:

$$\Psi(\mathbf{q}, z) = \overbrace{-D_1(z)\nabla_{\mathbf{q}}\phi^{(1)}(\mathbf{q})}^{\text{1LPT}} + \overbrace{D_2(z)\nabla_{\mathbf{q}}\phi^{(2)}(\mathbf{q})}^{\text{2LPT}}$$

$$\nabla^2\phi^{(1)} = \delta(\mathbf{q}),$$

$$D_1(t) = D_+(t),$$

$$\nabla^2\phi^{(2)} = \sum_{i<j} \left\{ \partial_i^2\phi^{(1)}\partial_j^2\phi^{(1)} - \left(\partial_{i,j}\phi^{(1)}\right)^2 \right\}, \quad D_2(t) \simeq -\frac{3}{7}D_1^2(t).$$

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# The simulations

- We used the G0TPM (Park et al 2005) and Gadget-3 (Springel 2005) TreePM codes
- $N$ -body only simulations (tests with gas in progress)
- WMAP5 (and 7) cosmology
- 1  $N_{\text{part}} = 2048^3$  (high res.) simulation, 2  $1024^3$ , many  $512^3$
- Varying the ICs:
  - 4 realisations (different random phase)
  - Initial redshift: 500, 100, 50, 23
  - Order of LPT: 1 or 2
  - Pre-initial configuration: grid or glass
- Two different box sizes: 256 and 768  $h^{-1}\text{Mpc}$  (aim: LSS)
  - mean particle separation of 0.5 and 1.5  $h^{-1}\text{Mpc}$  ( $512^3$ )

# Simulation parameters

| ID     | $N_p$ | $L_{\text{box}}$<br>( $h^{-1}\text{Mpc}$ ) | $z_{\text{ini}}$ | rms $\Psi$ | LPT | PreIC |
|--------|-------|--------------------------------------------|------------------|------------|-----|-------|
| Set 1: |       |                                            |                  |            |     |       |
| T2s    | 1024  | 256                                        | 100              |            | 2   | mesh  |
| T3s    | 512   | 256                                        | 100              |            | 2   | mesh  |
| T3f    | 512   | 256                                        | 100              |            | 1   | mesh  |
| T4s    | 512   | 256                                        | 50               |            | 2   | mesh  |
| T4f    | 512   | 256                                        | 50               |            | 1   | mesh  |
| T5s    | 512   | 256                                        | 23               |            | 2   | mesh  |
| T5f    | 512   | 256                                        | 23               |            | 1   | mesh  |
| T7     | 512   | 768                                        | 100              |            | 2   | mesh  |
| T8     | 512   | 768                                        | 50               |            | 2   | mesh  |
| T9     | 512   | 768                                        | 23               |            | 2   | mesh  |

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# Power spectrum

- Overdensity field:

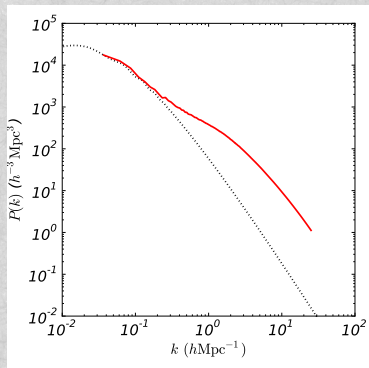
$$\delta(\mathbf{x}) = \frac{\rho(\mathbf{x}) - \bar{\rho}}{\bar{\rho}},$$

$$\delta(\mathbf{k}) = \frac{1}{(2\pi)^3} \int \delta(\mathbf{x}) e^{i\mathbf{k}\mathbf{x}} d^3\mathbf{x}$$

- Power spectrum:

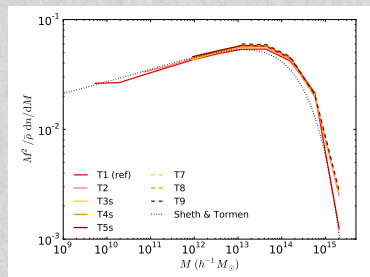
$$P(\mathbf{k}) = P(k) = \frac{1}{V} \langle |\delta(\mathbf{k})|^2 \rangle$$

- Power spectrum computed using TSC interpolation, on a  $N_{\text{grid}}^3 = 8N_{\text{part}}^3$  grid



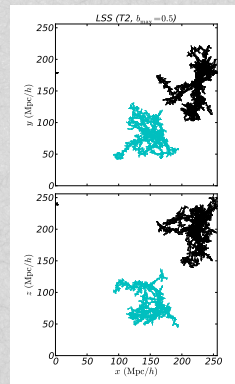
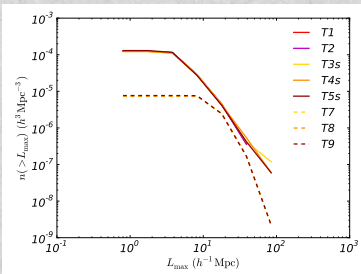
# Mass function

- Halo: non-linear, virialised object
- Halo mass function:  $\frac{dn}{dM}$ , number of haloes  $dn$  with mass between  $M$  and  $M + dM$
- Friends-of-friends (FOF, Davis et al 1985): groups together all particles within  $b$  times the mean interparticle distance.
- $b \approx 0.2$  (linking length) gives a “correct” mass function



# Maximal extent of LSS

- Apply FoF with varying  $b$  to the halo catalogue (Park et al 2012)
- Find  $b_{\max}$  that maximises the number of structures
- We found  $b_{\max} \approx 0.5\text{--}0.6$  for all simulations: apply the same  $b_{\max} = 0.55$
- Distribution of the maximal extent of LSS  $dn/dL_{\max}$



# Outline

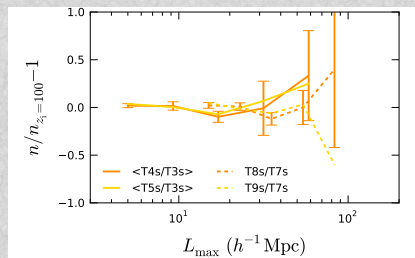
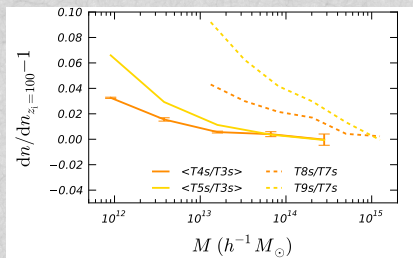
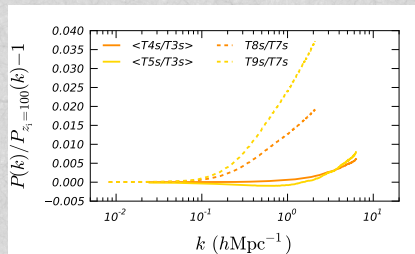
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# Results: Initial Redshift

Power spectrum, mass function & LSS extent

$$N = 512^3$$

Initial redshifts: 100 (ref), 50, 23

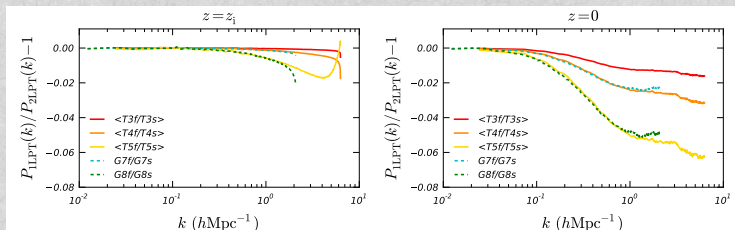


- Lower starting redshifts yield more low-mass haloes and extra small-scale power
- No clear effect for the size distribution of LSSs

# Results: Order of LPT

Power Spectrum (L'Huillier, Park & Kim 2014, New A 30, 79)

Initial redshift: 100, 50, 23 ( $256 h^{-1}\text{Mpc}$ )  
50, 23 ( $768 h^{-1}\text{Mpc}$ )

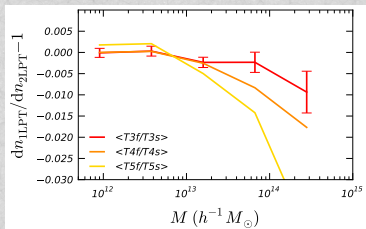


- 1LPT simulations have lower initial power on small scales
- This lack of power increases with starting redshift
- Independent of the resolution and code (G vs T simulations)
- Even  $z_{\text{ini}} = 100$  yields more than 1% difference: *need for 2LPT ICs*

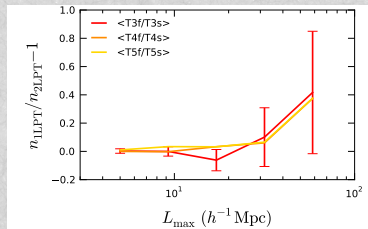
# Results: Order of LPT

Halo mass function & LSS extent (L'Huillier, Park & Kim 2014, New A 30, 79)

Initial redshift: 100, 50, 23 ( $256 h^{-1} \text{Mpc}$ )



Mass function



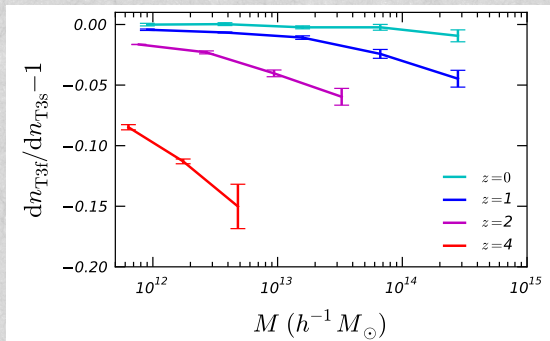
LSS size distribution

- Mass function: within 1% at low masses
- High masses underestimated in 1LPT simulations
- The underestimation is larger at lower starting redshifts
- LSS distribution: independent of the LPT order

# Results: Order of LPT

Redshift evolution of the mass function (L'Huillier, Park & Kim 2014, New A 30, 79)

$$z_{\text{ini}} = 100$$

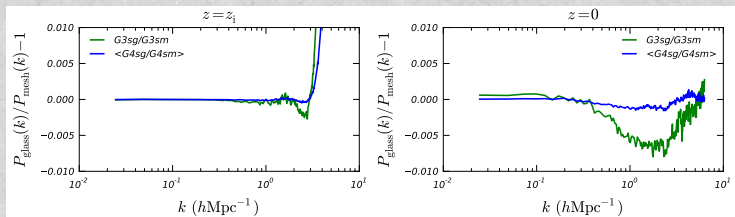


- At  $z > 0$ , the mass function is underestimated in 1LPT simulations
- The underestimation is larger at high mass
- Need for at least  $\approx 100$  expansion factors

# Results: Preinitial configuration

Power Spectrum (L'Huillier, Park & Kim 2014, New A 30, 79)

$z_i = 100$ ,  $z_i = 50$  (Gadget)

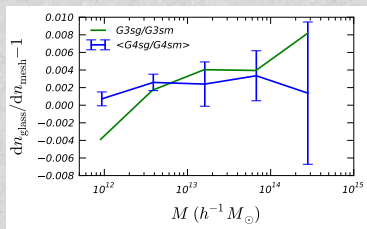


- Extra power on very small scales at initial redshift
- Vanishes by  $z = 0$
- At a given LPT order, initial power is independent of  $z_{\text{ini}}$
- At  $z = 0$ , all within 1%

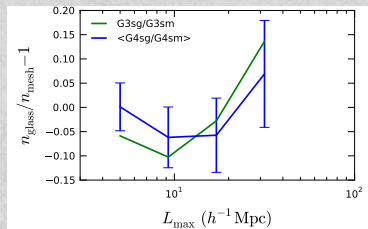
# Results: Preinitial configuration

Halo mass function & LSS extent (L'Huillier, Park & Kim 2014, New A 30, 79)

$z_i = 100$ ,  $z_i = 50$  (Gadget)



Mass function



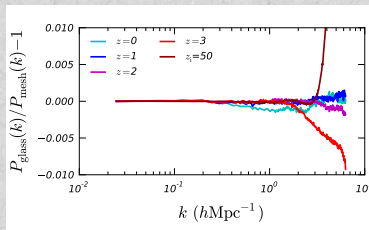
LSS size distribution

- Mass function: within 1% at low masses, large fluctuation at high masses
- No significant differences for the LSS size distribution

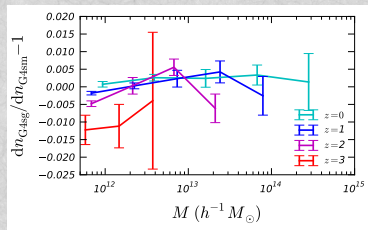
# Results: Preinitial configuration

Redshift evolution (L'Huillier, Park & Kim 2014, New A 30, 79)

$$z_{\text{ini}} = 50$$



Power spectrum



mass function

- No significant difference after  $z = 2$
- At  $z = 3$ : underestimation of the grid small scale power and the low-mass end of the mass function

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# Horizon run 4

Some propaganda

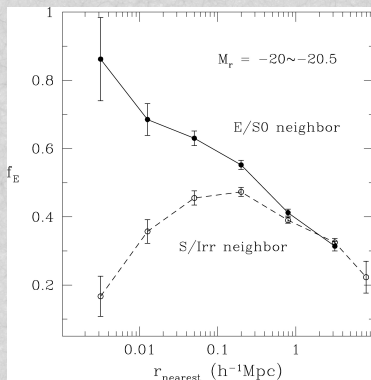
## Horizon run 4 (this background image)

- J. Kim, C. Park, S.W. Hong, H.S. Hwang, B. L'Huillier
- 8000 CPU cores, 50 days.
- Aim at creating mock catalogue for HectoMAP
- $L = 3.15 h^{-1}\text{Gpc}$ ,  $N = 6300^3$  ( $\bar{d} = 0.5 h^{-1}\text{Mpc}$ )
- 2LPT,  $z_{\text{ini}} = 100$ , 2000 timesteps
- 70 outputs, lightcone up to  $z = 1.39$
- Simulation achieved, haloes detected and (preliminary) merger tree built
- Applications: Galaxy interactions, clustering, semi-analytic models, lensing, ...

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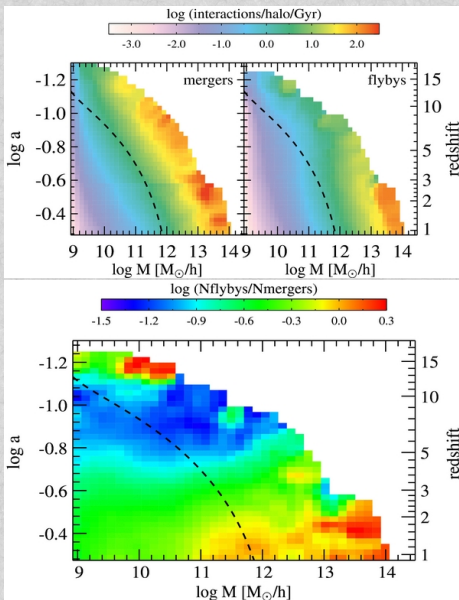
# Morphological transformation



Park, Gott & Choi (2008)

- SDSS DR4plus (LSS-DR4plus),  
 $15.5 < r_{\text{Pet}} < 17.6$ ,  $0.001 < z < 0.5$
- Fraction of elliptical (ETG) versus distance to nearest neighbour
- If the neighbour is an ETG: decreases with increasing distance
- If the neighbour is a LTG:
  - outside of  $R_{\text{vir},N}$ : same trend
  - Within  $R_{\text{vir},N}$ : the probability to be an ETG decreases with decreasing distance: *reversed morphological transformation?*
- Role of distant interactions

# Flybys in cosmological simulations



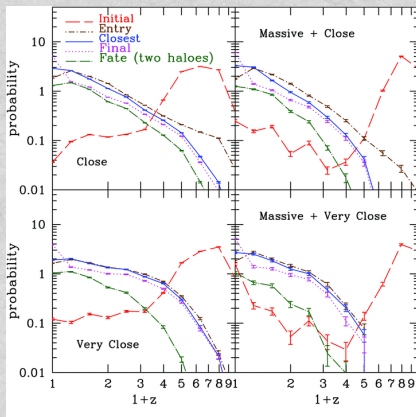
- Sinha & Holley-Bockelmann (2012): importance of flybys?
- $N$ -body simulation:
- Merger dominant at high  $z$
- For massive haloes ( $> 10^{11}$ ) and  $z < 2$ , flybys important
- Small box ( $50 h^{-1}\text{Mpc}$ : large-scale effects?)
- Down to  $z = 1$
- Observationally: close pairs as a proxy for merger rate. What about flybys? (cf. Tonnensen & Cen 2012)

# Pair interactions

Moreno (2012) using the Millennium simulation (Springel et al 2005): Interacting pairs: within  $d_{\text{crit}} = 0.2$  or  $1 h^{-1}\text{Mpc}$  (comoving). Introduced a 5-steps interaction scheme:

- Initial: when the two haloes are first detected
- Entry: when their separation is closer than  $d_{\text{crit}}$
- Closest: when the distance is the smallest
- Final: last time the 2 haloes are identified
- Fate: what happens to the pair: merges, absorbed by third party, or survives

# Pair interactions



- $M > 8.6 \times 10^{10} h^{-1} M_{\odot}$
- Close:  $d < 0.2 h^{-1} \text{Mpc}$
- Very close:  $d < 1 h^{-1} \text{Mpc}$
- Massive:  $M > 8.6 \times 10^{11} h^{-1} M_{\odot}$
- Also: separation, total mass, mass ratio, lifetime

Moreno et al (2012)

# The rates and types of halo interactions

L'Huillier, C. Park and J. Kim, in prepatation

## Means of galaxy evolution:

- Secular evolution: isolated galaxies
- Major merger have a dramatic impact (morphology transformation, significant mass increase) (Toomre & Toomre 1972)
- Minor mergers also matter: more frequent (Bournaud et al 2007)
- How about flybys? Not much studied (notable exception: Sinha & Holley-Bockelmann 2012)
- Role of the environment: field, groups and cluster

# The rates and types of halo interactions

L'Huillier, C. Park and J. Kim, in prepatation

## Means of galaxy evolution:

- Secular evolution: isolated galaxies
- Major merger have a dramatic impact (morphology transformation, significant mass increase) (Toomre & Toomre 1972)
- Minor mergers also matter: more frequent (Bournaud et al 2007)
- How about flybys? Not much studied (notable exception: Sinha & Holley-Bockelmann 2012)
- Role of the environment: field, groups and cluster

## Main questions

- How and how often do haloes interact?
- How does it change with redshift and with other properties (mass ratio, impact factor, environment)?

# Halo catalogues

## Catalogues

- Two catalogues of target and neighbour haloes defined by a mass cut
- Catalogue of target haloes (T):  $M > M_0 = 5 \times 10^{11} h^{-1} M_{\odot}$
- Catalogue of neighbour haloes (N):  $M > fM_0 = 2 \times 10^{11} h^{-1} M_{\odot}$ ;  $f = 0.4$  sets the minimum mass ratio
- Both catalogues are complete (more massive than the mass resolution)

# Method

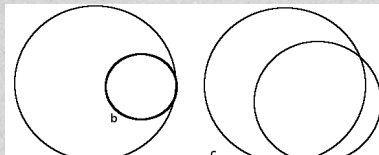
## Interactions

We define interactions pairs of targets and neighbours such as

- the target halo lies within the virial radius of its (closest) neighbour
- the neighbour satisfies:  $M_N > fM_T$  ( $f = 0.4$ )

Notes:

- At the moment, we don't consider multiple interactions: only the closest neighbour is considered
- An interaction may counted twice if the neighbour is also in the Target catalogue, and if the target is the closest neighbour of the neighbour satisfying the mass condition



## Method

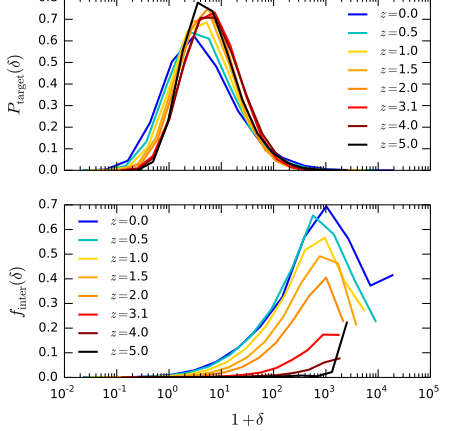
To quantify the environment:  $\rho_{20}$ : density over 20 neighbours

$$\rho_{20} = \sum_{i=1}^{20} M_i W(r_i, h),$$

where  $r_i$  is the distance to the  $i^{\text{th}}$  neighbour,  $M_i$  its mass,  $W$  the SPH spline kernel, and  $h$  the smoothing length.

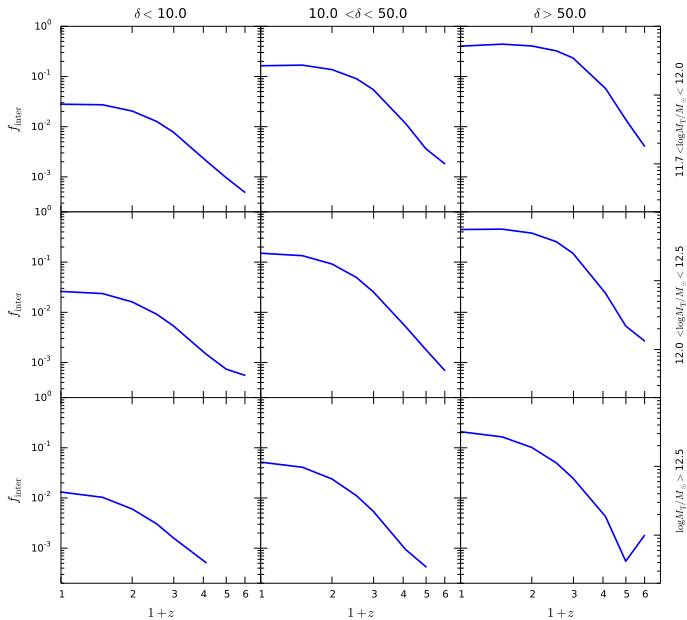
We are interested in the distribution  $dN = f(M_T, p, q, \delta, z) dM_T dp dq d\delta dz$ , where  $p = d/R_{\text{vir},N}$ ;  $q = M_N/M_T$ ;  $\delta = \rho_{20}/\bar{\rho} - 1$

5 parameters: we use different bins of  $\rho_{20}$  and  $M_T$ , at different  $z$ , and study the distribution of  $p$  and  $q$ .



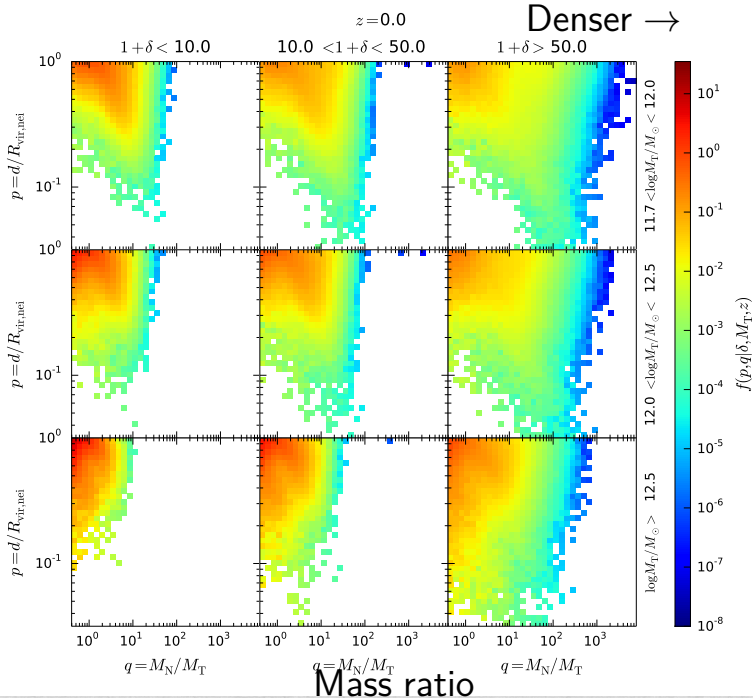
## Preliminary results!

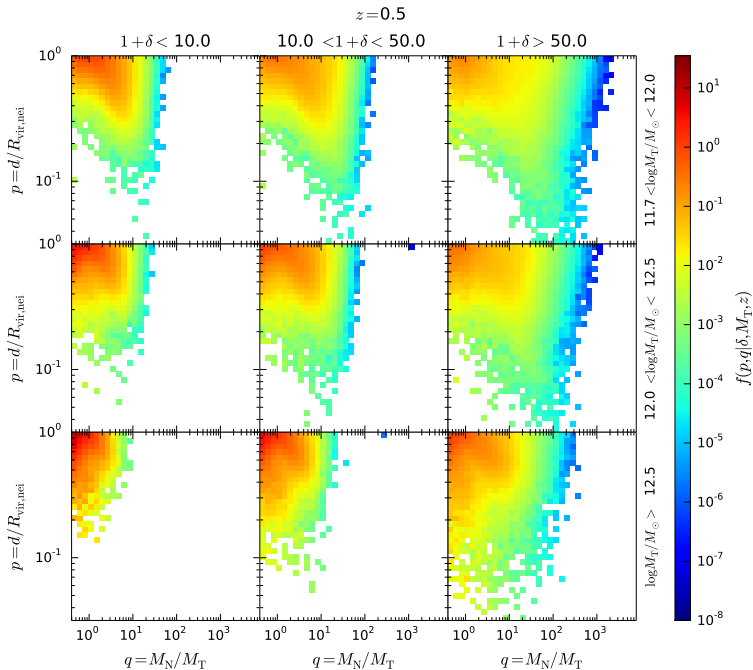
Denser  $\rightarrow$

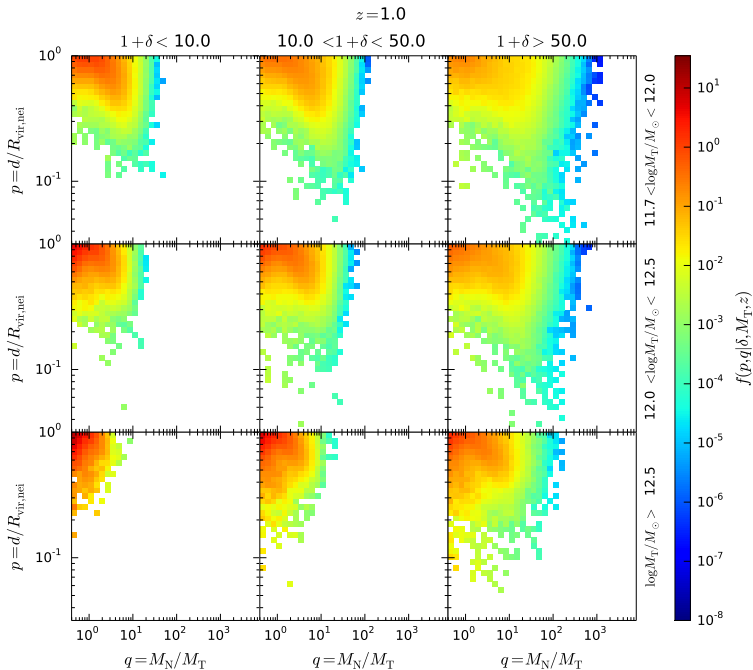


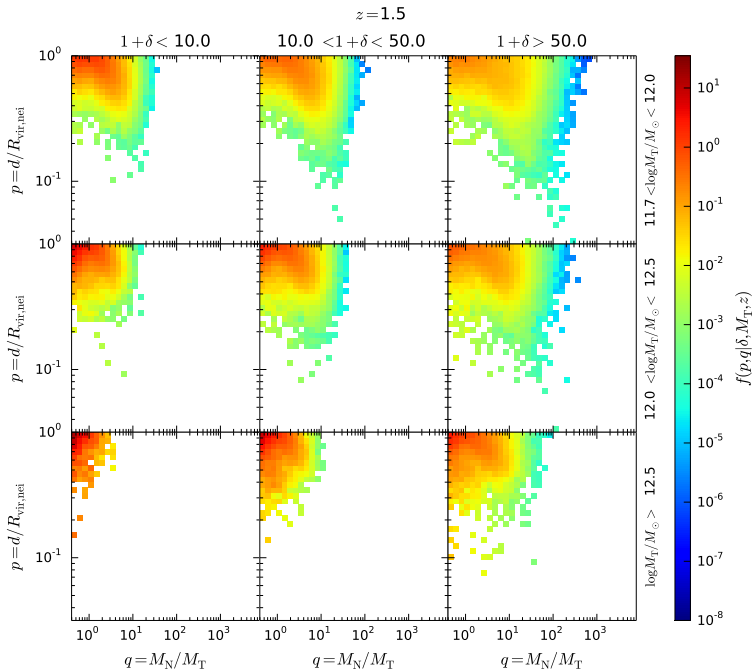
More massive  $\rightarrow$

Distance ratio

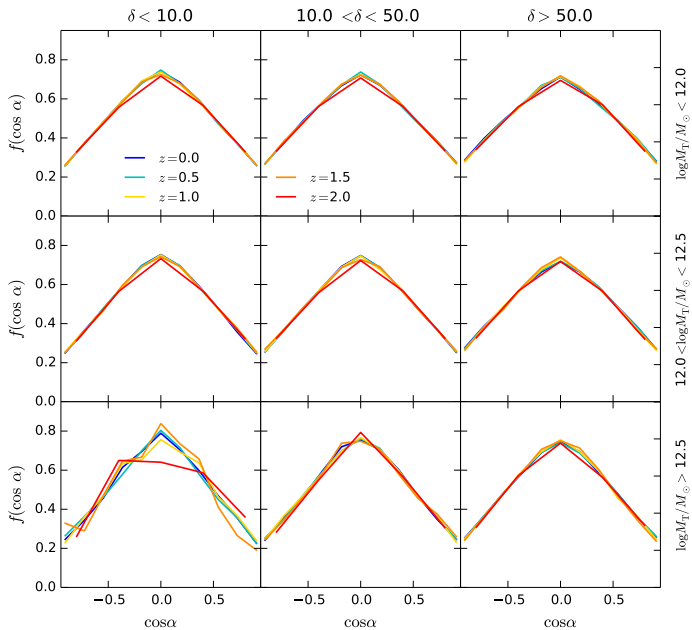


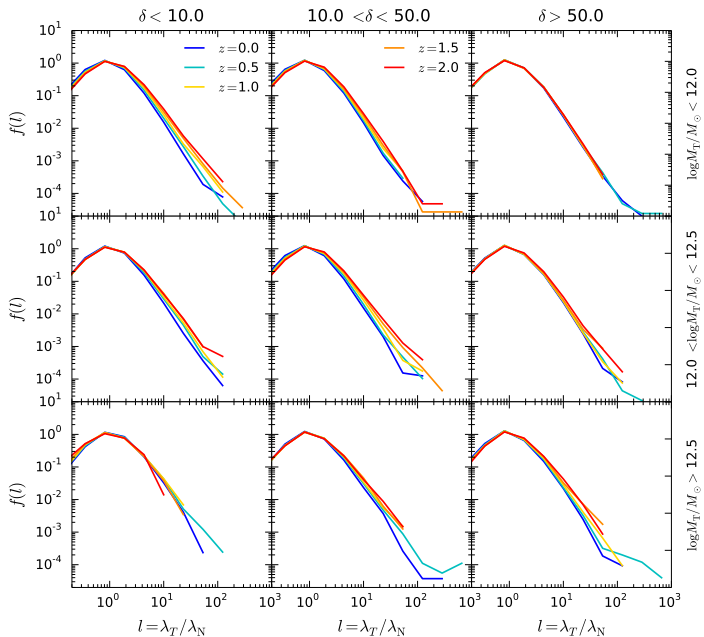






$$\alpha = (\mathbf{J}_N, \mathbf{r})$$





# Outline

- 1 Cosmological  $N$ -body simulations
- 2 Effects of the initial conditions
- 3 Applications: galaxy interactions in the Horizon run 4 cosmological simulation
- 4 Summary & Perspectives

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- 4 Summary & Perspectives
  - Summary (1)

# Summary & perspectives

## Summary (1): ICs

- Choice of the ICs important to reach 1% precision *even for the pure  $N$ -body case!*
- Size distribution of LSS not very sensitive to the ICs (small box)
- Glass pre-ICs have an excess of power at small scales at initial times, but vanishes with time
- 2LPT and high initial redshift are necessary to reach 1% accuracy:  $z_{\text{ini}} \approx 100$  for a mean particle separation of  $0.5 h^{-1}\text{Mpc}$ , at least 50 expansion factors
- Important for high-redshift studies

## Next

- ICs for the hydro case (in progress)
- Use of accurate large  $N$ -body simulations for galaxy evolution, study of the LSS, ...

# Summary (2): halo interactions

## Halo interaction

- Horizon run 4 provides very good statistics and allow for study of environmental effects

## Next

- Use of merger trees to distinguish the types (mergers vs. flybys)
- Need to quantify the strength of interactions in addition to the frequency
- Study of galaxy interaction in clusters
- Inclusion of hydrodynamics
- Formation of the large-scale structures
- Work in progress... stay tuned!

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감사합니다!