面向下一代大尺度巡天的超级数值模拟

- Hyper Millennium project
- PhotoNs code

报告人：王乔

合作者：李明、高亮、郭琦、裴文祥 et al.

2023 - 6 - 19 上海交通大学

中国科学院国家天文台
NATIONAL ASTRONOMICAL OBSERVATORIES, CAS

Large simulations are still demading for modern cosmology

- To understand complex physical processes related to various cosmic probes（BAO、RSD、Weak lensing and etc.）
- To meet the requirement of accurate Cosmology（1%）

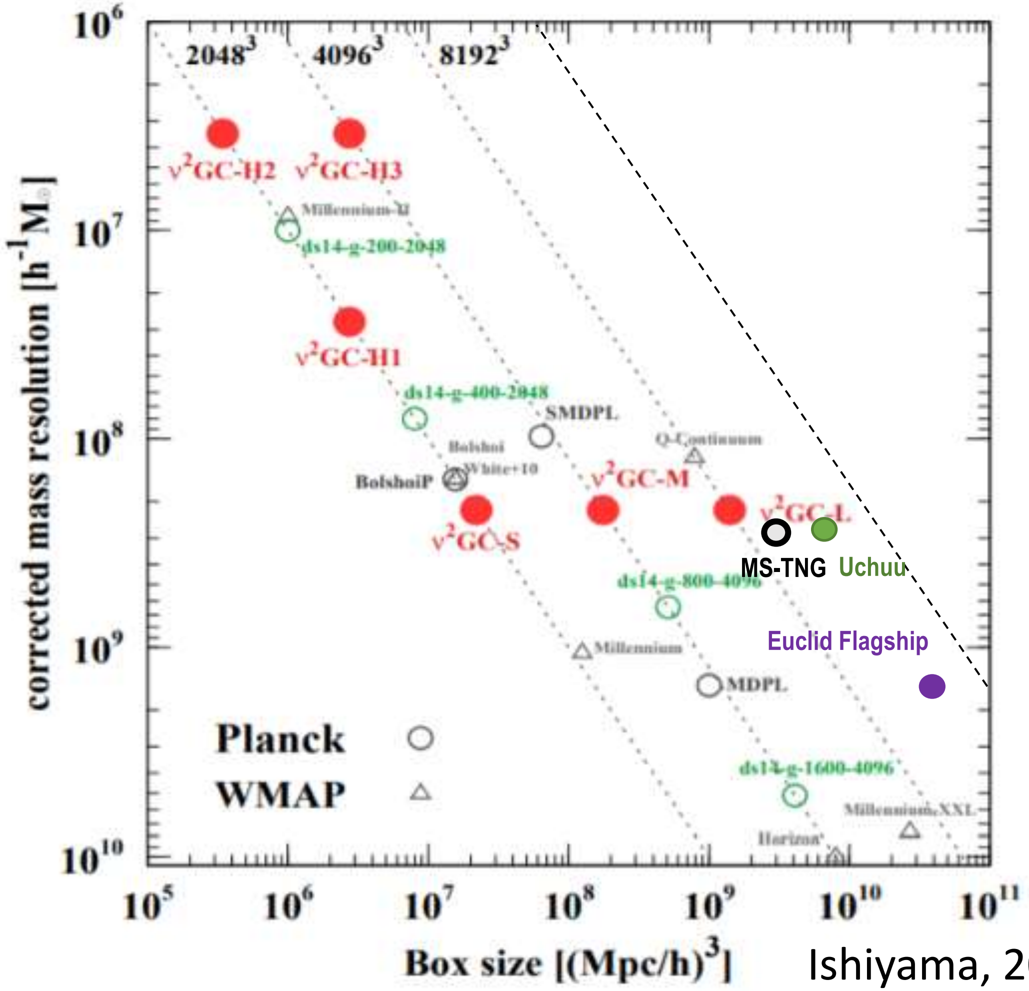
selection effects, systematic uncertainties, statistic uncertainties

New Generation Large-scale Surveys

Name	Sky coverage (degree)	Wavelength （nm）
CSST	17,500	255-1000
LSST	18,000	320-1050
EUCLID	15,000	550-920 1000-2000
WFIRST	2,400	927-2000

Tracers:
QSOs, LRGs(massive), ELGs(low masses), and etc.

art-of-the-state simulations



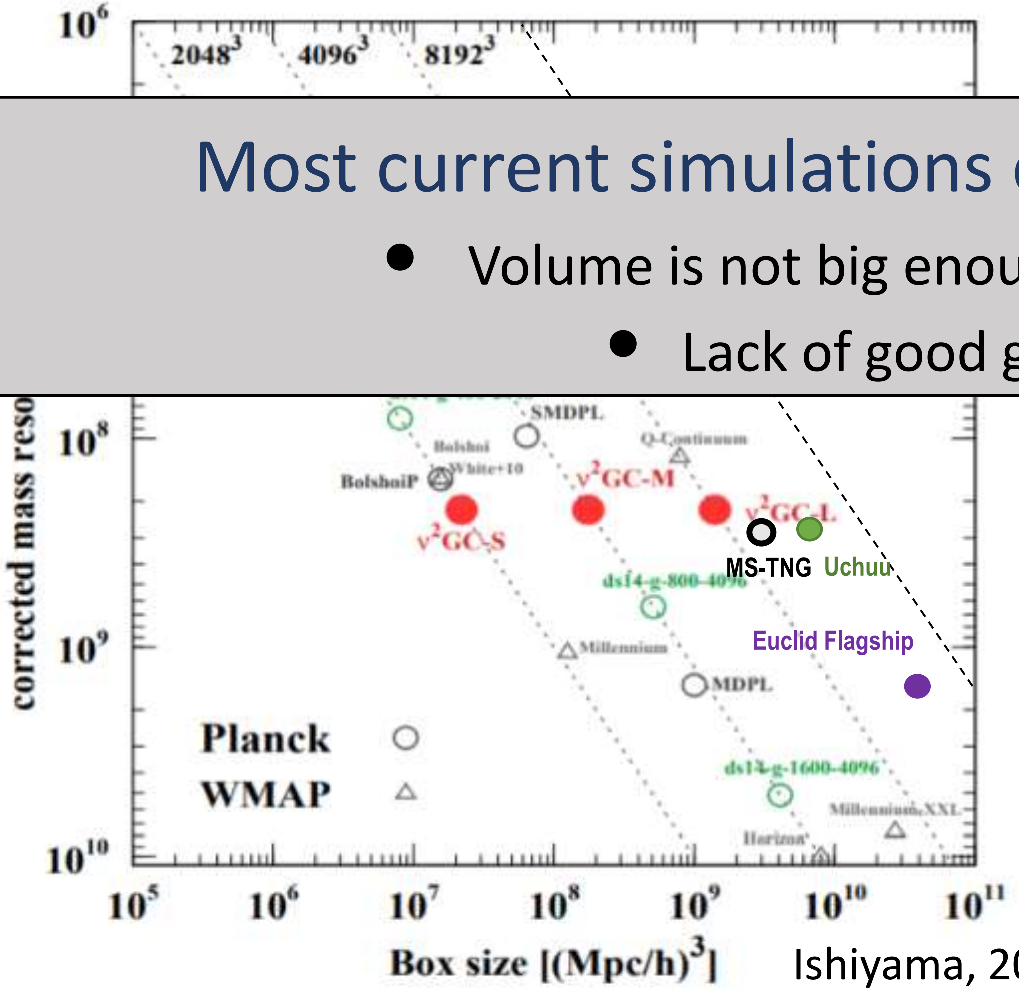
Ishiyama, 2016

Name	Code	L_{box} $[h^{-1}Mpc]$	N_p $[10^9]$	m_p $[h^{-1}M_\odot]$
Horizon Run 3	GOTPM	10815	370	2.5×10^{11}
Bolshoi PL	ART	250	8.6	1.6×10^{8}
Small MultiDark PL	GADGET-2	400	57	1.5×10^{9}
MultiDark PL	GADGET-2	1000	57	1.5×10^{9}
Big MultiDark PL	GADGET-2	2500	57	2.4×10^{10}
Huge MultiDark PL	GADGET-2	4000	69	7.9×10^{10}
Horizon-4Π	RAMSES	2000	69	7.8×10^{9}
DEUS FUR	RAMSES-DEUS	21000	550	1.2×10^{12}
Pangu	L-GADGET-2	1000	29	2.5×10^{9}
Tiangong Pathfinder	L-GADGET-3	1000	232	3.72×10^{8}
ν^2GC-L	GREEM	1120	550	2.2×10^{8}
Shin-Uchuu	GREEM	140	262	8.97×10^{5}
Uchuu	GREEM	2000	~2000	3.27×10^{8}
Euclid Flagship	PKDGRAV3	3780	~2000	$\sim 2.398 \times 10^{9}$
Euclid Flagship v2.0	PKDGRAV3	3600	~4000	$\sim 1 \times 10^{9}$
Q-Continuum	HACC	923	~550	1.05×10^{8}
Outer Rim	HACC	3000	~1070	1.85×10^{9}
Millennium	L-GADGET-2	500	10	8.6×10^{8}
Millennium-II	P-GADGET-3	100	10	6.9×10^{6}
Millennium-XXL	L-GADGET-3	3000	300	6.2×10^{9}

art-of-the-state simulations

Most current simulations can not meet the requirements

- Volume is not big enough/resolution is not high enough
- Lack of good galaxy formation models



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自主研发软件平台

2014 PhotoNs-1
天河-2平台
TreePM code

2016 新算法
PM-FMM

2017 太湖之光平台，1千万核心16万进程，测试10万亿模拟粒子，峰值到达21.3 Pflops

2018 PhotoNs-2
升级算法和并行策略。核心效率达到41Pflops

2019 “神威杯”
国产CPU并行应用挑战赛总决赛

2020 GPU平台
再次重写底层。

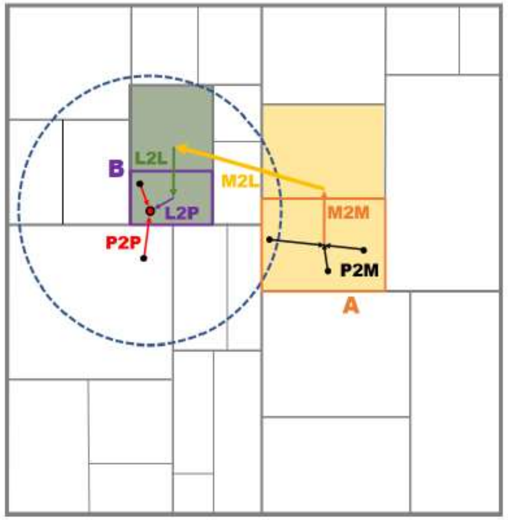
2021PhotoNs-3
完成2.1万亿规模再电离期宇宙学模拟，完备解析电离源的质量分辨能力

2022升级再电离期宇宙学模拟到3.1万亿

2023 Hyper Millennium 4.1万亿粒子规模，halo+subhalo finder,结合merger tree与半解析模拟

算法介绍

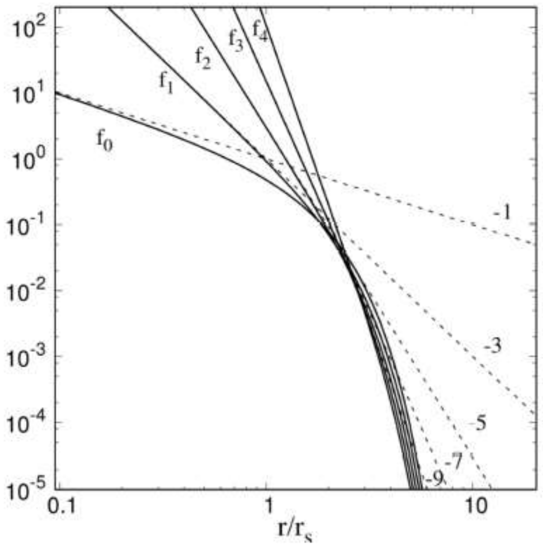
Particle-Mesh + Fast-Multipole-Method (PM-FMM)

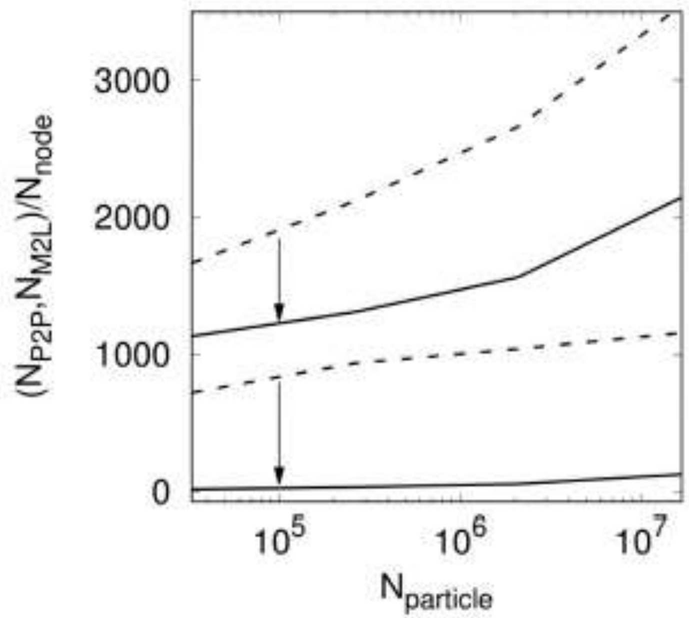


$$f_{(2)}(r) = \frac{3}{r^5}\text{erfc}\left(\frac{r}{2r_s}\right) + \frac{1}{\sqrt{\pi}}\exp\left(-\frac{r^2}{4r_s^2}\right) \times \left[\frac{3}{r_s r^4} + \frac{1}{2r_s^3 r^2}\right],$$

$$f_{(3)}(r) = -\frac{15}{r^7}\text{erfc}\left(\frac{r}{2r_s}\right) - \frac{1}{\sqrt{\pi}}\exp\left(-\frac{r^2}{4r_s^2}\right) \times \left[\frac{15}{r_s r^6} + \frac{5}{2r_s^3 r^4} + \frac{1}{4r_s^5 r^2}\right],$$

$$f_{(4)}(r) = \frac{105}{r^9}\text{erfc}\left(\frac{r}{2r_s}\right) + \frac{1}{\sqrt{\pi}}\exp\left(-\frac{r^2}{4r_s^2}\right) \times \left[\frac{105}{r_s r^8} + \frac{35}{2r_s^3 r^6} + \frac{7}{4r_s^5 r^4} + \frac{1}{8r_s^7 r^2}\right].$$





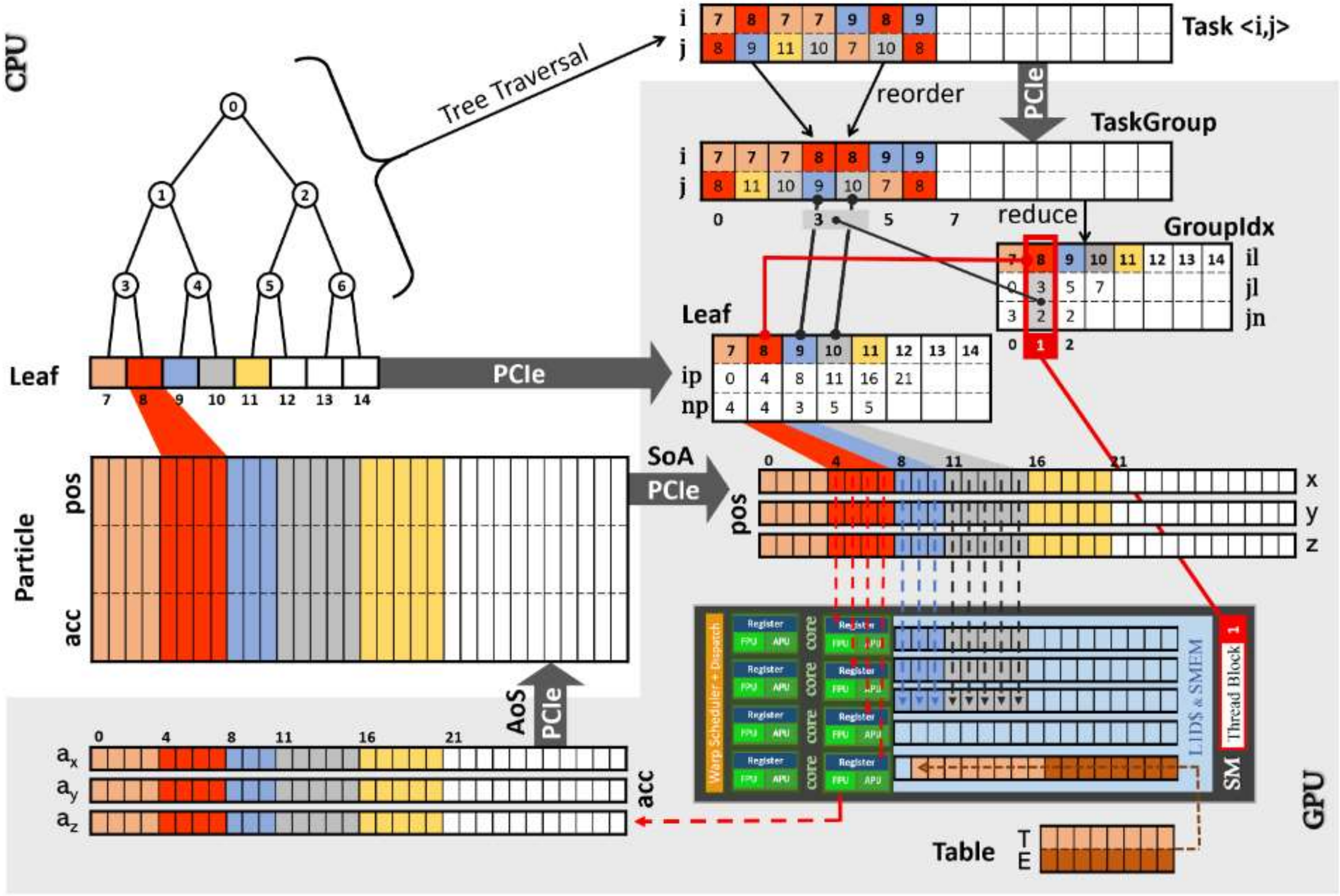
$O\left(\mathbf{N} * p + n \log_2 n + m \log_2 m\right)$

- PM-FMM 接近线性的时间复杂度，同时解耦了长短程的相互作用,极大地减少了通信和计算的总量

Q. Wang，2021

1.热点计算性能和优化手段

- 树遍历的过程中通过判定条件判断建立任务列表
- 根据公式推算以及NVProf等性能分析工具得出，一次P2P核心计算，访问6个float，至少86次浮点计算
- 实现数据传输与计算重叠
- 所有源叶节点中的粒子则依次被排序处理。这种任务分配方法使得所有线程的任务完全独立，最大化访存的连续性和局部性，可以充分利用Global Memory的访存合并、Shared Memory共享缓存以及Register

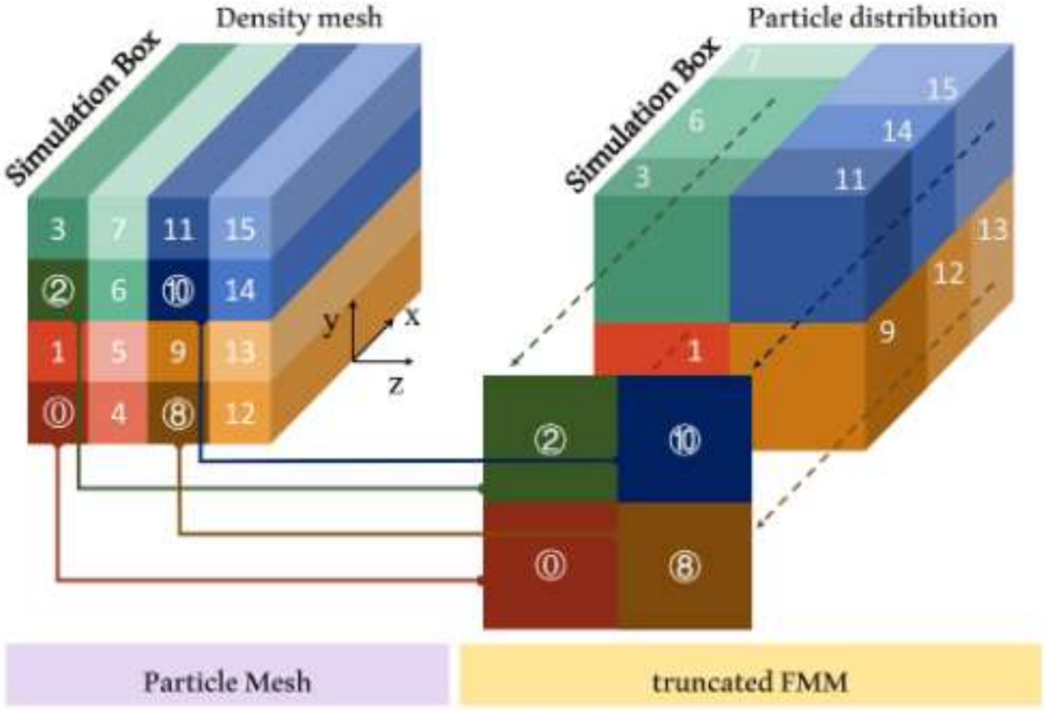


实测峰值性能~ 49%, 平均性能 ~ 36.5% [Q.Wang & C. Meng, 2021]

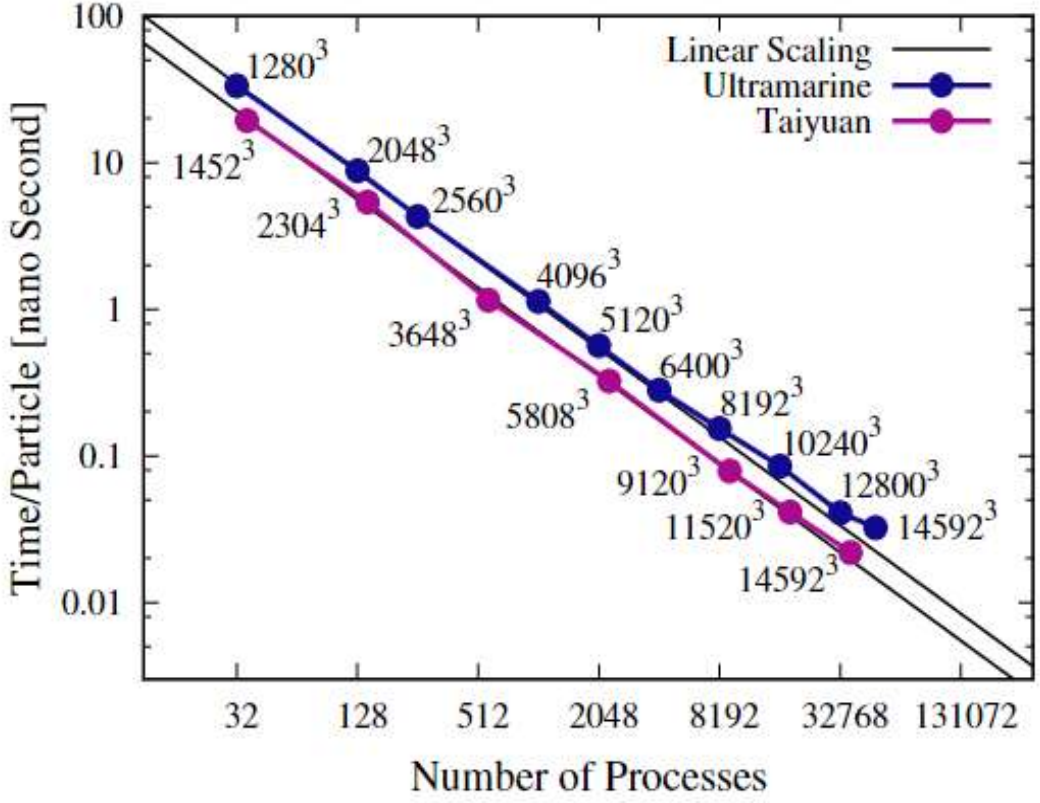
2.通信与区域分解的优化

- PM 和 FMM 的分解算法中，使用了不同的区域分解来实现
- PM 求解器执行数据和计算任务的分解
  - ✓ 对应Pencil状密度网格
  - ✓ 调用2DECOMP&FFT 库计算并执行 FFT 的全局通信
- FMM采用3D分解，优先进程组内的内存占用量均衡
  - ✓ 同组内的进程与硬件资源的绑定同样保持局部性，因为在不同的网络拓扑结构下，进程和计算资源的映射对通信性能至关重要

2.通信与区域分解的优化

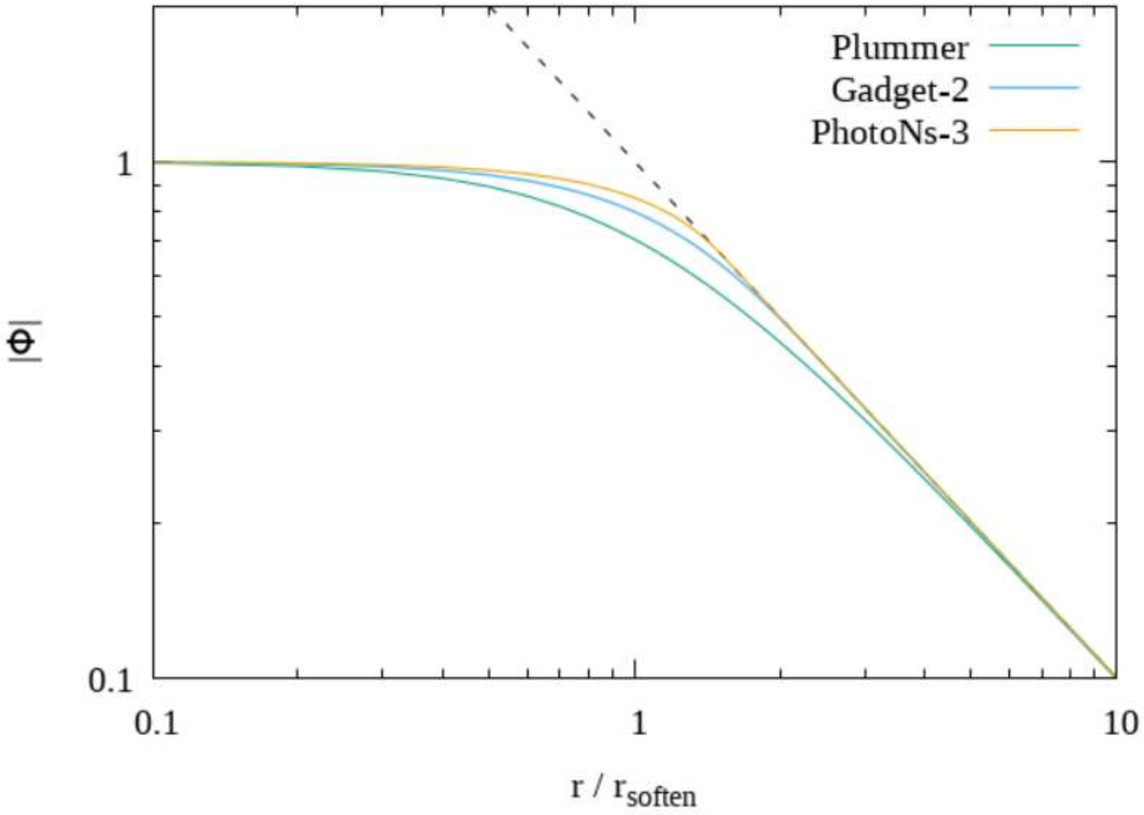


图表 4: 并行框架与区域分解 [Wang et al. 2022 MNRAS]



Wang, gao, meng, 2022

Softening of Gravitational force



Gravitational potential in Plummer, Gadget-2 and PhotoNs-3, respectively.

Gravitational force goes back to inverse-square law when r>1.5 Rsoft and it is proportional to r when r<1.5 Rs.

$$g(r) = \begin{cases} -G/r^2 & (r > \epsilon) \\ -Gr/\epsilon^3 & (r \leq \epsilon) \end{cases},$$

where $\epsilon = 1.5R_s$.

error in PM-FMM

Multipole Acceptance Criteria

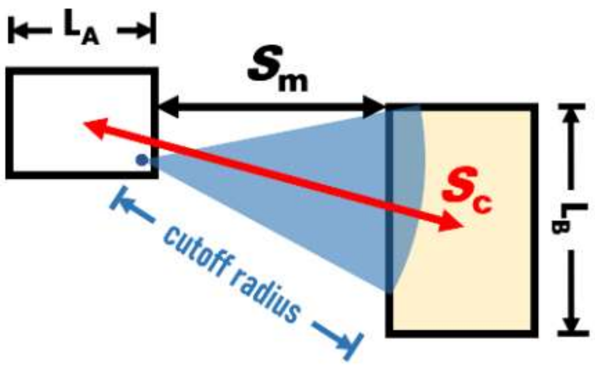


Figure 3: Multipole Acceptance Criteria. L_A is side length of sink (targeted) tree cell and L_B is the source one. The red arrow is the separation S_c between the centers of two nodes and S_m is minimum distance between tow boundaries of tree cells. Two boxes are still physically relevant despite S_c beyond the cutoff radius.

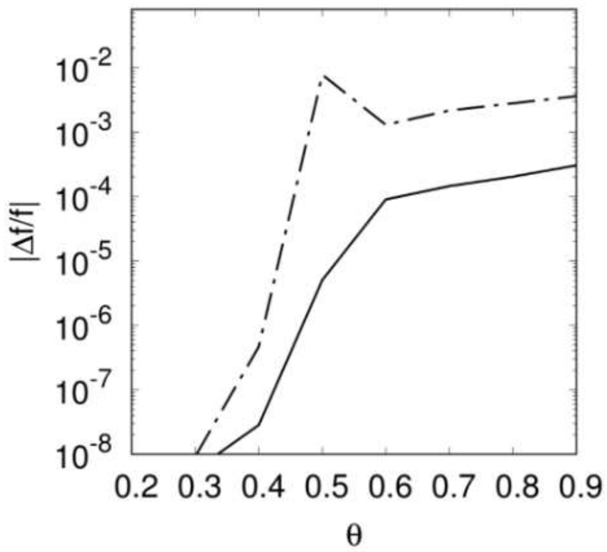
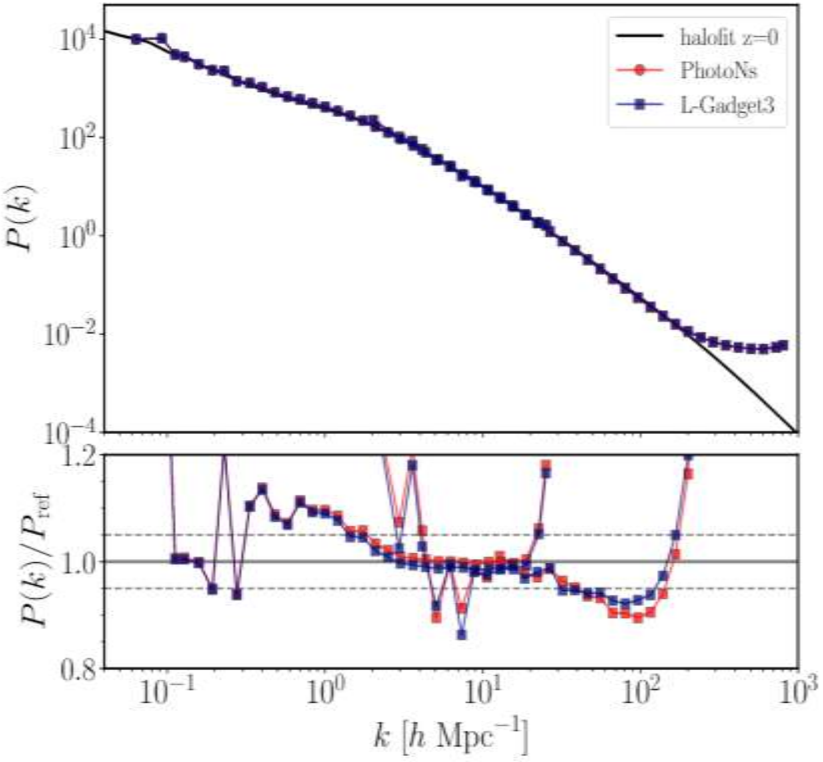


Figure 4: Relation of error to opening angle. Relative error of gravity or acceleration is calculated via truncated FMM upto hexpole. The solid curve denotes the rms error and dash-dotted curve denotes the maximum error of all particles.

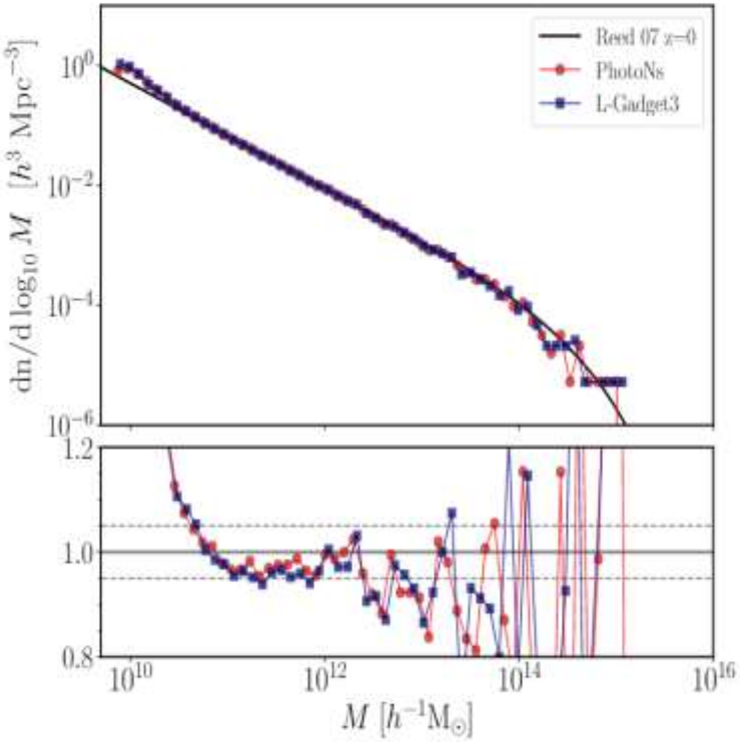
Wang Q, 2021

与L-Gadget3比较测试PhotoNs-3的计算精度和数值收敛性

- 使用相同的IC同时运行768^3，box=120Mpc/h模拟，比较两点相关和物质功率谱
- 不同程序之间P3/G3,在大尺度（k ≦ 1）上<2-3‰的差别，在k≦10的尺度上<1%，与Gadget4的比较有类似的结构。



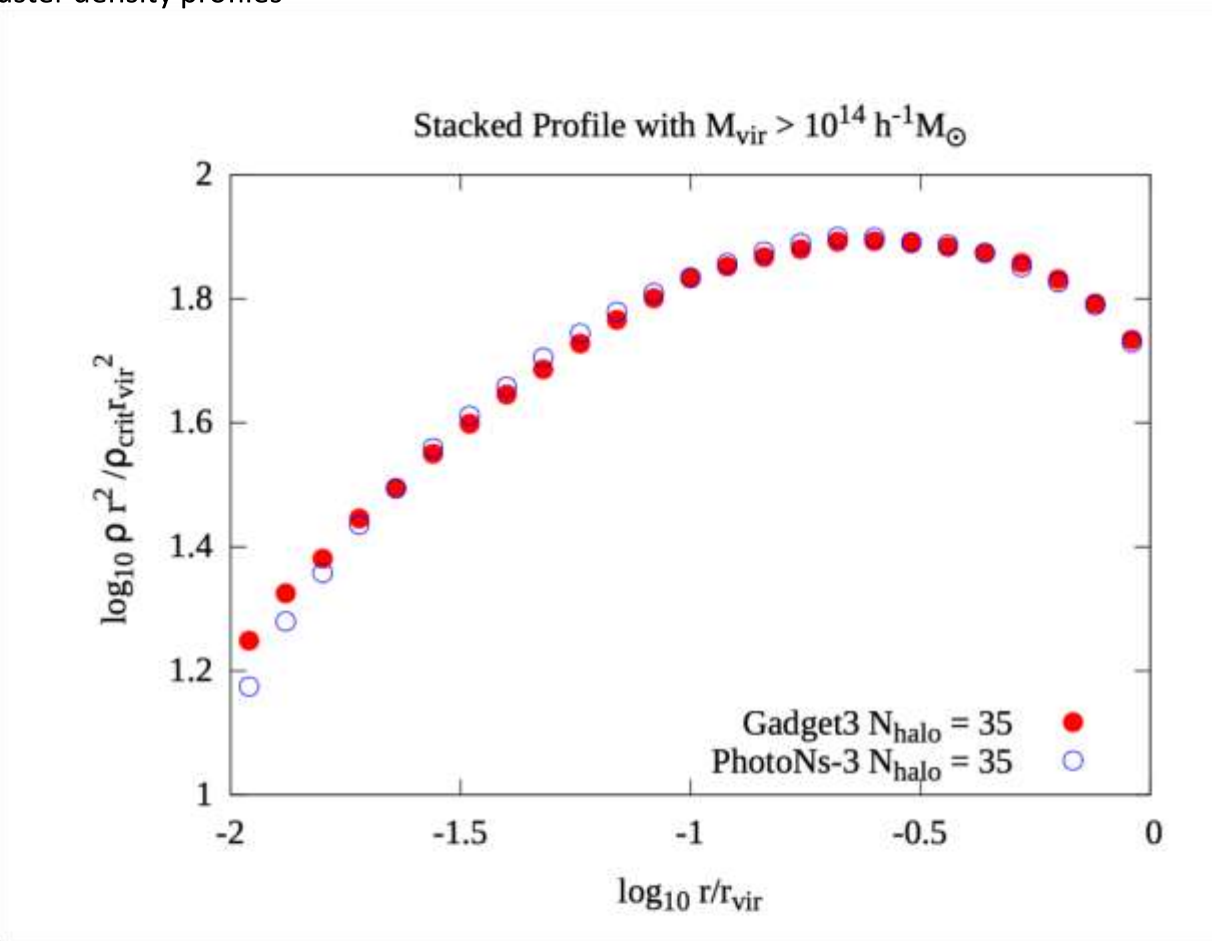
物质功率谱



暗晕质量函数

Comparison between PhotoNs and Gadget

Stacked cluster density profiles

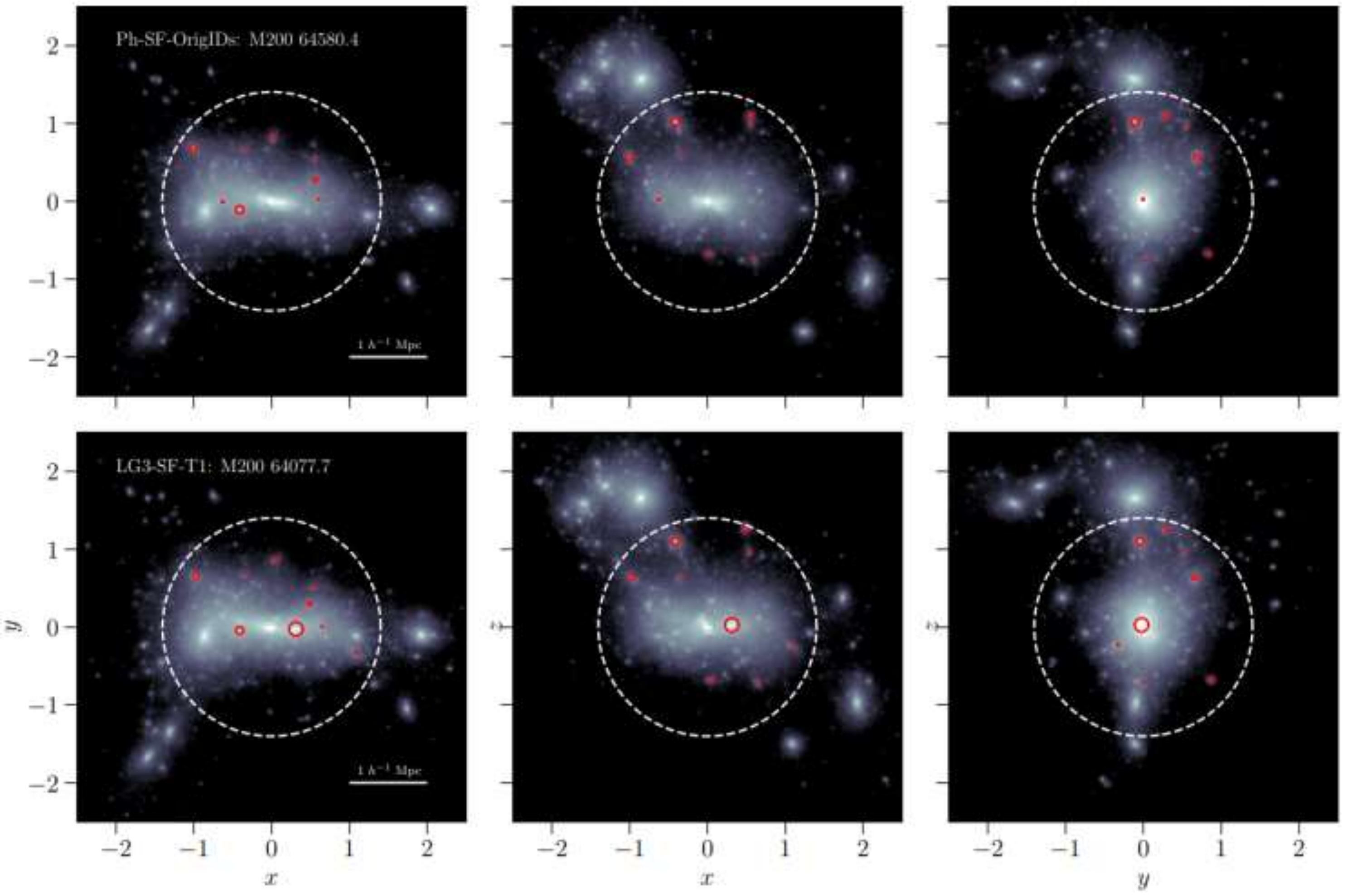


768^3 particles + 125Mpc/h

Comparison between PhotoNs and Gadget

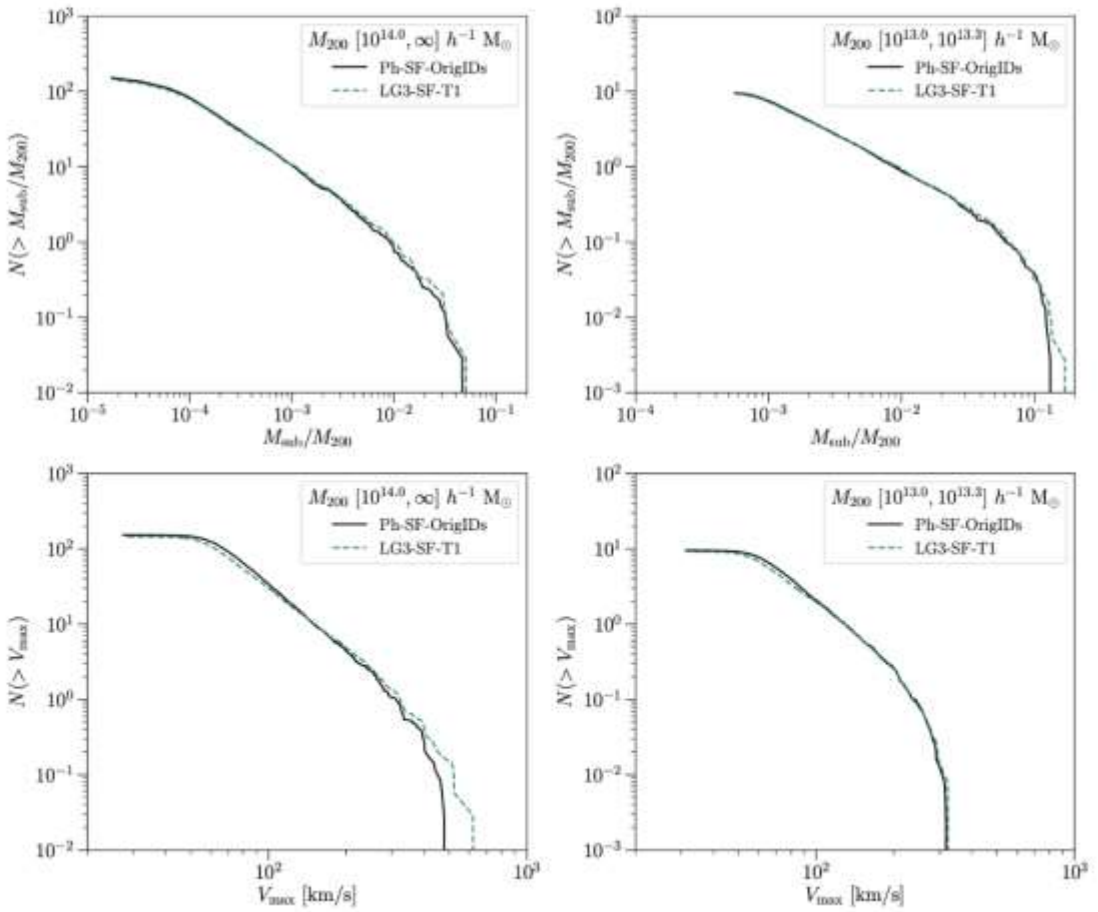
Projections of top 10 most massive subhalo in the most mass cluster

768^3particles + 125Mpc/h



Comparison between PhotoNs and Gadget

Subhalo mass functions



768^3 particles + 125Mpc/h

Hyper-Millennium run

Large volume + high resolution (z = 20 —0, 100 snapshots)

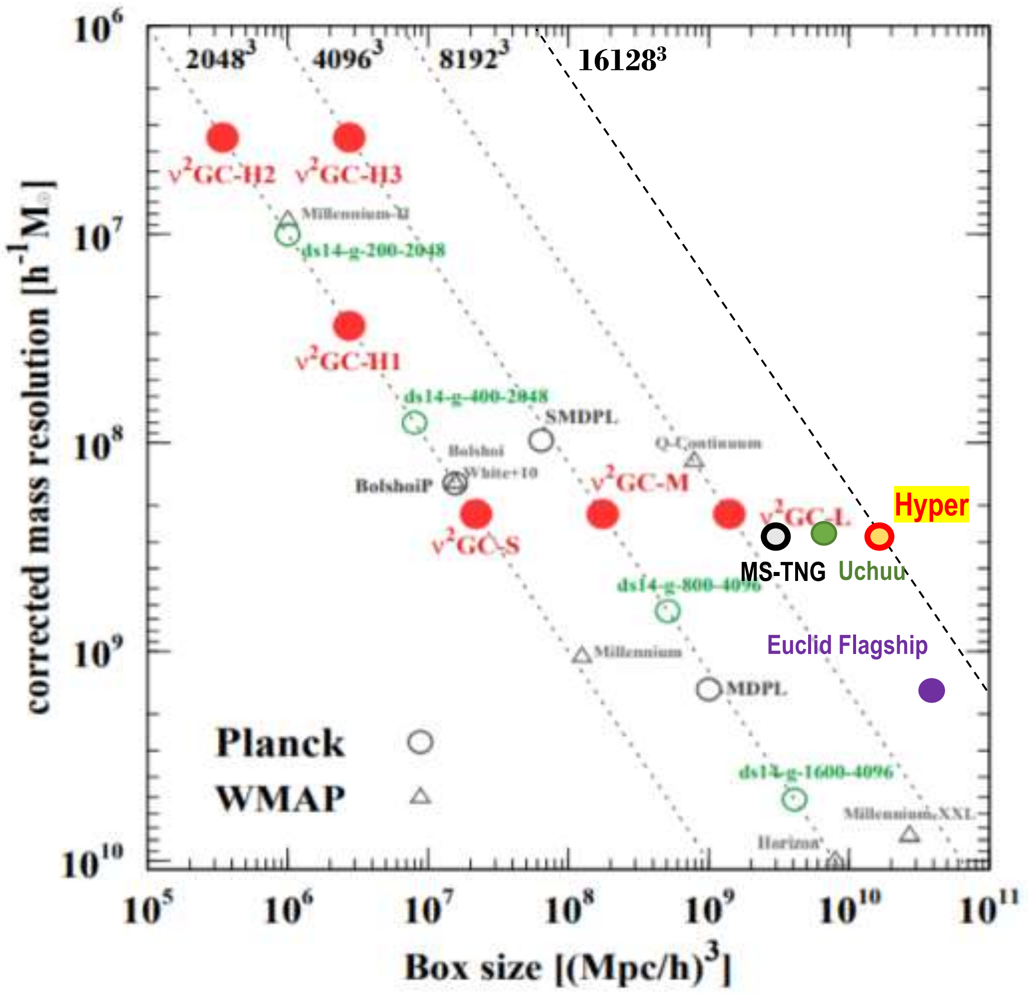
Ω_m	0.3111
Ω_Λ	0.6889
Ω_b	0.0490
h	0.6766
σ_8	0.8102
n_s	0.9665

	Hyper-Millennium
Volume	$2.5^3[h^{-3}\mathrm{Gpc}^3]$
Particles number	$16128^3 \sim 4.195 \times 10^{12}$
Particle mass	$3.21 \times 10^8 h^{-1}\mathrm{M}_\odot$

Largest ever N-body cosmological simulation

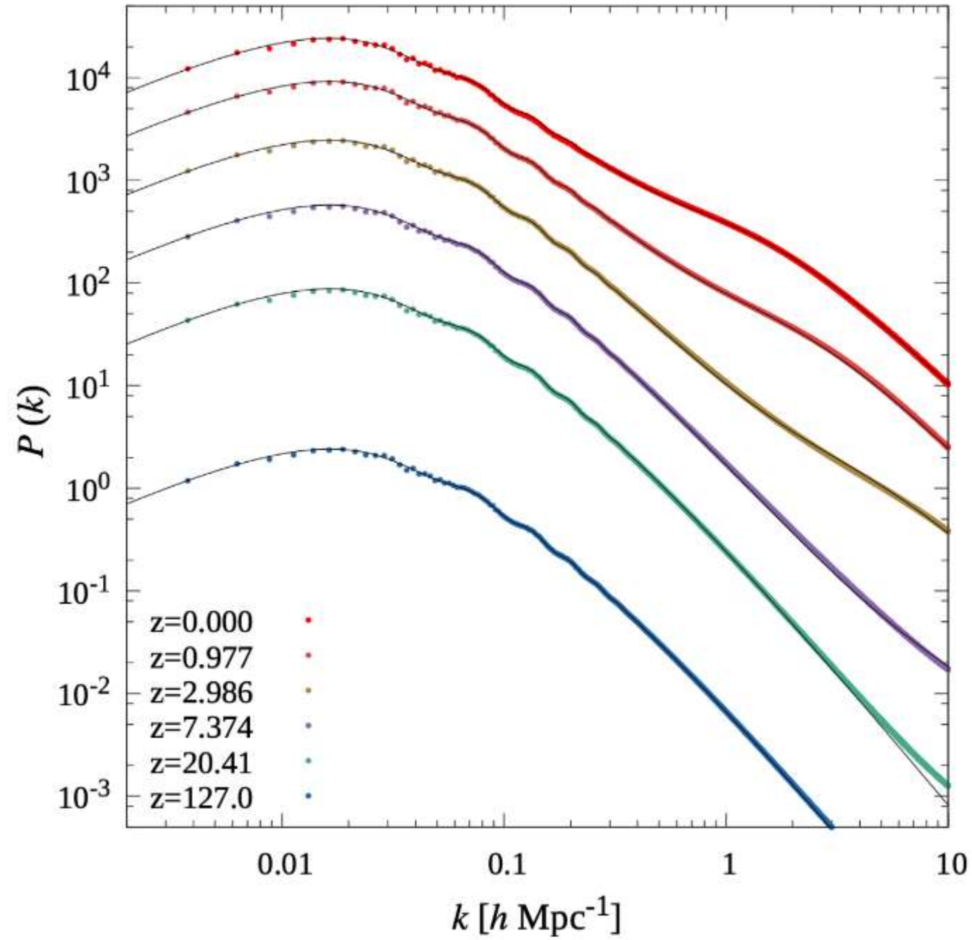
Volume is 125 times the Millennium simulation and the resolution is higher by a factor of 3

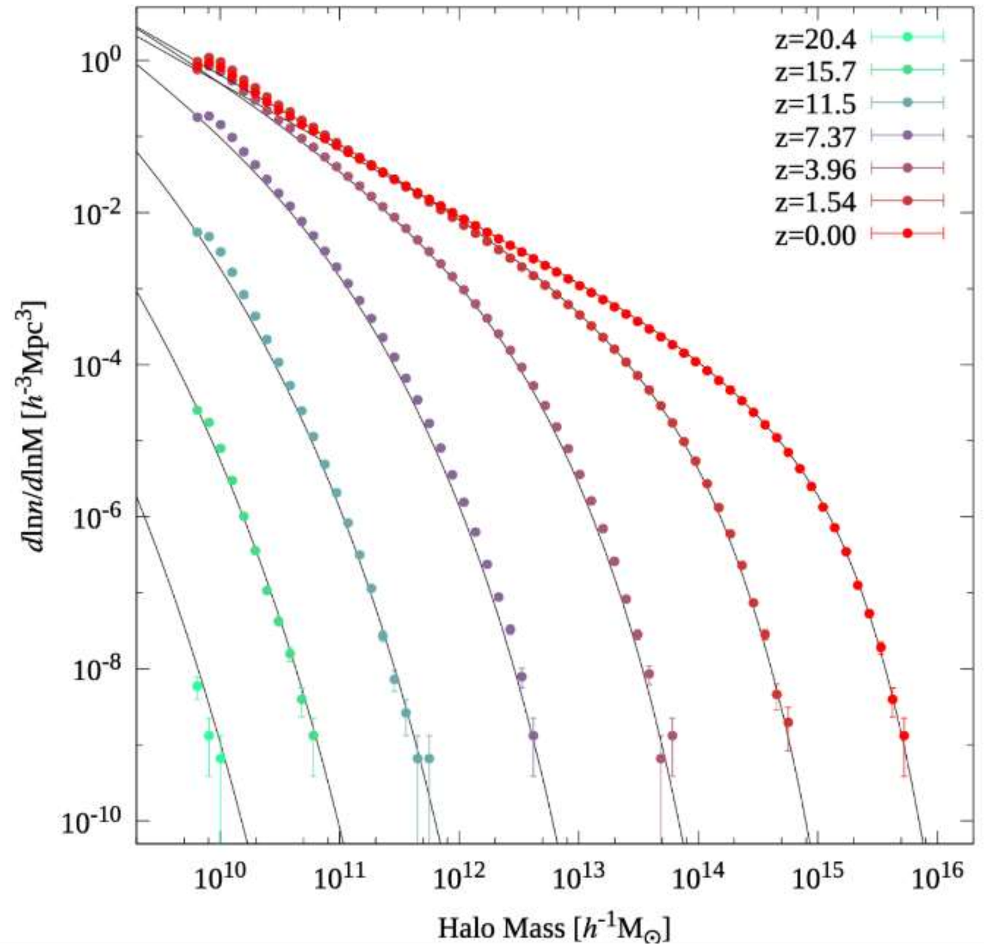
Hyper-Millennium run



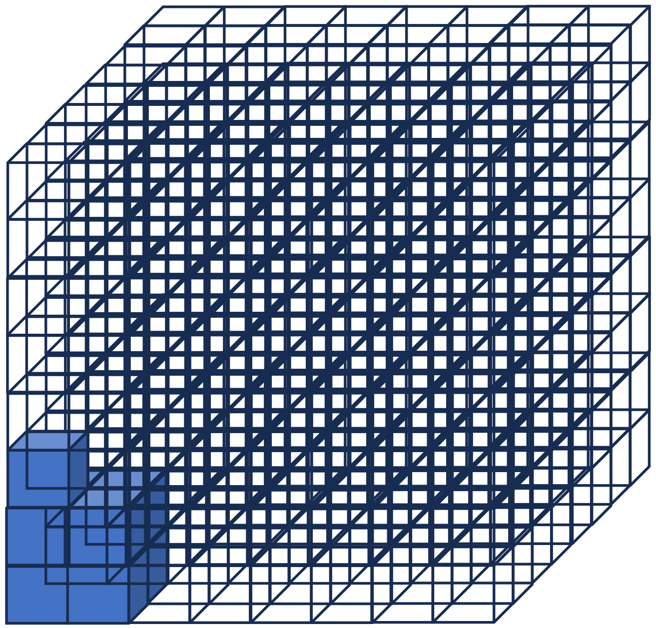
- 东方一号运行墙钟时间17.5天，13 PB的输出

Hyper-Millennium: Power specturm and the halo mass functions





Distributed data Post-processing



Codes validations are nearly finished
Massive postprocessing will start very soon and should be completed in this August.

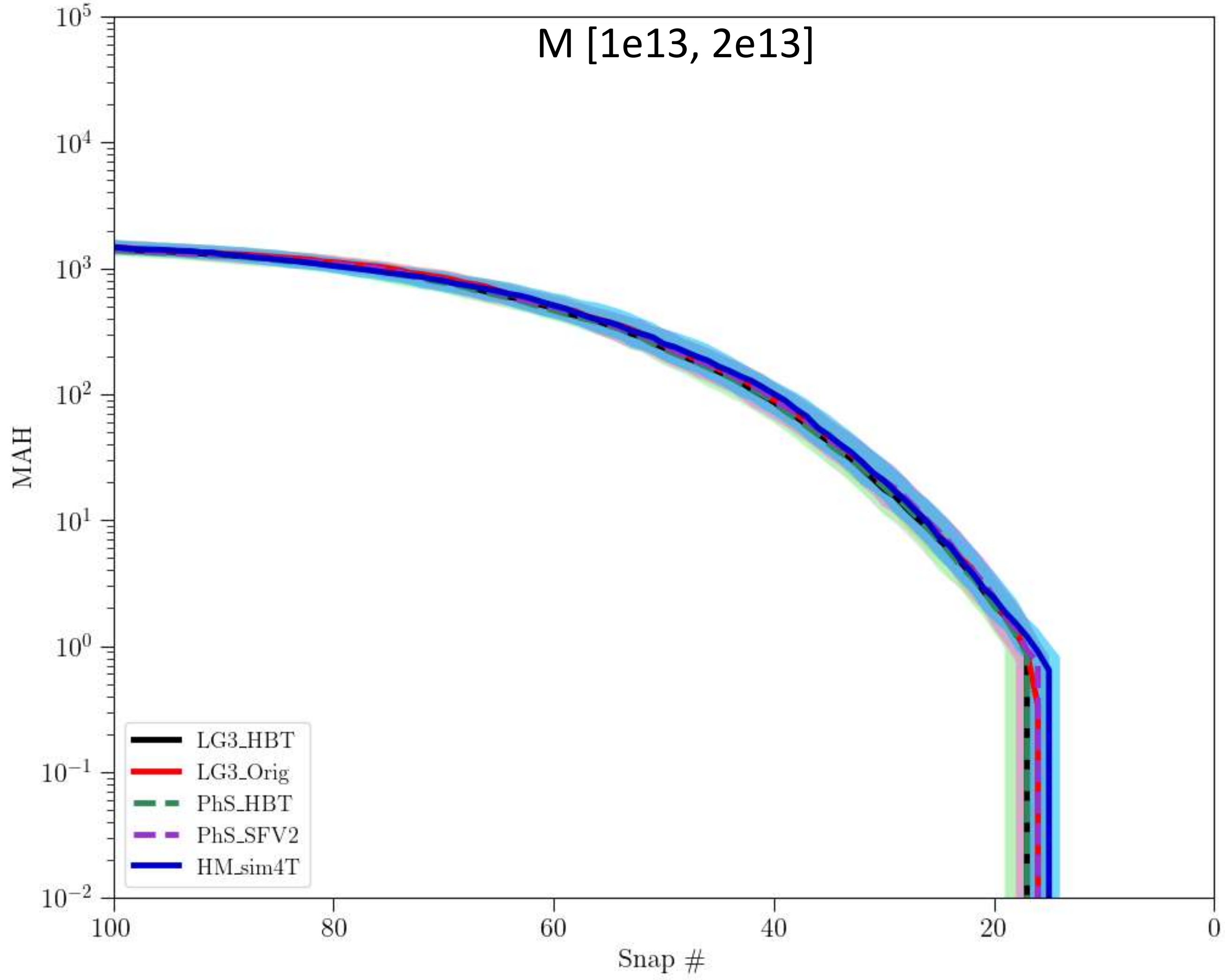
- Halo/subhalo are identified in $8 \times 8 \times 8$ =512 cubes (330Mpc/h on a side)

- Only inner 300Mpc/h are used. The cubes are combined later to obtain the complete catalogues/merging trees in the whole volume

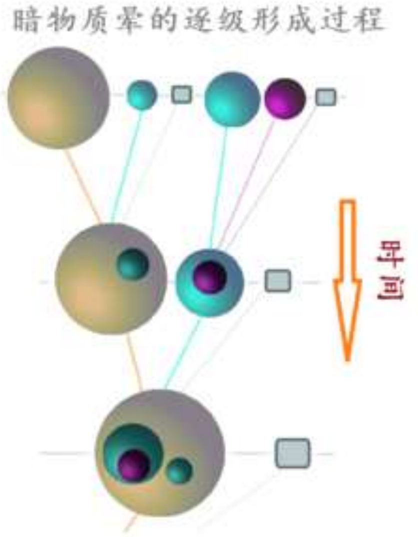
- In each cube, ~1TB for halo+subhalo catalogues in format of hdf5. ~500TB in total.
- MPA-tree ~50 TB

  Aux file ~ 350 TB

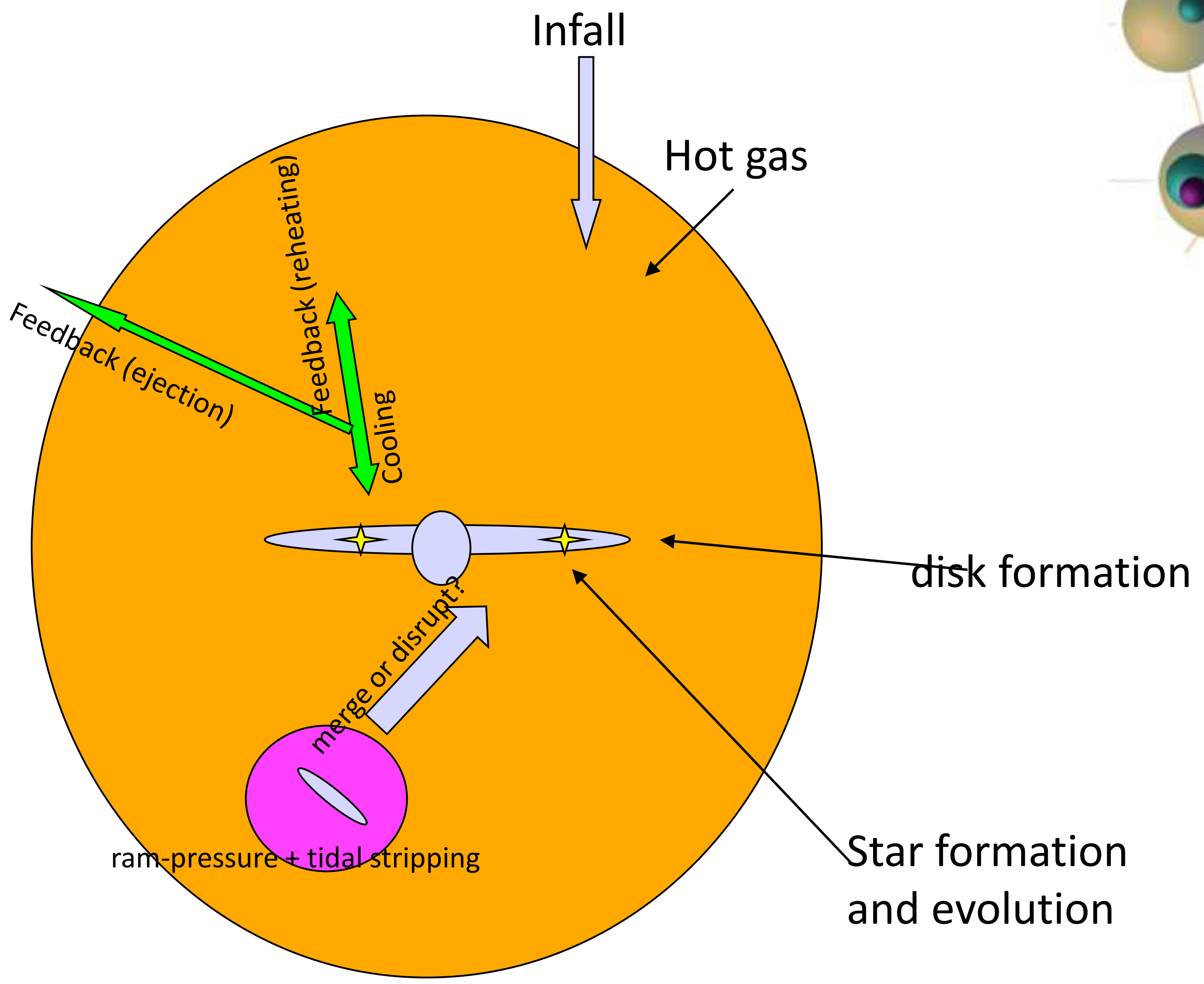
Halo Mass Accretion History



Galaxy formation models

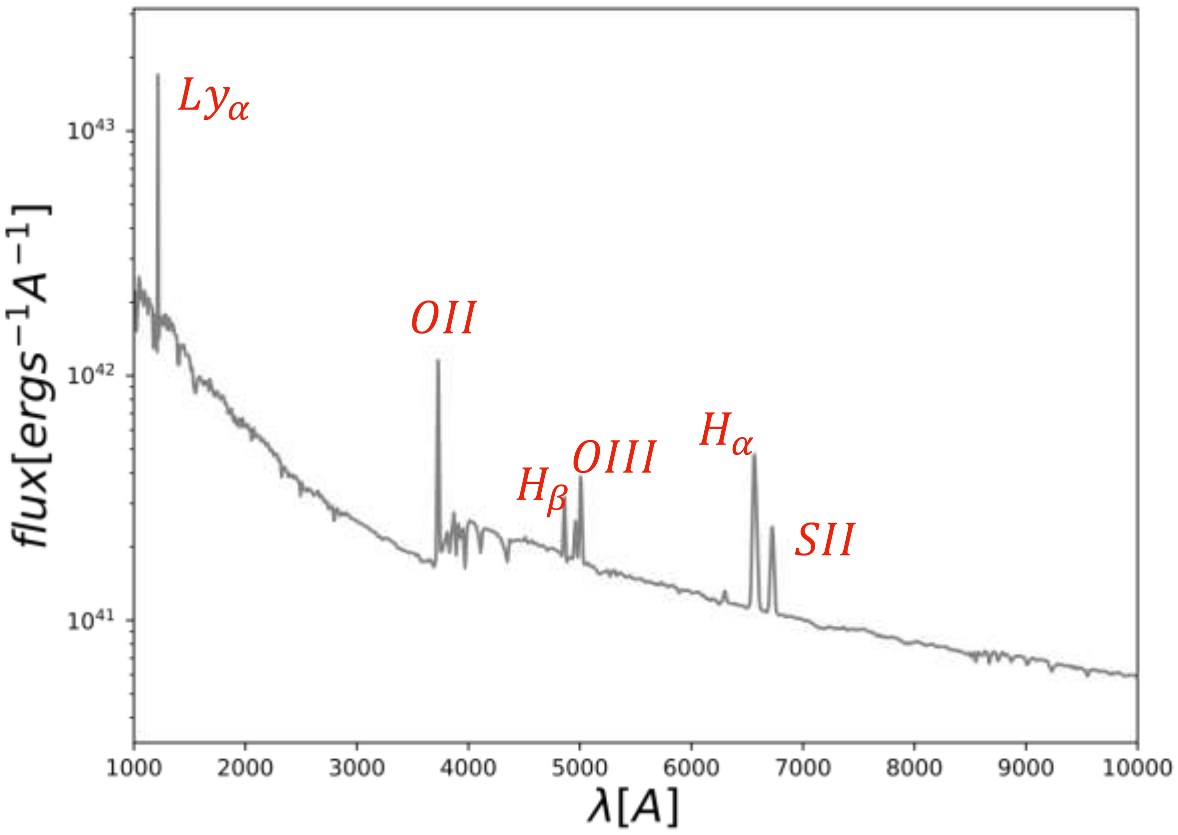


http://galformod.mpa-garching.mpg.de/mrobs/private/china.jsp



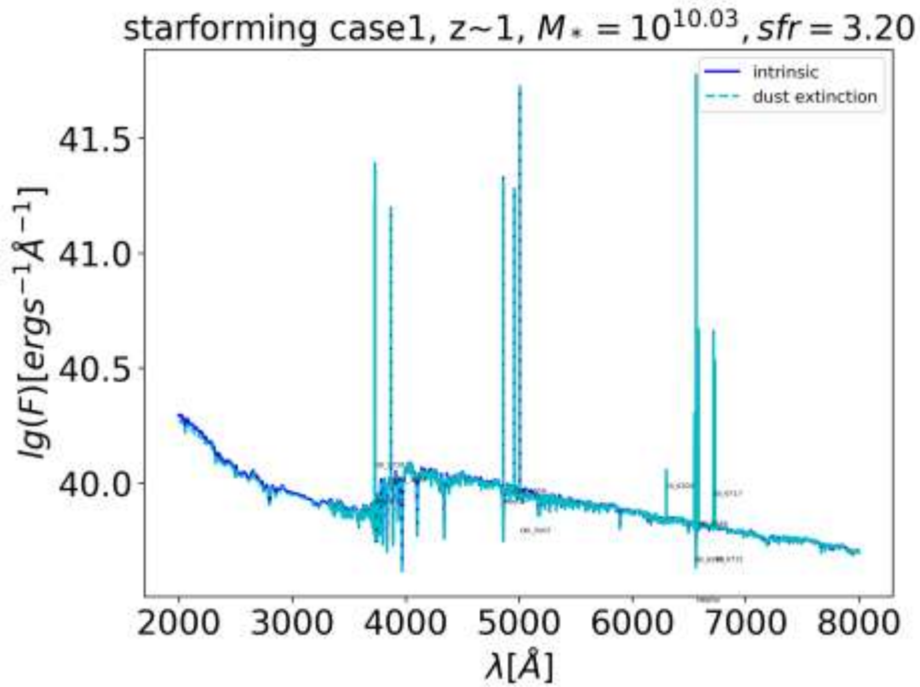
- Emission lines
  - Line ratios - CLOUDY13.03
    - geometry
    - chemical content
    - ionizing spectrum
    - metallicity (Z)
    - ionizing parameter (U)
    - Hydrogen density (n_H)

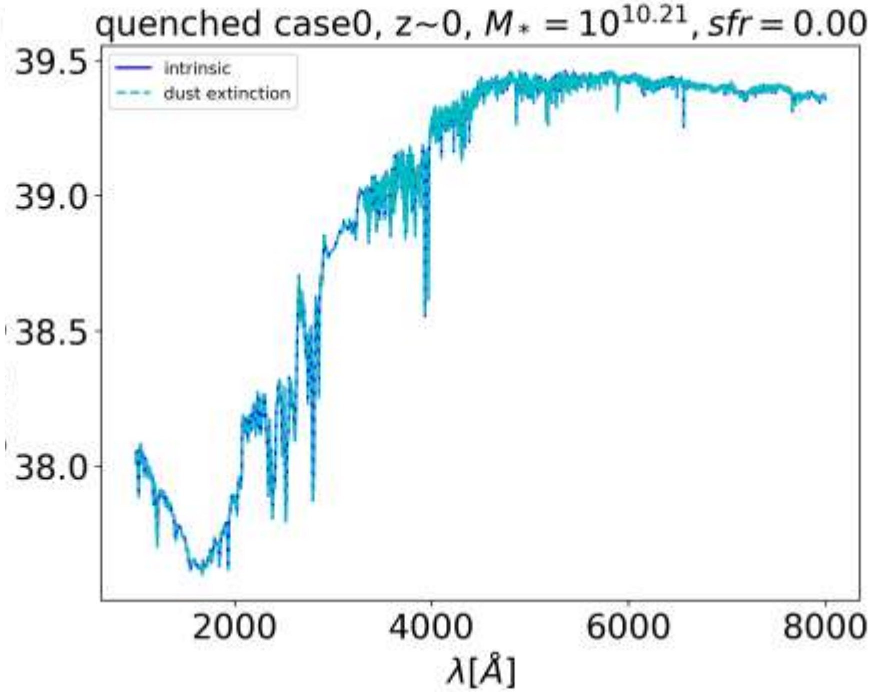
star forming galaxies at z~0



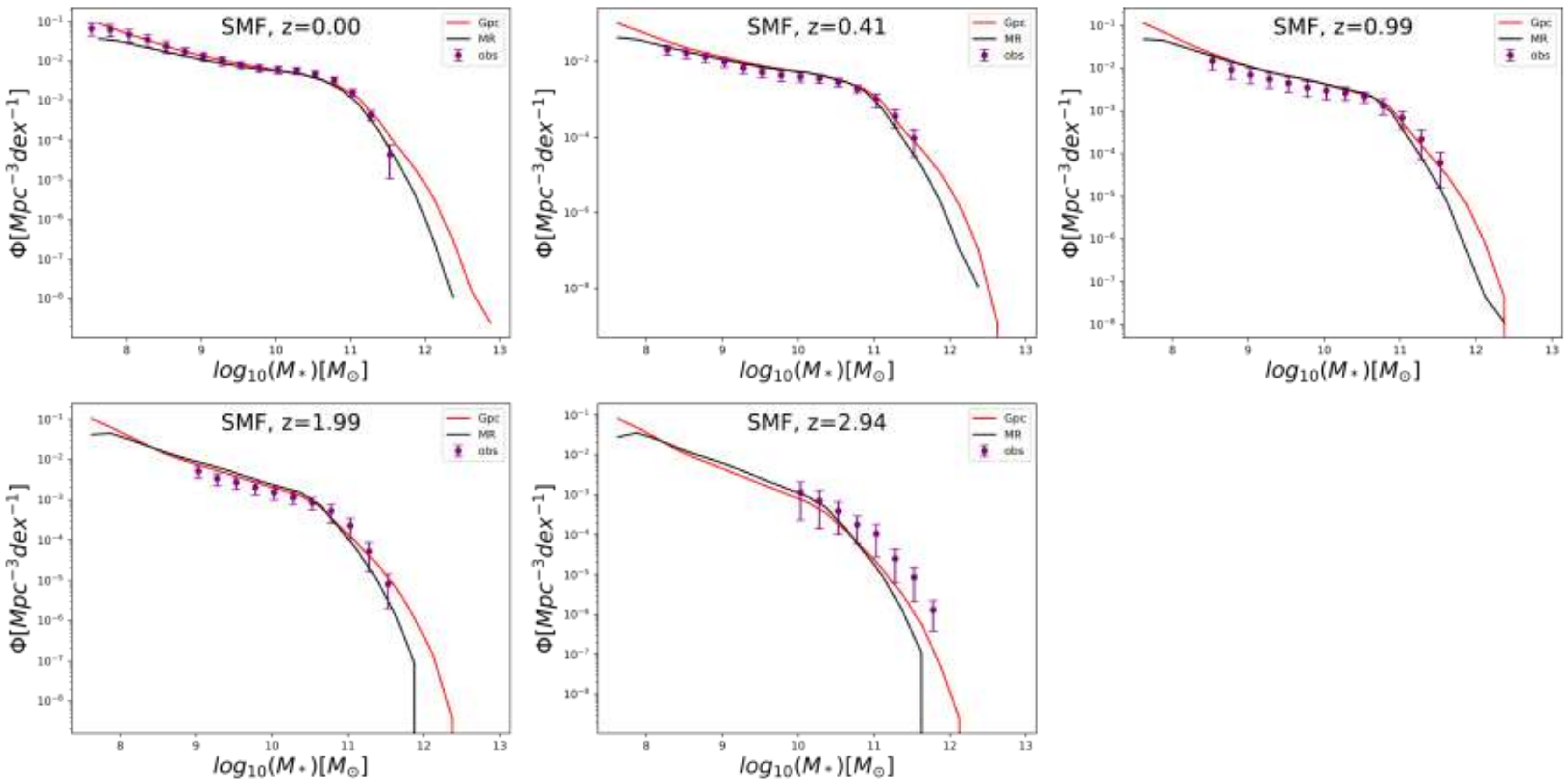
Wenxian Pei

Full Galaxy Spectrum

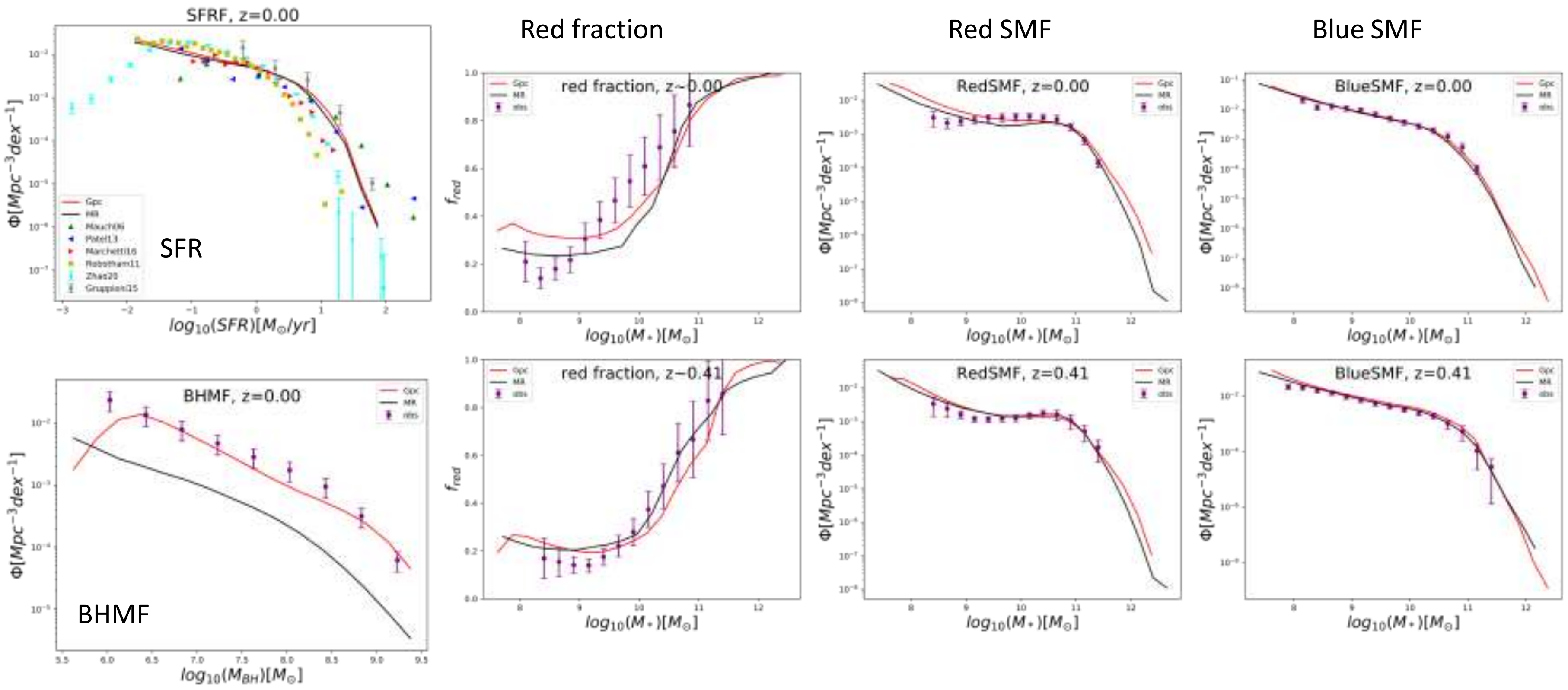




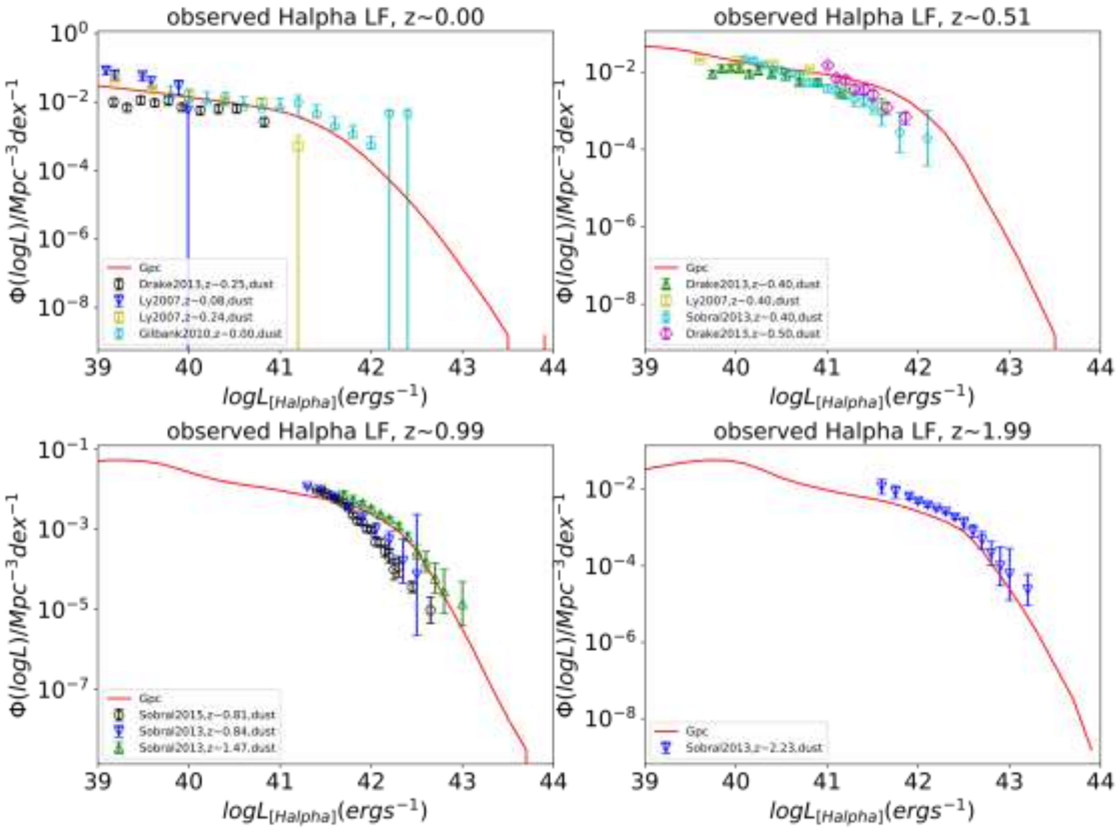
Reproduce stellar mass functions z=0—3



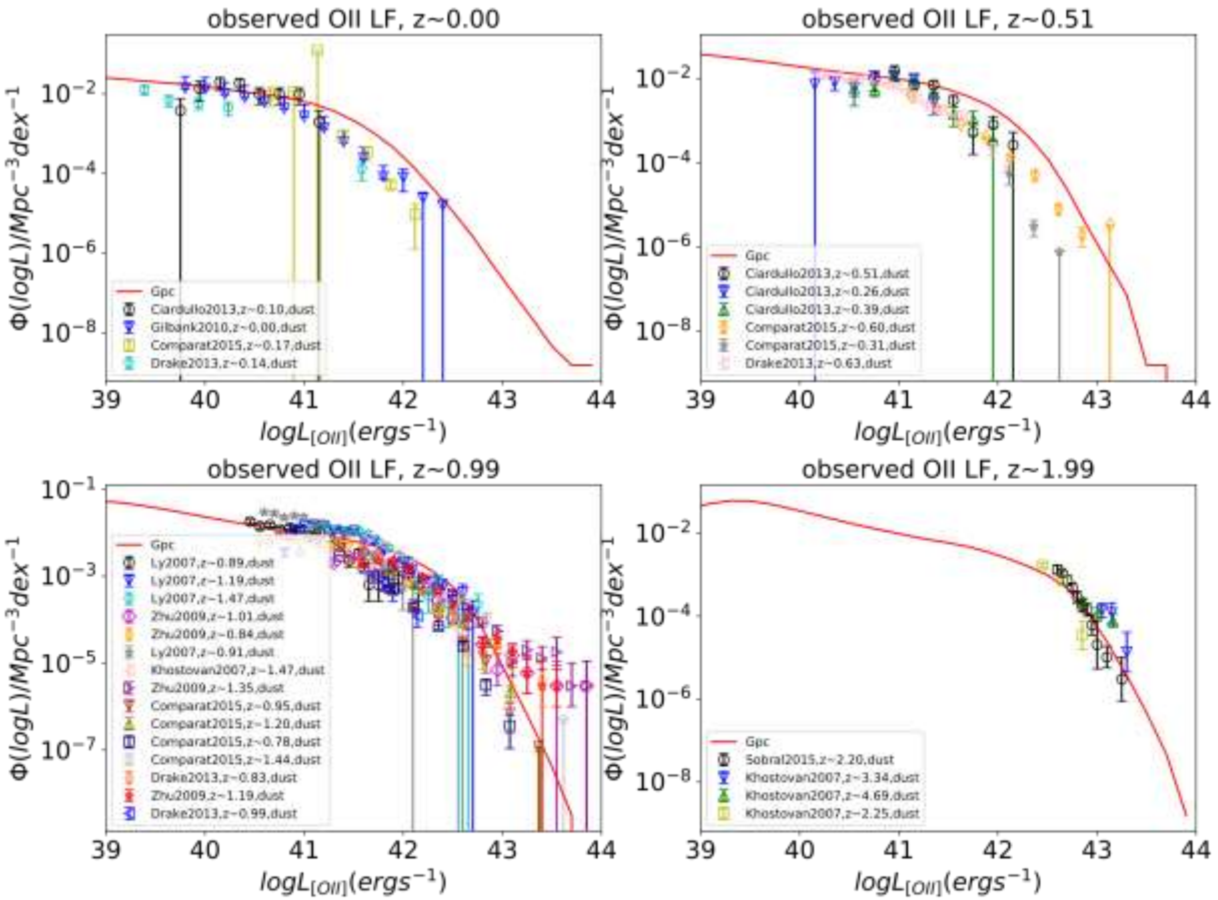
Reproduce various galaxy properties



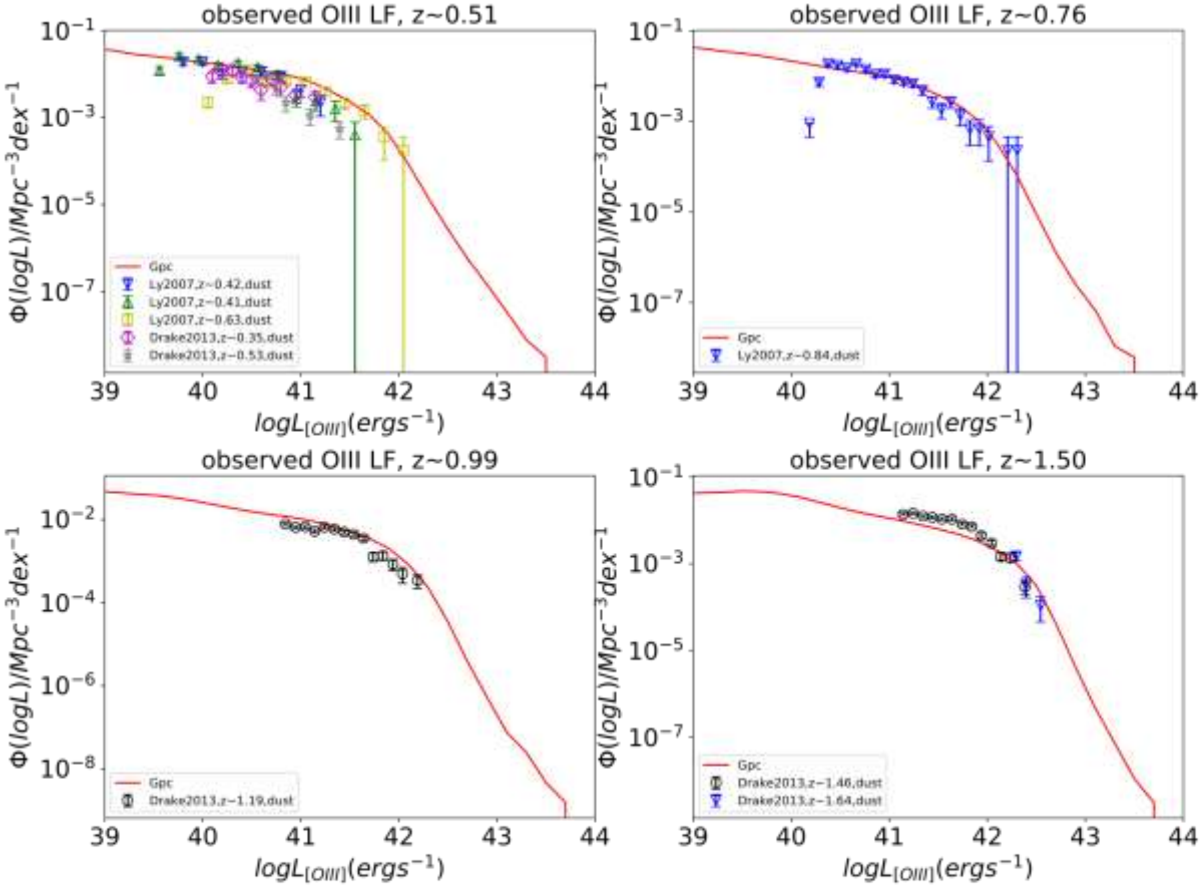
H_α Luminosity Function z=0—3



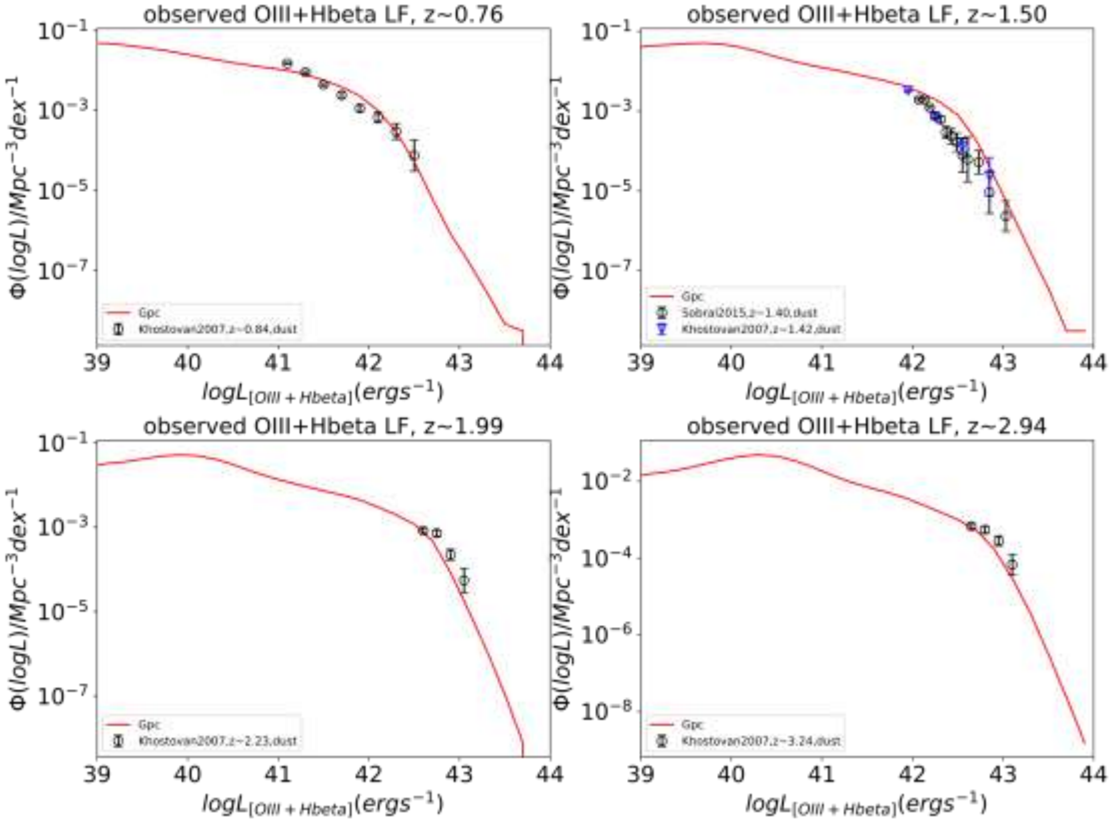
OII Luminosity Function z=0—3



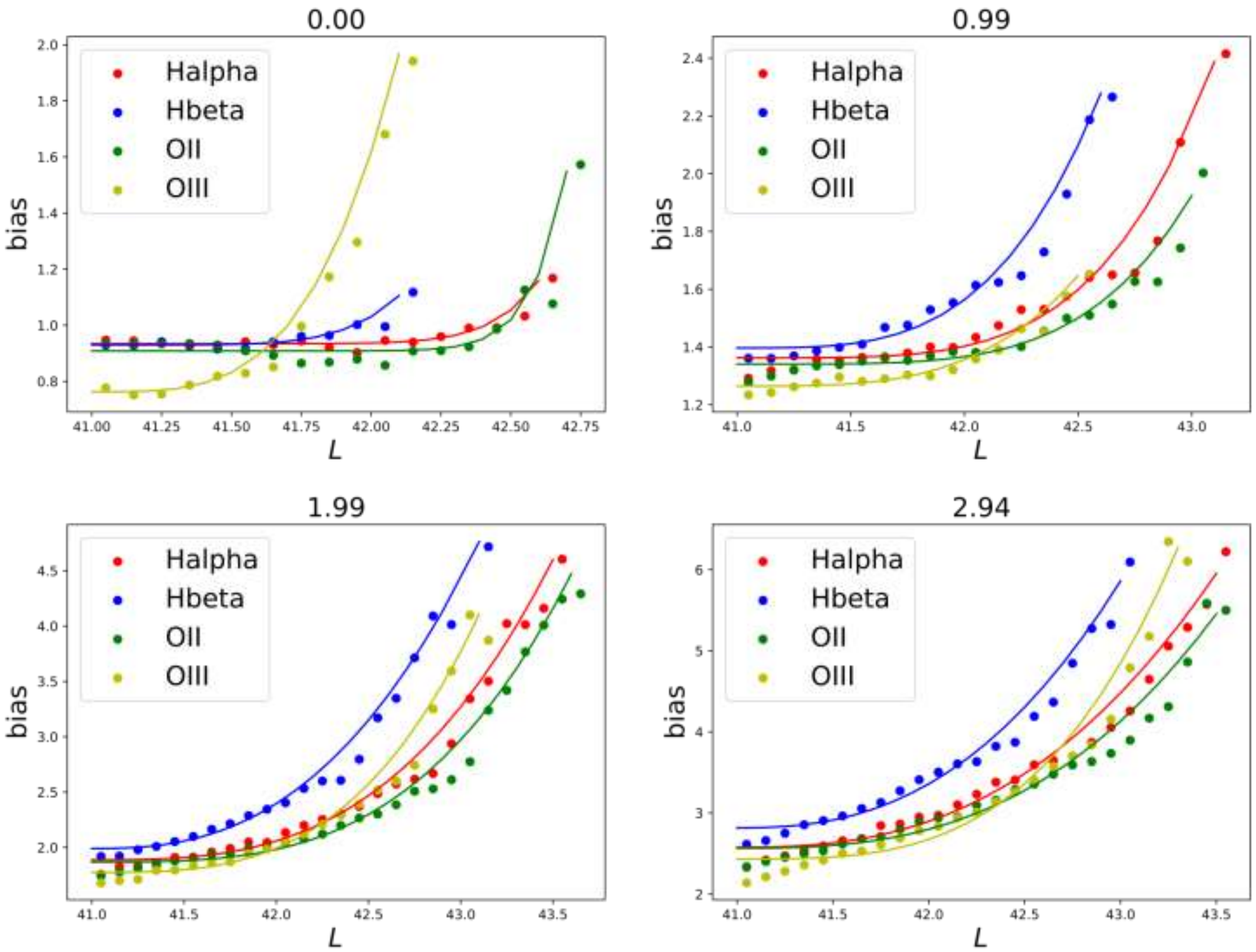
$OIII$ Luminosity Function z=0—3



$OIII + H_\beta$ Luminosity Function z=0—3



Bias as a function of luminosity and z



Summary

- Hyper—Millennium run--the largest ever N-body simulation

  4 trillion particles, $2.5^3 [h^{-3}\mathrm{Gpc}^3]$, particle mass 3.2d8Msun/h

- Improved Munich semi-analytical galaxy formation models
  - Convergence issue fixed
  - Ionization model + radiation transfer (galaxy emission lines)
  - Succeed in reproducing local and high redshift galaxy properties, especially including emission line luminosity functions of Halpha, Hbeta, OII, OIII, and AGN luminosities
- To come…
  - Halo/subhalo catalogues, merging trees (before this September)
  - Mocks (galaxy, Lensing) …
- Science ….

  BAO, RSD, Weaking lensing and other large scale structure studies….

谢谢！ 请批评指正！

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NATIONAL ASTRONOMICAL OBSERVATORIES, CAS