



数值模拟与模拟观测

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Outline

1. Introduction

2. Collisionless N-Body Simulations

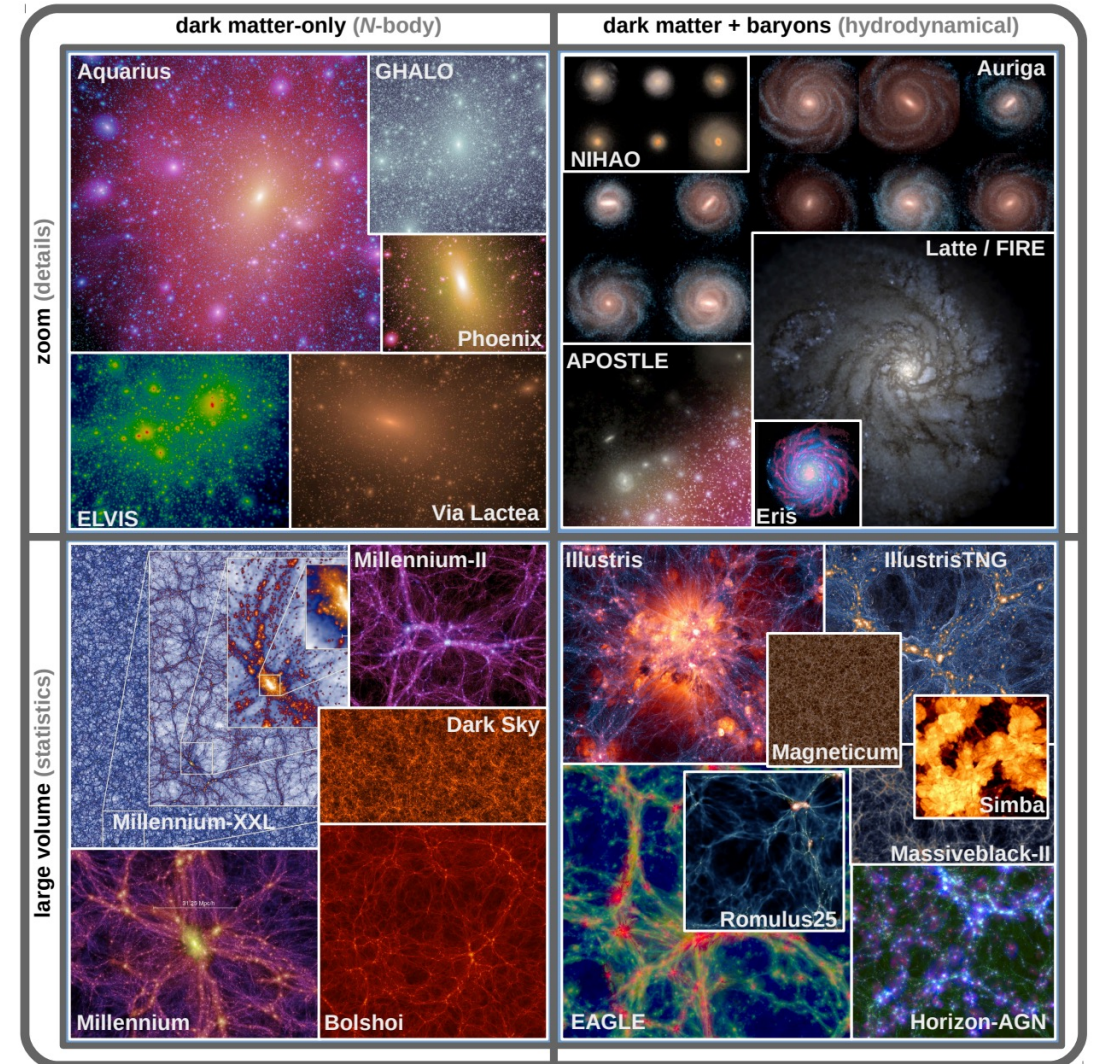
- Basic Idea
- Gravity Solvers & Parallelization
- Analysis, Success

3. Hydrodynamic Simulations

- Eulerian & Lagrangian solvers
- Baryonic Physics
- Analysis, Successes, Challenges

4. Mock Observations

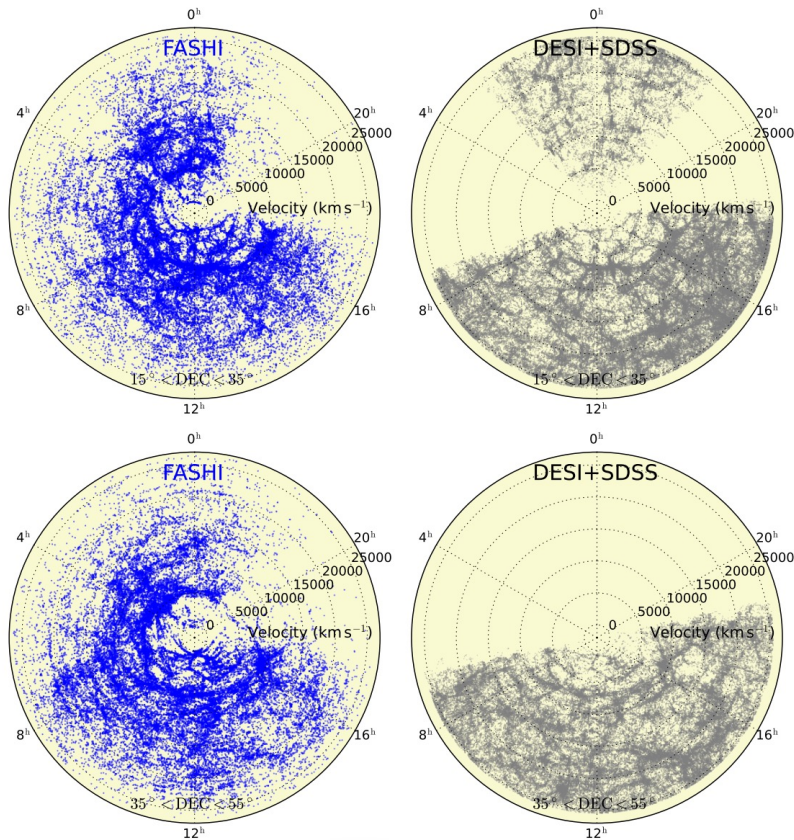
- Optical & HI



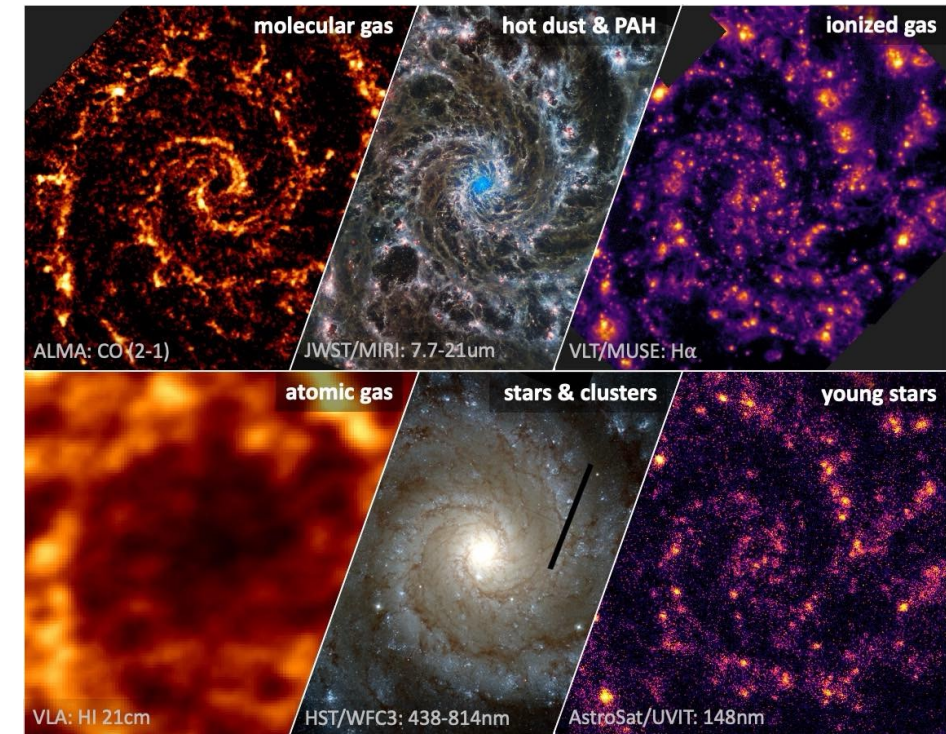
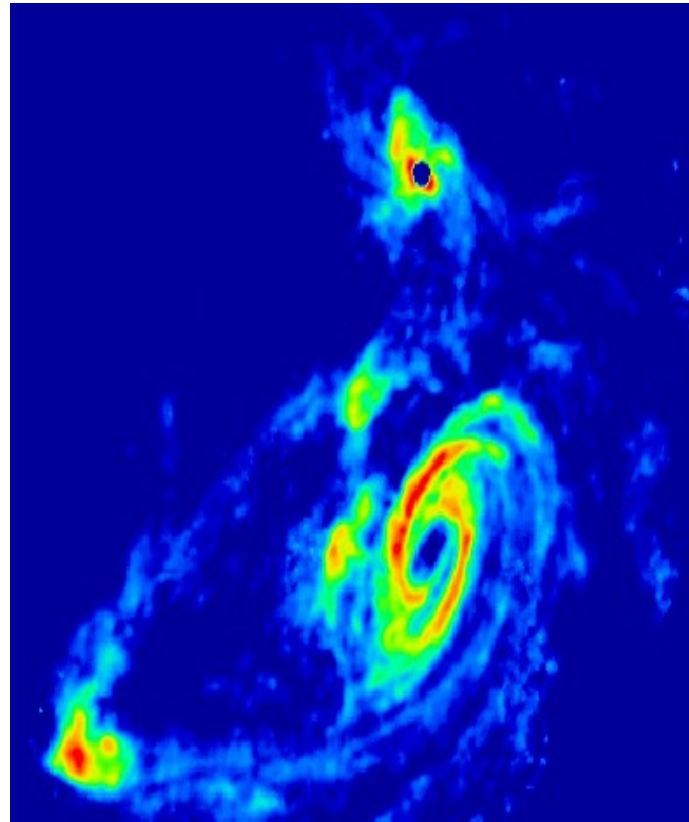
Vogelsberger et al. 2020

Introduction

HI星系观测是揭示暗物质属性、星系形成演化、宇宙重子循环的重要探针
观测结果蕴藏的物理过程与规律？



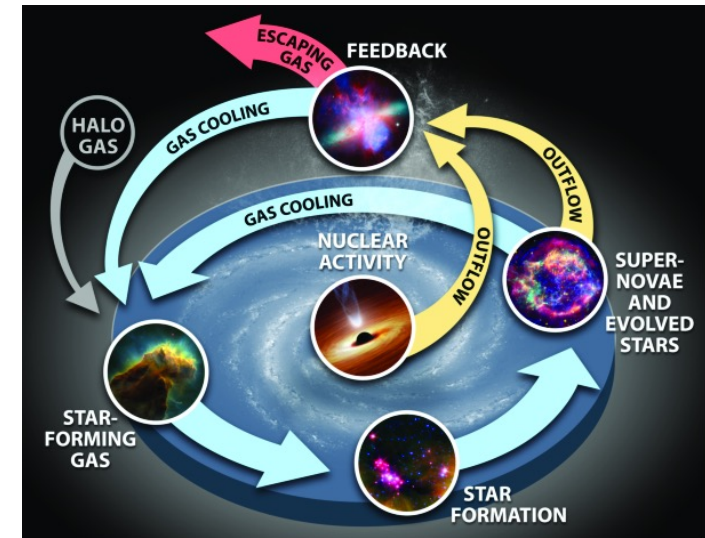
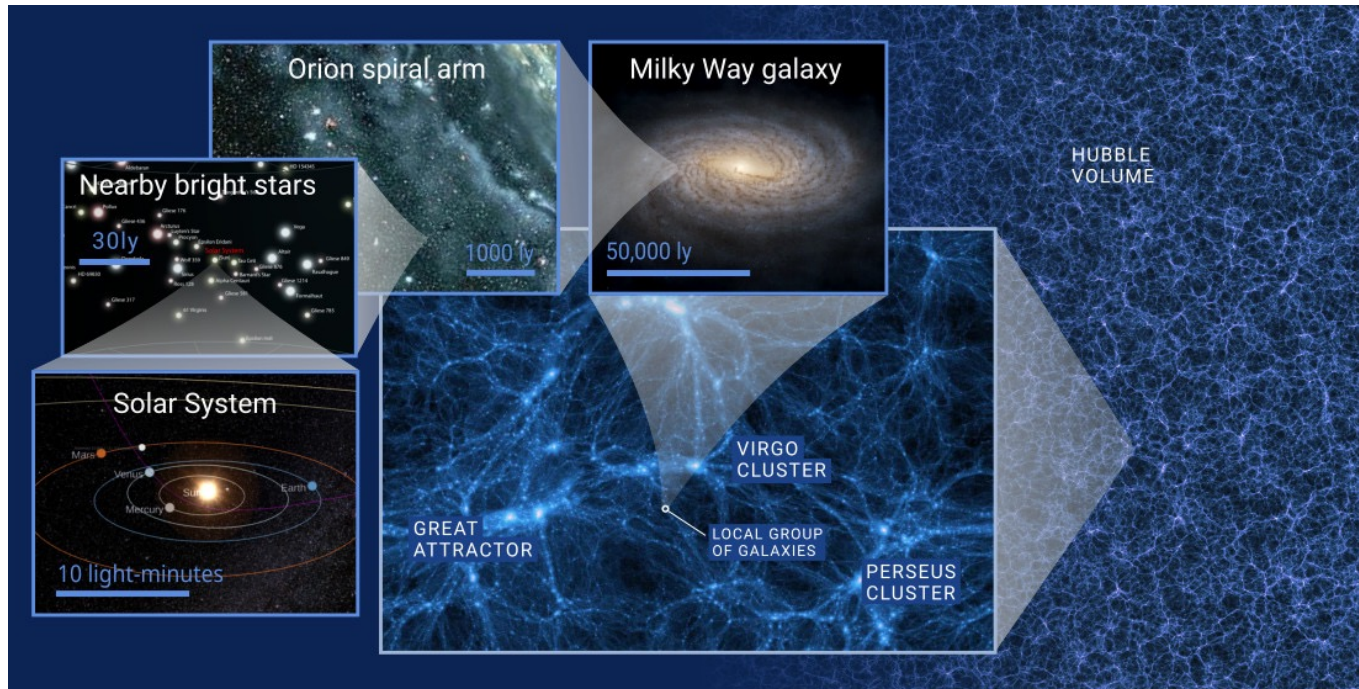
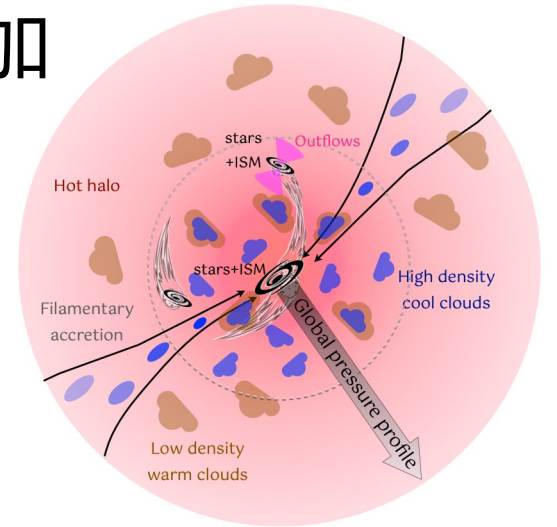
Zhang et al. 2026



Introduction

HI分布与动力学由宇宙网环境、暗物质势阱、气体冷却加热、恒星形成、恒星与黑洞反馈、相互作用等共同塑造：

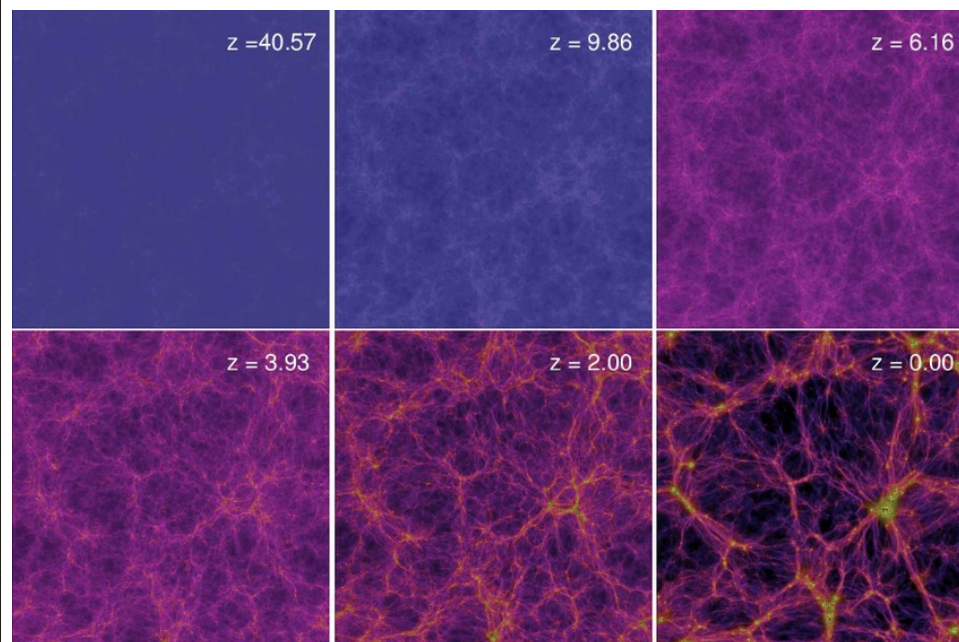
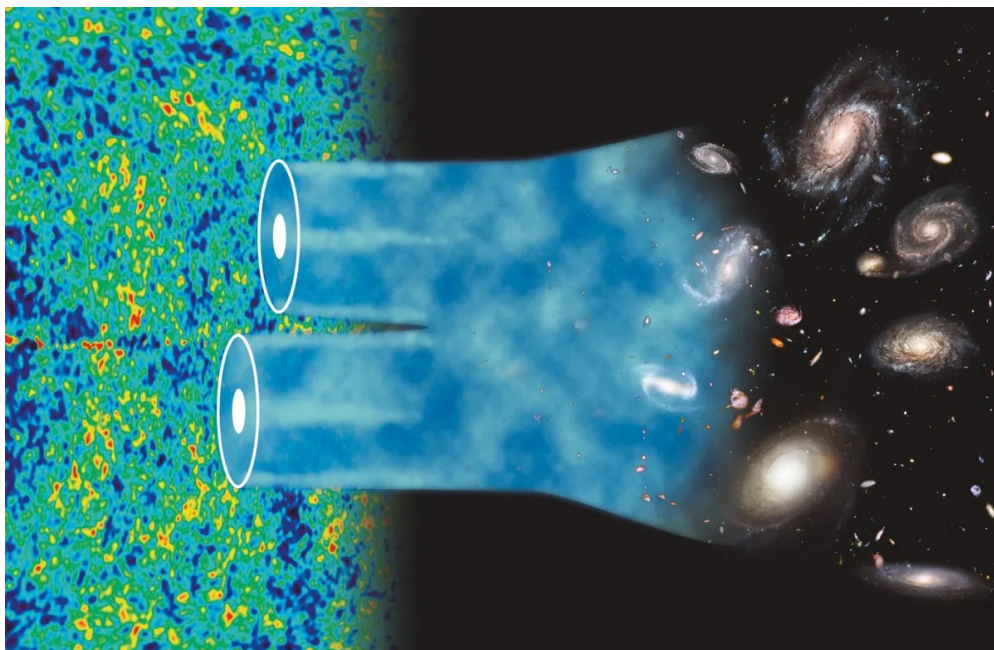
- 宇宙网、暗物质晕的形成演化
- 气体吸积，冷却凝聚，恒星形成，恒星与黑洞反馈
- 暗晕（星系）相互作用、并合



Introduction

➤ 宇宙网、暗物质晕的形成演化（引力主导）

引力驱动密度扰动发展到非线性阶段，演化出宇宙网络（暗物质与IGM）；
在高密区域产生脱离膨胀背景的引力束缚系统-暗物质晕



Introduction

➤ 暗晕中星系的形成与演化（引力与重子物理共同主导）

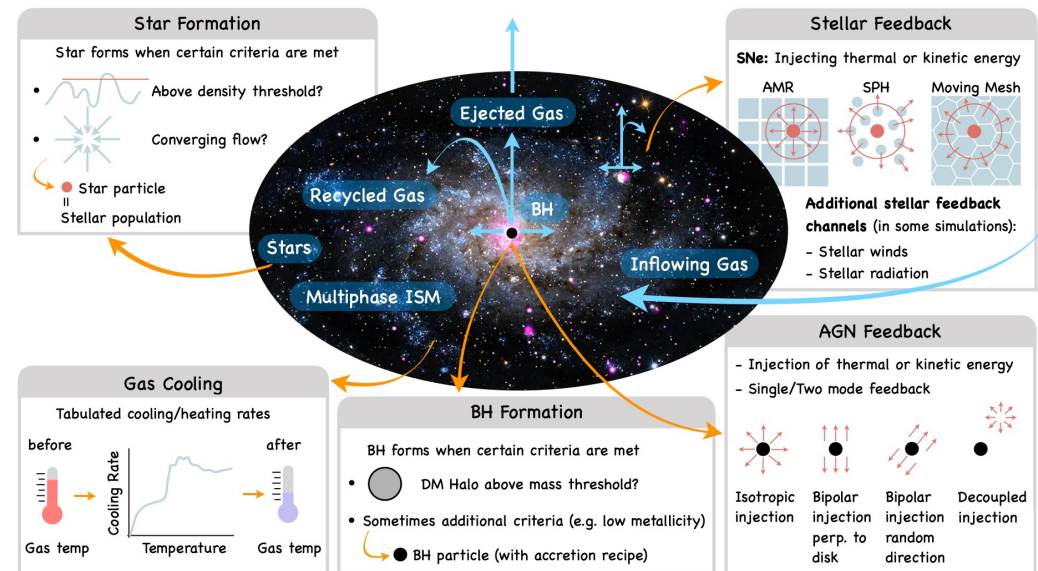
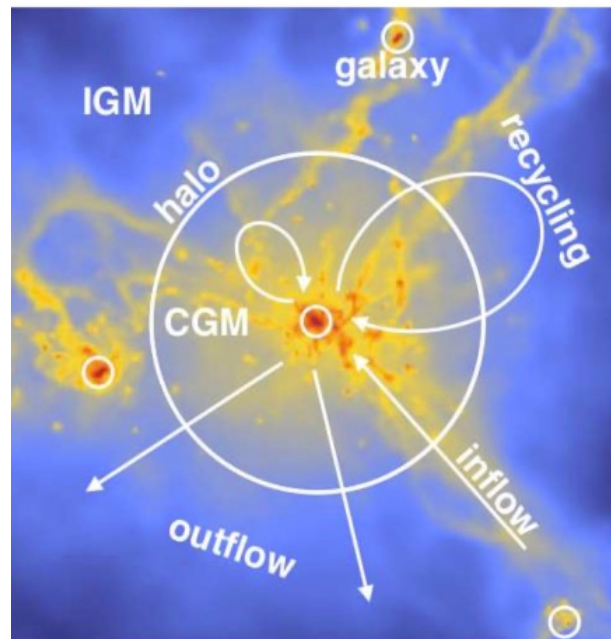
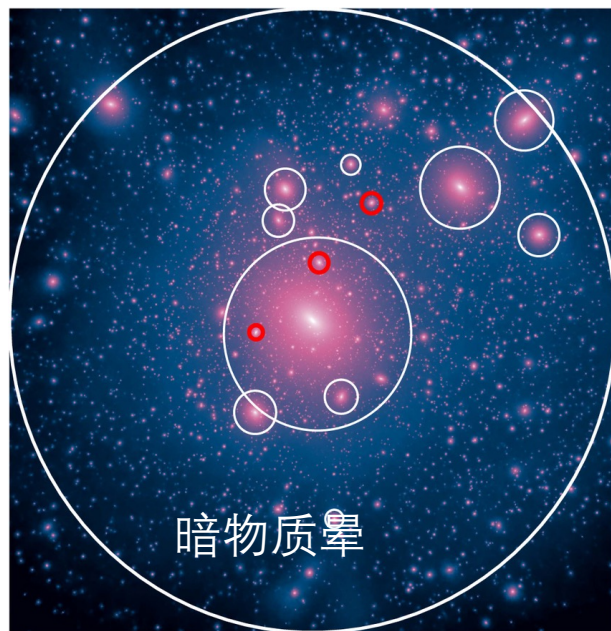


Fig. 2 Illustration of key baryonic processes in galaxies, using the Triangulum Galaxy (M33) as an example (Image credit: X-ray: X-ray)

arXiv: 2507.08925

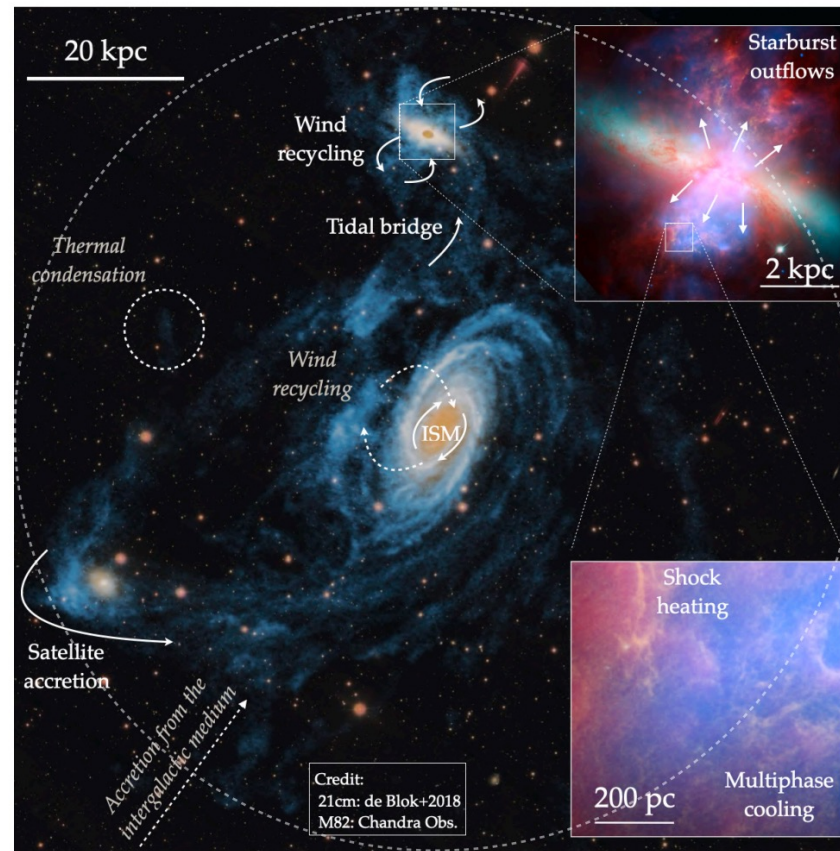
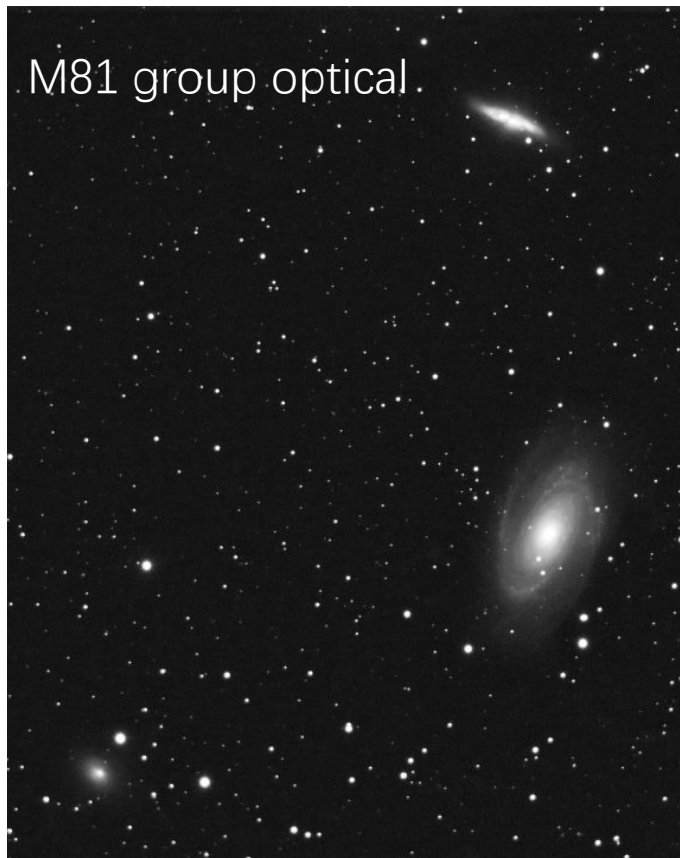
引力驱动重子气体进入暗晕，冷却聚集在暗晕中心，产生HI与H₂等，触发恒星形成

恒星与黑洞反馈加热与电离气体，驱动冷热气体外流

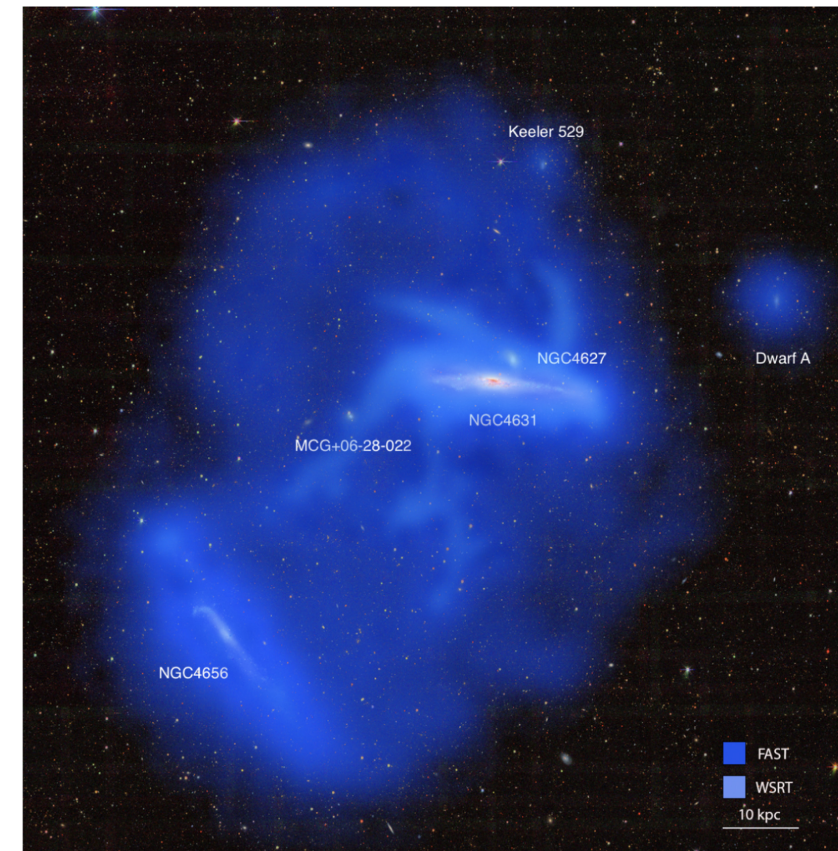
演化：继续形成恒星或恒星形成停止；与其他星系相互作用及并和

Introduction

➤ 星系相互作用、并合（引力与重子物理共同主导）



Chen & Zahedy 2024



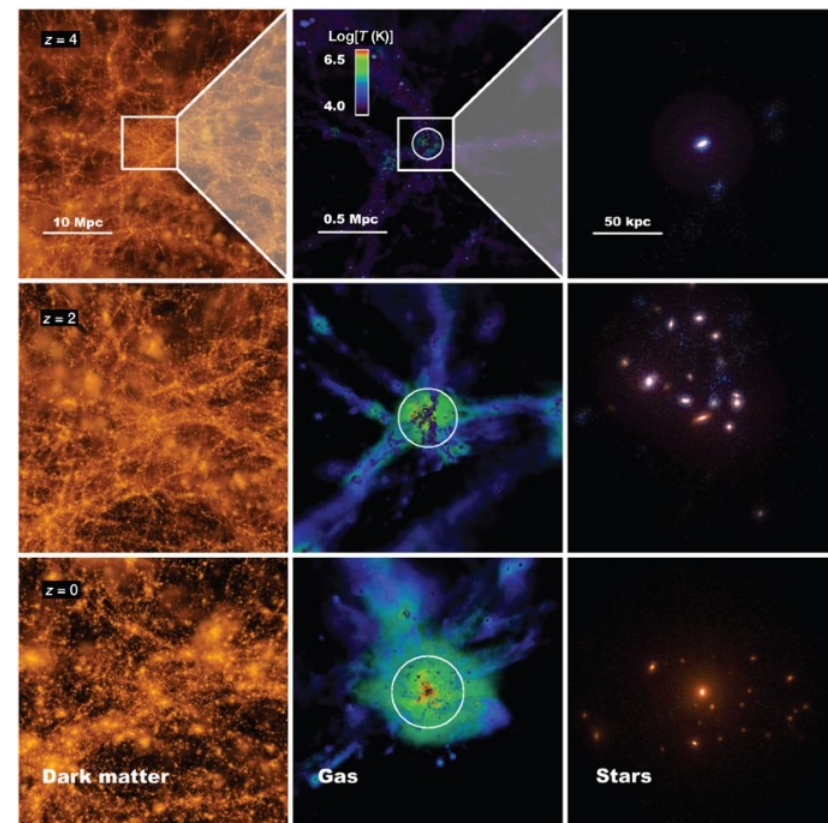
Wang J. et al. 2023

Introduction

宇宙结构、星系形成演化，HI分布与动力学，涉及多种非线性物理过程，诸多关键问题，仅靠解析理论无法得到准确答案

- 暗晕的具体形成、增长？内部结构？
- 暗晕如何吸积气体？HI与H₂的产生与比例？
- 恒星形成与停止？中心黑洞形成演化？
- 重子反馈对ISM的影响、重子循环过程？
- 星系相互作用与并合影响？
- 宇宙学模型与参数的影响？
- ...

1970年代起，数值模拟(数值求解相关非线性方程组)成为重要手段，与观测、解析理论联合，揭示物理规律



Introduction

近50年发展迅速，主要有N体模拟，N体+流体，纯流体；另：大体积， zoom-in, 单星系

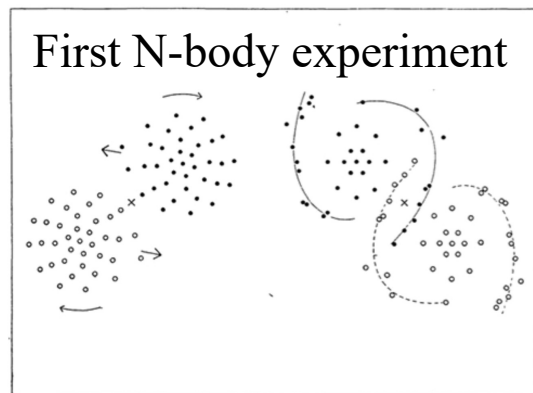
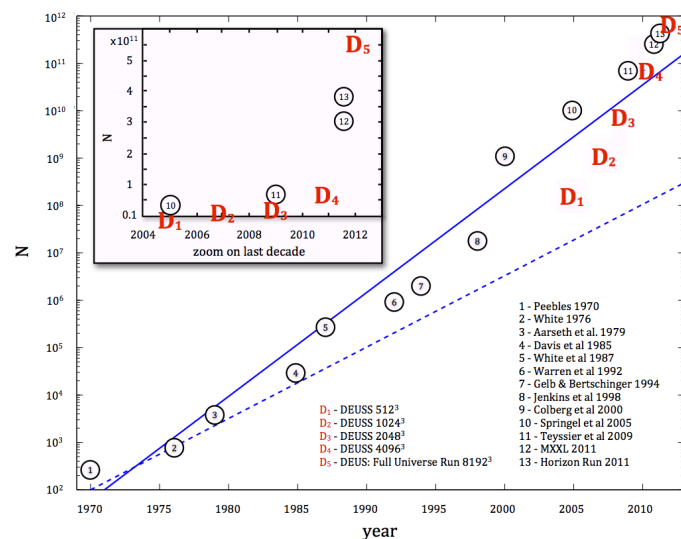


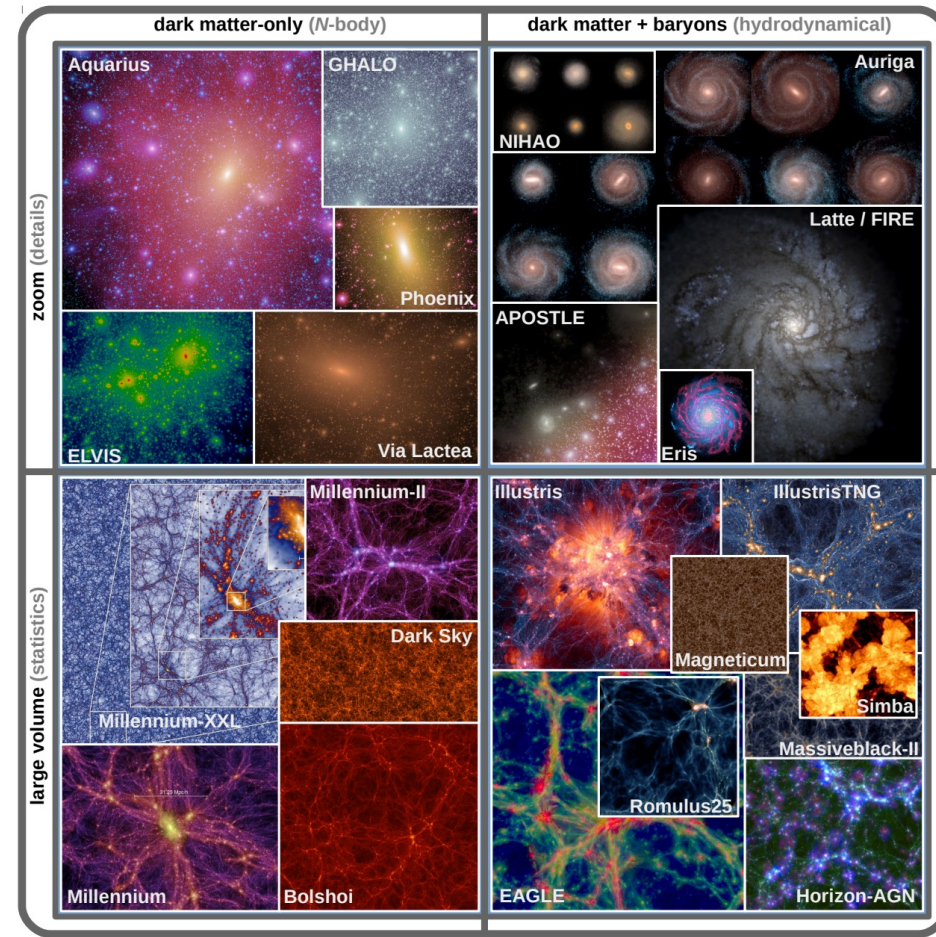
Fig. 1.5. The first N -body experiment of a galaxy encounter using 37 light bulbs for each galaxy by Holmberg. The tidal arms as a result of encounter is clearly visible on the RHS of the figure showing the final result of the experiment (or simulation). Figure adapted from Fig. 4(a) of [49].



number of particles in N-body simulations

zoom-in
模拟

大体积
模拟



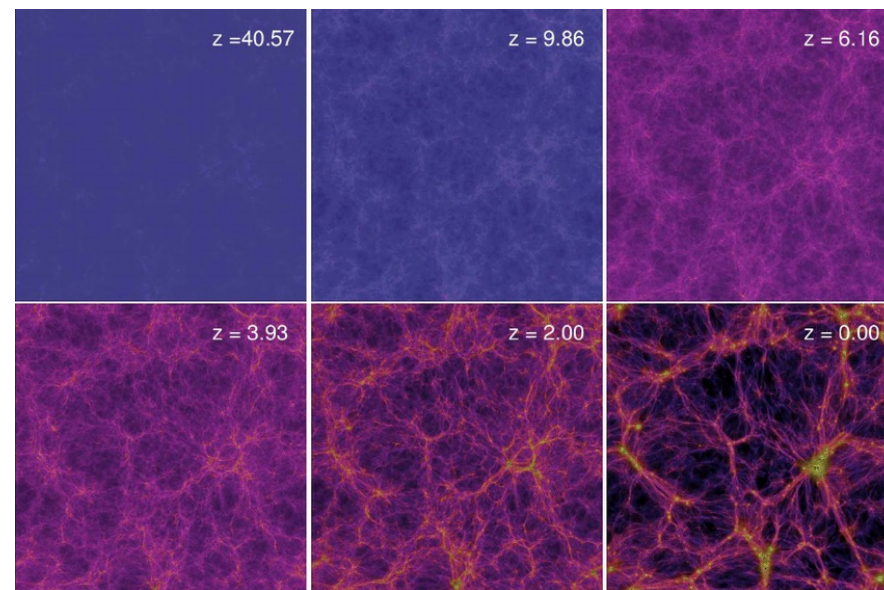
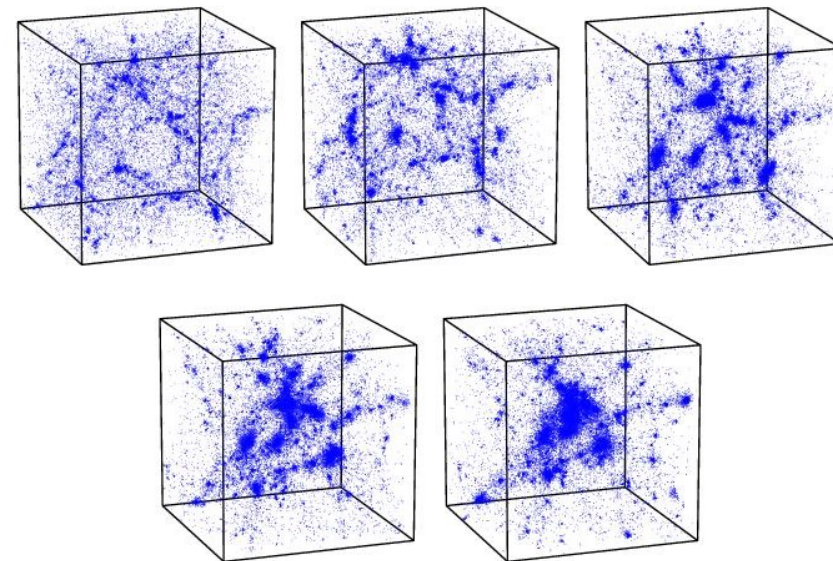
Visual representations of some selected recent simulations (arXiv:1909.07976)

2. Collisionless N-Body Simulations

2.1 Basic idea

In a simulation, mass distribution is represented by particles or sampled on a grid; motion of each mass element is traced numerically by accounting its interactions with other elements.

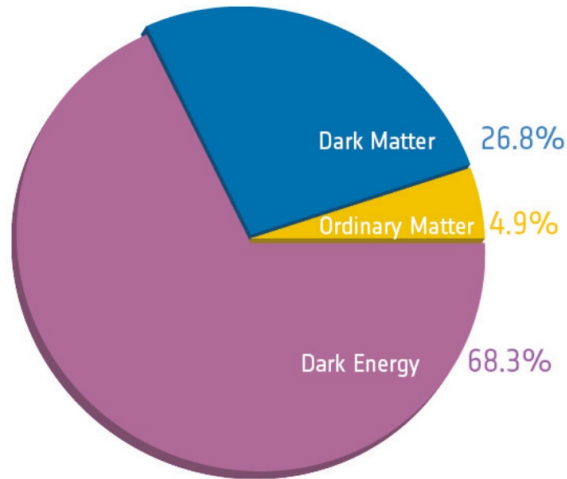
- Cosmological simulation tracks the evolution of a periodic (uniformly sampled) comoving cubical box with side length L
- N collisionless particles ($\sim 10^4$ in 1985; $\sim 4 \times 10^{12}$ in 2025) in the box, representing a sampling of the matter field



2. Collisionless N-Body Simulations

2.1 Basic idea

Λ **CDM** model assumes that dark matter is cold, with **negligible random motions** when decoupled from other matter, and **collisionless**



After Planck

Introducing phase-space density or distribution function of dark matter, $f = f(\mathbf{x}, \mathbf{p}, t)$

CDM is governed by cosmic Vlasov–Poisson equations

$$\frac{\partial f}{\partial t} + \frac{1}{ma^2} \mathbf{p} \cdot \nabla f - m \nabla \phi \cdot \frac{\partial f}{\partial \mathbf{p}} = 0$$

collisionless Boltzmann equation (CBE)

$$\nabla^2 \phi = 4\pi G a^2 (\rho(\mathbf{x}, t) - \bar{\rho})$$

$$\rho = \bar{\rho}(t)[1 + \delta(\mathbf{x}, t)], \quad \rho = \int f(\mathbf{x}, \mathbf{p}, t) d^3 p.$$

2. Collisionless N-Body Simulations

2.1 Basic Idea

The cosmic Vlasov–Poisson equations

$$\frac{\partial f}{\partial t} + \frac{1}{ma^2} \mathbf{p} \cdot \nabla f - m \nabla \phi \cdot \frac{\partial f}{\partial \mathbf{p}} = 0$$

collisionless Boltzmann equation (CBE)

$$\nabla_{\mathbf{x}}^2 \phi = 4\pi G \bar{\rho}(t) a^2 \delta(\mathbf{x}, t)$$

Poisson equation

$$\rho = \bar{\rho}(t)[1 + \delta(\mathbf{x}, t)], \quad \rho = \int f(\mathbf{x}, \mathbf{p}, t) d^3 p.$$

directly solving them in 7D space is difficult

N-Body methods as an efficient technique:

sample $f(\mathbf{x}, \mathbf{p}, t)$ by N phase-space points

$$f(\mathbf{x}, \mathbf{p}, t) \approx \sum_{i=1}^N m_i \delta^3(\mathbf{x} - \mathbf{x}_i(t)) \delta^3(\mathbf{p} - \mathbf{p}_i(t))$$

蒙特卡洛采样 (Monte Carlo Sampling)

solve CBE by Method of Characteristics

沿特征线 $\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{d\mathbf{x}}{dt} \cdot \frac{\partial f}{\partial \mathbf{x}} + \frac{d\mathbf{p}}{dt} \cdot \frac{\partial f}{\partial \mathbf{p}} = 0$



$$\frac{d\mathbf{x}_i}{dt} = \frac{\mathbf{p}_i}{m_i a^2}$$

$$\frac{d\mathbf{p}_i}{dt} = -m_i \nabla \phi$$

2. Collisionless N-Body Simulations

2.1 Basic Idea

$$\frac{\partial f}{\partial t} + \frac{1}{ma^2} \mathbf{p} \cdot \nabla f - m \nabla \phi \cdot \frac{\partial f}{\partial \mathbf{p}} = 0$$

$$\nabla_{\mathbf{x}}^2 \phi = 4\pi G \bar{\rho}(t) a^2 \delta(\mathbf{x}, t)$$

$$\frac{d\mathbf{x}_i}{dt} = \frac{\mathbf{p}_i}{m_i a^2}$$

$$\frac{d\mathbf{p}_i}{dt} = -m_i \nabla \phi$$

➤ N-Body methods as an efficient technique:

f is constant along any trajectory $\{\mathbf{x}(t), \mathbf{p}(t)\}$, the trajectories obtained by time integration of N points $\{\mathbf{x}_i, \mathbf{p}_i\}$ sampled from the f at time $t = t_{\text{initial}}$ form a representative sample of f at each time t

$$f(\mathbf{x}, \mathbf{p}, t) \approx \sum_{i=1}^N m_i \delta^3(\mathbf{x} - \mathbf{x}_i(t)) \delta^3(\mathbf{p} - \mathbf{p}_i(t))$$

problem reduces to **solving Poisson's Eq.** for a set of N particles and **advancing them forward in time according to the equations of motion** derived from the system's Hamiltonian

2. Collisionless N-Body Simulations

2.1 Basic Idea

problem reduces to **solving Poisson's Eq.** for a set of **N** particles and **advancing them forward in time according to the equations of motion**

$$\nabla_x^2 \phi = 4\pi G \bar{\rho}(t) a^2 \delta(\mathbf{x}, t)$$

$$\phi(\mathbf{x}_i) = -G \sum_{j \neq i} \frac{m_j}{\sqrt{|\mathbf{x}_i - \mathbf{x}_j|^2 + \epsilon^2}}$$

**Discrete
Poisson
Solver**

Hamilton Equation

$$\frac{d\mathbf{x}_i}{dt} = \frac{\mathbf{p}_i}{m_i a^2}$$

$$\frac{d\mathbf{p}_i}{dt} = -m_i \nabla \phi$$

Lagrangian Equation

$$\frac{d\mathbf{x}}{dt} = \frac{1}{a} \mathbf{v}$$

$$\frac{d\mathbf{v}}{dt} + \frac{\dot{a}}{a} \mathbf{v} = -\frac{\nabla \phi}{a}$$

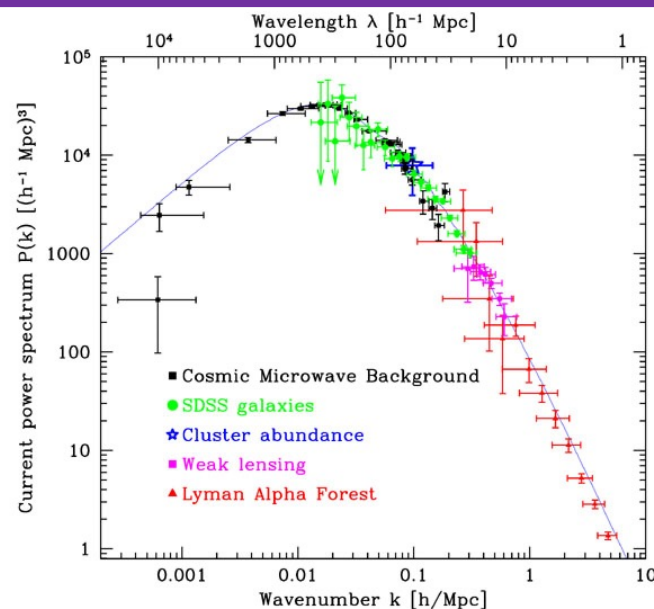
2. Collisionless N-Body Simulations

2.1 Basic Idea: Procedures

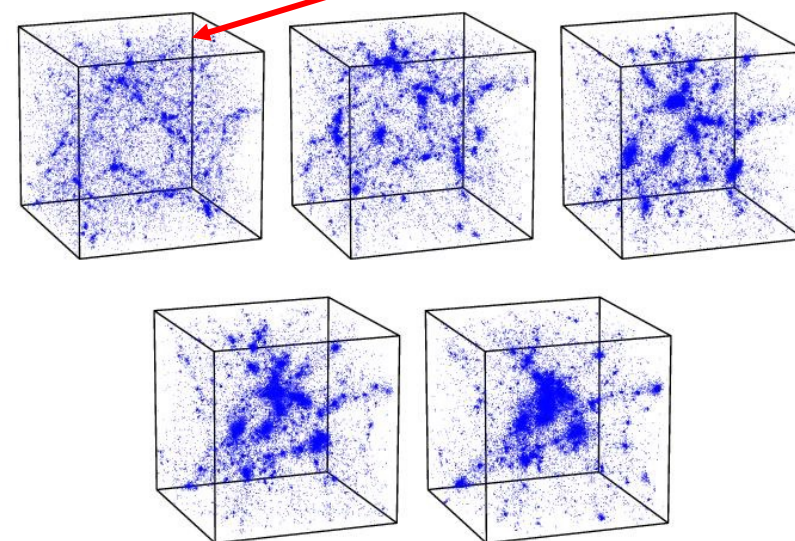
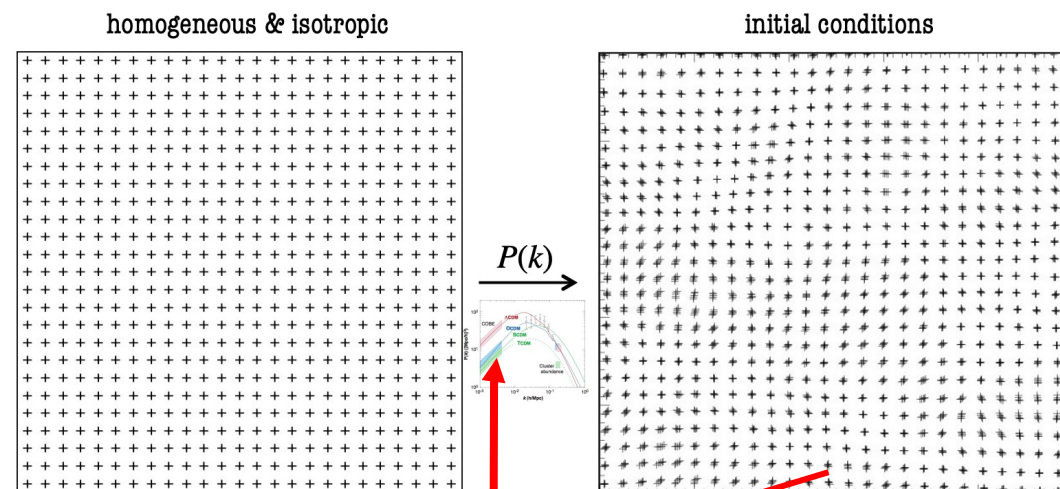
- Produce the initial conditions (position and velocity of particles) according to the chosen cosmology
- Trace the motions of particles

Produce the initial conditions

$$P_i(k) = Ak^n$$
$$P(k) = T^2(k)P_i(k)$$



Zel'dovich Approximation, 2LPT



2. Collisionless N-Body Simulations

b). Trace the motions of particles:

Time Discretization & Integration

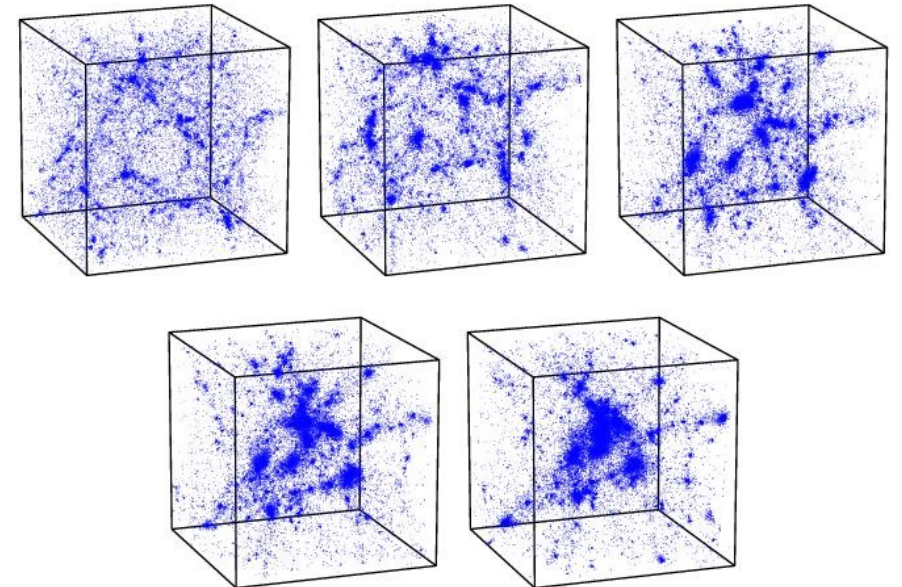
Suppose that at the **nth time step**, the time is t_n and the distribution of particles is given by $x_i(t_n)$, $v_i(t_n)$ where $i = 1, 2, \dots, N$. How to update?

simple 'Euler method' for a time step Δt

$$\begin{aligned}\vec{x}_i^{[n+1]} &= \vec{x}_i^{[n]} + \vec{v}_i^{[n]} \cdot \Delta t \\ \vec{v}_i^{[n+1]} &= \vec{v}_i^{[n]} + \vec{a}_i^{[n]} \cdot \Delta t\end{aligned}$$

relatively poor accuracy

$$\begin{aligned}\frac{d\mathbf{x}}{dt} &= \frac{1}{a}\mathbf{v} \\ \frac{d\mathbf{v}}{dt} + \frac{\dot{a}}{a}\mathbf{v} &= -\frac{\nabla\phi}{a}\end{aligned}$$



2.2 Gravity Solver

The efficiency of N-body simulation mainly depend on the specific Poisson/Gravity Solver

$$\phi(\mathbf{x}_i) = -G \sum_{j \neq i} \frac{m_j}{\sqrt{|\mathbf{x}_i - \mathbf{x}_j|^2 + \epsilon^2}}$$

ϵ : softening length
Plummer smoothing

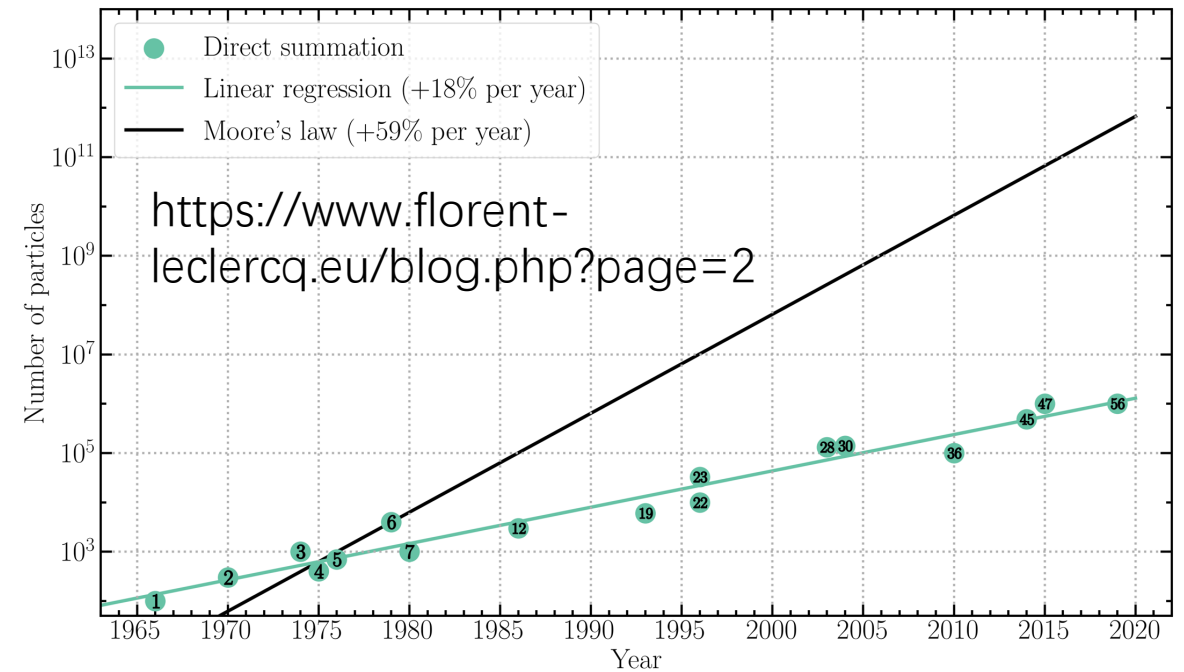
(a) Particle-Particle (PP) method

$$F_{ij} = Gm^2 \frac{\mathbf{x}_i - \mathbf{x}_j}{(\epsilon^2 + |\mathbf{x}_i - \mathbf{x}_j|^2)^{3/2}}$$

Pros: robust, accurate and completely general

Cons: **computation expansive** $O(N^2)$, too slow

preferred in simulation of star clusters



Evolution of the number of particles used in direct - body simulations as a function of year of publication.

2.2 Gravity Solver

(b) Particle-Mesh (PM) method $\sim N \cdot \log(N)$

(Hockney & Eastwood 1988)

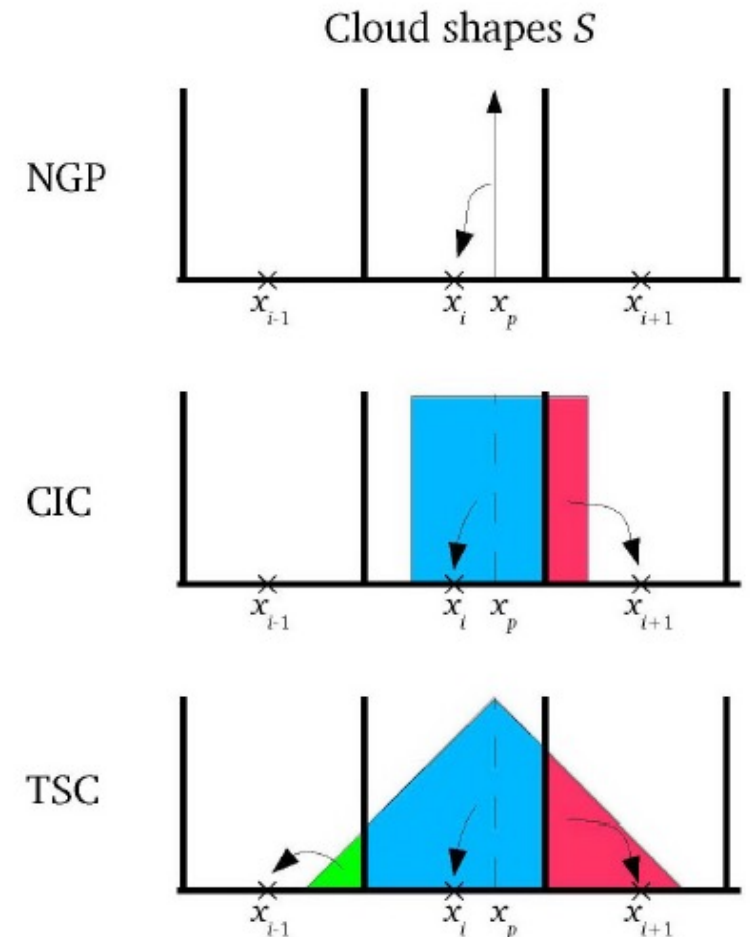
Mass assignment; Solving equation with FFT; Forces interpolation

- I. Divide computational box (size L) in grid of N_c^3 meshes of constant size L/N_c
- II. Compute mass density on mesh using interpolation schemes (Nearest Grid Point, Cloud in Cell, Triangular Shaped Cloud); Fourier transform

$$\rho(\vec{q}) = \frac{m}{L^3} \sum_{i=1}^N W(\vec{x}_i - \vec{X}_q)$$

- III. Solve for potential on mesh using the Poisson equation (in Fourier Space)

$$-k^2 \phi_{\vec{k}} = 4\pi G \rho_{\vec{k}}$$



2.2 Gravity Solver

(b) Particle-Mesh (PM) method $\sim N \cdot \log(N)$

(Hockney & Eastwood 1988)

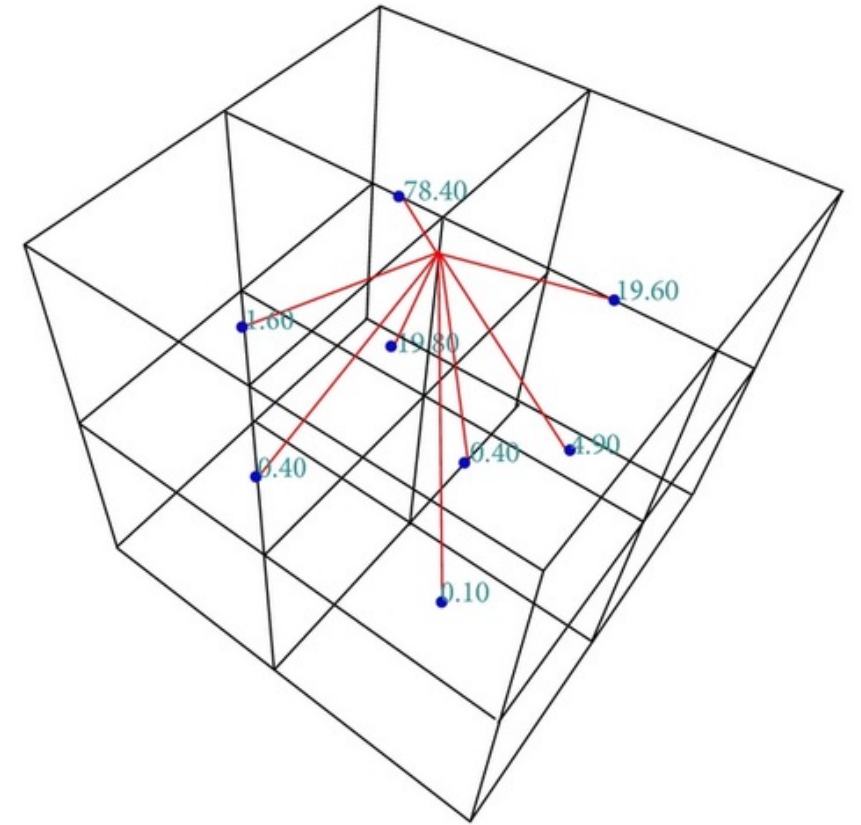
IV. Compute each particle acceleration using inverse interpolation scheme

$$F(\vec{x}_i) = \sum_{\vec{q}} W(\vec{x}_i - \vec{X}_q) F(\vec{q})$$

V. Update each particle velocity and position

Pros: Fast

Cons: Force resolution is limited by size of mesh



inverse Cloud in Cell in 3D

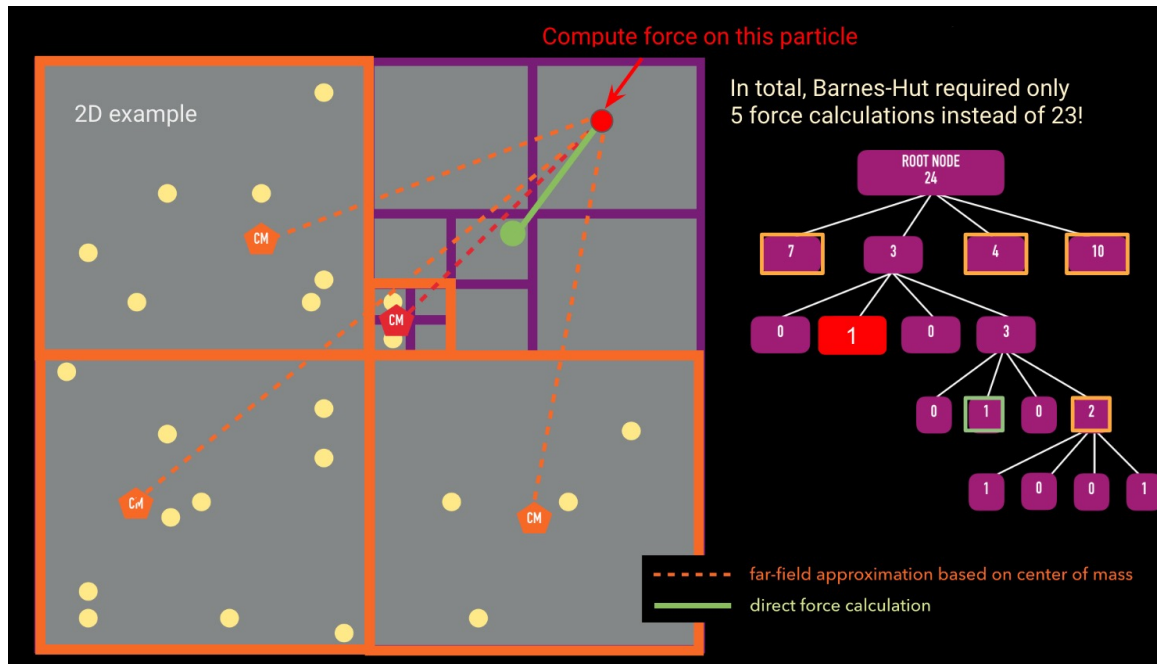
2.2 Gravity Solver

c) Tree(Tree-PM) method $O(N \cdot \log(N))$

e.g. Barnes & Hut (1986)

Octree, kd-tree

- Particles are grouped together systematically according to their distances to the particle for which the force is to be calculated.
- Force from each group is then replaced by its multipole expansion.
- A smaller number of multipole components for distant particles or more distant particles can be combined into larger groups.



to compute the force on particle i

LOOP over all cells of the lowest refinement level.

IF $|\vec{x}_i - \vec{x}_c| > l_c / \theta$ THEN

compute force due to this cell (using low-order multipole expansion)

ELSE

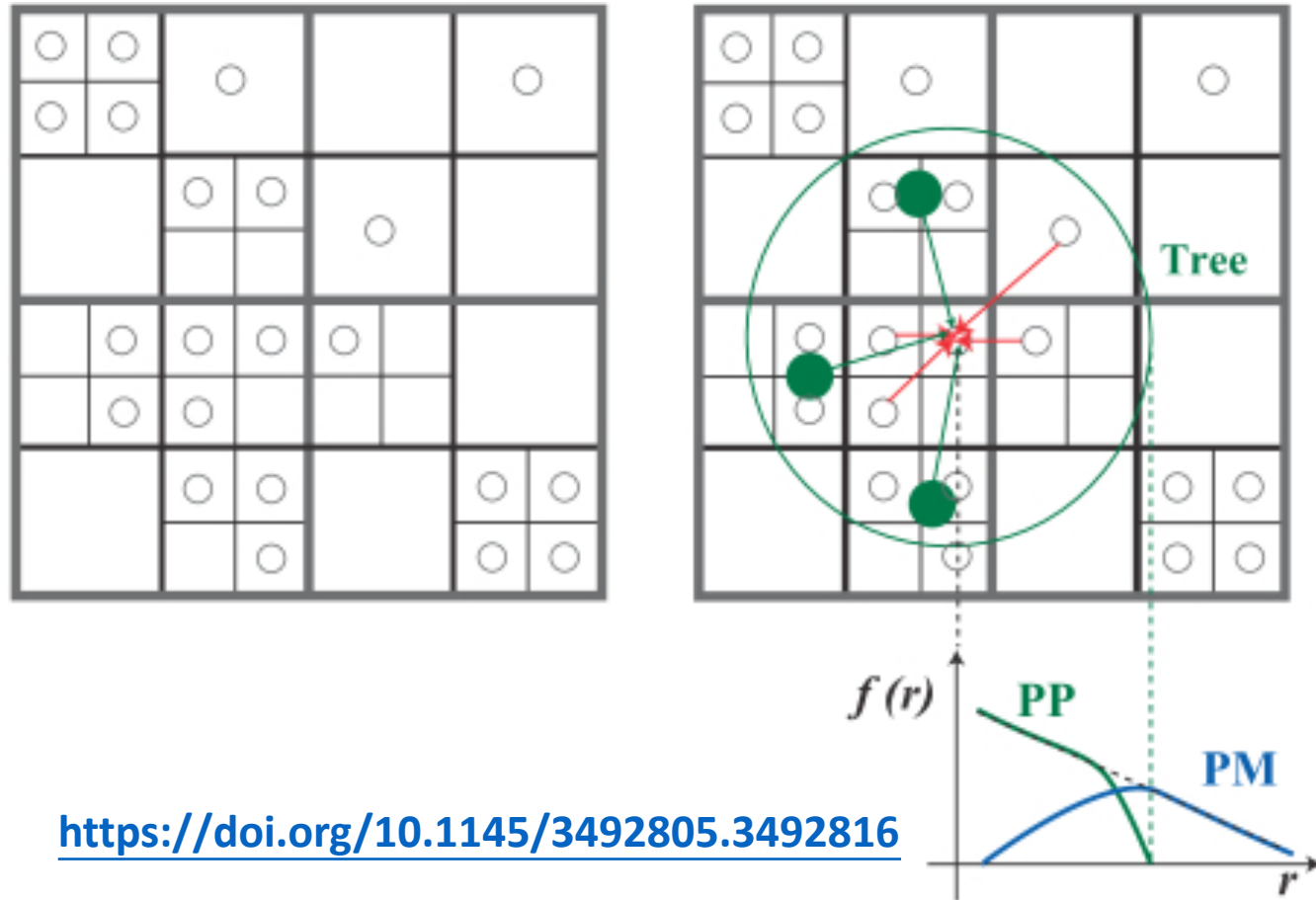
sum the contributions of its sub-cells

END IF

l_c the size of the cell, θ is a free parameter (opening-angle)

2.2 Gravity Solver

c) Tree(Tree-PM) method $O(N \cdot \log(N))$



<https://doi.org/10.1145/3492805.3492816>

The large open green circle shows the cutoff radius, in which the short-range forces are calculated by the tree algorithm. Green filled circles are the center of mass of tree nodes.

Green and red arrows indicate particle-multipole and particle-particle interactions, respectively. The PM algorithm is used to calculate the residual forces.

The functions for short and long ranges forces are illustrated in the bottom-right by green and blue curves.

2.2 Gravity Solver

(d) Particle-Particle-Particle-Mesh (P3M) method

Long distance: PM Short distance: P-P

(e.g. Efstathiou
1985; Couchman 1991)

e.g. short-range force

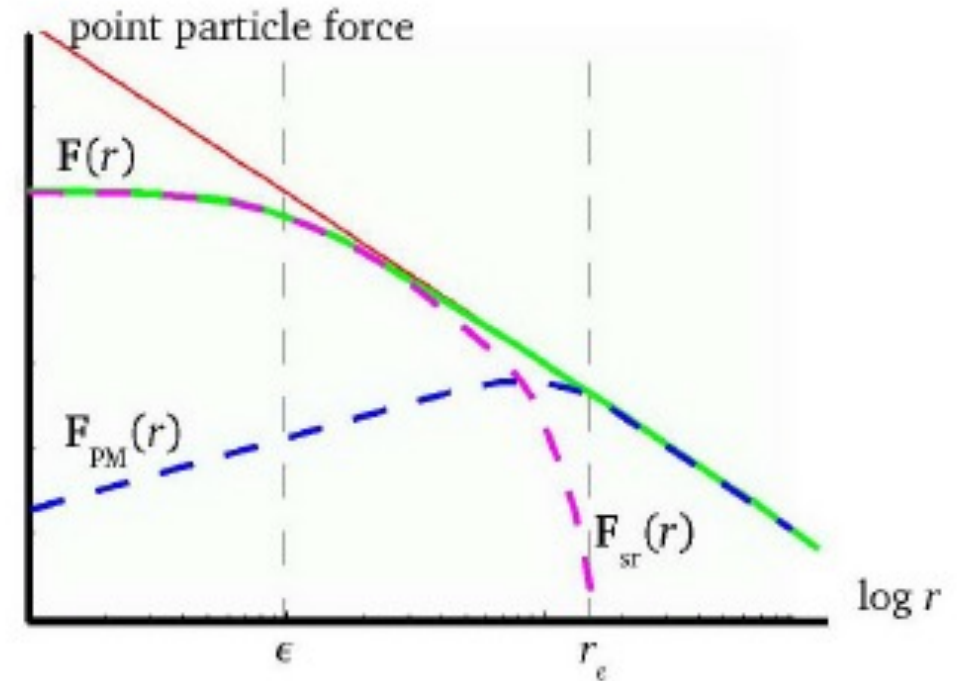
$$\mathbf{f}_i = \sum_{j \neq i}^N G m_j \frac{\mathbf{r}_j - \mathbf{r}_i}{(r^2 + \epsilon^2)^{3/2}} g_{\text{P3M}}(r),$$

cutoff function

$$g_{\text{P3M}}(r) = \begin{cases} 1 + \xi^3 \left(-\frac{8}{5} + \xi^2 \left(\frac{8}{5} + \xi \left(-\frac{1}{2} + \xi \left(-\frac{12}{35} + \xi \frac{3}{20} \right) \right) \right) \right) \\ - \zeta^6 \left(\frac{3}{35} + \xi \left(\frac{18}{35} + \xi \frac{1}{5} \right) \right), & (0 \leq \xi \leq 2), \\ 0, & (\xi > 2), \end{cases}$$

where $\xi = 2r/r_{\text{cut}}$ and $\zeta = \max(0, \xi - 1)$.

If particles are not strongly clustered, most particle pairs are solved using PM. Once particles become strongly clustered, code becomes effectively PP. ➔ adaptive P3M



2.2 Gravity Solver

Table 1: Major galaxy formation simulation codes

code name	gravity treatment ^a	hydrodynamics treatment ^b	parallelization technique ^c	code availability ^d	primary reference
ART	PM/ML	AMR	data-based	public	Kravtsov (1997) ²⁷
RAMSES	PM/ML	AMR	data-based	public	Teyssier (2002) ³⁸
GADGET-2/3	TreePM	SPH	data-based	public	Springel (2005) ³⁹
Arepo	TreePM	MMFV	data-based	public	Springel (2010) ⁴⁰
Enzo	PM/MG	AMR	data-based	public	Bryan et al. (2014) ⁴¹
ChaNGa ^e	Tree/FM	SPH	task-based	public	Menon et al. (2015) ^{42–44}
GIZMO ^f	TreePM	MLFM/MLFV	data-based	public	Hopkins et al. (2015) ⁴⁵
HACC	TreePM/P ³ M	CRK-SPH	data-based	private	Habib et al. (2016) ⁴⁶
PKDGRAV3	Tree/FM	—	data-based	public	Potter et al. (2017) ⁴⁷
Gasoline2	Tree	SPH	task-based	public	Wadsley et al. (2017) ⁴⁸
SWIFT	TreePM/FM	SPH	task-based	public	Schaller et al. (2018) ⁴⁹

^a PM: particle-mesh; TreePM: tree + PM, FM: fast multipole, P³M: particle-particle-particle-mesh; ML: multilevel; MG: multigrid

^b SPH: smoothed particle hydrodynamics, CRK-SPH: conservative reproducing kernel smoothed particle hydrodynamics, AMR: adaptive-mesh-refinement, MMFV: moving-mesh finite volume, MLFM/MLFV: mesh-free finite mass / finite volume

^c data-based: data parallelism focuses on distributing data across different nodes, which operate on the data in parallel; task-based: task parallelism focuses on distributing tasks concurrently performed

^d private: private code; public: publicly available code (in some cases with limited functionality)

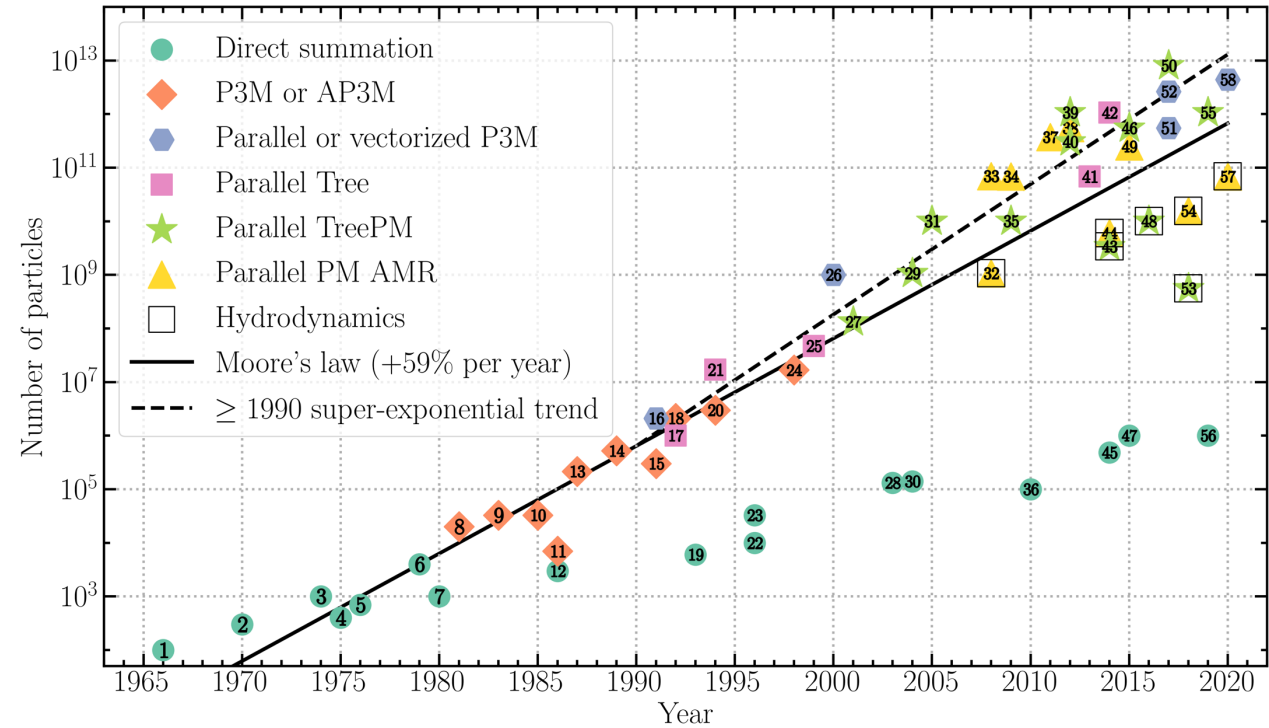
^e gravity solver is based on PKDGRAV3

^f based on the GADGET-3 code

2.3 Parallelization and Load balancing

number of particles used in N-body simulations

mass and force resolution is import!



Typical Resolution of Cosmological N-body Simulations			
Simulation	Box Size	Mass Resolution	Force Resolution
Quijote	1.0 Gpc/h	$6.5 \times 10^{11} M_{\odot}/h$	20 kpc/h
Millennium	0.5 Gpc/h	$8.6 \times 10^8 M_{\odot}/h$	5 kpc/h
Bolshoi	0.25 Gpc/h	$1.4 \times 10^8 M_{\odot}/h$	1 kpc/h
TNG300-Dark	0.205 Gpc/h	$5.9 \times 10^7 M_{\odot}/h$	1 kpc/h
TNG100-Dark	0.075 Gpc/h	$6.5 \times 10^6 M_{\odot}/h$	0.5 kpc/h
TNG50-Dark	0.035 Gpc/h	$4.5 \times 10^5 M_{\odot}/h$	0.2 kpc/h

估计1万亿粒子数的N体模拟所需要的资源？

单CPU FLOPS=核数*主频*CPU单个时钟周期浮点计算值（与cpu架构有关，4~32）

2.3 Parallelization and Load balancing

大规模N体模拟需要超算集群并行计算实现，部分会采用GPU加速
针对不同的超算硬件架构，优化并行计算策略

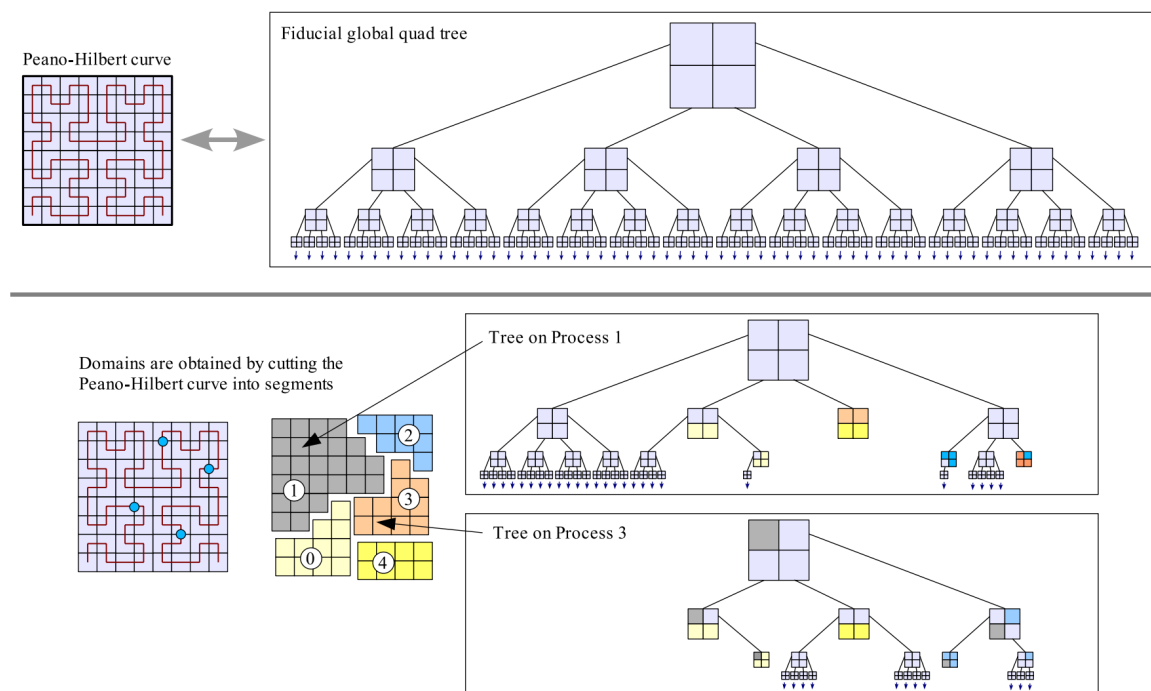
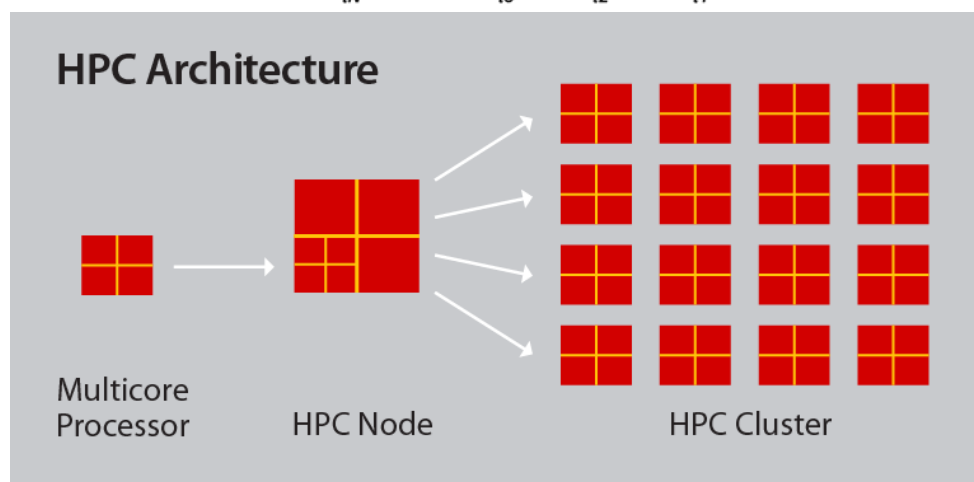
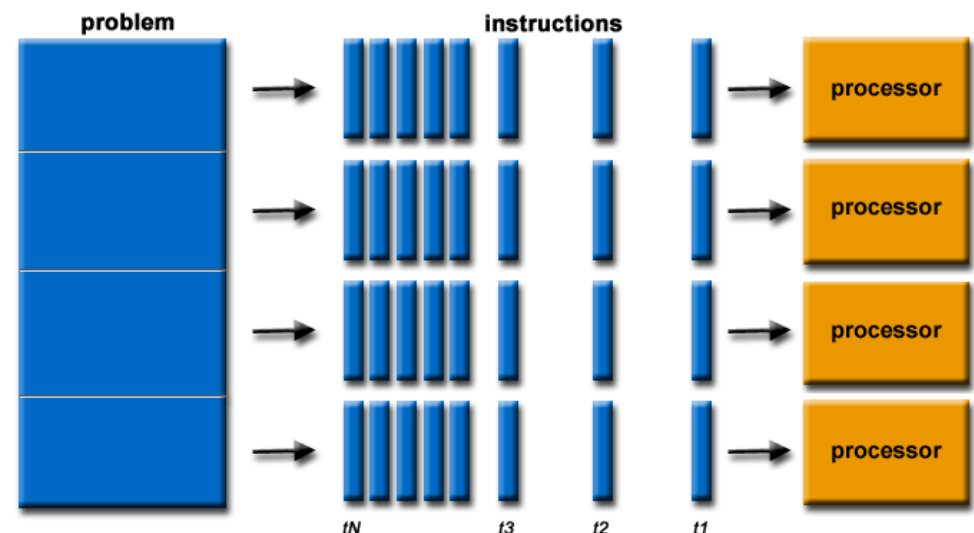
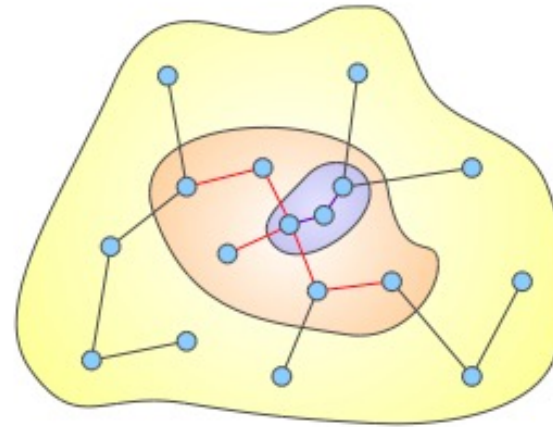
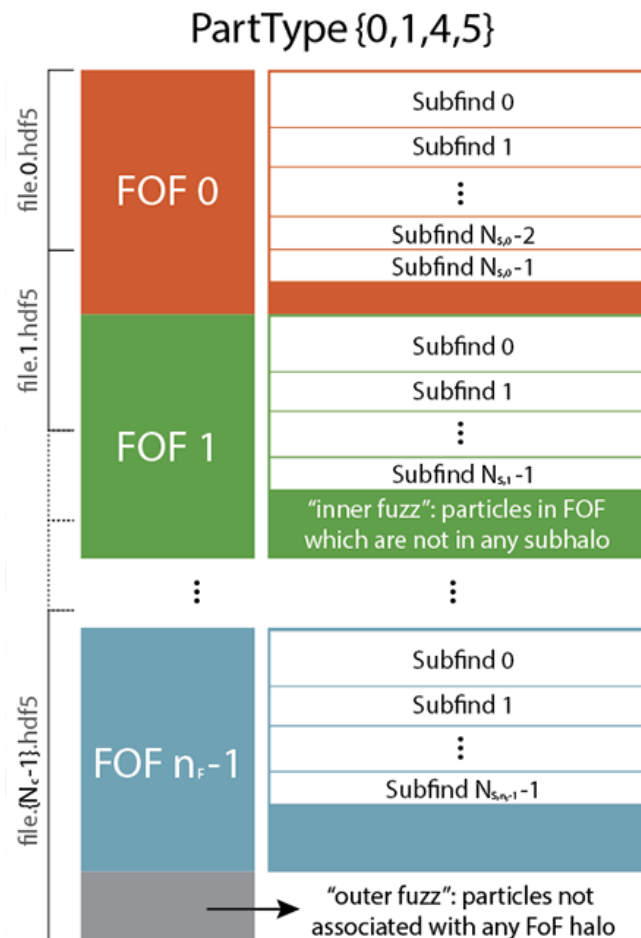


Illustration of the relation between the BH oct-tree and a domain decomposition based on a Peano-Hilbert curve (Volker Springel)

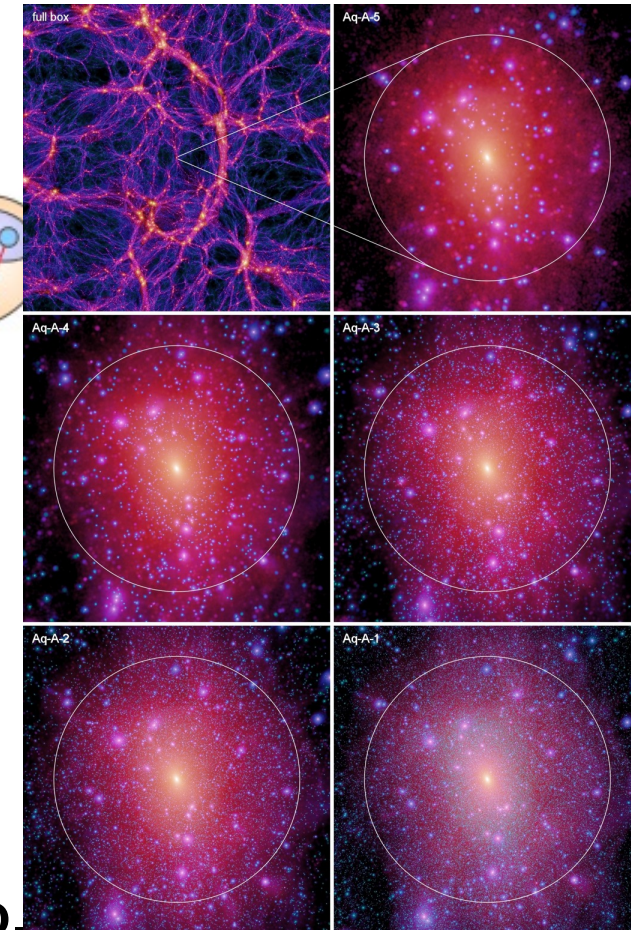
2. Collisionless N-Body Simulations: Analysis, Successes

output: information of particles (pos, velocity, mass) at different time snapshots

Halo Finder

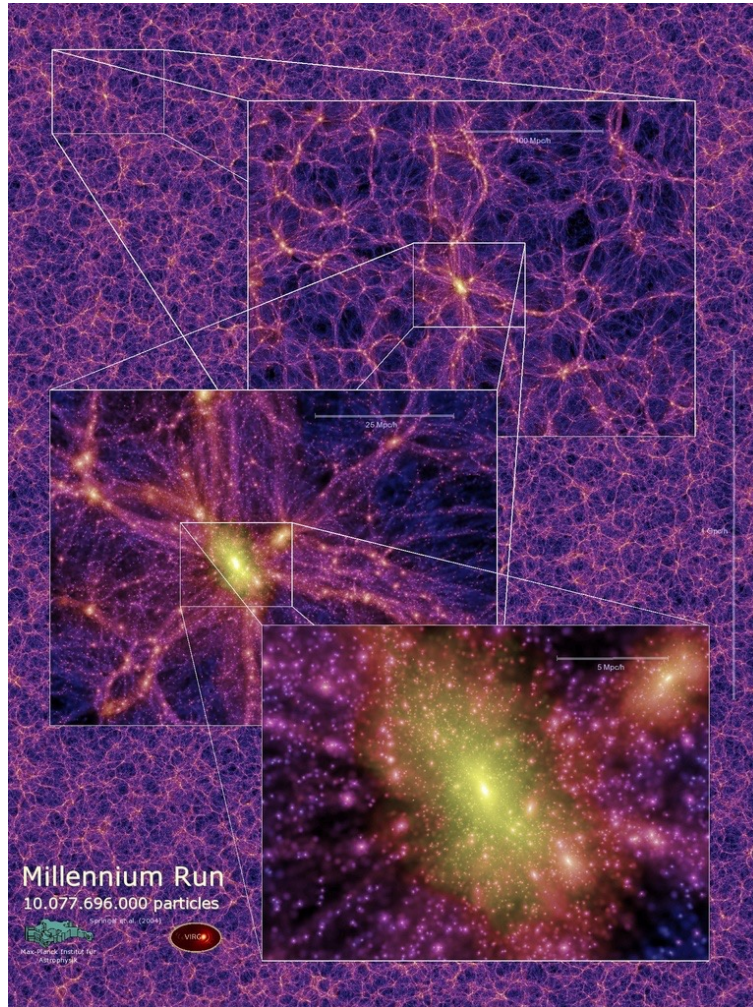


FOF groups with different linking lengths (yellow, orange, violet): substructures are defined as FOF groups which have a smaller linking length and lie inside a larger host halo.

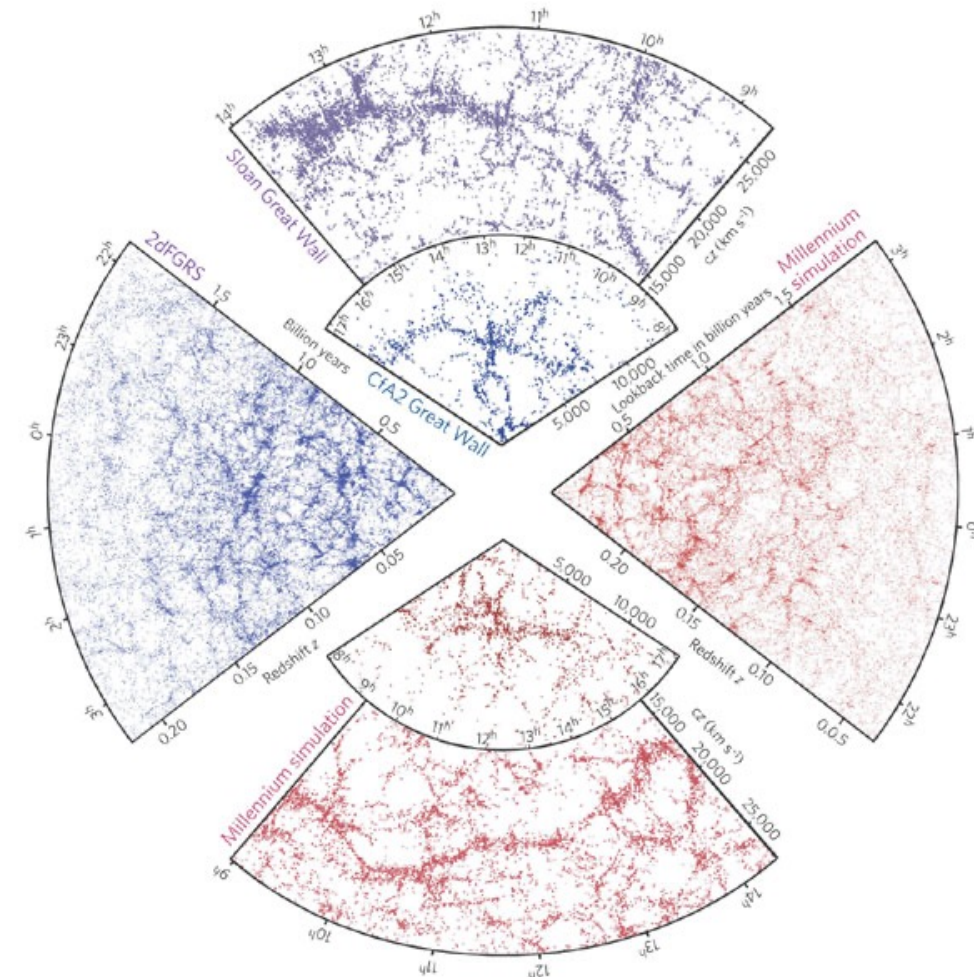


2. Collisionless N-Body Simulations: Analysis, Successes

formation & evolution of large scale structure, cosmic web, dark matter halos



<http://www.mpa.mpa-garching.mpg.de/gadget/>

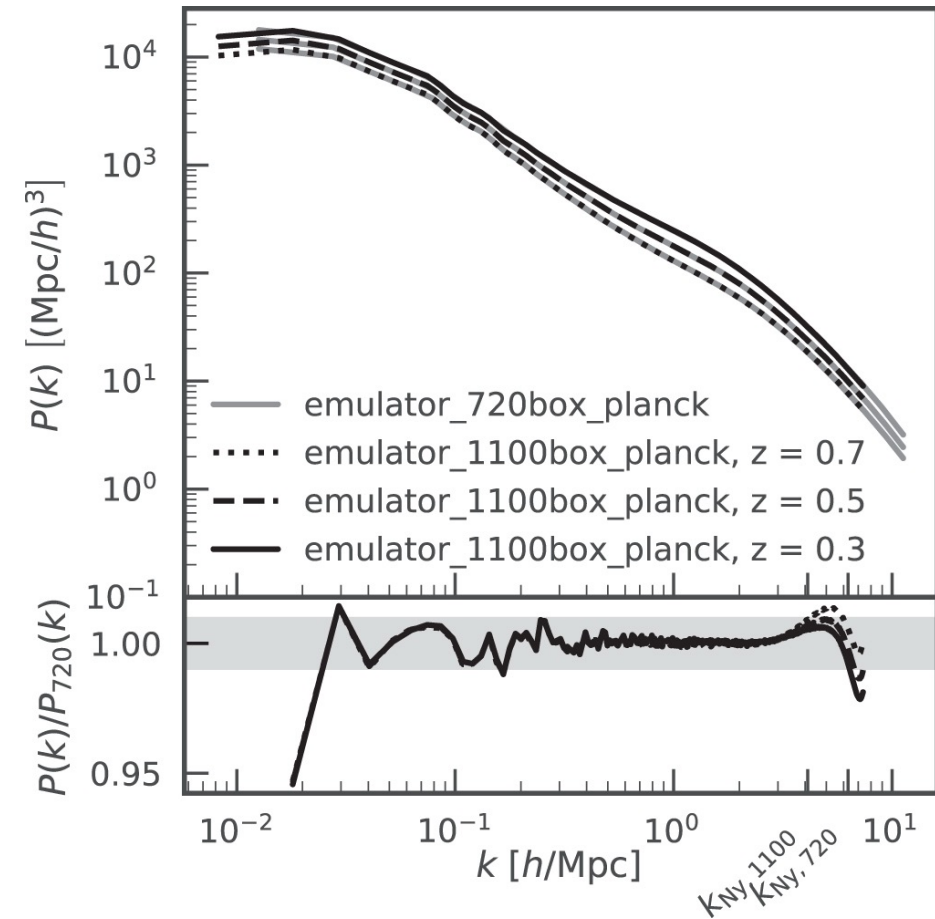
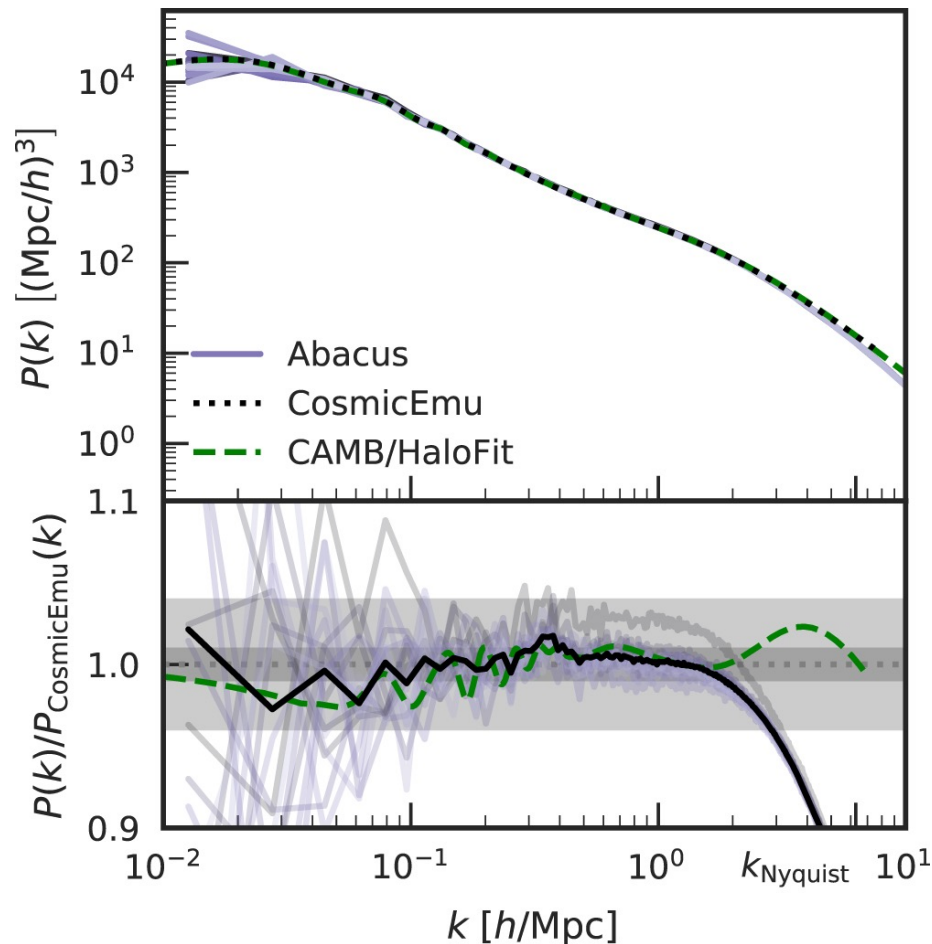


N-body simulation vs. observation

2. Collisionless N-Body Simulations: Analysis, Successes

evolution of non-linear, matter power spectrum

e.g. The Abacus Cosmos: A Suite of Cosmological N -body Simulations



2. Collisionless N-Body Simulations: Analysis, Successes

Properties of dark matter halos: internal structure and substructures

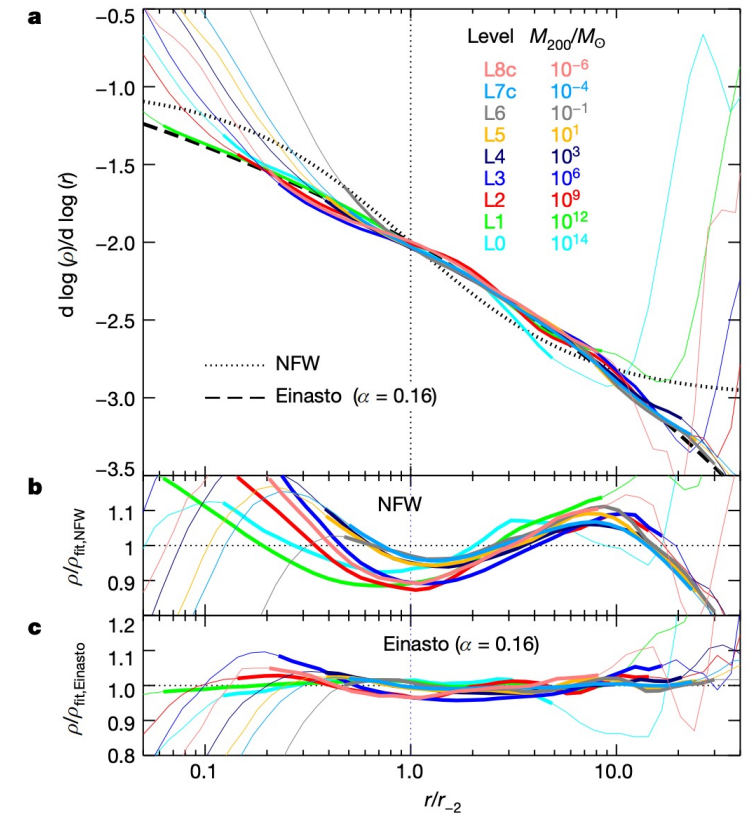
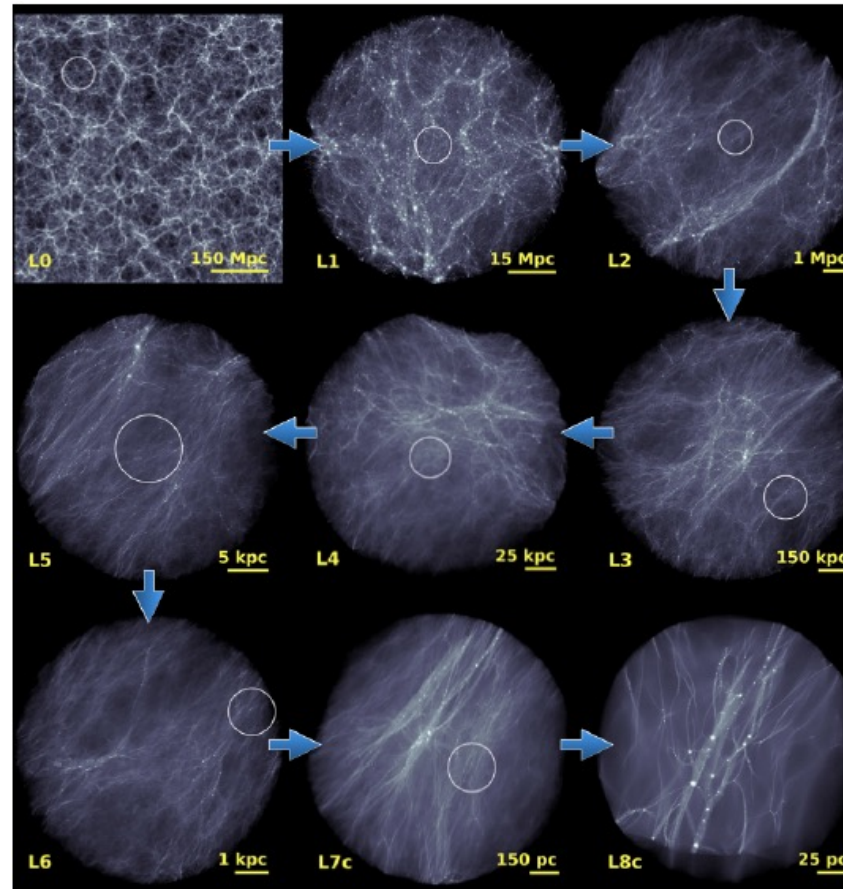
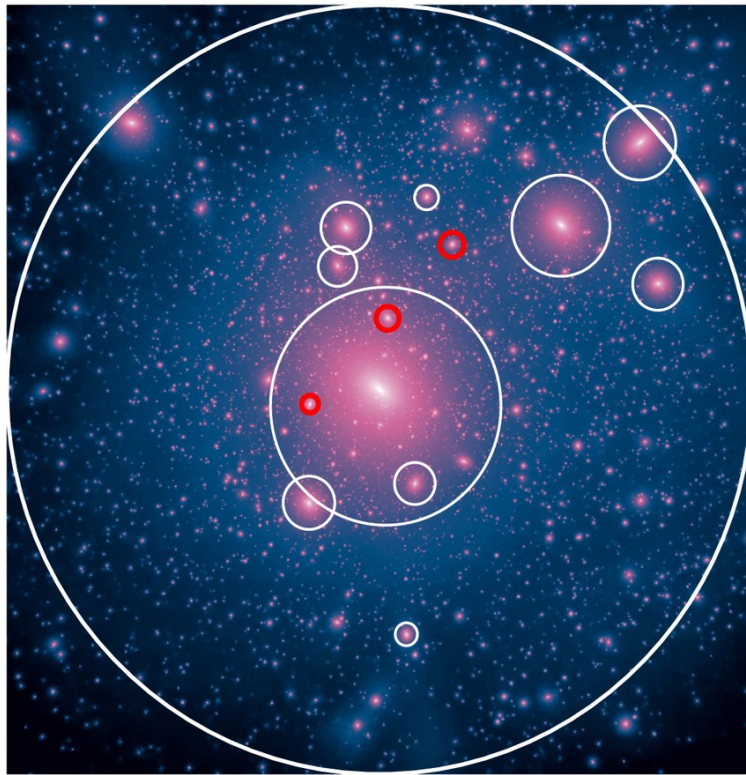
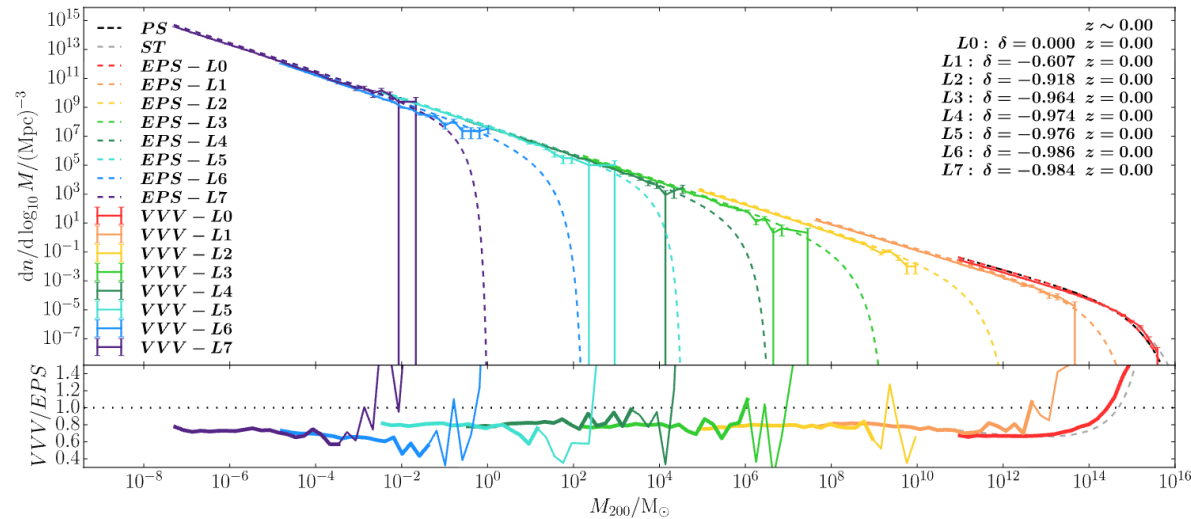


Fig. 2 | Density profiles for haloes with mass between that of the Earth and that of a rich galaxy cluster. As described in detail in the Methods section,

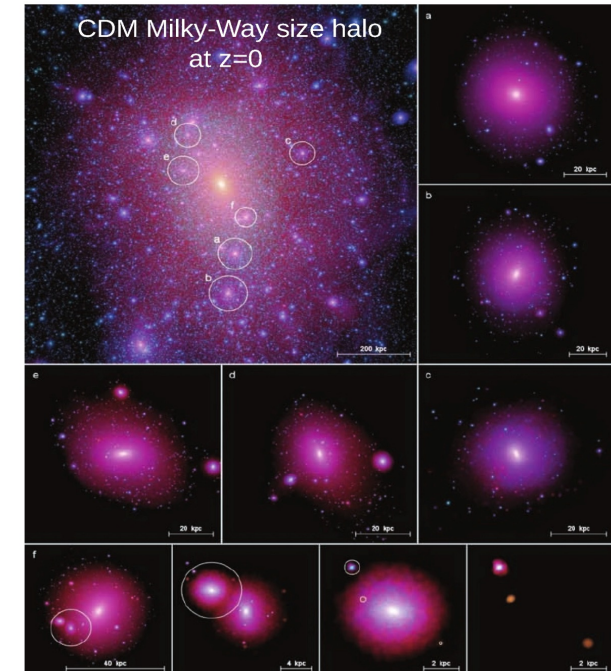
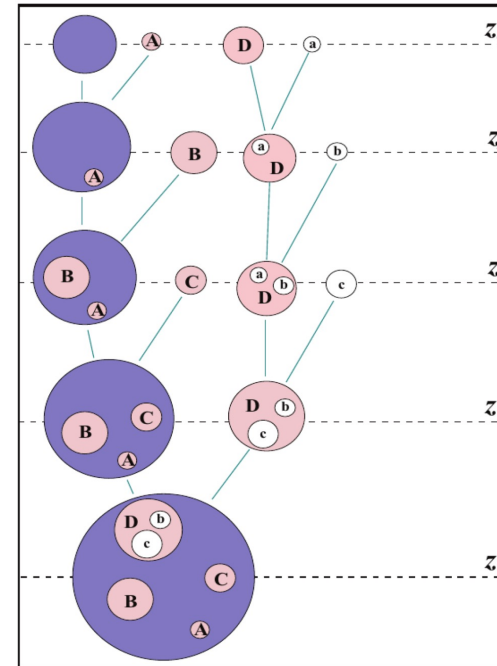
e.g. Wang Jie. et al., 2020, Nature . Zoom-in Simulations

2. Collisionless N-Body Simulations: Analysis, Successes

properties of dark matter halos: halo mass function, merge tree

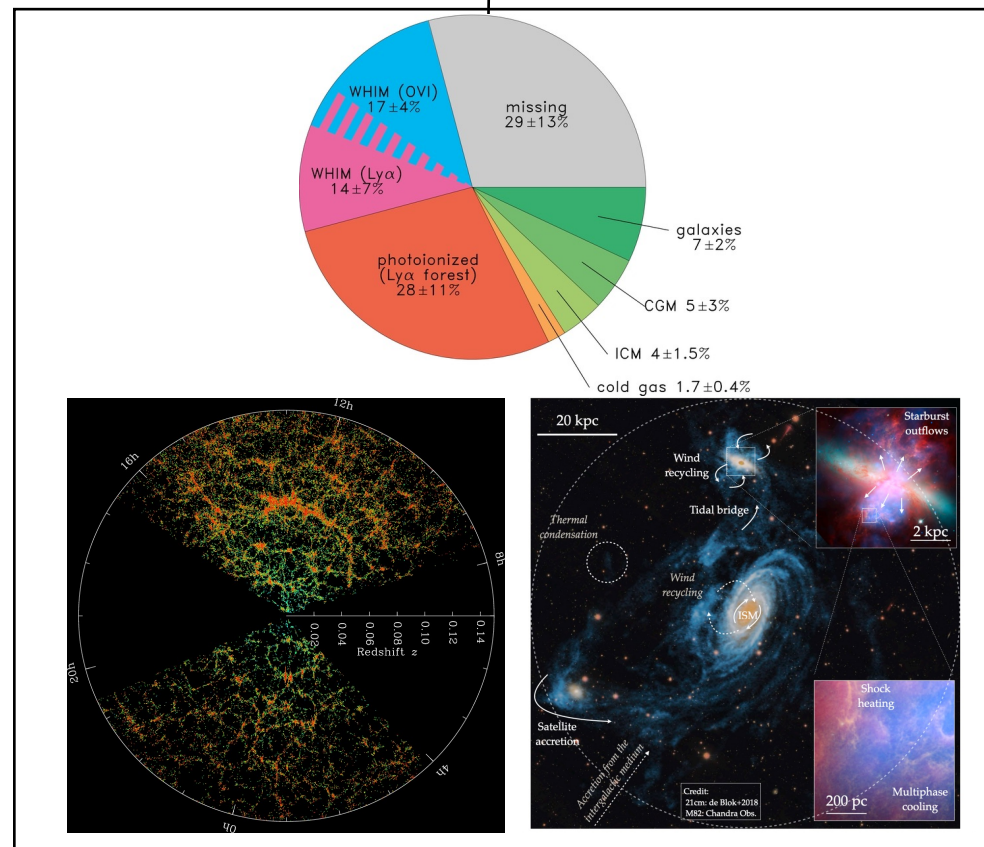
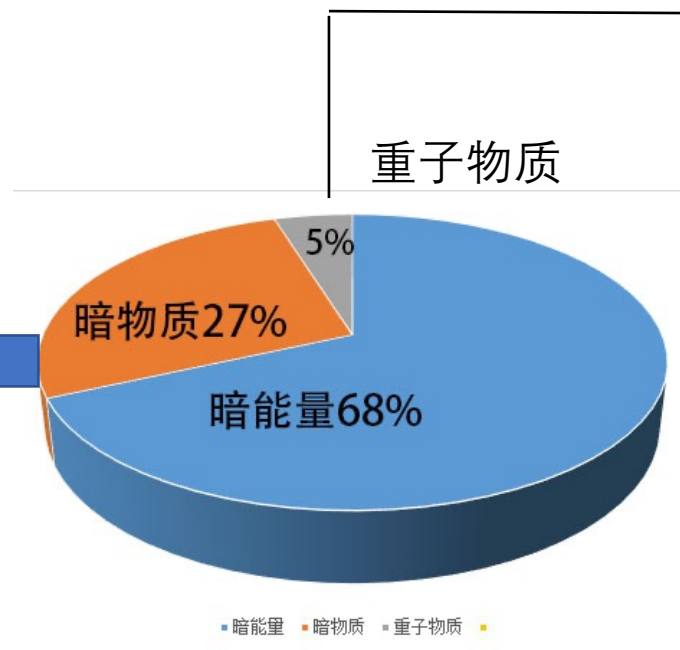
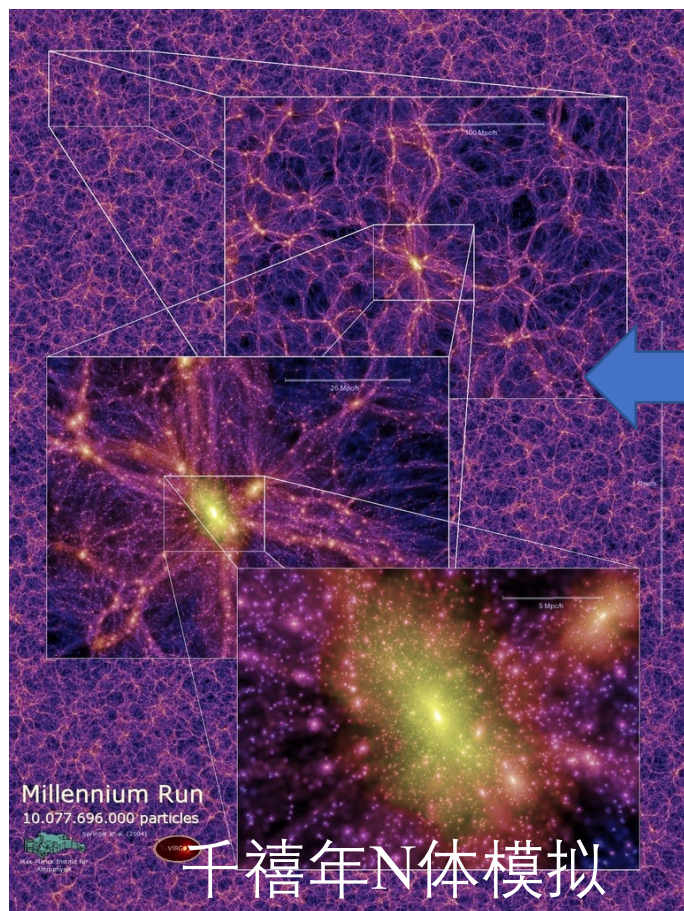


[doi: 10.1093/mnras/stae289](https://doi.org/10.1093/mnras/stae289)



3. Hydrodynamic Simulation (流体模拟)

N体模拟可以精确解析宇宙不同层级结构的形成演化，暗物质晕性质，但是观测信号主要来自恒星和气体

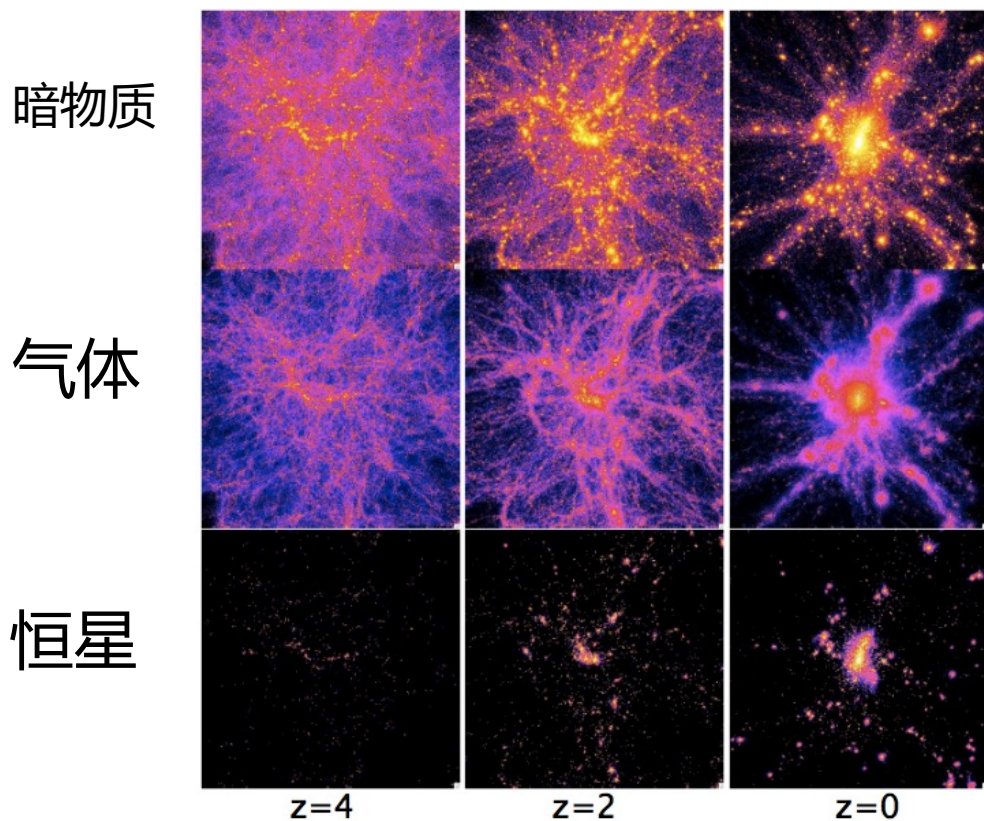


如何同时追踪重子气体，恒星，星系，黑洞的形成演化过程？

3. Cosmological Hydrodynamic Simulation (流体模拟)

N体 (暗物质) + 重子流体模拟

宇宙重子成分在与CMB脱耦后处于中性状态, 随后进入暗晕的部分气体逐渐转变为HI, H₂, 恒星



(1) 重子气体演化: 求解宇宙流体方程组

$$U_t + f(U)_x + g(U)_y + h(U)_z = F(t, U)$$

$$\begin{matrix} U & f & g & h \\ \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ E \end{pmatrix}, & \begin{pmatrix} \rho u \\ \rho u^2 + P \\ \rho uv \\ \rho uw \\ u(E + P) \end{pmatrix}, & \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + P \\ \rho vw \\ v(E + P) \end{pmatrix}, & \begin{pmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + P \\ w(E + P) \end{pmatrix}. \end{matrix}$$

$$E = \frac{P}{\gamma - 1} + \frac{1}{2}\rho(u^2 + v^2 + w^2)$$

$$F(t, U) = \begin{pmatrix} 0 \\ -\frac{\dot{a}}{a}\rho\mathbf{V} + \rho\mathbf{G} \\ -2\frac{\dot{a}}{a}E + \rho\mathbf{V} \cdot \mathbf{G} - \Lambda_{\text{net}} \end{pmatrix},$$

引力势, 与N体耦合
冷却加热

(2) + 气体冷却、恒星形成等物理过程

3.1 Hydrodynamic Solvers (流体方程求解方法)

(a) Eulerian (Grid/Mesh based, Finite Difference, Finite Volume)

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} + \frac{\partial G(U)}{\partial y} + \frac{\partial H(U)}{\partial z} = S$$

Space

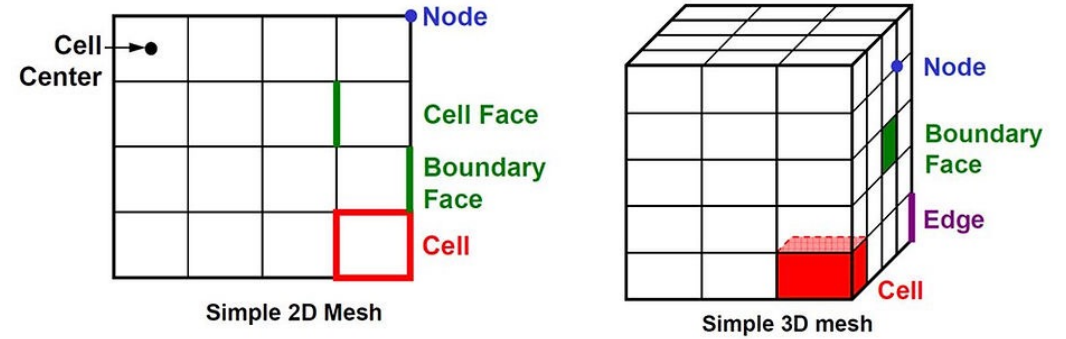
$$F(U)_{x,x=x_i} \simeq \frac{\hat{F}_{i+1/2} - \hat{F}_{i-1/2}}{\Delta x} \quad \text{accuracy is limited}$$

Time

$$U^{(1)} = U^n + \Delta t L(U^n, t^n)$$

$$U^{(2)} = \frac{3}{4}U^n + \frac{1}{4}U^{(1)} + \frac{1}{4}\Delta t L(U^{(1)}, t^n + \Delta t)$$

$$U^{n+1} = \frac{1}{3}U^n + \frac{2}{3}U^{(2)} + \frac{2}{3}\Delta t L(U^{(2)}, t^n + \frac{1}{2}\Delta t)$$

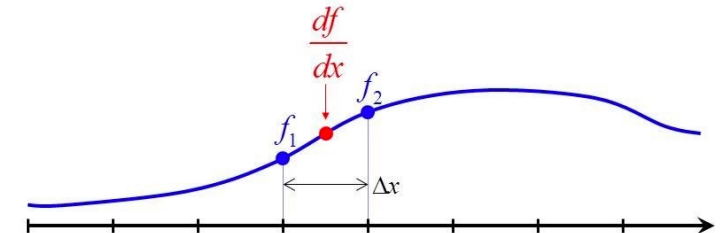


The Basic Finite-Difference Approximation



$$\frac{df_{1.5}}{dx} \approx \frac{f_2 - f_1}{\Delta x}$$

second-order accurate
first-order derivative



This is the only finite-difference approximation we will use in this course!

3.1 Hydrodynamic Solvers

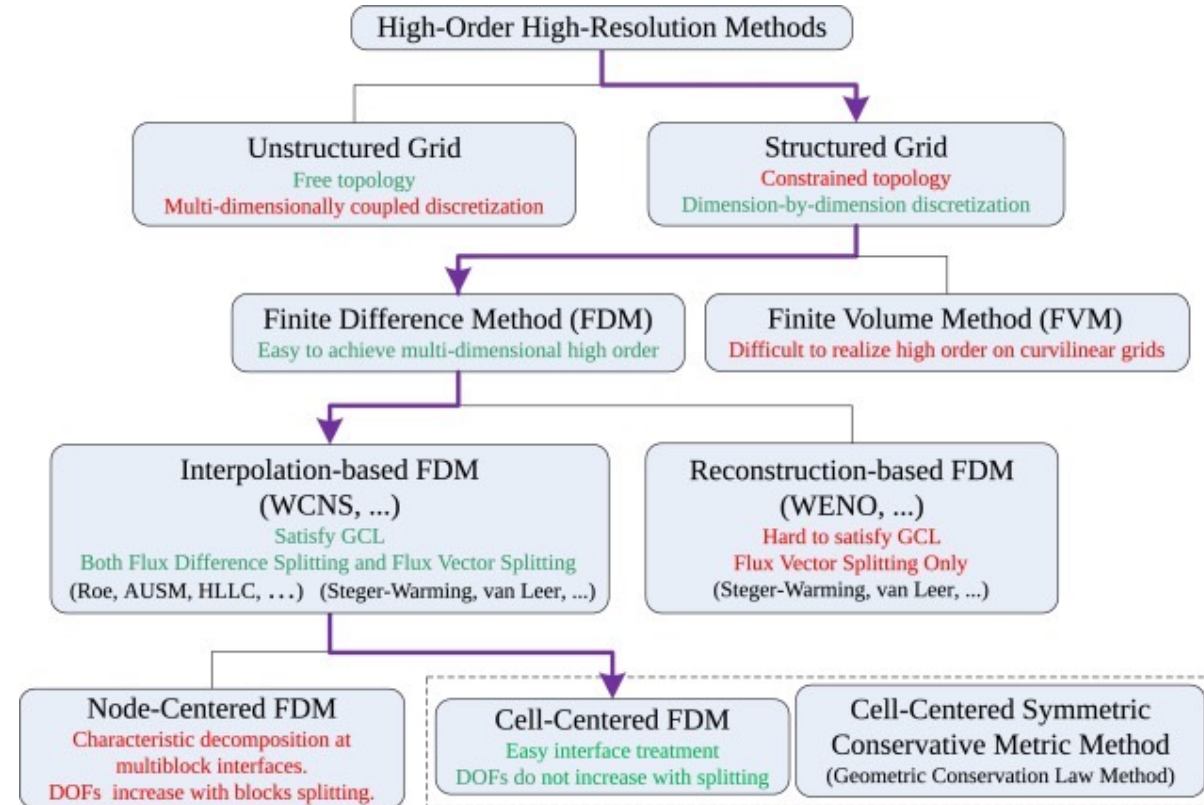
(a) Eulerian (Grid/Mesh based, Finite Difference, Finite Volume)

Different Finite Difference Schemes

$$\frac{d\phi}{dx} \approx \frac{\phi(x + \Delta x) - \phi(x)}{\Delta x} + \mathcal{O}(\Delta x) = \frac{\phi_{i+1} - \phi_i}{\Delta x}$$

$$\frac{d\phi}{dx} \approx \frac{\phi(x) - \phi(x - \Delta x)}{\Delta x} + \mathcal{O}(\Delta x) = \frac{\phi_i - \phi_{i-1}}{\Delta x}$$

$$\frac{d\phi}{dx} \approx \frac{\phi(x + \Delta x) - \phi(x - \Delta x)}{2\Delta x} + \mathcal{O}(\Delta x^2) = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}$$



shortcoming: resolution is limited for fixed grid/mesh

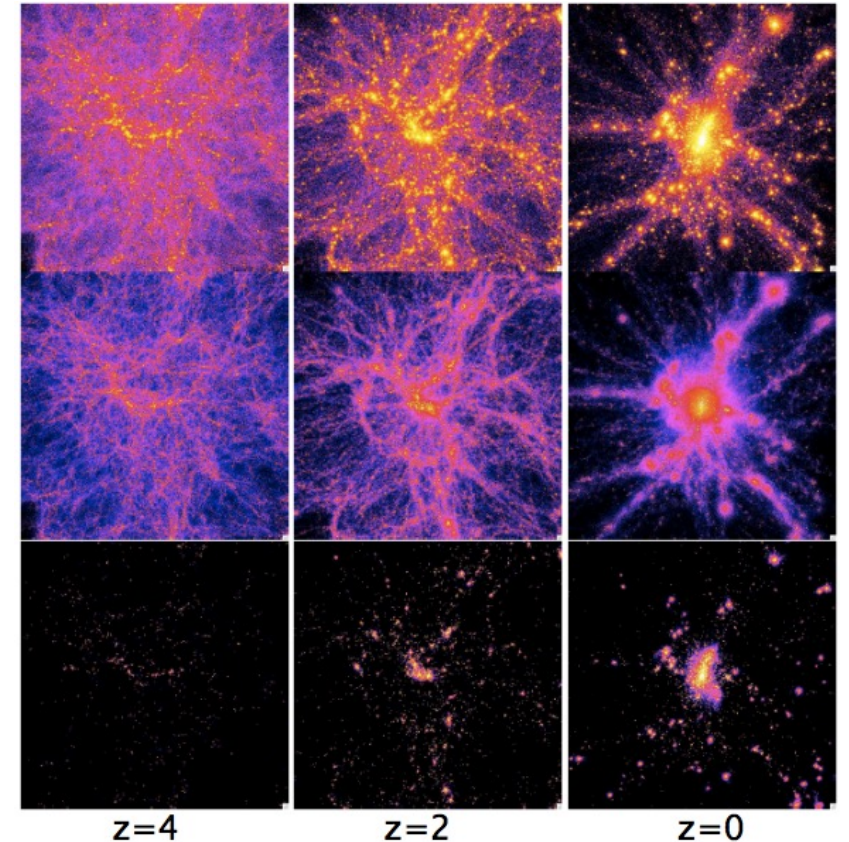
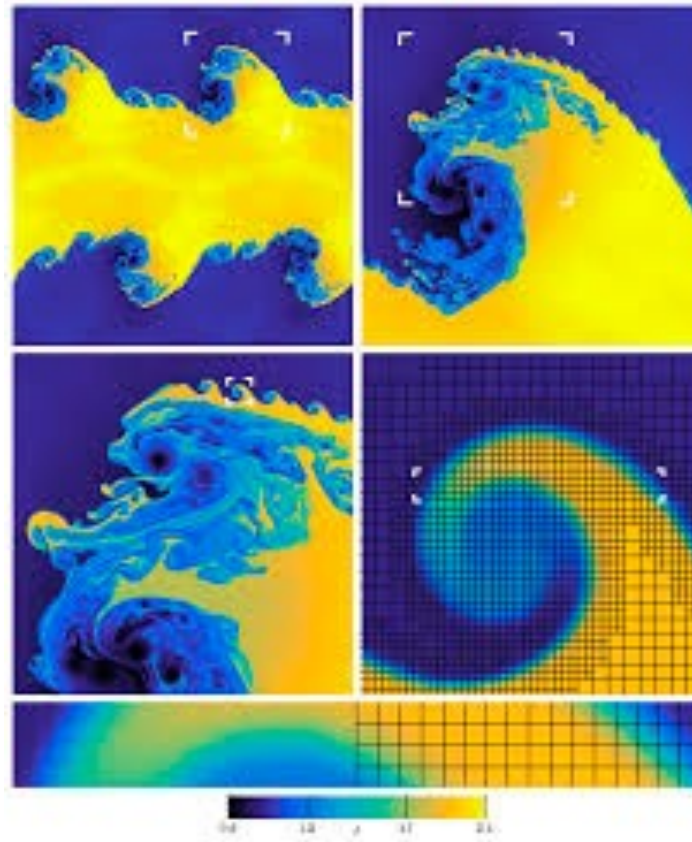
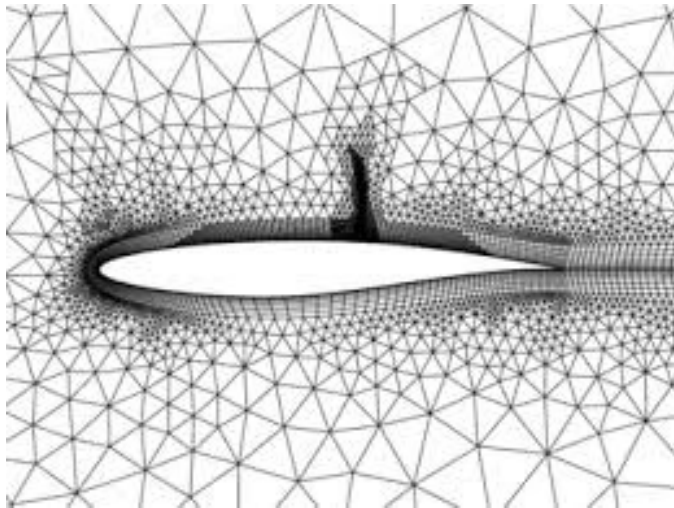
e.g. box size 100 Mpc/h, 1024^3 grid, $dx \sim 100$ kpc/h

3.1 Hydrodynamic Solvers

(a) Eulerian (Grid/Mesh based, Finite Difference, Finite Volume)

Adaptive Mesh Refinement (AMR), Moving Mesh

(自适应、动态网格，提高对高密度、结构形成区域的解析分辨能力)



3.1 Hydrodynamic Solvers

(b) Lagrangian (Smooth-Particle Hydrodynamics, SPH)

$$A(\mathbf{r}) = \int A(\mathbf{r}') \delta(\mathbf{r} - \mathbf{r}') d\mathbf{r}'$$

introduce a SPH kernel $W(\mathbf{r}, h)$ $\langle A(\mathbf{r}) \rangle = \int A(\mathbf{r}') W(\mathbf{r} - \mathbf{r}') d\mathbf{r}'$

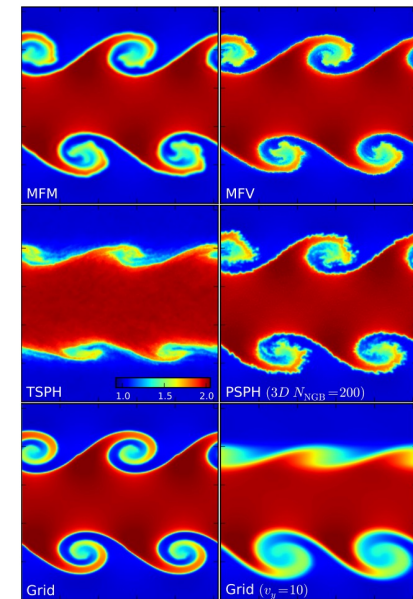
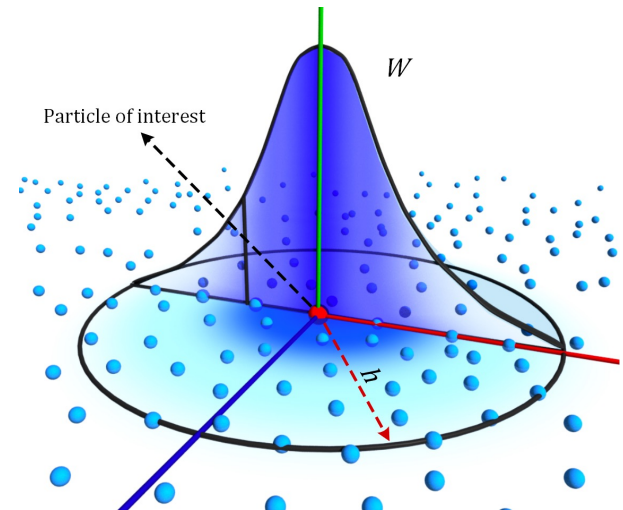
$$\int W(\mathbf{x}) d\mathbf{x} = 1, \quad \lim_{h \rightarrow 0} W(\mathbf{x}, h) = \delta(\mathbf{x}).$$

$$\int \frac{A(\mathbf{r}')}{\rho(\mathbf{r}')} W(\mathbf{r} - \mathbf{r}', h) \rho(\mathbf{r}') d\mathbf{r}'.$$

N sph particles

$$\langle A(\mathbf{r}) \rangle = \sum_{j=1}^N m_j \frac{A_j}{\rho_j} W(\mathbf{r} - \mathbf{r}_j, h), \quad \rho(\mathbf{r}) = \sum_{i=1}^N m_i W(\mathbf{r} - \mathbf{r}_i, h)$$

$$\frac{d\mathbf{v}_j}{dt} = - \sum_{i=1}^N m_i \left(\frac{P_j}{\rho_j^2} + \frac{P_i}{\rho_i^2} \right) \nabla_j W_{ij}$$



More: Volker Springel, ARA&A

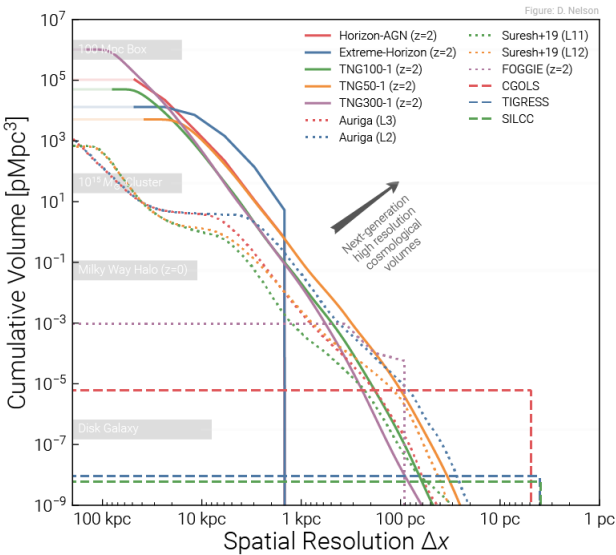
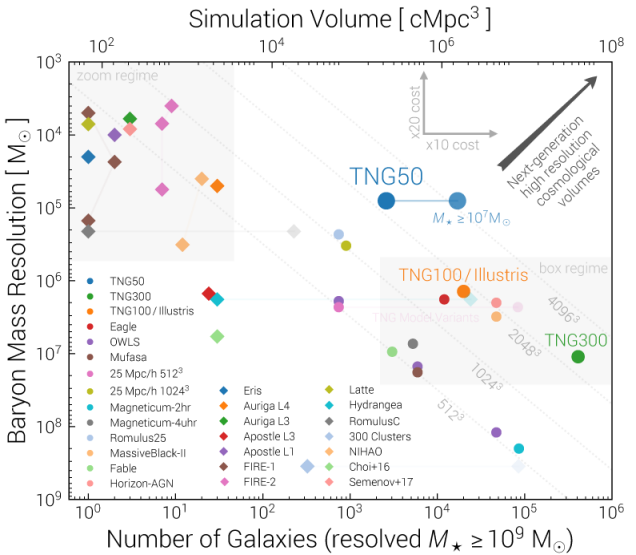
3.1 Hydrodynamic Solvers

代表性宇宙学模拟软件技术方法、流体模拟分辨率

Table 1: Major galaxy formation simulation codes

code name	gravity treatment ^a	hydrodynamics treatment ^b	parallelization technique ^c	code availability ^d	primary reference
ART	PM/ML	AMR	data-based	public	Kravtsov (1997) ²⁷
RAMSES	PM/ML	AMR	data-based	public	Teyssier (2002) ³⁸
GADGET-2/3	TreePM	SPH	data-based	public	Springel (2005) ³⁹
Arepo	TreePM	MMFV	data-based	public	Springel (2010) ⁴⁰
Enzo	PM/MG	AMR	data-based	public	Bryan et al. (2014) ⁴¹
ChaNGa ^e	Tree/FM	SPH	task-based	public	Menon et al. (2015) ^{42–44}
GIZMO ^f	TreePM	MLFM/MLFV	data-based	public	Hopkins et al. (2015) ⁴⁵
HACC	TreePM/P ³ M	CRK-SPH	data-based	private	Habib et al. (2016) ⁴⁶
PKDGRAV3	Tree/FM	—	data-based	public	Potter et al. (2017) ⁴⁷
Gasoline2	Tree	SPH	task-based	public	Wadsley et al. (2017) ⁴⁸
SWIFT	TreePM/FM	SPH	task-based	public	Schaller et al. (2018) ⁴⁹

^a PM: particle-mesh; TreePM: tree + PM, FM: fast multipole, P³M: particle-particle-particle-mesh; ML: multilevel; MG: multigrid
^b SPH: smoothed particle hydrodynamics, CRK-SPH: conservative reproducing kernel smoothed particle hydrodynamics , AMR: adaptive-mesh-refinement, MMFV: moving-mesh finite volume, MLFM/MLFV: mesh-free finite mass / finite volume
^c data-based: data parallelism focuses on distributing data across different nodes, which operate on the data in parallel; task-based: task parallelism focuses on distributing tasks concurrently performed
^d private: private code; public: publicly available code (in some cases with limited functionality)
^e gravity solver is based on PKDGRAV3
^f based on the GADGET-3 code



3.2 Baryonic Physics (重子物理过程)

1990s年的流体模拟表明在较大尺度($> \sim 10$ Mpc/h), 重子分布与暗物质接近。在中小尺度, 理论预期**冷却加热、恒星形成、恒星与黑洞反馈等物理过程**, 使重子与暗物质出现偏离; N体+流体+重子物理模拟是近30年的努力

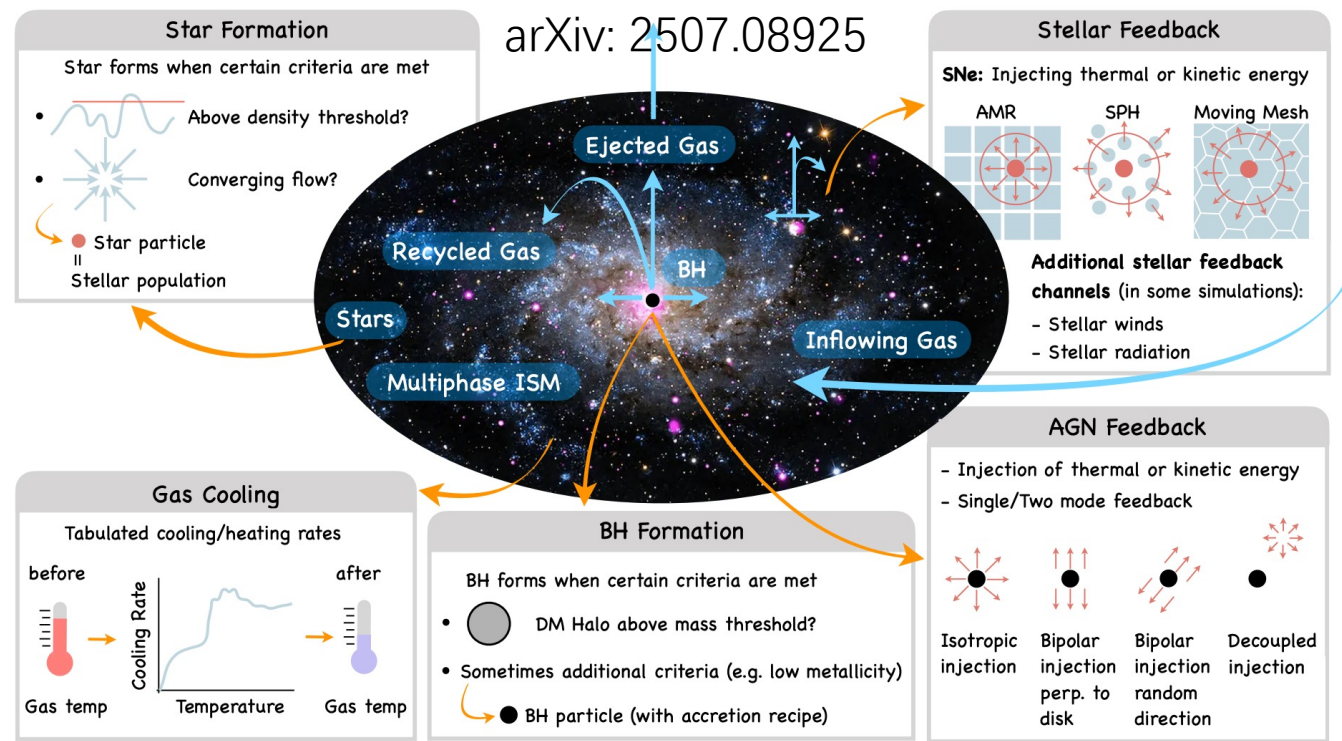
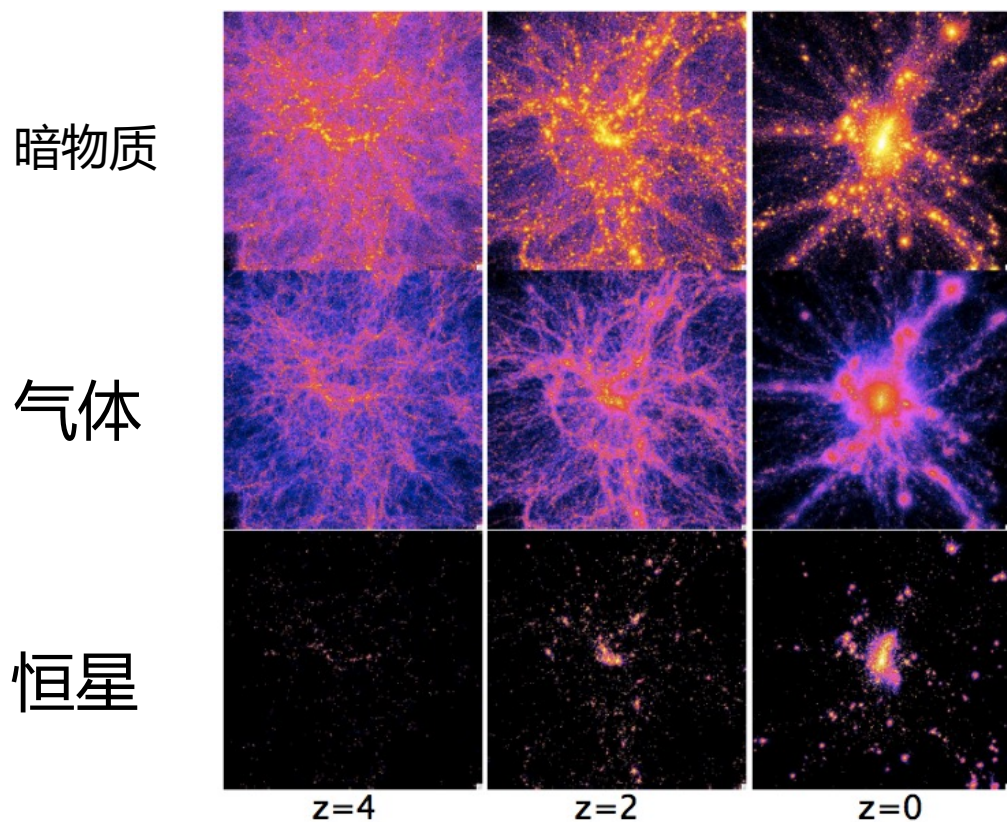


Fig. 2 Illustration of key baryonic processes in galaxies, using the Triangulum Galaxy (M33) as an example (Image credit: X-ray:

3.2 Baryonic Physics (重子物理过程)

模拟分辨率 $dx >$ 物理过程典型尺度, 用亚网格(sub-grid)模型近似处理

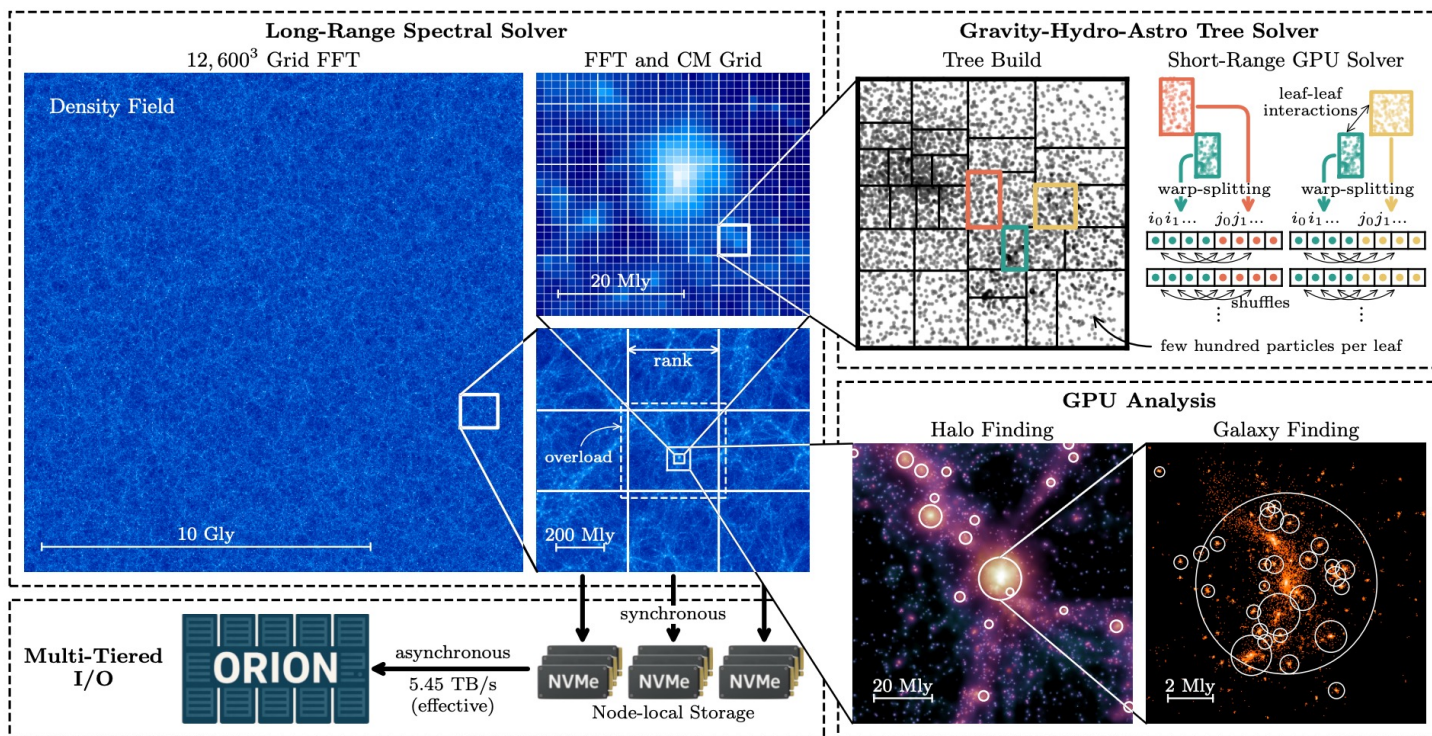
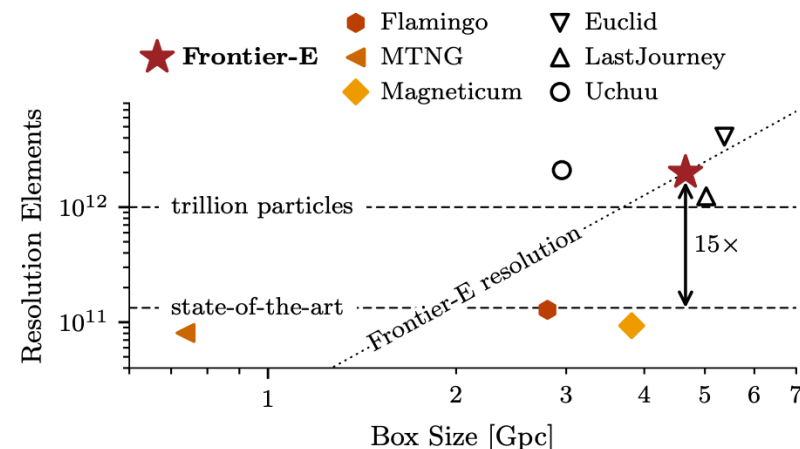
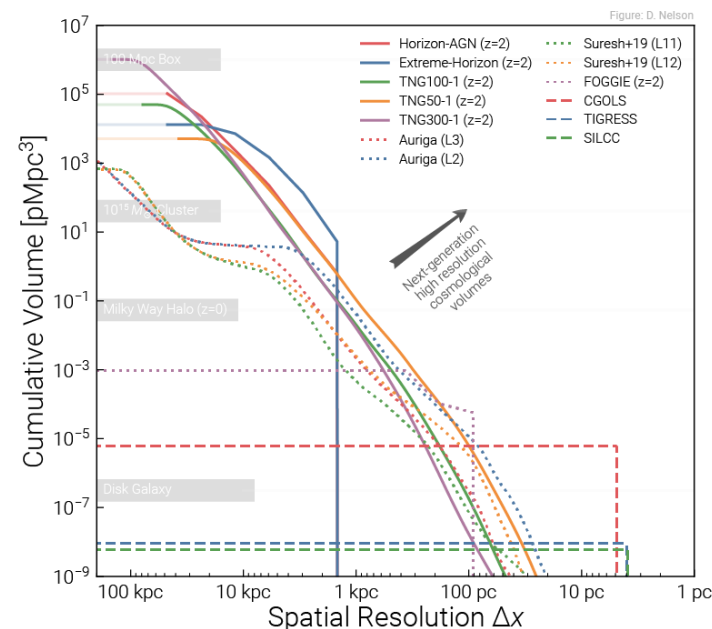
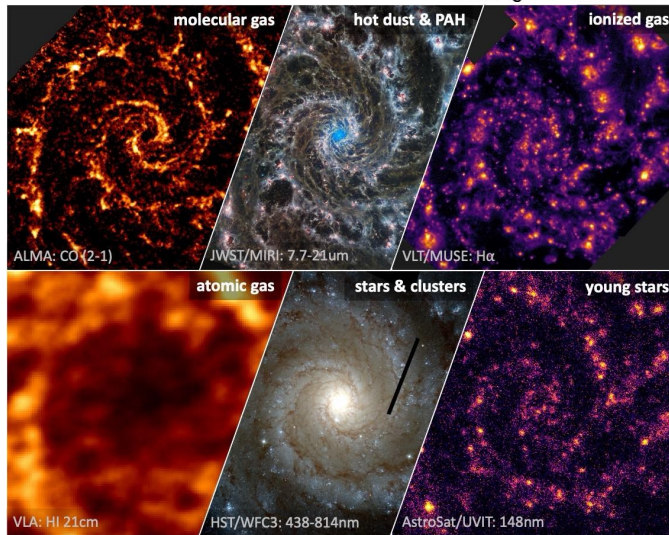
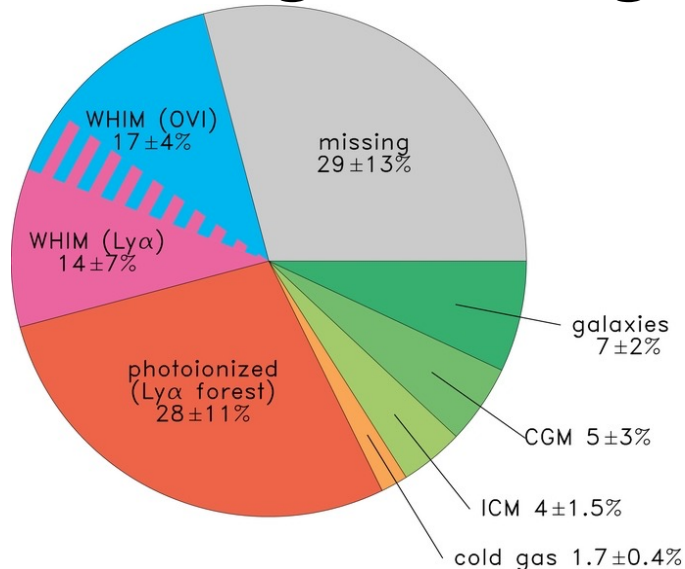


Figure 2: CRK-HACC architecture diagram of the primary simulation components, spanning gigalight-year volumes down to short-range forces acting on individual particles. The distributed long-range spectral FFT solver operates over the global domain across all nodes (top left). After k-d trees are constructed in chaining mesh bins, the entire overloaded rank is pushed to the GPU (top right), where short-range force operators process leaf-leaf interactions using warp-splitting kernels. Cluster-based in situ analysis is also GPU-accelerated (bottom right). Multi-tier I/O (bottom left) outputs data using synchronous writes to node-local NVMe SSDs, which bleed data to the PFS asynchronously. For Frontier-E, the time-to-solution contributions from the long-range solver, tree build, short-range solver, in situ analysis, and I/O were {1.7%, 1.7%, 79.6%, 11.6%, and 2.6%}, respectively. Over 90% of solver time was executed on the GPU; see Section 7.2.

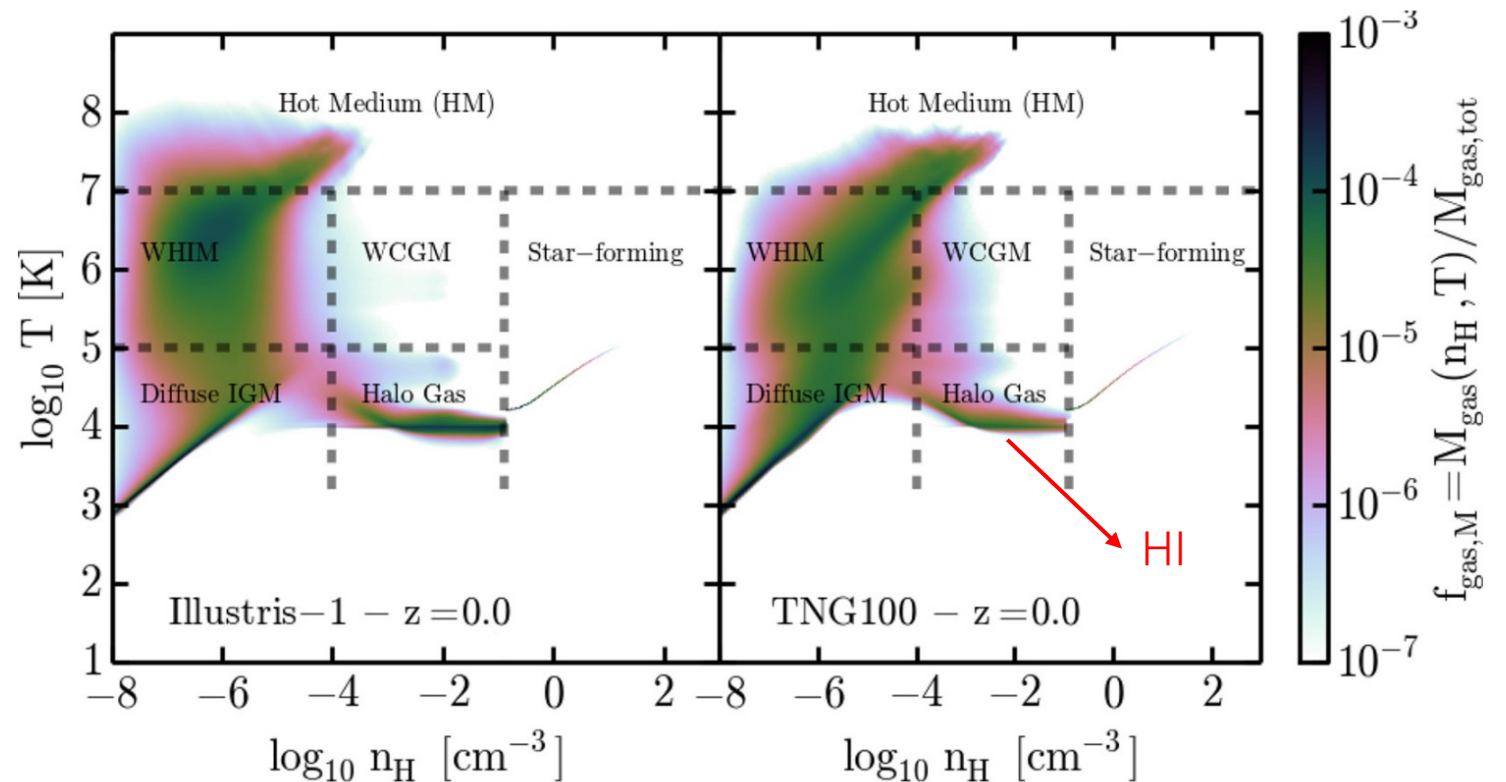


3.2 Baryonic Physics

➤ gas cooling & heating, metals, chemicals



引力加热，宇宙紫外背景加热，辐射冷却与加热综合作用下，重子气体处于多相状态



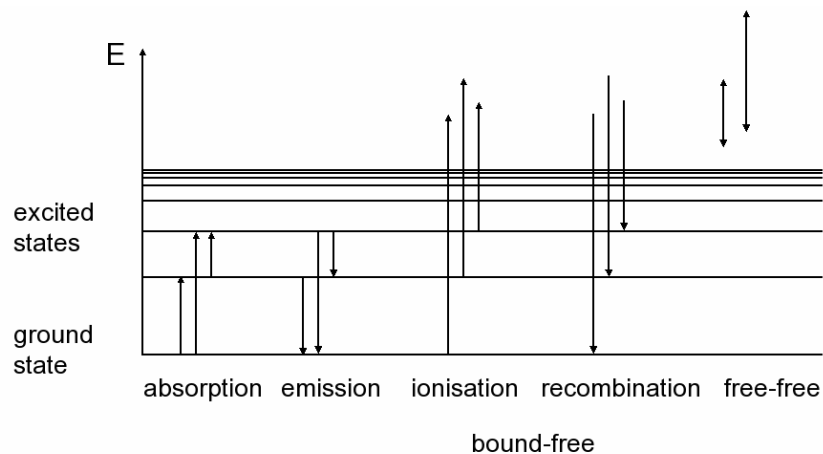
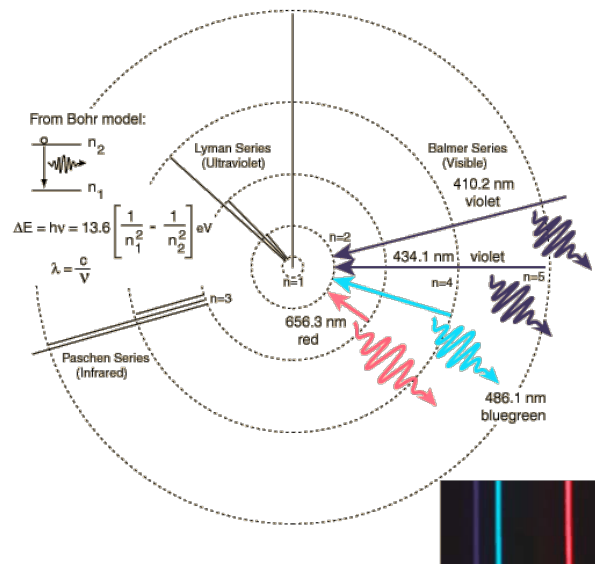
3.2 Baryonic Physics

➤ gas cooling & heating , metals, chemicals

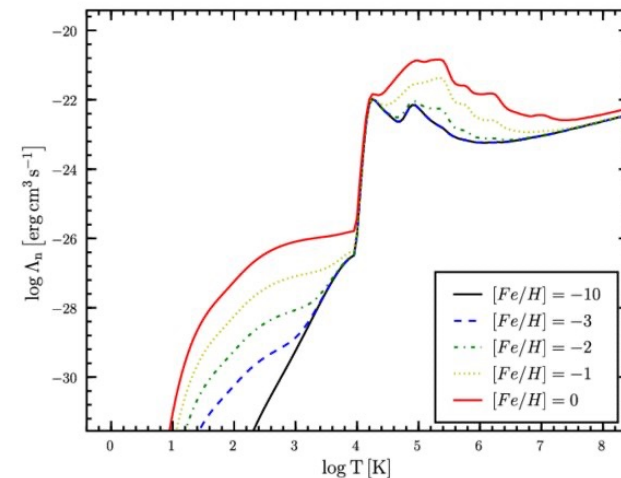
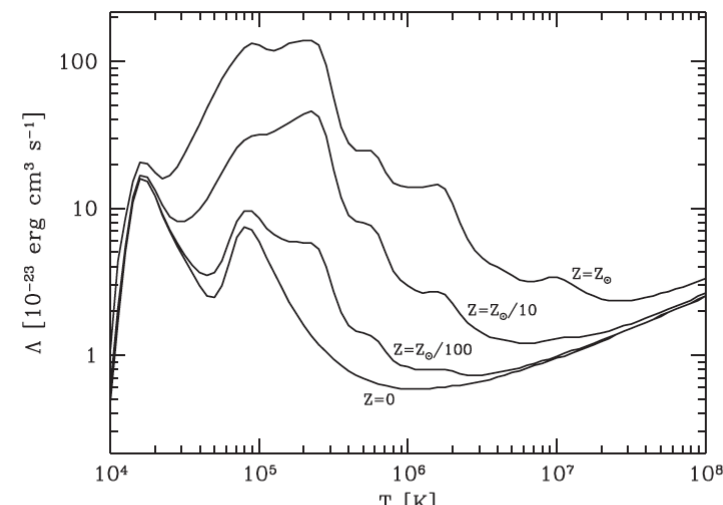
Calculation: energy loss due to cooling per unit volume

$$\Delta E = n^2 \Lambda(T, Z) \Delta t$$

- Atomic, molecular processes
- Compton scattering, Bound-bound, Bound-free, Free-bound, Free-free



Note: gas metallicity evolves in simulation.

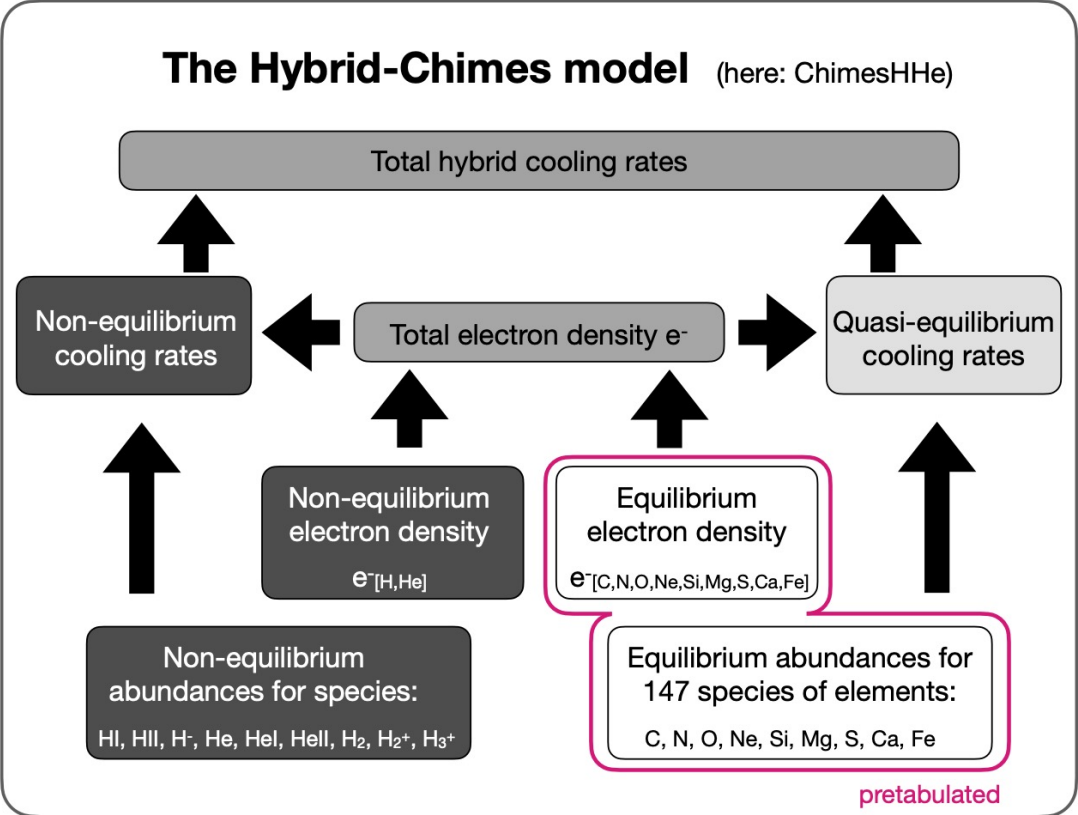


不同金属丰度冷却率

3.2 Baryonic Physics

➤ gas cooling & heating , metals, chemicals

Pretabulated cooling function from ISM-Chemical models

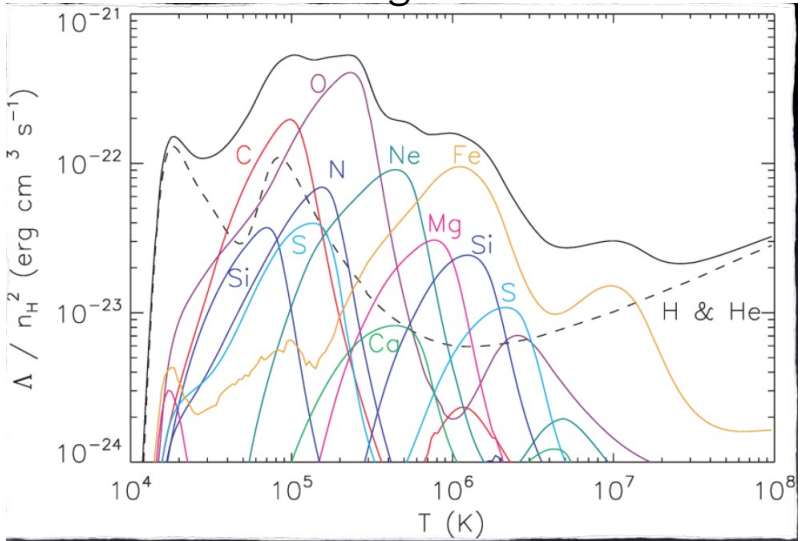


Ploeckinger et al. 2025

Table B1. Summary of primordial and molecular reactions.

Reaction no. ^a	Reaction	Reference ^b
1	$\text{H} + \text{e}^- \rightarrow \text{H}^- + \gamma$	1
2	$\text{H}^- + \text{H} \rightarrow \text{H}_2 + \text{e}^-$	2
3	$\text{H} + \text{H}^+ \rightarrow \text{H}_2^+ + \gamma$	3
4	$\text{H} + \text{H}_2^+ \rightarrow \text{H}_2 + \text{H}^+$	4
5	$\text{H}^- + \text{H}^+ \rightarrow \text{H} + \text{H}$	5
6	$\text{H}_2^+ + \text{e}^- \rightarrow \text{H} + \text{H}$	6
7	$\text{H}_2 + \text{H}^+ \rightarrow \text{H}_2^+ + \text{H}$	7
8	$\text{H}_2 + \text{e}^- \rightarrow \text{H} + \text{H} + \text{e}^-$	8
9	$\text{H}_2 + \text{H} \rightarrow \text{H} + \text{H} + \text{H}$	9, 10
10	$\text{H}_2 + \text{H}_2 \rightarrow \text{H}_2 + \text{H} + \text{H}$	11
11	$\text{H} + \text{e}^- \rightarrow \text{H}^+ + \text{e}^- + \text{e}^-$	12
13 ^c	$\text{H}^+ + \text{e}^- \rightarrow \text{H} + \gamma$	13

Richings et al. 2014



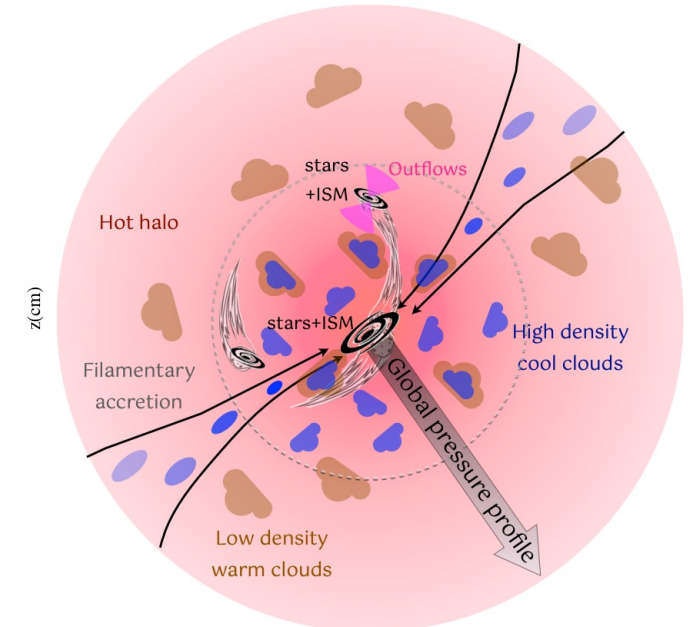
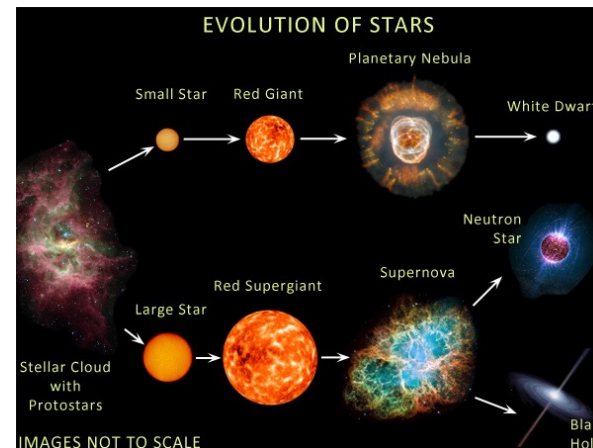
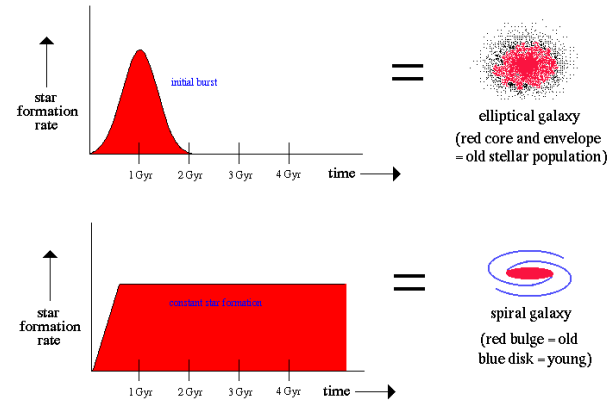
不同元素对冷却的贡献

3.2 Baryonic Physics

➤ Star formation, evolution and stellar feedback



Note: sub-grid physics models can vary significantly across different codes



3.2 Baryonic Physics

star formation sub-grid models

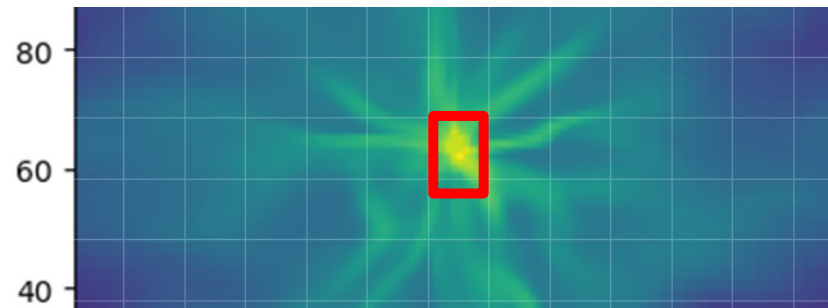
SF laws from obs. and theory

$$\Sigma_{\text{SFR}} \propto \Sigma_{\text{gas}}^N$$

$$\Sigma_{\text{SFR}} = \epsilon_{\text{ff}} \frac{f_{\text{mol}} \Sigma_{\text{gas}}}{t_{\text{ff}}}$$

$$t_{\text{ff}} = (3\pi/32G\rho_g)^{-1/2}$$

$$\epsilon_{\text{ff}} = \frac{t_{\text{ff}}(n_{\text{th}})}{t_{\text{dep},0}}$$



- **Gadget, Illustris, TNG series (gas res. $\sim 100\text{pc-kpc}$)**

$$\dot{m}_* = (1 - \beta) \frac{m_g}{t_*} \equiv \frac{m_g}{t_{\text{dep}}}, \quad n_{\text{th}} \sim 0.13 \text{ cm}^{-3}$$

$$t_{\text{dep},0} \sim 2.2 \text{ Gyr}$$

- **EAGLE (gas res. $\sim 100 \text{ pc- kpc}$)**

$$\dot{m}_* \equiv \frac{m_g}{t_g} = m_g \frac{\dot{\rho}_*}{\rho_g} = A (1 \text{ M}_{\odot} \text{ pc}^{-2})^{-n} m_g \left(\frac{\gamma}{G} f_g P_{\text{tot}} \right)^{(n-1)/2}$$

$$n_{\text{H}}^*(Z) = \min \left[0.1 \text{ cm}^{-3} \left(\frac{Z}{0.002} \right)^{-0.64}, 10 \text{ cm}^{-3} \right]$$

3.2 Baryonic Physics

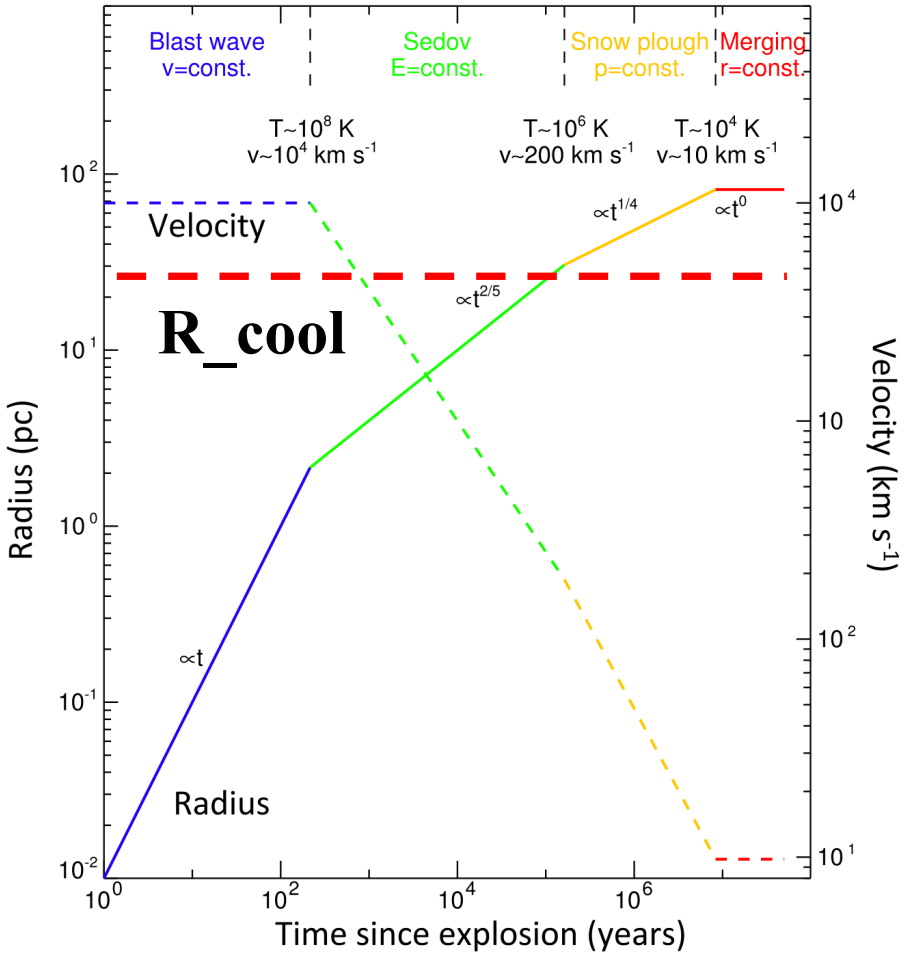
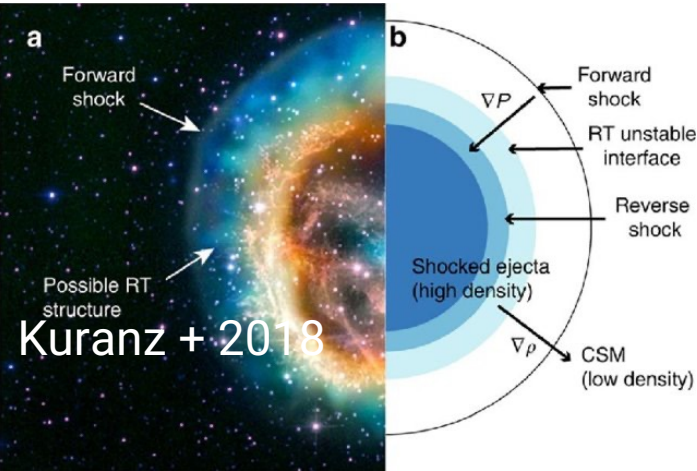
SNe feedback models

Resolution is often poor, must avoid over-cooling!

$$E_{\rm SN} = 10^{51} \rm{erg}$$

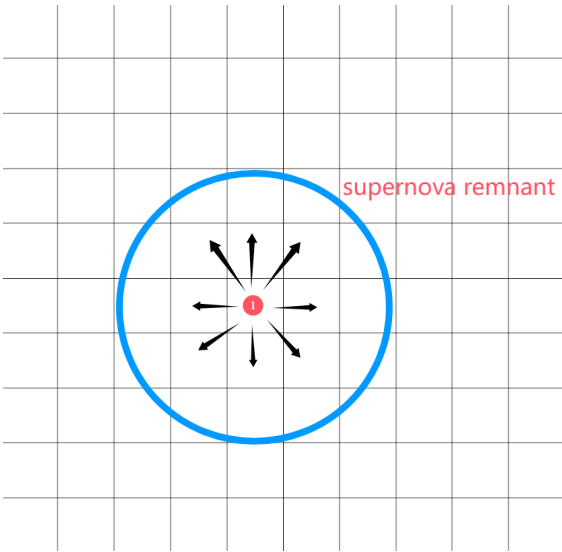
$$m_* \int_{m_d(t+\Delta t)}^{m_d(t)} \Phi(m) \, dm$$

同时向ISM反馈金属



Padmanabhan (2001)

$R_{\rm cool}(10^5 \rm{yr}) \sim 20 \rm{pc}$
 vs.
 TNG res. 100pc-kpc
 EAGLE res. 100 pc-kpc
 FIRE-2 res. 0.4-10 pc



3.2 Baryonic Physics

e.g. Varies sub-grid SN feedback models

EAGLE

Thermal only.
 Particles heated by $\Delta T_{\text{SF}} = 10^{7.5}$ K.
 Energy set by local ρ , Z .
 No hydrodynamic decoupling.
 Dalla Vecchia & Schaye (2012).

TNG

Thermal & kinetic.
 90% momentum, 10% thermal.
 η set by local metallicity.
 v_{wind} set by σ_{DM} , z .
 Wind elements decoupled.
 Pillepich et al. (2018).

SIMBA

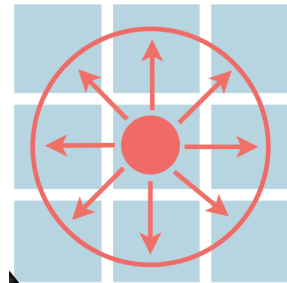
Thermal & kinetic.
 30% of wind particles injected "hot".
 $\eta(M_{\star})$ from FIRE (Anglés-Alcázar et al. 2017b).
 $v_{\text{wind}}(V_{\text{circ}})$ from FIRE (Muratov et al. 2015).
 Wind elements decoupled.
 Davé et al. (2019).

FIRE2

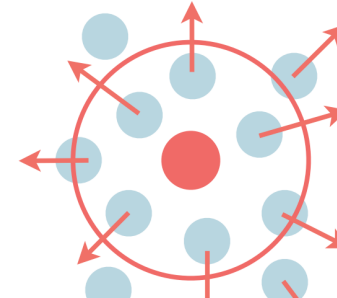
both momentum and thermal
 energy of mechanical ejecta

free parameters
 set by calibration

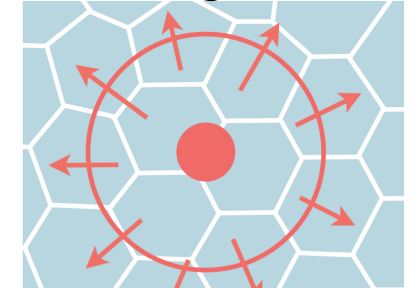
AMR



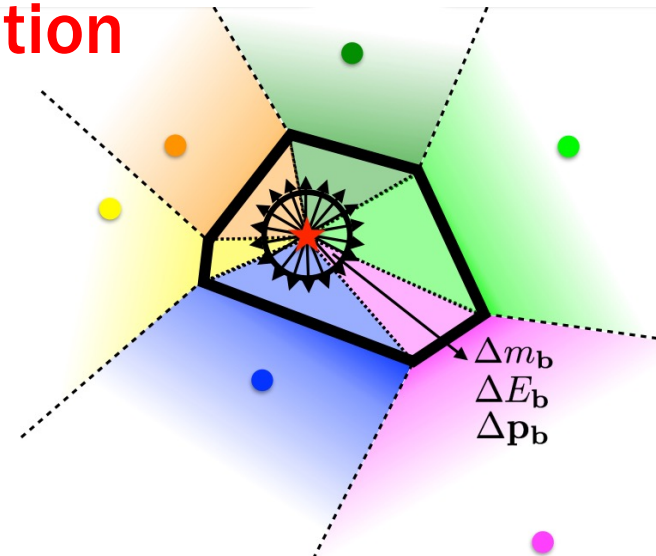
SPH



Moving Mesh



Feldmann & Bieri



Hopkins + 2017

4) Integrate ejecta over solid angle to faces

5) Verify conservation:

$$\begin{aligned} \sum \Delta E_b &= E_{\text{ej}} & \sum \Delta m_b &= m_{\text{ej}} \\ \sum \Delta p_b &= 0 & \sum |\Delta p_b| &= p_{\text{ej}} \end{aligned}$$

(correct faces if needed)

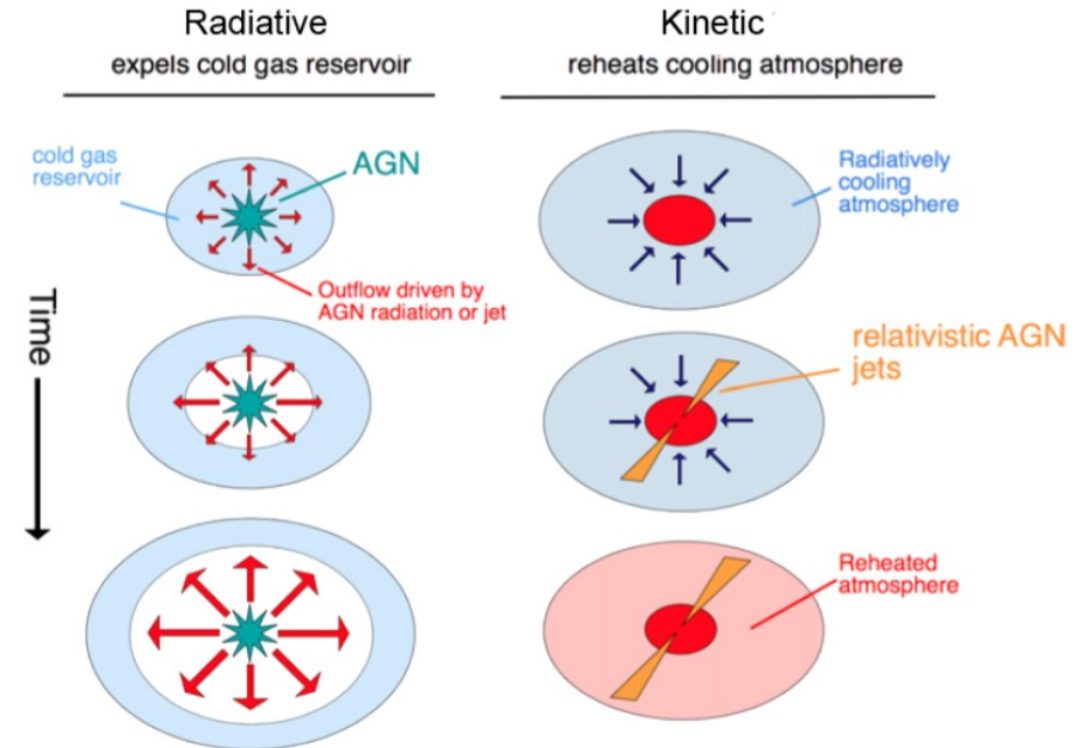
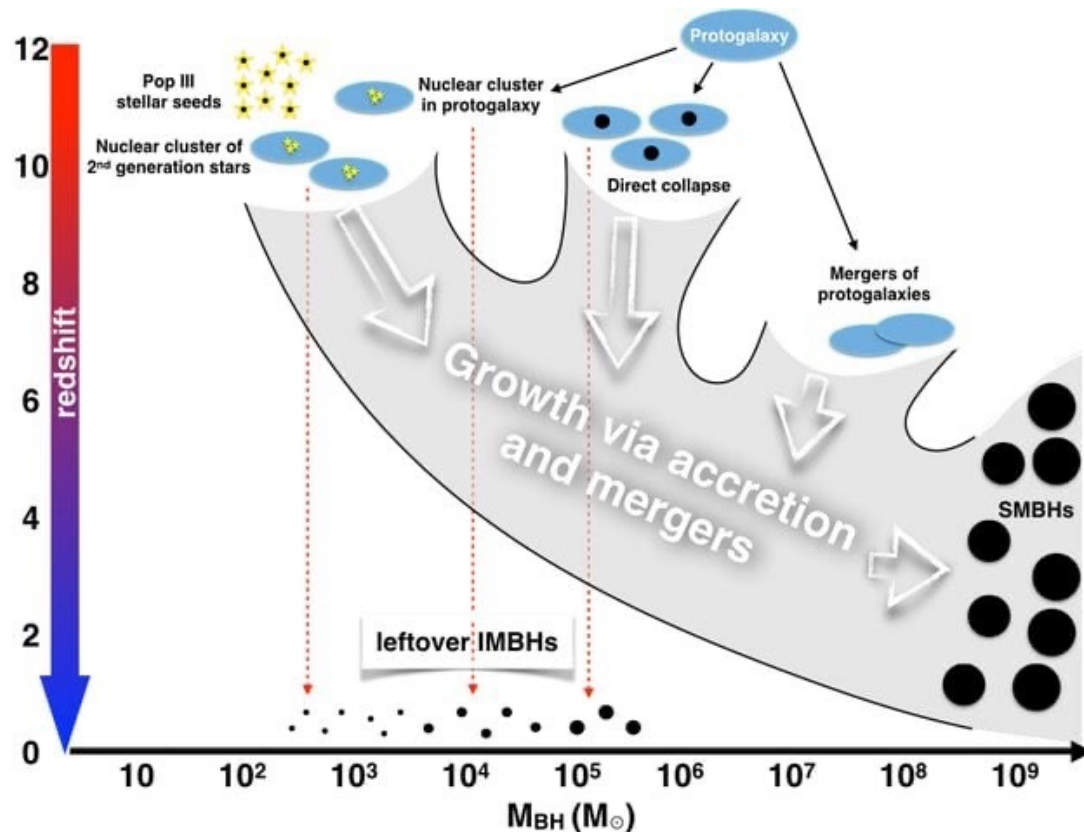
6) Boost back to "lab frame"
 (account for star-gas motion)

7) Couple ejecta fully-conservatively

3.2 Baryonic Physics

➤ Growth of supermassive black-hole and AGN feedback

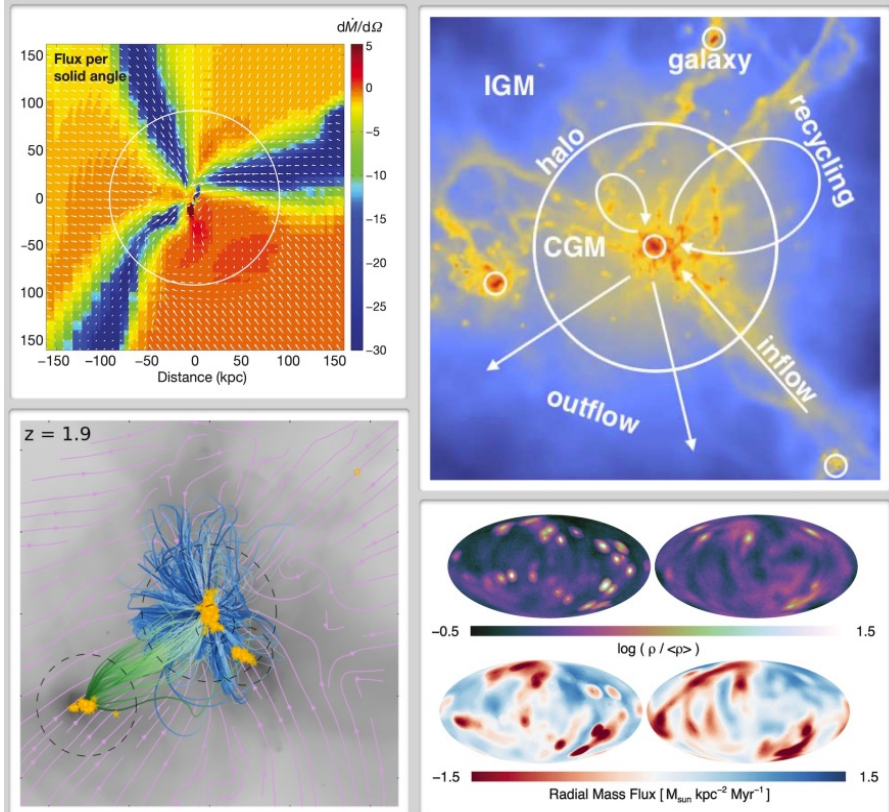
seed: $10^3 - 10^5 M_\odot$ accretion: Eddington, Bondi, ... feedback: radiation, thermal, kinetic



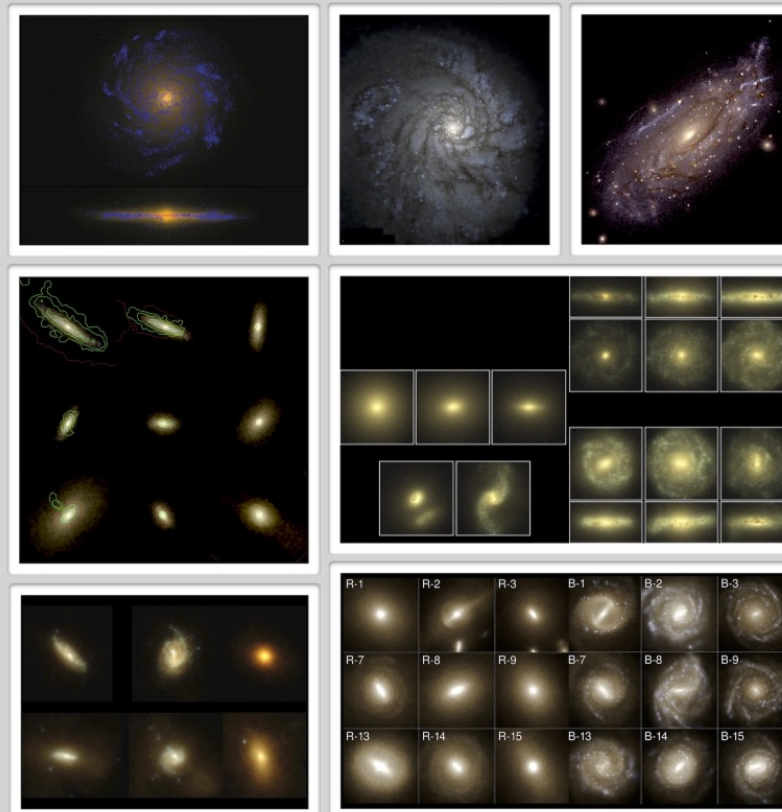
3. Cosmological/Galaxy Hydrodynamic Simulation: Successes

Advances in gravity/hydro solvers, baryonic physics and higher resolution have driven the ‘success’ of galaxy simulations over the past decade.

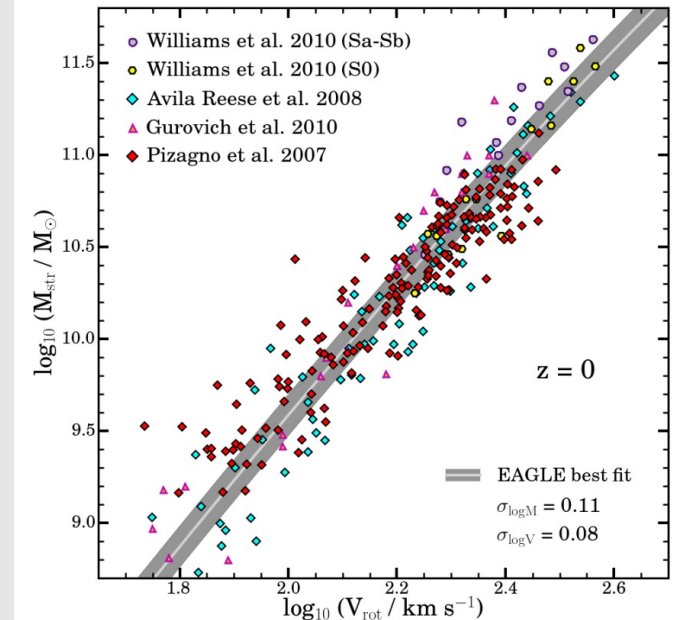
Baryonic Cycle



Morphology



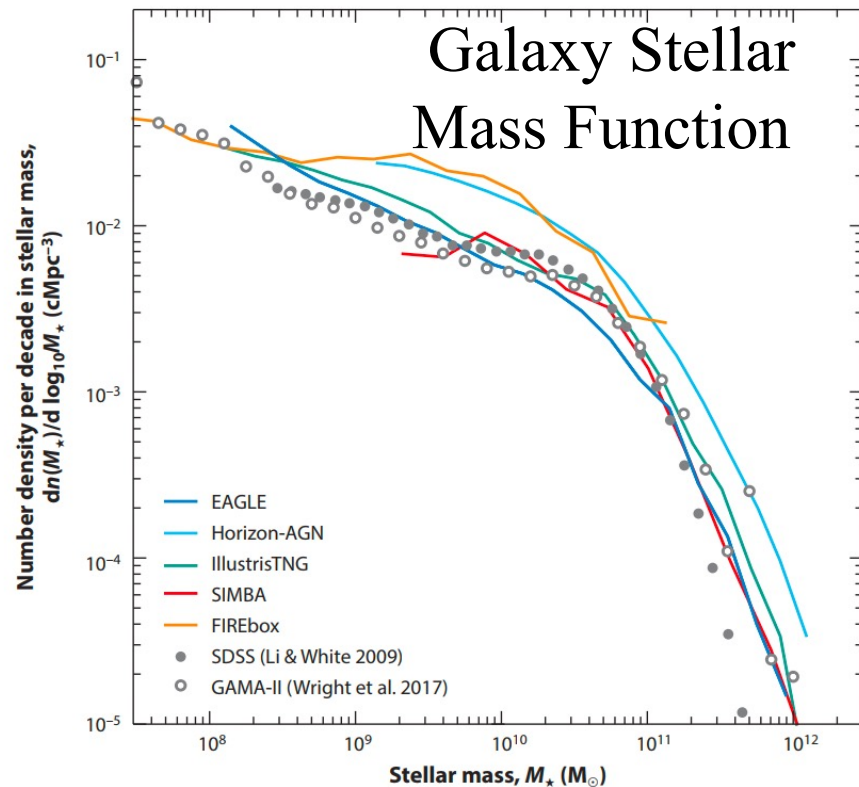
Scaling relations



Tully-Fisher relation

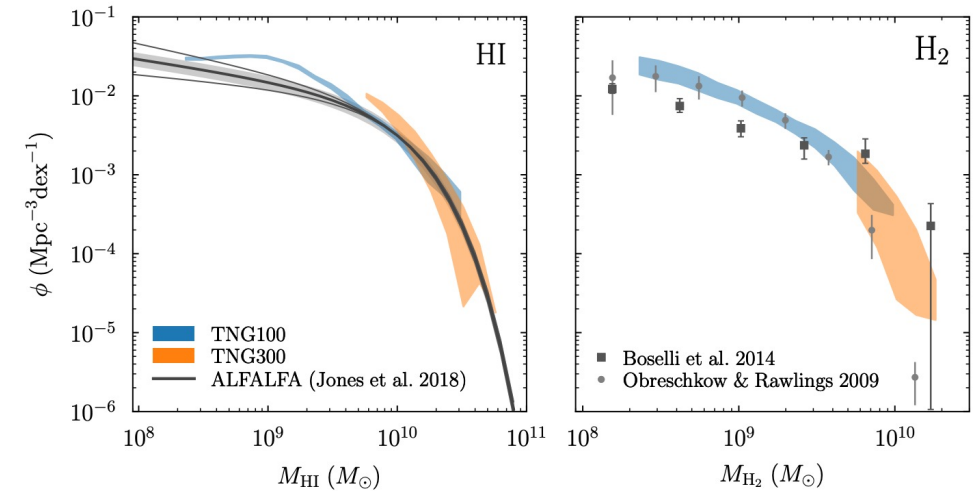
3. Cosmological/Galaxy Hydrodynamic Simulation: Successes

‘reproduce’ statistical properties
of stars and gas in galaxies

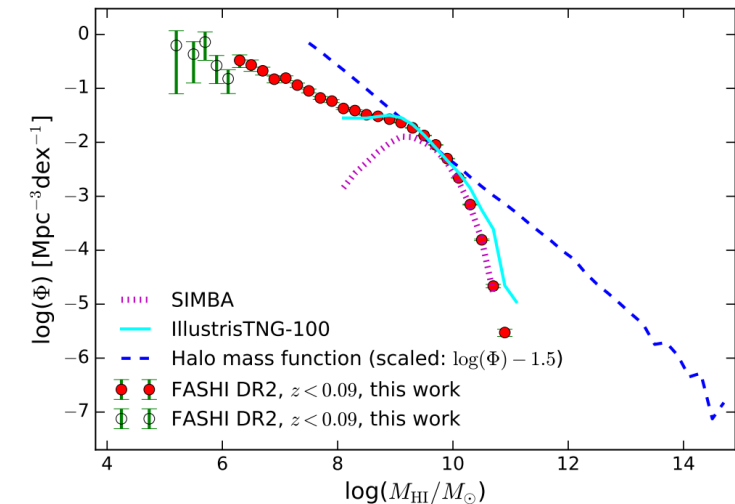


Crain & van de Voort 23

HI/H₂ mass
function



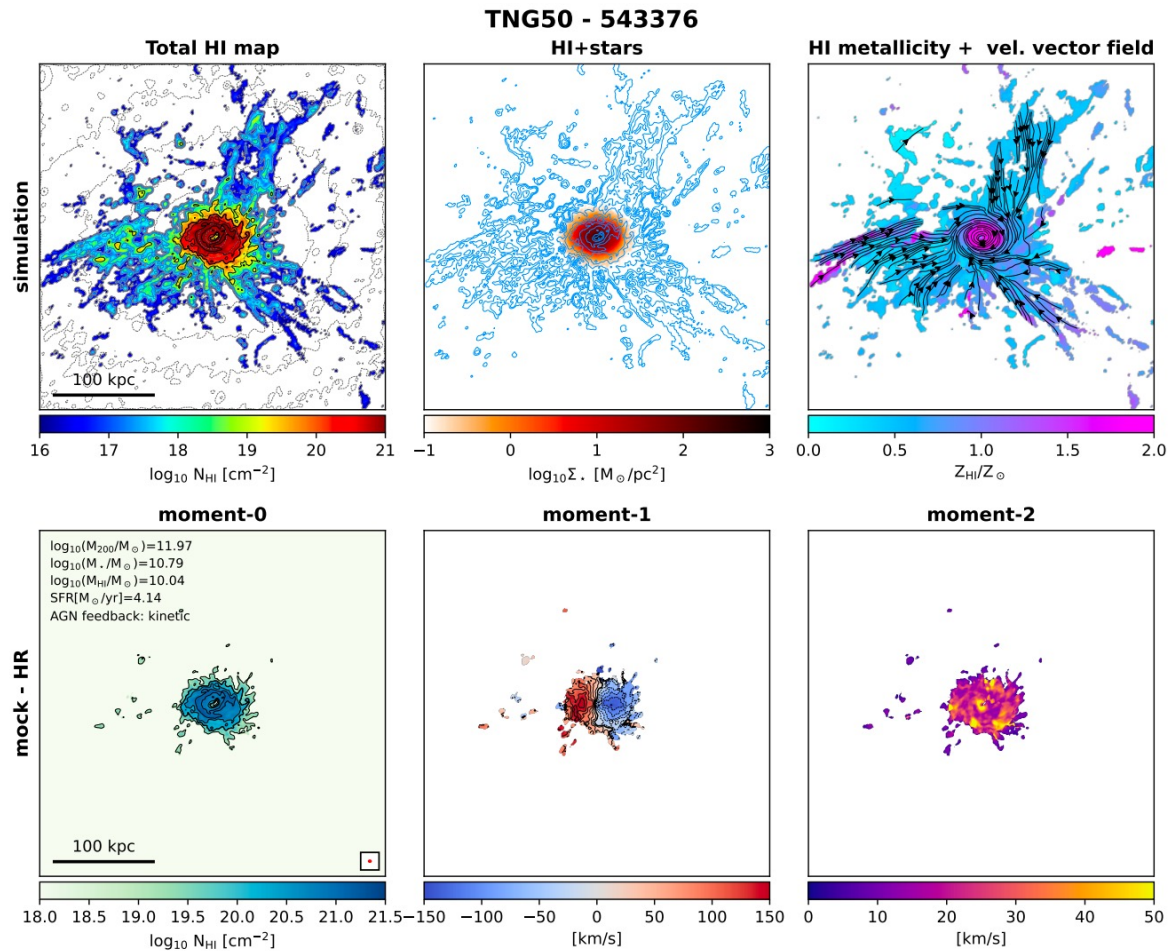
Diemer et al. arXiv:1902.10714



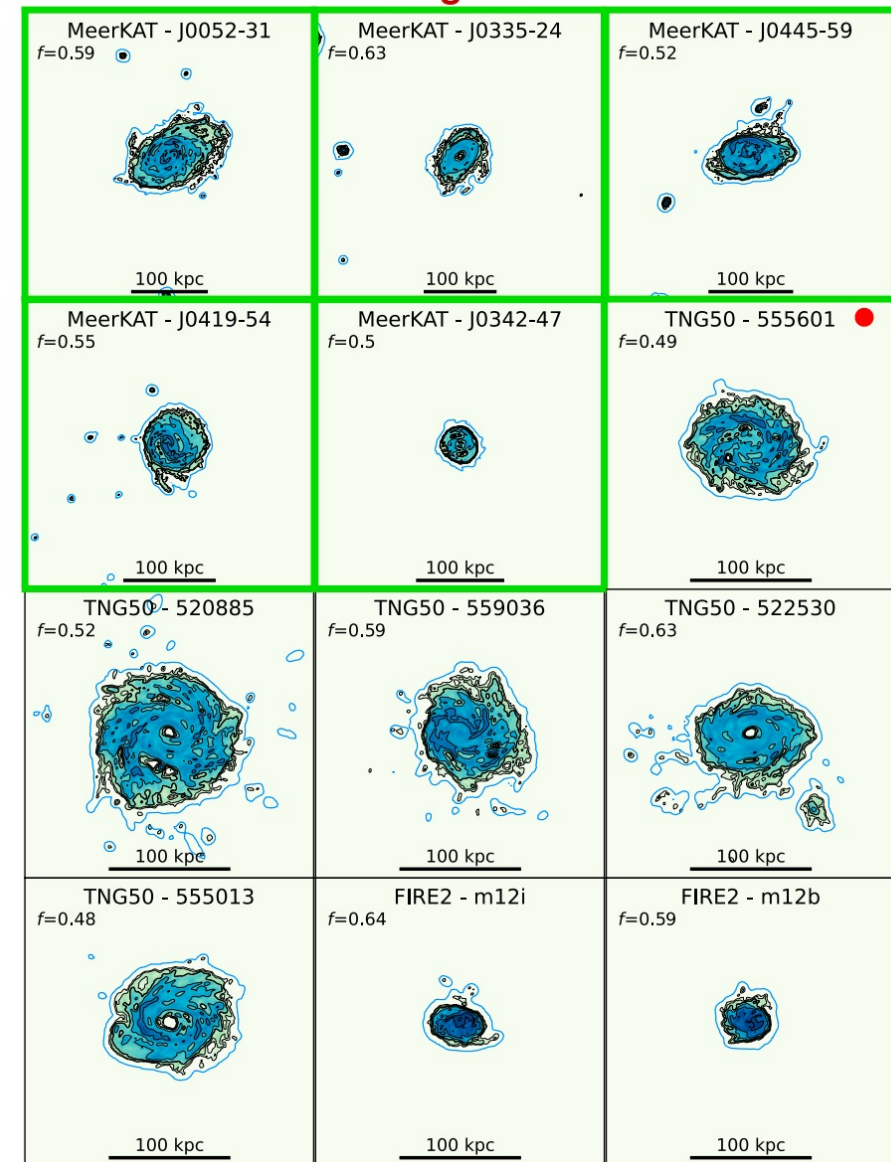
Zhang et al. 2026

3. Cosmological/Galaxy Hydrodynamic Simulation: Successes

detail HI distribution and dynamics in simulated galaxy



Regular

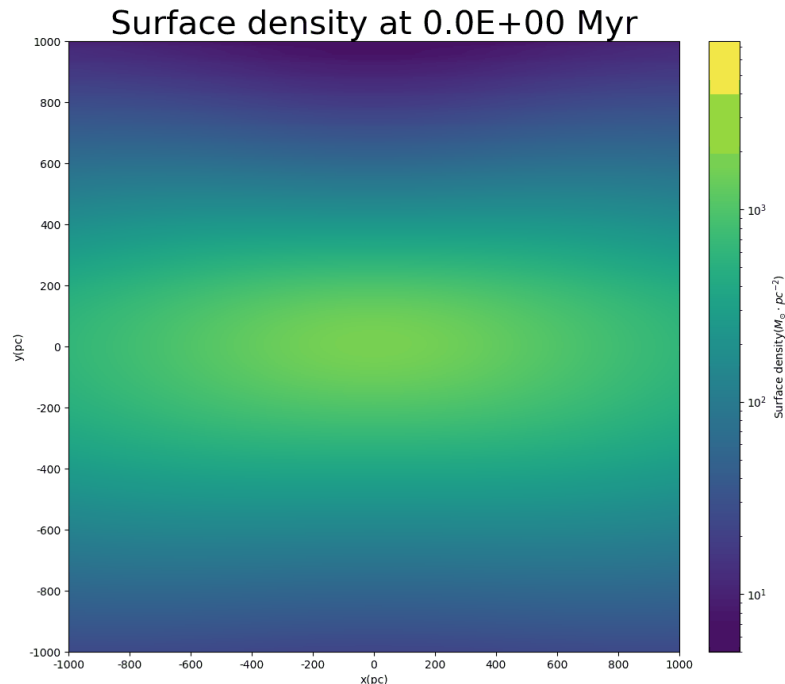


3. Cosmological/Galaxy Hydrodynamic Simulation: Successes

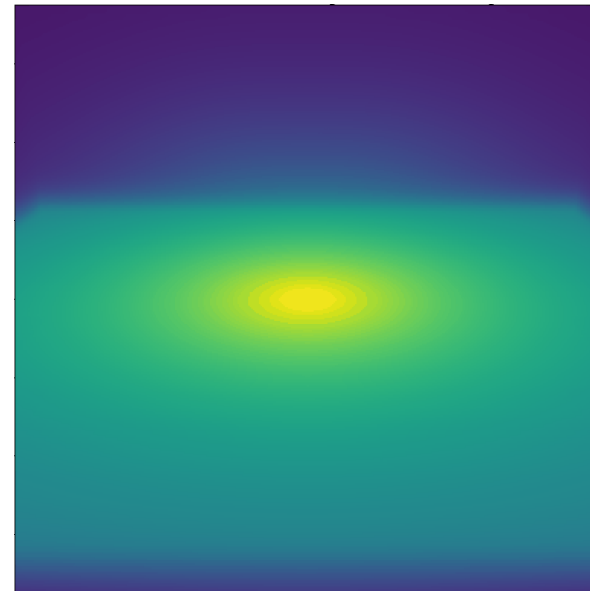
physics in the starburst and galactic wind in M82

Wang T.R., Zhu, et. al, 2026, MNRAS

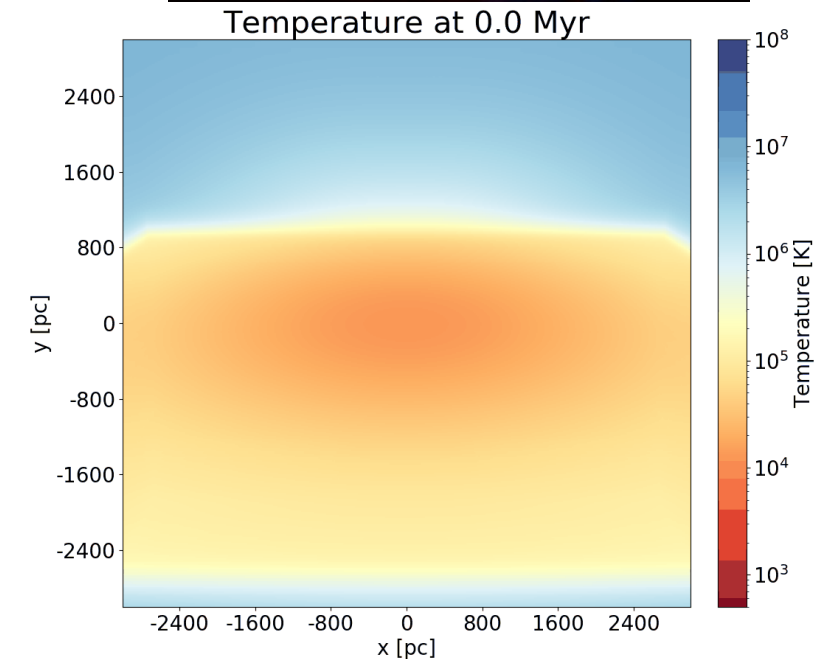
Li X.F., Zhu, et al. 2025, ApJ



Star (white dot) formation
in gas disc



density evolution



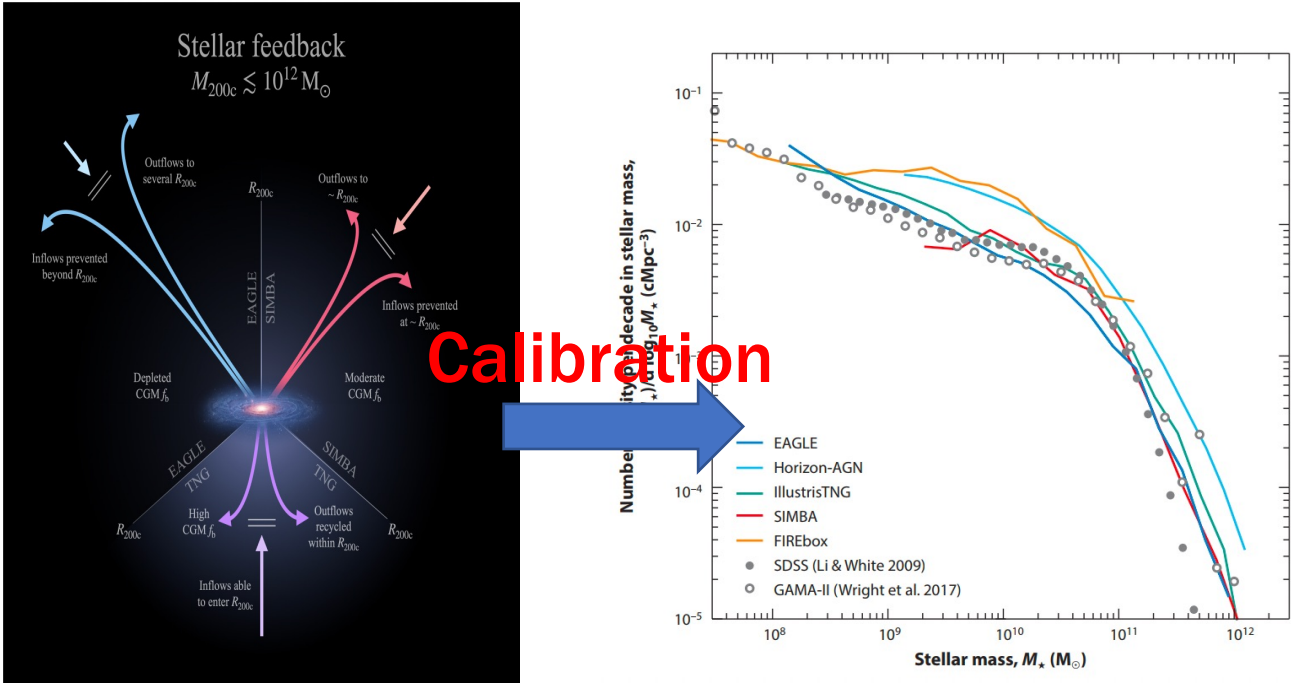
temperature

3. Cosmological/galaxy Hydrodynamic Simulation: Challenges

- Discrepancies in subgrid baryonic physics models across simulations
- Degeneracies between model parameters and numerical resolution
- Limited resolution or volume

.....

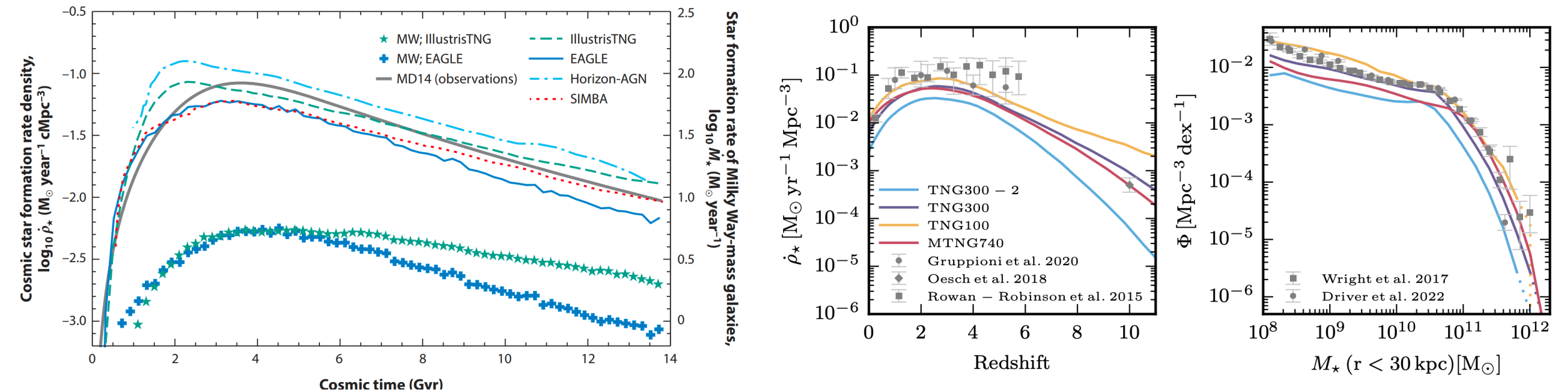
	EAGLE Schaye et al. (2015)	TNG100 Pillepich et al. (2018)	SIMBA Davé et al. (2019)
Box size	67.8 h ⁻¹ Mpc (REF) 16.9 h ⁻¹ Mpc (RECAL)	75 h ⁻¹ Mpc	50 h ⁻¹ Mpc
Element resolution	1.8 × 10 ⁶ M _⊙ (REF) 2.3 × 10 ⁵ M _⊙ (RECAL)	1.4 × 10 ⁶ M _⊙	1.8 × 10 ⁷ M _⊙
Hydrodynamics	Smooth particle hydrodynamics (SPH). GADGET-3 + ANARCHY. Springel (2005); Schaller et al. (2015).	Moving Voronoi Mesh (MVM). AREPO (with MHD). Springel (2010).	Meshless Finite Mass (MFM). GIZMO. Hopkins (2015, 2017).
Star formation	Informed by Kennicutt (1998). Density & Z criterion (Schaye 2004). Schaye & Dalla Vecchia (2008).	Informed by Kennicutt (1998). Density threshold. Springel & Hernquist (2003).	Informed by Kennicutt (1998). H ₂ -based criterion. Krumholz & Gnedin (2011).
Stellar feedback	Thermal only. Particles heated by ΔT _{SF} = 10 ^{7.5} K. Energy set by local ρ, Z. No hydrodynamic decoupling. Dalla Vecchia & Schaye (2012).	Thermal & kinetic. 90% momentum, 10% thermal. η set by local metallicity. v _{wind} set by σ _{DM} , z. Wind elements decoupled. Pillepich et al. (2018).	Thermal & kinetic. 30% of wind particles injected "hot". η(M _★) from FIRE (Anglés-Alcázar et al. 2017b). v _{wind} (V _{circ}) from FIRE (Muratov et al. 2015). Wind elements decoupled. Davé et al. (2019).
AGN feedback	Accretion: modified Bondi-Hoyle. Feedback: one mode, thermal only. Particles heated by ΔT _{AGN} = 10 ^{8.5} K. No directionality. No hydrodynamic decoupling. Schaye et al. (2015).	Accretion: modified Bondi-Hoyle. Low f _{Edd} : kinetic feedback. High f _{Edd} : thermal feedback. No directionality. No hydrodynamic decoupling. Weinberger et al. (2017).	Accretion: Bondi-Hoyle (hot), torque-limited (cold). Low f _{Edd} (jet-mode): kinetic & thermal. High f _{Edd} (radiative-mode): kinetic feedback. Outflows injected as bipolar. Jets are decoupled for 10 ⁻⁴ t _H (z). Anglés-Alcázar et al. (2017a).



3. Cosmological/galaxy Hydrodynamic Simulation: Challenges

e.g. Problem:

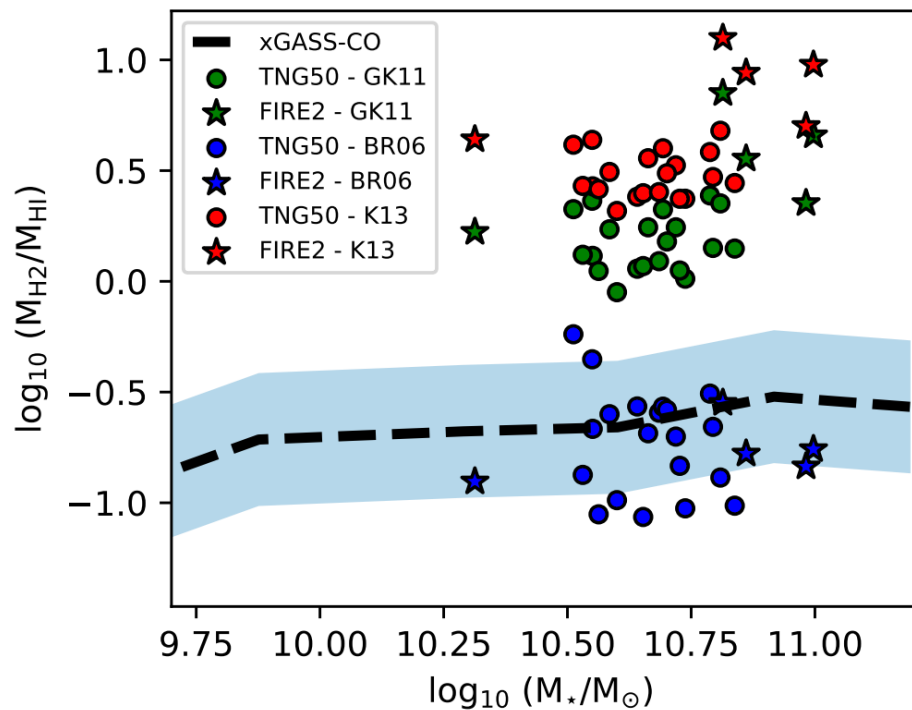
Significant discrepancies in SF predictions (e.g., CSFRD) across simulations
Lack of resolution convergence without retuning subgrid parameters



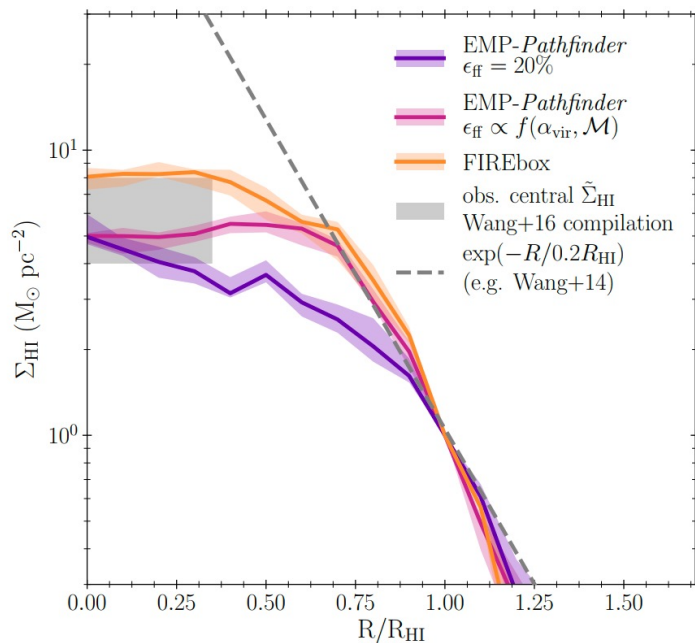
Name	BoxSize [comoving] [$h^{-1} \text{Mpc}$]	BoxSize [phys] [Mpc]	Volume [Mpc^3]	N_{ICs}	M_{dm} [$M_\odot$]	M_{baryon} [$M_\odot$]	$\epsilon_{\text{gas,min}}$ [kpc]	$\epsilon_{\text{dm},\star}$ [kpc]
MTNG740	500	740	4.0×10^8	2×4320^3	1.7×10^8	3.1×10^7	0.37	3.7
TNG300	205	300	2.7×10^7	2×2500^3	5.9×10^7	1.1×10^7	0.37	1.5
TNG300-2	205	300	2.7×10^7	2×1250^3	4.7×10^8	8.8×10^7	0.74	3.0
TNG100	75	110	1.6×10^6	2×1820^3	7.5×10^6	1.4×10^6	0.19	0.74

3. Cosmological/galaxy Hydrodynamic Simulation: Challenges

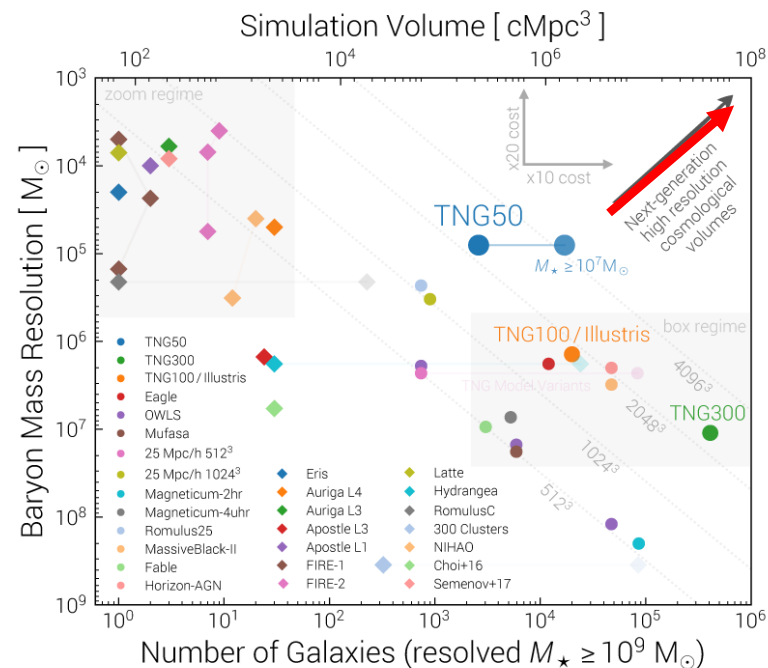
Discrepancies in cold gas properties: content, distribution, dynamics



Marasco et al. 2025



**HI surface density in EMP,
FIREbox simulations, vs. obs.**



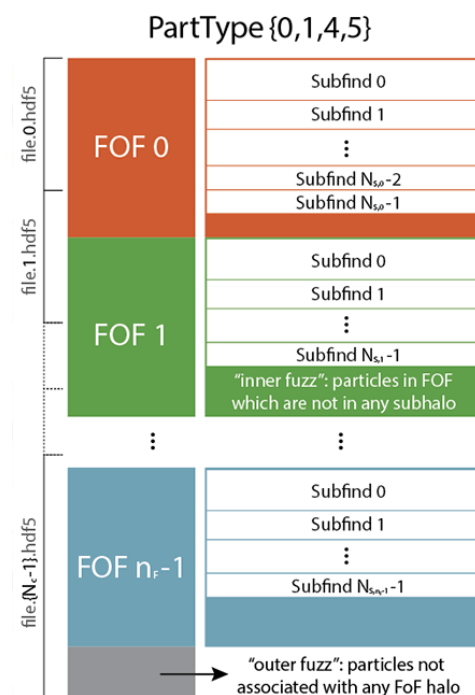
挑战与机遇并存：更高的模拟分辨率+更成熟可靠的重子物理模型，结合半解析方法，联合观测，有望揭示暗物质属性、星系形成演化、宇宙重子循环

4. Mock/Synthetic observations

数值模拟的关键作用是提供宇宙结构、星系非线性形成演化结果与观测比较。
但是要注意文献中模拟结果、统计数据与图的含义

模拟产生的直接数据

暗物质、恒星、气体粒子（网格）
的质量、位置、速度



数据分析

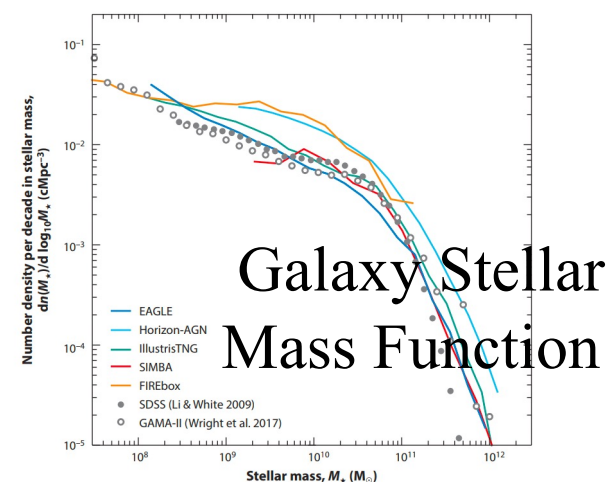
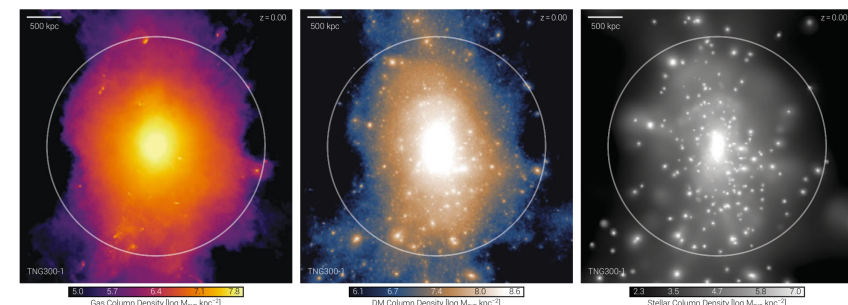
计算暗物质，恒星，气体的密度场，速度场 ...

统计暗晕质量，暗晕中恒星质量，气体质量 ...

....

绘图软件

可视化 “图像” 或统计量



往往没有考虑辐射传播、观测与仪器效应！

4. Mock/Synthetic observations

考虑地基光学望远镜终端在某一特定波长接收到恒星的辐射流量：



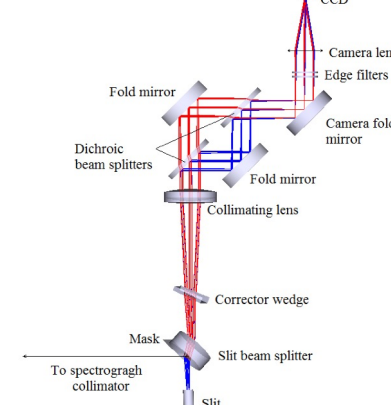
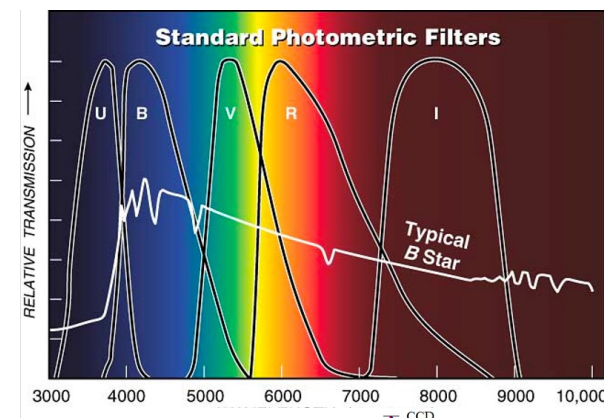
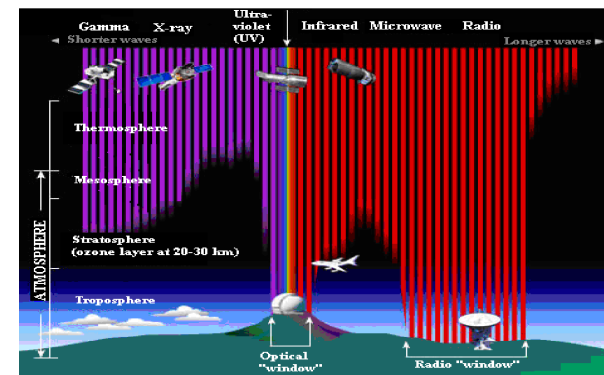
$$f_X = \int f_\lambda F_X(\lambda) R(\lambda) T(\lambda) d\lambda$$

滤光片在特定波段(band)的透射率
(transmission)

望远镜及终端的效率

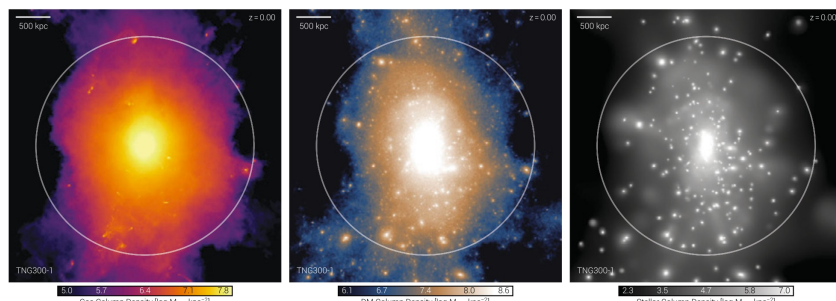
大气透射率

f_λ : 恒星的辐射，经传播路径上的尘埃/气体消光，到达大气层后流量

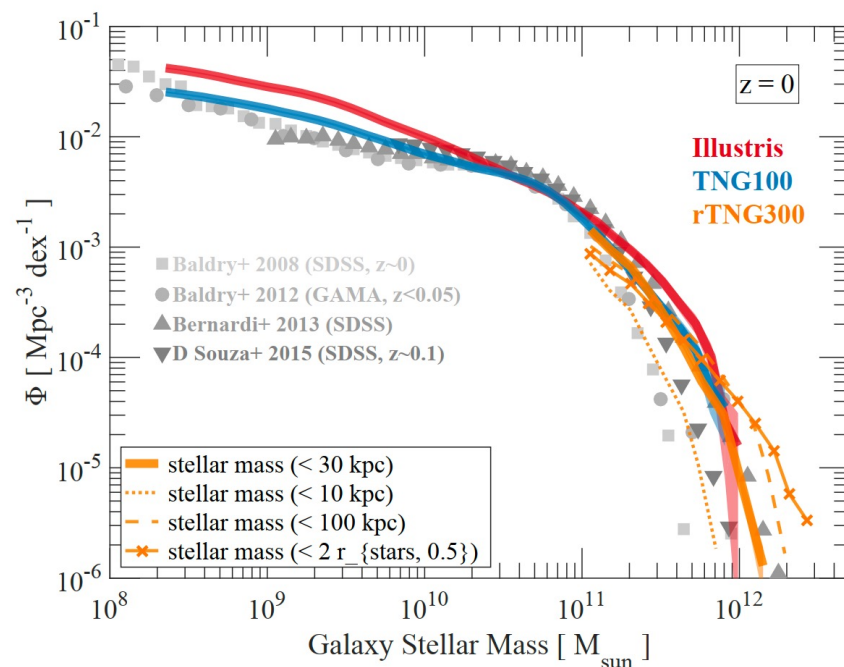


4. Mock/Synthetic observations

如何定义星系的恒星质量？



模拟



观测

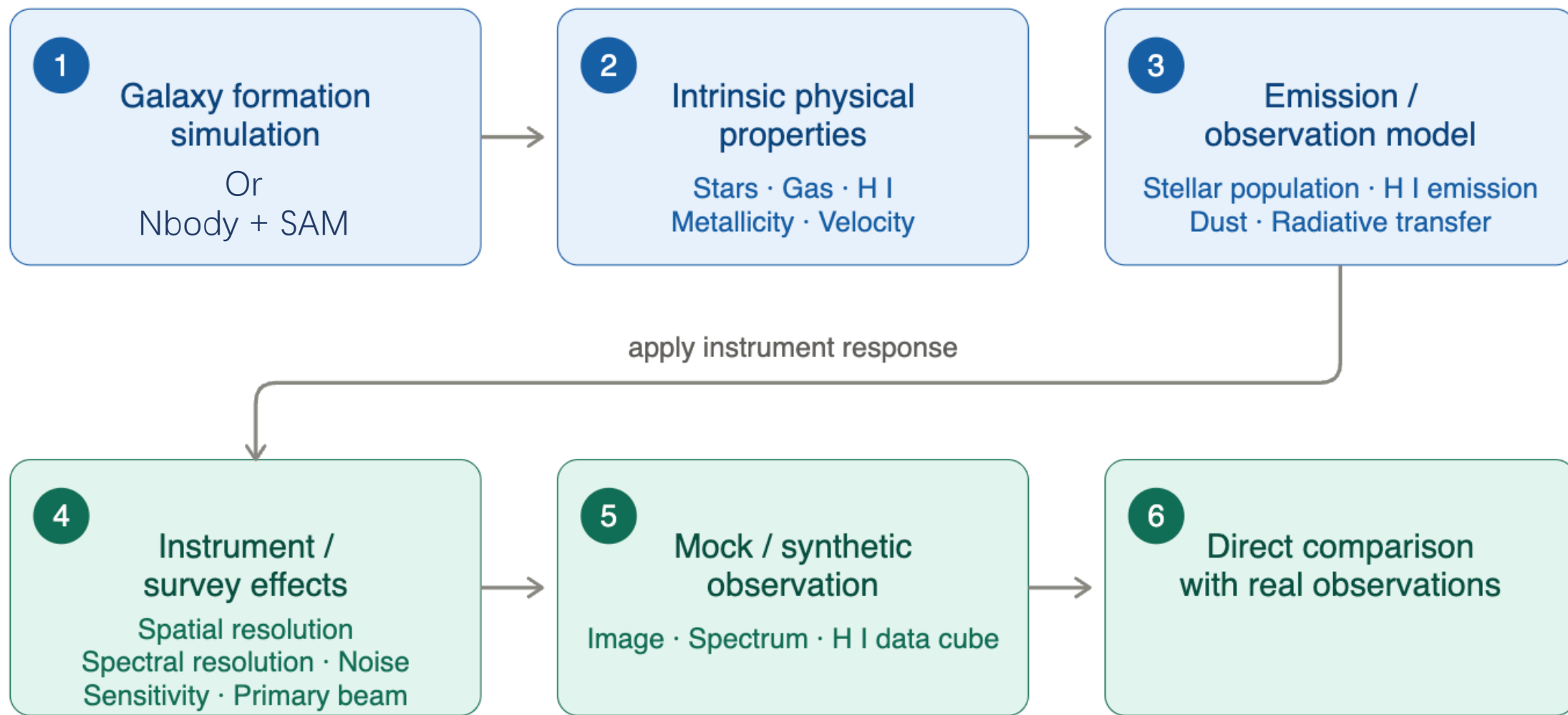


从光度推测恒星质量 (sed fitting)
(观测星等极限, 光纤覆盖, IMF, ...)

在将模拟结果与观测进行比较时, 需考虑观测效应

4. Mock/Synthetic observations

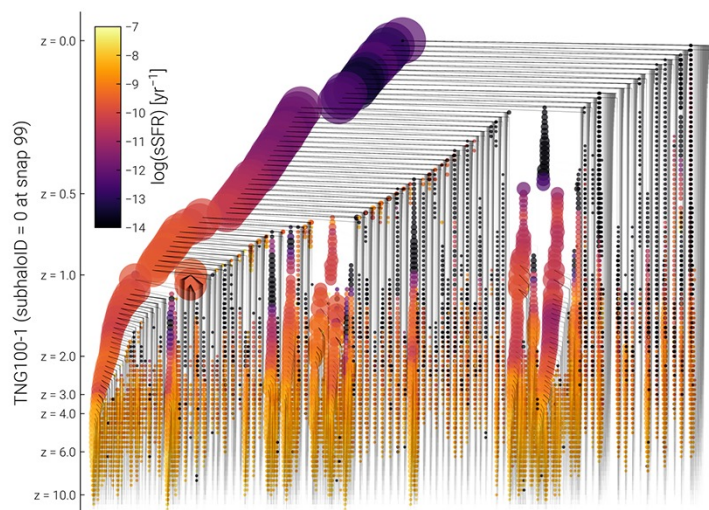
从数值模拟到模拟观测的主要流程



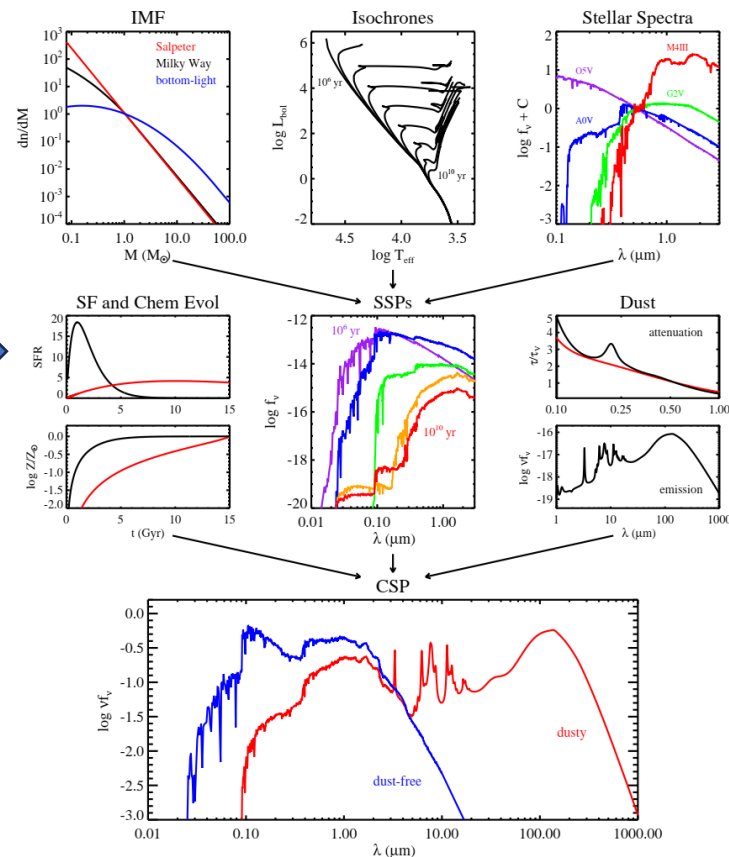
4. Mock/Synthetic observations

➤ Optical/IR (光学与红外) 星系成像流程

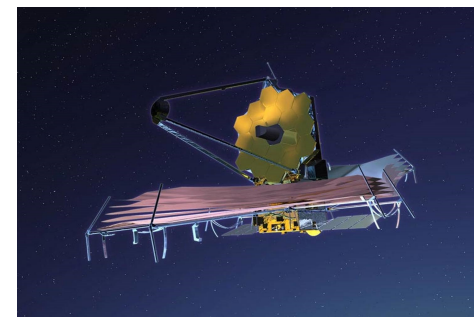
从halo/subhalo中所有恒星粒子的年龄信息，得到暗晕/星系的恒星形成历史



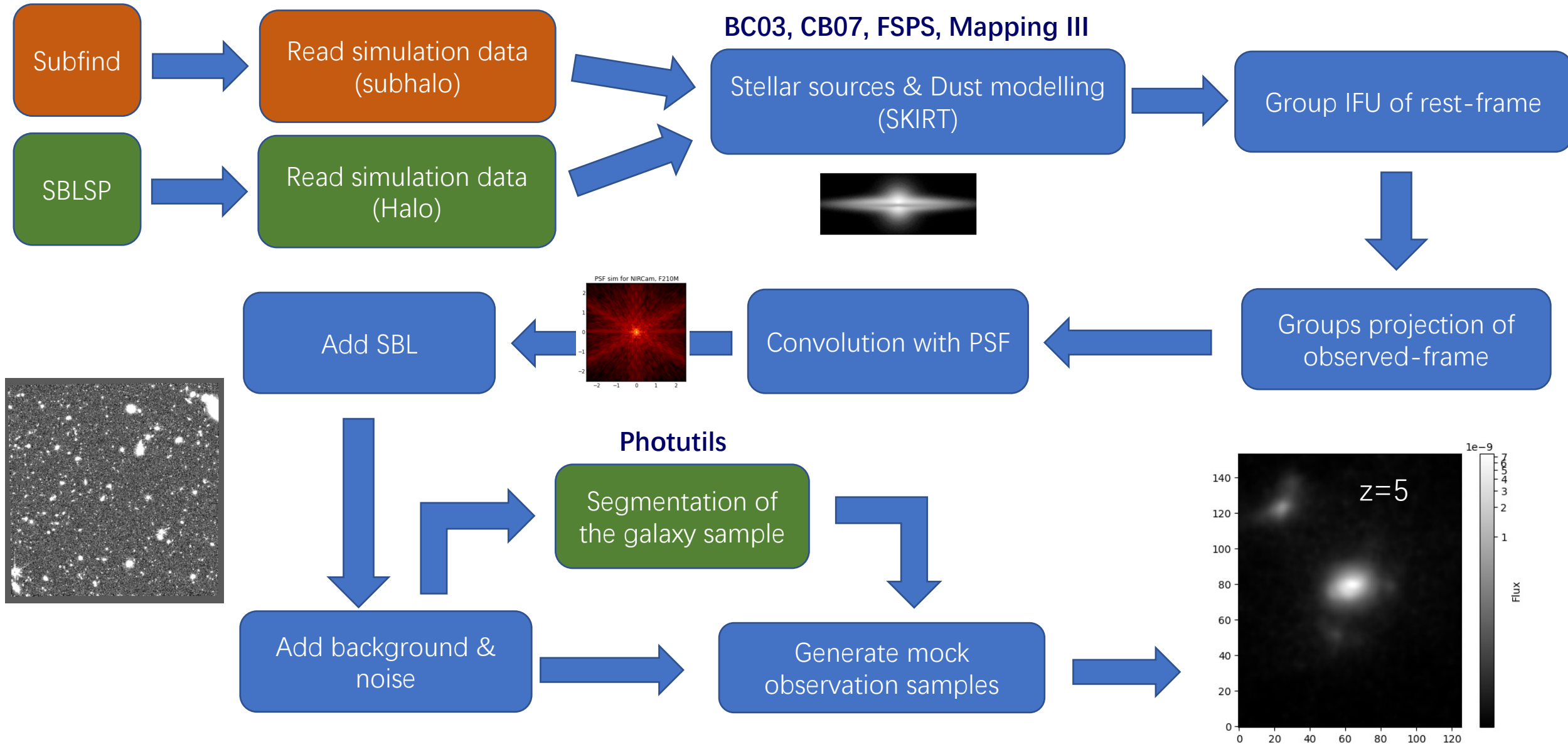
产生模拟辐射信号



投影、
积分



4. Mock/Synthetic observations



4. Mock/Synthetic observations

- HI Galaxy Synthetic observation
e.g., spatially resolved H I observations of nearby galaxies

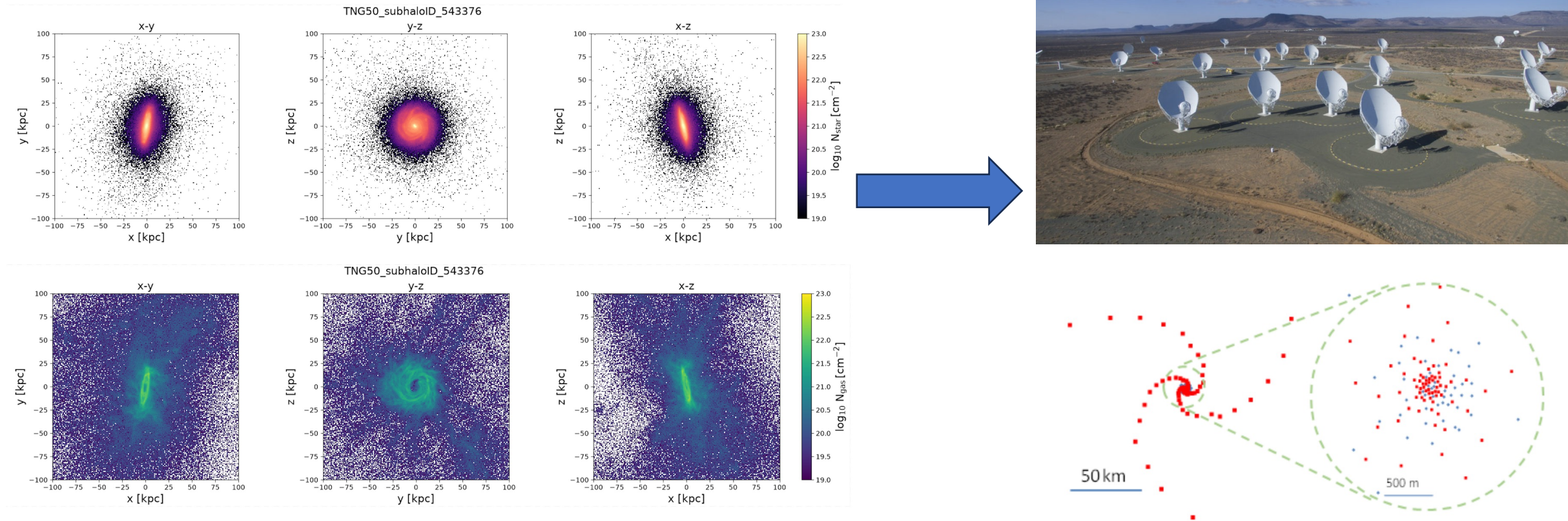


FIGURE 4. SKA1-MID array configuration and internal core

4. Mock/Synthetic observations

➤ HI Galaxy Synthetic observation , e.g. IllustrisTNG50+MeerKAT

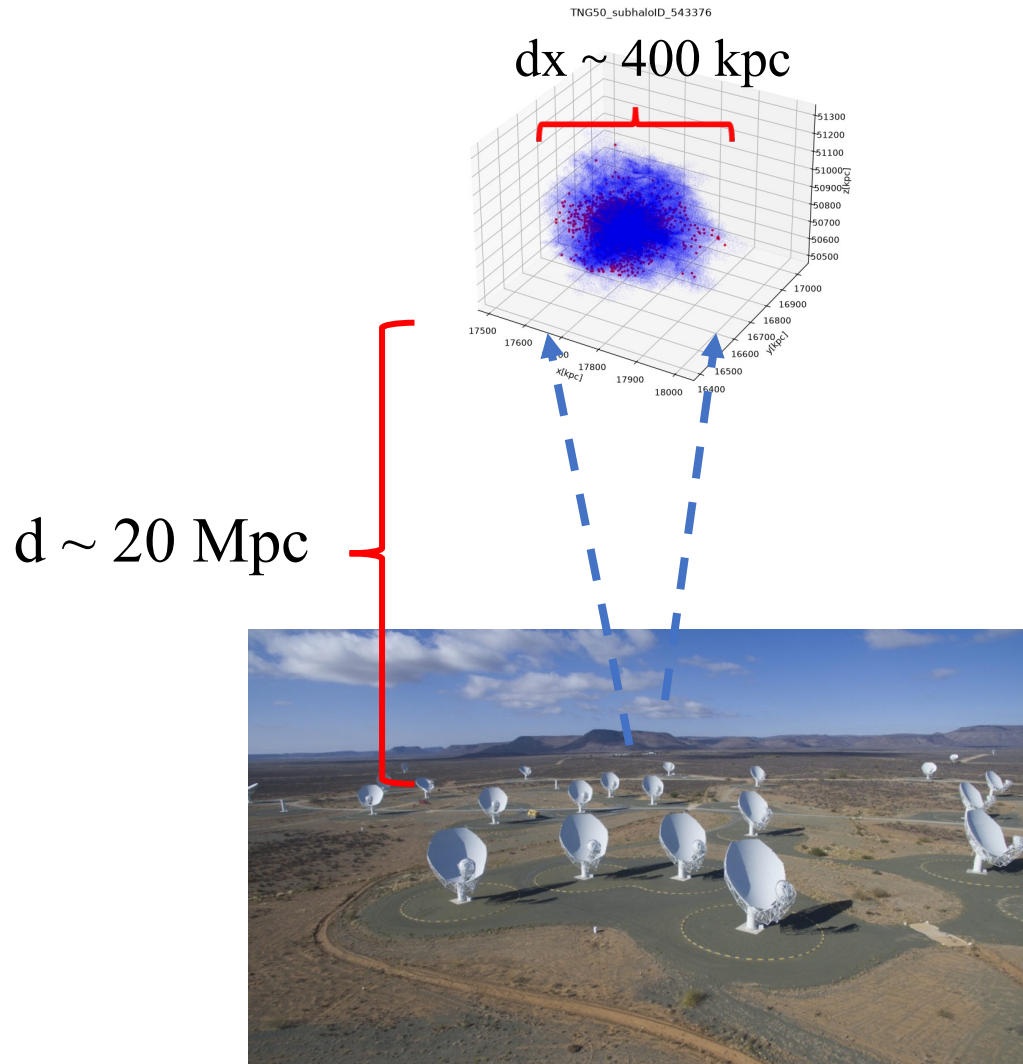


Table 2. Characteristic parameters for the HI datacubes of the observed and the simulated galaxy samples.

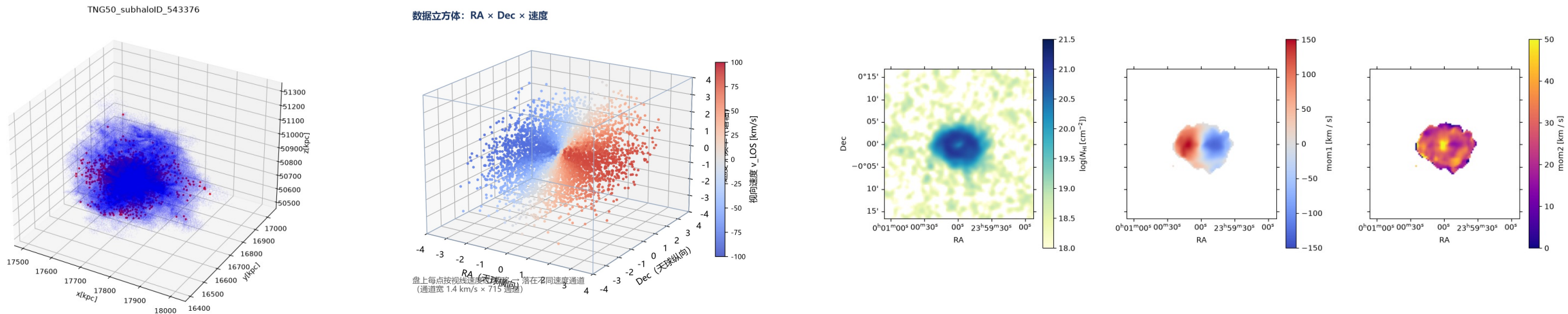
Parameter	unit	HR	LR
Field of view ^a	°	~ 1	~ 1
	kpc	~ 350	~ 350
Beam size ^b	"	26.4×18.2	65.3×64.0
	kpc	2.6×1.8	6.3×6.2
Beam PA	°	136	92
Pixel size	"	5	20
	kpc	0.5	1.9
Velocity range	km s^{-1}	± 500	± 500
Channel width ^c	km s^{-1}	1.4	1.4
σ_{rms} per channel	mJy beam^{-1}	0.15	0.25
Minimum N_{HI} ^d	cm^{-2}	5×10^{18}	1×10^{18}

Notes: ^a corresponding to the FWHM of the MeerKAT primary beam.

^b Sizes in kpc are based on a distance of 20 Mpc. ^c J0342-47 cubes have a different channel width of 5.5 km s^{-1} . ^d 3σ sensitivity integrated over 16 km s^{-1} . With respect to the values listed here, the rms noise per channel and the minimum detectable N_{HI} for J0342-47 are larger by 18 per cent (see text).

4. Mock/Synthetic observations

- HI Galaxy Synthetic observation , e.g. IllustrisTNG50+MeerKAT



读入气体粒子
信息, **计算HI**
质量、速度

坐标转换
观测视角

incl / az / pa

HI DataCube

距离、像素分
辨率, 平滑,
通道

beam + 噪声
+ 谱模型。。。.

FITS 立方体

(RA, Dec, 速
度)

4. Mock/Synthetic observations

模拟中单个气体粒子质量较大，且有些模拟（如TNG）不会直接计算HI，H₂比例，需后期根据模型计算

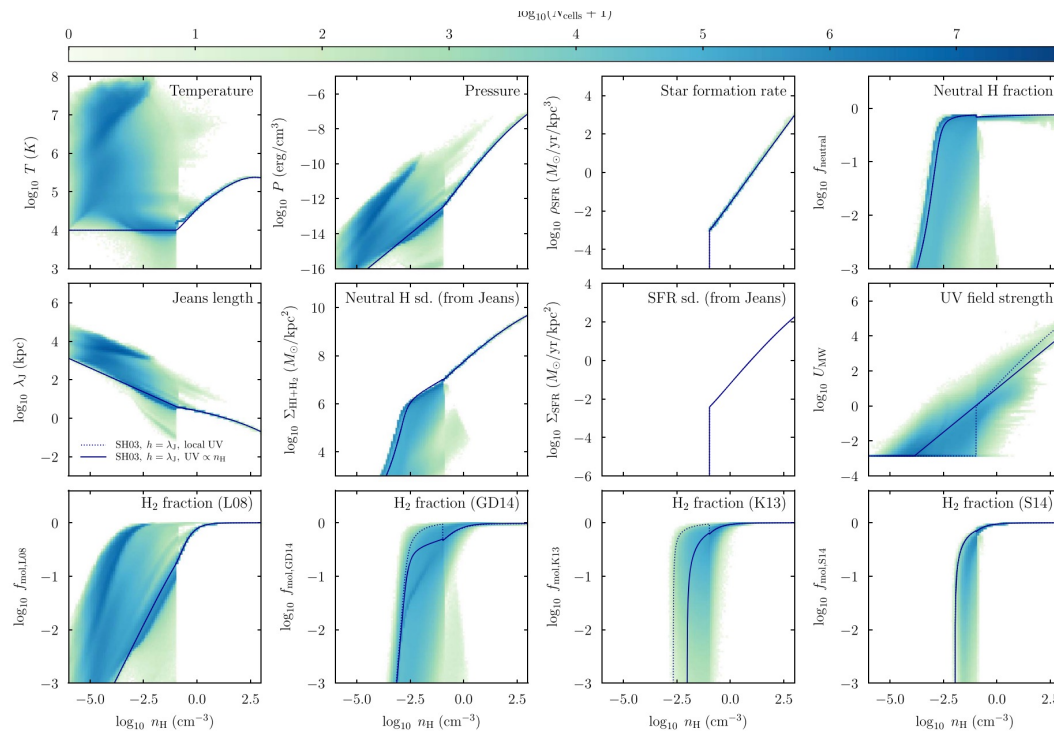
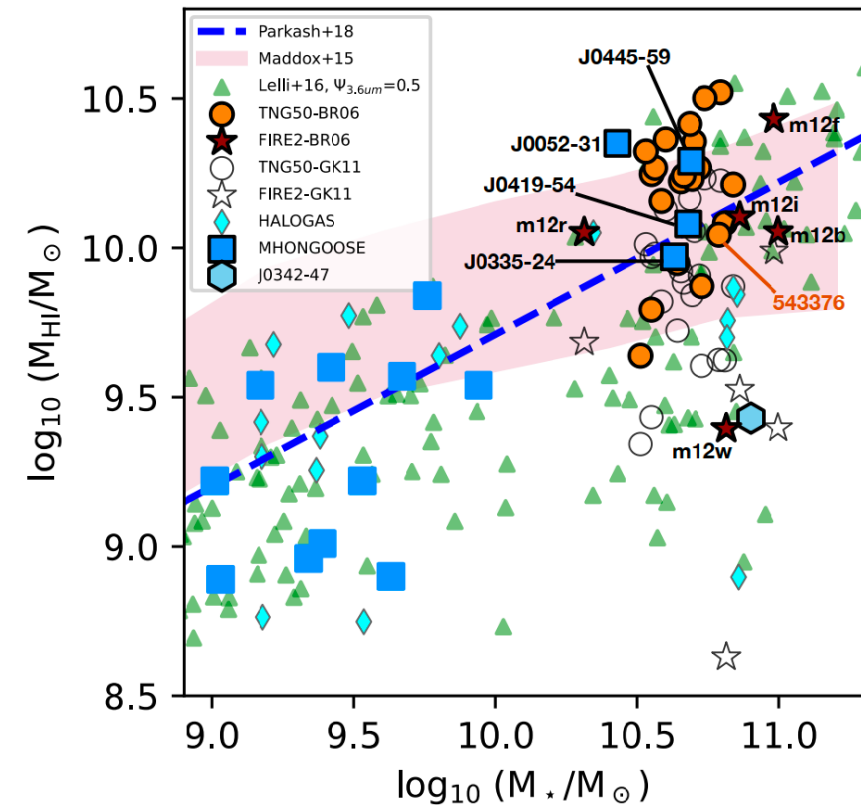
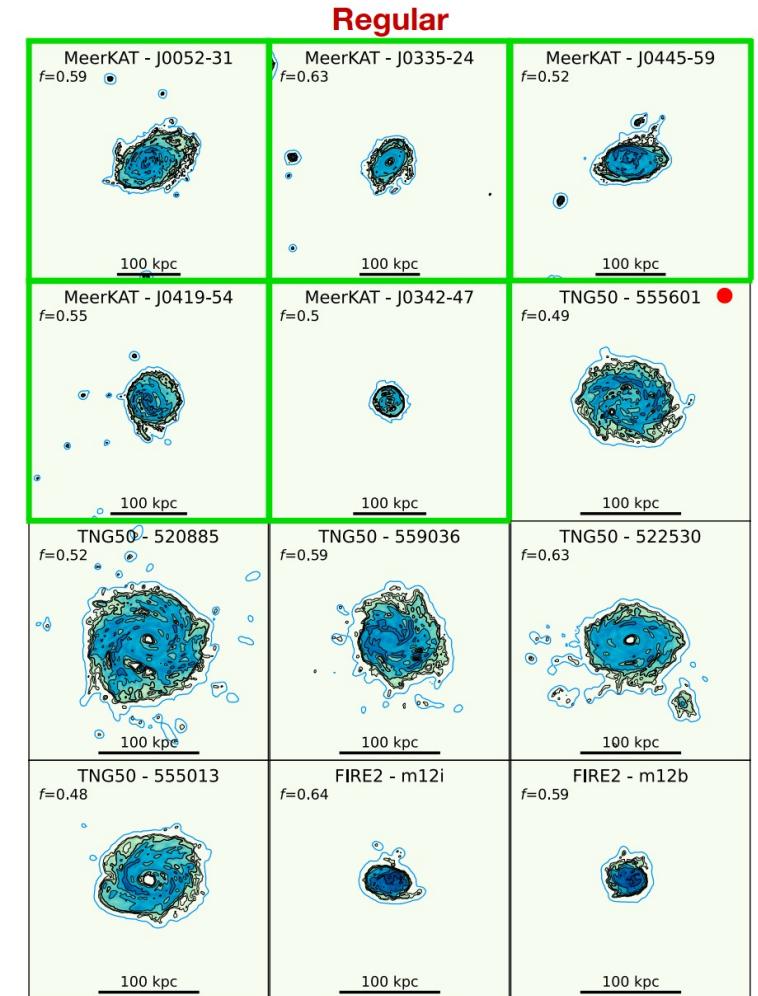
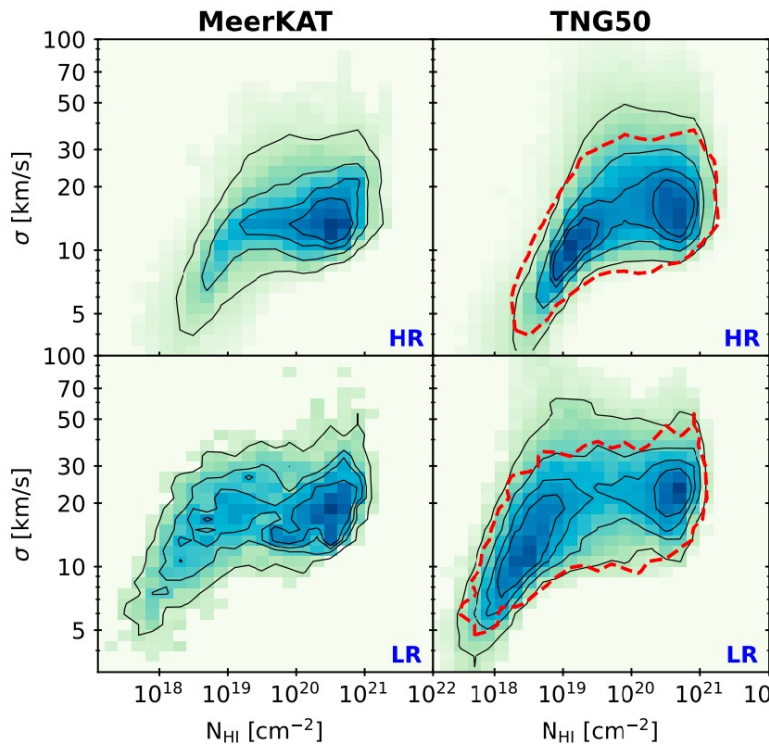
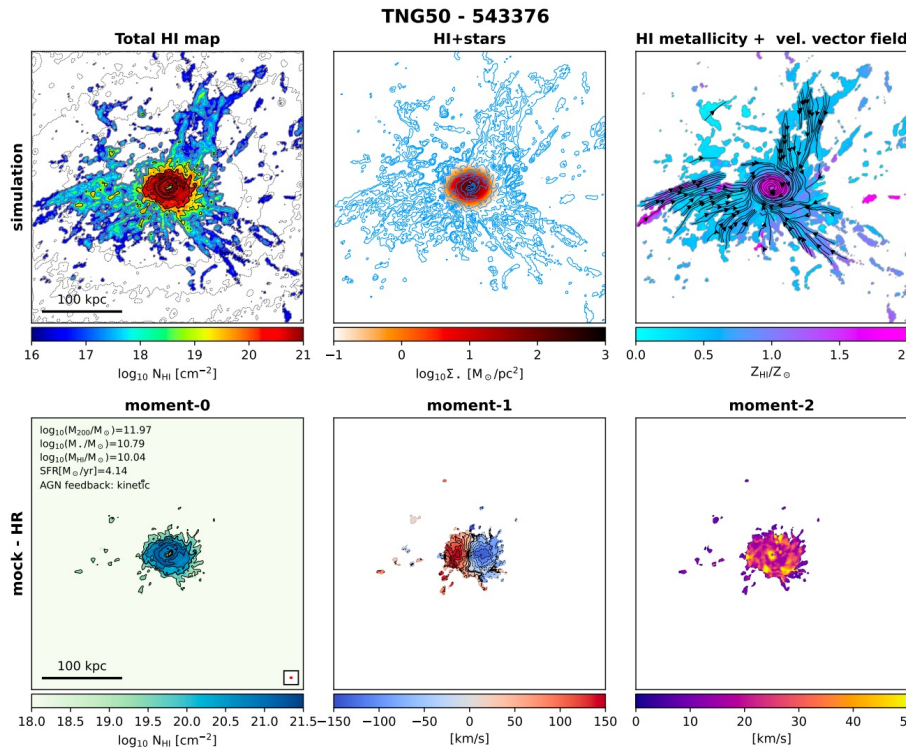


Figure 1. Physical conditions and the resulting molecular fractions as a function of density. In each panel, the histograms show the distribution of all gas cells in the analyzed galaxies in TNG100, about 1.2 billion cells. The solid blue lines represent the ISM model of SH03 (Section 2.2.1). Top row: At densities below the star formation threshold of $n_{\text{H}} = 0.106 \text{ cm}^{-3}$, hydrodynamics governs the state of the gas, leading to a range of temperatures and pressures. To guide the eye, the blue lines correspond to an ideal-gas equation of state with a temperature of 10,000 K. Above the threshold, the SH03 effective equation of state determines the temperature, pressure, and SFR. The top right panel shows the fraction of gas in neutral hydrogen, which is computed from the model of Behlmer et al. (2012) below



4. Mock/Synthetic observations

➤ HI Galaxy Synthetic observation , e.g. IllustrisTNG50+MeerKAT

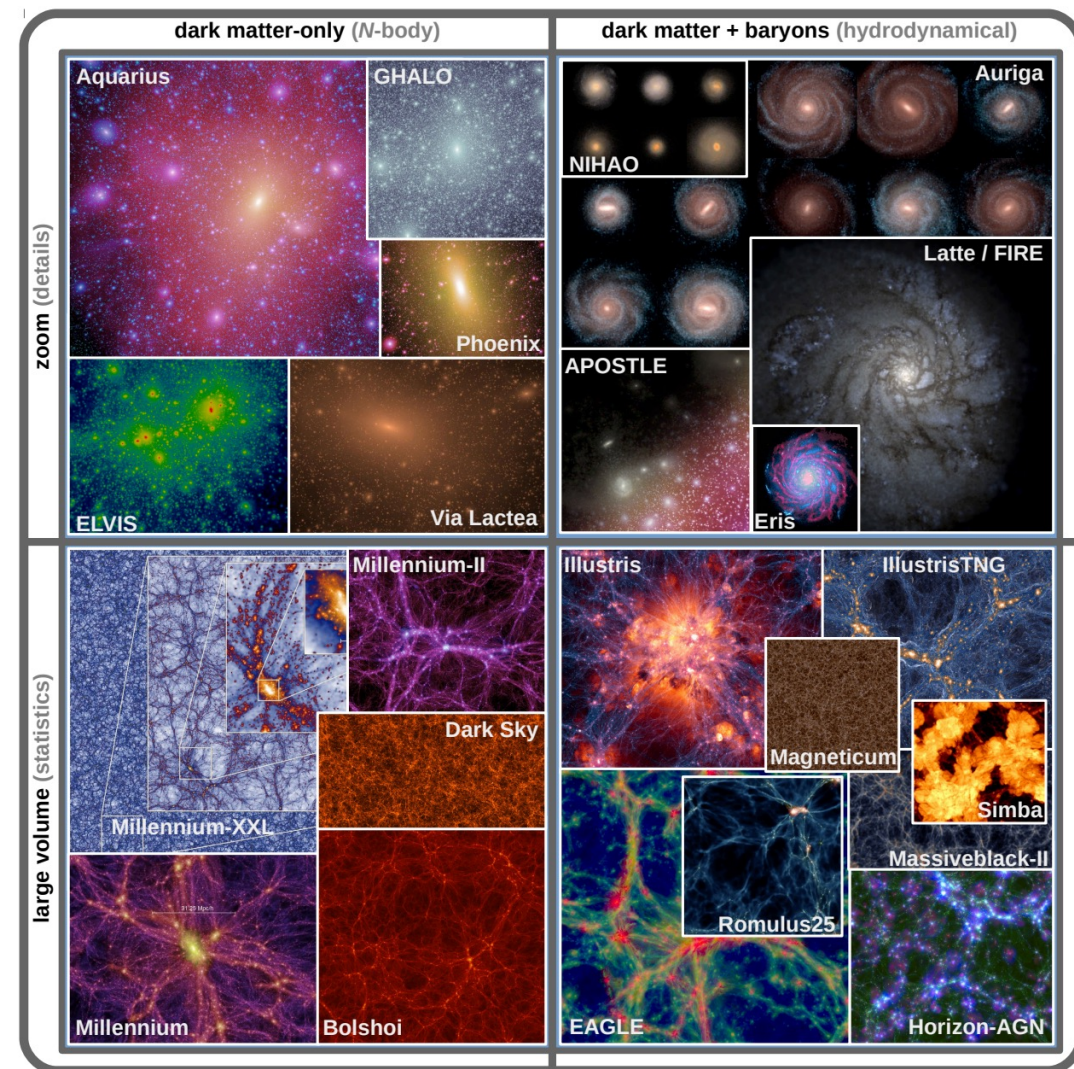


Marasco et al. 2025

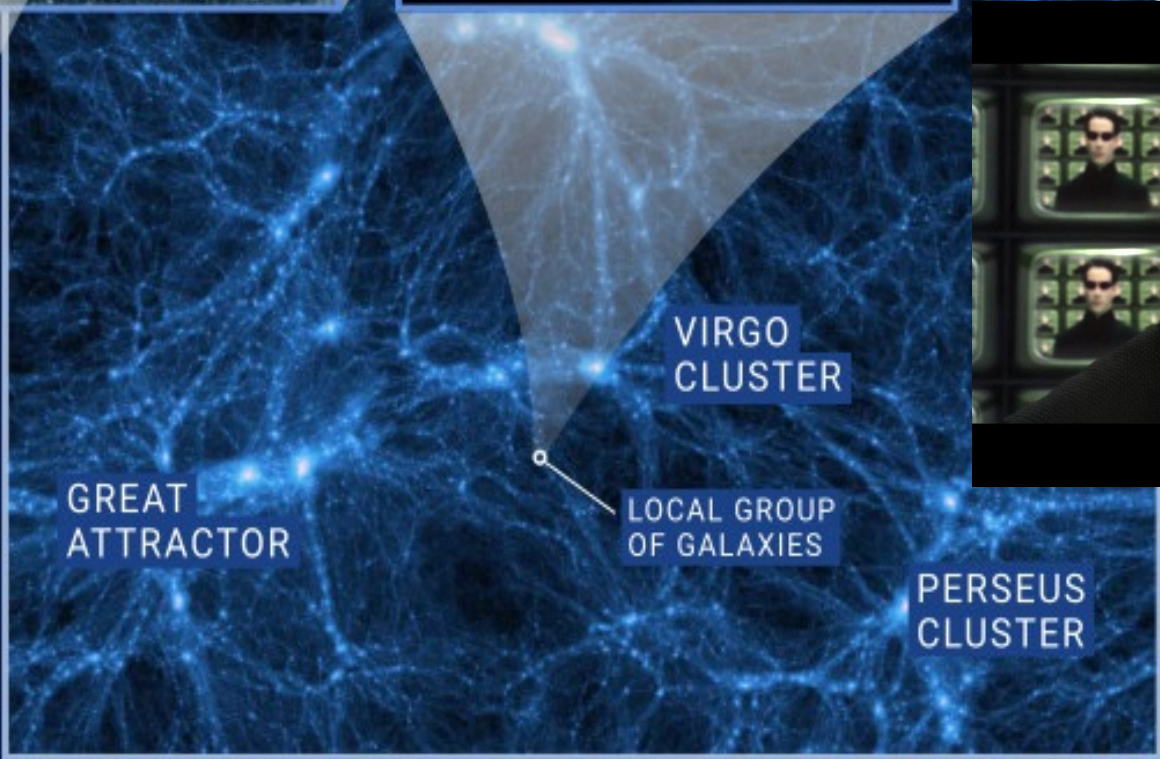
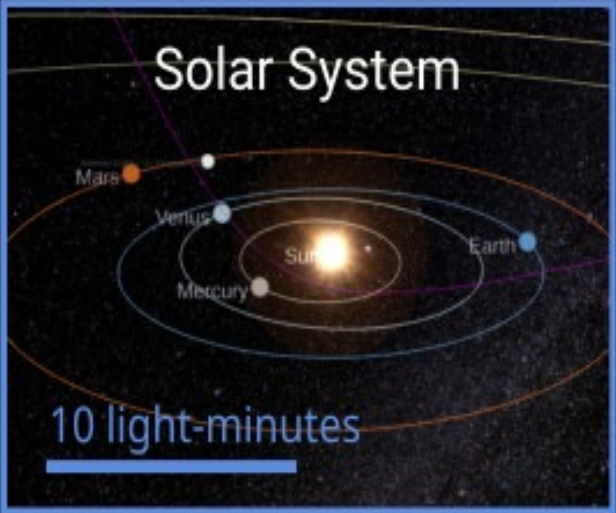
2D density histograms of column
density and second momen

Summary

- 数值模拟通过对暗物质、重子物质在宇宙结构、星系形成过程中非线性演化方程组数值求解，实现对过程的“全”追踪。
- 精确验证 Λ CDM宇宙及其结构形成理论框架，初步揭示重子物理细致过程，重子循环
- 目前的挑战：分辨率的限制，重子模型不确定，参数与分辨率的简并，大规模模拟对算法和硬件的需求...
- 在与观测比较时，需“公平”比较，模拟/合成观测很重要
- 与理论、观测联合，有望揭示暗物质属性、星系形成演化、重子循环



Vogelsberger et al. 2020



Thanks