Cosmological Hydrodynamical Simulations of Structure Formation

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Aknowldegements: Collaborators

- Tiziana Di Matteo, Rupert Croft, Yu Feng(Carnegie Mellon University, LBNL)
- Colin DeGraf (Cambridge)
- Stephen Wilkins (University of Sussex)
- Saili Dutta, Biprateep Dey, Sandeep Rana (NISER)

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Plan of the Talk

- Introduction
- Cosmological Simulations: A Tool for Studying Structure and Galaxy Formation
- Galaxy Formation and High and Low Redshifts
- Neutral Hydrogen in the local (and Post-Reionization) Universe
- Revisiting the pair-velocity correlation function relation as a probe of cosmology

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A Brief History of the Universe



http://map.gsfc.nasa.gov/

The Standard Model of Cosmology



http://www.esa.int/ESA (Planck Team 2013)

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The Standard Model of Cosmology



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The Standard Model of Cosmology: The ACDM model

- Big Bang followed by a brief period of inflation
- Matter/Energy density:



Planck Team 2013

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Structure Formation

Structure Formation: How can we explain the distribution and properties of objects that we see in the Universe?



Springel et al, 2004

2dF and SDSS survey

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Galaxy Formation and Cosmology

- Can we predict the number of spirals and elliptical galaxies?
- Can we predict the SEDs of galaxies and how they evolve across cosmic time?
- What are the important mechanisms affecting the formation and and evolution of galaxies?
- How do galaxies obtain gas and convert it to stars?
- What is the relation between galaxies and their host dark matter halos?
- Observational Cosmology is currently putting constraints at the percent level.

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Limitations are due to poor understanding of galaxy formation.

Schecter Functions: Mass Functions



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Baryonic Effects: The Galaxy Stellar Mass Function



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Mutch et al 2013

Baryonic Effects on Structure Formation

The Halo Mass Function:

$$\frac{dn}{d\log_{10}M} = \frac{M}{\rho} \frac{d\ln\sigma^{-1}}{d\log_{10}M} f(\sigma)$$
(2)



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The Need for Cosmological Simulations

- ► Fluctuations amplifier: Gravity ⇒ long range force
- Non-linear process ⇒ Evolution of *ρ* at different scales are coupled.
- Exact Force Computation \Rightarrow Expensive $\sim O(N^2)$
- Use approximate algorithms which scale as $\sim O(N \log N)$

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Particle Dynamics in an Expanding Universe EOM Physical Coordinates

$$\ddot{\mathbf{r}}(t) = \ddot{a}(t)\mathbf{x}(t) + 2\dot{a}(t)\dot{\mathbf{x}}(t) + a\ddot{\mathbf{x}}(t) = -\nabla\Phi_{tot} = -\nabla(\Phi_{av} + \phi)$$

$$\nabla_r^2 \Phi_{tot} = \nabla_r^2(\Phi_{av} + \phi) = 4\pi G\rho - \Lambda = (4\pi G\bar{\rho} - \Lambda) + 4\pi G\bar{\rho}\delta$$

$$\rho(\mathbf{r}) = \sum_i m_i \delta_D^3(\mathbf{r} - \mathbf{r}_i) \qquad \delta(\mathbf{r}, t) = \frac{\rho(\mathbf{r}, t) - \bar{\rho}(t)}{\bar{\rho}(t)}$$
(3)

EOM Comoving Coordinates: $\mathbf{r} = \mathbf{a}(t)\mathbf{x}$

$$\ddot{\mathbf{x}} + 2\frac{\dot{a}}{a}\dot{\mathbf{x}} = -\frac{\nabla_r \phi(\mathbf{x}, t)}{a} = -\frac{\nabla_x \phi(\mathbf{x}, t)}{a^2}$$

$$\nabla_x^2 \phi = 4\pi G a^2 \bar{\rho} \delta = \frac{3}{2} H_0^2 \Omega_{nr} \frac{\delta}{a} \qquad \rho = \bar{\rho}(1+\delta)$$

$$\rho(\mathbf{x}) = \sum_i m_i \delta_D^3(\mathbf{x} - \mathbf{x}_i) \approx \sum_i m_i W(\mathbf{x} - \mathbf{x}_i, \epsilon) \qquad (4)$$

Friedmann Equation:

$$\frac{\dot{a}^2}{a^2} + \frac{k}{a^2} = H_0^2 \left[\Omega_{rad} \left(\frac{a_0}{a} \right)^4 + \Omega_{nr} \left(\frac{a_0}{a} \right)^3 + \Omega_{\Lambda} \right]$$
(5)

Basic Equations The Linear Limit

$$\ddot{\delta} + 2\frac{\dot{a}}{a}\dot{\delta} = 4\pi G\bar{\rho}_{nr}\delta \tag{6}$$

$$\delta_{\mathbf{x}}(t) = \int \frac{d^{3}\mathbf{k}}{(2\pi)^{3}} \delta_{\mathbf{k}}(t) \exp(i\mathbf{k}.\mathbf{x})$$
(7)
$$\delta_{\mathbf{k}}(t) = \int \frac{d^{3}\mathbf{x}}{V} \delta_{\mathbf{x}}(t) \exp(-i\mathbf{k}.\mathbf{x})$$
(8)

$$\ddot{\delta}_{\mathbf{k}} + 2\frac{\dot{a}}{a}\dot{\delta}_{\mathbf{k}} = 4\pi G\bar{\rho}_{nr}\delta_{\mathbf{k}}$$
⁽⁹⁾

Hubble's parameter $H(a) = \dot{a}/a$ is a solution (decaying). Second solution can be constructed using the Wronskian.

$$X = 1 + \Omega_{nr} \left(\frac{1}{a} - 1\right) + \Omega_{\Lambda}(a^2 - 1)$$

$$b(t) \propto \frac{X^{1/2}}{a} \int^a \frac{da}{X^{3/2}}$$
(10)

Approximate N-Body techniques: Grid Based Methods

- EOM is simple to integrate $\Rightarrow \mathcal{O}(N)$.
- ► Time consuming part is the force calculation due to gravitational interaction $\Rightarrow O(N^2)$.
- *O*(*N*²) ⇒ due to pairwise interaction of gravity and its long-range nature.
- N-Body methods: resort to quicker and approximate techniques to compute the gravitational interactions between particles.
- Also need to soften forces since systems are collisionless.

- Broadly 2 methods to compute interactions (third hybrid one)
- Important: need to also assign size to particles, since we are dealing with a collisionless system.

Eulerian or Grid Based methods (PM)

Method One: solve the Poisson Equation to get the potential (hence force):

$$\nabla^2 \phi(\mathbf{r}) = 4\pi G \rho(\mathbf{r}) \tag{11}$$

 $-k^2 \phi_k \propto \rho_k$ In Fourier space (12)

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Use the $\mathcal{O}(N \log N)$ Fast Fourier Transform to do the forward and inverse transform.

PM Method Continued

Pros

- $\mathcal{O}(N \log N) \Rightarrow$ extremely fast.
- Simple to implement, algebraic equations.
- Easy to Parallelise with MPI (not OpenMP)
- Periodic Boundary Conditions from FFT.

Cons

- Resolution limit \Rightarrow grid size.
- Parallisation limited to slab parallisation in FFTW.

Remedy

- Use PencilFFT for further parallisation (See Blue Waters Simulation by Feng et al)
- Adaptive meshes which adjust to local density, AMR
- ART (Kravtsov, Klypin, Kokhlov), MLAPM (Knebe et al), Nyx (Almgren et al), Enzo (Bryan, Norman et al)

Lagrangian or Particle Based methods (BH-Tree)

- Compute direct forces in real space.
- ► Approximation: Structure the entire mass distribution into groups nested into larger groups ⇒ Tree.
- Can keep the monopole term or higher order multipoles (expensive)
- Pros:
 - Scales as O(N log N)
 - Extremely Accurate
- Cons:
 - $\blacktriangleright\,$ Slower than PM by $\sim 100\,$
 - Consumes more memory
 - Need to add terms due to periodic boundary conditions.

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- Remedy:
 - Combine with PM to get both speed and accuracy, TPM: Bode & Ostriker TreePM:Bagla 2002

BH-Tree



Figure : BH-Quad Tree: Credits cs.cmu.edu

- Cell Opening Criterion $\theta < L/D$, Choice of $\theta < 1.0$
- Other Multipole Methods (not covered) Fast Multipole Method (memory intensive)

TreePM Method: Bagla



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Cosmological Simulations of Galaxy Formation

• N-Body simulations \Rightarrow predict the distribution of dark matter halos.

- For Galaxy Formation need Baryonic processes
- For the rest of the talk we use Gadget (Springel 2002) which includes:
 - TreePM gravity solver (Bagla 2002, NK& Bagla 2009)
 - ► Smoothed Particle Hydrodynamics (SPH) ⇒ evolution of baryons
 - ► Heating/Cooling ⇒ external radiation background
 - Subgrid recipes for star formation, feedback, metal enrichment (Springel & Hernquist 2003)
 - Subgrid recipes for the growth of Super Massive Blackholes (SMBH) and feedback (DiMatteo, Springel & Hernquist 2005

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Details of SMBH model

- Origins of SMBH are still not known.
- ► $M_{\text{seed}} = 5 \times 10^5 h^{-1} M_{\odot}$ inserted in FOF halo with mass $M_{\text{halo}} \ge 5 \times 10^{10} h^{-1} M_{\odot}$ if it does not contain one.
 - PopIII stars $M_{\rm BH} \sim 10^2 M_{\odot}$ at $z \sim 30$ (Bromm and Larson 2004).
 - Direct collapse of gas $M_{\rm BH} \sim M_{\rm seed}$ (Bromm and Loeb 2003).
- Black hole growth through Bondi-Hoyle accretion

$$\dot{M}_{\rm BH} = \alpha \frac{4\pi G^2 M_{\rm\scriptscriptstyle BH}^2 \rho}{\left(c_{\rm\scriptscriptstyle S}^2 + v^2\right)^{3/2}}$$

BH mergers if $v < c_s$ within ϵ

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Black hole radiates with a bolometric luminosity

$$L_{\rm bol} = \eta \dot{M}_{\rm BH} c^2 \qquad \eta = 10\%$$

5% of liberated energy couples to surrounding gas.

Requirements for a Cosmological Simulation

- $L_{box} \Rightarrow$ larger than the nonlinear scale at the epoch of interest.
- $N_{part} \Rightarrow$ large so as to sufficiently resolve an object of interest.

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Part I: Super Massive Blackholes and Galaxy Formation



NGC 5128

Guiltekin et al 2009

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- Origins of SMBH are still not known.
- Two possible mechanisms to produce $M_{\rm seed} \sim \times 10^5 h^{-1} M_{\odot}$
 - PopIII stars $M_{\rm BH} \sim 10^2 M_{\odot}$ at $z \sim$ 30 (Bromm and Larson 2004).
 - Direct collapse of gas $M_{
 m BH} \sim M_{
 m seed}$ at $z \sim$ 12 (Bromm and Loeb 2003).

Structure Formation at $z \sim 6$

- ► Observations of *z* ~ 6 quasars (~ 30) suggest that they are powered by 10⁹*M*_☉ blackholes (Fan et al 2006)
- Abundances \implies hosts halos $M_{\rm halo} \sim 10^{13} M_{\odot}$.
- Extremely rare: $n \sim a$ few Gpc⁻³.
- ▶ SED of quasars \implies fully developed by $z \sim 6$ (Wang et al 2008).
- Question: How can we form such extreme objects so rapidly (< 1 billion years)
- What about properties of host galaxies ?

Molecular Gas and Star Formation in $z \sim$ 6 QSO hosts

- ► CO \implies trace molecular gas for host galaxies: $M_{\rm mol} \sim 10^{10} M_{\odot}$ (Wang et al 2010, 2011)
- FIR \implies SFR $\sim 10^2 10^3 M_{\odot}.yr^{-1}$ for quasar hosts.

J1048+4637 $z_{co} = 6.2284$



Figure : Wang et al, 2010

The MassiveBlack (-II) Simulation

Run	N _{part}	L _{box} (Mpc/h)	ϵ (kpc/h)	N _{cores}	Zf	$\begin{array}{c} \text{CPU Hours} \\ \times 10^6 \end{array}$
MB	$\begin{array}{c} 2\times 3200^3\\ 2\times 1792^3\end{array}$	533	5.0	98304	4.75	7
MB-II		100	1.85	24576	0.0625	21

 \sim 350 Tb of data generated.

- Gadget3: DM, Gas, Star, Black Holes and Feedback
- Cosmology: WMAP7
- Halofinder: SUBFIND with 20 bound particles.



Figure : NICS, University of Tennessee

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Team: NK, Di Matteo, Croft, Feng, Degraf...

Visualisation: The first Terapixel Image



Figure : Feng, Croft, DiMatteo, NK et al 2011

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See: http://gigapan.com/gigapans/76215/

Growth of Blackhole through cold flows



Figure : DiMatteo, NK, DeGraf, Feng, Croft et al (2012)

Growth of Blackhole through cold flows



Figure : DiMatteo, NK, DeGraf, Feng, Croft et al (2012)

Growth of Black Hole and its Host Galaxy



Figure : NK, Feng, DeGraf, DiMatteo, Croft, (2012)

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High-z BH Luminosity Function



Figure : DeGraf, DiMatteo, NKet al (2012)

Evolution of SFR Density



Figure : NK, DiMatteo, Croft, et al (2014)

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Dusty Galaxies at High Redshift



Figure : Wilkins et al 2017

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Cosmic Spectral Energy Distribution of Galaxies



Figure : NK, DiMatteo, Croft, et al (2014)

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Galaxy Stellar Mass Function



Left: Wilkins, DiMatteo, Croft, **NK** et al (2013) Right: **NK**, DiMatteo, Croft, et al (2014)

Comparison



Schaye et al (2015)

Evolution of Neutral Hydrogen (HI)



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Ali & Bharadwaj 2005

Basic Ingredients of Galaxy Formation

▶ Fuel: Cold Gas (*HI* and *H*₂)

Star Formation: Conversion of cold gas into stars $SFR(t) \propto \rho_{gas}^{\gamma}$

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• Stellar Mass:
$$M_{\star}(t) = \int^{t} SFR(t') dt'$$

The Kennicutt-Schmidt Law



Bigiel et al 2008



Leroy et al 2008



Leroy et al 2008



Leroy et al 2008

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Leroy et al 2008

HI and Galaxy Formation



Madau and Dickinson. 2014

HI and Galaxy Formation



Madau and Dickinson. 2014

HI and Galaxy Formation



Rhee et al. 2018

21cm Cosmology



Figure : Busca et al 2013

- Current estimates on Ω_{HI} based on DLAs and direct detection in the local Universe.
- The neutral fraction has remained consistent with a constant value of Ω_{HI} ~ O(10⁻³) z > 1 with large errors.
- SFR determined out to redshift ~ 8, however measurements of cold gas in galaxies have been made out to only z = 0.37. (Lah et. al 2009)

- A census of cold gas is crucial for galaxy formation models at moderate redshifts.
- Clustering of HI selected galaxies \Rightarrow halo occupation.

Neutral Fraction



Khandai et al 2012 See also Papastergis et al 2012 Padmanabhan et al 2017

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Detection of HI in the DEEP2 field with GBT



Figure : Khandai et al. 2012

Local Surveys and Observed Galaxy Occupation

$$\mathsf{HALO} \iff \mathsf{GALAXY} \text{ (stars)} \iff \mathsf{GALAXY} \text{ (HI)}$$

• Halo based models \Rightarrow useful for Intensity Mapping signal at $z \ge 1$.

- Semianalytical models in principle predict HI in Galaxies
- Need a robust relation between starlight and cold gas (available only locally).

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ALFALFA + SDSS

The ALFALFA and SDSS Surveys



Right Ascension

ALFALFA and SDSS



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ALFALFA and SDSS



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ALFALFA and SDSS



ALFALFA

SDSS

ALFALFA Completeness



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Estimates of the HI Mass Function



2dF

► The 1/ V_{max} method (Schmidt 1968) $\phi^j = \sum \frac{1}{v_{max,i}^j}$

 The 2D Stepwise Max Likelyhood method (Loveday 2000)

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$$p_i(M^i, w_{50}^i | D_i) = rac{\phi(M^i, W_{50}^i)}{\int_0^\infty \int_{M_{lim}^i}^\infty \phi dM dW}$$

The HI Mass Function



Dutta, NK, Dey 2019

The HIMF for Different Populations



M_r

The HI Mass Function: 1.5σ sample



Dutta, NK, Dey 2019

Contribution to Ω_{HI}

 $\Omega_{HI} \propto M_* \phi_*$

region	$\Omega_{HI}[10^{-4}h_{70}^{-1}]$	$\Omega_{HI}/\Omega_{HI}^{total}$
total	4.894 ± 0.424	1.00
bright blue	$2.243 \pm 0.174 \; (1.057 \pm 0.095)$	0.458 (0.216)
faint blue	$1.317 \pm 0.299~(2.202 \pm 0.296)$	0.269 (0.450)
bright red	$0.668 \pm 0.079~(0.560 \pm 0.071)$	0.136 (0.114)
bright bluer	$0.207 \pm 0.064 \; (0.333 \pm 0.426)$	0.042 (0.068)
faint bluer	$0.078 \pm 0.014 \; (0.328 \pm 0.048)$	0.016 (0.067)
faint red	$0.032 \pm 0.014 \; (0.099 \pm 0.022)$	0.007 (0.020)
dark	0.329 ± 0.237	0.067

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Dutta, NK, Dey 2019

Dusty Red Galaxies



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Conditional HI Mass Function



Dutta and NK(in prep)

Conditional HI Mass Function



Dutta and NK(in prep)

Distribution of $\Omega_{\rm HI}$ in the color-magnitude plane of galaxies



 $M_r - 5log_{10}(h_{70})$

Dutta and NK(in prep)

The HI Velocity Width Function



Dutta and **NK**(in prep)

Abundance Matching ALFALFA and SDSS





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The Pair-Velocity - Correlation Function Relation

On large (linear) scales, pair conservation equation leads to:

$$-\frac{v_p(r)}{Hr} = \frac{2}{3}\bar{\xi}(r)f \qquad f = \frac{d\ln b}{d\ln a} \simeq \Omega_m^{0.6} \tag{15}$$

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Peebles 1980



Rana and NK(in progress)



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Rana and NK(in progress)