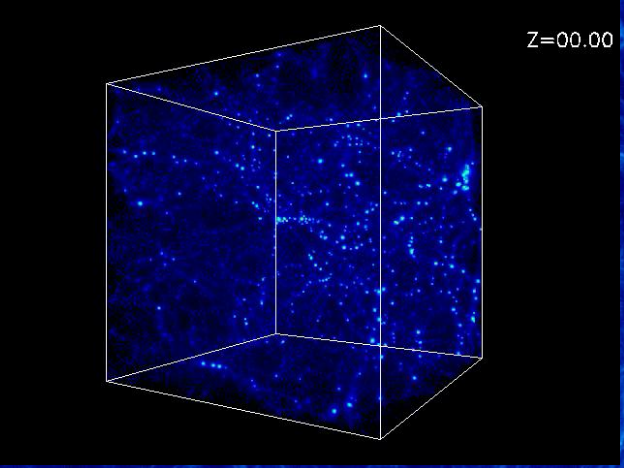


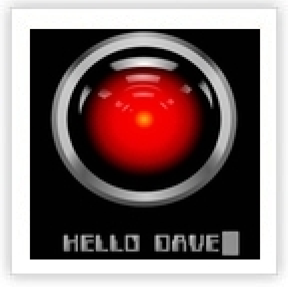
Supercomputación en Cosmología:
El Laboratorio Virtual del Universo

Gustavo Yepes

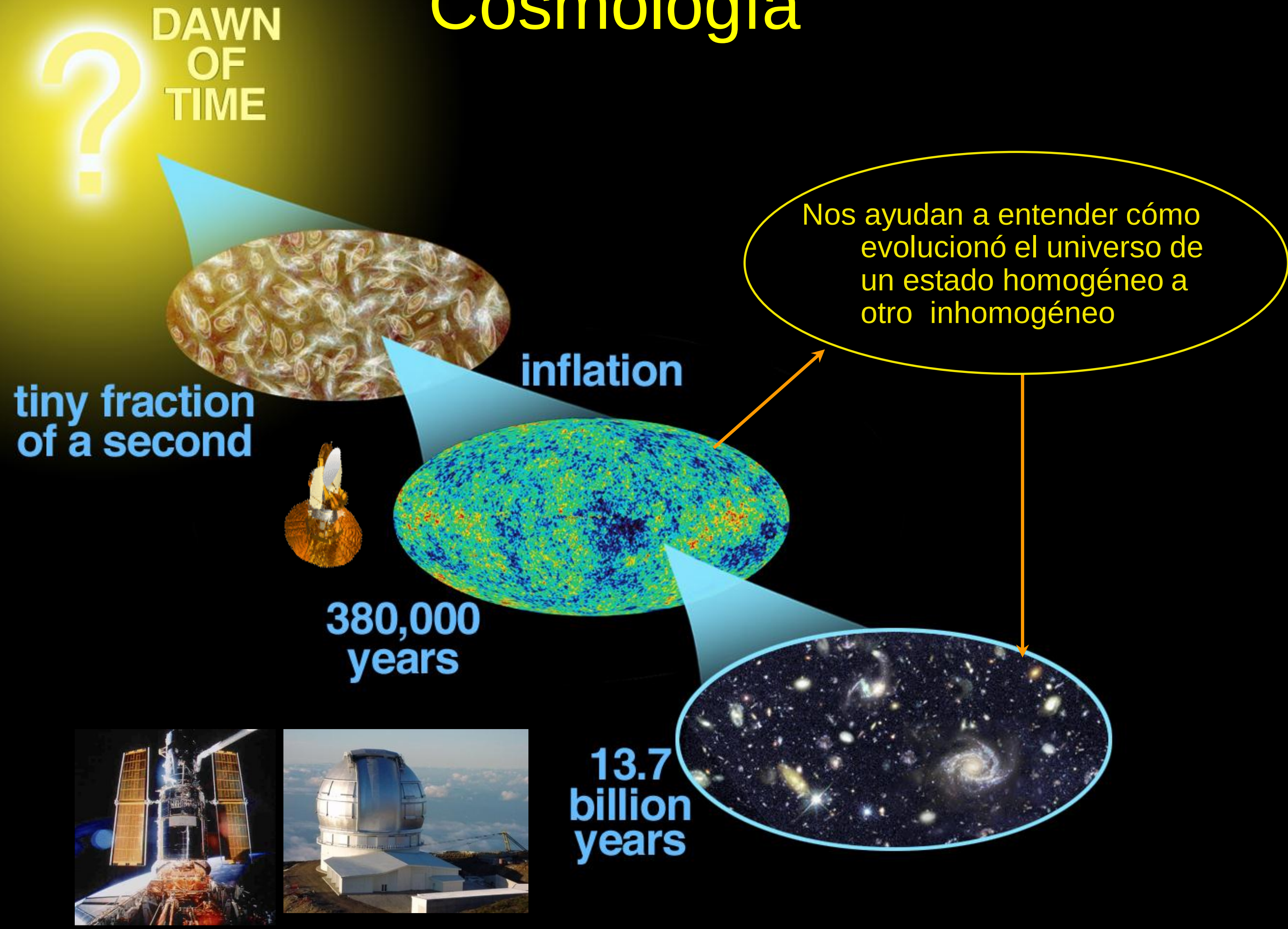
Universidad Autónoma de Madrid

http://astro.ft.uam.es/marenostrum

Fronteras de la Computación
Benasque Julio 2011



Por qué es necesaria la simulación numérica en Cosmología

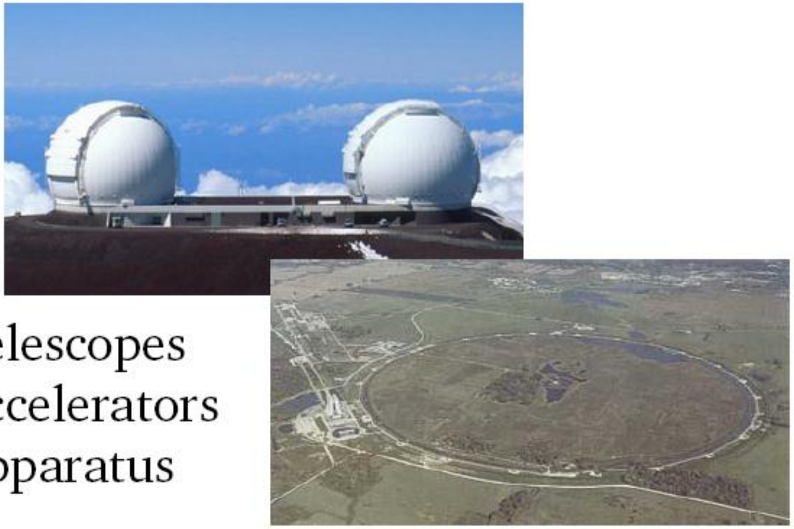


Nos ayudan a entender cómo evolucionó el universo de un estado homogéneo a otro inhomogéneo

COSMOLOGIA: UNA CIENCIA EXPERIMENTAL

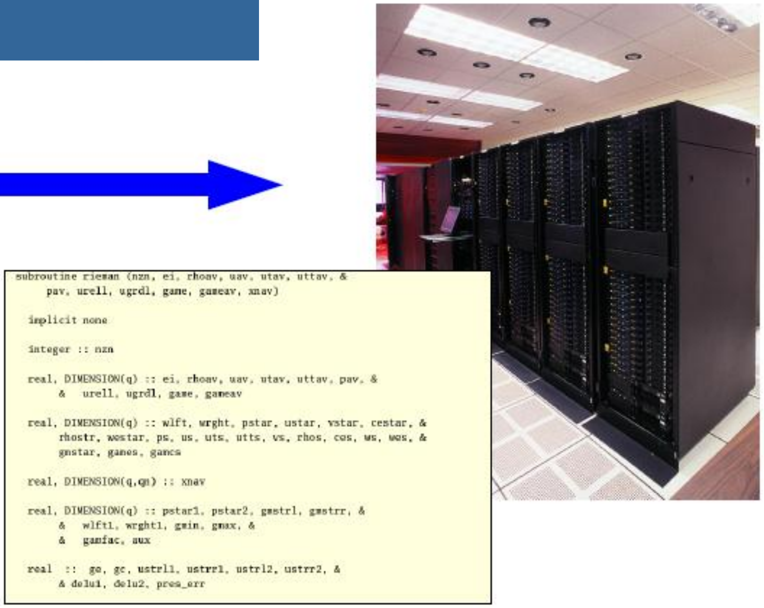
Universo Real **Universo Virtual**

Analogías

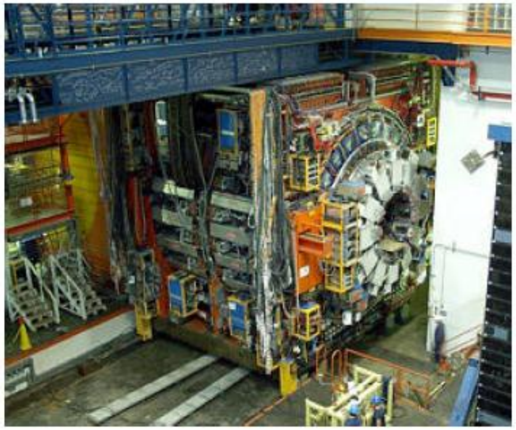


Telescopes
Accelerators
Apparatus

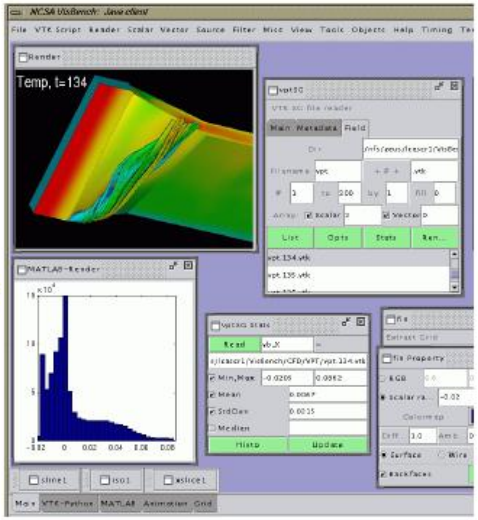
Fast computers+
Simulation codes



```
subroutine rieman (nzn, ei, rhoav, uav, utav, uttav, &
     pav, urell, ugrdl, game, gameav, xnav)

  implicit none

  integer :: nzn

  real, DIMENSION(q) :: ei, rhoav, uav, utav, uttav, pav, &
       &   urell, ugrdl, game, gameav

  real, DIMENSION(q) :: wlft, wrght, pstar, ustar, vstar, cestar, &
       rhostr, westar, ps, us, uts, utts, vs, rhos, ces, ws, wes, &
       gmstar, games, gamcs

  real, DIMENSION(q,qn) :: xnav

  real, DIMENSION(q) :: pstar1, pstar2, gmstrl, gmstrr, &
       &   wlft1, wrght1, gmin, gmax, &
       &   gamfac, aux

  real  ::  ge, gc, ustrl1, ustrr1, ustrl2, ustrr2, &
       & delu1, delu2, pres_err
```

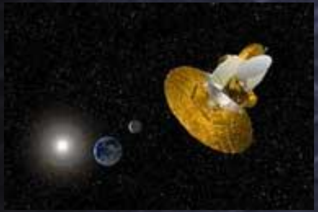


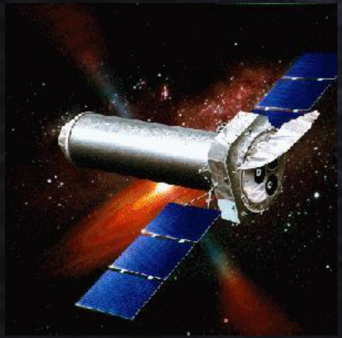
Cameras
Detectors

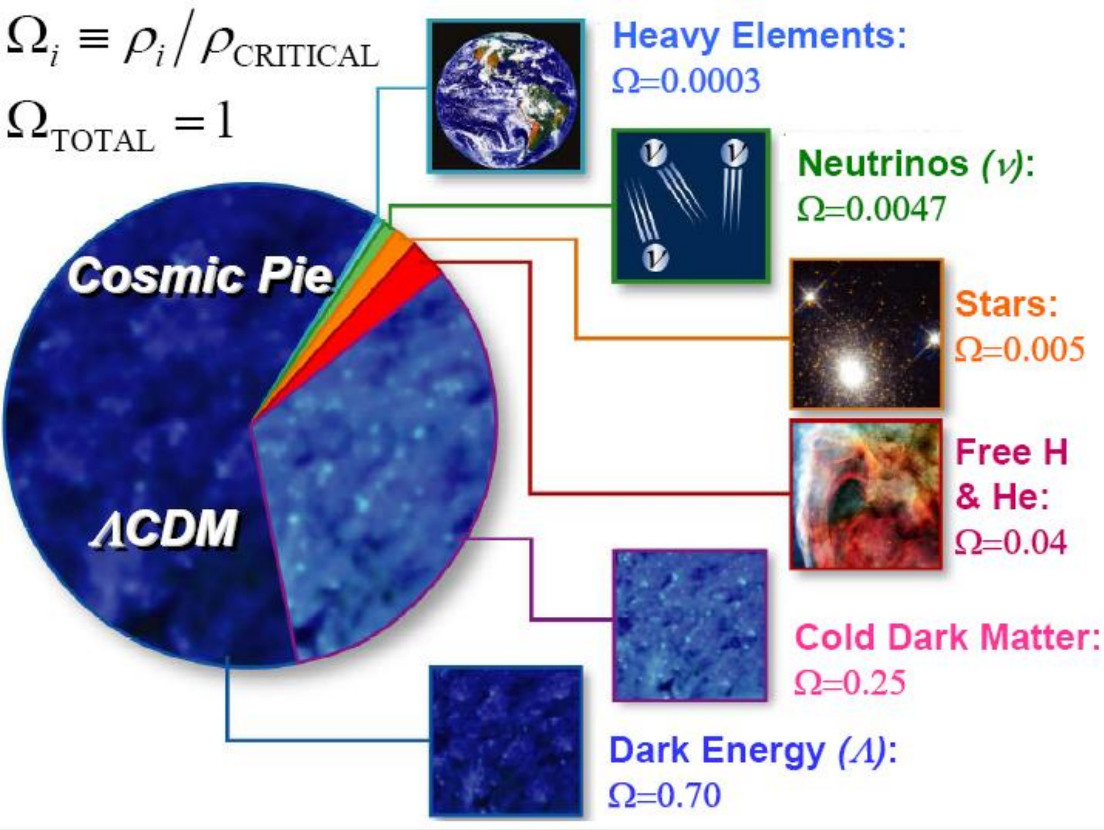


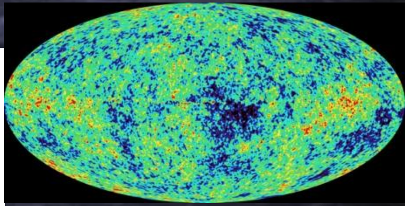
Analysis software

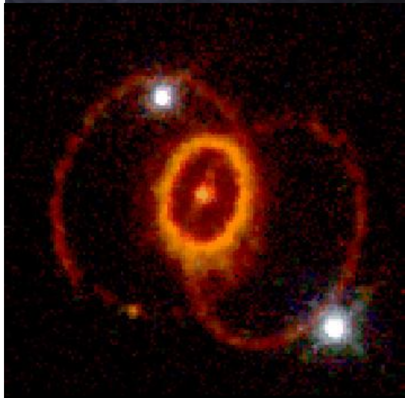
Los Ingredientes del Universo

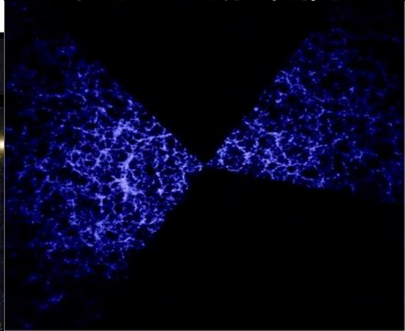




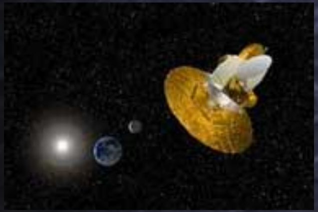


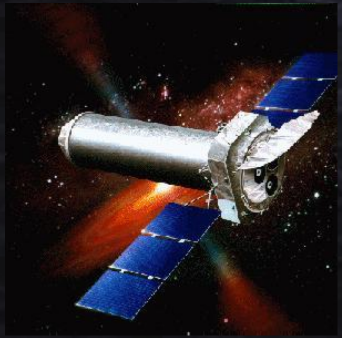


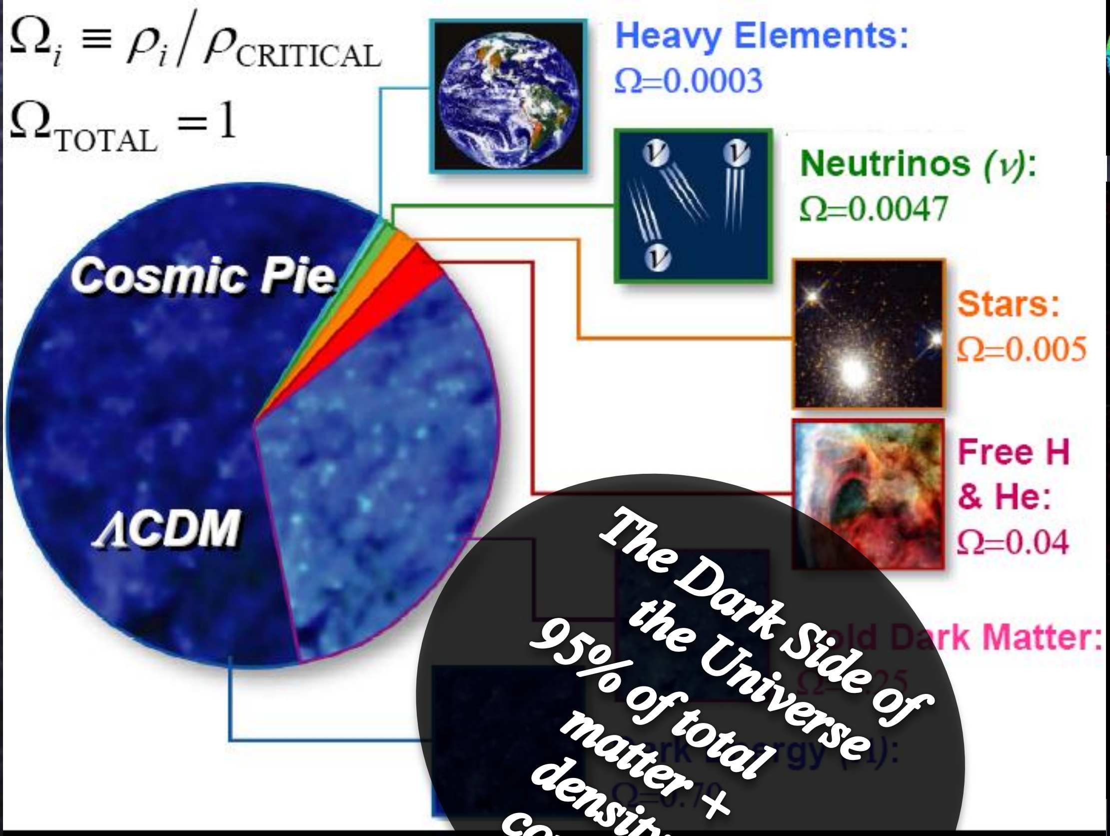




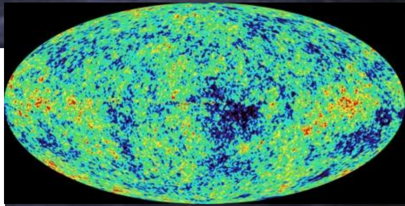
Los Ingredientes del Universo

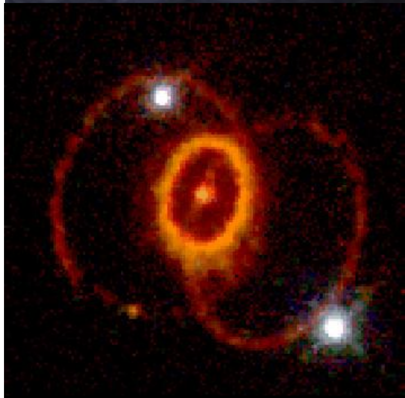


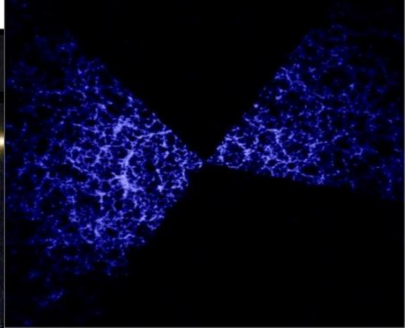




The Dark Side of the Universe
95% of total matter + density content





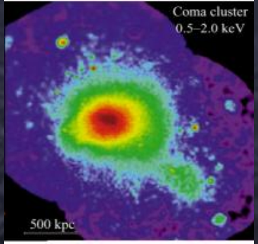


Evidencias de Existencia de Materia Oscura

- Curvas de rotación planas en galaxias espirales

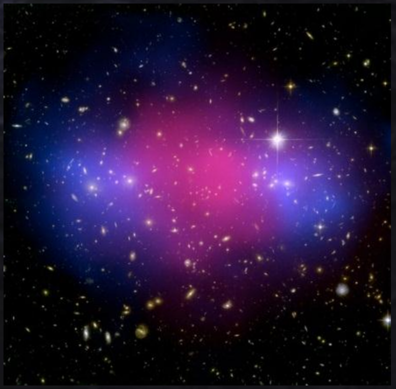
Galaxias elípticas: dispersión de velocidades de las estrellas

- Emisión de rayos X en cúmulos de galaxia



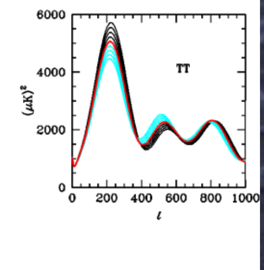
- Bullet Cluster

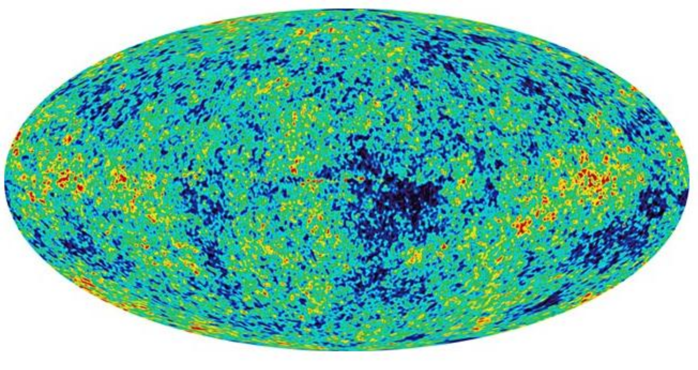
- Lentes Gravitatorias en cúmulos de galaxias



Energía Oscura

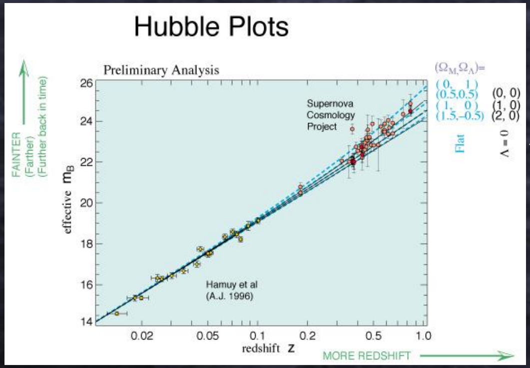
- Determinación de la geometría del universo y materia total contenida
- Universo Plano $\Omega=1$
- . $\Omega_m = 0.27\text{-}0.30$
- 70-80% restante?

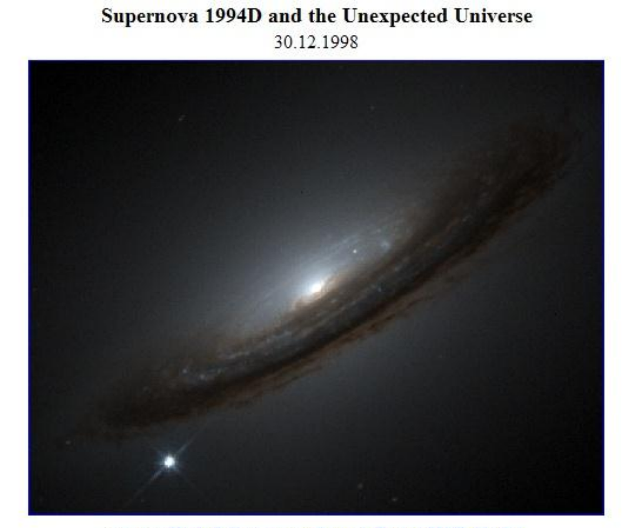




Expansión acelerada:
Existencia de un fluido
con $\rho=-\omega p$

Constante cosmológica
u otro campo cosmico
Quintaesencia,



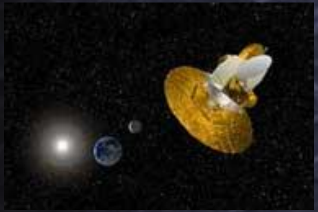


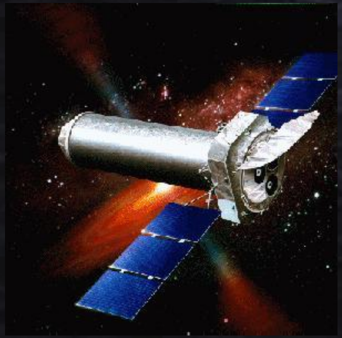
Supernova 1994D and the Unexpected Universe

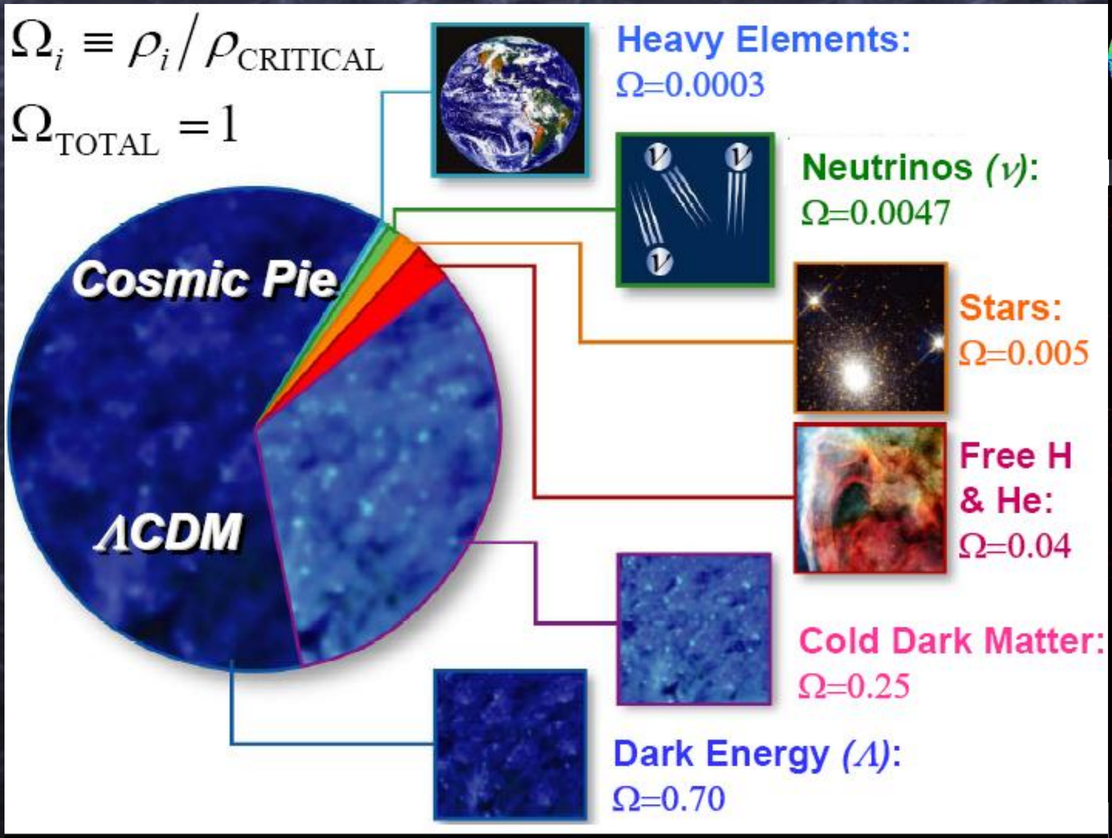
30.12.1998

Credit: High-Z Supernova Search Team, HST, NASA

Los Ingredientes del Universo







$\Omega_i \equiv \rho_i / \rho_{\text{CRITICAL}}$

$\Omega_{\text{TOTAL}} = 1$

Cosmic Pie

ΛCDM

Heavy Elements: $\Omega = 0.0003$

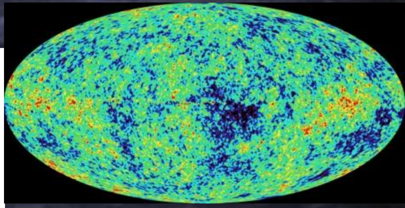
Neutrinos (ν): $\Omega = 0.0047$

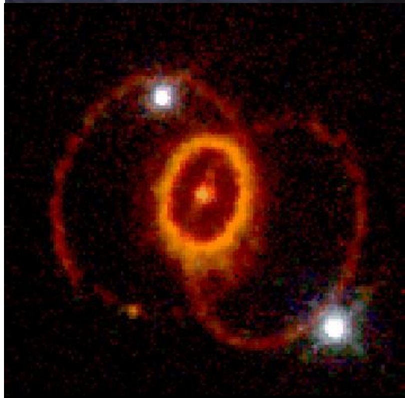
Stars: $\Omega = 0.005$

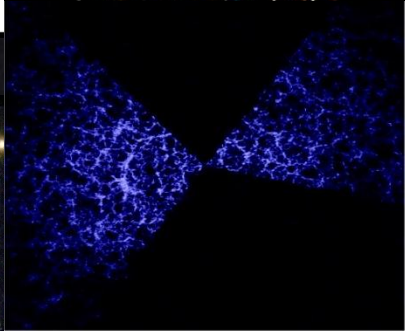
Free H & He: $\Omega = 0.04$

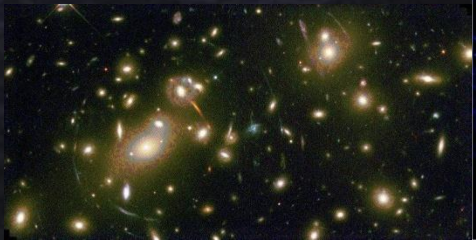
Cold Dark Matter: $\Omega = 0.25$

Dark Energy (Λ): $\Omega = 0.70$

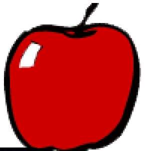


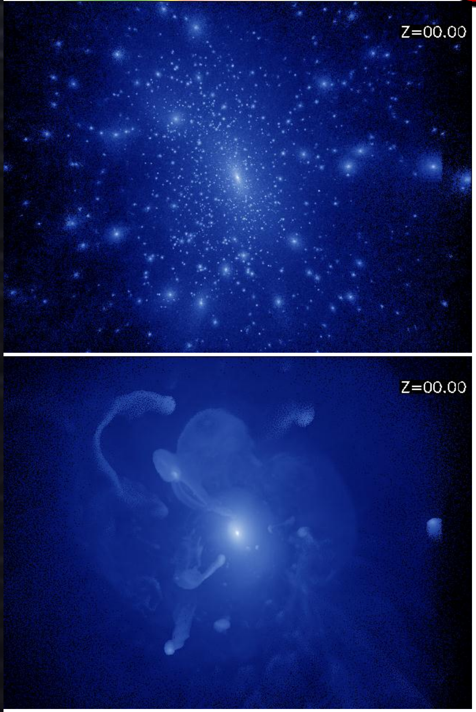






PROCESOS FISICOS MAS RELEVANTES





equations that govern evolution

- *Gravity is the king*

  gravity is by far the strongest force on the large scales. gravitational interactions are modelled using Newton's laws

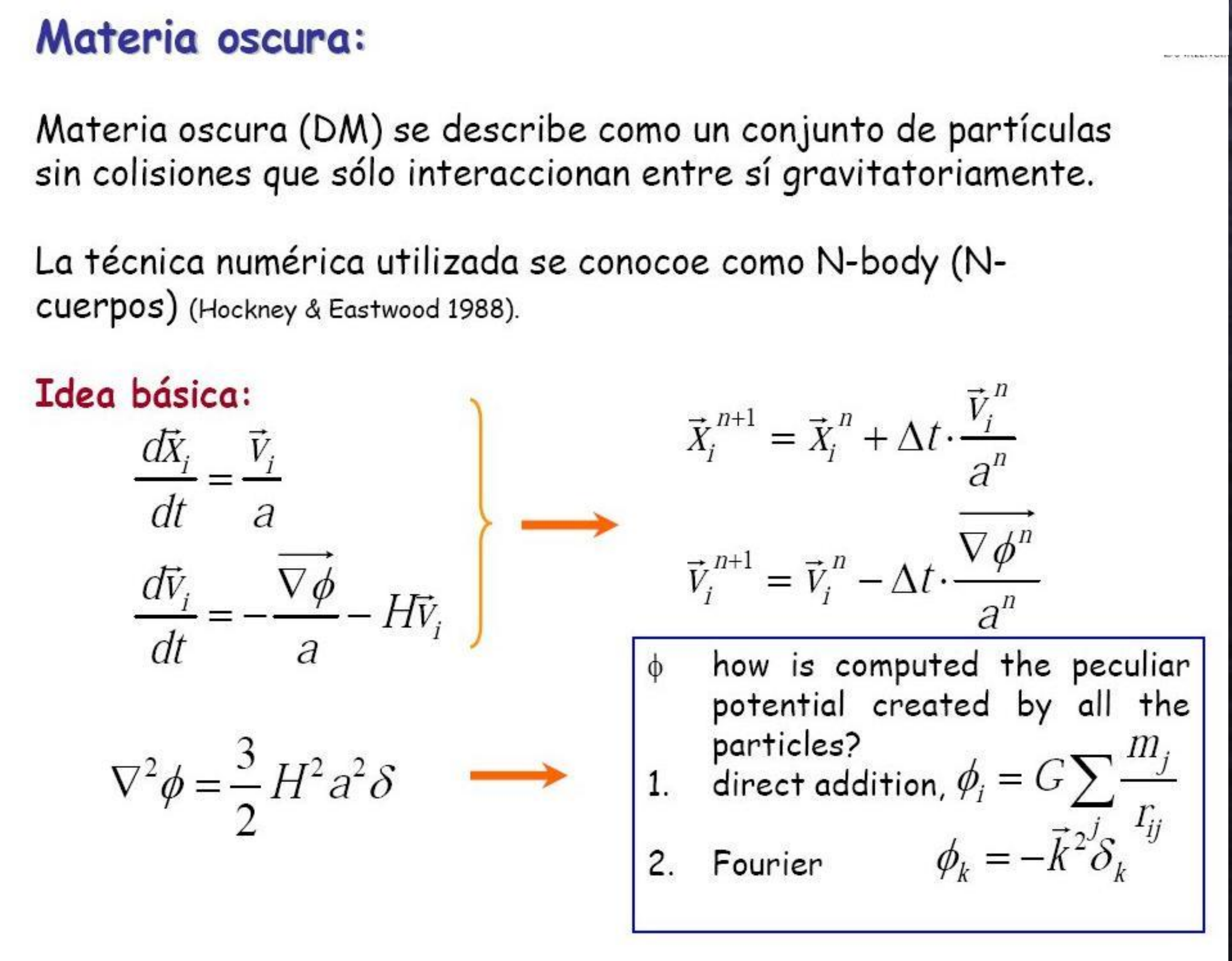
- *Other forces may need to be included depending on the composition of the Universe and scales considered*

  ordinary matter, the baryons, experiences pressure forces if compressed to sufficiently high densities. these "hydrodynamic" forces are included in simulations that include baryons

- *The equations are solved in expanding system of coordinates (because Universe expands)*

Una guia rápida de los métodos numéricos en cosmologia.

Simulación de la evolución gavitacional
Método N-cuerpos



Materia oscura:

Materia oscura (DM) se describe como un conjunto de partículas sin colisiones que sólo interaccionan entre sí gravitatoriamente.

La técnica numérica utilizada se conocoe como N-body (N-cuerpos) (Hockney & Eastwood 1988).

Idea básica:

$$\left.\begin{aligned}\frac{d\vec{x}_i}{dt}&=\frac{\vec{v}_i}{a}\\ \frac{d\vec{v}_i}{dt}&=-\frac{\overrightarrow{\nabla\phi}}{a}-H\vec{v}_i\end{aligned}\right\}\longrightarrow\begin{aligned}\vec{x}_i^{\,n+1}&=\vec{x}_i^{\,n}+\Delta t\cdot\frac{\vec{v}_i^{\,n}}{a^n}\\ \vec{v}_i^{\,n+1}&=\vec{v}_i^{\,n}-\Delta t\cdot\frac{\overrightarrow{\nabla\phi^n}}{a^n}\end{aligned}$$

$$\nabla^2\phi=\frac{3}{2}H^2a^2\delta\longrightarrow$$

ϕ how is computed the peculiar potential created by all the particles?

1. direct addition, $\phi_i = G\sum_j \frac{m_j}{r_{ij}}$
2. Fourier $\phi_k = -\vec{k}^2\delta_k$

Simulación de la evolución gavitacional
Métodos de N-cuerpos

- **Particle-Particle:**
  - Easiest of all methods. newtonian differential
  - Scale as order N^2
  - Easy to parallelize an not too large N.

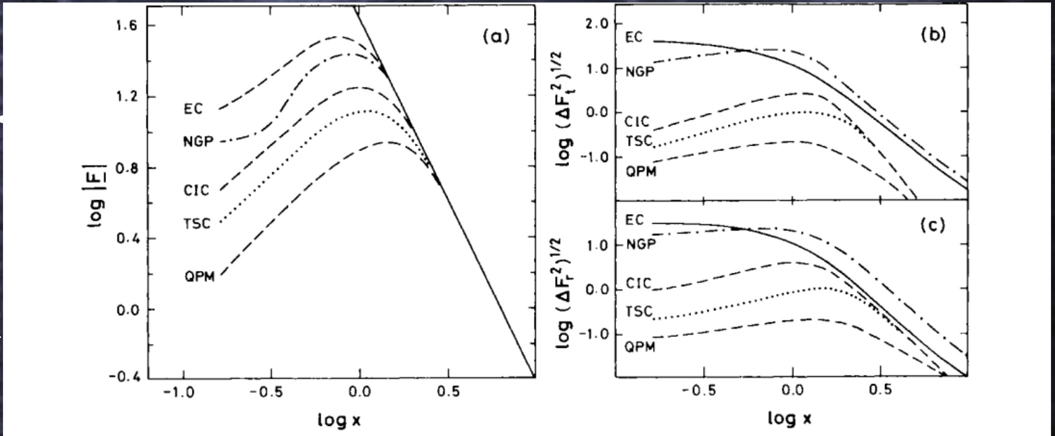
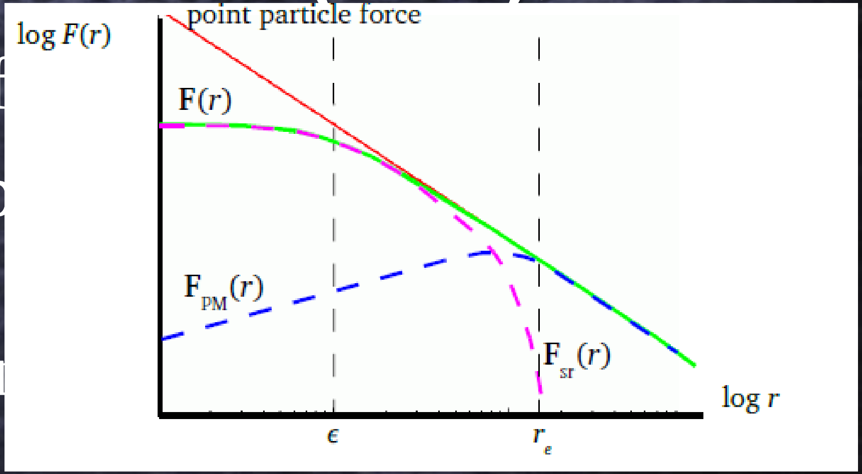


Figure 2 (*a*) The mean interparticle force as a function of separation in mesh spaces for several particle-mesh schemes. The solid line in (*a*) shows the unsoftened force. The other panels show the rms fluctuations in the tangential (*b*) and radial (*c*) directions [reproduced from Efstathiou et al. (1985), with permission].

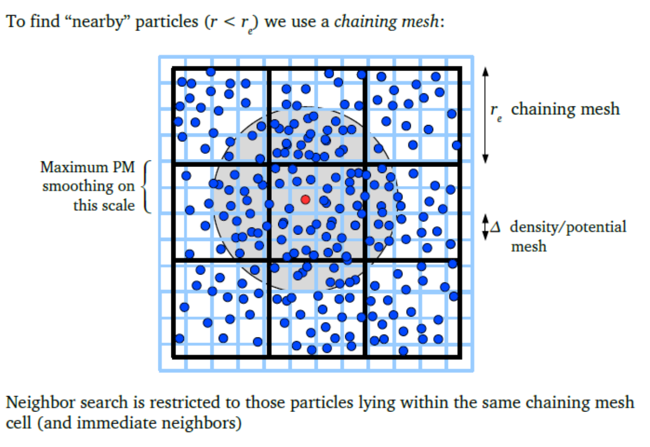
- **Particle-Mesh.**
  - Mean field approximation: particles do not feel each other but interact only through the mean gravitational field computed in a mesh.
  - Different interpolation techniques between particles and mesh: NGP, CIC , TSC..
  - Use FFT to solve Poisson equation. Very fast and parallel using periodic boundary conditions.

Simulación de la evolución gavitacional
Métodos de N-cuerpos

- **Particle-Particle-Particle-Mesh (P^3M):**
  - PM force accuracy only f
  - Gravitational clustering p gradients: poor resolution too small compared with r
  - Possible <u>Solution:</u>
    - Increase the number of cells.
    - Divide the net force in Short-range (PM). Neighbour search



To find “nearby” particles ($r < r_e$) we use a *chaining mesh*:

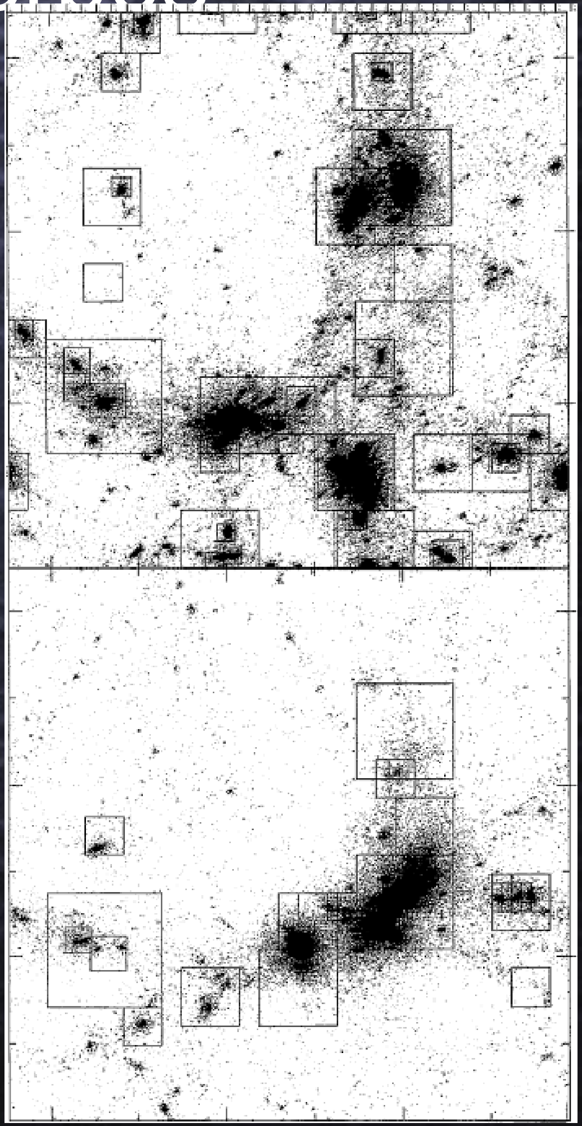


Neighbor search is restricted to those particles lying within the same chaining mesh cell (and immediate neighbors)

Simulación de la evolución gavitacional
Métodos de N-cuerpos

- **Adaptive P^3M:**
  - Basic idea: for those P^3M chaining mesh cells whose calculation time would be dominated by the particle-particle sum, process further with a finer potential mesh before computing PP force.

Example cold dark matter structure formation calculation with AP3M(from Couchman 1991)



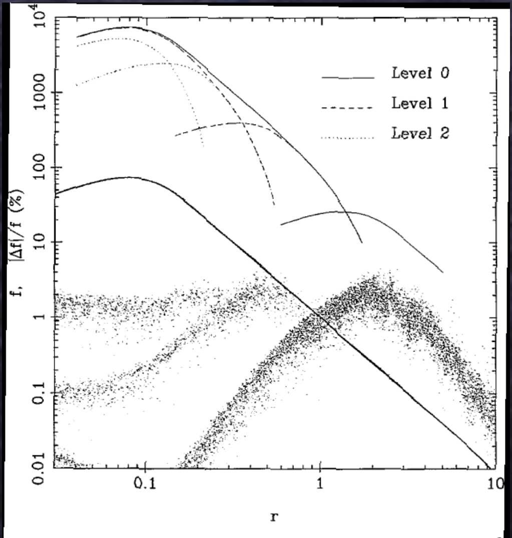
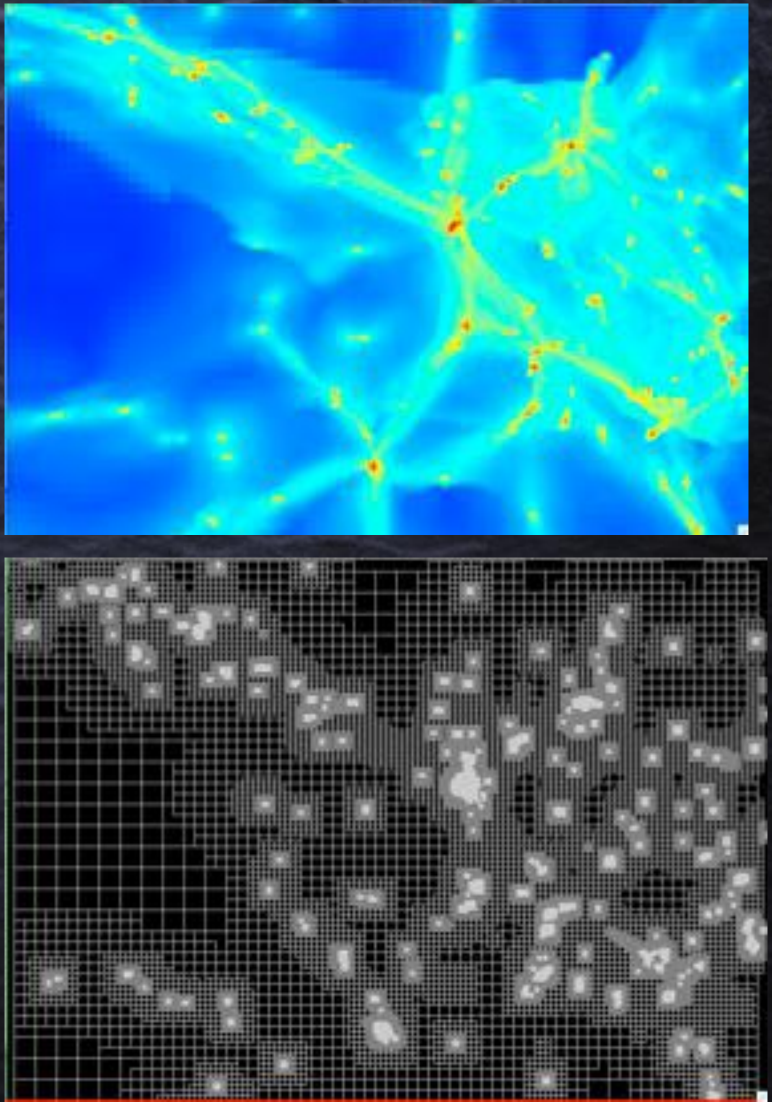


FIG. 1.—The pairwise force as a function of radius calculated on a 32^3 periodic mesh with two levels of refinement. The heavy continuous line is the calculated force, and the dots indicate the modulus of the error in the force. The curves at the top of the plot indicate the components of the force (× 100) calculated from the base mesh (level 0), the refinements, and the corresponding direct sums.

Simulación de la evolución gavitacional
Métodos de N-cuerpos

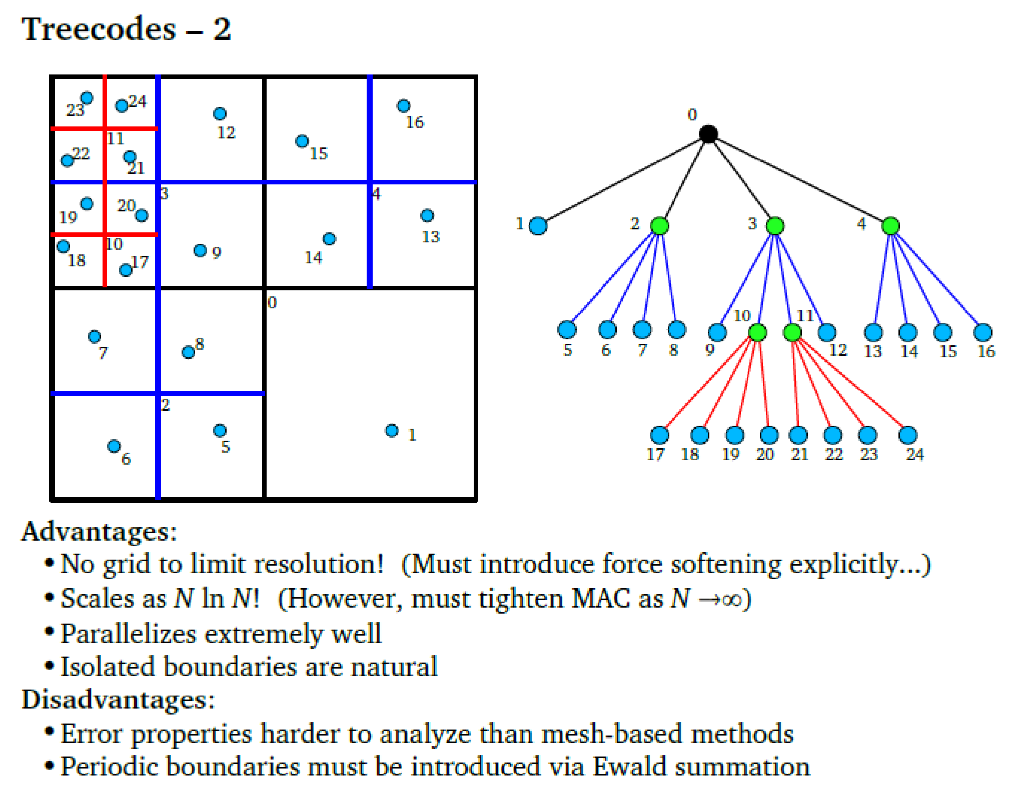
- **ADAPTIVE MESH REFINEMENT (AMR)**
- Use staggered meshes to compute poisson’s equation in different levels: PM is used at level 0 and then cells are refined depending on density. Typically each cell is recursively refined if the number of particle per cell exceed some threshold (around 10 particles). Main problem is the bookkeeping of the mesh structure. Easy to implement hydrodynamics.



•RAMSES cosmological simulation:
•Density and mesh structure

Simulación de la evolución gavitacional
Métodos de N-cuerpos

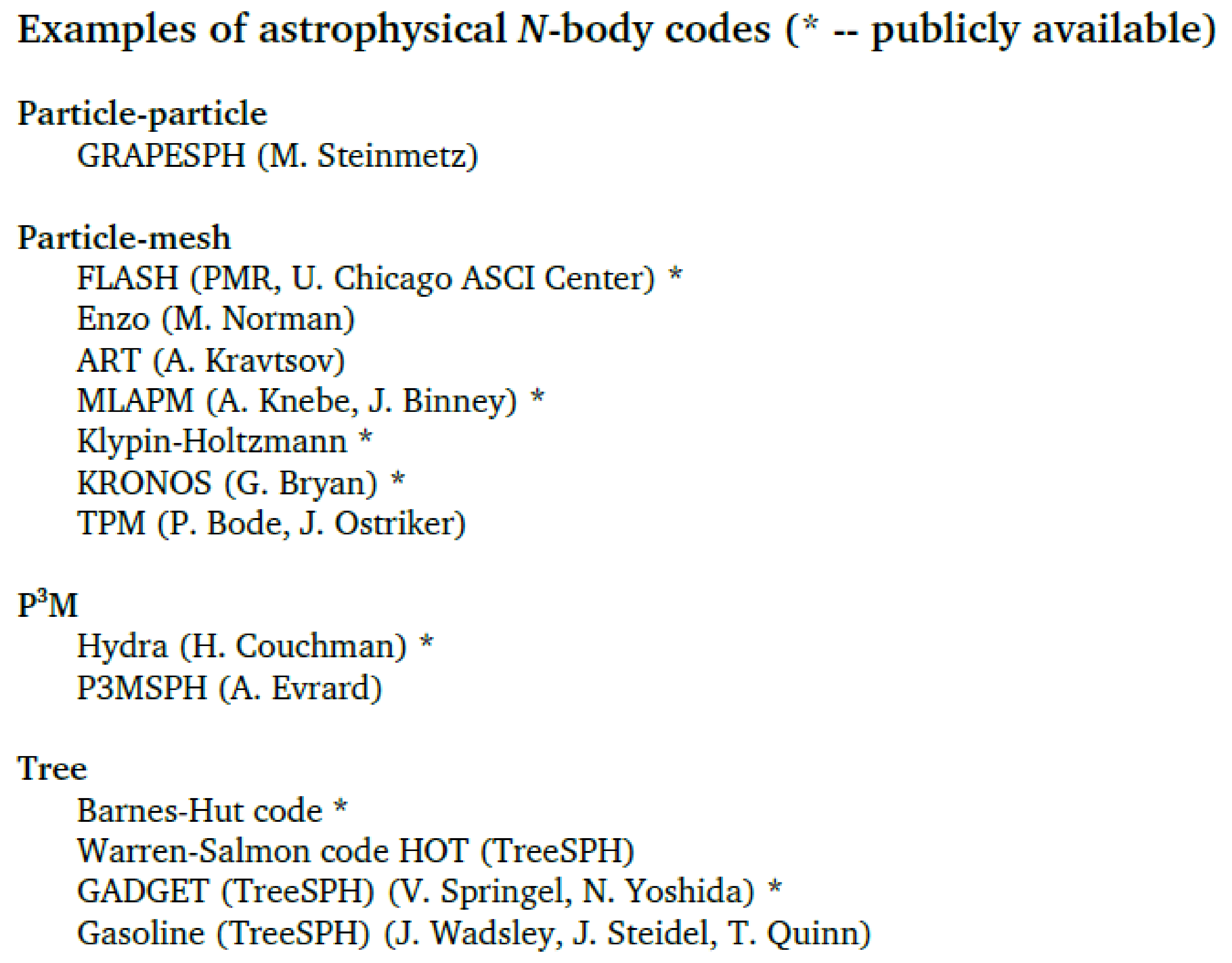
- **TREE METHODS.**
  - Do not used any mesh at all. Only particle-particle force
  - Easy to implement boundary conditions.
  - Store particles in a tree data structure Particles are at leaves of tree; parent nodes store total mass of children.
  - When the force on a particle is needed we traverse tree, starting at the root.
  - If a node is terminal (leaf node), directly sum the force from the particle at that node.
  - If not, ask: is the monopole (or quadrupole, ...) of the node an adequate
  - approximation to the force from the child particles?
    - (i) If yes, use the approximate force and stop traversing this branch.
    - If no, traverse the children.



Treecodes – 2

Advantages:
- No grid to limit resolution! (Must introduce force softening explicitly...)
- Scales as $N \ln N$! (However, must tighten MAC as $N \rightarrow \infty$)
- Parallelizes extremely well
- Isolated boundaries are natural

Disadvantages:
- Error properties harder to analyze than mesh-based methods
- Periodic boundaries must be introduced via Ewald summation



Examples of astrophysical *N*-body codes (* -- publicly available)

Particle-particle
- GRAPESPH (M. Steinmetz)

Particle-mesh
- FLASH (PMR, U. Chicago ASCI Center) *
- Enzo (M. Norman)
- ART (A. Kravtsov)
- MLAPM (A. Knebe, J. Binney) *
- Klypin-Holtzmann *
- KRONOS (G. Bryan) *
- TPM (P. Bode, J. Ostriker)

P^3M
- Hydra (H. Couchman) *
- P3MSPH (A. Evrard)

Tree
- Barnes-Hut code *
- Warren-Salmon code HOT (TreeSPH)
- GADGET (TreeSPH) (V. Springel, N. Yoshida) *
- Gasoline (TreeSPH) (J. Wadsley, J. Steidel, T. Quinn)

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GRAPE Board

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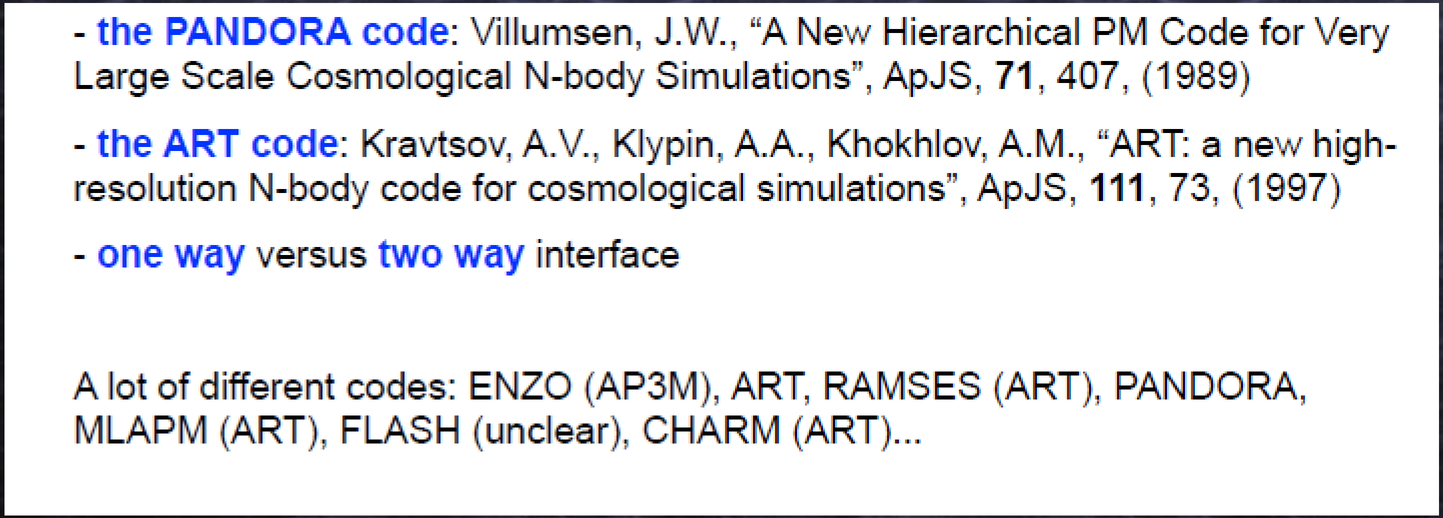
Examples of astrophysical *N*-body codes (* -- publicly available)

N body with Adaptive Mesh Refinement

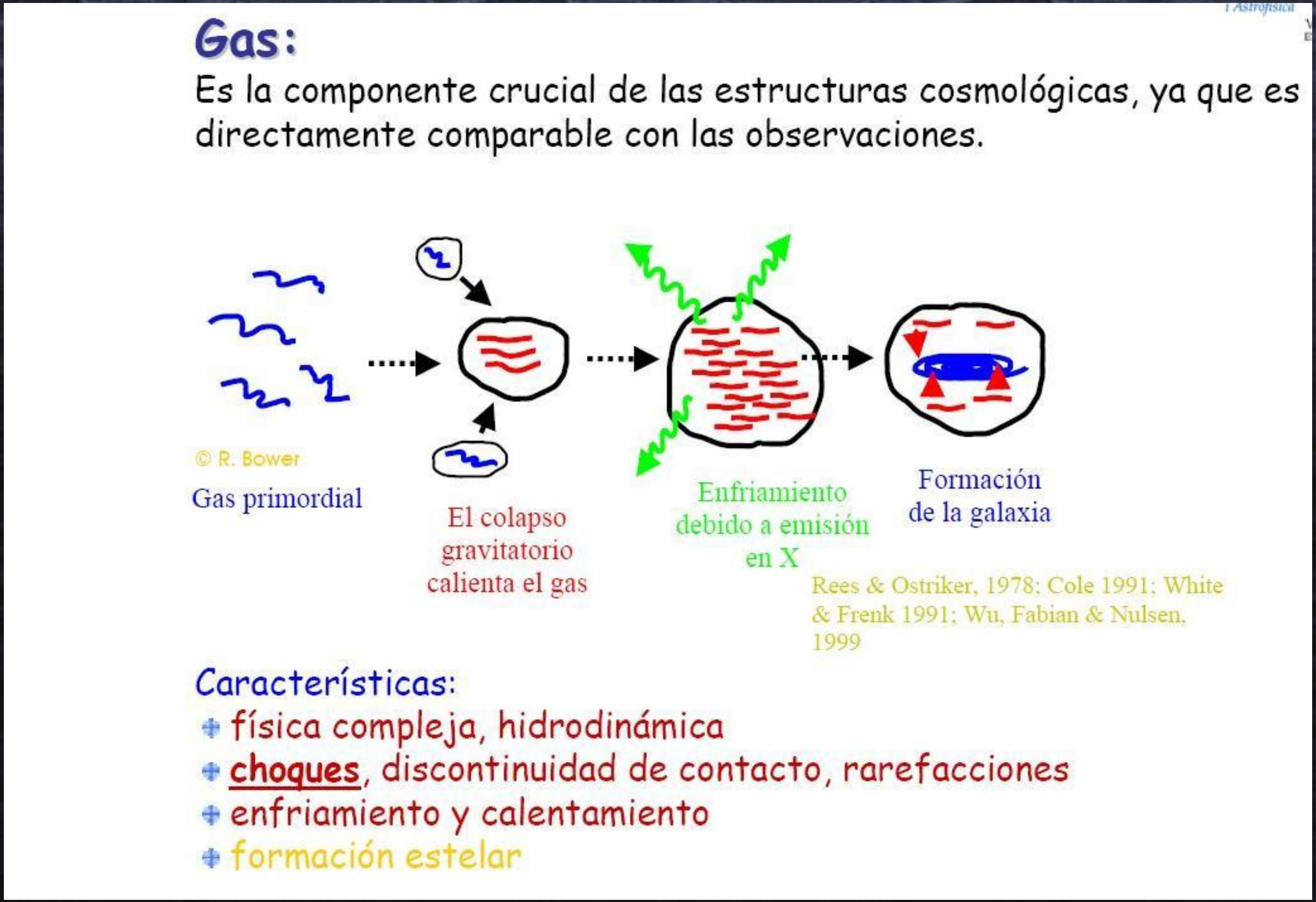


- **the PANDORA code**: Villumsen, J.W., “A New Hierarchical PM Code for Very Large Scale Cosmological N-body Simulations”, ApJS, **71**, 407, (1989)
- **the ART code**: Kravtsov, A.V., Klypin, A.A., Khokhlov, A.M., “ART: a new high-resolution N-body code for cosmological simulations”, ApJS, **111**, 73, (1997)
- **one way** versus **two way** interface

A lot of different codes: ENZO (AP3M), ART, RAMSES (ART), PANDORA, MLAPM (ART), FLASH (unclear), CHARM (ART)...

•NEMO: a compilation of   N-body free software:
http://carma.astro.umd.edu/nemo/
ASTROSIM wiki:
http://www.astrosim.net

DINÁMICA DE GASES EN COSMOLOGIA



Gas:

Es la componente crucial de las estructuras cosmológicas, ya que es directamente comparable con las observaciones.

© R. Bower

Gas primordial

El colapso gravitatorio calienta el gas

Enfriamiento debido a emisión en X

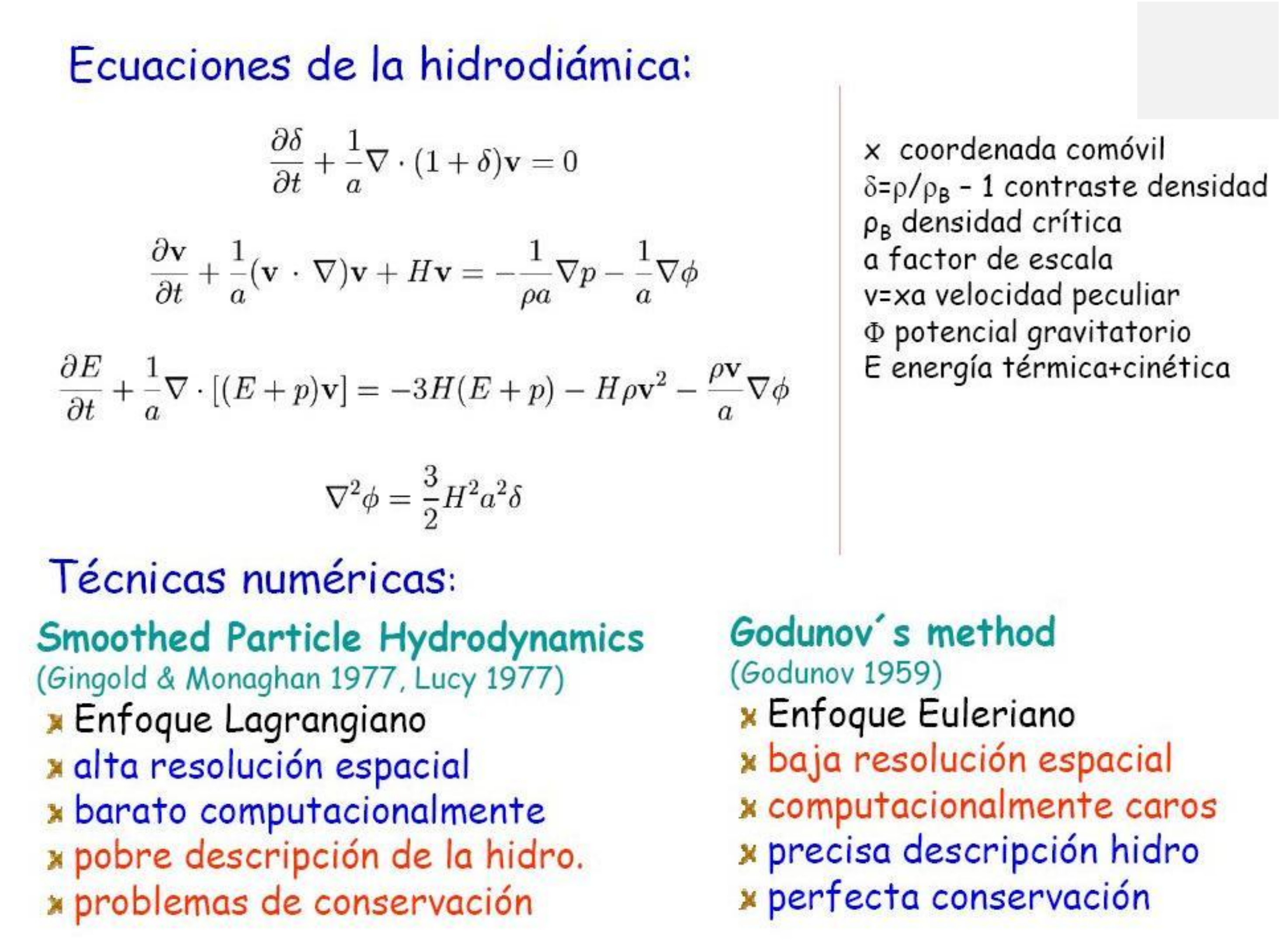
Formación de la galaxia

Rees & Ostriker, 1978; Cole 1991; White & Frenk 1991; Wu, Fabian & Nulsen, 1999

Características:

- física compleja, hidrodinámica
- **choques**, discontinuidad de contacto, rarefacciones
- enfriamiento y calentamiento
- formación estelar

DINÁMICA DE GASES EN COSMOLOGIA



Ecuaciones de la hidrodiámica:

$$\frac{\partial \delta}{\partial t} + \frac{1}{a}\nabla \cdot (1+\delta)\mathbf{v} = 0$$

$$\frac{\partial \mathbf{v}}{\partial t} + \frac{1}{a}(\mathbf{v} \cdot \nabla)\mathbf{v} + H\mathbf{v} = -\frac{1}{\rho a}\nabla p - \frac{1}{a}\nabla \phi$$

$$\frac{\partial E}{\partial t} + \frac{1}{a}\nabla \cdot [(E+p)\mathbf{v}] = -3H(E+p) - H\rho\mathbf{v}^2 - \frac{\rho\mathbf{v}}{a}\nabla\phi$$

$$\nabla^2\phi = \frac{3}{2}H^2 a^2 \delta$$

x coordenada comóvil
$\delta=\rho/\rho_B$ - 1 contraste densidad
ρ_B densidad crítica
a factor de escala
v=xa velocidad peculiar
Φ potencial gravitatorio
E energía térmica+cinética

Técnicas numéricas:

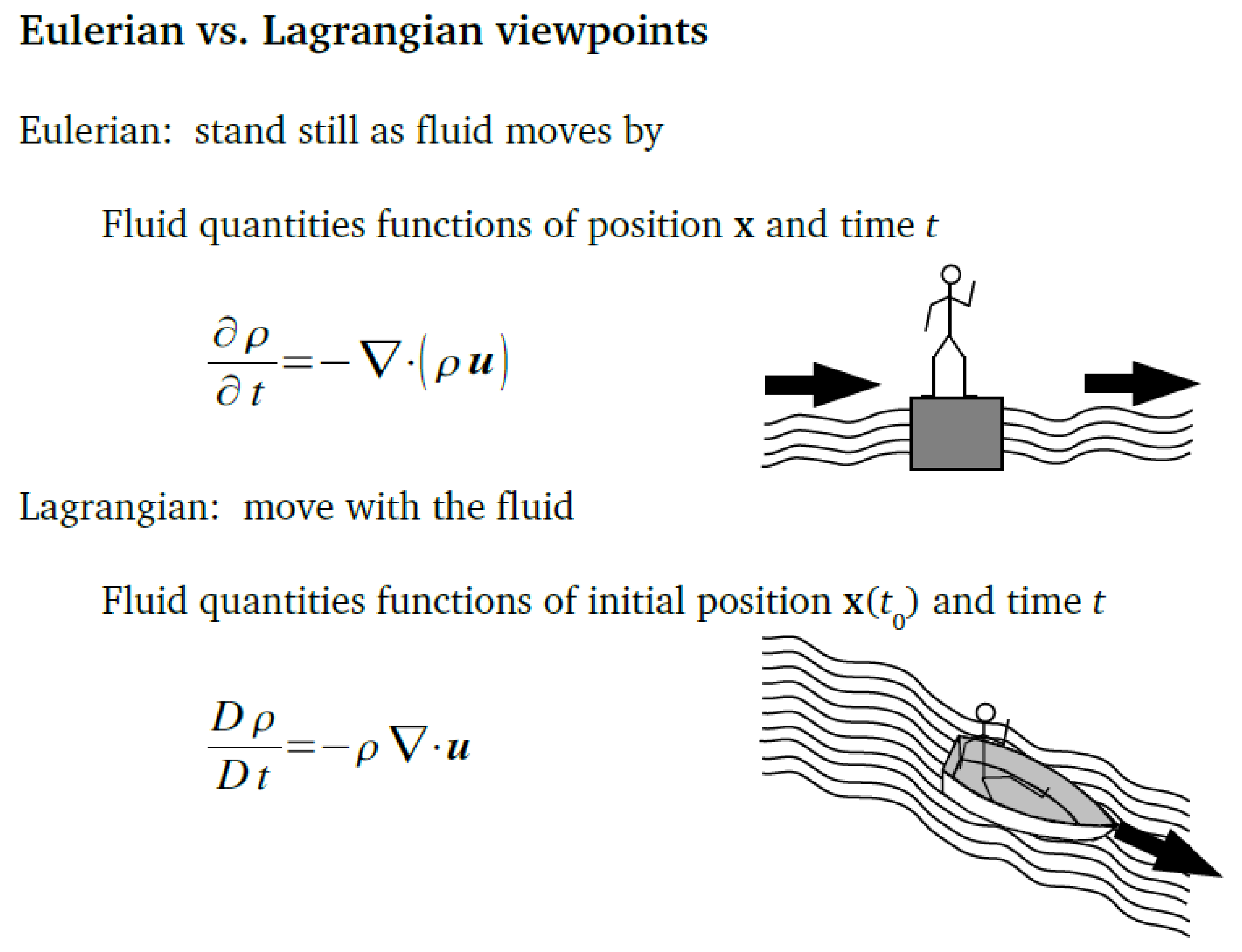
Smoothed Particle Hydrodynamics
(Gingold & Monaghan 1977, Lucy 1977)

- Enfoque Lagrangiano
- alta resolución espacial
- barato computacionalmente
- pobre descripción de la hidro.
- problemas de conservación

Godunov´s method
(Godunov 1959)

- Enfoque Euleriano
- baja resolución espacial
- computacionalmente caros
- precisa descripción hidro
- perfecta conservación

DINÁMICA DE GASES EN COSMOLOGIA



Eulerian vs. Lagrangian viewpoints

Eulerian: stand still as fluid moves by

Fluid quantities functions of position **x** and time t

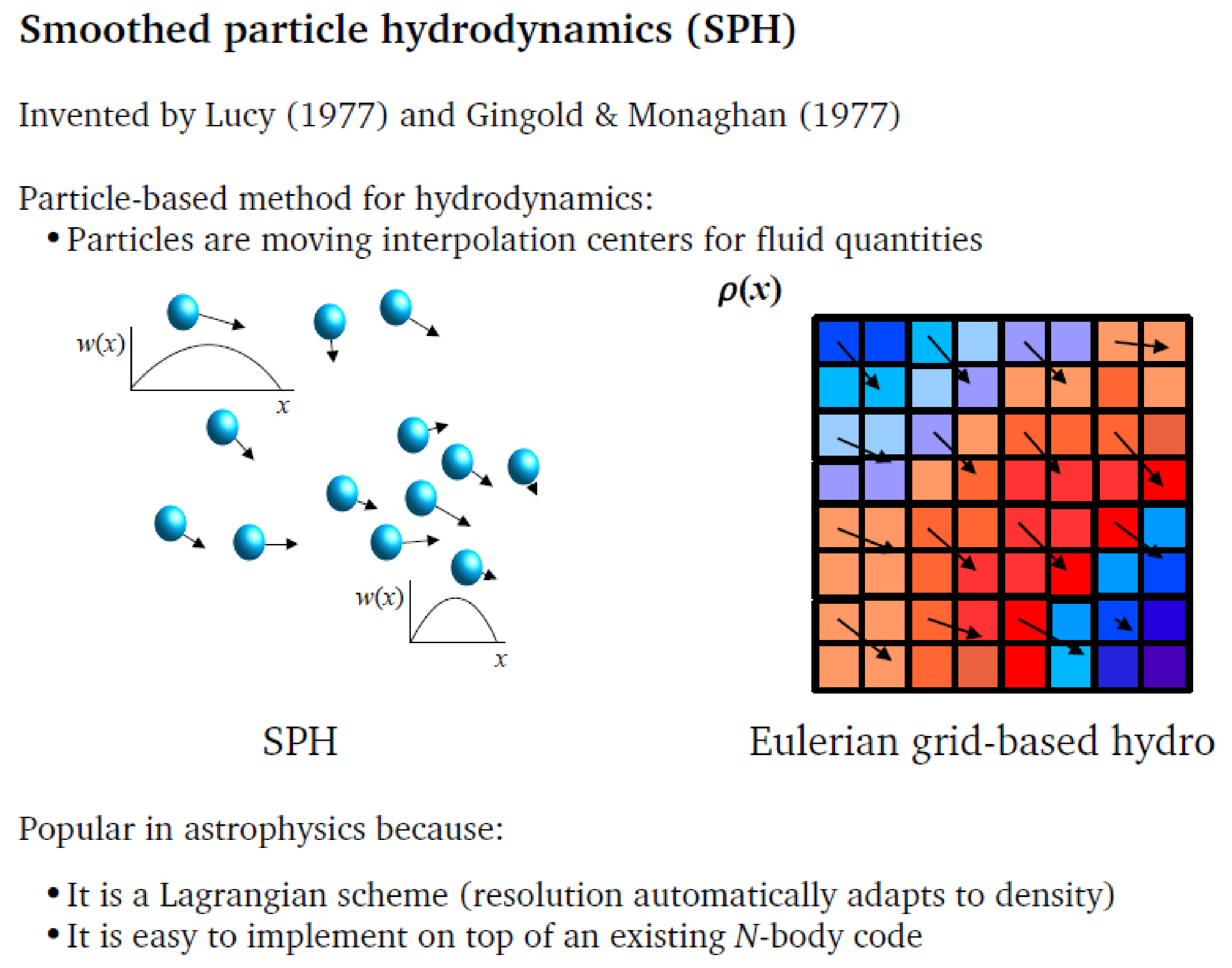
$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \boldsymbol{u})$$

Lagrangian: move with the fluid

Fluid quantities functions of initial position $\mathbf{x}(t_0)$ and time t

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \boldsymbol{u}$$

DINÁMICA DE GASES EN COSMOLOGIA



Smoothed particle hydrodynamics (SPH)

Invented by Lucy (1977) and Gingold & Monaghan (1977)

Particle-based method for hydrodynamics:

- Particles are moving interpolation centers for fluid quantities

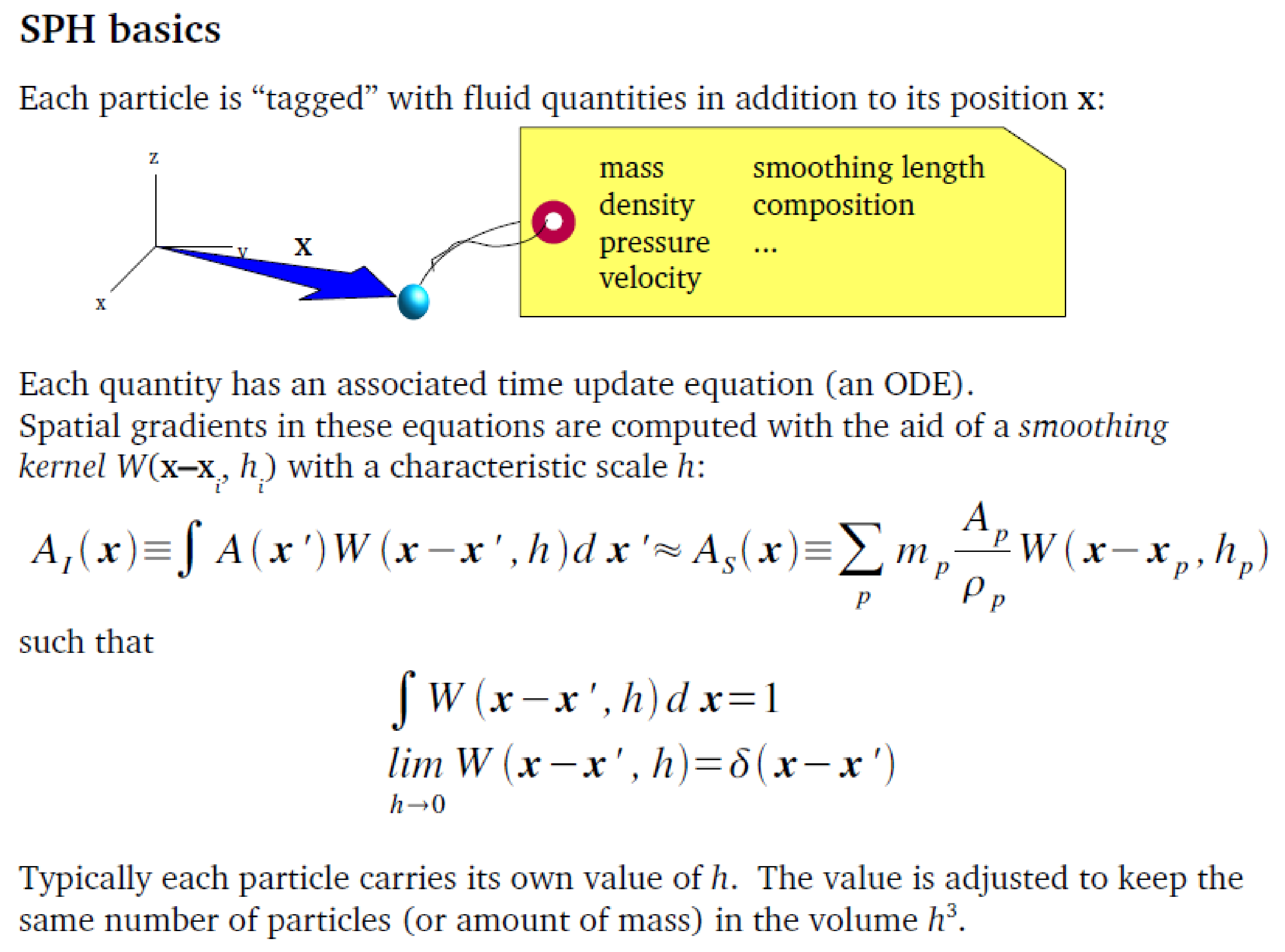
SPH

Eulerian grid-based hydro

Popular in astrophysics because:

- It is a Lagrangian scheme (resolution automatically adapts to density)
- It is easy to implement on top of an existing *N*-body code

DINÁMICA DE GASES EN COSMOLOGIA



SPH basics

Each particle is "tagged" with fluid quantities in addition to its position **x**:

mass
density
pressure
velocity
smoothing length
composition
...

Each quantity has an associated time update equation (an ODE).
Spatial gradients in these equations are computed with the aid of a *smoothing kernel* $W(\mathbf{x}-\mathbf{x}_i, h_i)$ with a characteristic scale h:

$$A_I(\mathbf{x}) \equiv \int A(\mathbf{x}')\,W(\mathbf{x}-\mathbf{x}', h)\,d\mathbf{x}' \approx A_S(\mathbf{x}) \equiv \sum_p m_p \frac{A_p}{\rho_p} W(\mathbf{x}-\mathbf{x}_p, h_p)$$

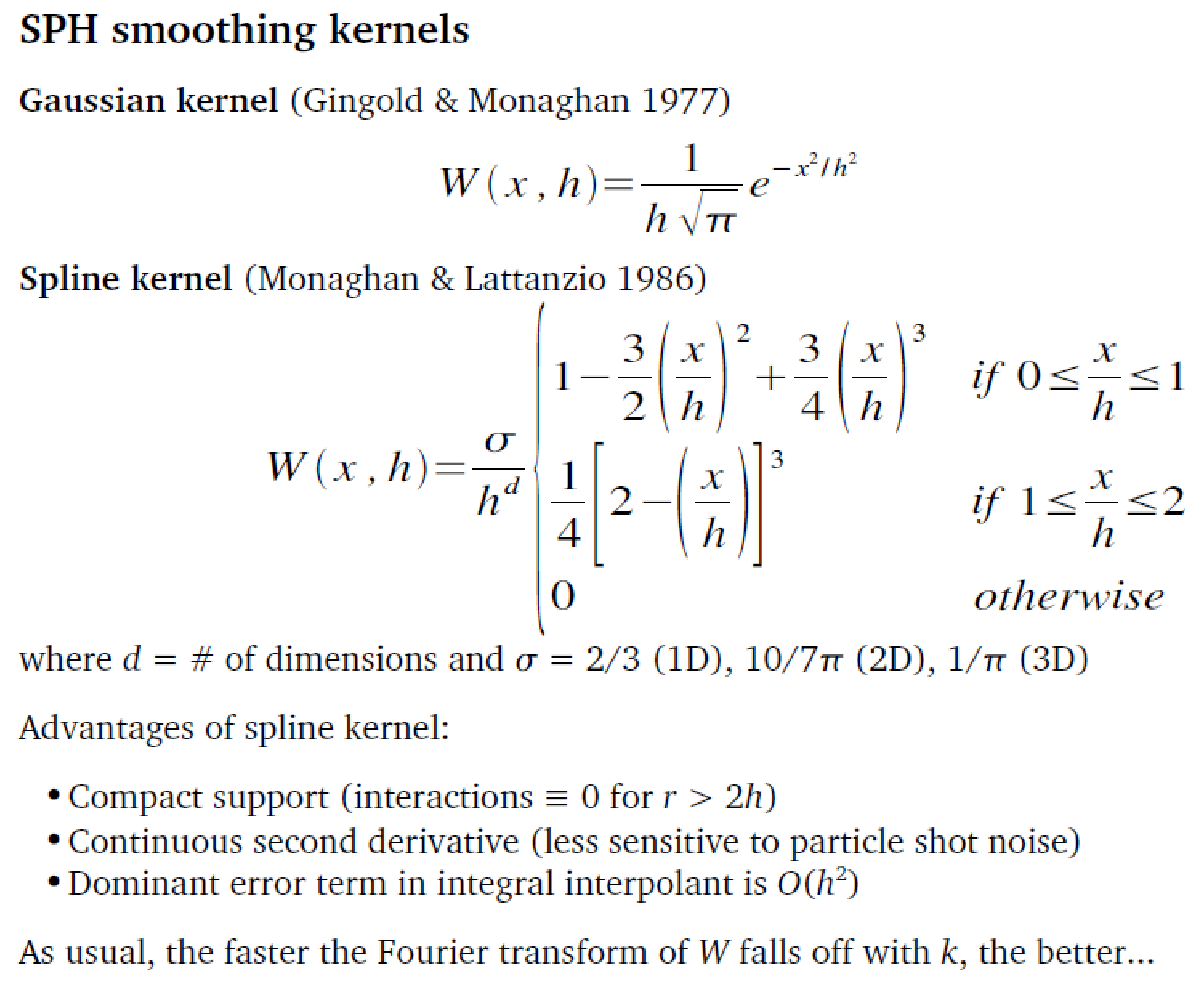
such that

$$\int W(\mathbf{x}-\mathbf{x}', h)\,d\mathbf{x} = 1$$

$$\lim_{h \to 0} W(\mathbf{x}-\mathbf{x}', h) = \delta(\mathbf{x}-\mathbf{x}')$$

Typically each particle carries its own value of h. The value is adjusted to keep the same number of particles (or amount of mass) in the volume h^3.

DINÁMICA DE GASES EN COSMOLOGIA



SPH smoothing kernels

Gaussian kernel (Gingold & Monaghan 1977)

$$W(x,h)=\frac{1}{h\sqrt{\pi}}e^{-x^2/h^2}$$

Spline kernel (Monaghan & Lattanzio 1986)

$$W(x,h)=\frac{\sigma}{h^d}\begin{cases}1-\frac{3}{2}\left(\frac{x}{h}\right)^2+\frac{3}{4}\left(\frac{x}{h}\right)^3 & \text{if } 0\le\frac{x}{h}\le 1\\ \frac{1}{4}\left[2-\left(\frac{x}{h}\right)\right]^3 & \text{if } 1\le\frac{x}{h}\le 2\\ 0 & \text{otherwise}\end{cases}$$

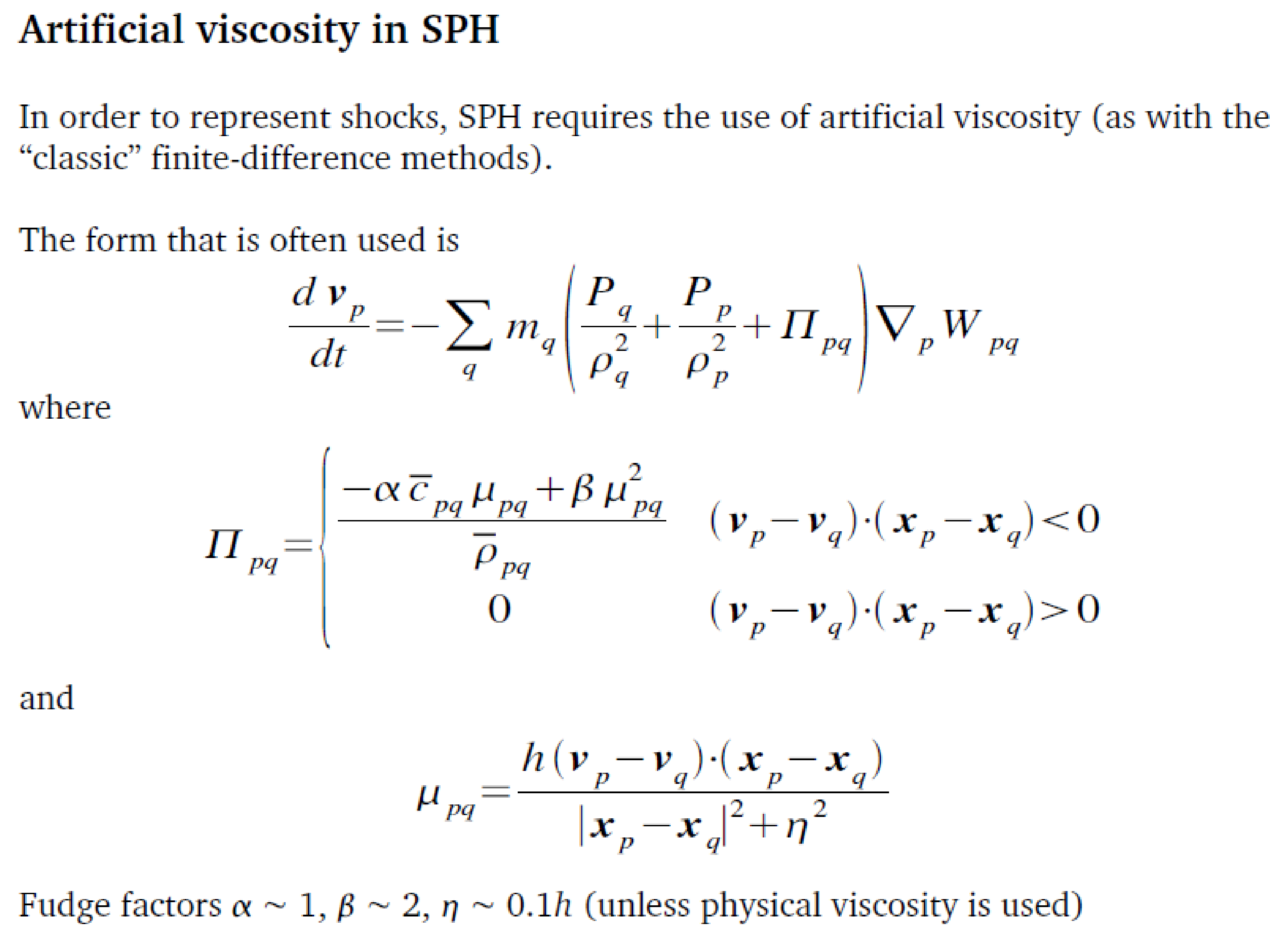
where d = # of dimensions and $\sigma = 2/3$ (1D), $10/7\pi$ (2D), $1/\pi$ (3D)

Advantages of spline kernel:

- Compact support (interactions $\equiv 0$ for $r > 2h$)
- Continuous second derivative (less sensitive to particle shot noise)
- Dominant error term in integral interpolant is $O(h^2)$

As usual, the faster the Fourier transform of W falls off with k, the better...

DINÁMICA DE GASES EN COSMOLOGIA



Artificial viscosity in SPH

In order to represent shocks, SPH requires the use of artificial viscosity (as with the “classic” finite-difference methods).

The form that is often used is

$$\frac{d\mathbf{v}_p}{dt} = -\sum_q m_q \left(\frac{P_q}{\rho_q^2} + \frac{P_p}{\rho_p^2} + \Pi_{pq} \right) \nabla_p W_{pq}$$

where

$$\Pi_{pq} = \begin{cases} \dfrac{-\alpha\, \bar{c}_{pq}\, \mu_{pq} + \beta\, \mu_{pq}^2}{\bar{\rho}_{pq}} & (\mathbf{v}_p - \mathbf{v}_q)\cdot(\mathbf{x}_p - \mathbf{x}_q) < 0 \\ 0 & (\mathbf{v}_p - \mathbf{v}_q)\cdot(\mathbf{x}_p - \mathbf{x}_q) > 0 \end{cases}$$

and

$$\mu_{pq} = \frac{h\,(\mathbf{v}_p - \mathbf{v}_q)\cdot(\mathbf{x}_p - \mathbf{x}_q)}{|\mathbf{x}_p - \mathbf{x}_q|^2 + \eta^2}$$

Fudge factors $\alpha \sim 1$, $\beta \sim 2$, $\eta \sim 0.1h$ (unless physical viscosity is used)

DINÁMICA DE GASES EN COSMOLOGIA

- EULERIAN BASED CFD
  - Basically all modern CFD is based on grid-based methods.
    - Solve the gasdynamical equations for volume averaged gas quantites. Integral form of equations. No gradients. No artificial viscosity needed.
    - Captures shocks more accurately.
    - Huge industry of mathematical algorithms for CFD.
    - Used only recently in Cosmology due to the problem of gravitational evolution: Need gravity solvers in AMR.

DINÁMICA DE GASES EN COSMOLOGIA

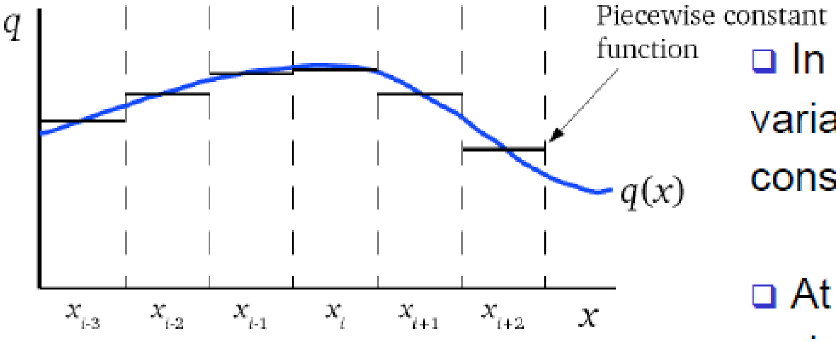
Solving equation of gasdynamics

a crash course in shock-capturing Eulerian methods

$$\frac{\partial \rho}{\partial t} + \nabla \rho \mathbf{u} = 0,$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla \Phi - \frac{\nabla P}{\rho},$$

$$\frac{\partial E}{\partial t} + \nabla \cdot [(E + P)\mathbf{u}] = -\rho \mathbf{u} \cdot \nabla \Phi.$$



- ❑ Some other schemes (e.g., Lax-Wendroff) were proposed but none were really satisfactory
- ❑ In 1959, Godunov proposed a radically different scheme for solving these equations
- ❑ In the original Godunov's method variables were assumed to be constant in each cell.
- ❑ At each cell interface the fluxes of variables are computed by solving the Riemann boundary problem

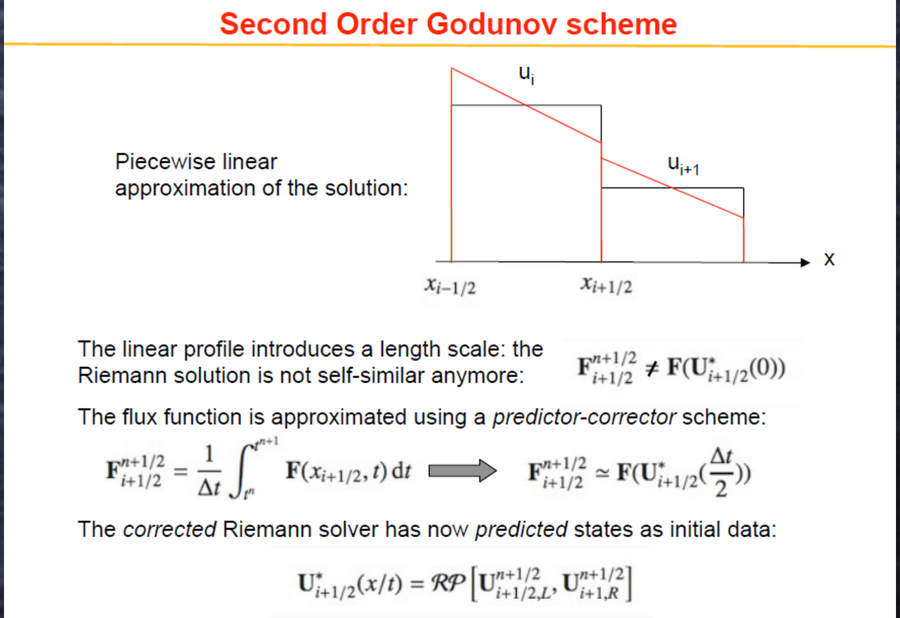
Sergei Konstantinovich Godunov

Sergei Konstantinovich Godunov

Born	17th July, 1929 Moscow

DINÁMICA DE GASES EN COSMOLOGIA

Bram Van Leer



Second Order Godunov scheme

Piecewise linear approximation of the solution:

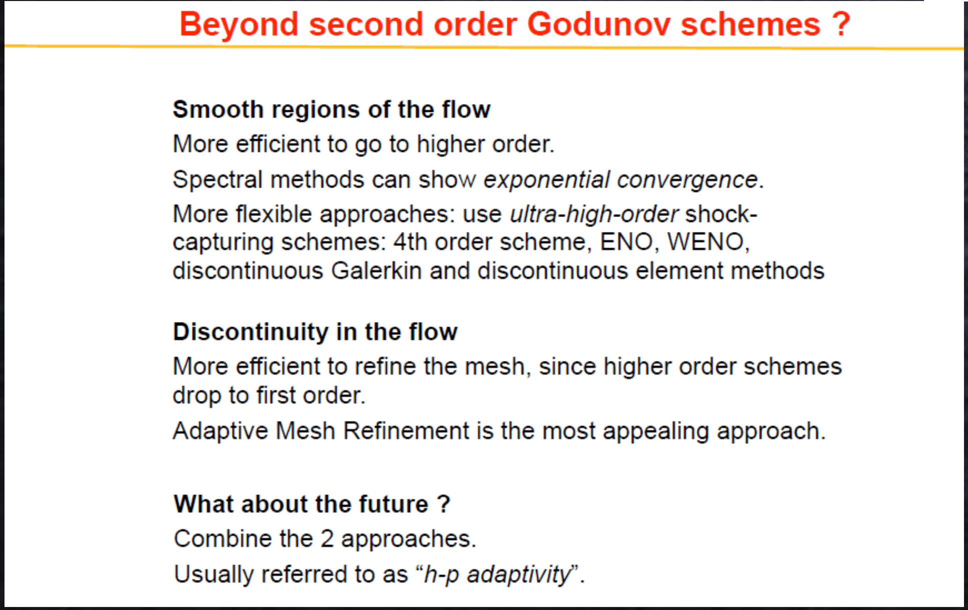
The linear profile introduces a length scale: the Riemann solution is not self-similar anymore: $\mathbf{F}^{n+1/2}_{i+1/2} \neq \mathbf{F}(\mathbf{U}^*_{i+1/2}(0))$

The flux function is approximated using a *predictor-corrector* scheme:

$$\mathbf{F}^{n+1/2}_{i+1/2} = \frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} \mathbf{F}(x_{i+1/2}, t)\,\mathrm{d}t \Longrightarrow \mathbf{F}^{n+1/2}_{i+1/2} \simeq \mathbf{F}(\mathbf{U}^*_{i+1/2}(\frac{\Delta t}{2}))$$

The *corrected* Riemann solver has now *predicted* states as initial data:

$$\mathbf{U}^*_{i+1/2}(x/t) = \mathcal{RP}\left[\mathbf{U}^{n+1/2}_{i+1/2,L}, \mathbf{U}^{n+1/2}_{i+1,R}\right]$$



Beyond second order Godunov schemes ?

Smooth regions of the flow

More efficient to go to higher order.

Spectral methods can show *exponential convergence*.

More flexible approaches: use *ultra-high-order* shock-capturing schemes: 4th order scheme, ENO, WENO, discontinuous Galerkin and discontinuous element methods

Discontinuity in the flow

More efficient to refine the mesh, since higher order schemes drop to first order.

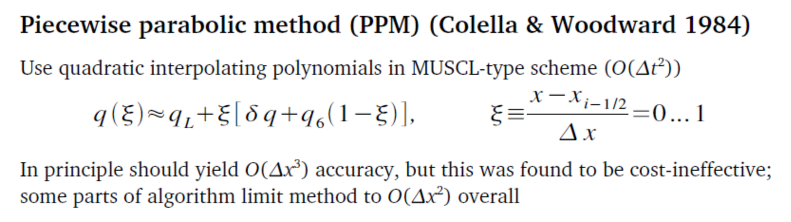
Adaptive Mesh Refinement is the most appealing approach.

What about the future ?

Combine the 2 approaches.

Usually referred to as "*h-p adaptivity*".

- State of the ART: PPM



Piecewise parabolic method (PPM) (Colella & Woodward 1984)

Use quadratic interpolating polynomials in MUSCL-type scheme ($O(\Delta t^2)$)

$$q(\xi) \approx q_L + \xi[\delta q + q_6(1-\xi)], \qquad \xi \equiv \frac{x - x_{i-1/2}}{\Delta x} = 0 \ldots 1$$

In principle should yield $O(\Delta x^3)$ accuracy, but this was found to be cost-ineffective; some parts of algorithm limit method to $O(\Delta x^2)$ overall

Cosmological Numerical codes

- SPH + Tree:
  - GASOLINE, GADGET, TREESPH
- SPH + AP3M:
  - Hydra, P-DEVA
- AMR (gas+n-body)
  - RAMSES, ART, ENZO, FLASH

See:

http://www.astrosim.net

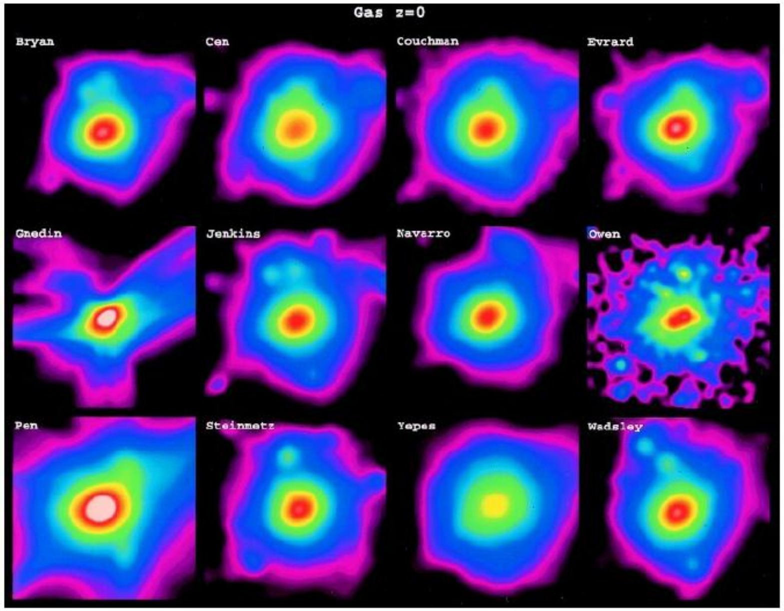
How well different simulation codes compare?

- ❑ a more general how do we know that the codes work as they should in the situations where we do not have analytic solution? (modeling these situations is of course the whole point of doing simulations!)
  - ➢ *convergence studies for a given code – keep increasing resolution until results converge*
  - ➢ *cross-comparison of codes (e.g., Frenk et al. 1999; Knebe et al. 1999; Knebe et al. 2001; Heitmann et al. 2005; O'Shea et al. 2005)*

Different hydrodynamical simulation codes are broadly in agreement, albeit with substantial scatter and differences in detail

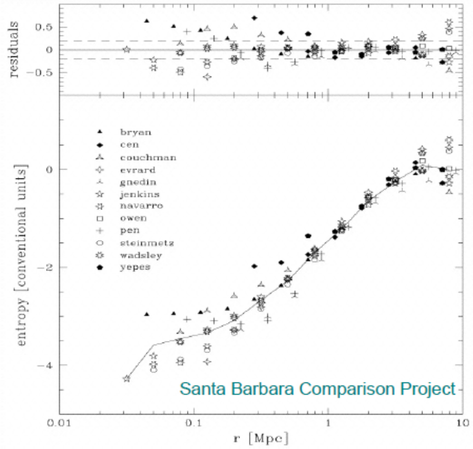
THE SANTA BARBARA CLUSTER COMPARISON PROJECT

Frenk, White & 23 co-authors (1999)



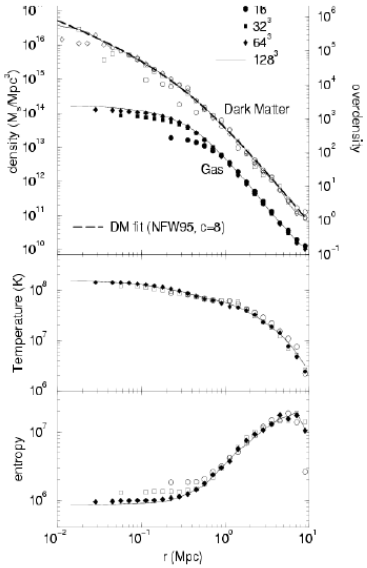
Mesh codes appear to produce higher entropy in the cores of clusters

RADIAL ENTROPY PROFILE



Ascasibar, Yepes, Müller & Gottlöber (2003):
More accurate SPH simulations also seem to develop an entropy core

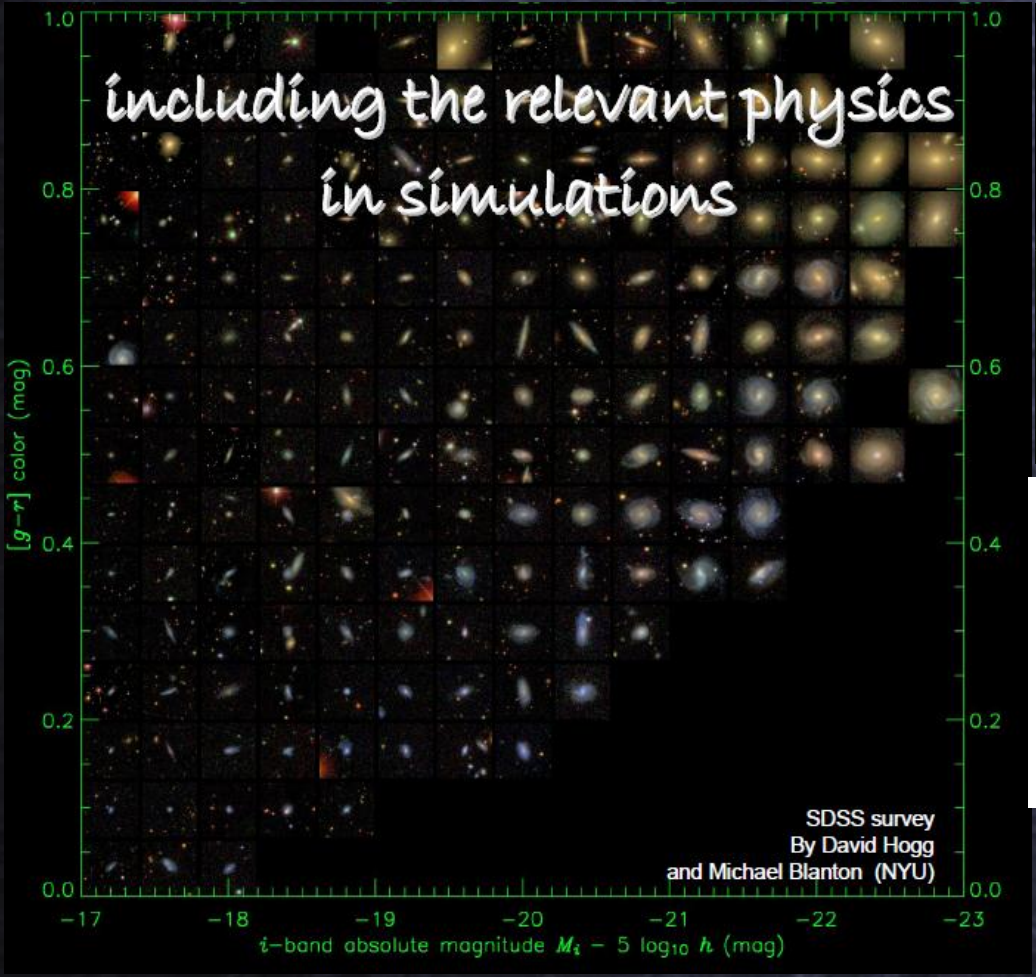
Bryan & Norman 1997



Additional physics

- Baryonic matter is subject to many different processes due to electromagnetic and strong interactions:
  - Radiative atomic cooling and UV heating.
  - Gravothermal catastrophies
  - Star formation
  - Feedbacks: thermal injection by exploding stars and metal enrichments.
  -

including the relevant physics in simulations



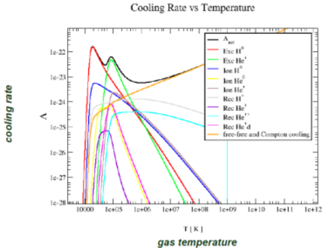
SDSS survey
By David Hogg
and Michael Blanton (NYU)

some of these processes are poorly understood

HST image of the Antennae galaxies

gas cooling rates for primordial gas composition

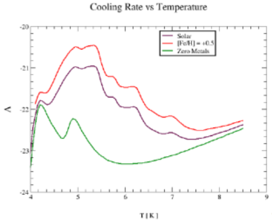
Cooling Rate vs Temperature



Dopita & Sutherland 20

dependence of cooling rate on metallicity

Cooling Rate vs Temperature



Sutherland & Dopita 1993, ApJS

Given the rates, how is cooling included in the simulations?

$$\frac{\partial \rho}{\partial t} + \nabla \rho \mathbf{u} = 0,$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla\Phi - \frac{\nabla P}{\rho},$$

$$\frac{\partial E}{\partial t} + \nabla\cdot[(E+P)\mathbf{u}] = -\rho\mathbf{u}\cdot\nabla\Phi + (\Gamma - \mathrm{L}),$$

$$\nabla^2\Phi = 4\pi G(\rho_{tot} + 3P_{tot}/c^2) - \Lambda,$$

$$\varepsilon = \frac{1}{\gamma-1}\frac{P}{\rho},$$

❑ net cooling/heating modify the internal energy of the gas and hence the total energy $E=v^2/2+\varepsilon$

❑ so cooling/heating is included as sink/source term on r.h.s. of the energy equation

❑ the only subtlety is that the rate of energy change (e.g., cooling time) can be much shorter than local dynamical time which sets the integration step of the hydro equations

starformation in simulations

HST image of the Antennae galaxies

Once a stellar particle is formed it is assigned mass, time of birth, metallicity of the parent cell, etc. These properties allow then to model spectra of galaxies and to calculate its optical properties (luminosity, colors,…)

starformation can be assume to occur over some time, rather than instantly

$$\Delta m_{\rm SF} = m_*(\Delta t/t_{\rm dyn})[(t - t_*)/t_{\rm dyn}]\ \exp\left[-(t - t_*)/t_{\rm dyn}\right]$$

which allows to spread heating due stellar feedback over time

$$\Delta E_{\rm SN}/\Delta t = (\Delta m_{\rm SF}/\Delta t)c^2\epsilon_{\rm SN}$$
$$\Delta E_\nu/\Delta t = (\Delta m_{\rm SF}/\Delta t)c^2\epsilon_{\rm UV}\,g_\nu$$

$$\epsilon_{\rm SN} = 10^{-4.5} \qquad \epsilon_{\rm UV} = 10^{-4.0}$$

star formation in nutshell

convert gas mass into collisionless stellar particles in cold, dense regions according to rate:

$$\dot\rho_* = C_*\left(\frac{\rho_{\rm gas}}{\rho_0}\right)^\alpha, \quad T < T_*, \quad \rho_{\rm gas} > \rho_*$$

sometimes compression condition is enforced to form stellar particles only in the regions of converging flow

$$\nabla\cdot\boldsymbol{v} < 0$$

normalization C is chosen so that the empirical Kennicutt's star formation law is reproduced:*

$$\Sigma_{\rm SFR} = (2.5\pm0.7)\times10^{-4}\left(\frac{\Sigma_{\rm gas}}{1\ {\rm M_\odot pc^{-2}}}\right)^{1.4\pm0.15}\ {\rm M_\odot yr^{-1}kpc^{-2}}$$

Tag all mesh cells (or gas particles in an SPH simulation) for which the following set of conditions is satisfied:

$$\nabla\cdot\boldsymbol{v} < 0 \Rightarrow \text{contracting}\ ,$$

$$t_{\rm cool} < t_{\rm dyn} \equiv \sqrt{\frac{3\pi}{32G\rho_{\rm tot}}} \Rightarrow \text{cooling rapidly}$$

$$m_b > m_J \quad \Rightarrow \text{gravity unstable}$$

Take mass from the gas mass of the cell and convert it into a stellar particle:

$$\Delta m_b = -m_b\,\Delta t/t_{\rm dyn} \quad \text{and} \quad m_* = +m_b\,\Delta t/t_{\rm dyn}$$

Stellar particles are assigned the momentum and position of their parent cell (or gas particle). Subsequently, they are followed as collisionless particles along with DM particles using standard N-body techniques.

Computational Resources

Gravity:

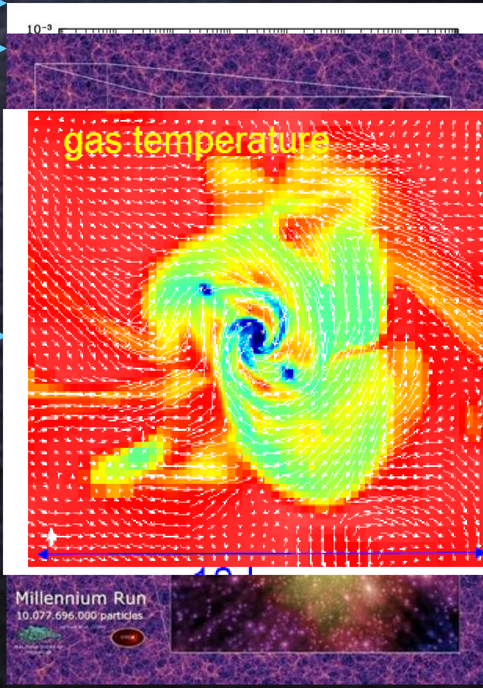
- N-body method ($O(N^2)$)
- New algorithms (tree, pm, etc) can scale as O (N log N)
- MPI implementations of N-body algorithms using domain decomposition
- Cold Dark matter *fluctuations have contribution at all scales*:
    - Need to resolve many scale lenghts simultaneously,
    - $N > 10^{11}$ partícles
    - RAM Memory > 10 Tbytes
    - Large number of processors.> 5,000

Gas dynamics:

- AMR and SPH codes
- More demanding than pure N-body due to Courant Condition
- Very large dynamical range and strong shocks show up in the fluid.

Data Storage and Visualization

- Huge datasets generated (4 dimensional problem)
- Need of access to large storage systems.
- Parallel codes for visualization of billions of computational elements.



Moore’s Law for Cosmological N-body Simulations

Moore`s Law:

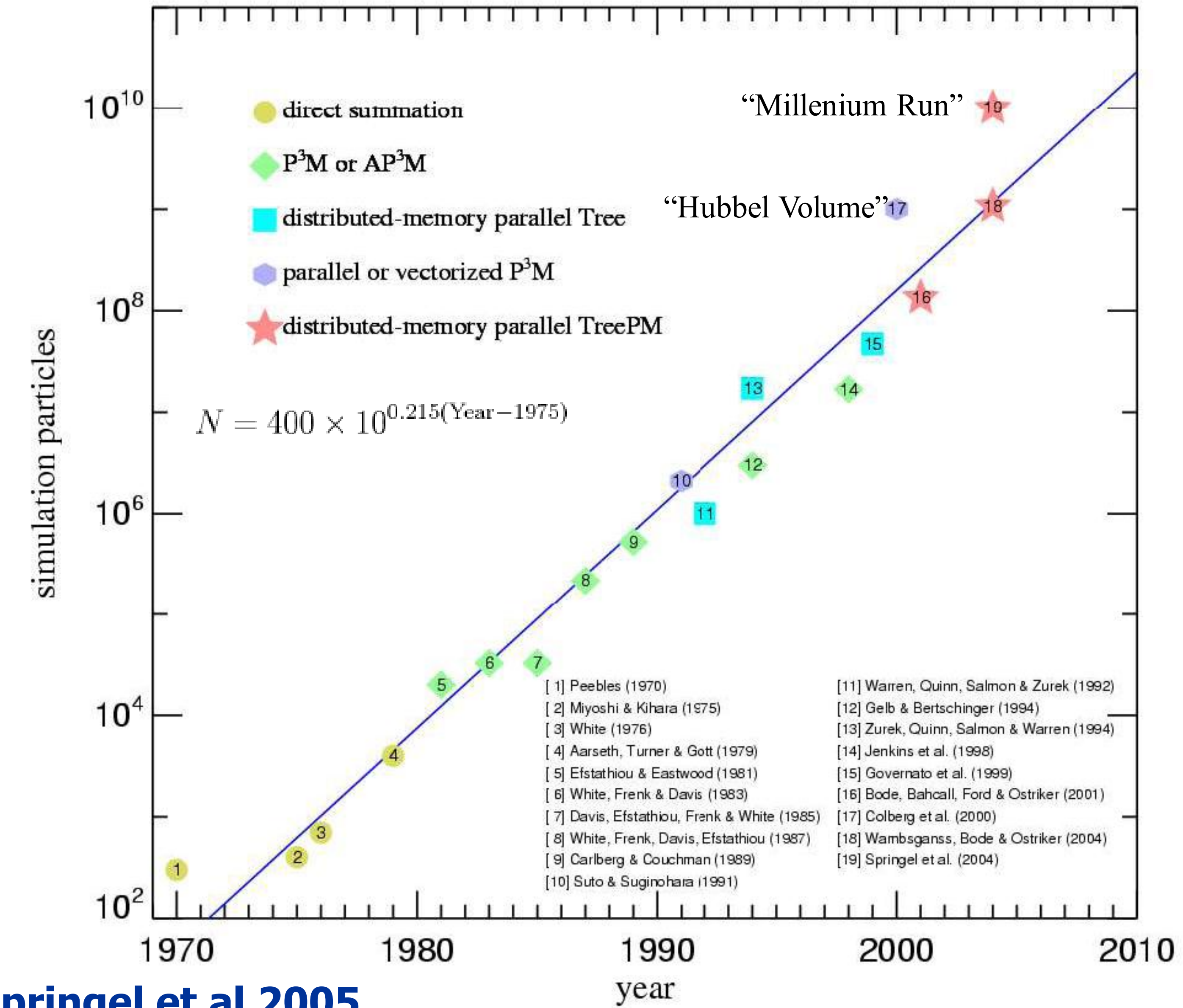
Capacity of processors double every 18 months

N.Body simulations double the number of particles every 16.4 months

Extrapolating:

10^{10} partículas in 2008

…but it was done in 2004



Springel et al 2005

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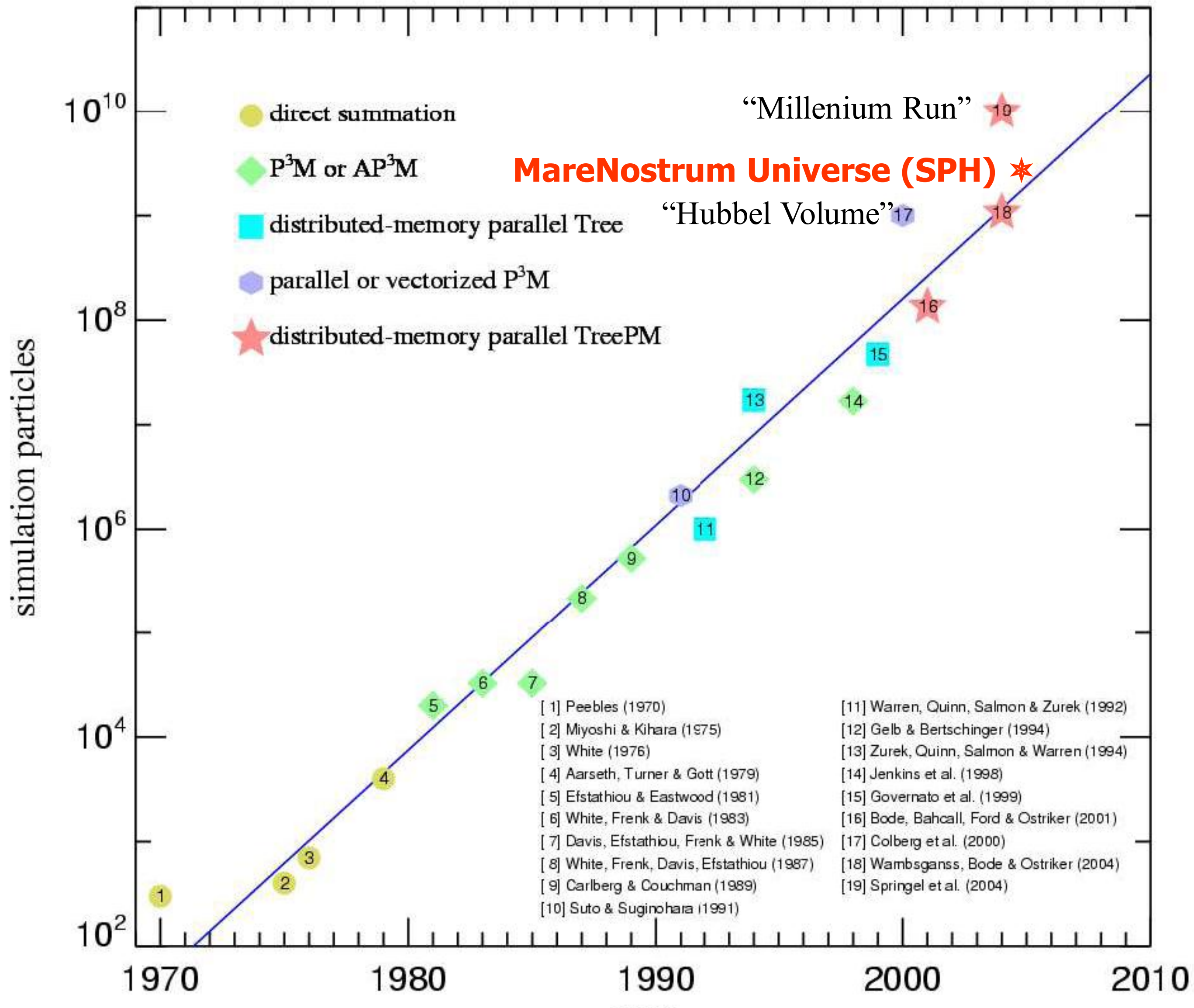

Springel et al 2005

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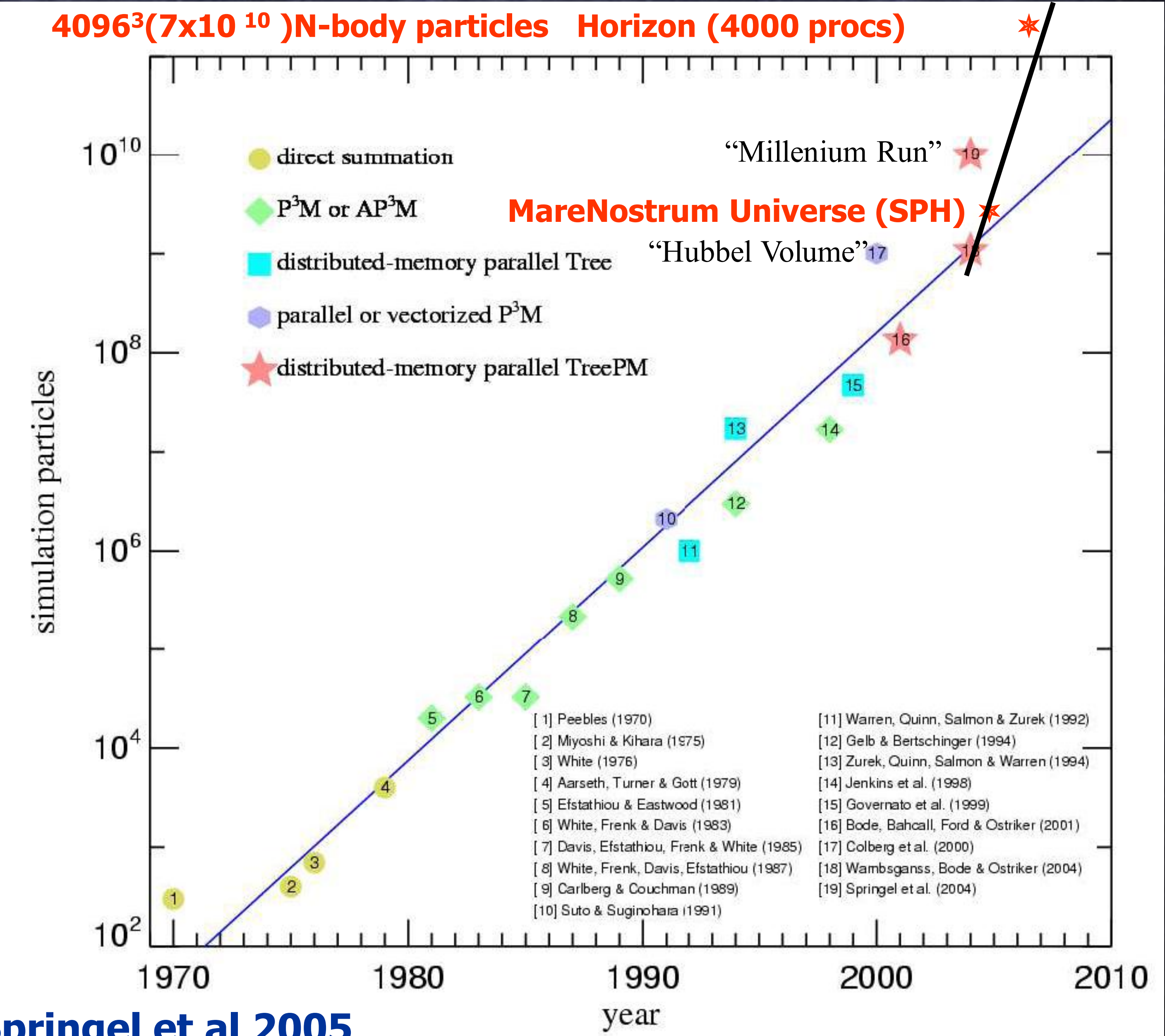
10^{10} partículas in 2008

…but it was done in 2004

In fact it is possible to do 10^{11} in 2008

An order of magnitude over less than 2 years



$4096^3 (7\times10^{10})$N-body particles Horizon (4000 procs)

MareNostrum Universe (SPH)

Springel et al 2005

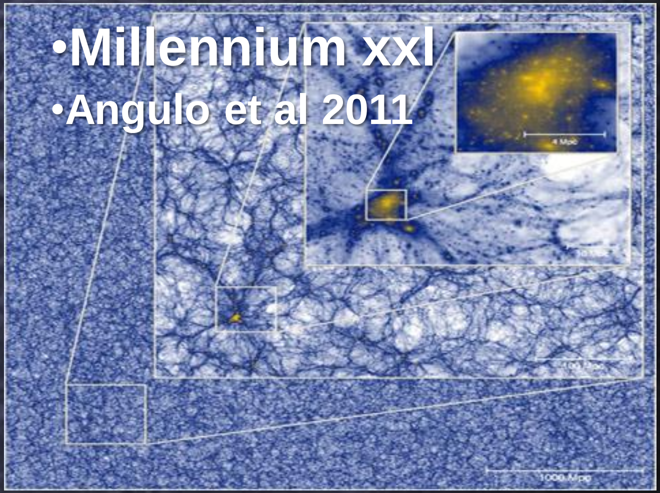
Collisionless N-body Simulations

Millennium Run

Springel et al 05

Millennium Run II

Springel et al 08



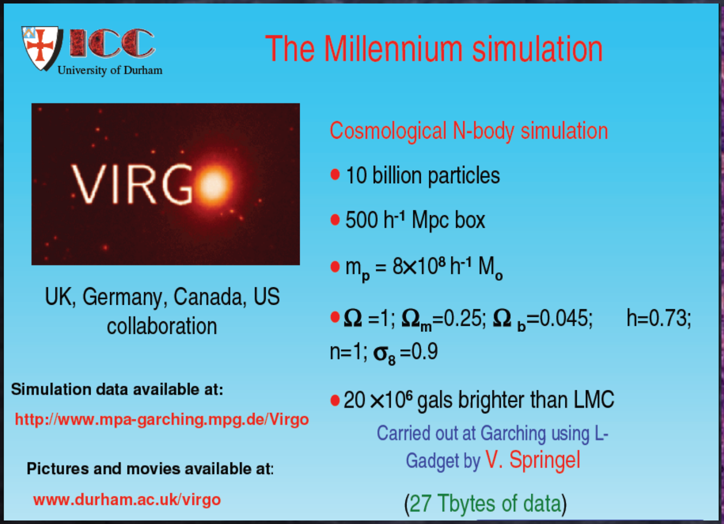
- **Millennium xxl**
- **Angulo et al 2011**

- **Bolshoi and**
- **Multidark Run**
- **Klypin et al 2011. 1Gpc**

- Millennium I (WMAP1): 500 /h Mpc 10 billion particles
- Millennium II (WMAP1) 100/h Mpc 10 billion particle
- Millenium XXL (WMAP1) 3 /h Gpc 303 billion particles
- Bolshoi (WMAP5) 250/h Mpc 8 billion particles
- Multidark (WMAP7) 1Gpc/h 8 billion particles

- Mass resolution:
- MI: $8x10^8$ Msun/h
- MII: $7x10^6$ Msun/h
- Bolshoi: 1.3×10^8 Msun/h
- Multidark: $8.3x10^9$ Msun/h

•Collisionless N-body Simulations



ICC University of Durham

The Millennium simulation

VIRGO

UK, Germany, Canada, US collaboration

Simulation data available at:

http://www.mpa-garching.mpg.de/Virgo

Pictures and movies available at:

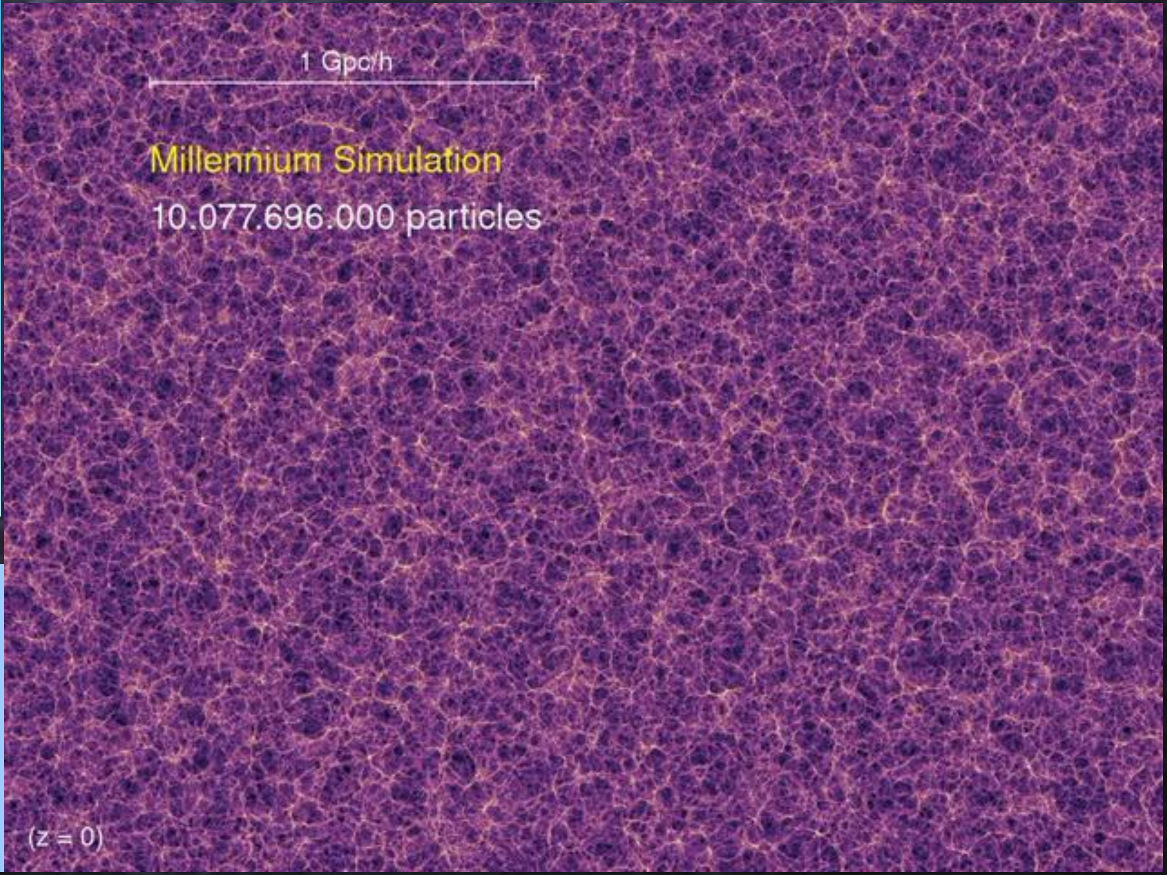
www.durham.ac.uk/virgo

Cosmological N-body simulation

- 10 billion particles
- 500 h^{-1} Mpc box
- $m_p = 8\times10^8 h^{-1} M_o$
- $\Omega=1$; $\Omega_m=0.25$; $\Omega_b=0.045$; $h=0.73$; $n=1$; $\sigma_8=0.9$
- 20×10^6 gals brighter than LMC

Carried out at Garching using L-Gadget by V. Springel

(27 Tbytes of data)



IBM Regatta p690+ cluster

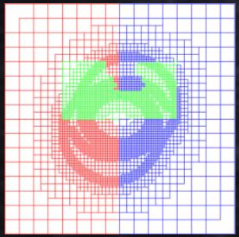
- •512 Power4 processors
- •1 Tbyte RAM
- •500 wall clock hours
- •300,000 HOURS CPU

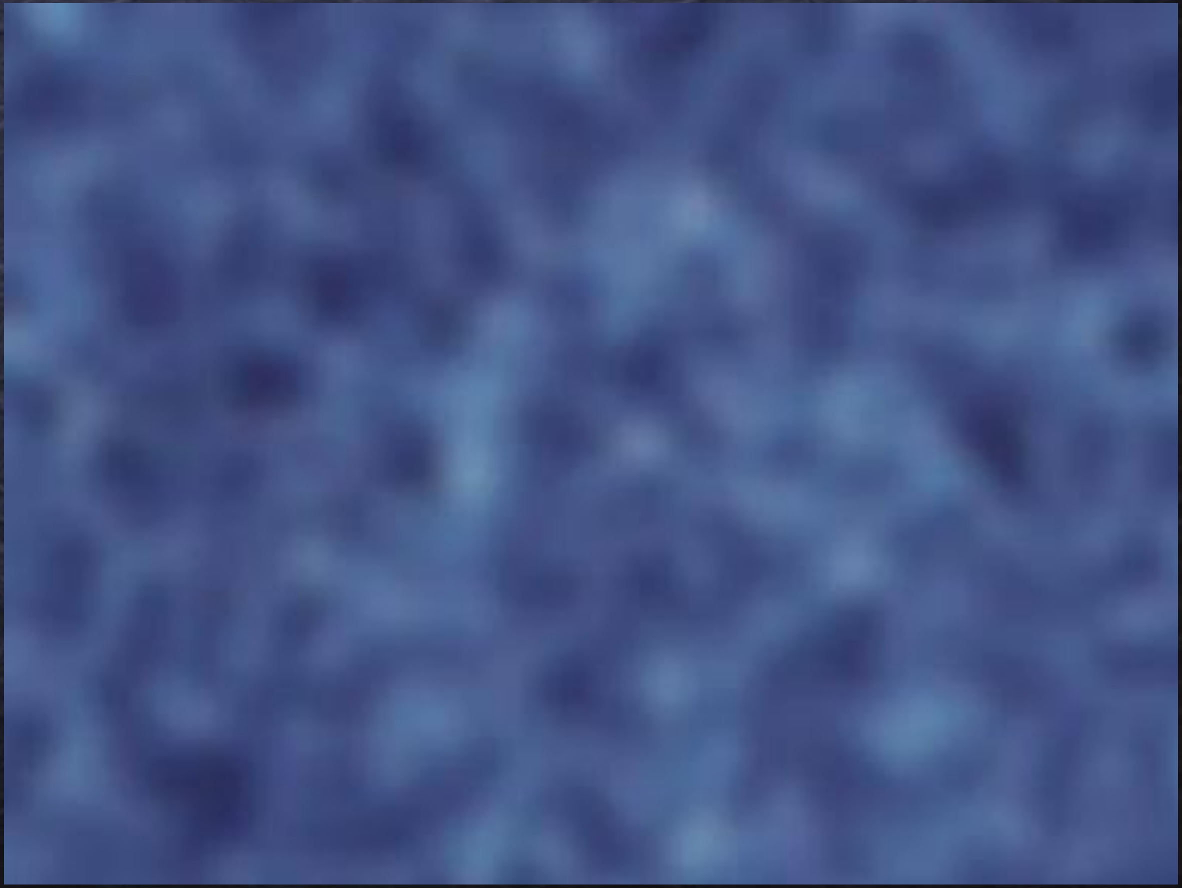
•Collisionless N-body Simulations

PROJET
HORIZON

HORIZON SIMULATION
(2008)
70 BILLION PARTICLES
2 GPC VOLUME

RAMSES amr code





Collisionless N-body Simulations

AIP Leibniz-Institut für Astrophysik Potsdam

US University of Sussex

UAM UNIVERSIDAD AUTONOMA DE MADRID

IFCA Instituto de Física de Cantabria

J-UNIVERSE

- Largest simulated volume ever made:
  - ☐ 6/h Gpc = 20 billons light-years
- ☐ Second largest number of particles
  - ☐ 6000^3 ~ 216 billion particles
- ☐ Covers all the universe from z=1
- ☐ N-body simulation CUBEP^{3}M code
- ☐ Use 8000 nodes of Juropa:
  - ☐ Node=8 Cpus and 24 Gbytes
- ☐ Each snapshot = 6 Tbytes.

- **2012**, > 4 trillion particles could be possible with new PFLOP computers (NCSA BM Blue-Waters)

Collisionless N-body Simulations
Single dark matter object formation

Via L

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Amount

But…

Highly

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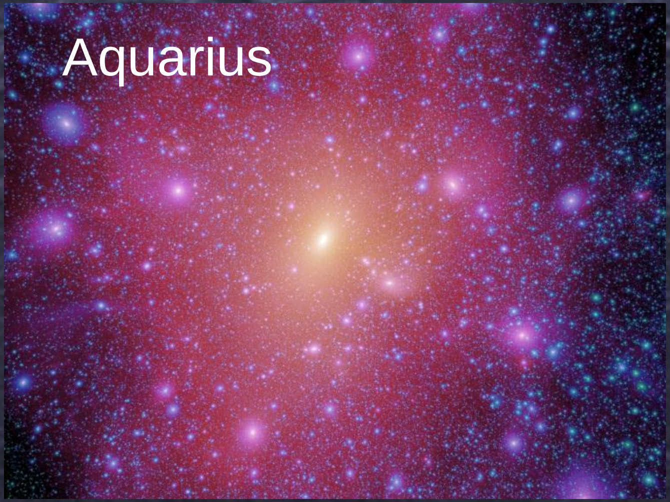
Collisionless N-body Simulations
Single dark matter object formation


Via Lactea


Aquarius


GHALO

A Milky Way size Cold Dark Matter halo formation:
More than a billion particles in one object.
Detailed study of the phase space of the invisible dark matter
Amount of substructures surviving in the formation process of
But…
Highly unrealistic because there is no visible matter in these simulations.

Grand Challenges in Computational Cosmology

- Most of the information from the Universe comes from the tiny fraction of normal matter: baryons
  - Galaxies detected from light coming from the stars inside.
  - Gas in galaxy clusters is detected by X-ray emission.
  - Intergalactic gas is measured from features in light from QSO
- Realistic simulations would require inclusion of dissipational component: gas
  - Gasdynamical simulations in dark matter dominated models need more than an order of magnitude larger computational resources than pure N-body

Grand Challenges in Computational Cosmology

- **Galaxy formation does not involve only gravity and gasdynamics :**
  - **but** more complex physics:
    - *Cooling, heating, star formation, supernova explosions,feedbacks,.*
- **Extreme Computing intensive simulations**
    - Larger scale range in density, space and time
    - Strong time constrains due to cooling and star formation.
    - Huge Problems with scaling and load/balancing in MPI.
      - *E.g. GADGET scales well only for few dozens of processors.*
    - OpenMP or MPI+OpenMP codes can perform better
- **More information to store and post-process.**

Grand Challenges in Computational Cosmology

Simulating the structure formation in the Universe is one of the most complex computational problems that exceeds the technical and human capacity of an individual research group:

As in observational astronomy: (e.g. ESO)

- Need to establish large international collaborations to join efforts.
  - One example is the VIRGO collaboration: (UK, Germany, US, Canada)
  - Or the HORIZON Project (France)

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UAM UNIVERSIDAD AUTONOMA DE MADRID

The MareNostrum Numerical Cosmology Project

IUB

האוניברסיטה העברית בירושלים
The Hebrew University of Jerusalem

THE UNIVERSITY OF CHICAGO

NM STATE NEW MEXICO STATE UNIVERSITY

- International collaboration to take advantage of the uprecedented computing power of *MareNostrum* to create:

Grand Challenge Cosmological Simulations

- Different scales and physics:
  - **Large Scale Structure (adiabatic physics)**
    - *X-ray Clusters. SZ effect, baryon distribution at Large Scales*
  - **Galaxy formation: (including star formation)**
    - *High redshift objects*
    - *Faint objects in different environments*
  - **Our Local Universe (DECI)**
    - *Simulate our local neighbourhood:*
      - *The Local Group + Local Supercluster*


Copyright 2005, Barcelona Supercomputing Center - BSC

People behind

- Collaborators

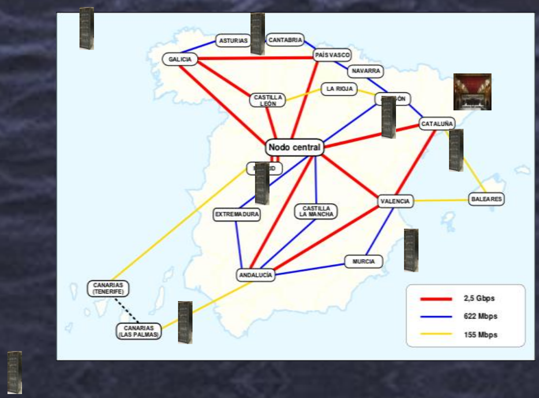
- **Gustavo Yepes**
- Raúl Sevilla
- Luis Martínez
- F. Sembolini
- A. Knebe
- S. Knollmann
- A. di Cintio
- E. Carlesi
- J. Vega

- **Stefan Gottlöber**
- Arman Khalatyan
- Christian Wagner
- J. Forero
- N. Libeskind

- Andrey Kravtsov (Chigago)
- Anatoly Klypin (NMSU)
- Matthias Hoëft (IU)
- Yehuda Hoffman (HU)
- Massimo Meneghetti (ITA)
- Andreas Faltenbacher (USC)
- Viktor Turchanikov (IAM)
- Fernando Atrio (USAL)
- Manolis Plionis (NOA)
- Oliver Zhan (CfA)
- F. Prada (IAA)
- …

Computational Resources

Barcelona



Madrid

Jülich

LRZ
Munich

DEISA

DISTRIBUTED EUROPEAN INFRASTRUCTURE FOR SUPERCOMPUTING APPLICATIONS

Jülich

Munich

Barcelona

DECI PROJECTS:

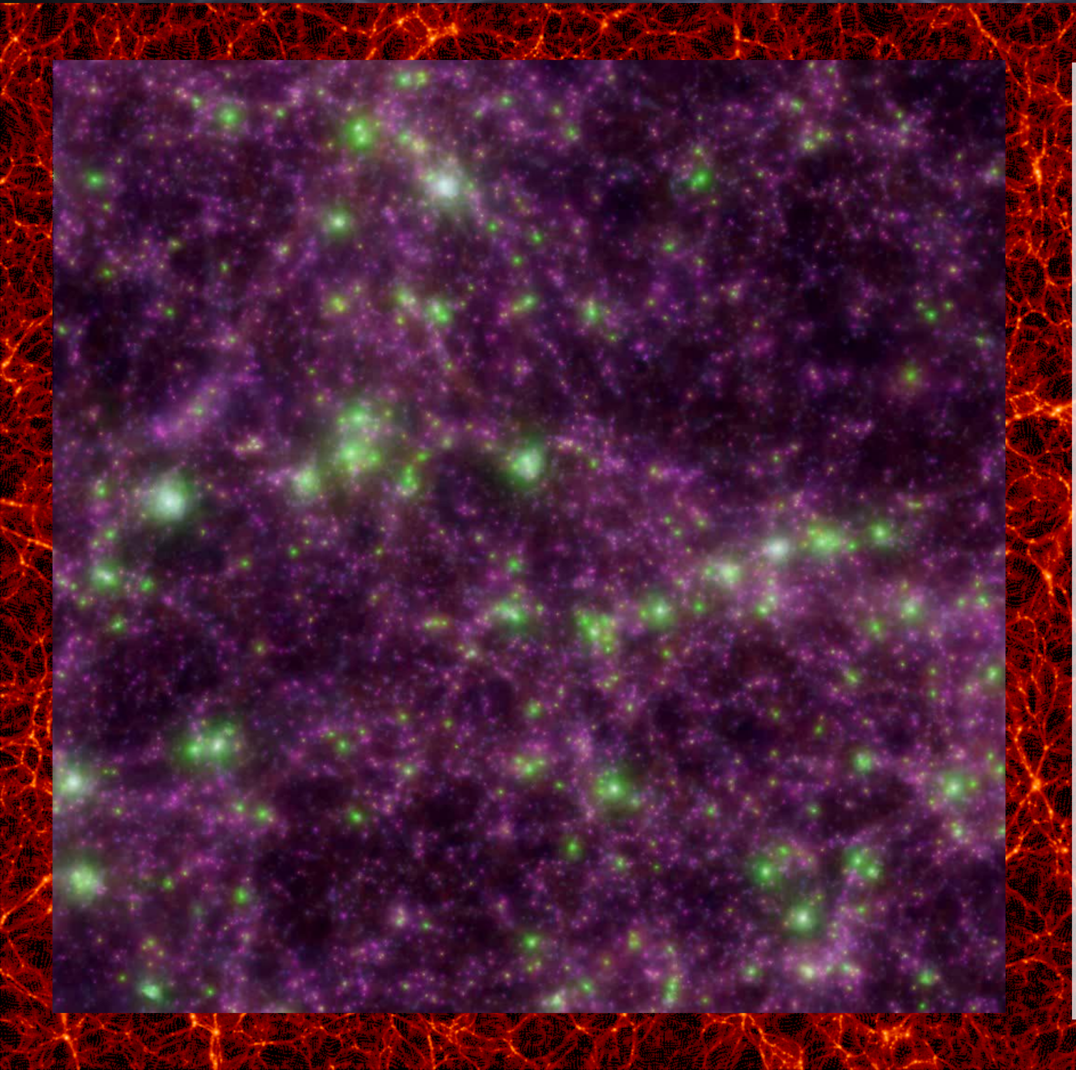
SIMU-LU (2006)	***SIMUGAL-LU (2008)***
10^6 CPUH	*10^6 CPUH*


CURIE: 1.6 PFLOPS

- **Most powerful supercomputer in Europe**

- **2011. 5,000,000 CPU hours project grant**

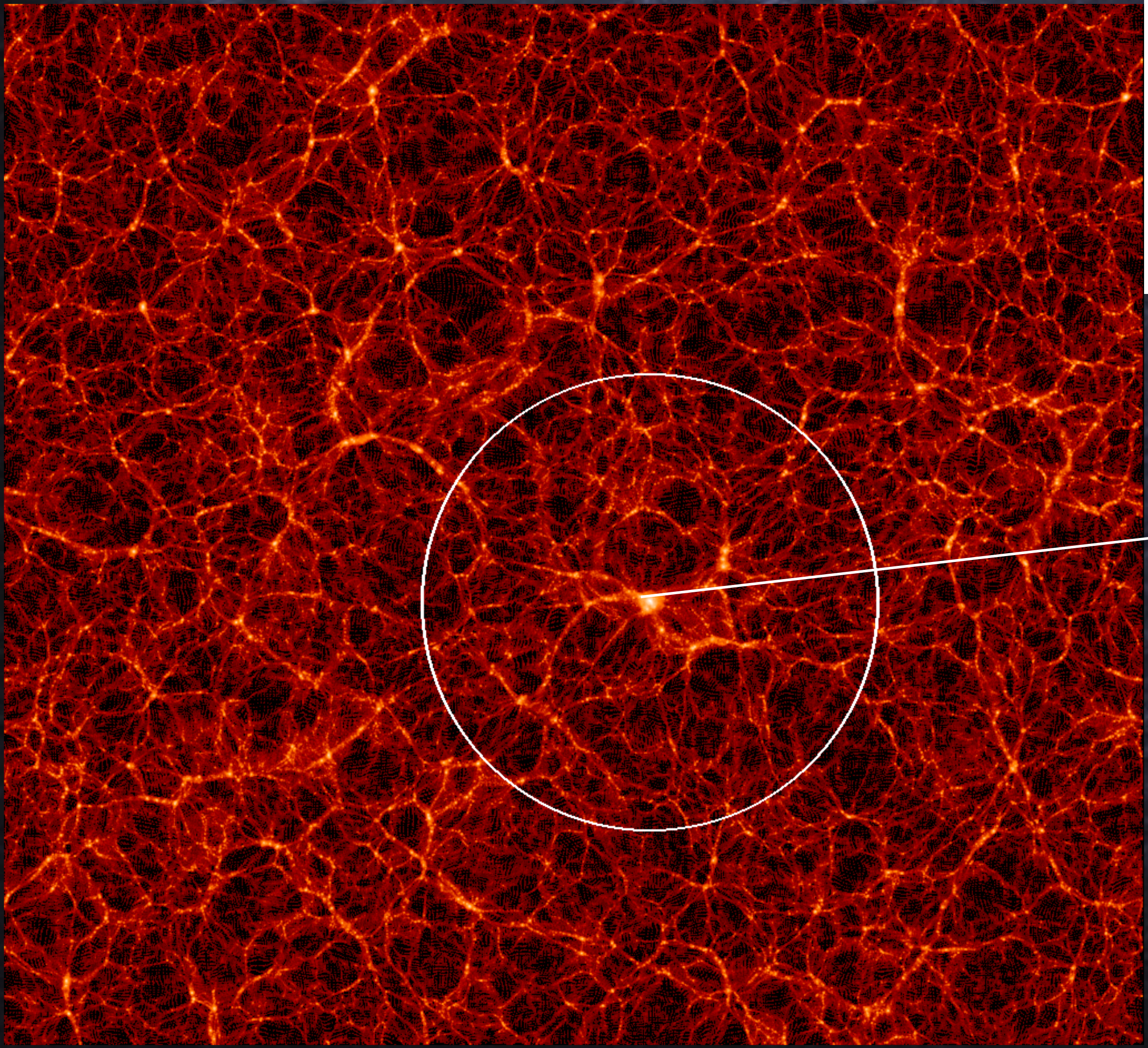
The *MareNostrum Universe* TREEPM+SPH simulation

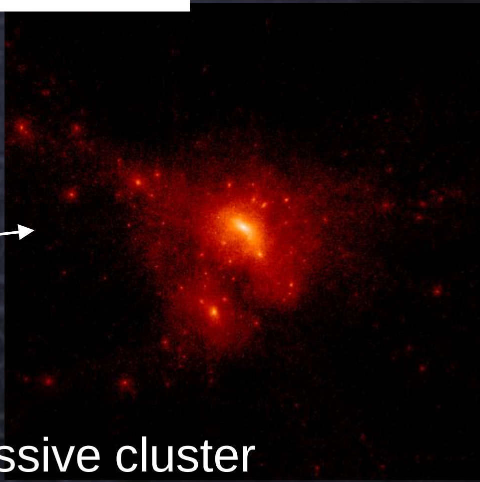


- ΛCDM model (WMAP1)
- 500/h Mpc^3 volume
- **GADGET 2 code (Springel 2005)**
- Adiabatic SPH+TREEPM Nbody
  - 1024^3 FFT for the PM force.
  - 15 kpc force resolution.
- 2x1024^3 dark and sph particles
  - $10^{9.33}$ partículas
  - 8x10^9 $M_\odot$ dark matter
  - 10^9 $M_\odot$ for gas particles
- 1 million dark halos bigger than a typical galaxy (10^{12} Mo)
- Simulation done at *MareNostrum*
  - 512 processors (1/20th total power)
  - 1Tbyte ram
  - 500 wallclock hrs (29 cpu years)
  - Output: 8600 Gbytes of data.
  - Same computing power than the Millenium Run.

Clusters of galaxies

- 30 clusters with $M_{vir} > 10^{15} h^{-1} \mathrm{M}_\odot$
- 4000 clusters with $M_{vir} > 10^{14} h^{-1} \mathrm{M}_\odot$





Most massive cluster

$$M_{vir} = 2.5 \times 10^{15} h^{-1} \mathrm{M}_\odot$$
$$r_{vir} = 2.8 h^{-1} \mathrm{Mpc}$$

THE MUSIC PROJECT

Compile an extended sample of high-resolution radiative gasdynamical resimulations of clusters:

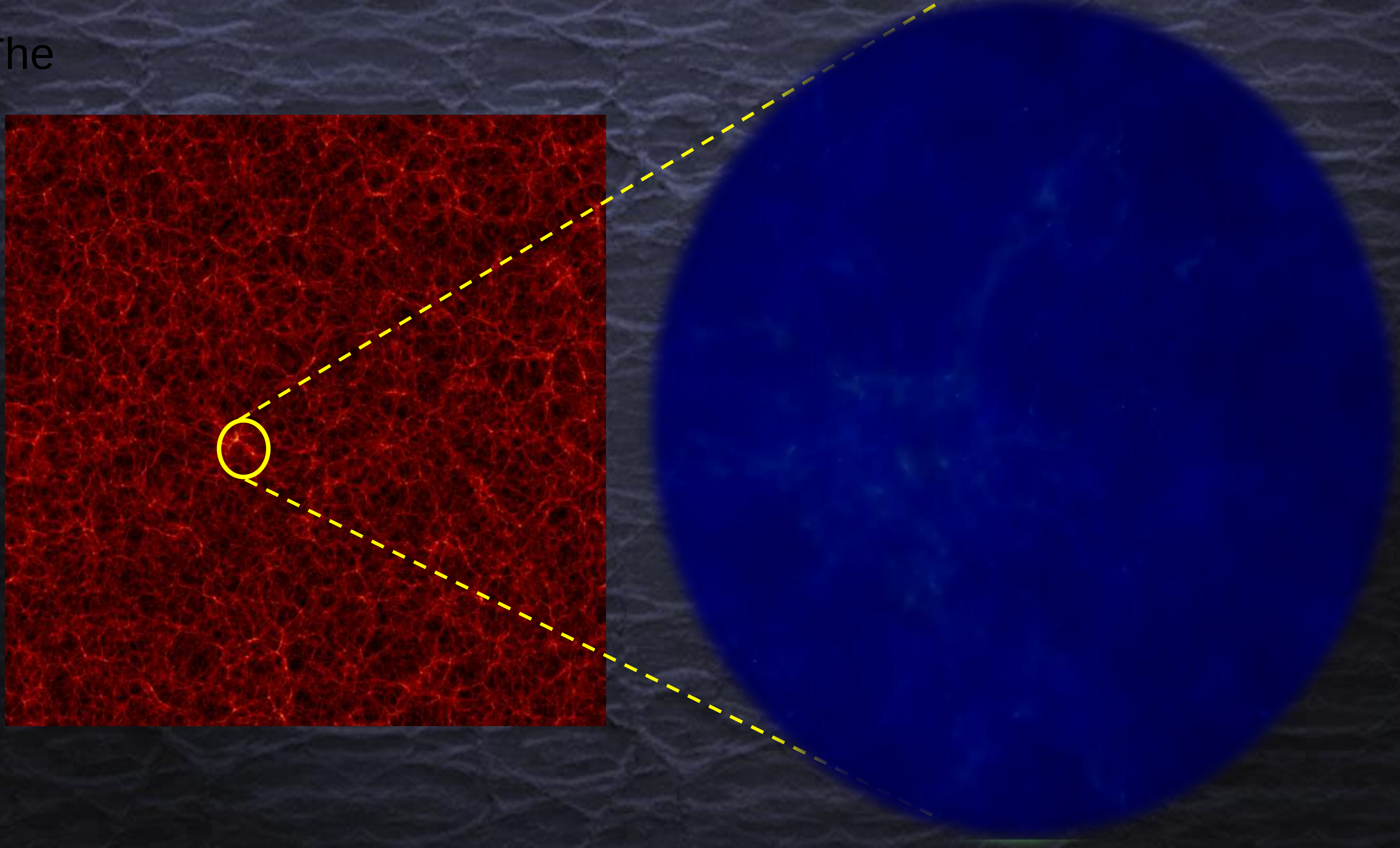
http://music.multidark.org

Two selection criteria:

- Based on the dynamical state:
  - Bullets vs. Relaxed cluster (from MN simulation)
- A complete volume limited sample:
  - Selection of all clusters above a given mass cutoff.
  - Extracted from large N-body volumes: MULTIDARK simulation.

MUSIC CLUSTERS

- The

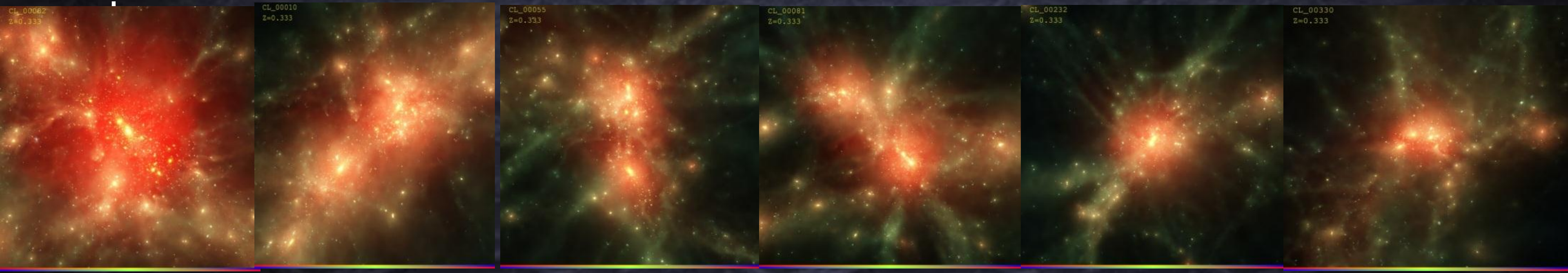


- We selected all the cluster-size halos more massive than $M > 10^{15}\ h^{-1}\ M_{sun}$ *(282)* at z=0

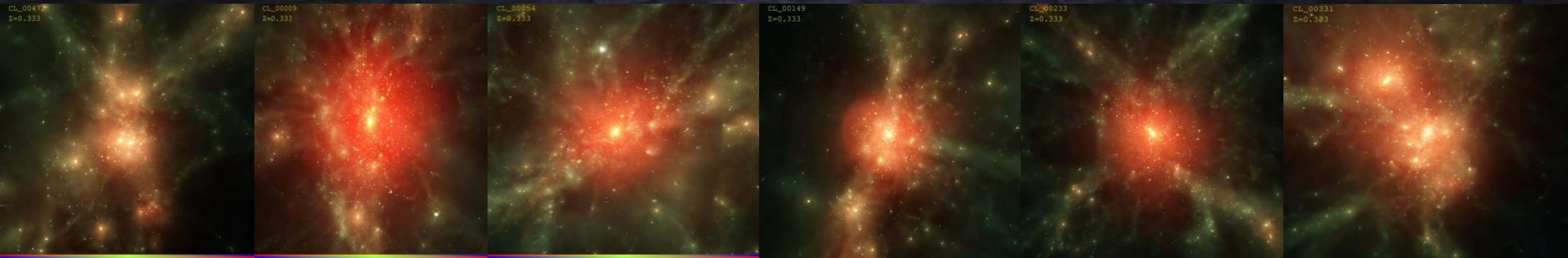
•MUSIC-1: Resimulated Marenostrum

•bullets and relaxed cluster samples

- **164** selected clusters resimulated using TreePM_SPH GADGET code.
- **8 times** more particles (**m_{DM}=1.03 x 10^9 h^{-1} M_{sun}** and **m_{gas}=1.82 x 10^8 h^{-1} M_{sun}**) than original MNU simulation.
- radiative physics (i.e cooling , UV photoionization, star formation and SN thermal and kinetic feedbacks in form of galactic winds)
- The most massive clusters of the dataset ($2 \cdot 10^{15}$ h^{-1} M_{sun}: 6 million particles (DM+gas+stars)
- The less massive (10^{14} h^{-1} M_{sun}) about 1 million particles
- The gravitational smoothing was set to an effective Plummer ε=6 h^{-1}



•top : bullet-like resimulated clusters bottom: relaxed resimulated clusters



The MareNostrum
GALAXY FORMATION SIMULATION

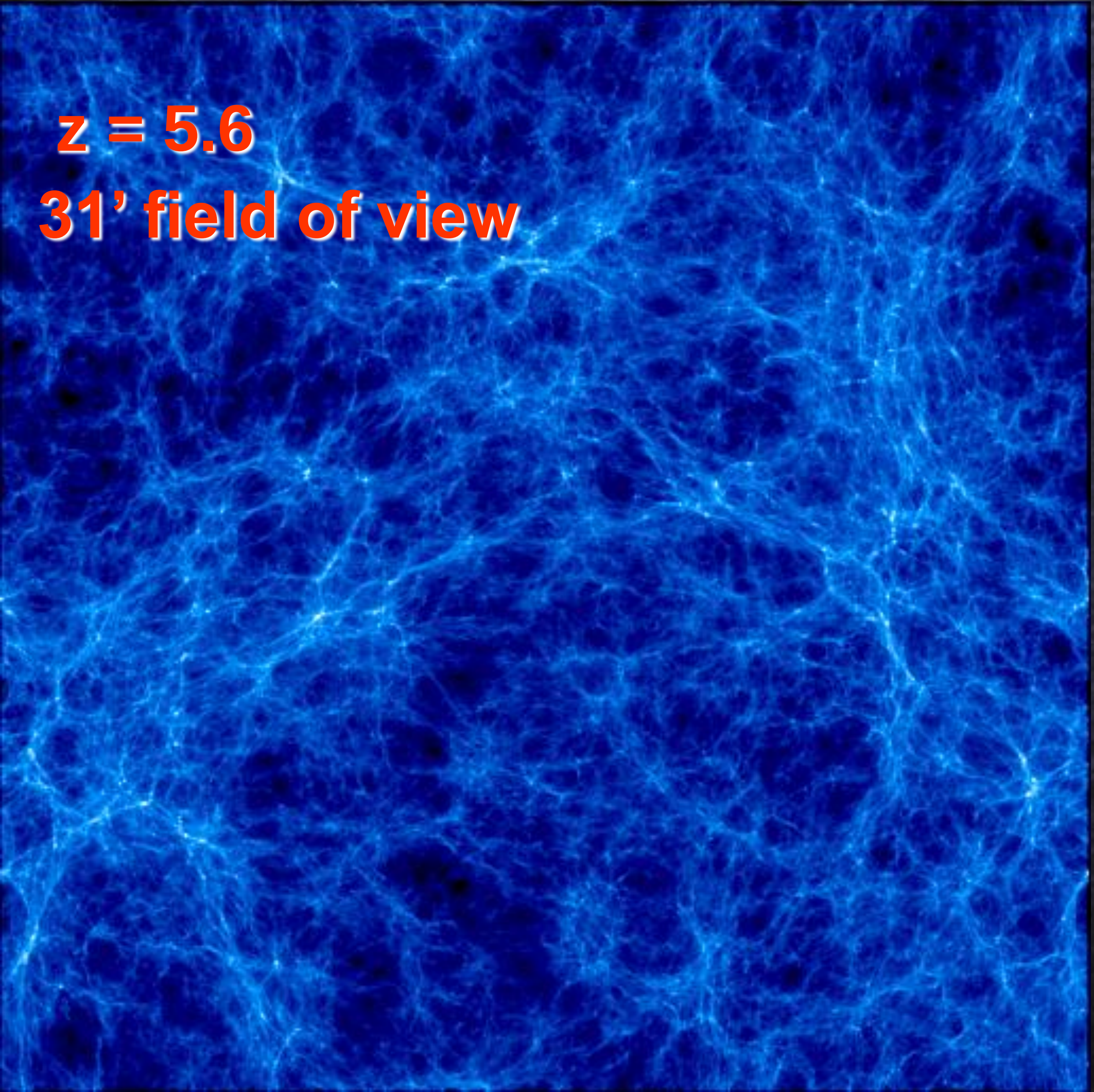
•Gasdynamics and N-body with 2 billion particles

+

•Detailed modelling of baryonic physics.

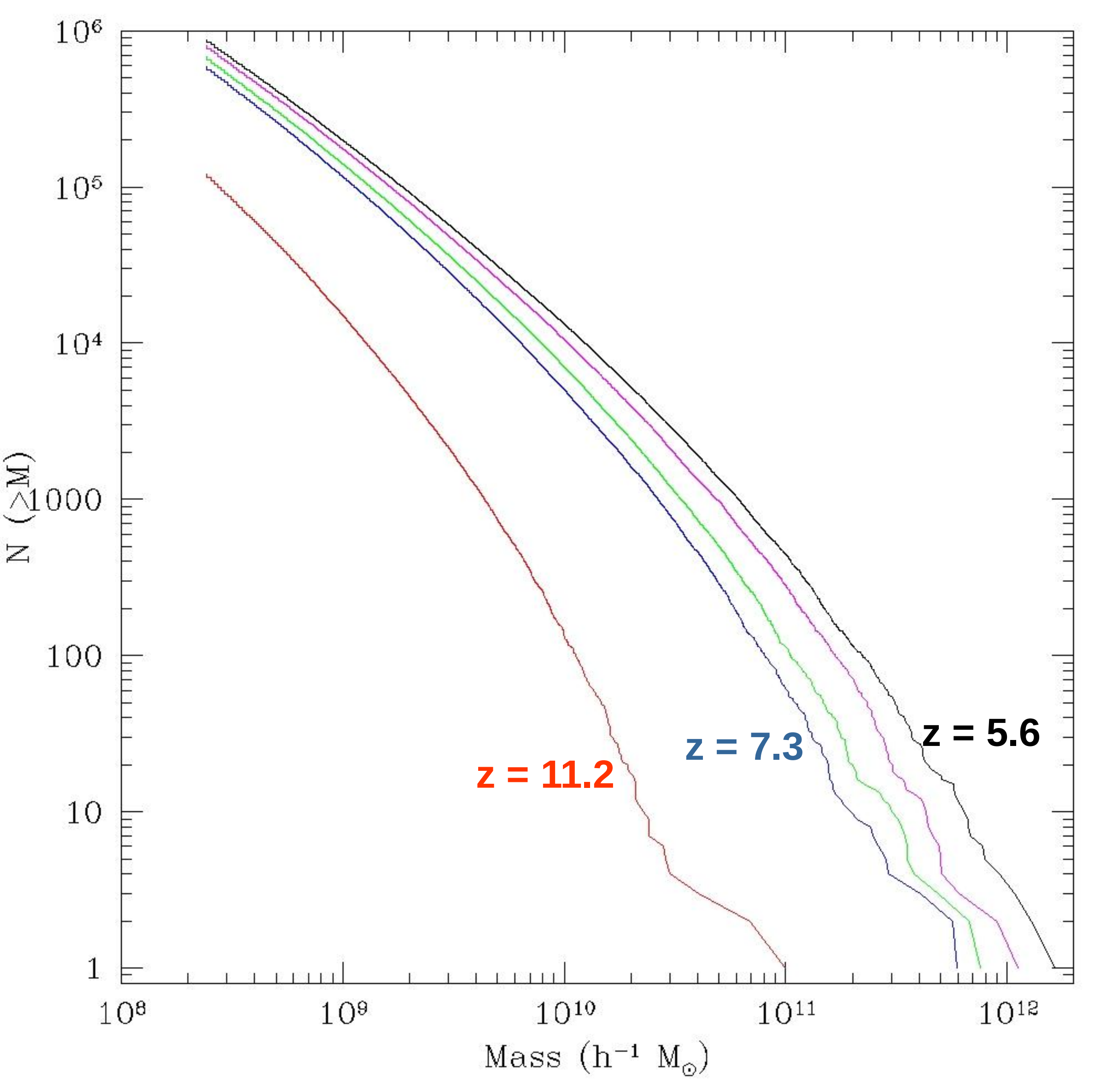
- To study in detail the galaxy formation process we need to account at least for
  - *Radiative and Compton cooling*
  - *UV-photoionization*
  - *Multiphase ISM.*
  - *Star Formation.*
  - *Star-Gas backreactions*.
- Use Springel-Hernquist (2003) implementation of multiphase SPH modeling in GADGET-2.

• MareNostrum galaxy formation simulation



- Box 50/h Mpc
- 2x 10^9 gas+dark
- LCDM model
- M_{gas}=1.4 x10^6 Msun
- Mdark=10^7 Msun.
- Mhalos > 10^9 Msun
- Gas density

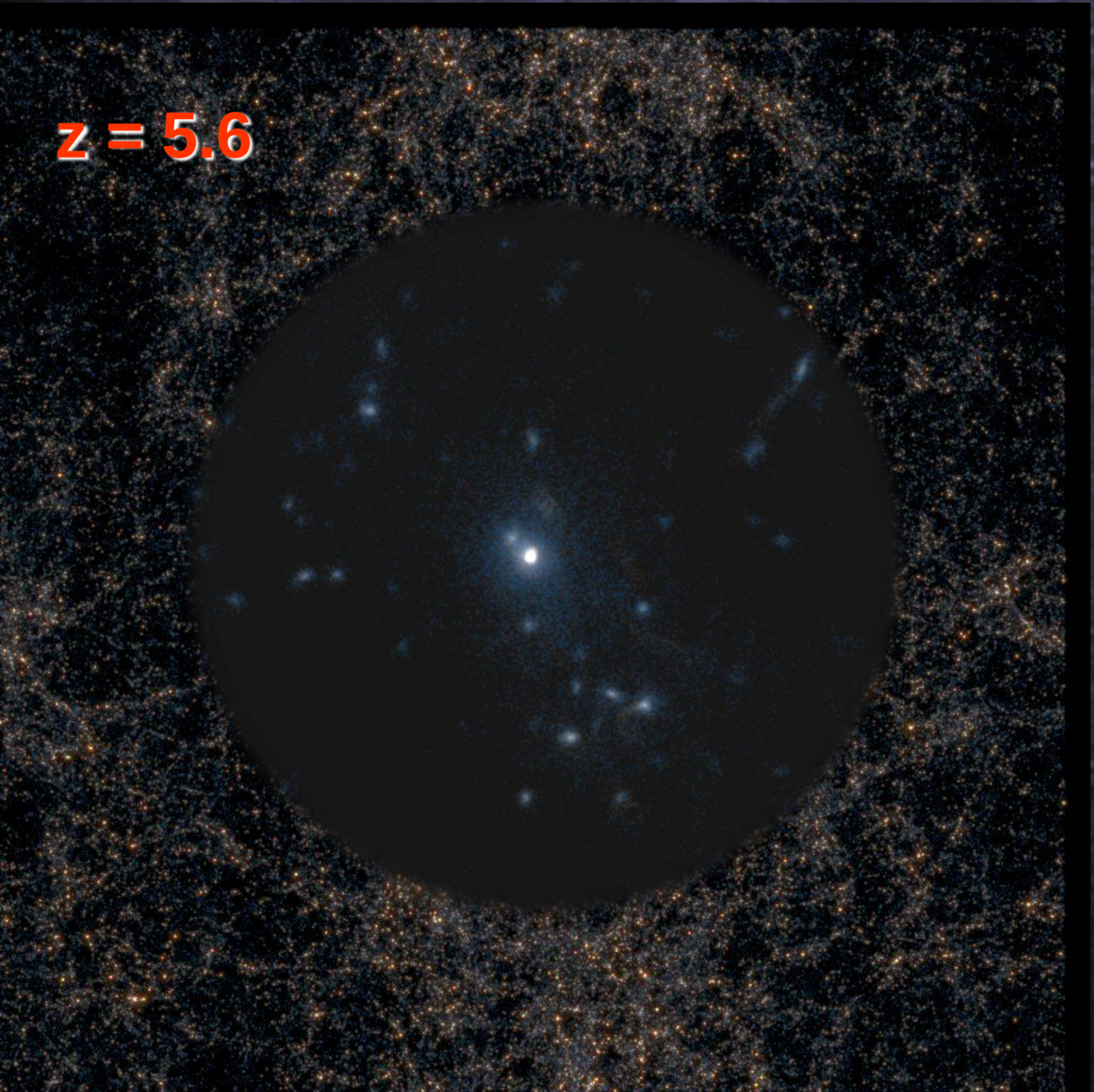
• MareNostrum galaxy formation simulation



- Box 50/h Mpc
- 2x 10^9 gas+dark
- LCDM model
- Mgas=1.4 x10^6 Msun
- Mdark=10^7 Msun.
- Mhalos > 10^9 Msun

- Mass Function

MareNostrum galaxy formation simulation



- Box 50/h Mpc
- 2x 109 gas+dark
- LCDM model
- Mgas=1.4 x106 Msun
- Mdark=8x106 Msun.
- Mhalos > 109 Msun
- Star density

Fraction stars = 0.74%
Comoving Luminosity density:
ρ_U = 7.6x10^7 Lsun/Mpc^3
ρ_B = 1.3x10^8
ρ_R = 1.0x10^8
ρ_I = 7.2x10^7
ρ_K = 2x10^7

CODE COMPARISON

- **MNCP GADGET (SPH)**
- **800 processors of MN**
- **Resolution: 500 pc.**
- **400 YEARS of CPU**
- **http://astro.ft.uam.es/marenostrum**

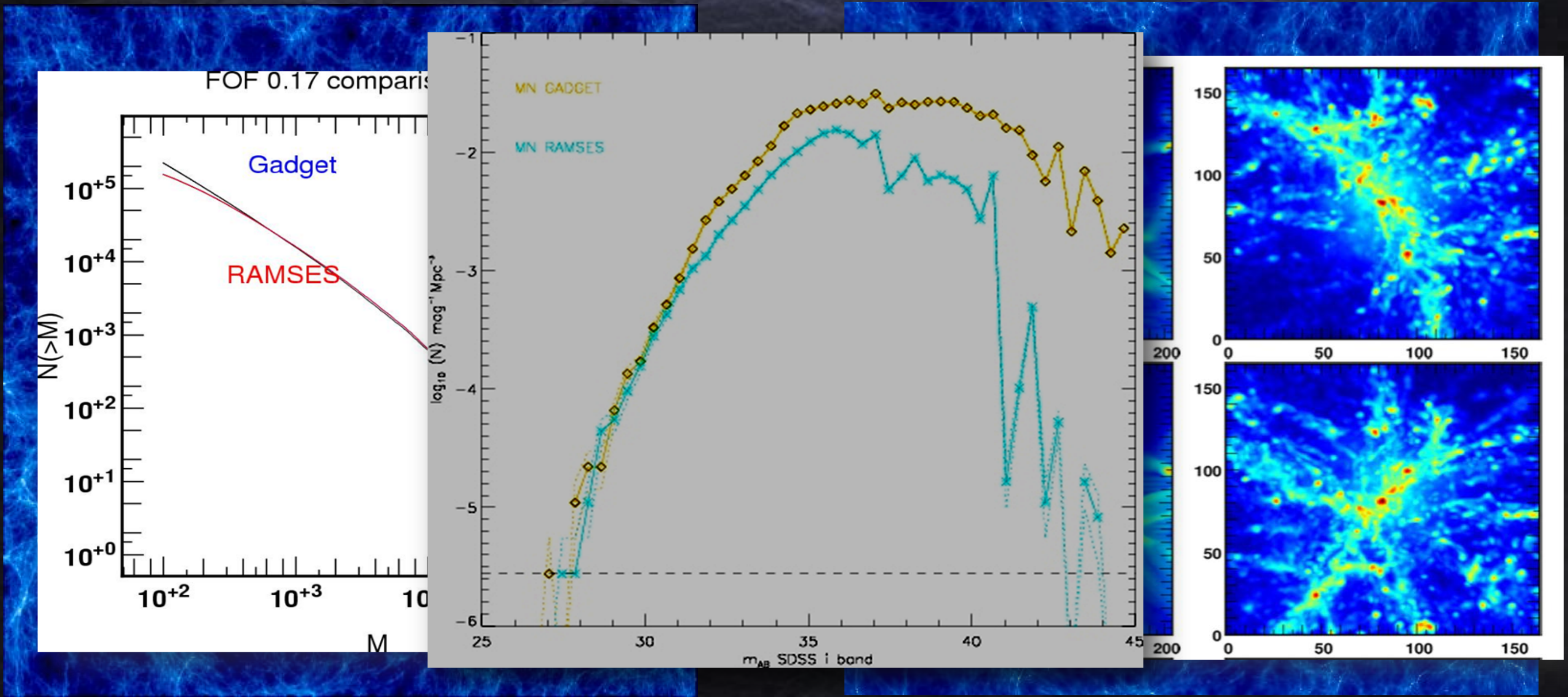
HORIZON -RAMSES (AMR)

More than 2000 processors

Resolution: 2 kpc

150 YEARS CPU

http://www.projet-horizon.fr



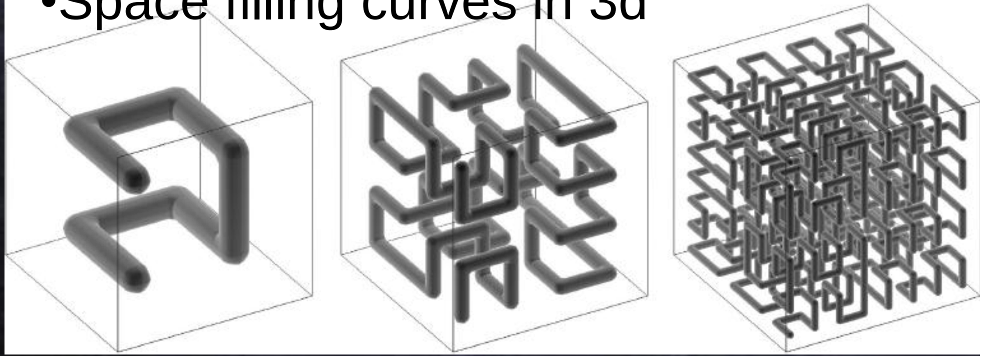
Towards Petaflop scaling

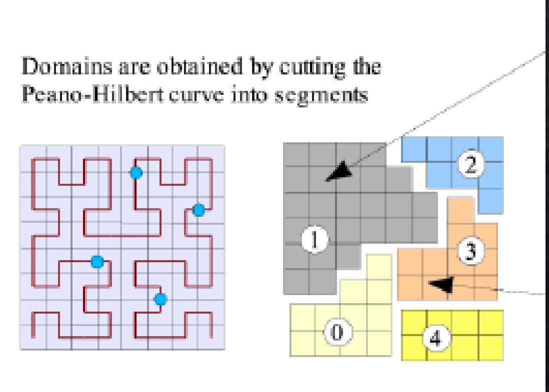
New algorithms for efficient domain decompositon in 3D:

Need to distribute particles that are closed in space between processors.

Keeping a good load/balance

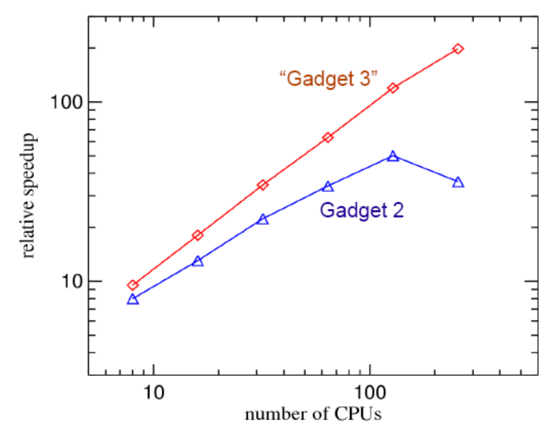
- Space filling curves in 3d





Domains are obtained by cutting the Peano-Hilbert curve into segments

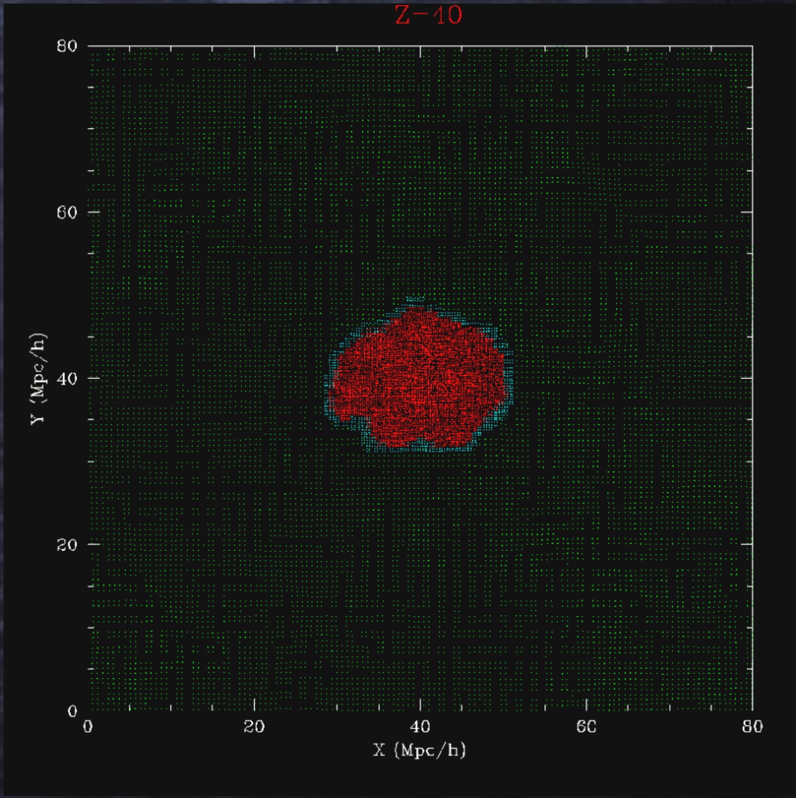
- Better scaling with number of processors when improved domain decomposition algorithms are used



- **Still a long way to achieve proper scaling in hundred of thousands of procesors of PFLOP machines..**

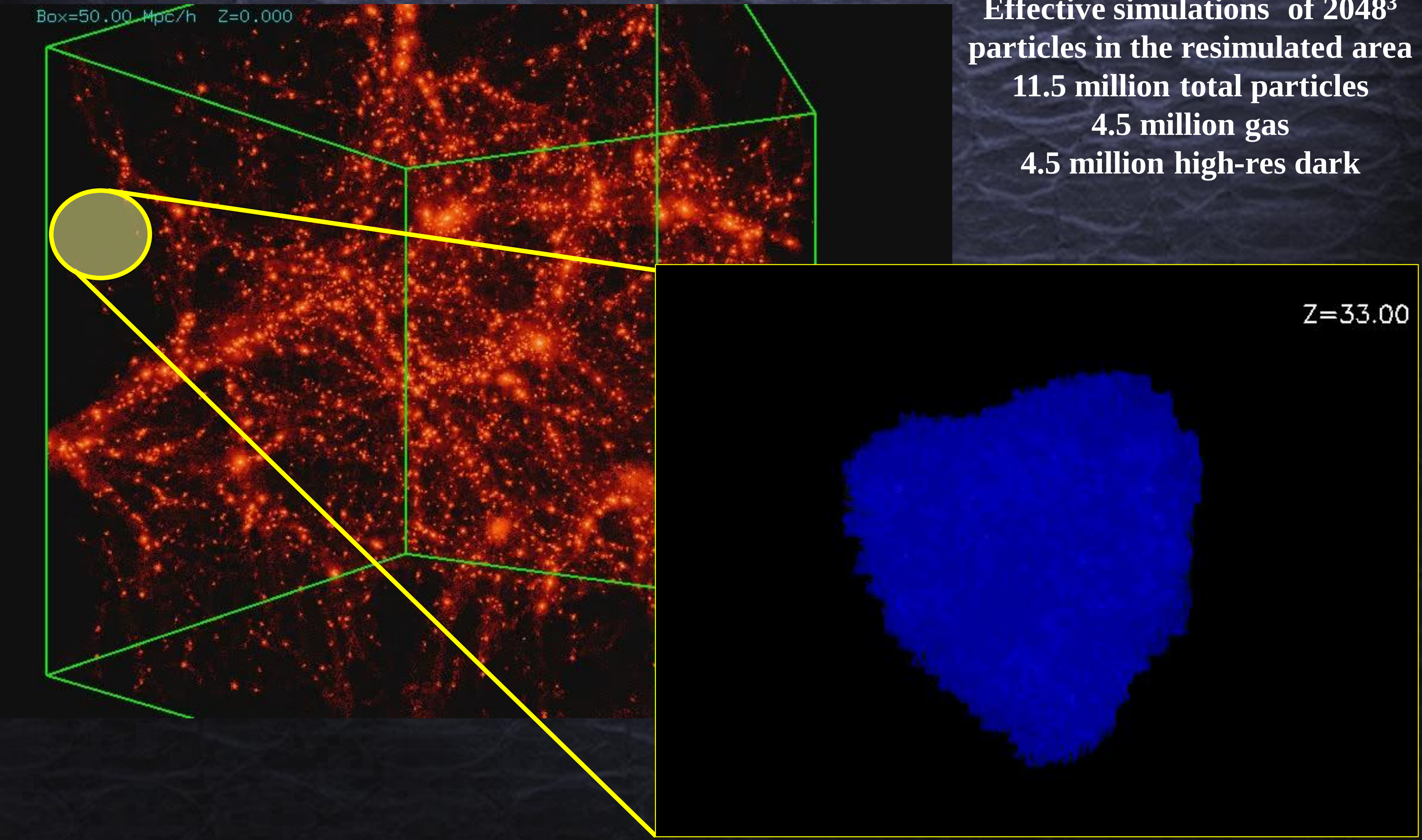
AN ALTERNATIVE: MULTIMASS TECHNIQUE

- Adaptive multi-mass to achieve high resolution:
- Re-Simulated areas from large computational boxes by resampling particles of increasing mass away from the refined region:
  - Original initial conditions up to 4096^3 particles in a big box.
  - Trace back particles of selected objects to identify region to be resimulated with very high resolution
  - **Very easy way of parallelization.**

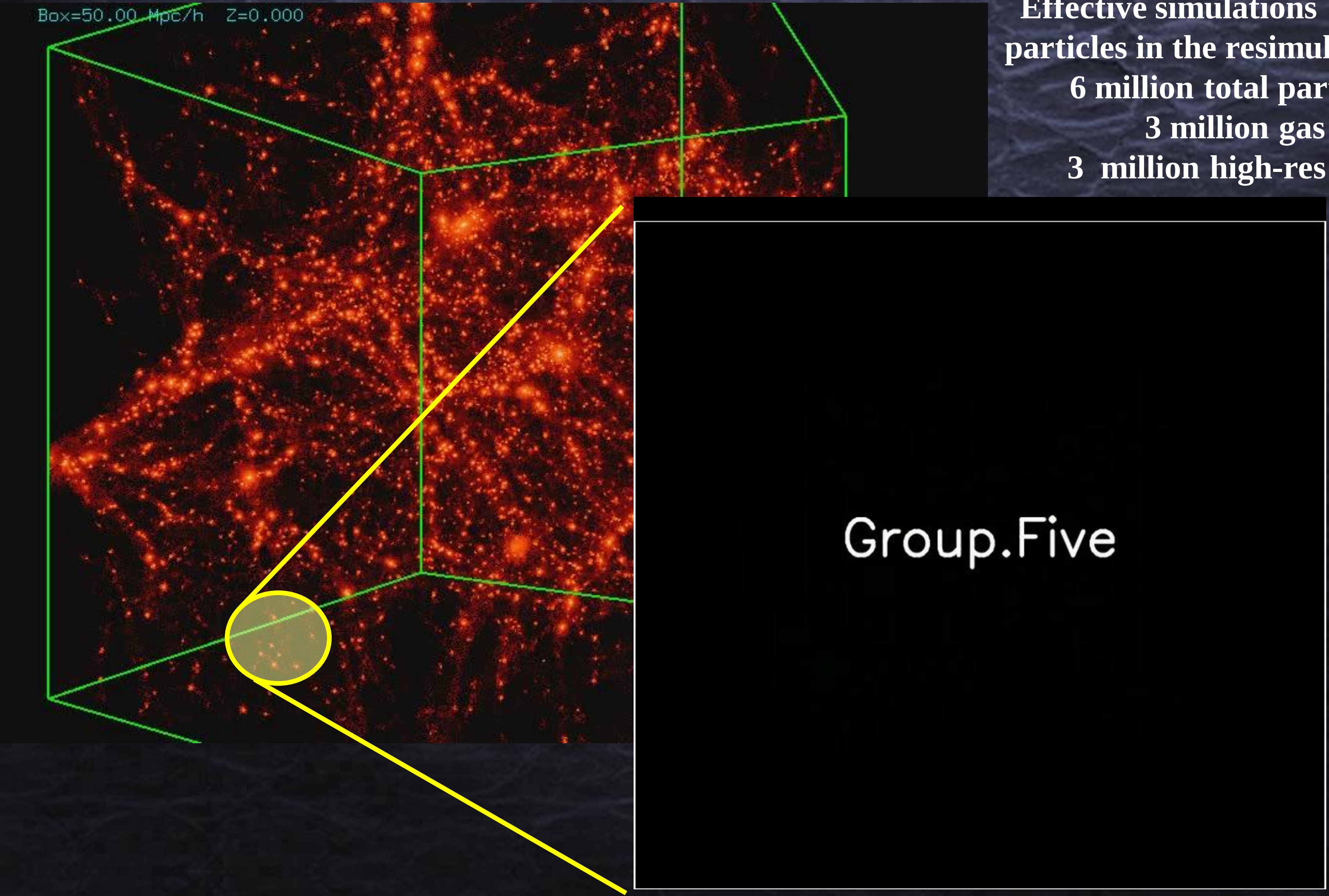


COSMIC VOIDS:

Effective simulations of 2048^3 particles in the resimulated area
11.5 million total particles
4.5 million gas
4.5 million high-res dark

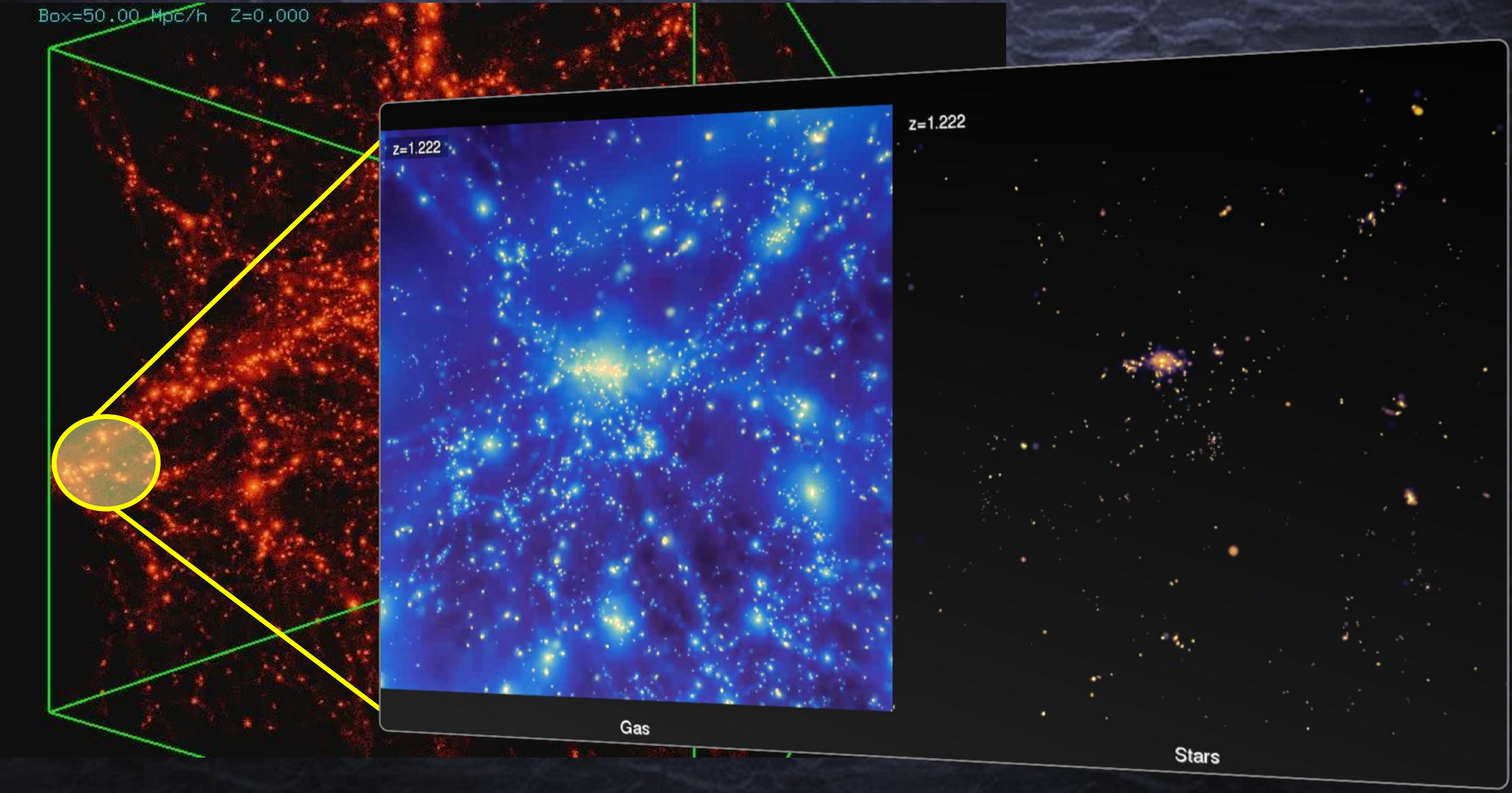


GALAXY GROUPS:

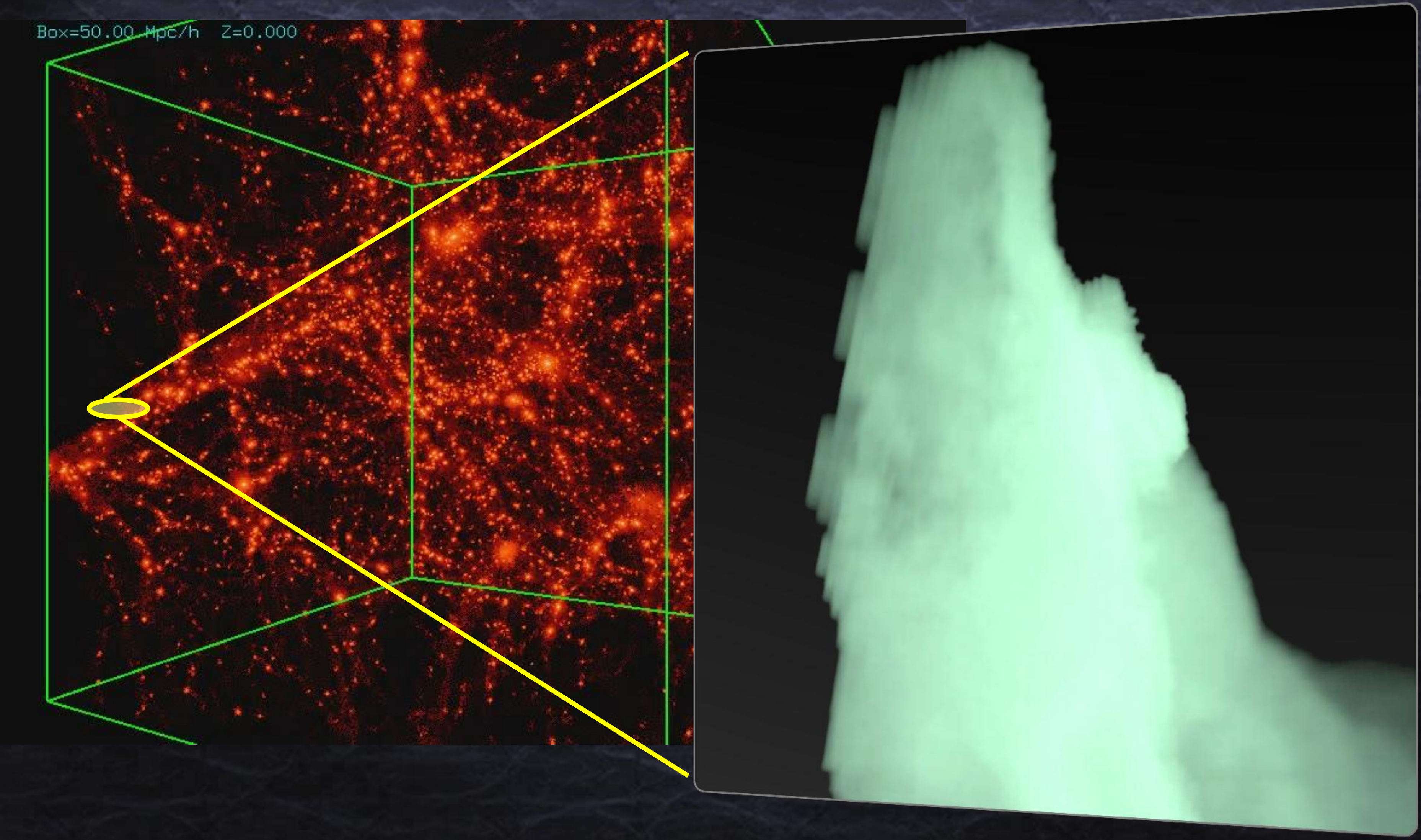


Effective simulations of 1024^3 particles in the resimulated area
6 million total particles
3 million gas
3 million high-res dark

GALAXY CLUSTERS



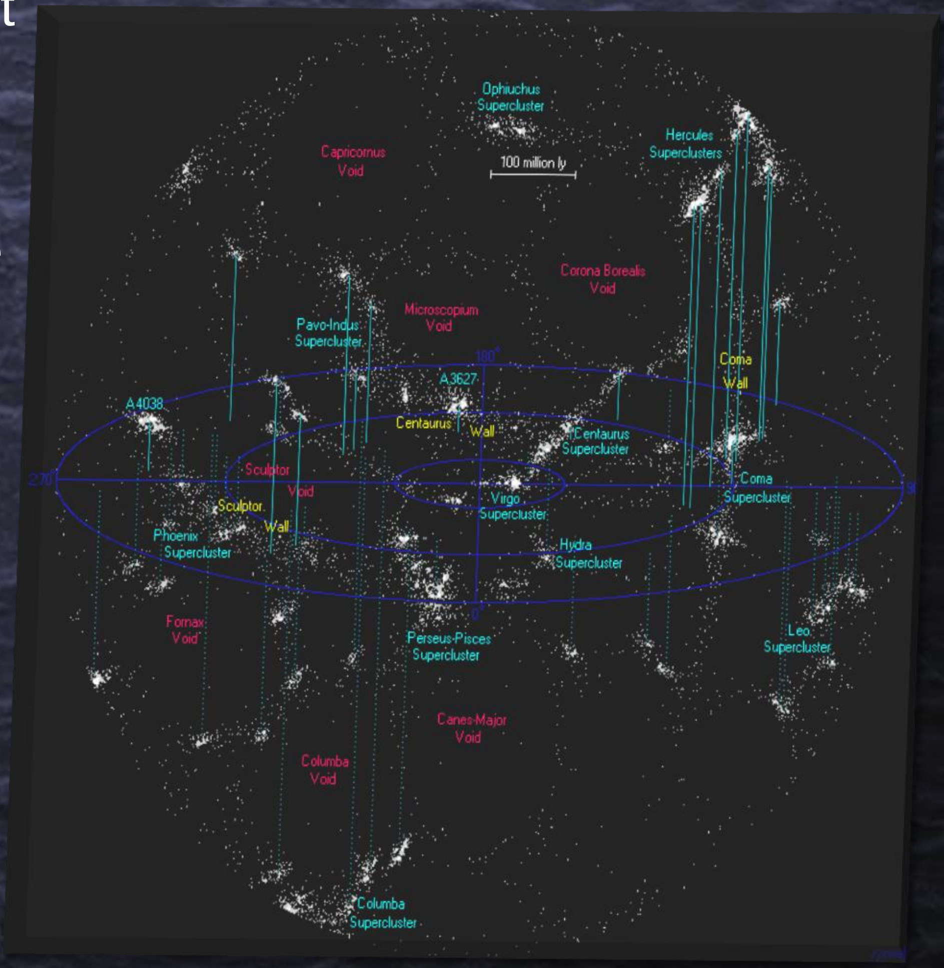
DISK GALAXIES

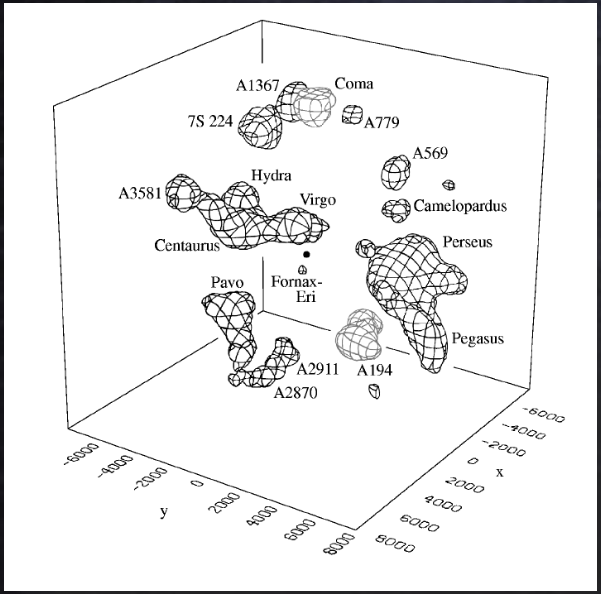


- Governato, GASOLINE code

Simulating the Local Universe

- Our Local neighborhood is the most well know piece of the universe . Thus, an ideal place to test models against observations.
- But it is not a representative volume of the universe. It is dominated by large mass concentrations Virgo, Local Supercluster, Coma, G.A).
- Cosmic variance has to be beaten when doing Near field cosmology





CLUES

Constrained Local UniversE Simulations

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The Hebrew University of Jerusalem

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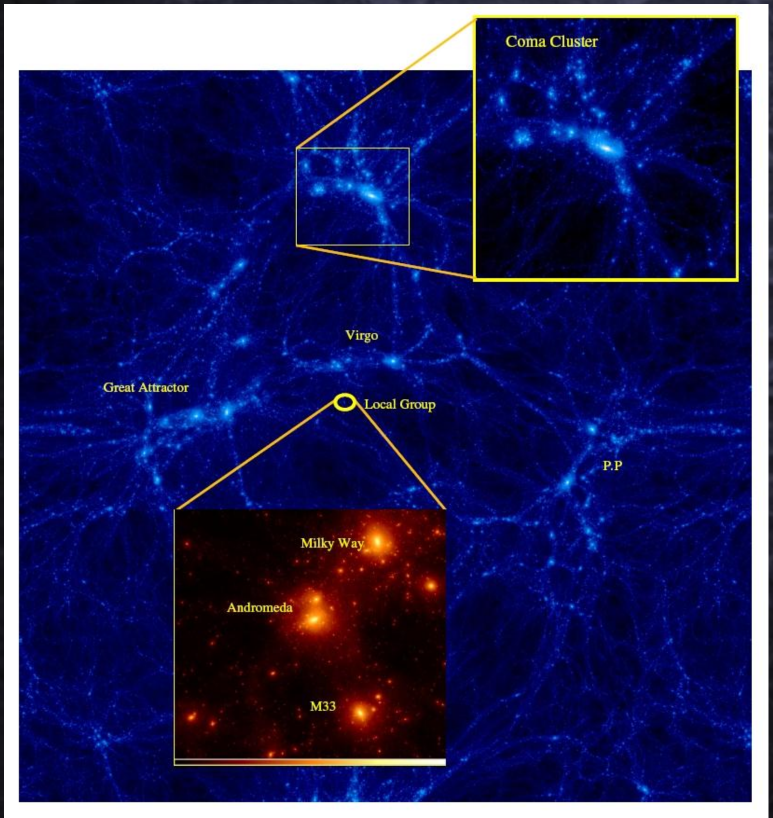
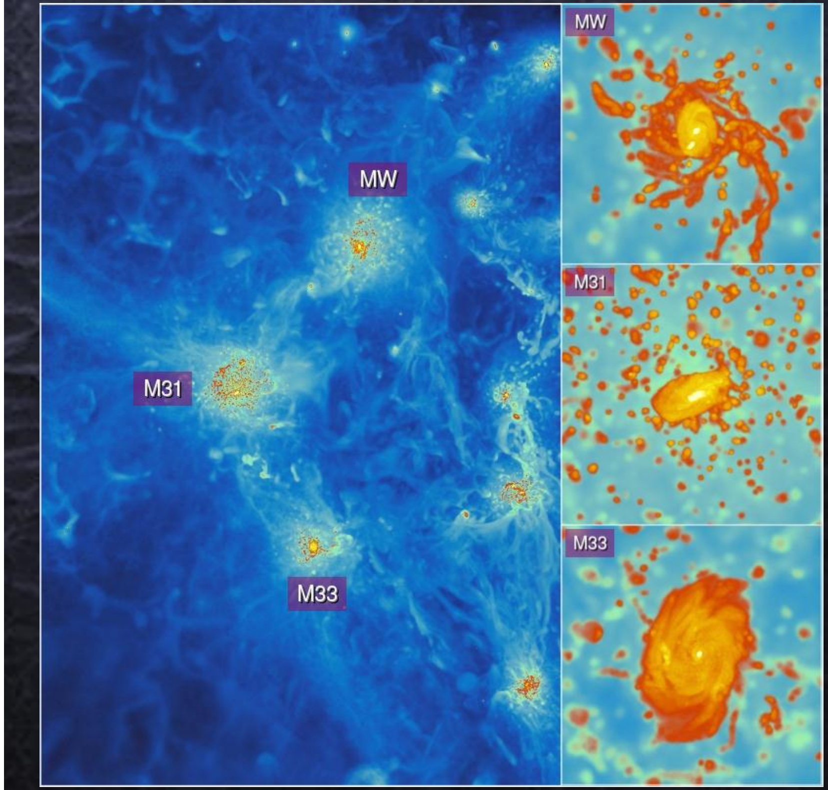
http: //www.clues-project.org





Constrained Simulations of the Local Universe

The perfect tool to study the formation of individual objects, that look like those close to us, starting from cosmological initial conditions and in a realistic environment.

  - ***Eg. Virgo, Coma, the Local filament .. or the Local Group.***

- **An excellent laboratory to investigate how dark matter is distributed and structured in a similar environment than our own galaxy.**

Observational Constrains

- **Mass and velocity constrains**

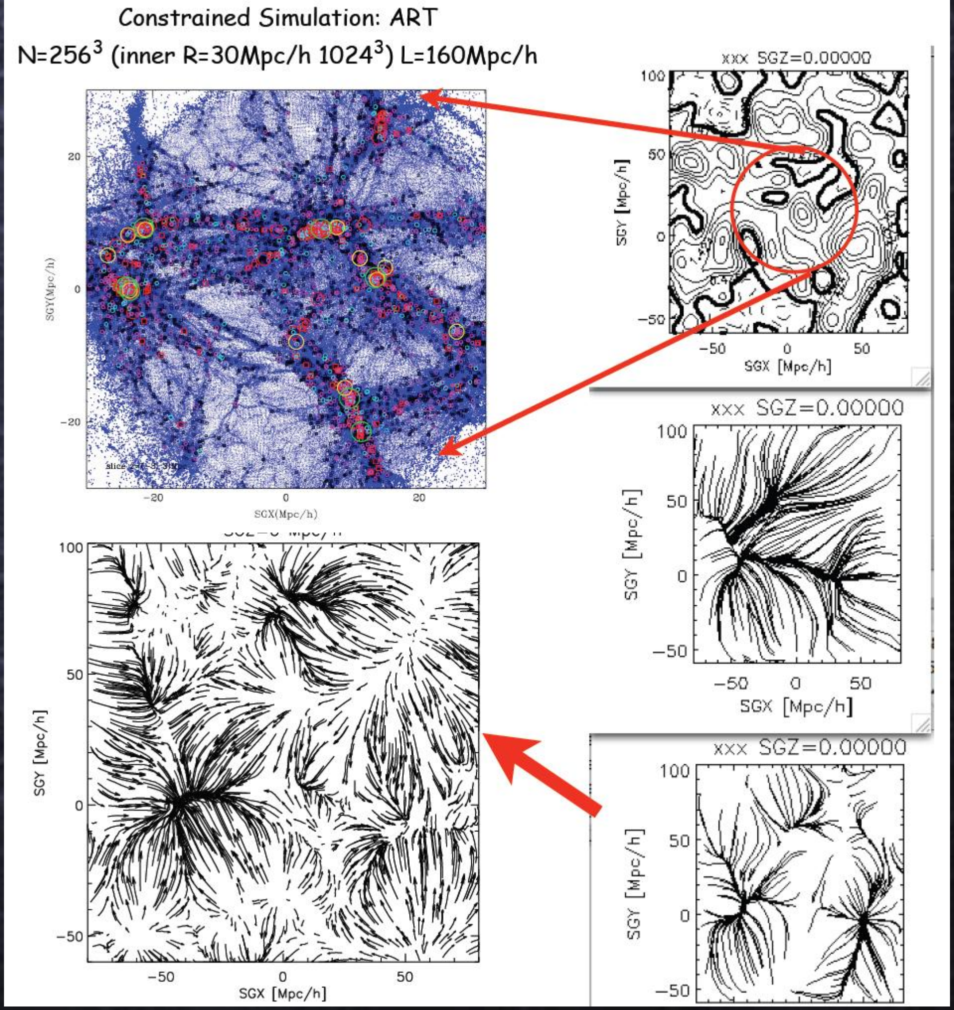
- Masses of nearby X-ray clusters
  - *Reiprich & Bohringer 2002*

- Peculiar Velocities taken from
  - *MARK3, SBF (large scale)*
- *(YH, Klypin,Gottlober,Kravtsov ,2002)*

+

  - *Karantchenstev et al. (LG)*

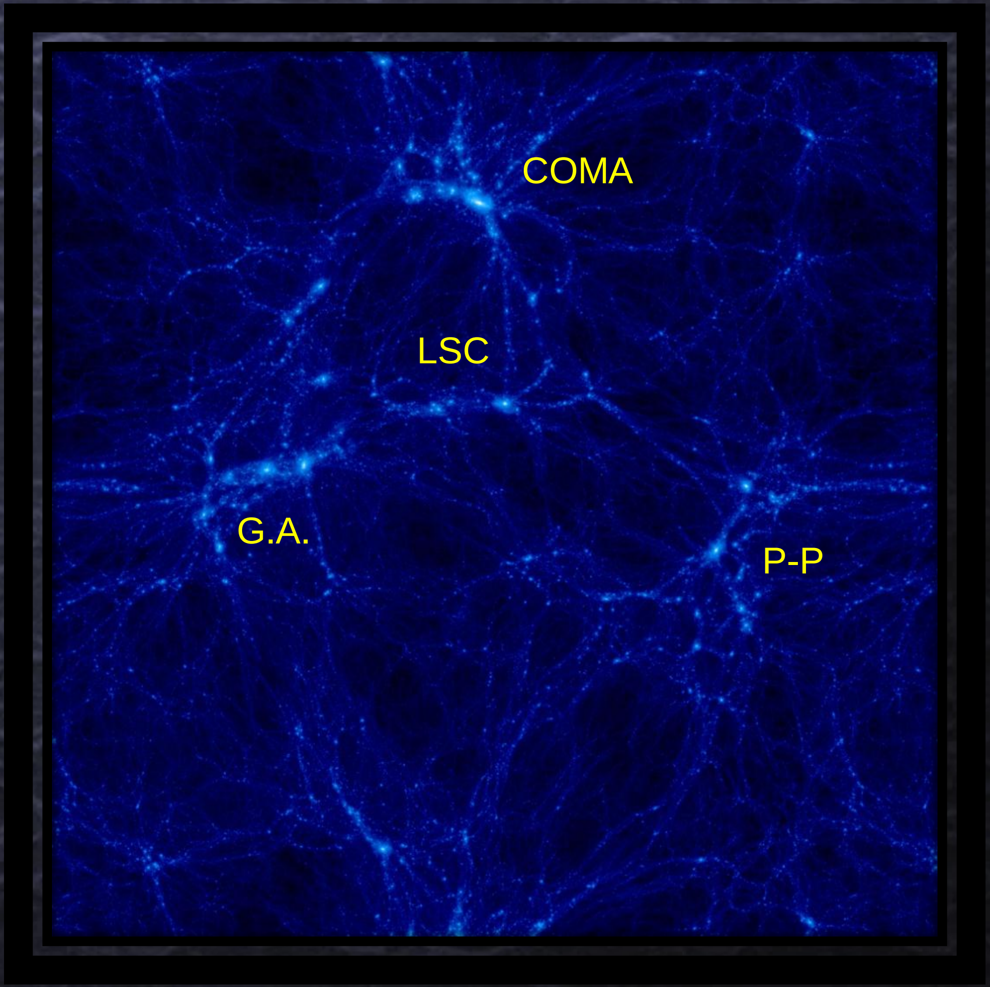
- ***Cosmological Model:***
  - *WMAP3 parameters*



Simulated Volumes

- Box 160/h Mpc:
- CS: 256^3 density field
    - COMA, LSC, PP, GA, Virgo

- Resimulated box with much higher resolution:
    - Make random realization of LCDM P(K) in a 4096^3 mesh.
    - Substitute fourier modes corresponding to those from the 256^3 CR.
    - Apply Zeldovich approx to find displacement fields
    - Fill box with arbitrary number of particles up to the 4096^3 maximum.

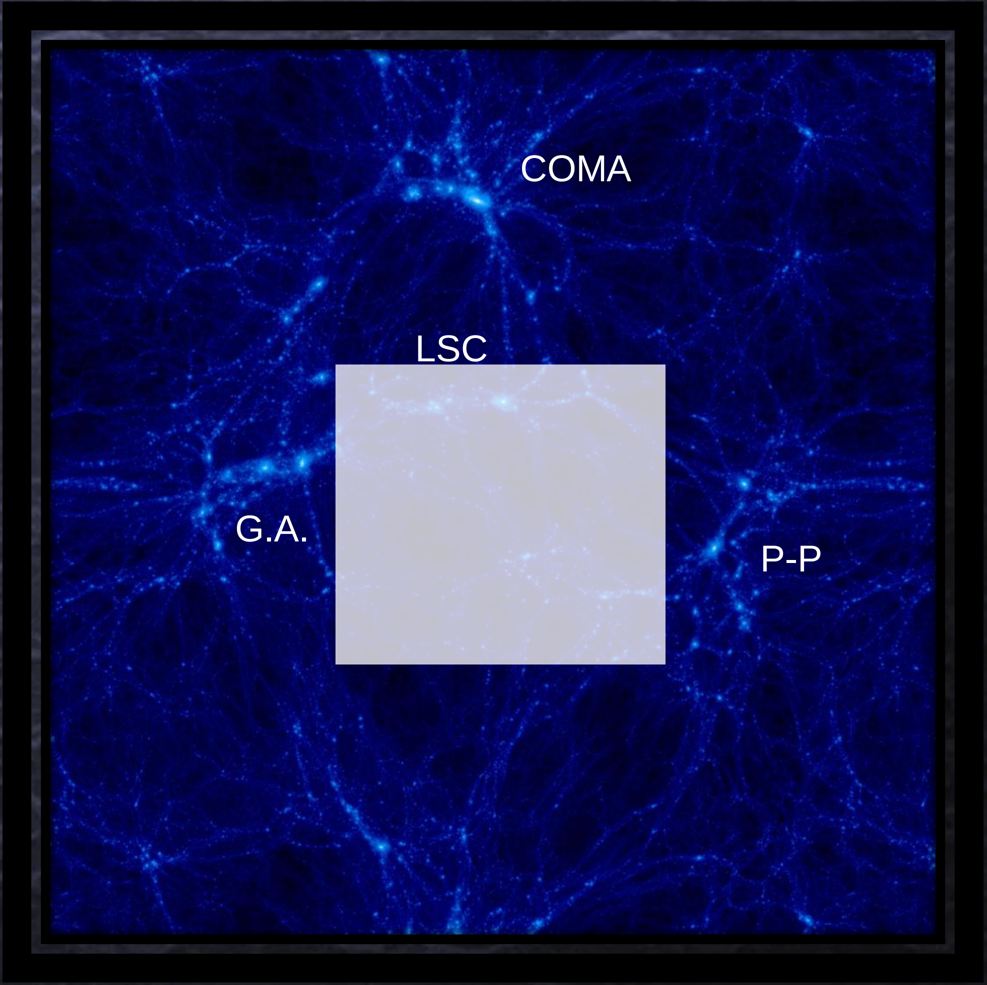


Simulated Volumes

- Box 160/h Mpc:
- CS: 256^3 density field
  - COMA, LSC, PP, GA, Virgo

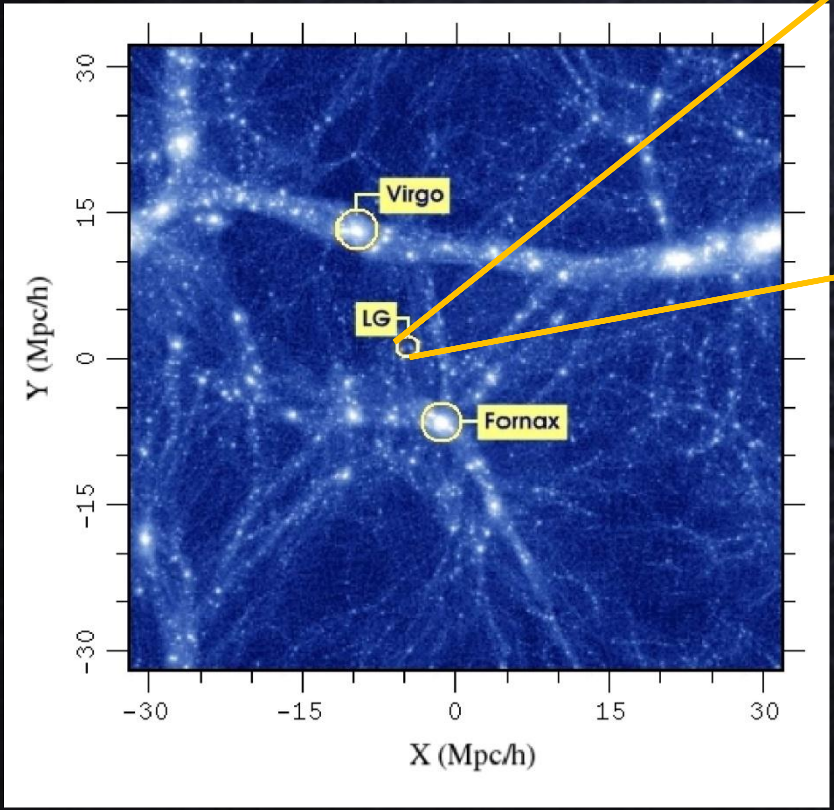
- Our biggest runs:

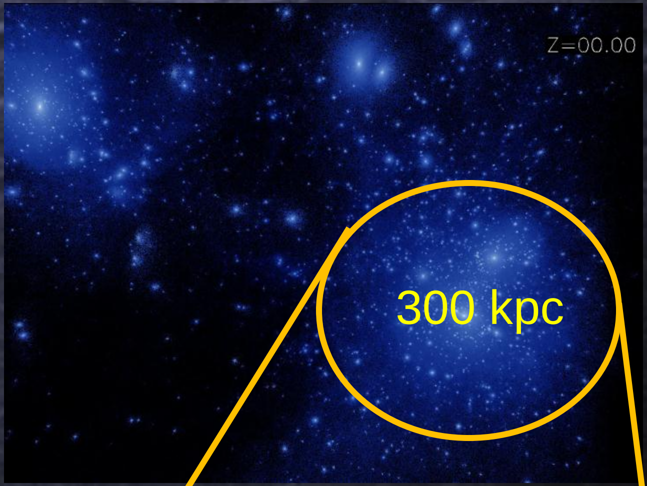
- 1024^3 particles filling the box
  - 1.2 kpc, 2.5×10^8 Msun
- Resimulated area around LSC
  - 4096^3 particles (4×10^6 $M_{\odot}$),
  - 300 pc resolution.
  - 300 million particles total.
  - ART N-body code.



DECI SIMU-LU
Simulating the Local Universe

Simulations including observational constrains in the initial conditions from the distribution of galaxies in our neighbourhood (R <100Mpc) can reproduce the mass structures observed around us





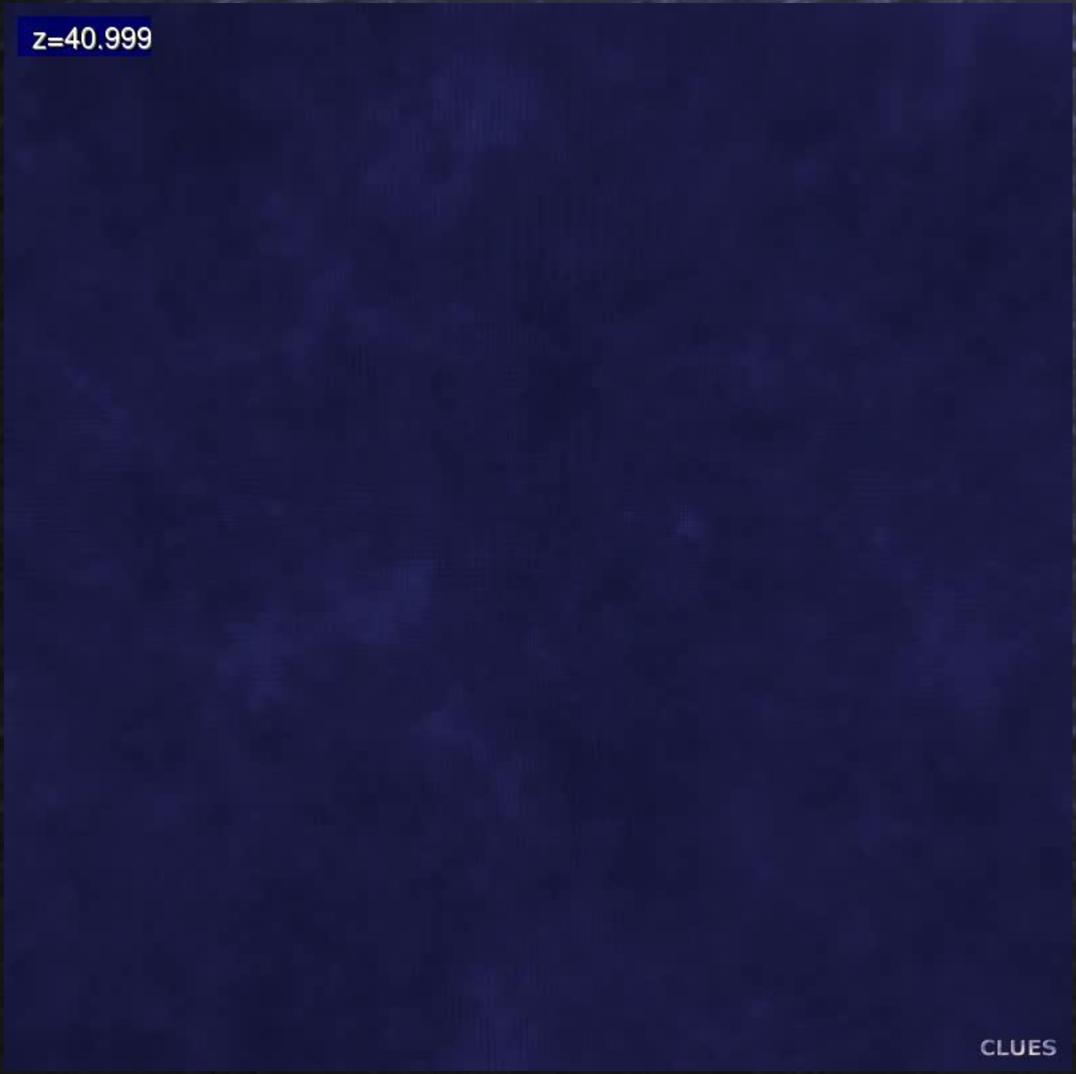
- 250K Msun:
- 4096^3 effective particles
- ~ $7 x 10^{10}$ in whole box. Only 60 million with zoomed simu.

Galaxy formation in the LG

- Overall, the Local Group object found in the constrained simulation looks quite realistic
  - *Environment, internal dynamics, halo structures*
- It can be used as a cosmological lab for galaxy formation to test different modeling of the various baryonic processes: ("gastrophysics") and compare results with observations:

Disk structure, Star formation history, HI and metal distributions, Local UV sources, surviving satellites…

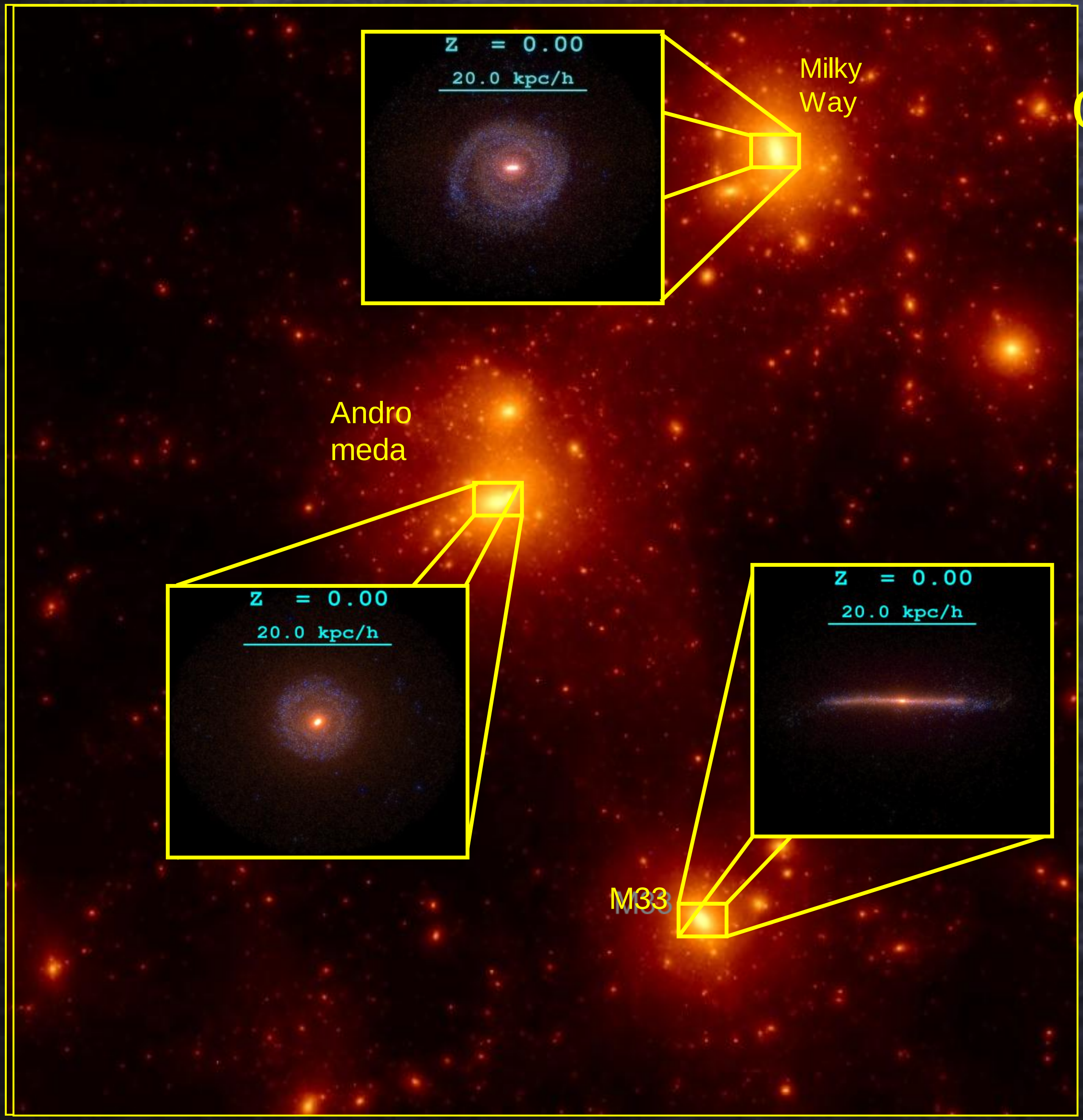
CLUES GAS SIMULATION



Gastrophysical simulation of the WMAP3 LG:

- **High resolution run with 4096^3 mass refinement.**
  - ***100 pc smoothing,***
  - ***34,000 M_{θ} SPH particle.***
  - ***17,000 M_{θ} STAR particle***
- **SPH simulation using GADGET2**
- **UV standard photoionization scheme H&M**
- **Multiphase medium + winds S&H 2003.**
- **Bruzual & Charlot 2003 SPSM.**
- **Primordial composition cooling.**

CLUES GAS SIMULATIONS



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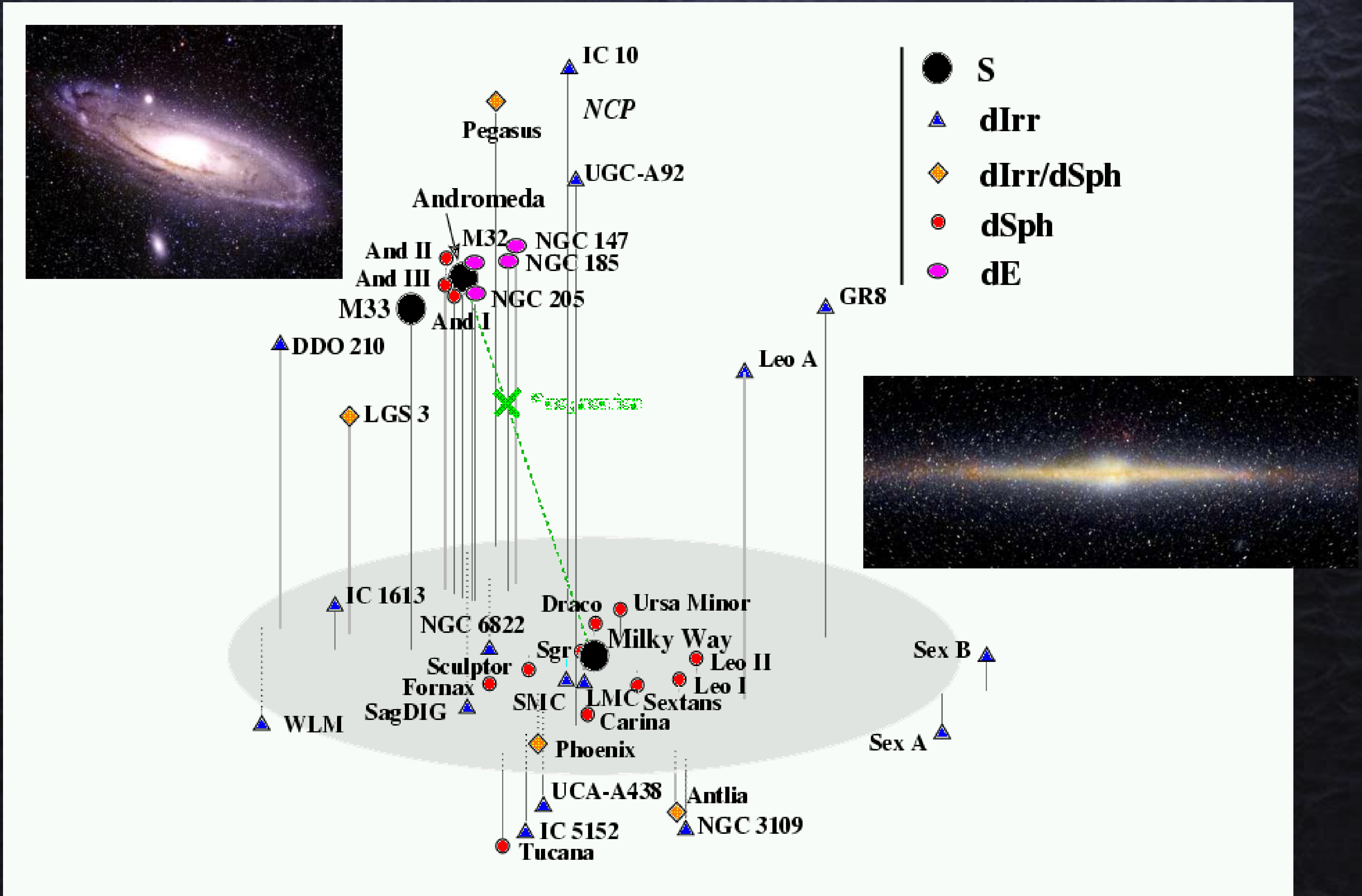
- **Primordial composition cooling.**

EL GRUPO LOCAL:
LABORATORIO DE MATERIA OSCURA



CDM Has a Missing Satellite Problem

•Springel et al. 2001

- CDM predicts large numbers of subhalos (~100-1000 for a Milky Way-sized galaxy)
- Milky Way only has 23 known satellites
- What happened to the rest of them?

CDM Has a Missing Satellite Problem

- Springel et al. 2001

- CDM predicts large numbers of subhalos (~100-1000 for a Milky Way-sized galaxy)
- Milky Way only has 23 known satellites
- What happened to the rest of them?

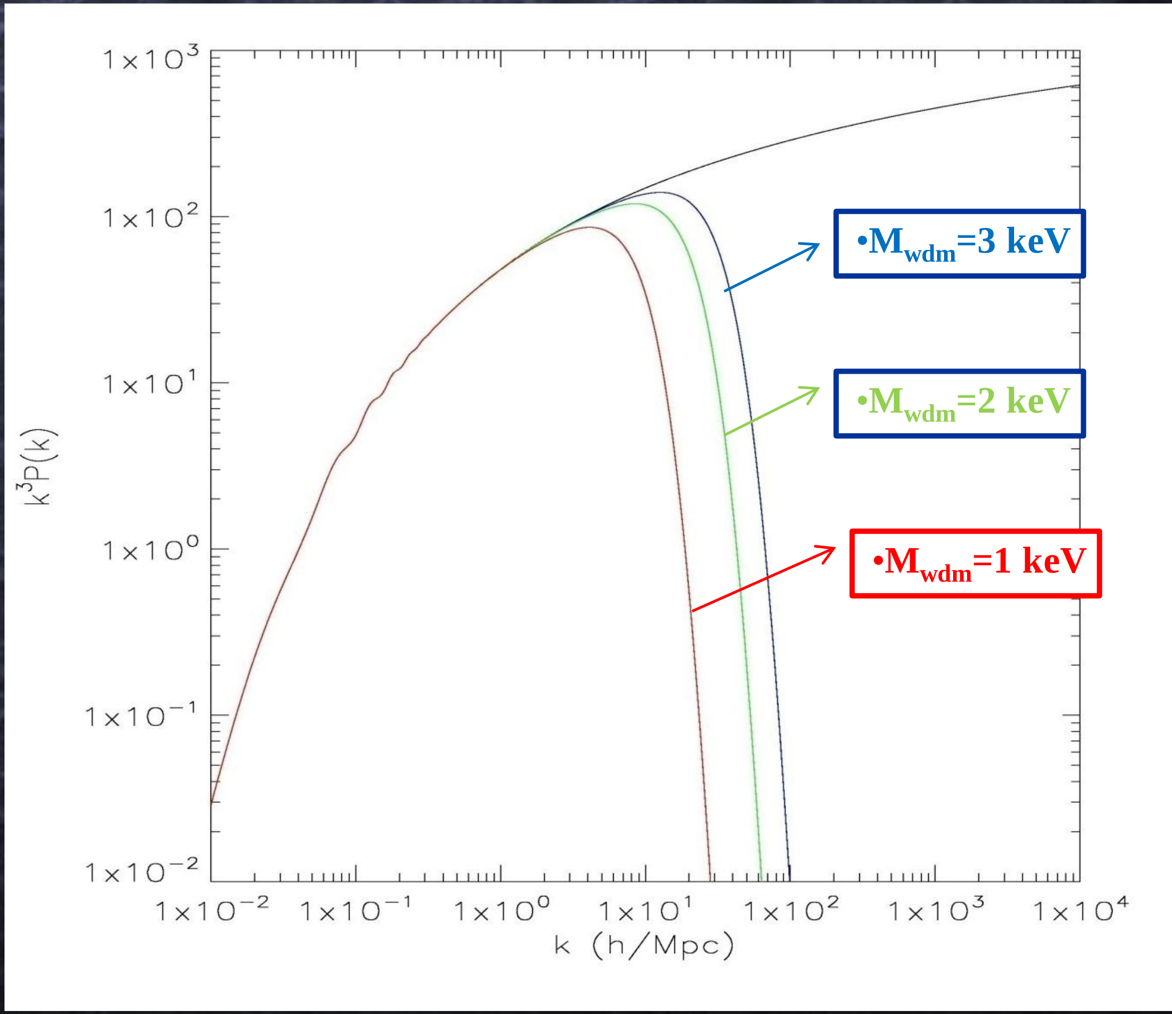
What Does This Problem Tell Us?

- Two basic sets of possible solutions:
  - Modifications to CDM
    - What modifications? Power spectrum, DM particle mass/decay/interaction cross-section?
  - Astrophysics prevents stars from forming in most low-mass halos
    - What astrophysics? Reionization, feedback, winds?

NATURE OF THE DARK MATTER
Cold DM vs Warm DM

- WDM particles:
- M_{wdm} = 3keV – 1 keV

- Comparison with ΛCDM:
    - density profiles
    - substructure mass functions
-



MILKY WAY IN CDM vs WDM

SUMARIO

- **La Creación de Universos Virtuales realistas en una de las herramientas fundamentales para considerar a la Astrofísica y la Cosmología como verdaderas ciencias experimentales:**
  - *Es el laboratorio natural donde hacer experimentos con las componentes del universo y sus interacciones físicas.*
  - *Nos permite adentrarnos en épocas todavía no accesibles a la observación y predecir que podemos esperar* ver.
- **Las simulaciones cosmológicas son uno de los desafíos computacionales más importantes. Debido a que la gravedad es una fuerza no saturante, es muy difícil derivar algoritmos capaces de distribuir los elementos computacionales que describen los distintos fluidos de forma eficiente entre miles o decenas de miles de procesadores**
  - *Es necesario realizar un trabajo de desarrollo de códigos paralelos considerable.*
  - *El paralelismo en este campo está en sus comienzos, menos de 10 años de vida…*
  - *Grid super-computing puede ayudar a resolver el problema..*
  -
- **The MareNostrum Numerical Cosmology Project, pretende unir esfuerzos a nivel internacional para abordar problemas de *grand challenge* que necesitan de capacidades computacionales extremas y de recursos humanos suficientes para el análisis de los datos numéricos.**

MNCP

GRACIAS POR SU ATENCIÓN

http://www.clues-project.org

http://astro.ft.uam.es/marenostrum

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