Numerical simulations in cosmology:

Review + cookbook

C Pichon

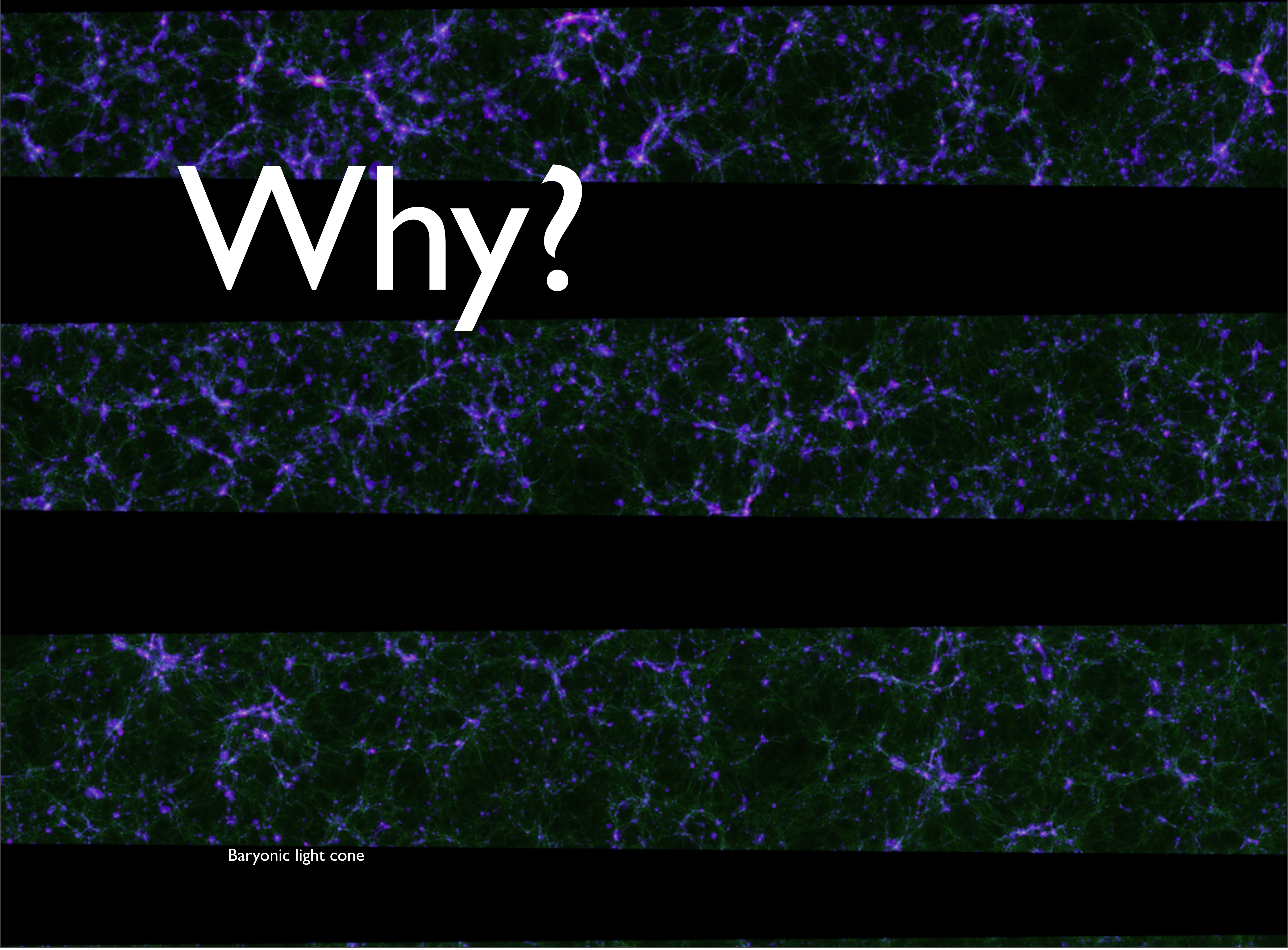
(largely inspired by lectures of Teyssier, Springel, White...)

Outline

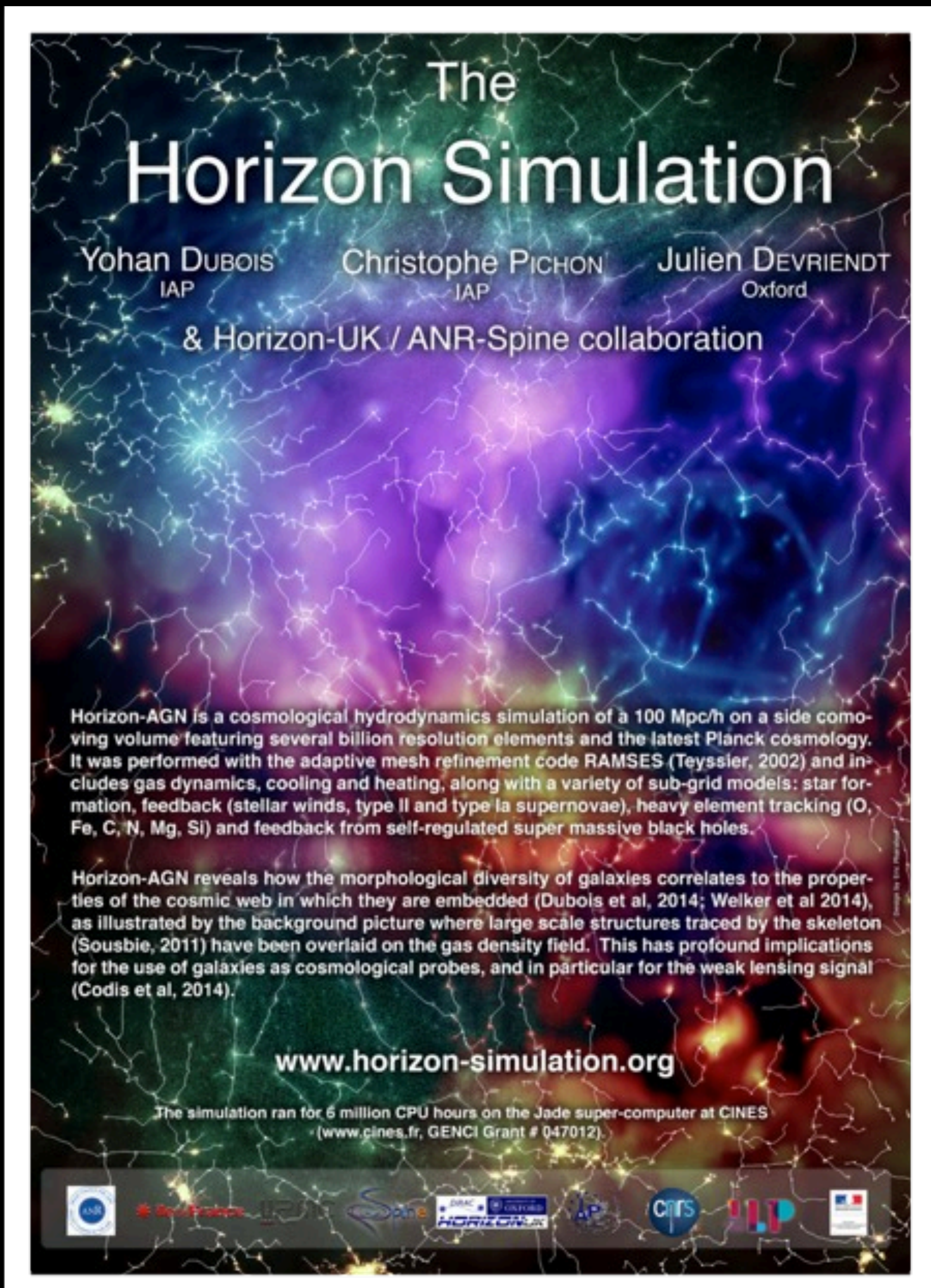
- What are cosmo sim?
- Why do cosmo sim?
- How is it done?
- Where we are today?

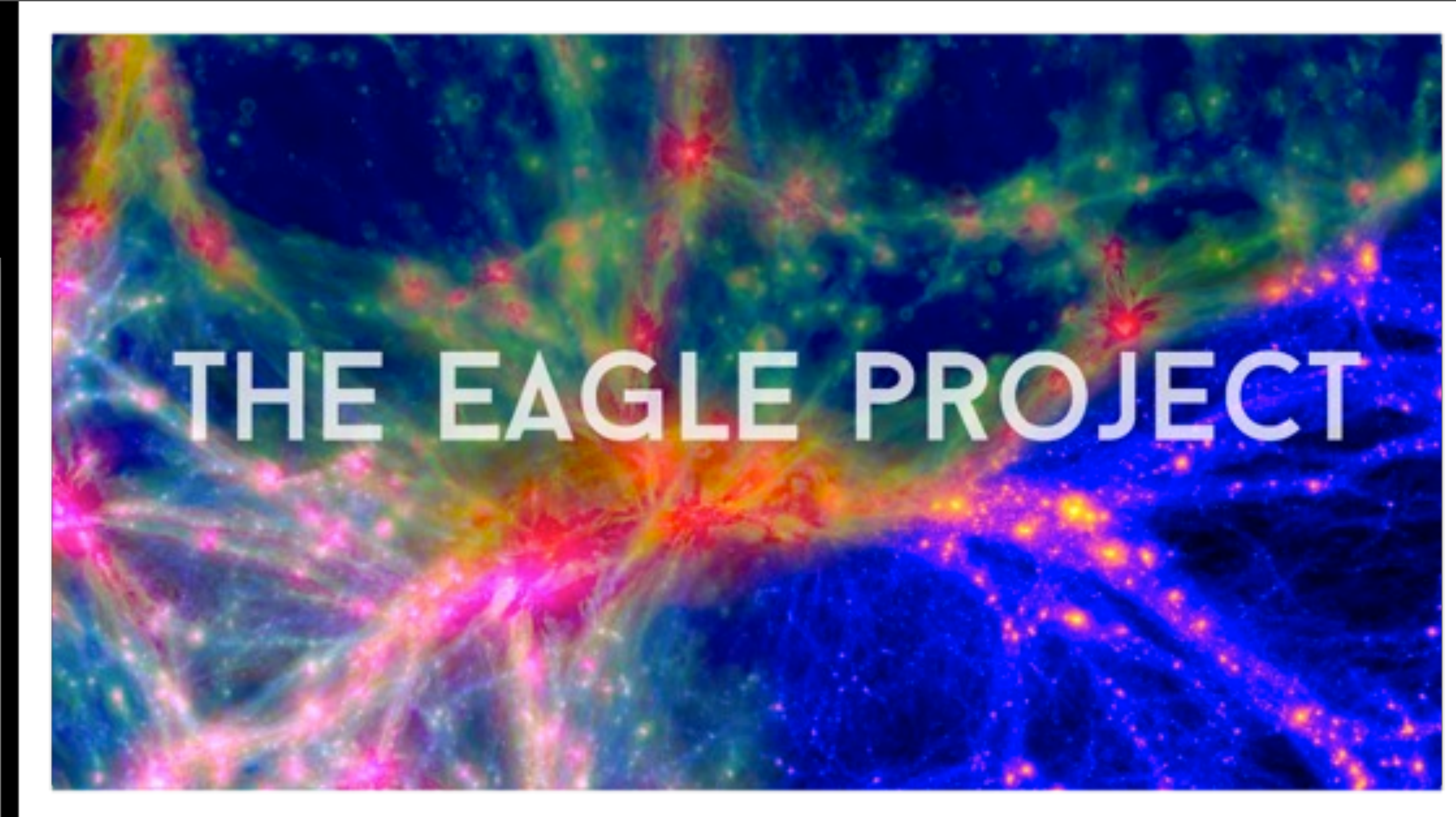

What?

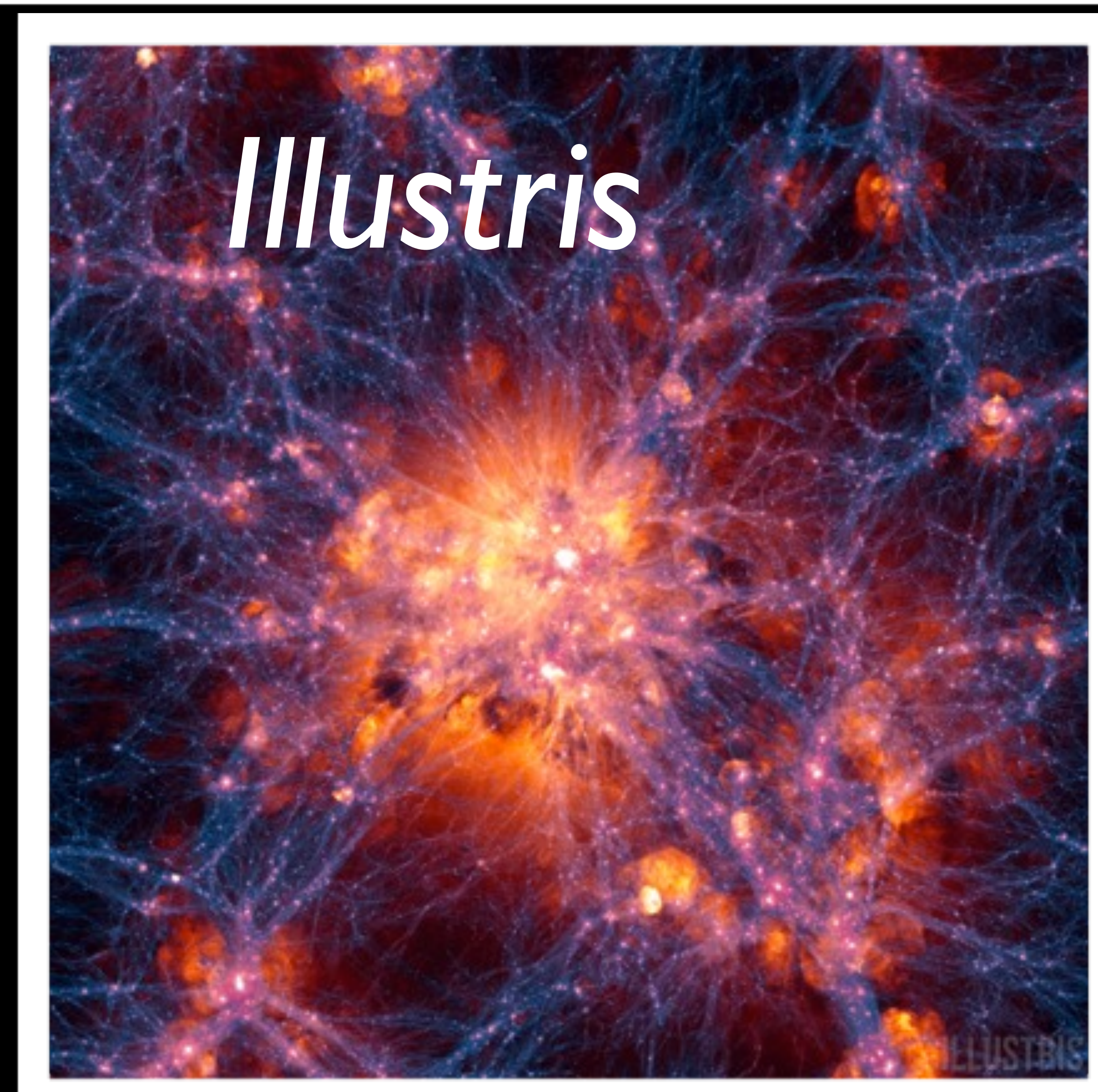
Why?



Baryonic light cone


The
Horizon Simulation
Yohan Dubois
IAP
Christophe Pichon
IAP
Julien Devriendt
Oxford
& Horizon-UK / ANR-Spine collaboration
Horizon-AGN is a cosmological hydrodynamics simulation of a 100 Mpc/h on a side comoving volume featuring several billion resolution elements and the latest Planck cosmology. It was performed with the adaptive mesh refinement code RAMSES (Teyssier, 2002) and includes gas dynamics, cooling and heating, along with a variety of sub-grid models: star formation, feedback (stellar winds, type II and type Ia supernovae), heavy element tracking (O, Fe, C, N, Mg, Si) and feedback from self-regulated super massive black holes.
Horizon-AGN reveals how the morphological diversity of galaxies correlates to the properties of the cosmic web in which they are embedded (Dubois et al, 2014; Welker et al 2014), as illustrated by the background picture where large scale structures traced by the skeleton (Sousbie, 2011) have been overlaid on the gas density field. This has profound implications for the use of galaxies as cosmological probes, and in particular for the weak lensing signal (Codis et al, 2014).
www.horizon-simulation.org
The simulation ran for 6 million CPU hours on the Jade super-computer at CINES
(www.cines.fr, GENCI Grant # 047012).


THE EAGLE PROJECT


Illustris

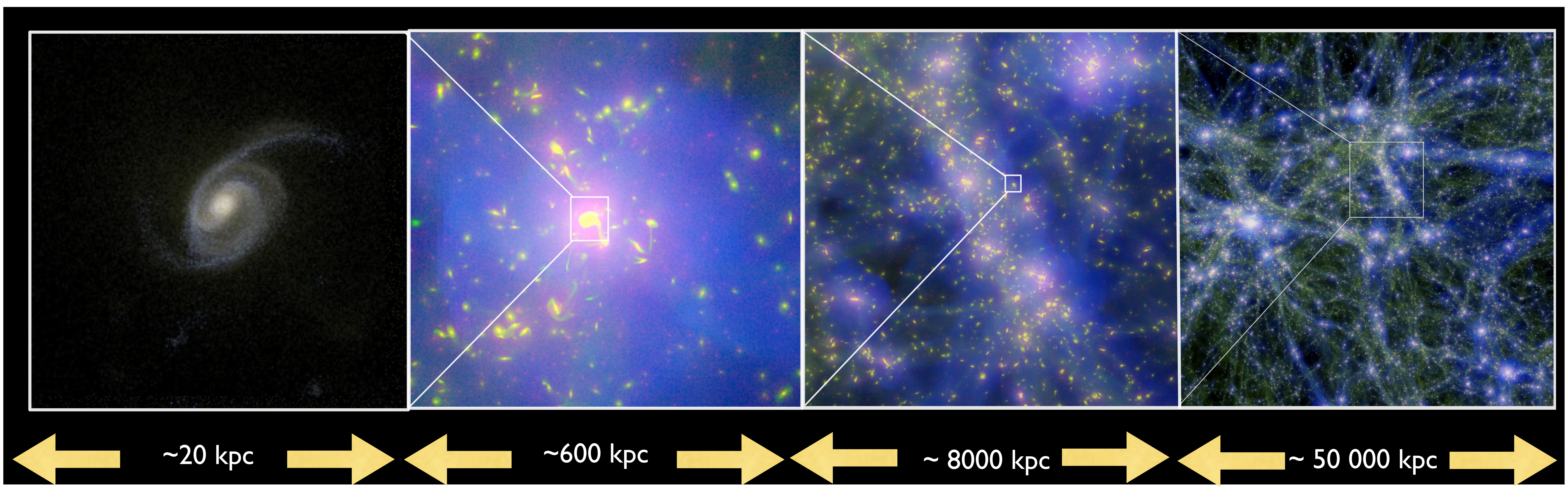
Why simulate structure formation ?

* to understand effects of **non-linear** processes on cosmology/galaxies

* to connect the early universe to ***statistical*** surveys at low redshifts

* to validate upcoming instruments via **mocks**

* to explore the subtle effect of **alternative theory of gravity**



Why?

PROS

- properly account for scale coupling/ anisotropy
- allow for visualisation of the effect of complex processes
- decide quantitatively which non-linear process dominates
- make (large) virtual data sets/ surveys;
- validate inverse methods;
- build realistic estimators/ model biases;
- calibrate new instrument:

  how well can we measure things from

  a given *incomplete* survey?
- estimate error bars/covariance matrices;
- validate perturbation theory

CONS

- Most players *present* a very skewed view of success/failure
- Simulations can easily be Garbage In Garbage Out
  *Sometimes, domain of scientific interest =0
- Misleading because *too* convincing compared to thought experiments
- Chaotic solution possibly driven by algorithmic limitation
- Sociologic bias towards runaway: code validation sporadic
- A lot of work !

  * write a code
  * validate the code
  * run the simulations : big mock data (@ IAP ~ PB)
  * validate the simulation
  * produce virtual observables
  * write the estimator
  * validate the estimator
  * explore domain of relevance
  * study biasses

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- v

- b

- c

- e

- v

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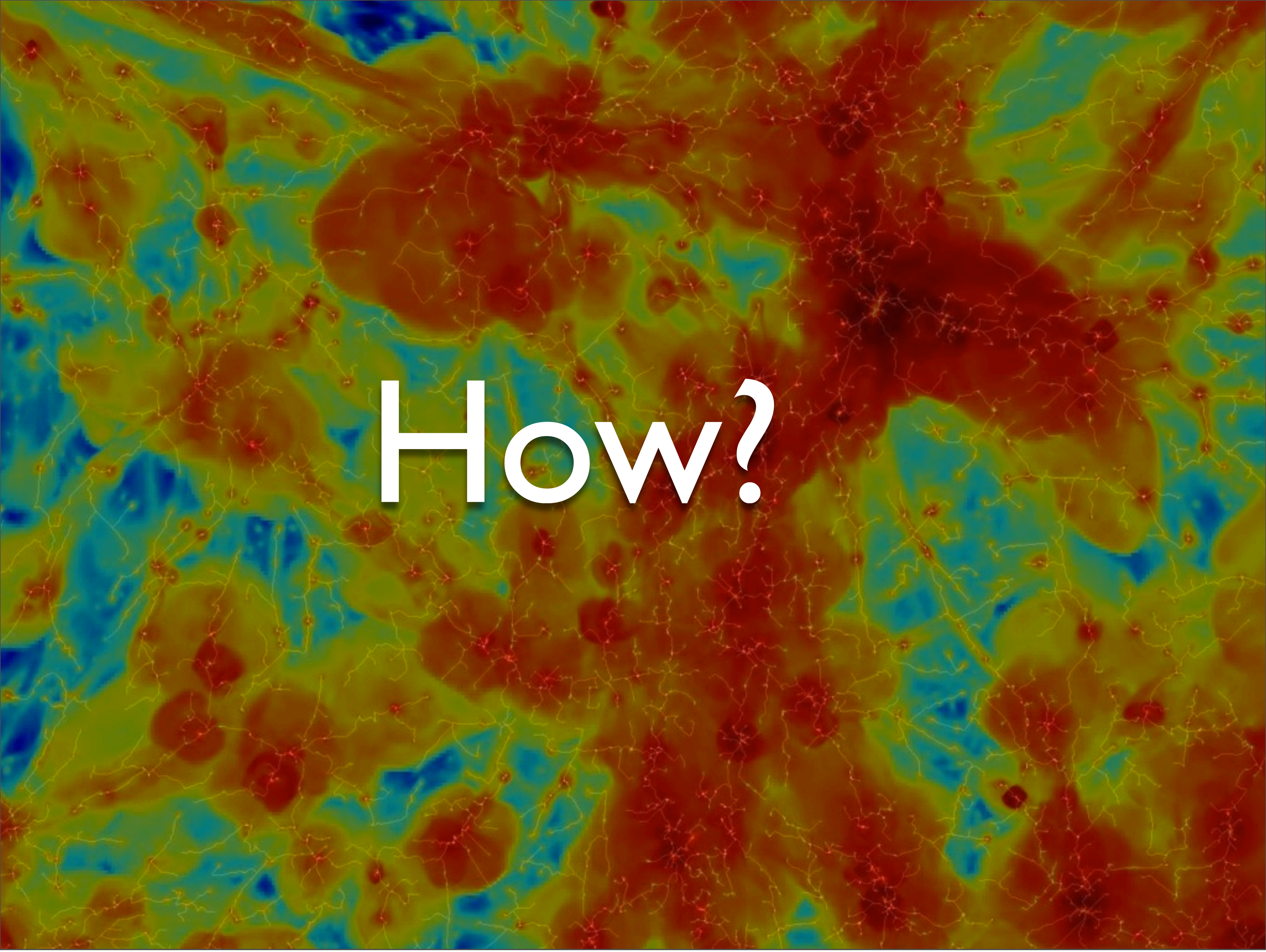
How?

Account for cosmic expansion

$$\frac{\partial f}{\partial t} + \mathbf{u}.\nabla f - \nabla\Phi.\nabla_u f = 0$$

$$\frac{\partial \rho_\mathrm{b}}{\partial t} + \nabla.(\rho_\mathrm{b}\mathbf{u}) = 0$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}.\nabla).\mathbf{u} = -\nabla\Phi - \frac{\nabla p}{\rho_\mathrm{b}}$$

$$\frac{\partial \varepsilon}{\partial t} + \mathbf{u}.\nabla\varepsilon = -\frac{p}{\rho_\mathrm{b}}\nabla.\mathbf{u}$$

$$p = (\gamma - 1)\varepsilon\rho_\mathrm{b}$$

$$\nabla^2\Phi = 4\pi G\left[\int f d^3u + \rho_\mathrm{b}\right]$$

- voids repel,
- gas shocks
- if collapse, fate final

(cooling catastrophy)

super co-moving variables

$$d\tilde{t} = H_0 \frac{dt}{a^2}$$

$$\tilde{x} = \frac{1}{a}\frac{x}{L}$$

$$\tilde{\rho} = a^3 \frac{\rho}{\Omega_0 \rho_\mathrm{c}}$$

$$\tilde{p} = a^5 \frac{p}{\Omega_0 \rho_\mathrm{c} H_0^2 L^2}$$

$$\tilde{\mathbf{u}} = a \frac{\mathbf{u} - H\mathbf{x}}{H_0 L}$$

$$\tilde{\nabla}^2\tilde{\Phi} = \frac{3}{2} a\Omega_0(\tilde{\rho} - 1)$$

Martel & Shapiro (1998)

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Dynamics is Hamiltonian

HAMILTONIAN SYSTEMS AND SYMPLECTIC INTEGRATION

$$H(\mathbf{p}_1, \ldots, \mathbf{p}_n, \mathbf{x}_1, \ldots, \mathbf{x}_n) = \sum_i \frac{\mathbf{p}_i^2}{2m_i} + \frac{1}{2}\sum_{ij} m_i m_j \phi(\mathbf{x}_i - \mathbf{x}_j)$$

If the integration scheme introduces non-Hamiltonian perturbations, a completely different long-term behaviour results.

The Hamiltonian structure of the system can be preserved in the integration if each step is formulated as a *canoncial transformation*. Such integration schemes are called *symplectic*.

Poisson bracket:

$$\{A, B\} \equiv \sum_i \left(\frac{\partial A}{\partial \mathbf{x}_i}\frac{\partial B}{\partial \mathbf{p}_i} - \frac{\partial A}{\partial \mathbf{p}_i}\frac{\partial B}{\partial \mathbf{x}_i} \right)$$

Hamilton's equations

$$\frac{\mathrm{d}\mathbf{x}_i}{\mathrm{d}t} = \{\mathbf{x}_i, H\}$$

$$\frac{\mathrm{d}\mathbf{p}_i}{\mathrm{d}t} = \{\mathbf{p}_i, H\}$$

Liouville (N point PDF conservation)

$$z \equiv (\mathbf{r}, \mathbf{v}) \qquad \partial_t f_n + \{f_n, H_n\}_n = 0$$

N point function

$$f_1(z) = n \int f_n(z, z_2, \cdots, z_n) dz_2 \cdots dz_n$$

$$f_2(z, z') = n(n-1) \int f_n(z, z', z_3, \cdots, z_n) dz_3 \cdots dz_n$$

...

BBGKY hierarchy

$$\partial_t f_1 + \{f_1, H_1\} = \int \Big\{ f_1(z) f_1(z') - f_2(z, z'), H_2(z, z') \Big\} dz'$$

long range force /short timescale limit (mean free path ~ system)

$$\mathrm{DM} \implies f_2(z, z') = f_1(z) f_1(z')$$

short + long range force /long timescale limit

$$\mathrm{Hydro} \implies \int \Big\{ f_1(z) f_1(z') - f_2(z, z'), H_2(z, z') \Big\} dz' = \frac{\partial f}{\partial t}_{\mathrm{col}}$$

CBE/Vlazof equation

$$\partial_t f + \{f, H\} = \partial_t f + \mathbf{v}\cdot\nabla f + \nabla\psi\cdot\nabla_v f = 0$$

mass

moments yield **Jeans** Hierarchy

$$\partial_t \rho + \rho\nabla\cdot\mathbf{v} = 0$$

Euler

$$\partial_t \mathbf{v} + \frac{1}{\rho}\nabla\cdot\mathbf{P} + \nabla\psi = 0$$

$$\partial_t \mathbf{P} + (\mathbf{P} + \mathbf{P}^T)\cdot\nabla\mathbf{v} + \frac{1}{\rho}\nabla\cdot\mathbf{Q} = \mathbf{0}$$

$$\cdots$$

$$\partial_t \mathbf{Q}_n + \sum_p C_n^p \mathbf{Q}_n \nabla\cdot\mathbf{Q}_{n-p} + \frac{1}{\rho}\nabla\cdot\mathbf{Q}_{n+1} = \mathbf{0}$$

Where generalized Heat tensor obey

$$\cdots$$

$$\mathbf{P} = \mathbf{Q}_2\,, \quad \rho\bar{\mathbf{v}} = \int d^3\mathbf{v} f(\mathbf{r},\mathbf{v})\mathbf{v}$$

$$\partial_t \equiv \frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla$$

$$\mathbf{Q}_n \equiv \int d^3\mathbf{v} f(\mathbf{r},\mathbf{v})(\mathbf{v}-\bar{\mathbf{v}})\otimes\ldots(\mathbf{v}-\bar{\mathbf{v}})_n$$

Collisions : $\mathbf{P} = p(\rho, T)\mathbf{1}$

Ideal gas : $p(\rho, T) = (\gamma - 1)\rho u$

The baryons in the universe can be modelled as an *ideal* gas

BASIC HYDRODYNAMICAL EQUATIONS

Euler equation:	$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\frac{\nabla P}{\rho} - \nabla\Phi$
Continuity equation:	$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho\nabla\cdot\mathbf{v} = 0$

trace of second moment equation

First law of thermodynamics:	$\frac{\mathrm{d}u}{\mathrm{d}t} = -\frac{P}{\rho}\nabla\cdot\mathbf{v} - \frac{\Lambda(u,\rho)}{\rho}$

Closure

Equation of state of ideal monoatomic gas:	$P = (\gamma - 1)\rho u\ , \qquad \gamma = 5/3$

The dynamics of structure formation is driven by gravity

Gravity
general relativity, but Newtonian approximation in expanding space usually sufficient

Hydrodynamics
shock waves
radiation processes
star formation
supernovae,
black holes, etc...

dark matter is collisionless

Monte-Carlo integration as an **N-body system**

3N **coupled**, non-linear differential equations of second order

Problems:

- N is very large
- All equations are coupled to each other

One challenge is to separate the important from the unimportant

Two conflicting requirements complicate the study of **hierarchical** structure formation

DYNAMIC RANGE PROBLEM FACED BY COSMOLOGICAL SIMULATIONS

Want **small particle mass** to resolve internal structure of halos

Want **large volume** to obtain respresentative sample of universe

need large **N**

where N is the particle number

Currently $N \sim 10^{10}$ on very large scales

Problems due to a small box size:

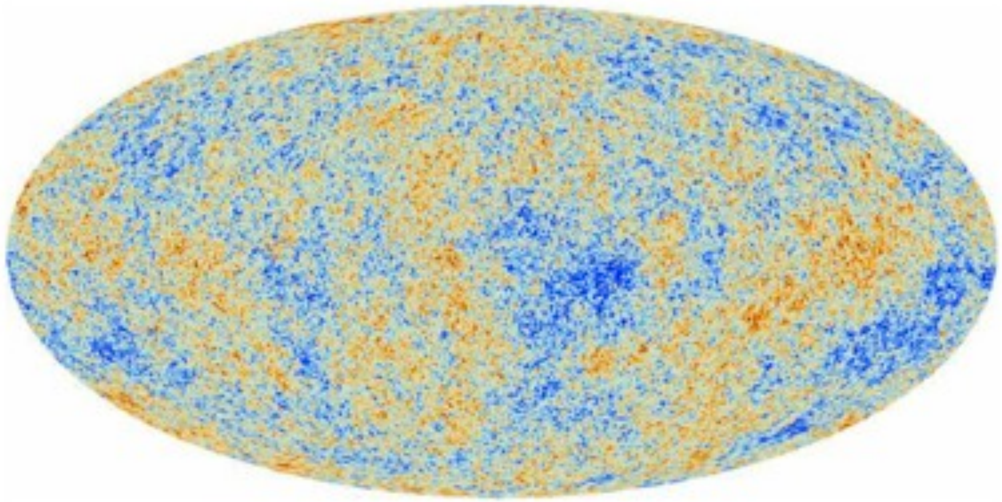
- Fundamental mode goes non-linear soon after the first halos form. ⇨ Simulation cannot be meaningfully continued beyond this point.
- No rare objects (the first halo, **rich** galaxy clusters, etc.)

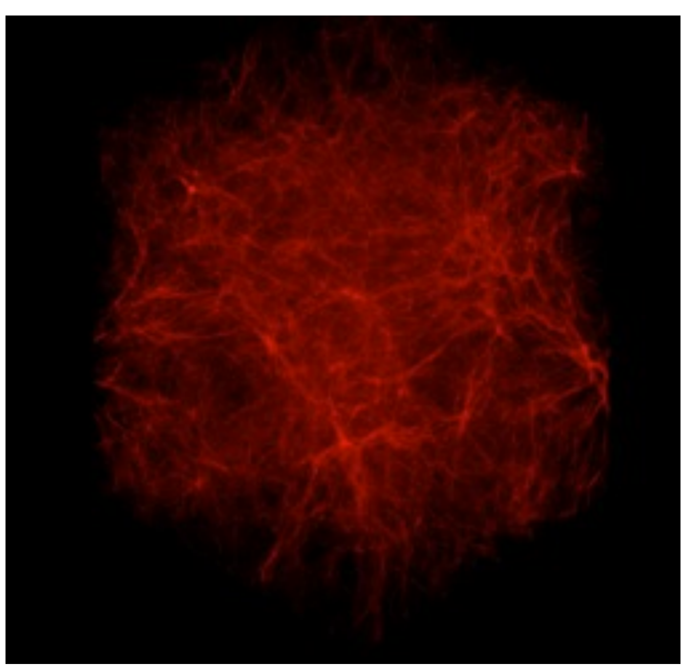
Problems due to a large particle mass:

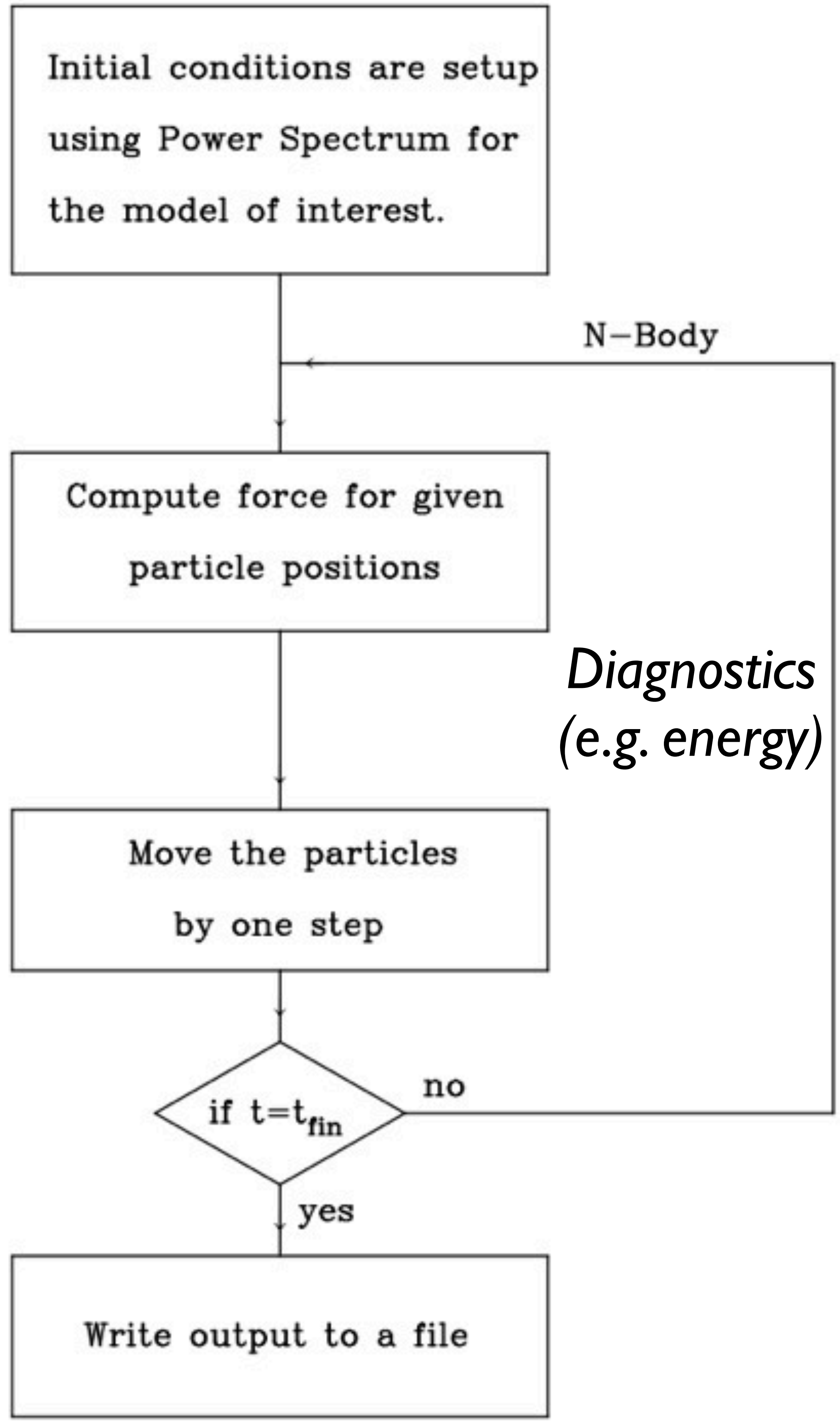
- Physics cannot be resolved.
- Small galaxies are missed.

At any given time, halos exist on a large range of mass-scales !

Flow Chart for N-body



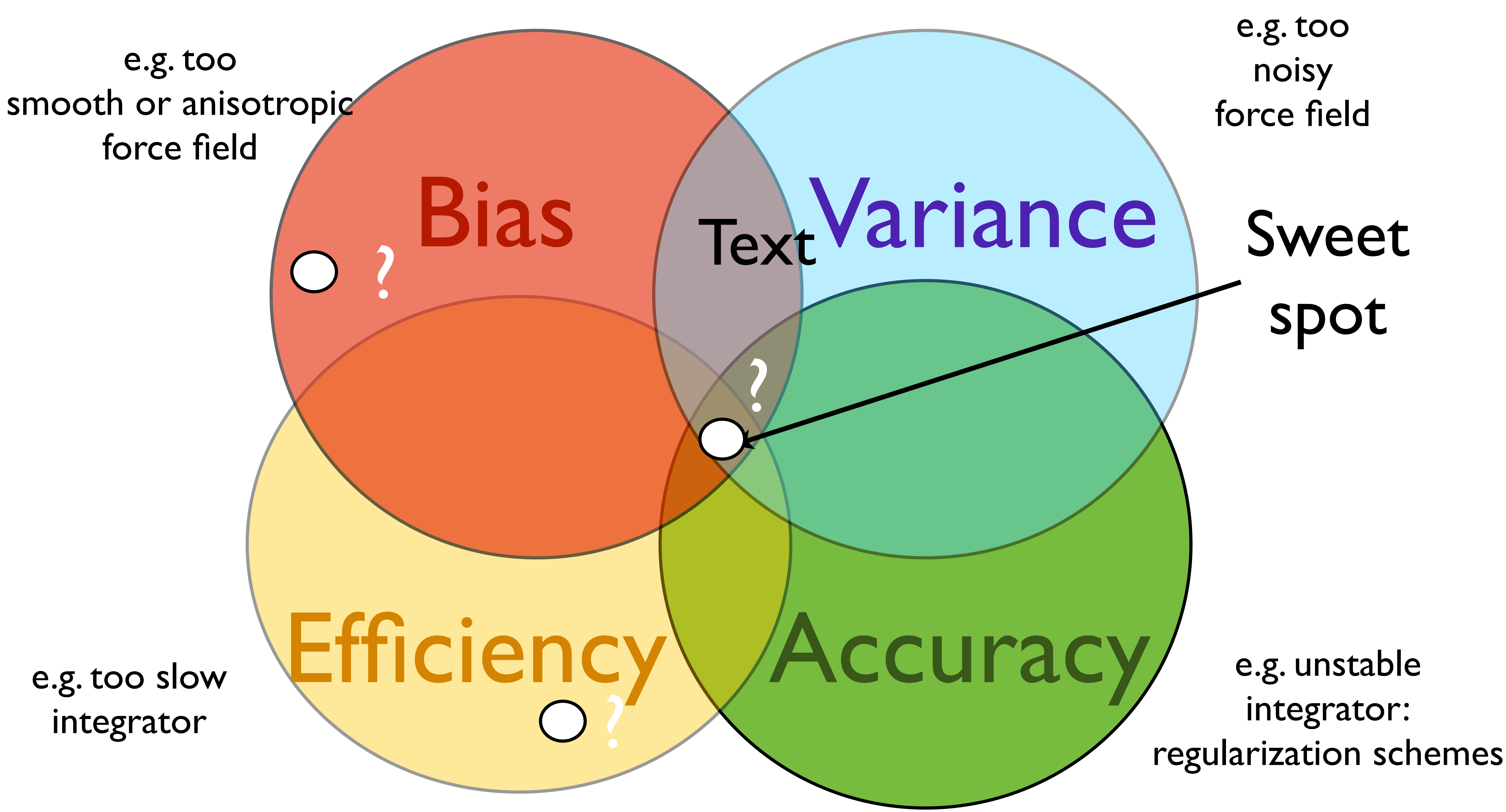




From the point of view of the theory of estimation/numerical analysis/computational geometry....

Discretize + control errors

Optimal (DM+*hydro*) code



Dark matter evolution

- Dynamics in a expanding universe
- Cosmological initial conditions
- Multi-scale dynamics
- Multigrid Poisson solver
- Symplectic integrators
- Zoom simulations

$$\tilde{\nabla}^2\tilde{\Phi} = \frac{3}{2}a\Omega_0(\tilde{\rho} - 1)$$

Initial conditions for LSS

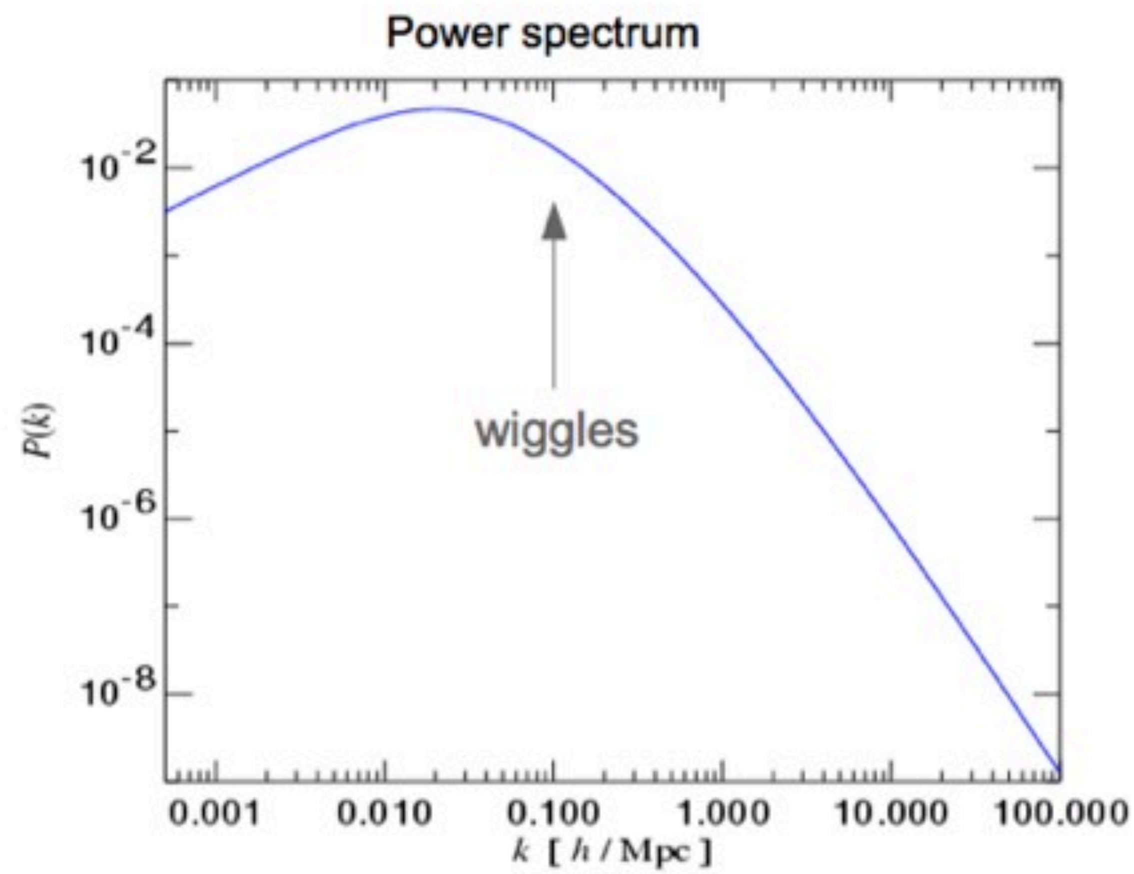
The linear theory power spectrum can be computed accurately

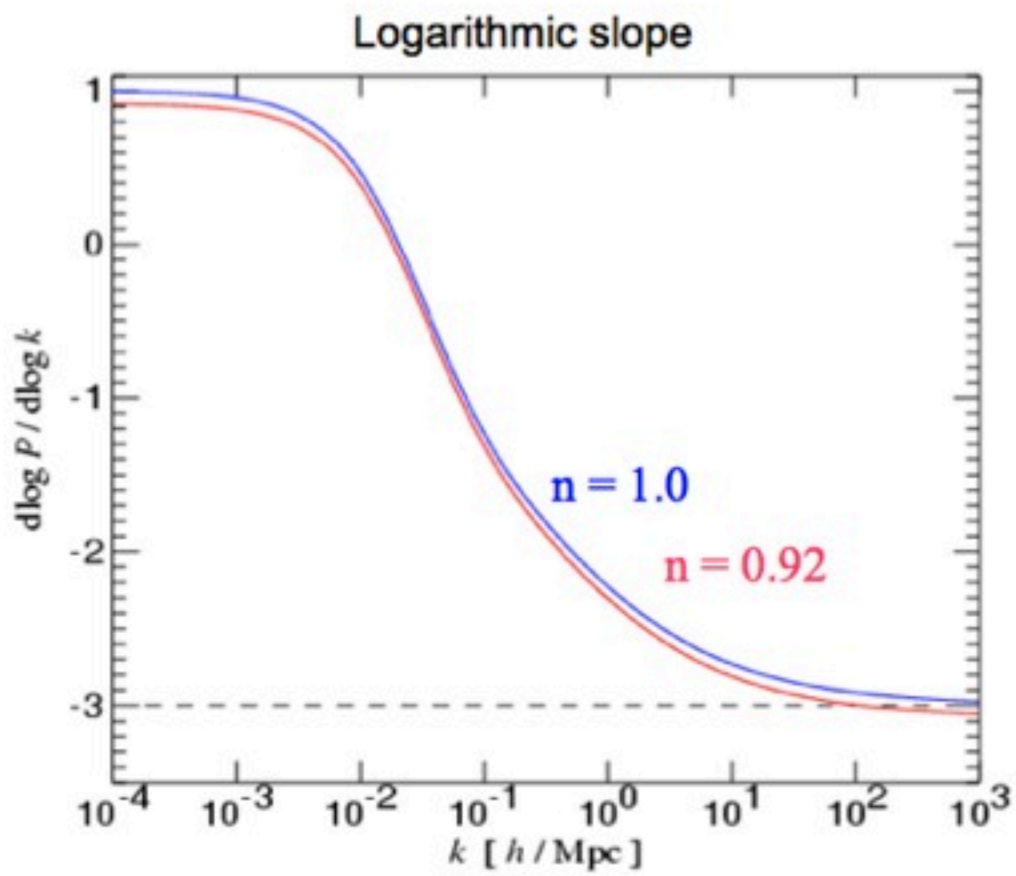
THE APPROXIMATE SHAPE OF THE LINEAR POWER SPECTRUM

$$P(k) = A \frac{k^n}{\{1 + [ak/\Gamma + (bk/\Gamma)^{3/2} + (ck/\Gamma)^2]^\nu\}^{1/\nu}}$$

Standard LCDM:

$$\begin{aligned} n &= 1.0 \\ \Gamma &= 0.21 \\ a &= 6.4\ h^{-1}\mathrm{Mpc} \\ b &= 3.0\ h^{-1}\mathrm{Mpc} \\ c &= 1.7\ h^{-1}\mathrm{Mpc} \\ \nu &= 1.13 \end{aligned}$$



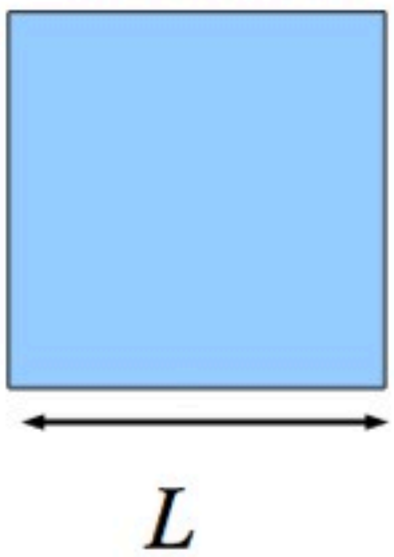


One usually assigns random amplitudes and phases for individual modes in Fourier space

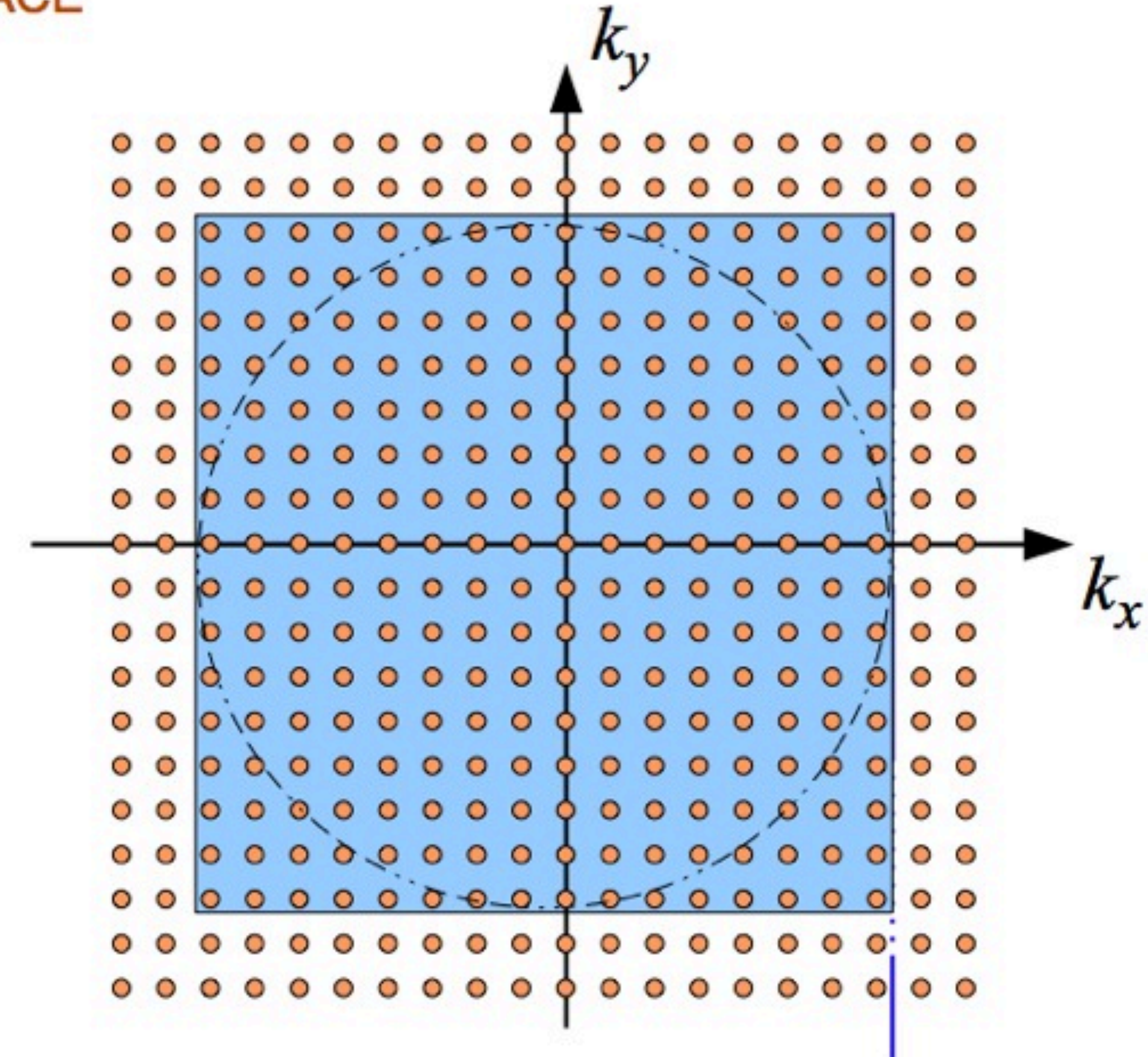
GENERATING THE FLUCTUATIONS IN K-SPACE

Hanning Filter:avoid anisotropic long waves

Simulation box



sampled with N^2 points



$$k_{\mathrm{Nyquist}} = \frac{2\pi}{L}\,\frac{N}{2}$$

$$\delta_{\mathbf{k}} = B_{\mathbf{k}} \exp^{\mathrm{i}\,\phi_{\mathbf{k}}}$$

For each mode, draw a random phase, and an amplitude from a Rayleigh distribution.

$$\left\langle \delta_{\mathbf{k}}^2 \right\rangle = P(k)$$

or equivalently filter white noise (phases) with $\sqrt{P_k}$

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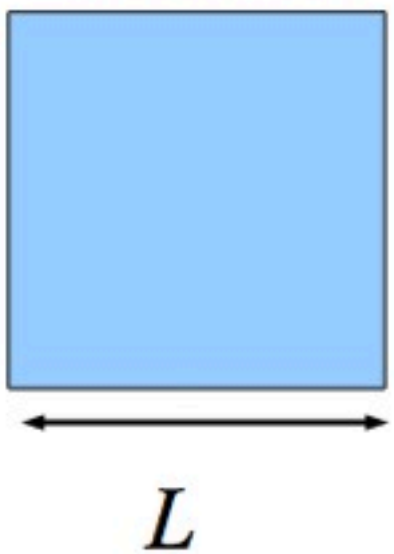

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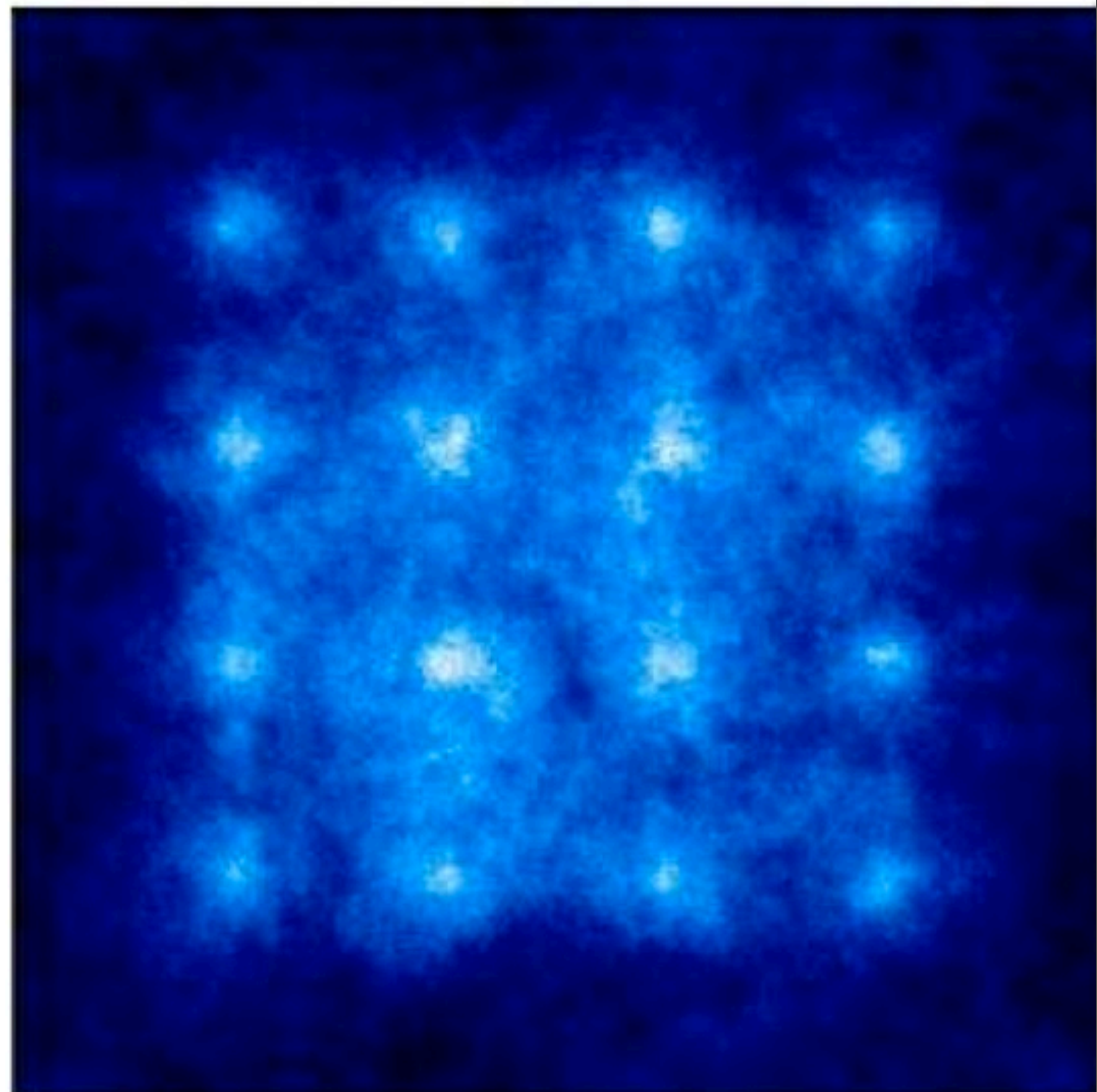

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Initial conditions for LSS

Using the Zeldovich approximation, the density fluctuations are converted to displacements of the unperturbed particle load

SETTING INITIAL DISPLACEMENTS AND VELOCITIES

Zeldovich's Lagrangian version of linear theory implies:

The force field simply follows from the initial realization of density fluctuations

Particle displacements:

$$\mathbf{d} = \mathbf{x} - \mathbf{x}_0 = -\frac{\nabla \Phi}{4\pi G \bar{\rho} a^2}$$

Particle velocities:

$$\mathbf{v} = \frac{a\dot{D}}{D}\mathbf{d}$$

Note: Particles move on straight lines in the Zeldovich approximation.

Force field estimation

Force solver using Fourier analysis

Use of Fast Fourier Transform to solve for the Poisson equation

Poor's man Poisson solver:

$$\frac{\partial^2 \Phi}{\partial x^2} = \rho \qquad -k^2 \tilde{\Phi}(k) = \tilde{\rho}(k) \qquad \tilde{G}(k) = -\frac{1}{k^2}$$

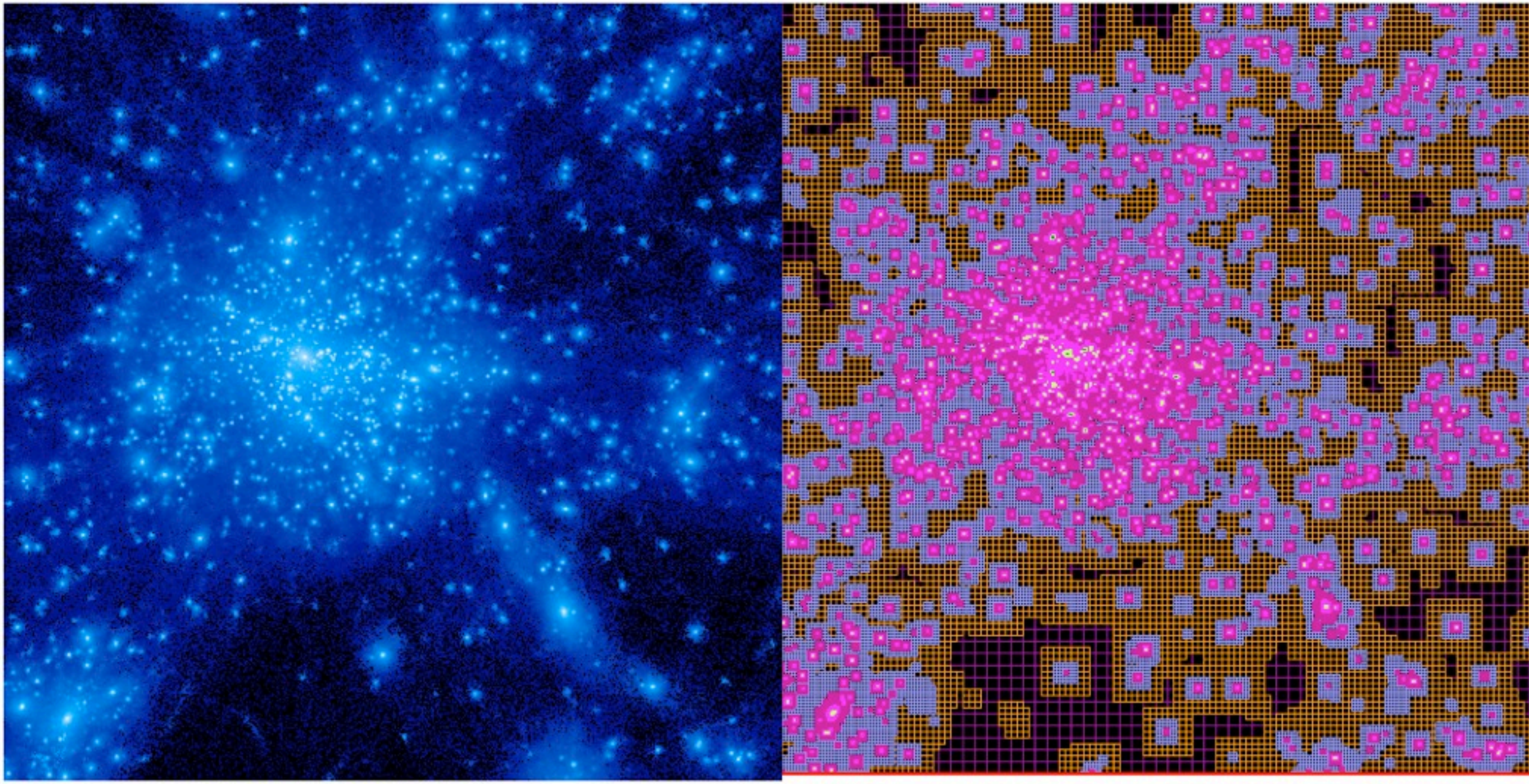
$$\frac{\partial \Phi}{\partial x} = -F \qquad -ik\tilde{\Phi}(k) = \tilde{F}(k) \qquad \tilde{D}(k) = -ik$$

Using finite difference approximations:

$$\Phi_{i+1} - 2\Phi_i + \Phi_{i-1} = \rho_i \Delta_x^2 \qquad \tilde{G}(k) = -\frac{\Delta x^2/4}{\sin(\frac{k\Delta x}{2})^2}$$

$$-(\Phi_{i+1} - \Phi_{i-1}) = F_i \Delta_x \qquad \tilde{D}(k) = -i\frac{\sin(k\Delta x)}{\Delta x}$$

Adaptive Mesh Refinement



Cosmology with AMR

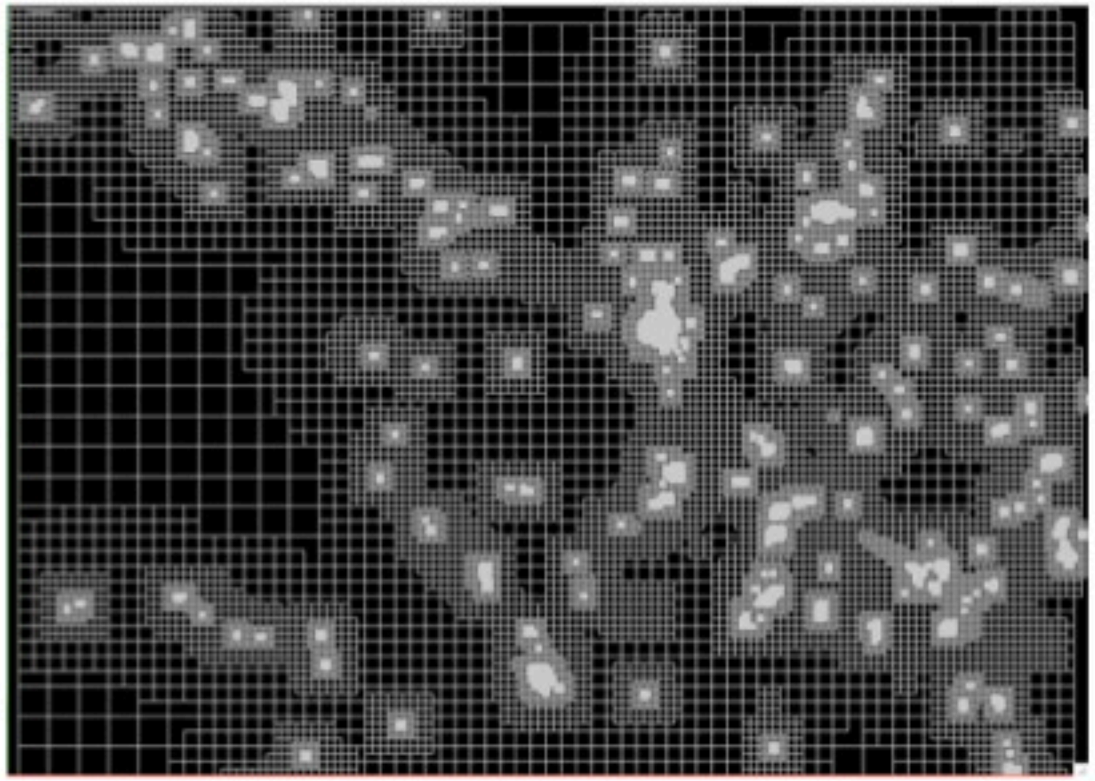
Particle-Mesh on AMR grids:
Cloud size equal to the local mesh spacing

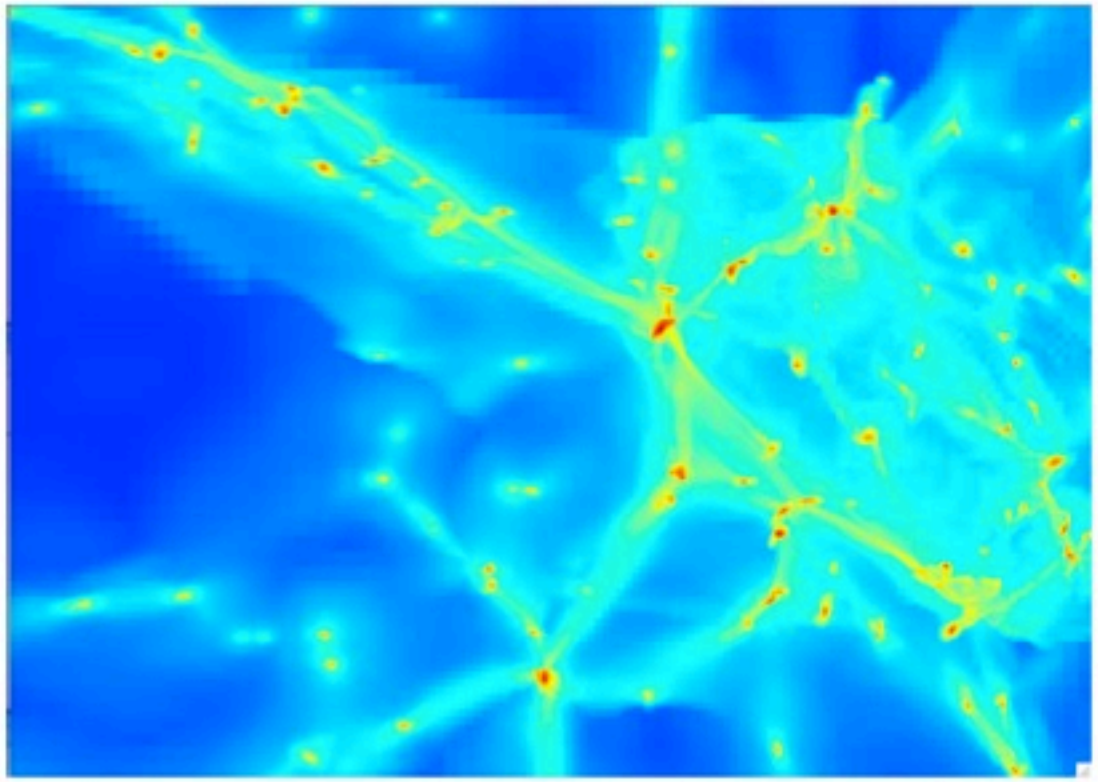
Poisson solver on the AMR grid
Multigrid or Conjugate Gradient
Interpolation to get Dirichlet boundary conditions (one way interface)

Quasi-Lagrangian mesh evolution:
roughly constant number of particles per cell

$$n = \frac{\rho_{DM}}{m_{DM}} + \frac{\rho_{gas}}{m_{gas}} + \frac{\rho_*}{m_*}$$

Trigger new refinement when n > 10-40 particles. The fractal dimension is close to 1.5 at large scale (filaments) and is less than 1 at small scales (clumps).





Relaxation solvers for the Poisson equation

Solve the linear system $\Delta_{ij}\Phi_j = \rho_i$ with arbitrary mesh geometry.

Simplest scheme: the Jacobi method (in 2D).

$$\phi_{i,j}^{n+1} = \frac{1}{4}\left(\phi_{i+1,j}^{n} + \phi_{i-1,j}^{n} + \phi_{i,j+1}^{n} + \phi_{i,j-1}^{n}\right) - \frac{1}{4}\rho_{i,j}$$

Converge very slowly for long wavelength and large grids.

Very sensitive to the initial guess.

Faster convergence is obtained for Gauss-Seidel "over-relaxation" method with red-black ordering.

$$\phi_{i,j}^{n+1} = \omega\phi_{i,j}^{n} + (1-\omega)\phi_{i,j}^{n+1} \quad \text{with} \quad 1 < \omega < 2$$

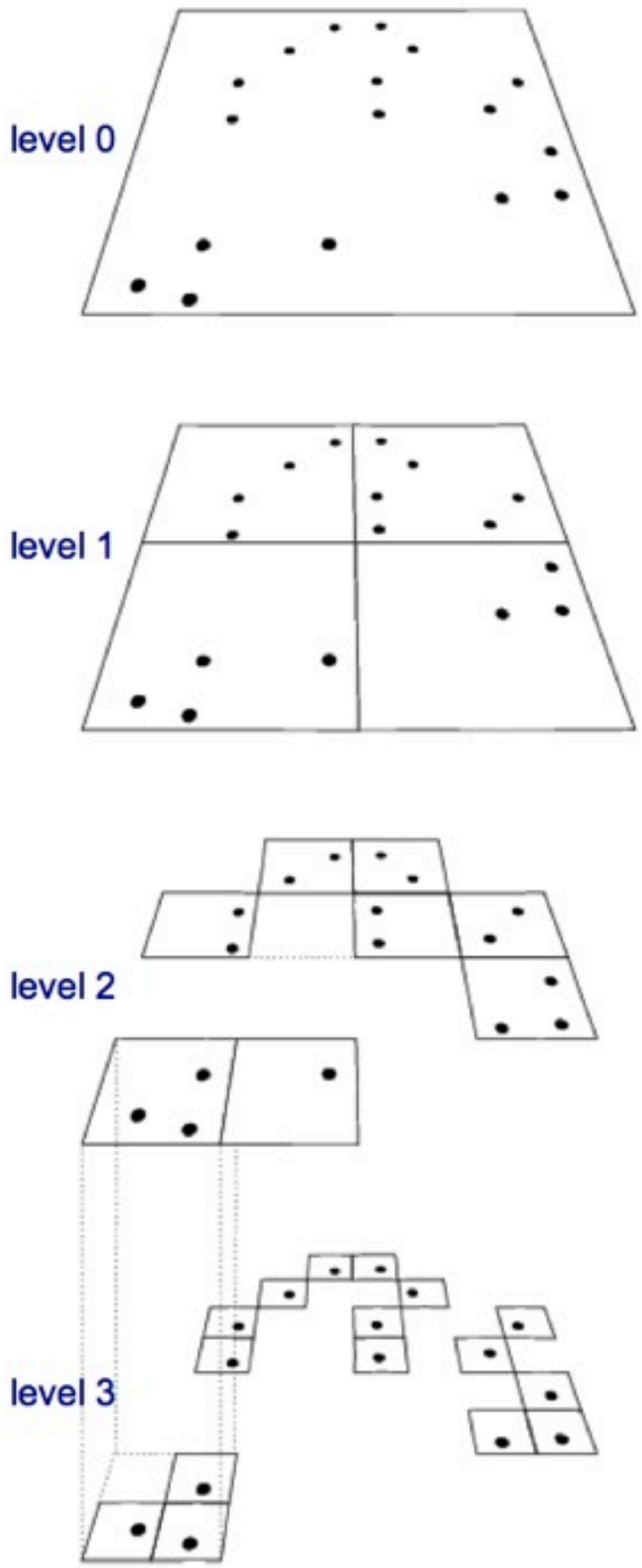
Fastest convergence for $\omega \simeq \dfrac{2}{1+\alpha\frac{\pi}{N}}$

Similar performance with the Conjugate Gradient method. For a NxN grid: exact convergence in N^2 iterations,

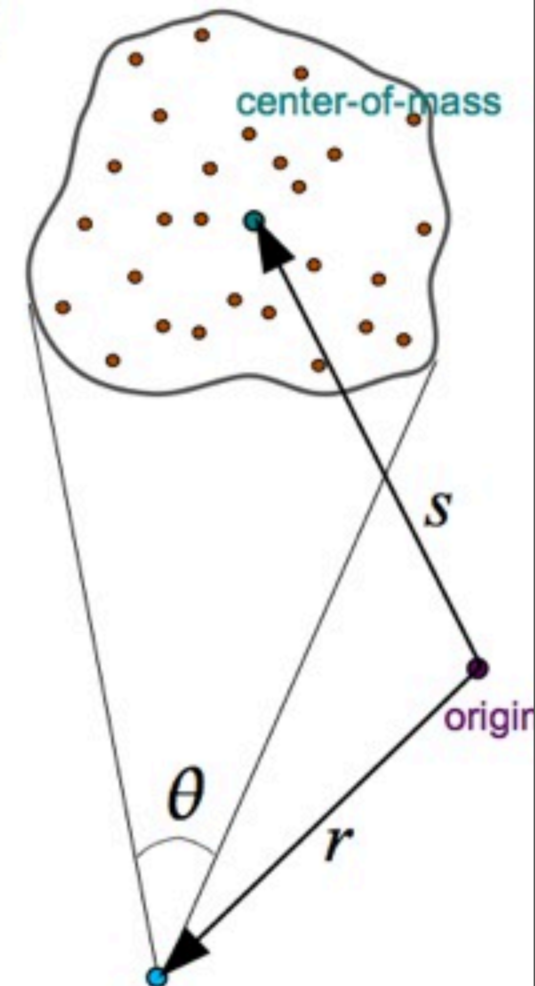
In practice, order N iterations are necessary to reach the level of truncation errors.

Tree algorithms

Oct-tree in two dimensions



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



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

We expand:

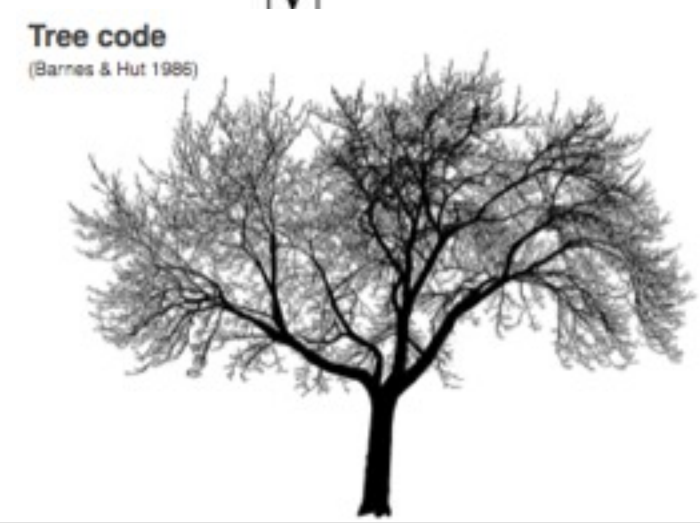
$$\frac{1}{|\mathbf{r} - \mathbf{x}_i|} = \frac{1}{|(\mathbf{r} - \mathbf{s}) - (\mathbf{x}_i - \mathbf{s})|}$$

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

and obtain:

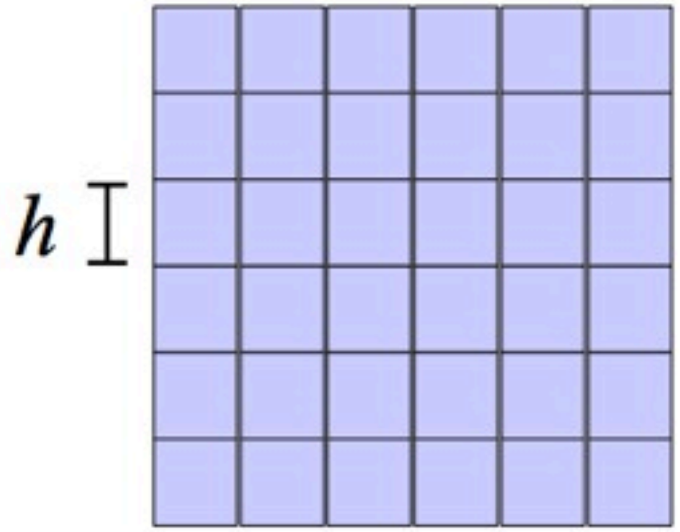
$$\frac{1}{|\mathbf{y} + \mathbf{s} - \mathbf{x}_i|} = \frac{1}{|\mathbf{y}|} - \frac{\mathbf{y} \cdot (\mathbf{s} - \mathbf{x}_i)}{|\mathbf{y}|^3} + \frac{1}{2} \frac{\mathbf{y}^T \left[3(\mathbf{s} - \mathbf{x}_i)(\mathbf{s} - \mathbf{x}_i)^T - \mathbf{I}(\mathbf{s} - \mathbf{x}_i)^2\right] \mathbf{y}}{|\mathbf{y}|^5}$$

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



Volker Springel

Density assignment



$\{\mathbf{x}_m\}$ set of discrete mesh centres

Give particles a "shape" S(x). Then to each mesh cell, we assign the fraction of mass that falls into this cell. The overlap for a cell is given by:

$$W(\mathbf{x_m} - \mathbf{x}_i) = \int_{\mathbf{x_m}-\frac{h}{2}}^{\mathbf{x_m}+\frac{h}{2}} S(\mathbf{x}' - \mathbf{x}_i)\,\mathrm{d}\mathbf{x}' = \int \Pi\left(\frac{\mathbf{x}' - \mathbf{x_m}}{h}\right) S(\mathbf{x}' - \mathbf{x}_i)\,\mathrm{d}\mathbf{x}'$$

The assignment function is hence the convolution:

$$W(\mathbf{x}) = \Pi\left(\frac{\mathbf{x}}{h}\right) \star S(\mathbf{x})$$

where

$$\Pi(x) = \begin{cases} 1 & \text{for } |x| \leq \frac{1}{2} \\ 0 & \text{otherwise} \end{cases}$$

The density on the mesh is then a sum over the contributions of each particle as given by the assignment function:

$$\rho(\mathbf{x_m}) = \frac{1}{h^3} \sum_{i=1}^{N} m_i\, W(\mathbf{x}_i - \mathbf{x_m})$$

Commenly used particle shape functions and assignment schemes

Name	Shape function S(x)	# of cells involved	Properties of forc
NGP Nearest grid point	$\delta(\mathbf{x})$	$1^3 = 1$	piecewise constant in cells
CIC Clouds in cells	$\frac{1}{h^3}\Pi\left(\frac{\mathbf{x}}{h}\right) \star \delta(\mathbf{x})$	$2^3 = 8$	piecewise linear, continuous
TSC Triangular shaped clouds	$\frac{1}{h^3}\Pi\left(\frac{\mathbf{x}}{h}\right) \star \frac{1}{h^3}\Pi\left(\frac{\mathbf{x}}{h}\right)$	$3^3 = 27$	continuous first derivative

Note: For interpolation of the grid to obtain the forces, the same assignment function needs to be used to ensure momentum conservation. (In the CIC case, this is identical to tri-linear interpolation.)

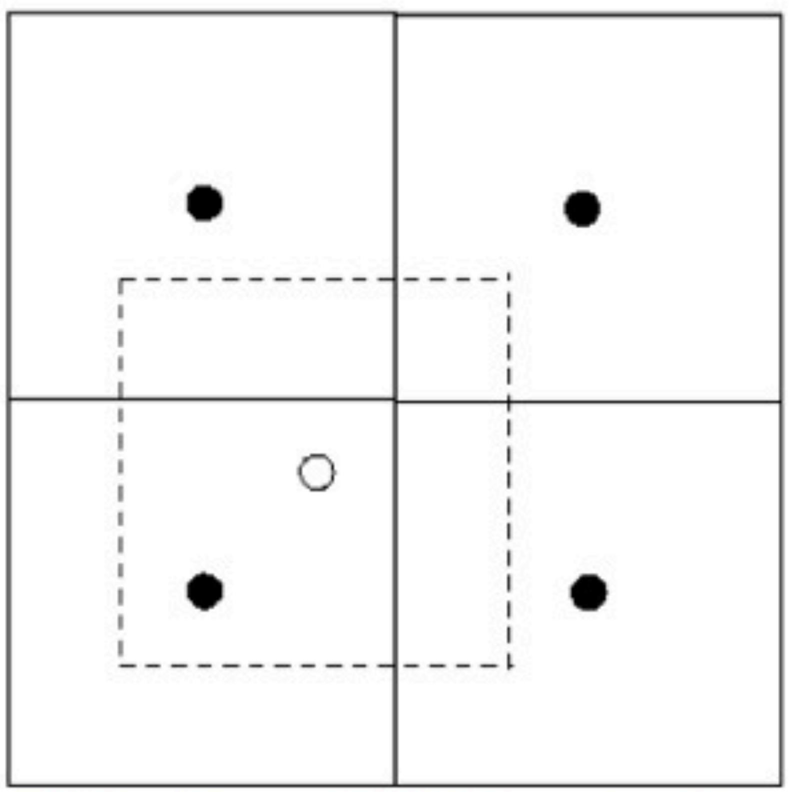
Force interpolation schemes

Use another interpolation scheme to get the mesh force at particle positions.

$$F(x_p) = m_p \sum W^F(x_p - x_i) F_i$$

Momentum conservation is enforced if:

- 2 interacting particles see equal but opposite forces
- no self-forces



"Cloud-In-Cell" interpolation

Poisson equation $\Delta_{ij}\Phi_j = \rho_i$

Gradient of the potential $F_i = -\nabla_{ij}\Phi_j$

Self-force for particle p: $\partial F(x_p) =$

$$-m_p^2 \sum_i \sum_j W^F(x_p - x_i) \left(\nabla.\Delta^{-1}\right)_{ij} W^\rho(x_p - x_j)$$

Self-force is zero if operator is antisymmetric and force and mass assignment schemes are equal.

Symplectic Time Integrator

Phase space: $q = \mathbf{x}_p \quad p = \mathbf{v}_p$ $\qquad \dot{q} = p$

Hamiltonian: $\mathcal{H}(q,p) = p^2/2 + \Phi(q)$ $\qquad \dot{p} = -\frac{\partial \Phi}{\partial q}$

The exact solution of an Hamiltonian system is energy-conserving and volume-preserving in phase-space (incompressible fluid in phase space).

The energy and the volume in phase-space are time-invariants.

$$\mathbf{z} = (q,p) \qquad \mathbf{f}(\mathbf{z}) = (p, -\partial\Phi/\partial q) \qquad \dot{\mathbf{z}} = \mathbf{f}(\mathbf{z})$$

Show that $\nabla \cdot \mathbf{f} = 0$ and $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H} = 0$

Using Reynold's transport theorem in phase-space, show that the time derivative of any Lagrangian volume in phase-space is zero.

Classical First Order Time Integrators

For a symplectic map $\mathbf{z}(t) = \mathcal{F}(\mathbf{z}_0)$

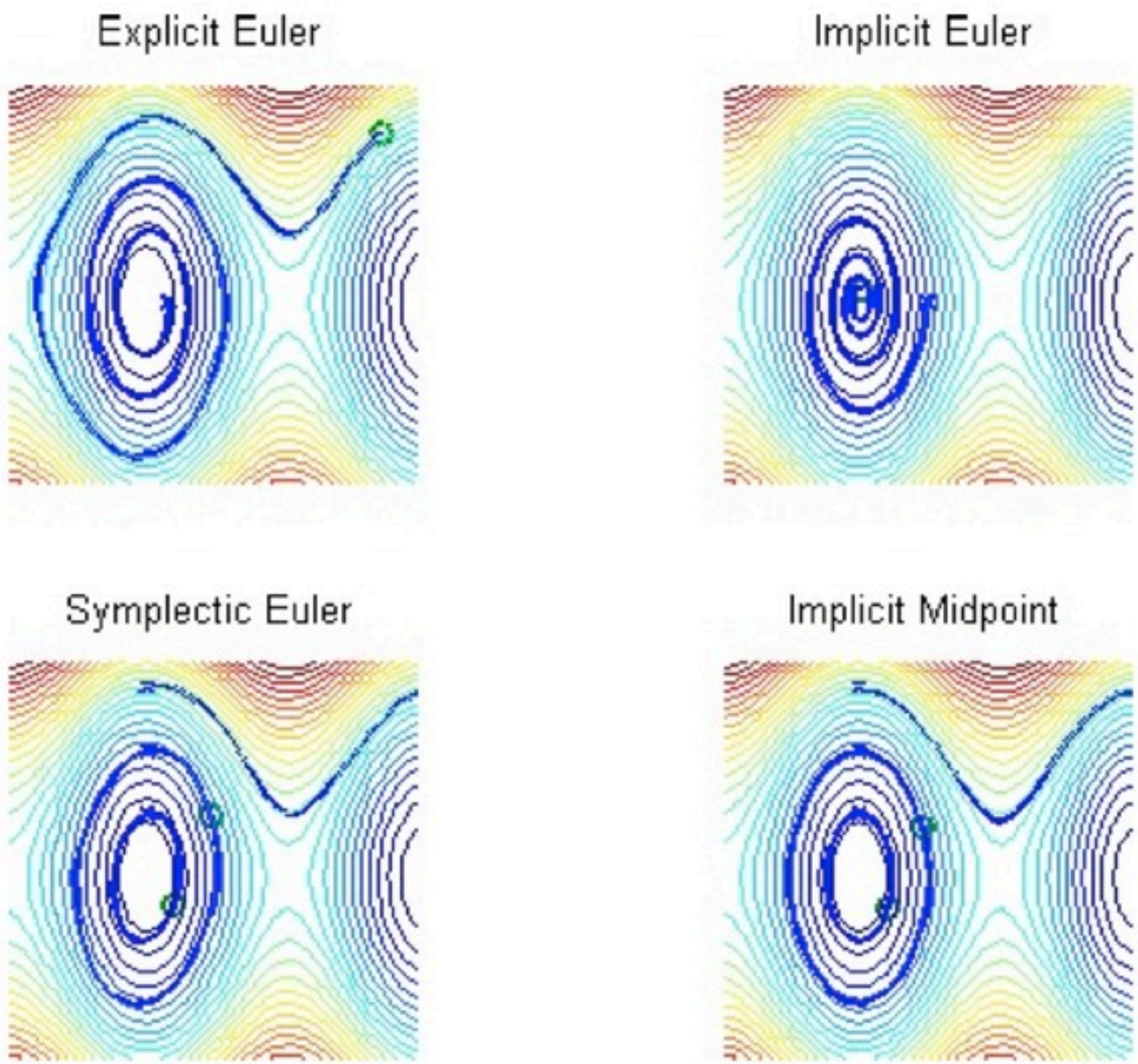
the volume in phase-space is preserved if $\det \frac{\partial \mathcal{F}}{\partial \mathbf{z}} = 1$

- Explicit Euler: $\mathbf{z}^{n+1} = \mathbf{z}^n + \Delta t \mathbf{f}(\mathbf{z}^n)$ $\quad \det \frac{\partial \mathcal{F}}{\partial \mathbf{z}} = 1 + \Delta t^2 \frac{\partial^2 \Phi}{\partial q^2}$

- Implicit Euler: $\mathbf{z}^{n+1} = \mathbf{z}^n + \Delta t \mathbf{f}(\mathbf{z}^{n+1})$ $\quad \det \frac{\partial \mathcal{F}}{\partial \mathbf{z}} = \frac{1}{1 + \Delta t^2 \frac{\partial^2 \Phi}{\partial q^2}}$

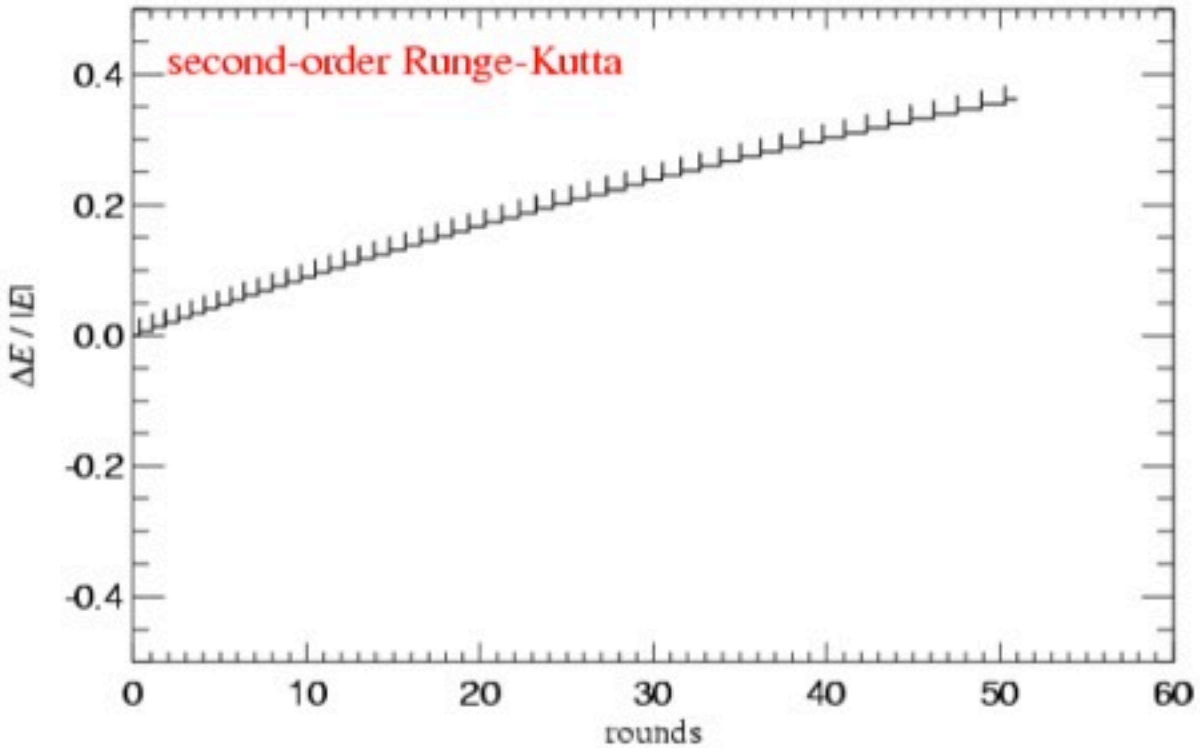
- Symplectic Euler: $\mathbf{z}^{n+1} = \mathbf{z}^n + \Delta t \mathbf{f}(q^n, p^{n+1})$ $\quad \det \frac{\partial \mathcal{F}}{\partial \mathbf{z}} = 1$

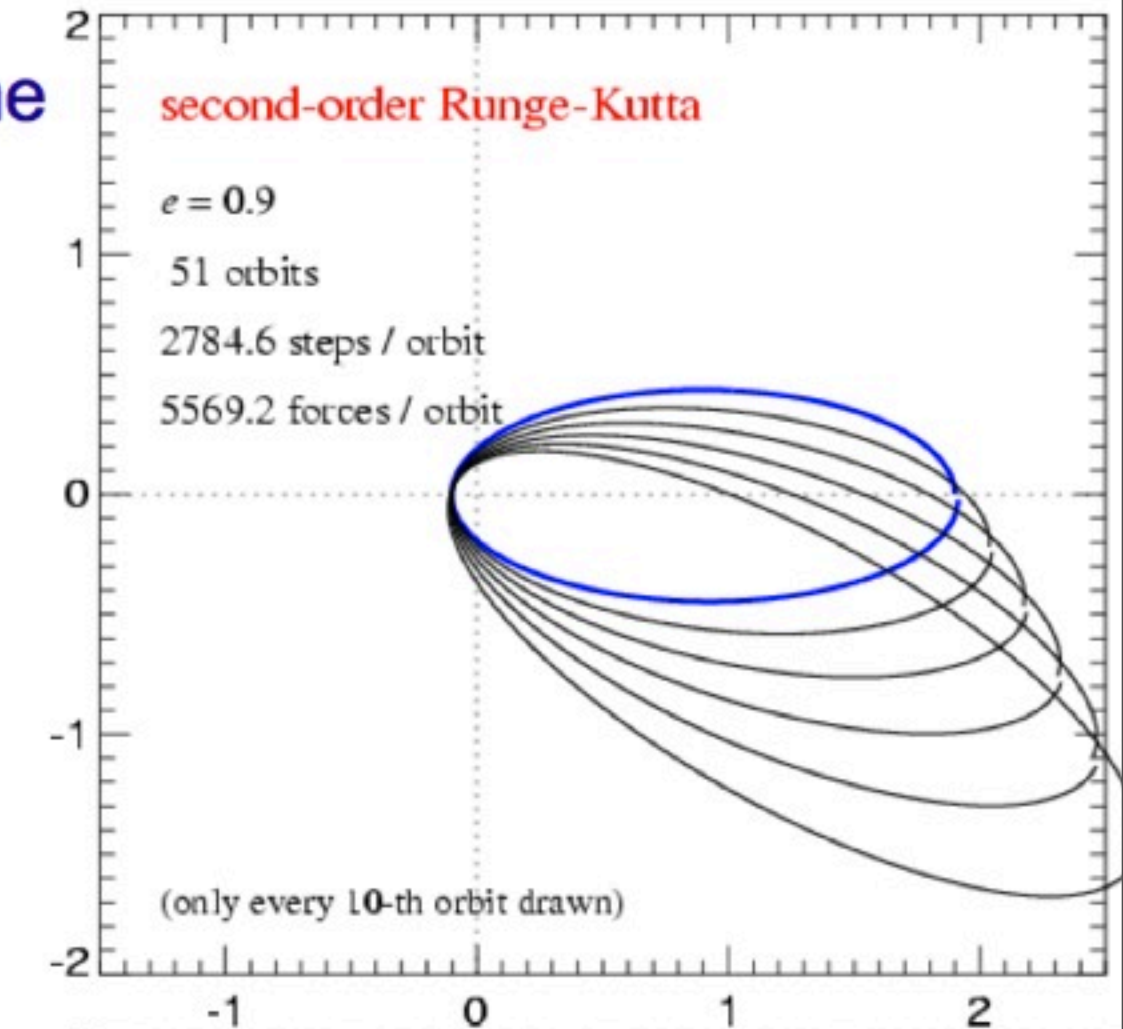
Why use a symplectic integrator ?

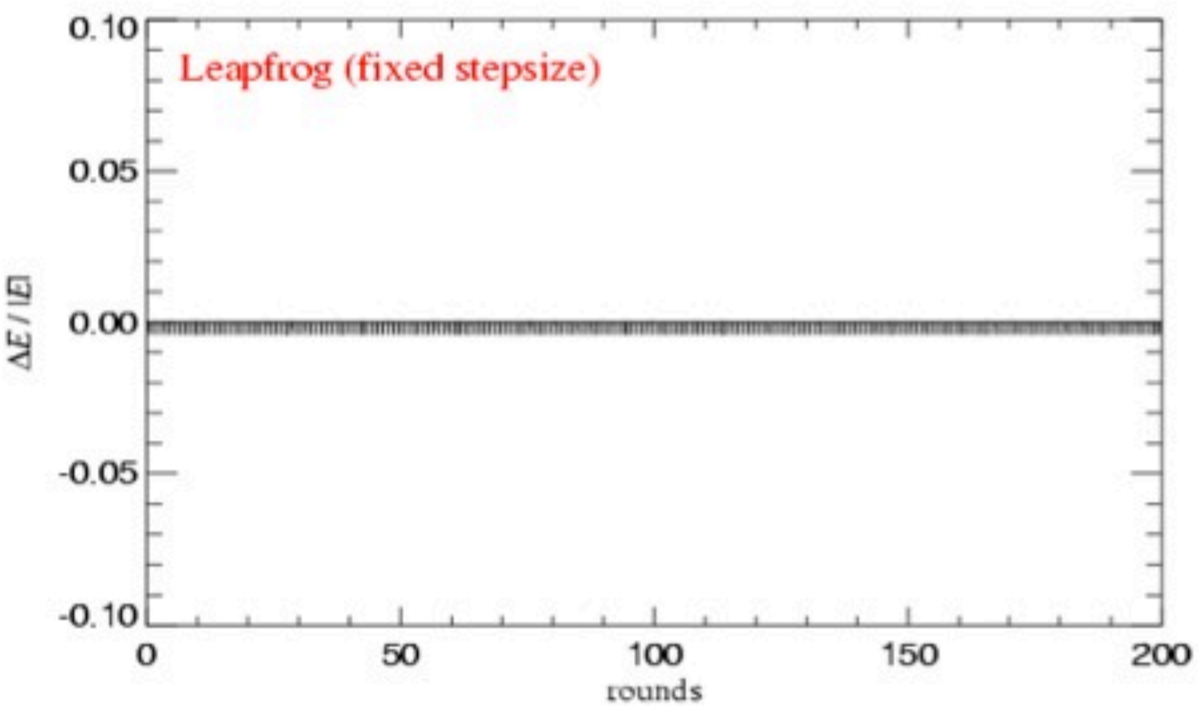


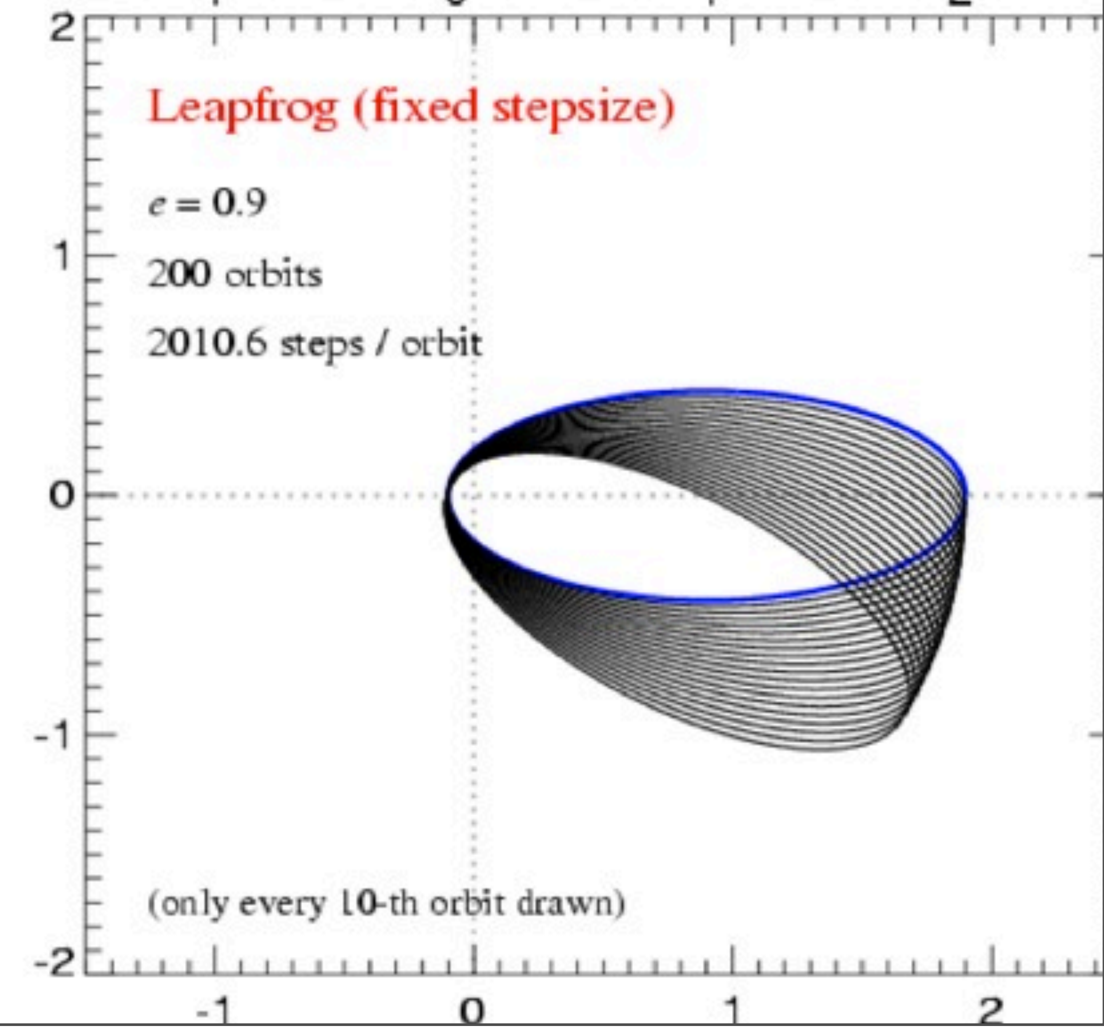
When compared with an integrator of the same order, the leapfrog is highly superior

INTEGRATING THE KEPLER PROBLEM

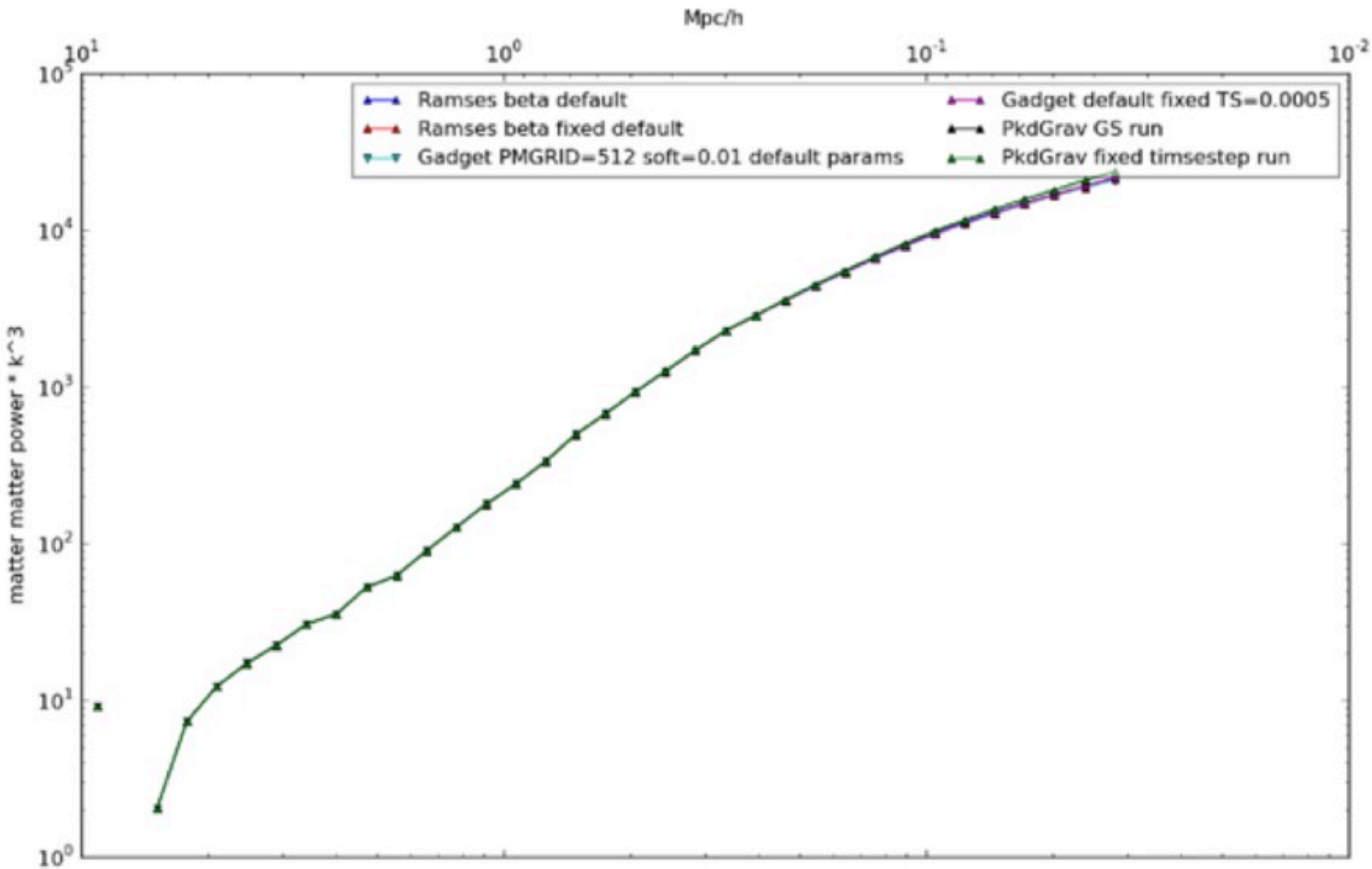






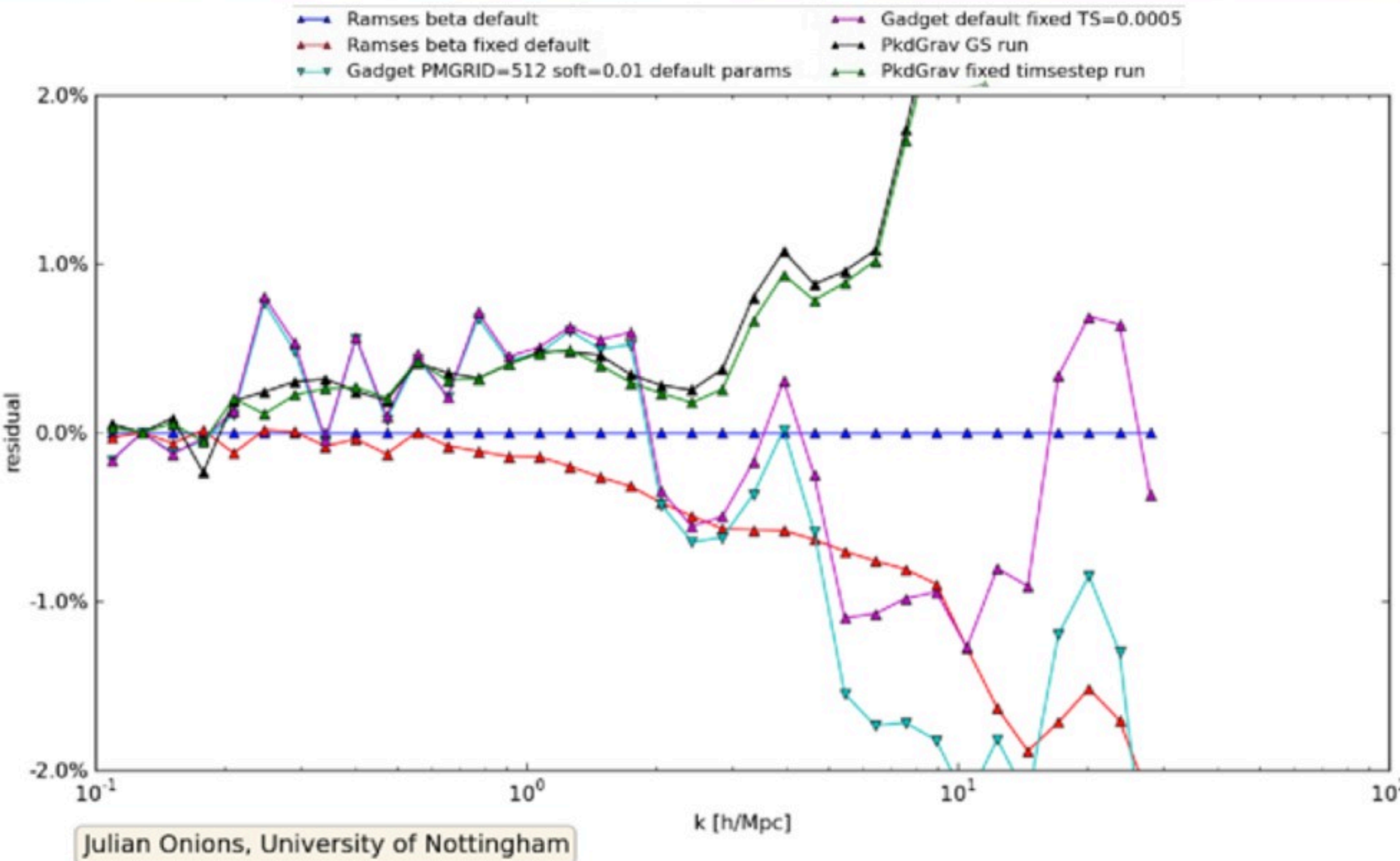


Precision computational cosmology



Cosmological Simulation Working Group (Euclid Consortium)

Precision computational cosmology



Cosmological Simulation Working Group (Euclid Consortium)

Baryons

- Multi-scale, multi timescale **hydro-dynamics**
- Optimal discretization of partial differential equations
  - *SPH & finite volume methods*
  - *Shock preserving algorithms*
- Subgrid physics: effective laws for unresolved scales
- Subgrid physics: effective laws for unresolved processes:

star formation,dust, magnetic fields, AGN, cosmic rays...

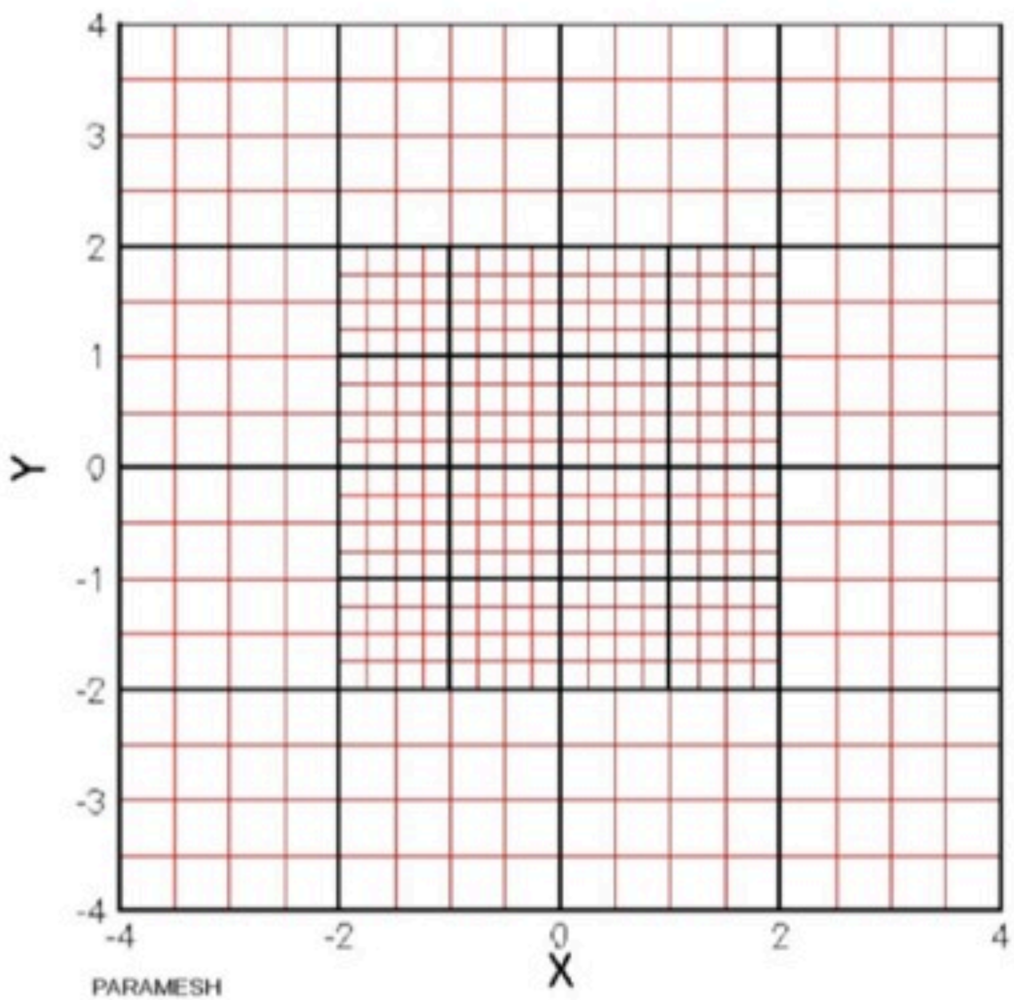
Numerical methods to discretize a fluid

Eulerian:

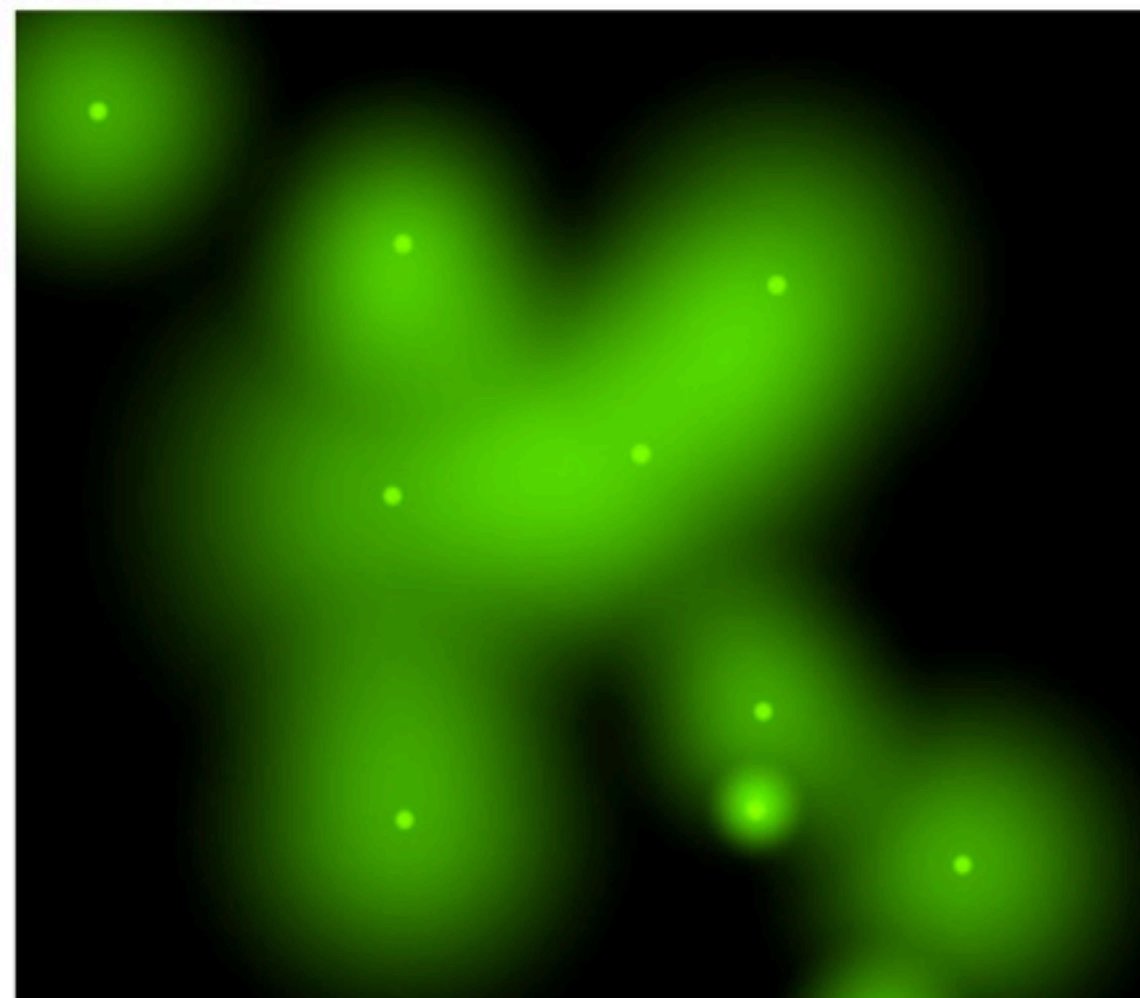
- discretization of *space*
- AMR
  (Adaptive Mesh Refinement)

Lagrangian:

- discretization of *mass*
- SPH
  (Smoothed Particle Hydrodynamics



grid refine if necessary

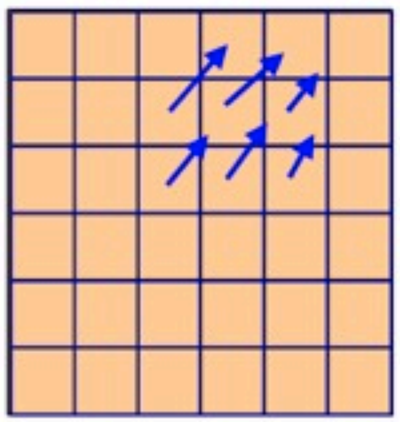


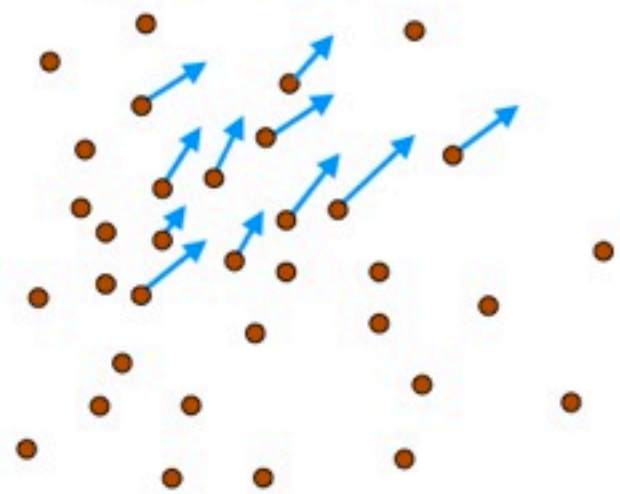
volume of sphere decreases if necessary

What is smoothed particle hydrodynamics?

DIFFERENT METHODS TO DISCRETIZE A FLUID

Eulerian	Lagrangian
discretize space	**discretize mass**
representation on a mesh (volume elements)	representation by fluid elements (particles)





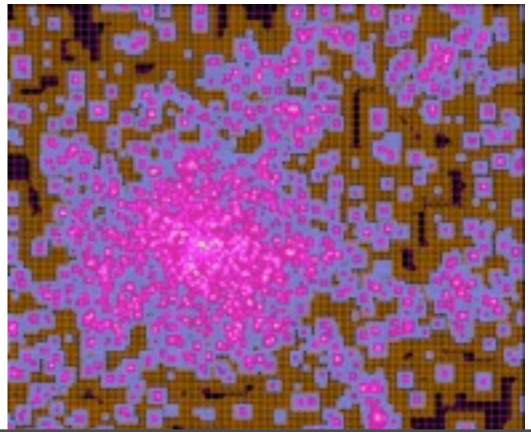
principle advantage:

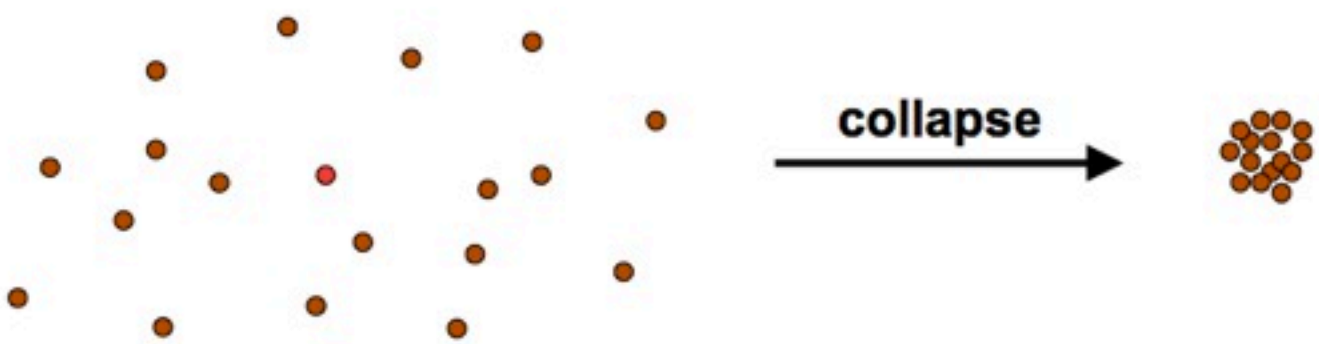
high accuracy (shock capturing), low numerical viscosity

principle advantage:

resolutions adjusts automatically to the flow

Quantifiable error budget





What is smoothed particle hydrodynamics?

BASIC EQUATIONS OF SMOOTHED PARTICLE HYDRODYNAMICS

Each particle carries either the energy or the entropy per unit mass as independent variable

Density estimate $\rho_i = \sum_{j=1}^{N} m_j W(|\mathbf{r}_{ij}|, h_i)$ → **Continuity equation automatically fulfilled.**

→ $P_i = (\gamma - 1)\rho_i u_i$

Euler equation

$$\frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = -\sum_{j=1}^{N} m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} + \Pi_{ij} \right) \nabla_i \overline{W}_{ij}$$

(Artificial viscosity: $+\Pi_{ij}$)

First law of thermodynamics

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = \frac{1}{2}\sum_{j=1}^{N} m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} + \Pi_{ij} \right) \mathbf{v}_{ij} \cdot \nabla_i \overline{W}_{ij}$$

The isothermal Euler equations

Unlike dark matter, perfect fluid **cannot** shell cross

$$\partial_t f_{\rm col} \neq 0$$

contact/rarefaction/shock waves are created

Let's look at a 1D toy model of 2 cells

Primitive form with primitive variables $\mathbf{W} = (\rho, u)$

$$\partial_t \rho + u \partial_x \rho + \rho \partial_x u = 0$$

$$\partial_t u + u \partial_x u + \frac{a^2}{\rho} \partial_x \rho = 0$$

a is the isothermal sound speed

The isothermal wave equation

We linearize the isothermal Euler equation around some equilibrium state.

$$\mathbf{W} = \mathbf{W_0} + \Delta\mathbf{W}$$

Using the system in primitive form, we get the ***linear*** system:

$$\partial_t \Delta\mathbf{W} + \mathbf{A_0}\partial_x \Delta\mathbf{W} = 0$$

where the constant matrix has 2 real eigenvalues and 2 eigenvectors

$$\mathbf{A_0} = \begin{Bmatrix} u & \rho \\ \frac{a^2}{\rho} & u \end{Bmatrix} \qquad \begin{aligned} \lambda^+ &= u + a \\ \lambda^- &= u - a \end{aligned} \qquad \begin{aligned} \Delta\alpha^+ &= \frac{1}{2}\left(\Delta\rho + \rho\frac{\Delta u}{a}\right) \\ \Delta\alpha^- &= \frac{1}{2}\left(\Delta\rho - \rho\frac{\Delta u}{a}\right) \end{aligned}$$

The previous system is equivalent to 2 independent *scalar linear* PDEs.

$$\partial_t \Delta\alpha^+ + (u + a)\partial_x \Delta\alpha^+ = 0$$

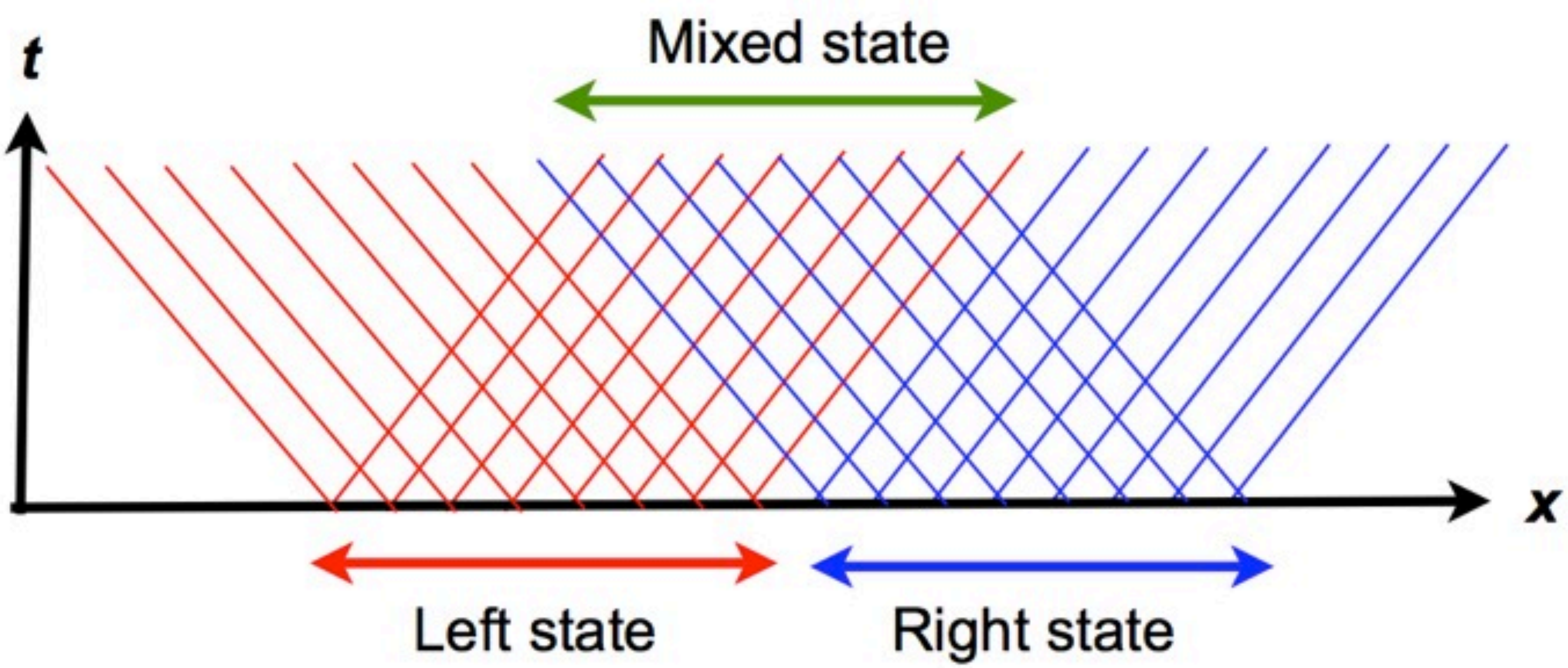
$$\partial_t \Delta\alpha^- + (u - a)\partial_x \Delta\alpha^- = 0$$

$\Delta\alpha^+$ ($\Delta\alpha^-$) is a Riemann invariant along characteristic curves moving with velocity $u + a$ $(u - a)$

Riemann problem for isothermal waves

finite volume scheme = field variables are constant/cell

Initial conditions are defined by 2 semi-infinite regions with pieceweise constant initial states $(\Delta\rho_R, \Delta u_R)$ and $(\Delta\rho_L, \Delta u_L)$



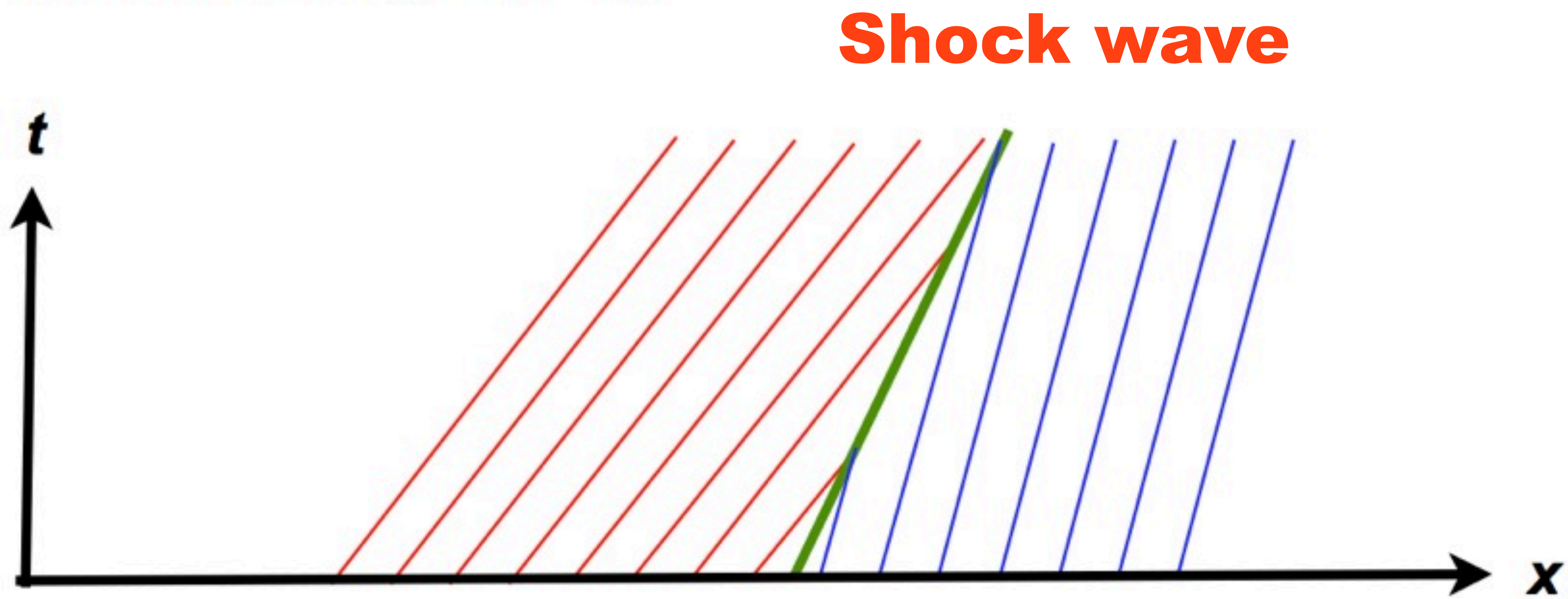
"Star" state is obtained using the 2 Riemann invariants.

$$u - a < \frac{x}{t} < u + a$$

$$\Delta\rho^* = \Delta\alpha_L^+ + \Delta\alpha_R^-$$

$$\Delta u^* = \frac{a}{\rho}(\Delta\alpha_L^+ - \Delta\alpha_R^-)$$

Initial conditions are defined by 2 semi-infinite regions with pieceweise constant initial states u_R and u_L.

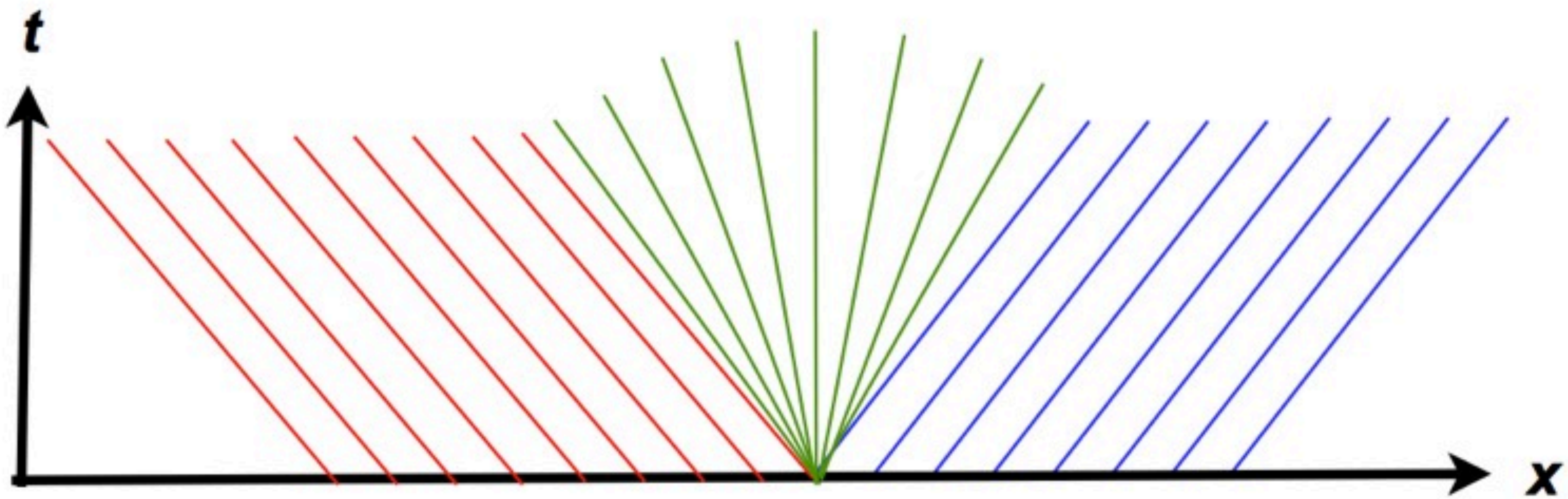


Case 1: $u_L > u_R$

Formation of a shock with velocity $S = \dfrac{u_L + u_R}{2}$

Solution: If $x < St$ then $u(x,t) = u_L$ else $u(x,t) = u_R$

Rarefaction wave



Case 2: $u_L < u_R$

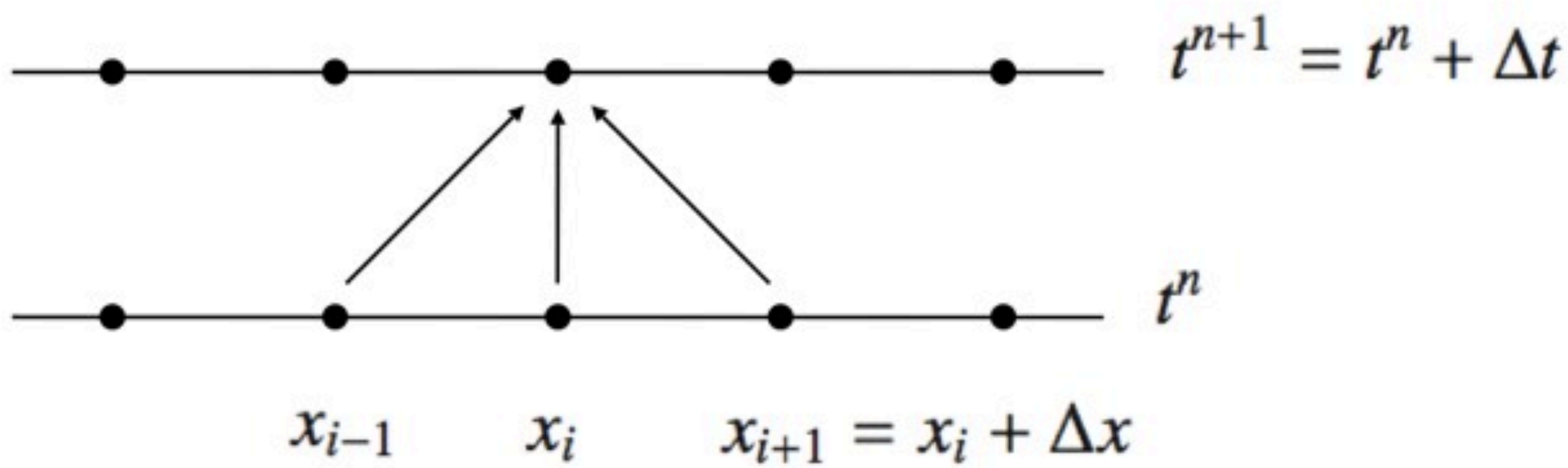
Characteristics are diverging: a rarefaction wave fills the gap.

Solution: If $x < u_L t$ then $u(x,t) = u_L$

If $u_L t < x < u_R t$ then $u(x,t) = \dfrac{x}{t}$

If $x > u_R t$ then $u(x,t) = u_R$

Finite difference scheme



$$u_i^n = u(x_i, t^n) \qquad \partial_x u \simeq \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} \qquad \partial_t u \simeq \frac{u_i^{n+1} - u_i^n}{\Delta t}$$

Finite difference approximation of the advection equation

$$\partial_t u + a\partial_x u = 0 \quad \Longrightarrow \quad \frac{u_i^{n+1} - u_i^n}{\Delta t} + a\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = 0$$

The Modified Equation

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = 0$$

Taylor expansion in time up to second order

$$u_i^{n+1} = u_i^n + \Delta t\left(\frac{\partial u}{\partial t}\right) + \frac{(\Delta t)^2}{2}\left(\frac{\partial^2 u}{\partial t^2}\right)$$

Taylor expansion in space up to second order

$$u_{i+1}^n = u_i^n + \Delta x\left(\frac{\partial u}{\partial x}\right) + \frac{(\Delta x)^2}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)$$

$$u_{i-1}^n = u_i^n - \Delta x\left(\frac{\partial u}{\partial x}\right) + \frac{(\Delta x)^2}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)$$

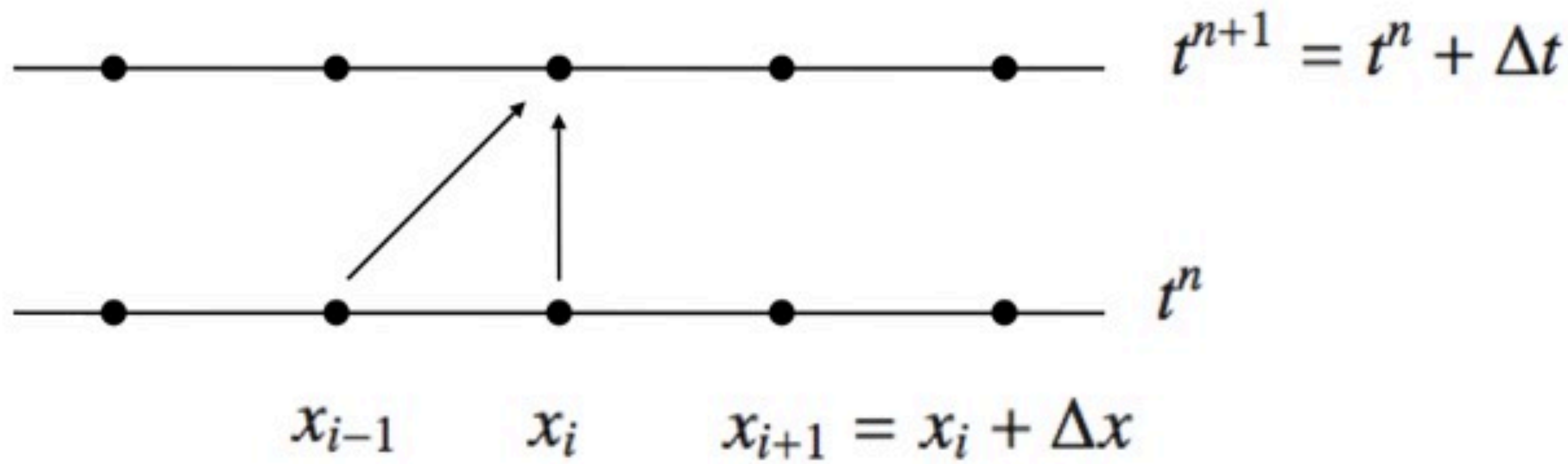
The advection equation becomes the advection-diffusion equation

$$\left(\frac{\partial u}{\partial t}\right) + a\left(\frac{\partial u}{\partial x}\right) = -\frac{\Delta t}{2}\left(\frac{\partial^2 u}{\partial t^2}\right) + O(\Delta t^2, \Delta x^2)$$

$$\left(\frac{\partial u}{\partial t}\right) + a\left(\frac{\partial u}{\partial x}\right) = -a^2\frac{\Delta t}{2}\left(\frac{\partial^2 u}{\partial x^2}\right) + O(\Delta t^2, \Delta x^2)$$

Negative diffusion coefficient: the scheme is *unconditionally unstable*

The Upwind scheme



a>0: use only upwind values, discard downwind variables

$$\partial_x u \simeq \frac{u_i^n - u_{i-1}^n}{\Delta x} \quad \Rightarrow \quad \frac{u_i^{n+1} - u_i^n}{\Delta t} + a\frac{u_i^n - u_{i-1}^n}{\Delta x} = 0$$

Taylor expansion up to second order:

$$\left(\frac{\partial u}{\partial t}\right) + a\left(\frac{\partial u}{\partial x}\right) = -\frac{\Delta t}{2}\left(\frac{\partial^2 u}{\partial t^2}\right) + a\frac{\Delta x}{2}\left(\frac{\partial^2 u}{\partial x^2}\right) + O(\Delta t^2, \Delta x^2)$$

Upwind scheme is stable if C<1, with $C = a\frac{\Delta t}{\Delta x}$

$$\left(\frac{\partial u}{\partial t}\right) + a\left(\frac{\partial u}{\partial x}\right) = a\frac{\Delta x}{2}(1 - C)\left(\frac{\partial^2 u}{\partial x^2}\right) + O(\Delta t^2, \Delta x^2)$$

The advection-diffusion equation

Finite difference approximation of the advection equation:

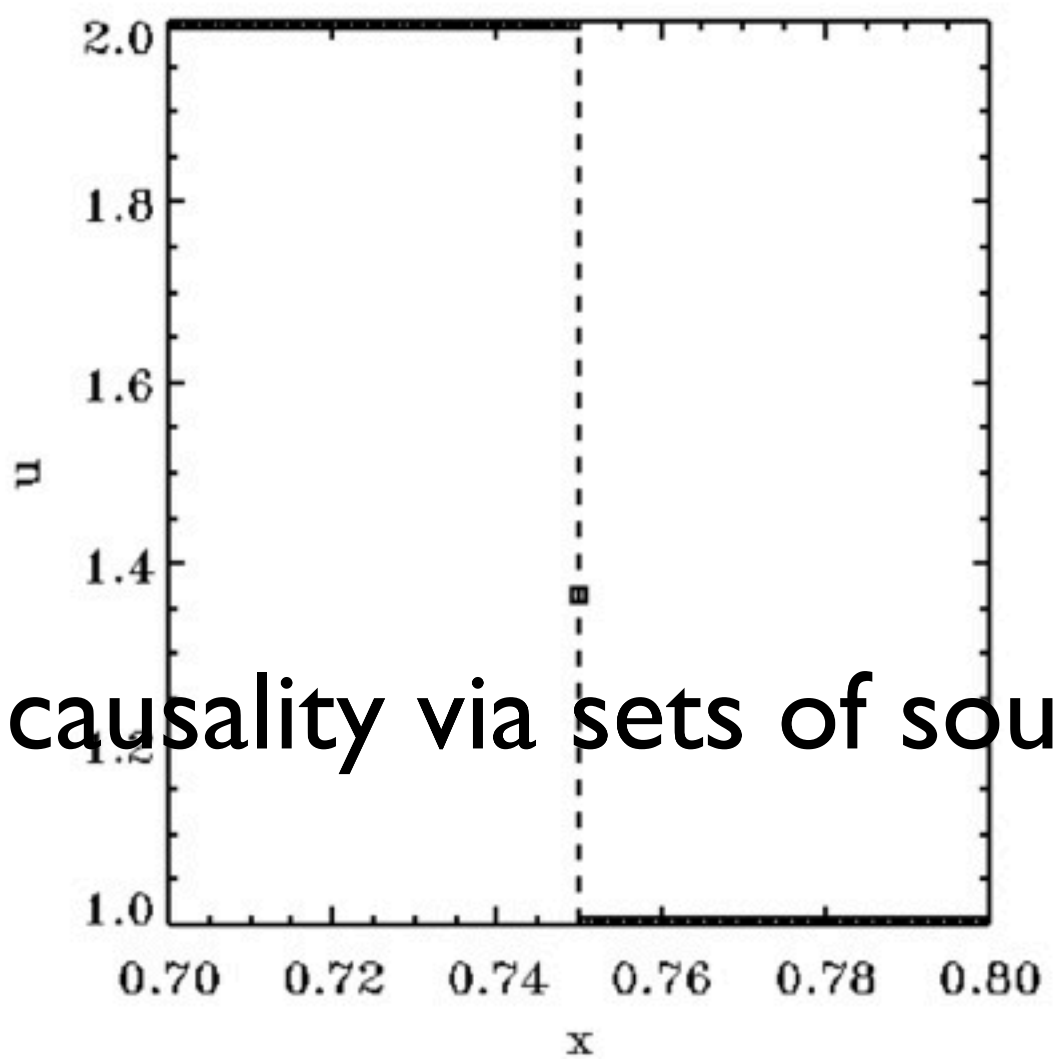
$$\left(\frac{\partial u}{\partial t}\right) + a\left(\frac{\partial u}{\partial x}\right) = \eta\left(\frac{\partial^2 u}{\partial x^2}\right)$$

Central differencing unstable: $\eta < 0$

Upwind differencing is stable: $\eta > 0$ $\quad \eta = a\frac{\Delta x}{2}(1 - C)$

Smearing of initial discontinuity:

"numerical diffusion"

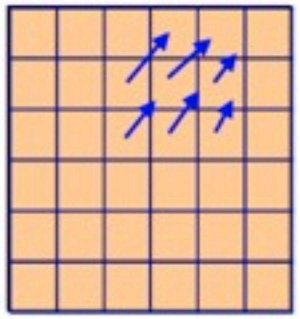


respect causality via sets of sound wave.

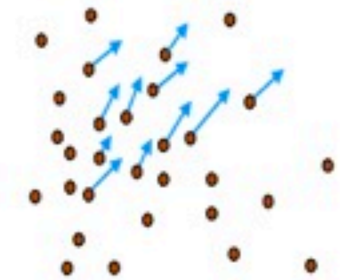
Thickness increases as $\sqrt{\eta t}$

There are principal differences between SPH and Eulerian schemes

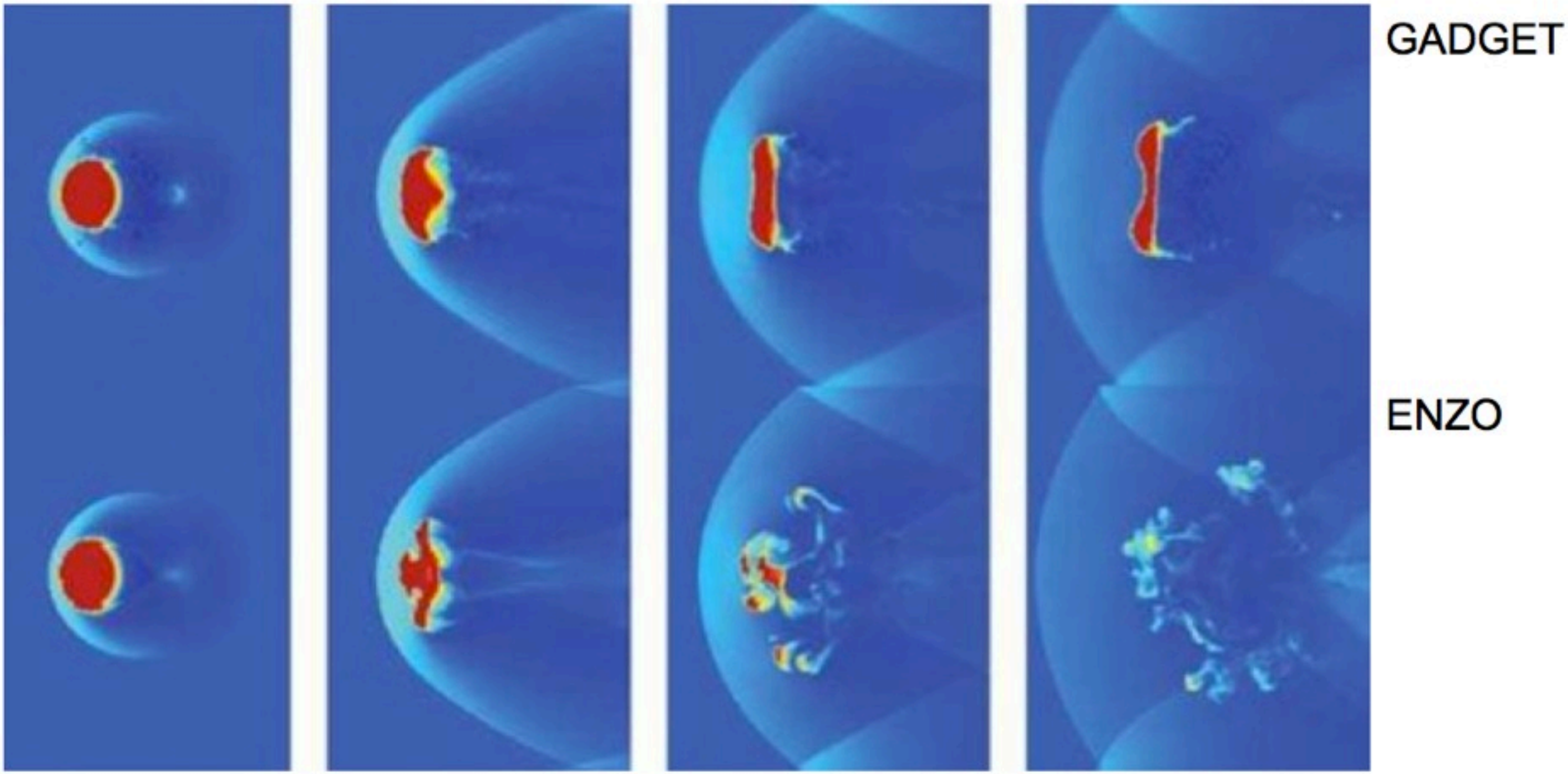
FUNDAMENTAL DIFFERENCE BETWEEN SPH AND MESH-HYDRODYNAMICS



Eulerian	Lagrangian
not Galilean invariant	**Galilean invariant**
sharp shocks and contact discontinuities (best schemes resolve fluid discontinuities it in one cell)	**shocks broadened over roughly 2-3 smoothing lengths** (post-shock properties are correct though)
mixing happens implicitly at the cell level (can providure closure for turbulence, but will also be a source of spurious mixing entropy from advection errors)	**mixing entirely suppressed at the particle-level** (no spurious entropy production, but fluid instabilities may be suppressed)
self-gravity of the gas needs to be done on a mesh (but dark matter must still be represented by particles)	**self-gravity of the gas naturally treated with the same accuracy as the dark matter**
low numerical viscosity	**requires artificial viscosity (lowers Reynolds numbers heavily)**



Galaxy formation codes: a few facts.



SPH (here GADGET2) cannot capture fluid instability correctly.

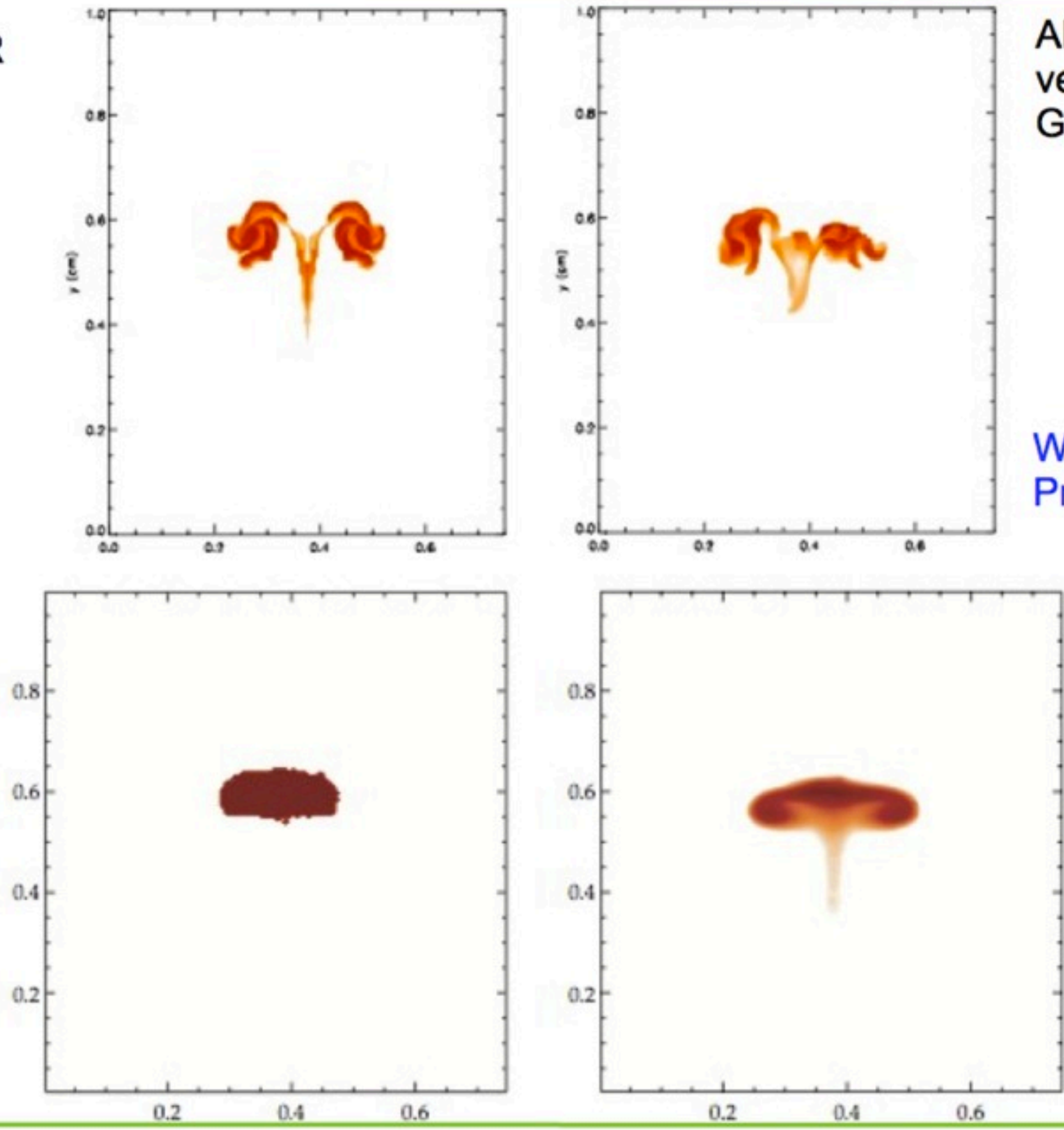
Blobs of gas survives for an artificial (infinite ?) long time to KH instability.

Agertz et al. (2007)

Galaxy formation codes: a few facts.

AMR

AMR with horizontal velocity: not strictly Galilean invariant



Wadsley et al. (2008), Price (2008)

standard SPH: strictly Galilean invariant

SPH with explicit entropy and mass diffusion

The case for grids in cosmological simulations

Dark matter dynamics modeled using the Particle Mesh technique.

- High resolution is obtained using adaptively refined grids
- Refinements triggered by the local particle density: ensures low collision rates and high resolution
- Adaptive force softening (the local mesh size) but non-uniform force (poor energy conservation at coarse-fine boundaries)
- Multigrid solver for the Poisson equation is O(N)

Fluid dynamics modeled using finite-volume schemes.

- developed decades go by an army of applied mathematicians and computational physicists
- Very good knowledge of the error budget
- Adaptive Mesh Refinement methodology for Godunov schemes invented in the late 1980's by Colella and co-workers
- High-order methods are required (at least second order)
- One looses one order of accuracy at coarse-fine boundaries

Where we are?

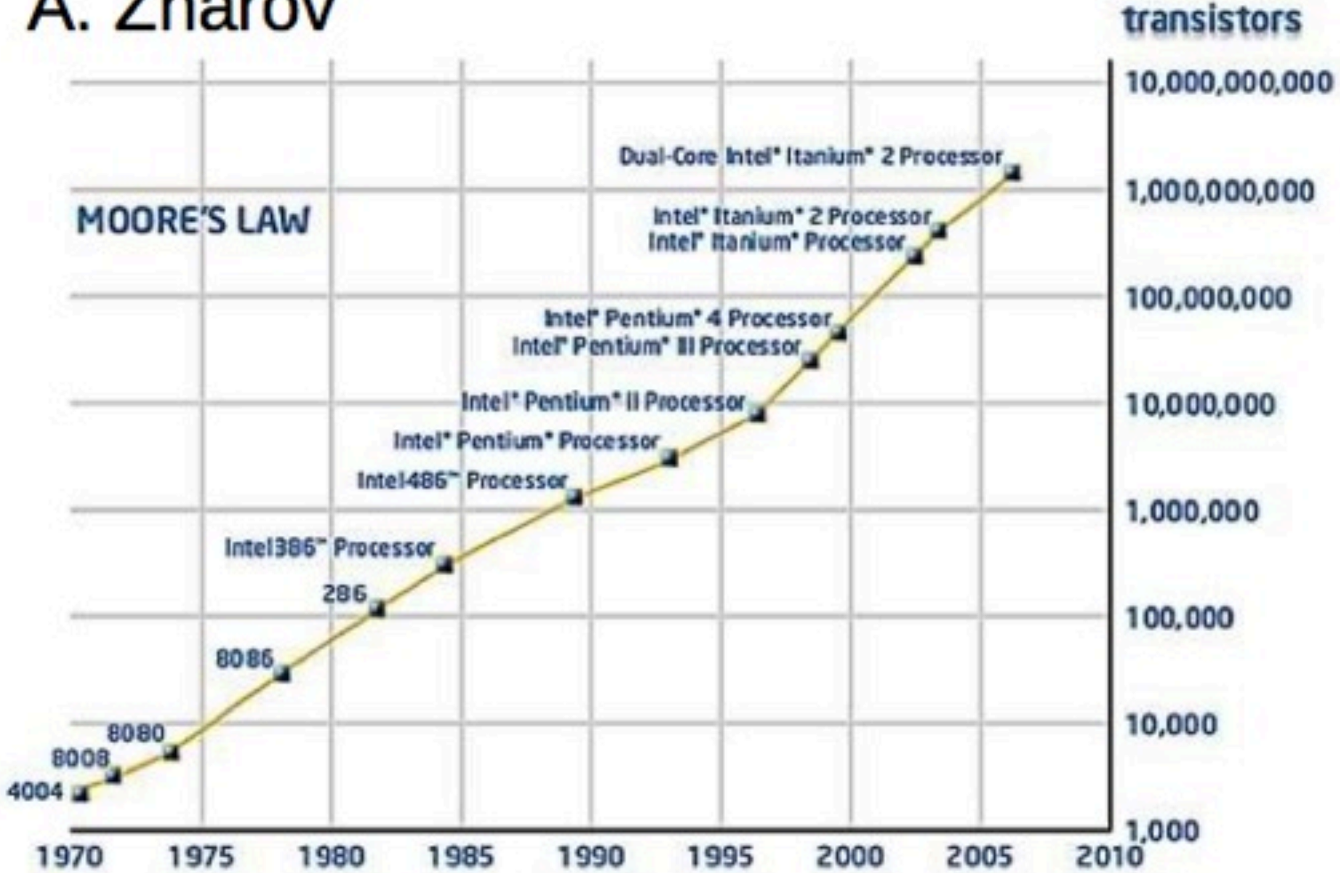
- **produce good looking galaxies :-)**
- **get correctly the *stellar mass* of galaxies :-(**

The Future

Develop algorithms for exploiting exaflop supercomputing

Exponential growth of computing power over 40 years

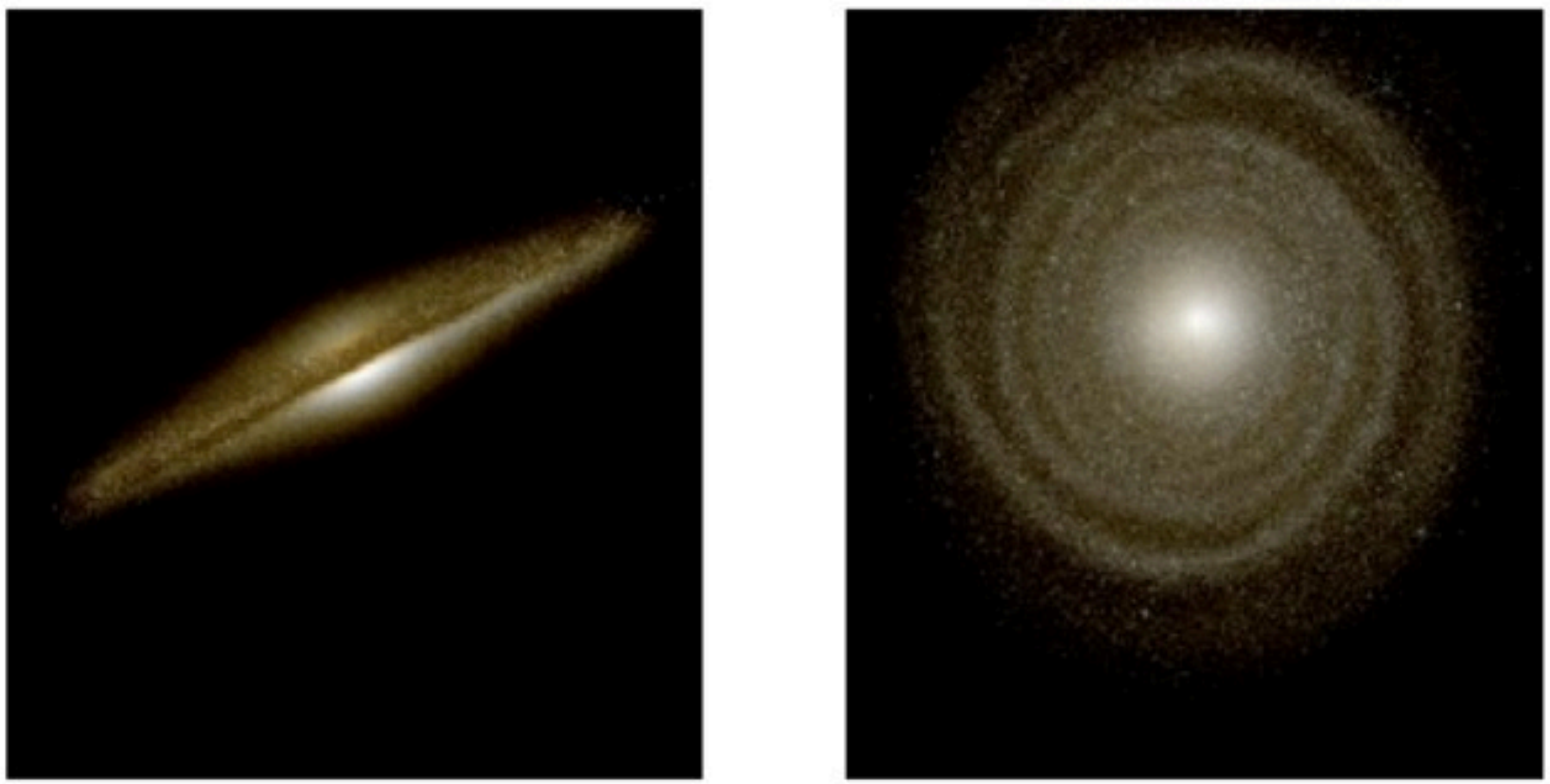
A. Zharov



- **Tianhe-2 in China**
- 3,120,000 cores
- 34 Petaflops
- 1,300 Tb of RAM
- 390 million dollars

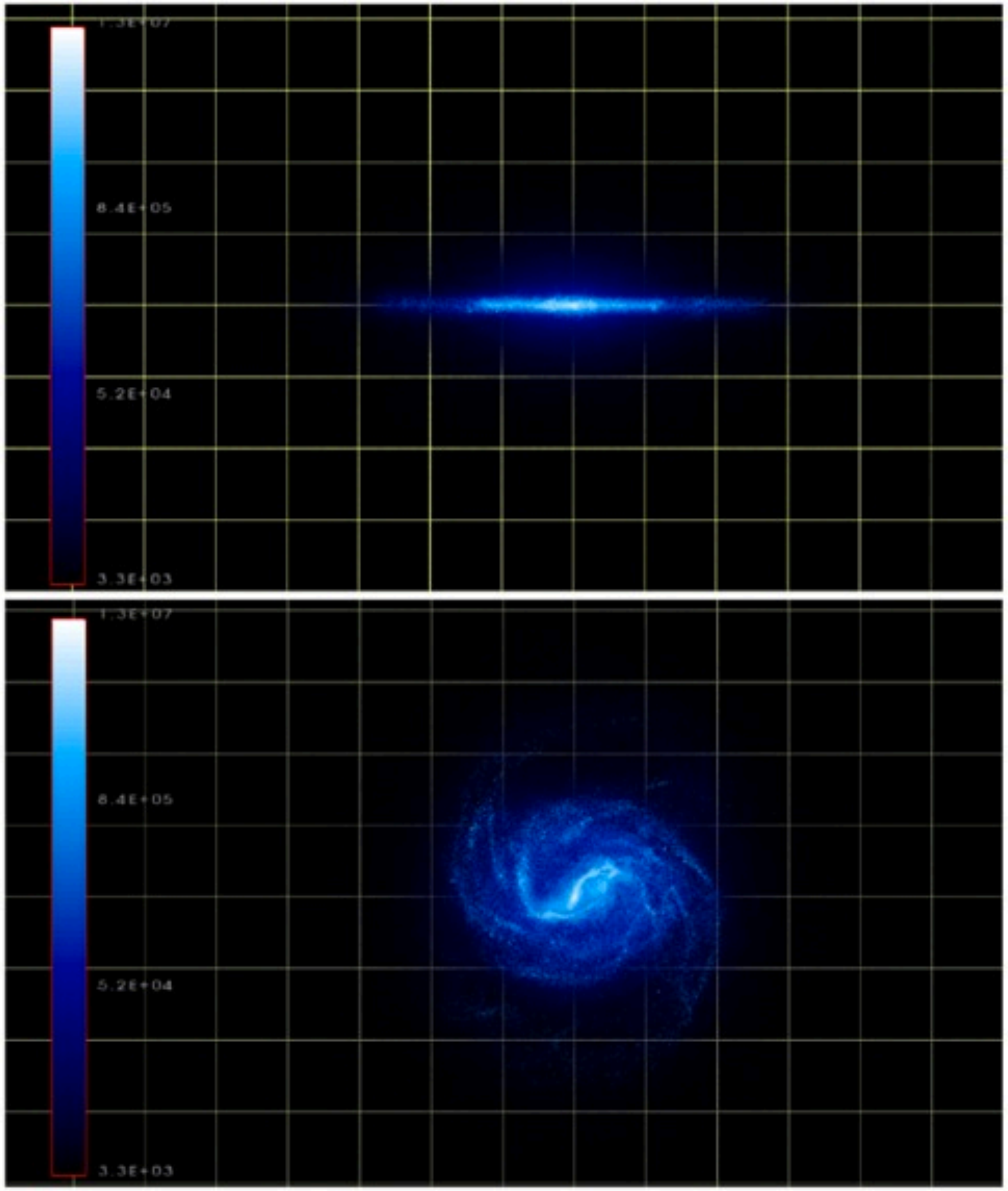
Exaflop limit is expected to be reached by 2020

Modern galaxy formation simulations

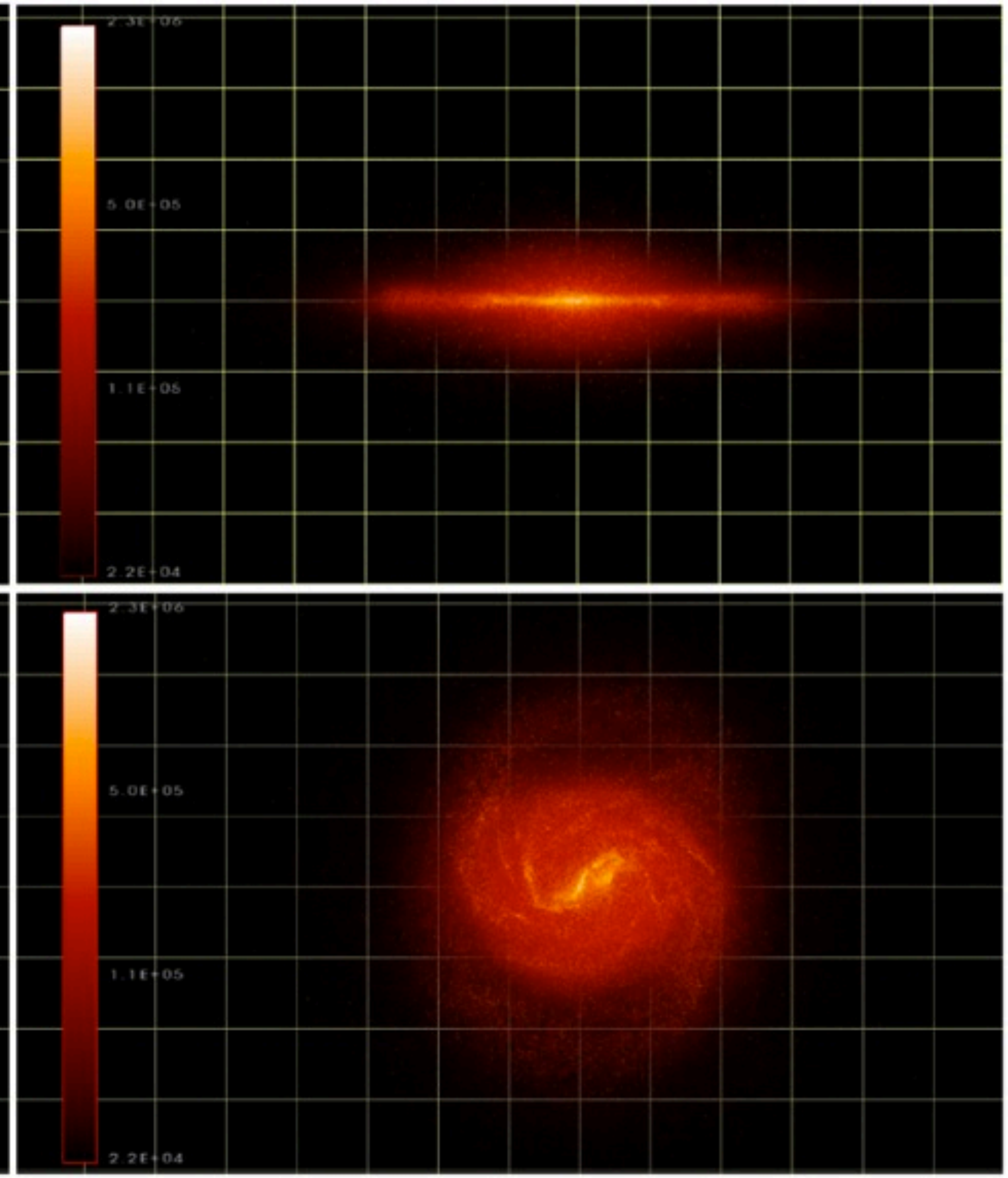


Mock gri SDSS composite image with dust absorption based on Draine opacity model.

NGC4622 as seen from HST

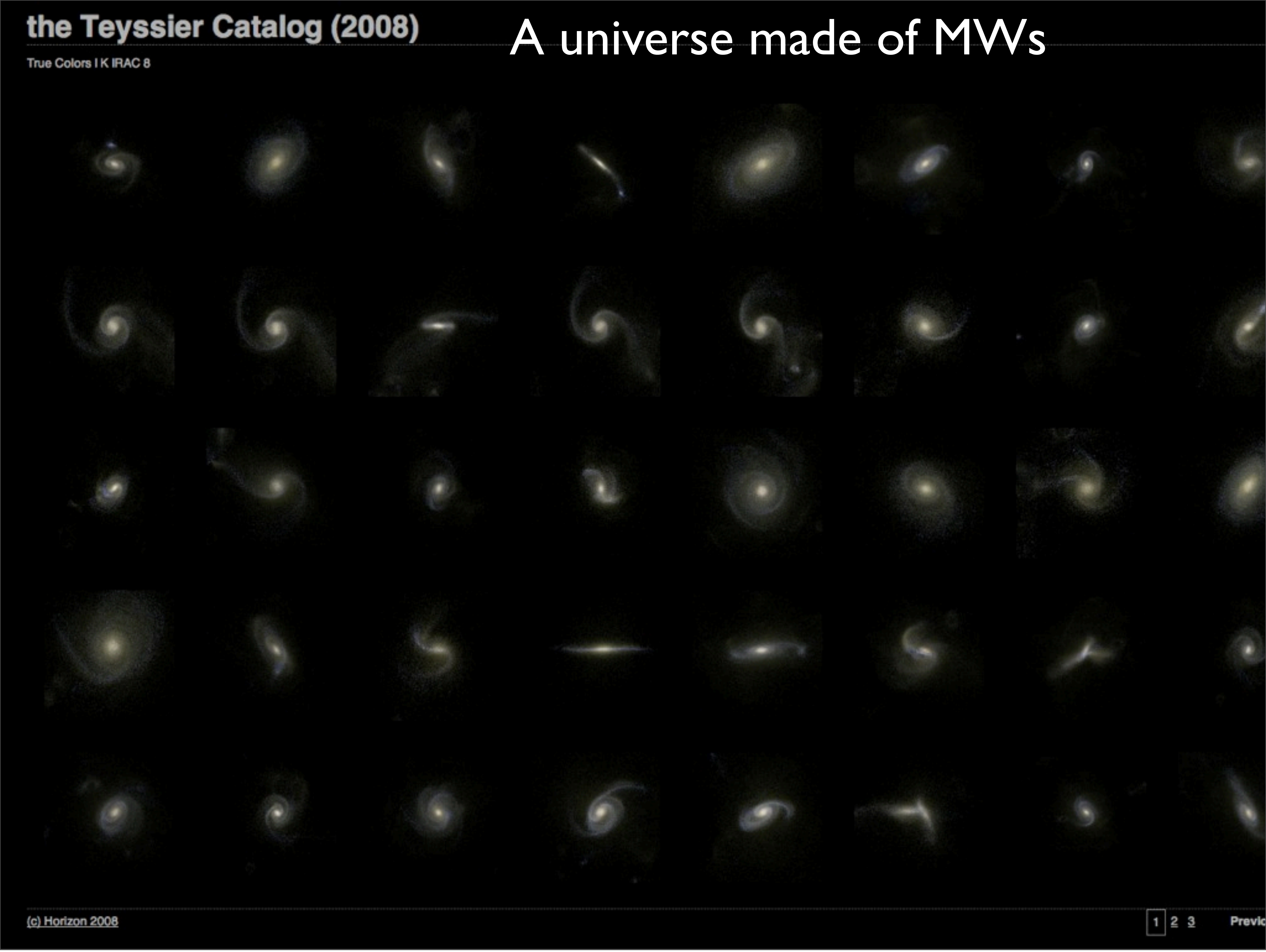


(a) U-band luminosity. Units scale from $3.3 \cdot 10^3 L_\odot$ to $1.3 \cdot 10^7 L_\odot$.

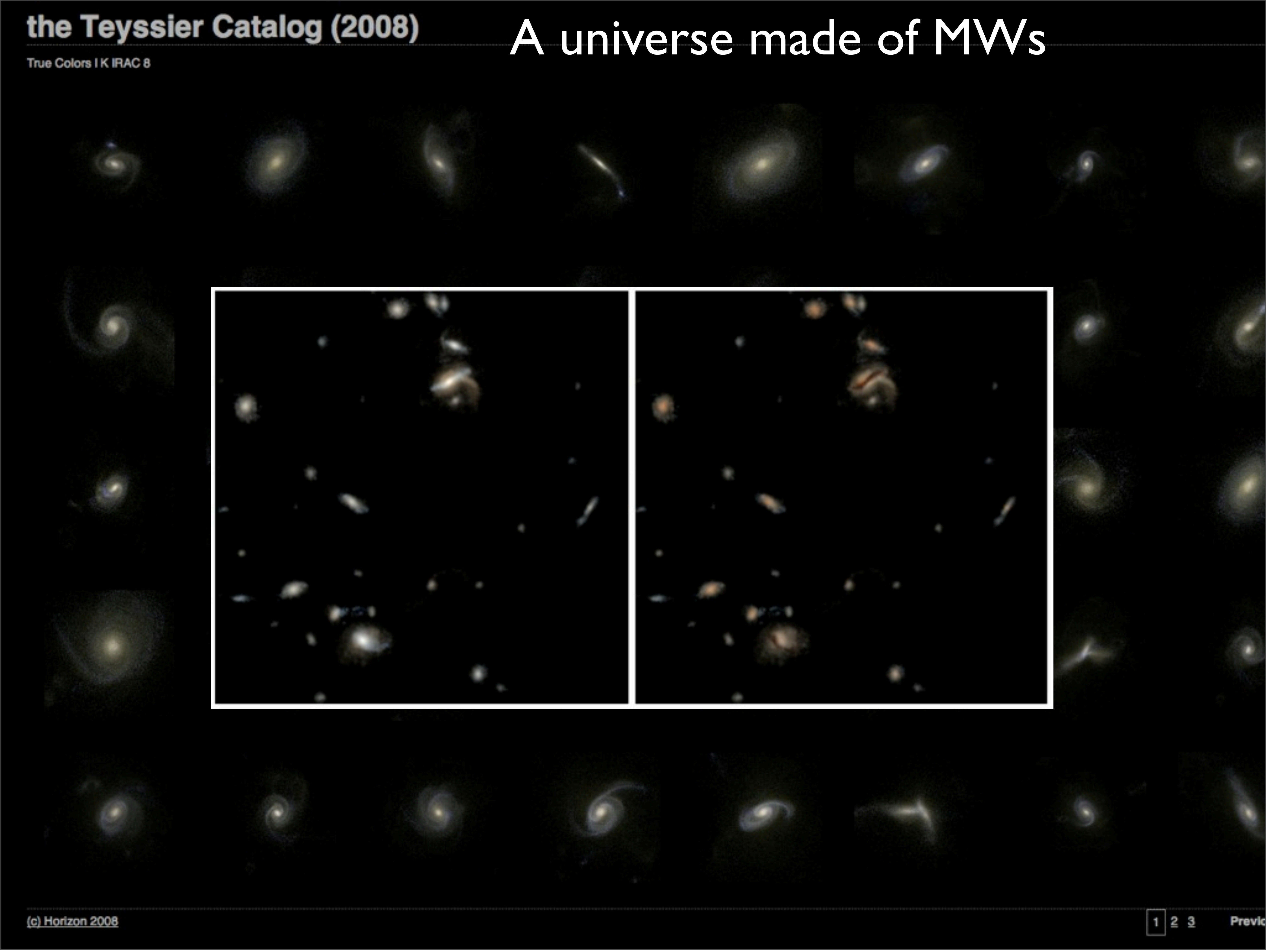


(b) K-band luminosity. Units scale from $2.2 \cdot 10^4 L_\odot$ to $2.3 \cdot 10^6 L_\odot$

A universe made of MWs



A universe made of MWs



Direct simulations of star formation in cosmological volumes have proven to be very difficult

COMMON HEADACHES OF SIMULATORS OF GALAXY FORMATION

- Cooling catastrophe & overproduction of stars
- Thermal supernova-feedback fails to regulate star formation, and fails to explain metal enrichment of the IGM
- Collapse of gas halted by numerical resolution not by physics
- The real structure of the ISM is known to be multi-phase

➤ *- Hybrid multi-phase model for the ISM*
- Inclusion of galactic winds

And the simulations are very expensive:

- **Required dynamic range is huge**

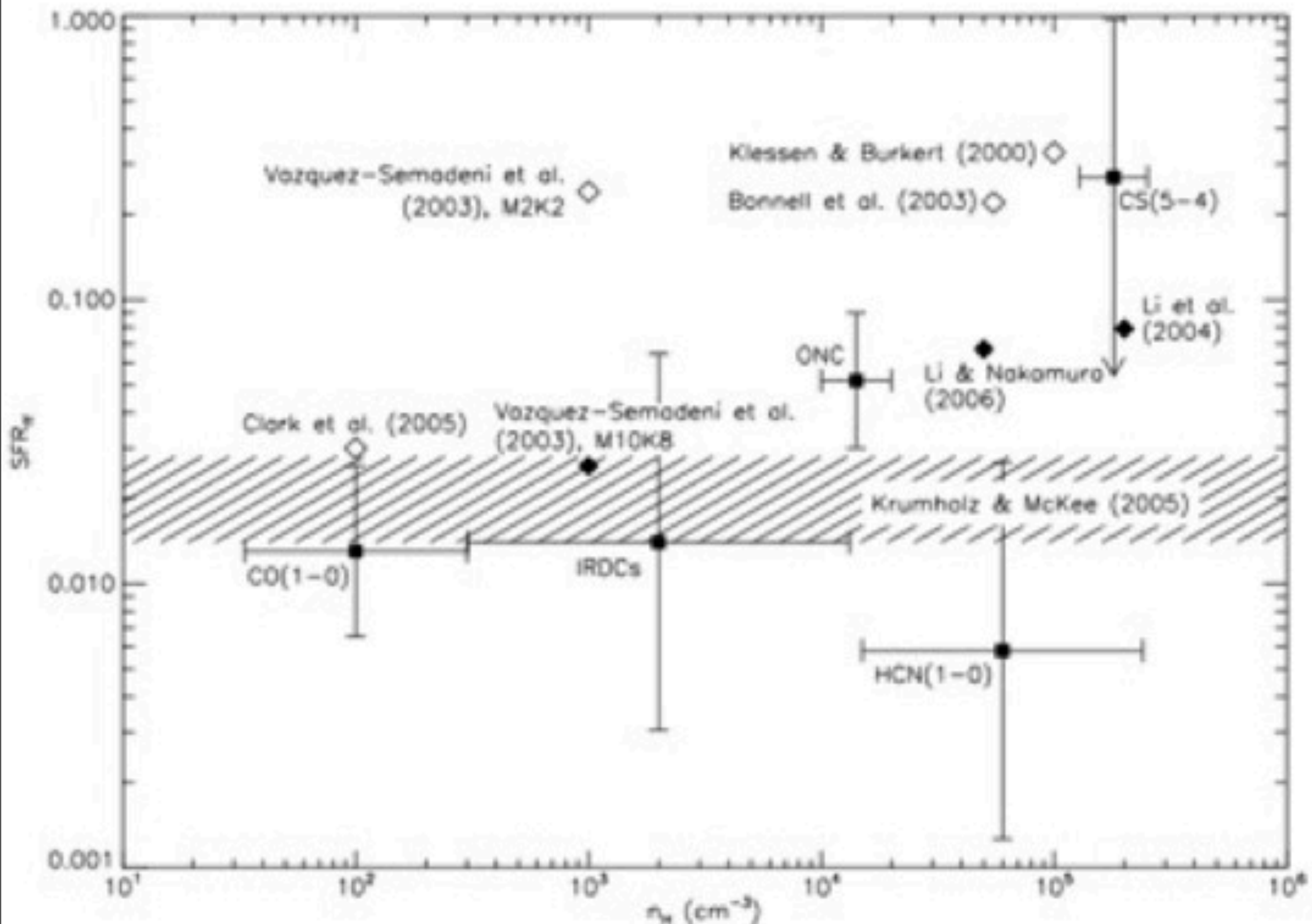
  To resolve ***all*** the star formation, one needs:

  $L \sim 100$ Mpc/h
  $m_{gas} \sim 10^6\ M_\odot$/h

  ➤ $\sim 10^{11}$ simulation particles

➤ *Comprehensive set of simulations on interlocking scales*

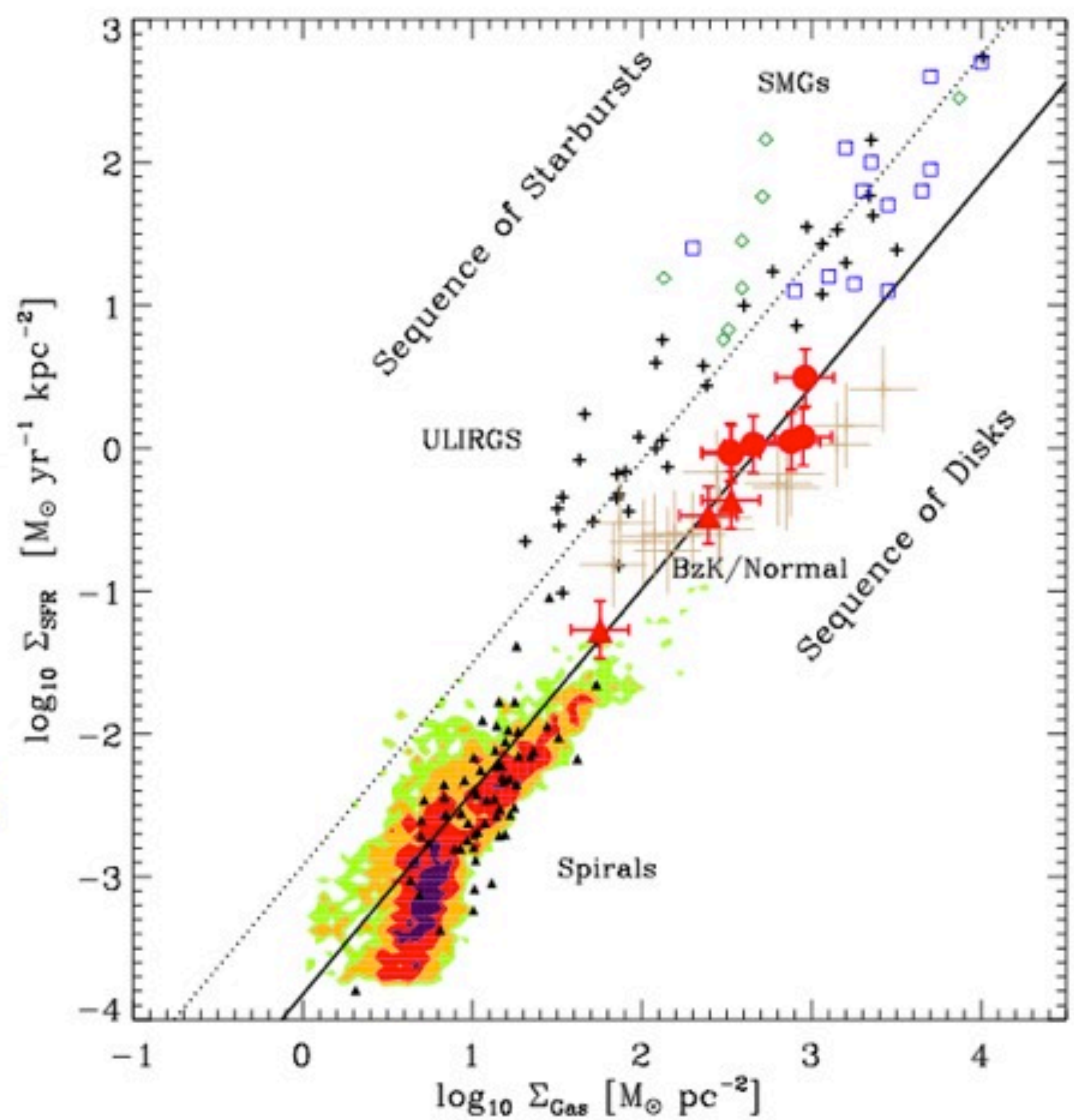
Star formation recipe



Schmidt law for star formation:

$$\dot{\rho}_* = \epsilon_* \frac{\rho_g}{t_{\rm ff}} \text{ for } \rho > \rho_*$$

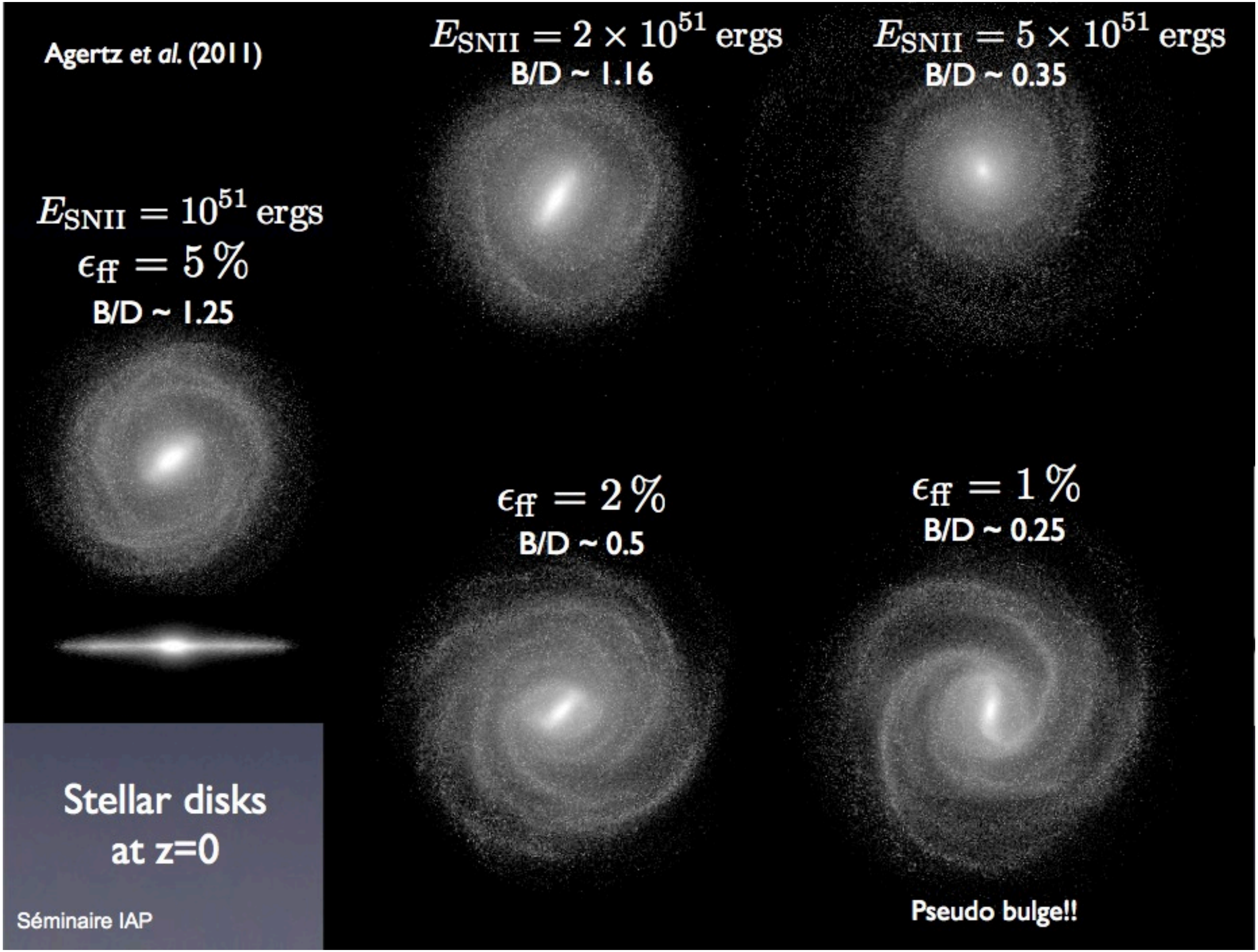
Krumholz & Tan (2007)



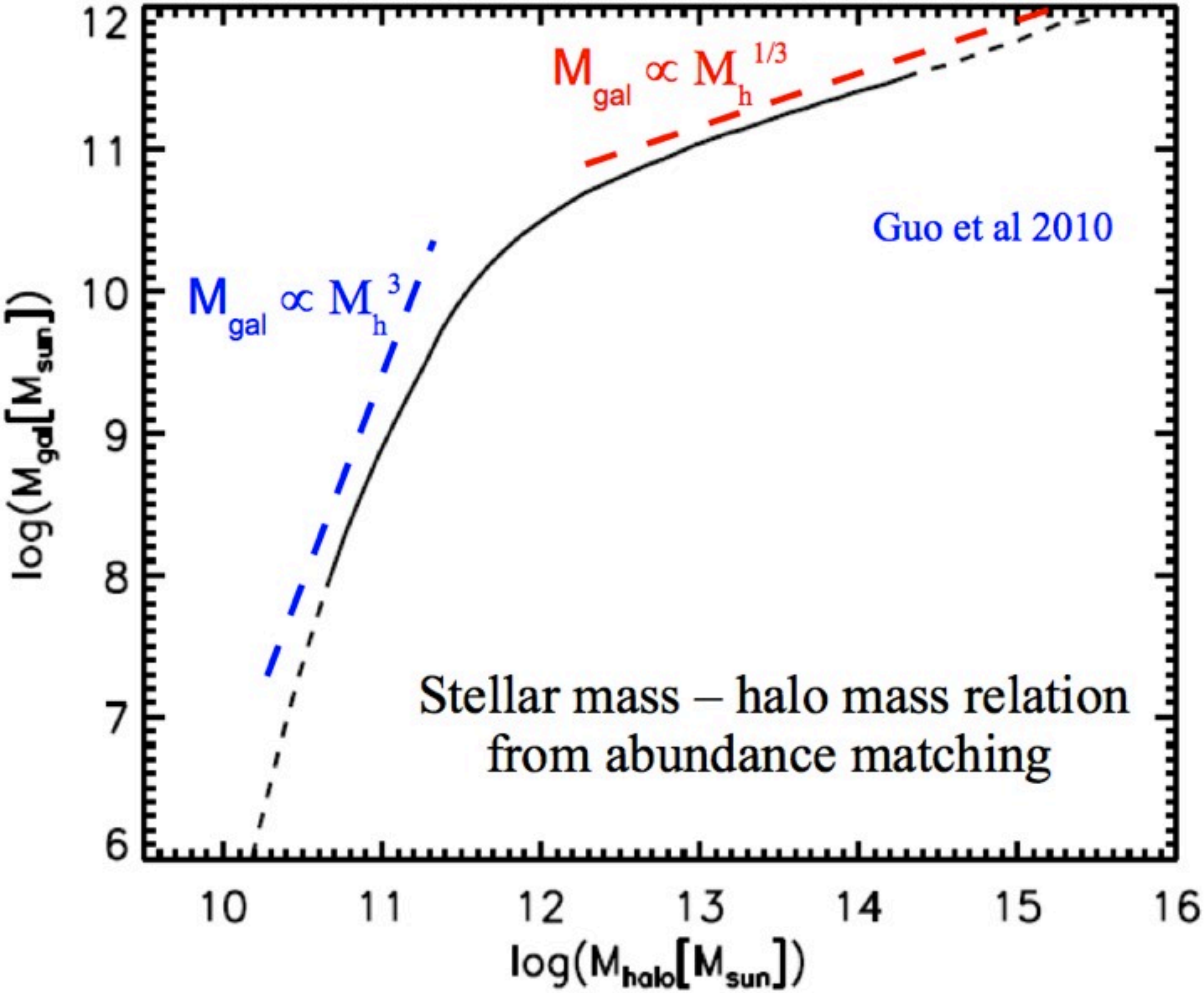
Parameters are calibrated on the Kennicutt (1998) relation

$$\Sigma_{\rm SFR} = (2.5 \pm 0.7) \times 10^{-4} \left(\frac{\Sigma_{\rm gas}}{\rm M_\odot pc^{-2}} \right)^{1.4}$$

Daddi et al. (2010)



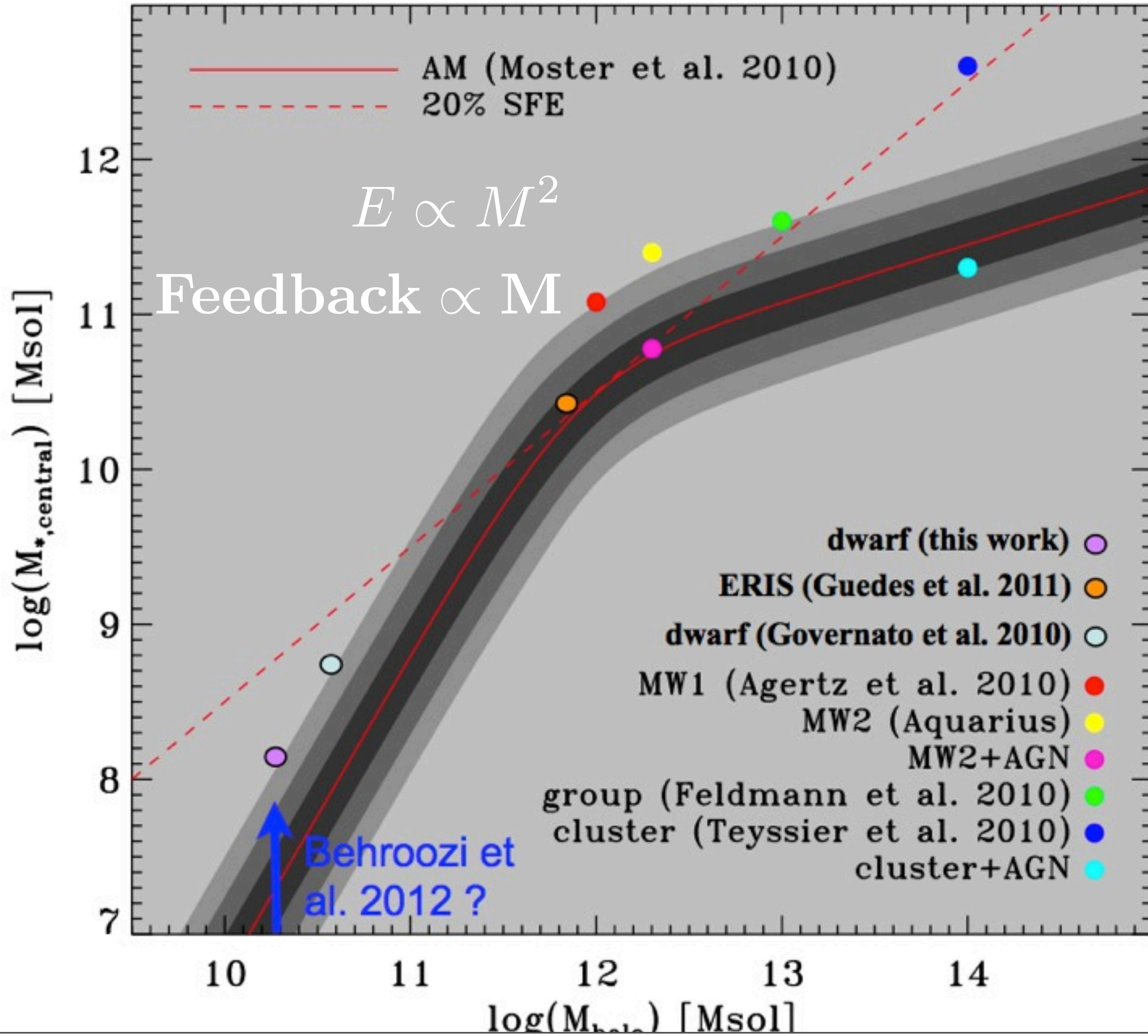
Agertz et al. (2011)
$E_{\rm SNII} = 2 \times 10^{51}$ ergs
B/D ~ 1.16
$E_{\rm SNII} = 5 \times 10^{51}$ ergs
B/D ~ 0.35
$E_{\rm SNII} = 10^{51}$ ergs
$\epsilon_{\rm ff} = 5\,\%$
B/D ~ 1.25
$\epsilon_{\rm ff} = 2\,\%$
B/D ~ 0.5
$\epsilon_{\rm ff} = 1\,\%$
B/D ~ 0.25
Stellar disks
at z=0
Séminaire IAP
Pseudo bulge!!



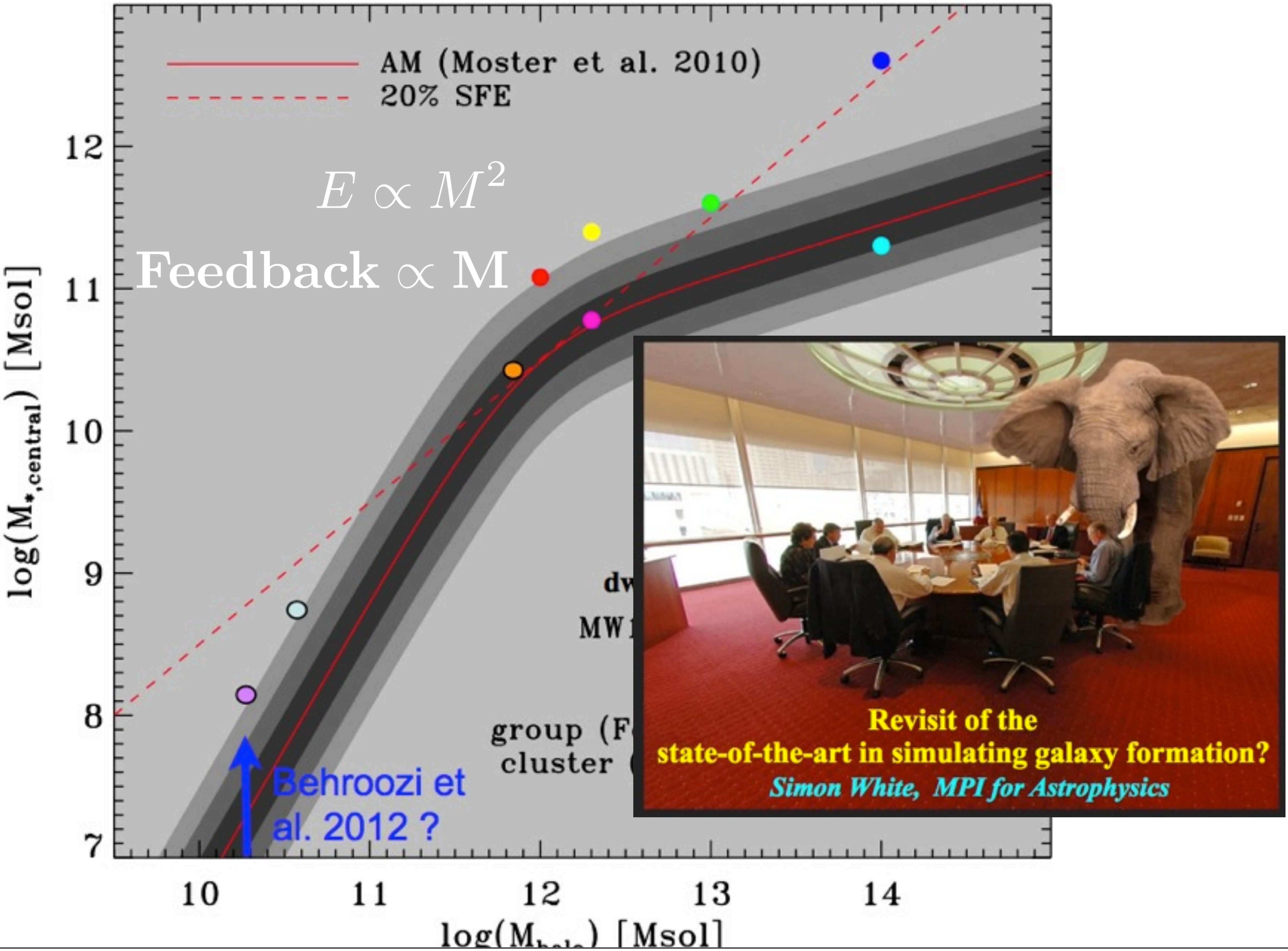
The stellar mass of the central galaxy increases rapidly with halo mass at small halo mass, but slowly at large halo mass

The characteristic halo mass at the bend is $5 \times 10^{11}\ M_{\odot}$

Constraints from abundance matching



Constraints from abundance matching




Clusters?
276.44 h^-1 kpc

Sink-particles and a simple parameterization of the accretion rate are used to model the growth of black holes

THE IMPLEMENTED BLACK HOLE ACCRETION MODEL

Growth of Black Holes

Bondi-Hoyle-Lyttleton type accretion rate parameterization:

$$\dot{M}_{\rm B} = \alpha \times 4\pi R_{\rm B}^2 \, \rho \, c_s \simeq \frac{4\pi\alpha G^2 M_\bullet^2 \, \rho}{(c_s^2 + v^2)^{3/2}}$$

Limitation by the Eddington rate:

$$\dot{M}_\bullet = \min(\dot{M}_{\rm B}, \dot{M}_{\rm Edd})$$

Feedback by Black Holes

Standard radiative efficiency:

$$L_{\rm bol} = 0.1 \times \dot{M}_\bullet \, c^2$$

Thermal coupling of some fraction of the energy output to the ambient gas:

$$\dot{E}_{\rm feedback} = f \times L_{\rm bol} \qquad f \simeq 5\%$$

Implementation in SPH simulation code

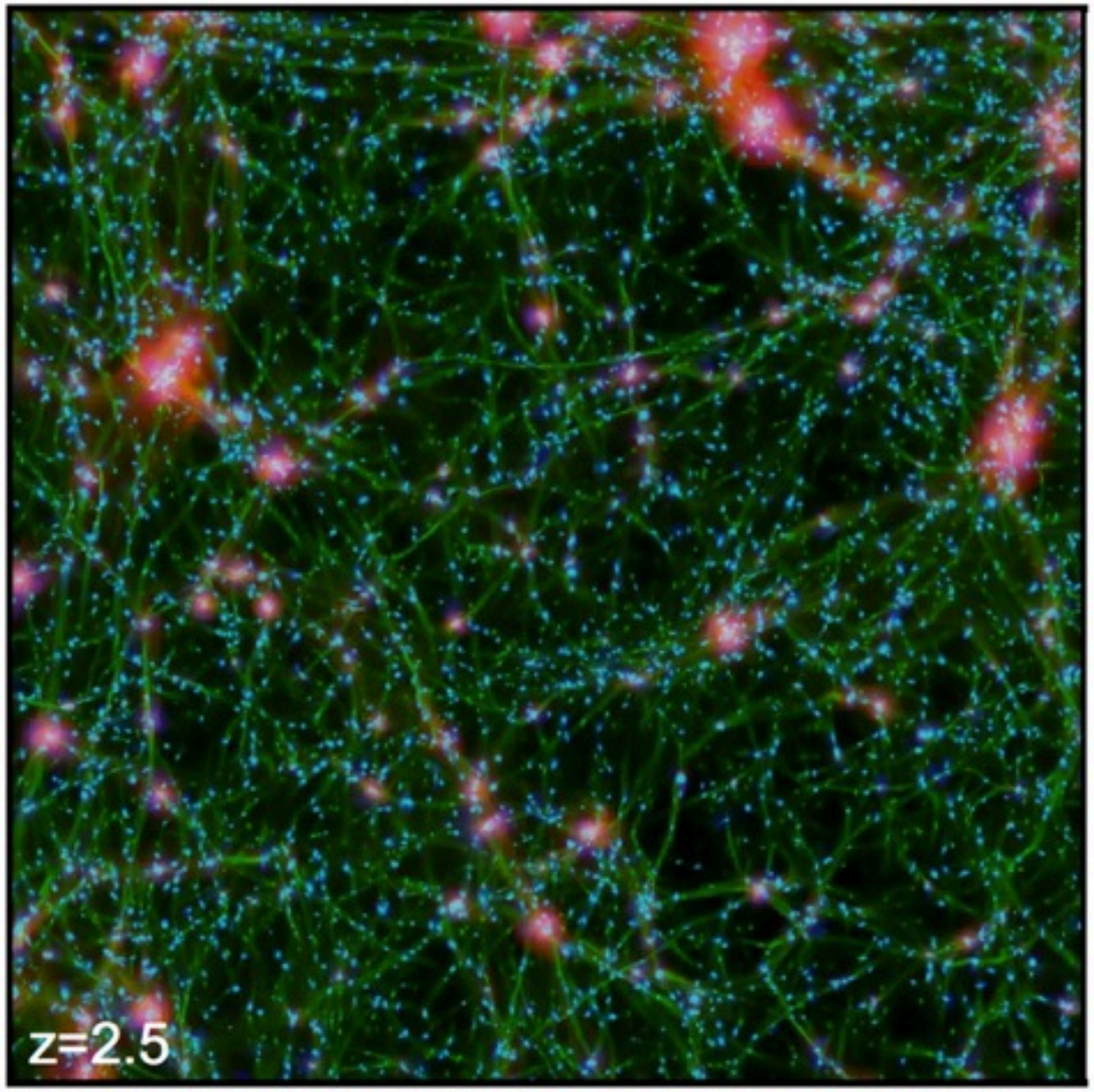
Additions in the parallel GADGET-2 code:

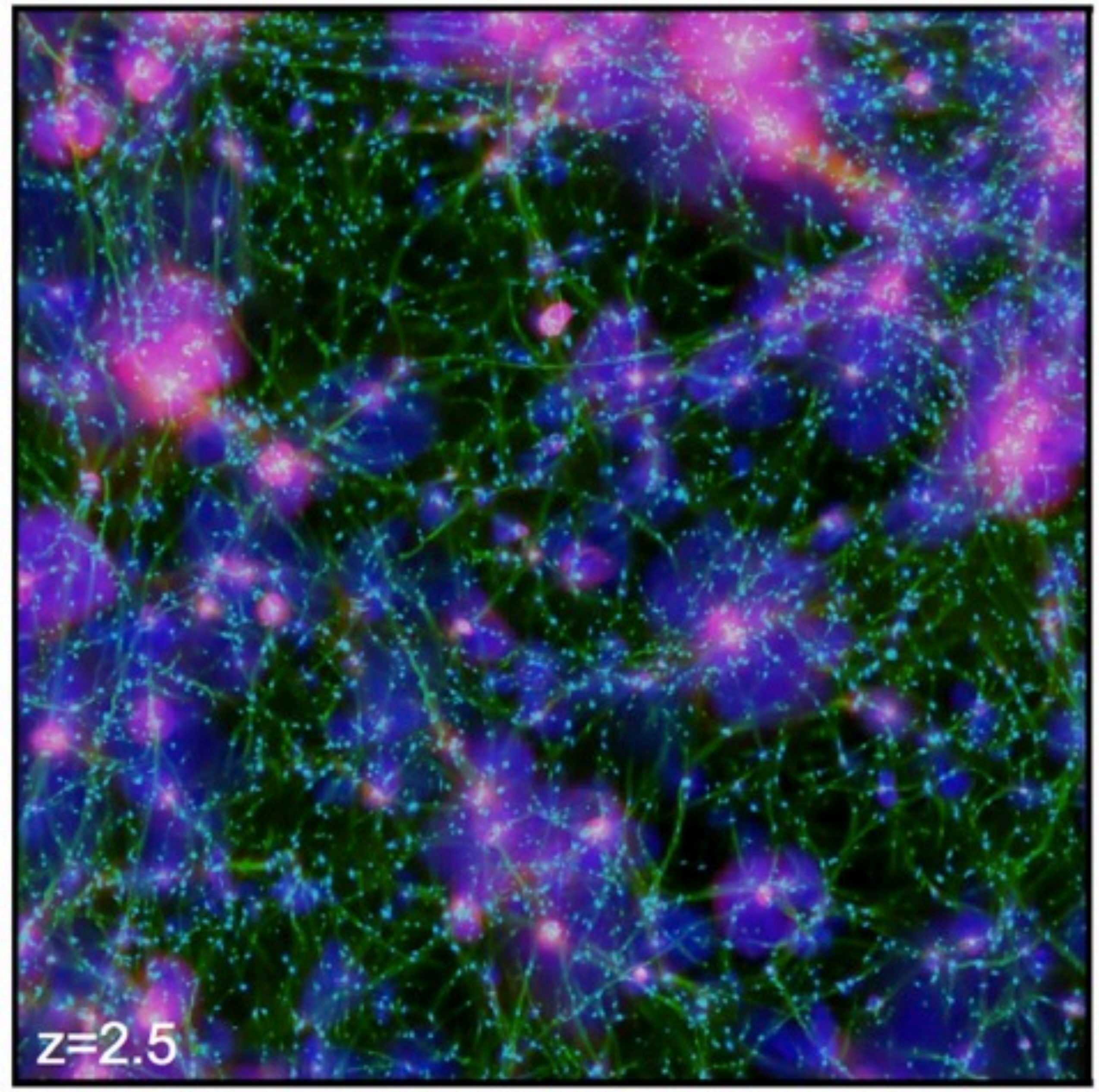
- BH sink particles swallow gas stochastically from their local neighbourhoods, in accordance with the estimated BH accretion rate
- Feedback energy is injected locally into the thermal reservoir of gas
- On-the-fly FOF halo finder detects emerging galaxies and provides them with a seed black hole
- BHs are merged if they reach small separations and low enough relative speeds

Green: gas density / Red: temperature / Blue: metallicity

Without AGN

With AGN





Clusters?

Galaxy formation and accretion on supermassive black holes appear to be closely related

BLACK HOLES MAY PLAY AN IMPORTANT ROLE IN THEORETICAL GALAXY FORMATION MODELS

Observational evidence suggests a link between BH growth and galaxy formation:

- M_B-σ relation
- Similarity between cosmic SFR history and quasar evolution

Theoretical models often assume that BH growth is self-regulated by **strong** feedback:

- Blow out of gas in the halo once a crtitical M_B is reached
  Silk & Rees (1998), Wyithe & Loeb (2003)

Feedback by AGN may:

- Solve the cooling flow riddle in clusters of galaxies
- Explain the cluster-scaling relations, e.g. the tilt of the L_x-T relation
- Explain why ellipticals are so gas-poor
- Drive metals into the IGM by quasar-driven winds
- Help to reionize the universe and surpress star formation in small galaxies

▷ ***Galaxy formation models need to include the growth and feedback of black holes !***

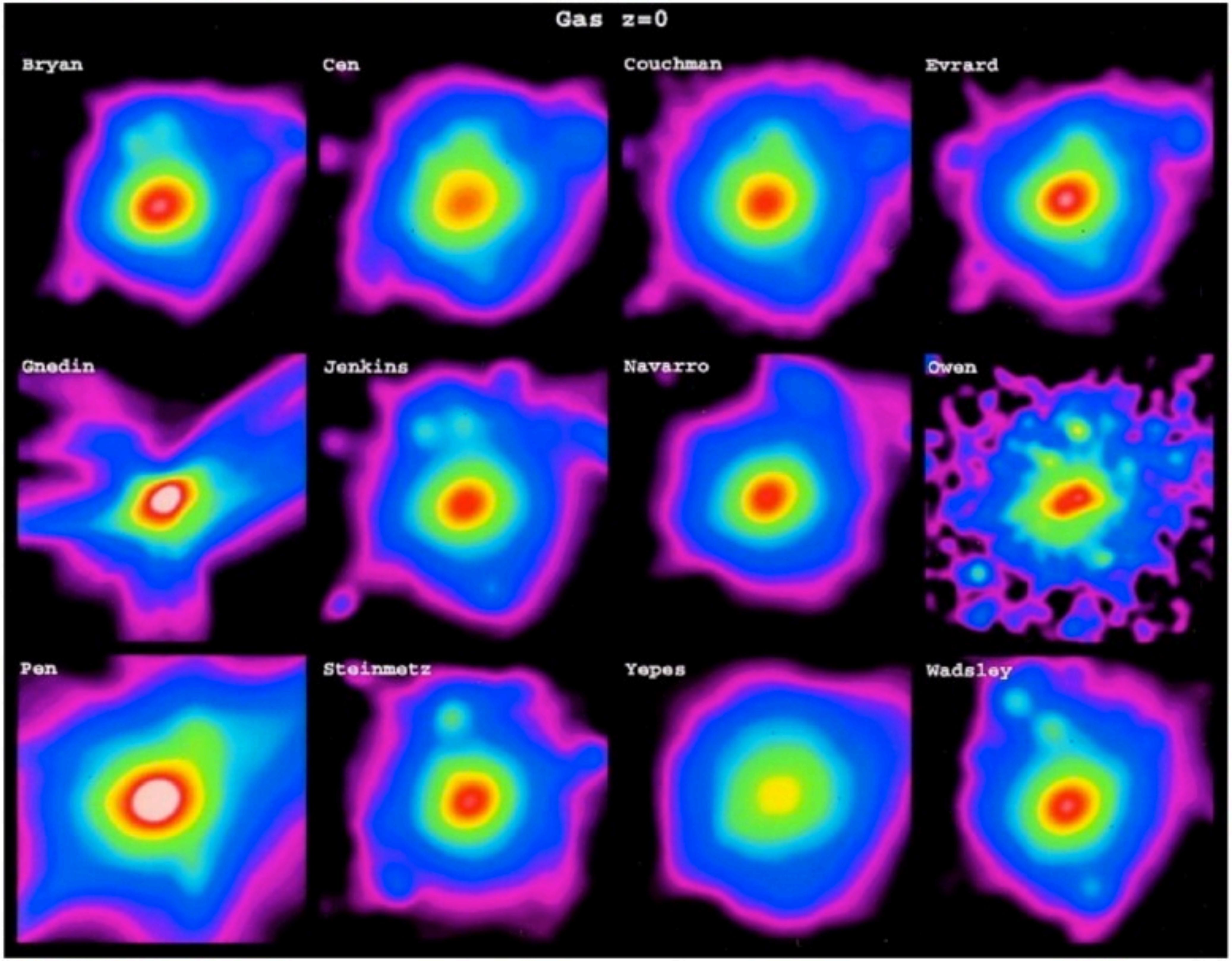
▷ ***This also applies to simulations !***

Volker Springel

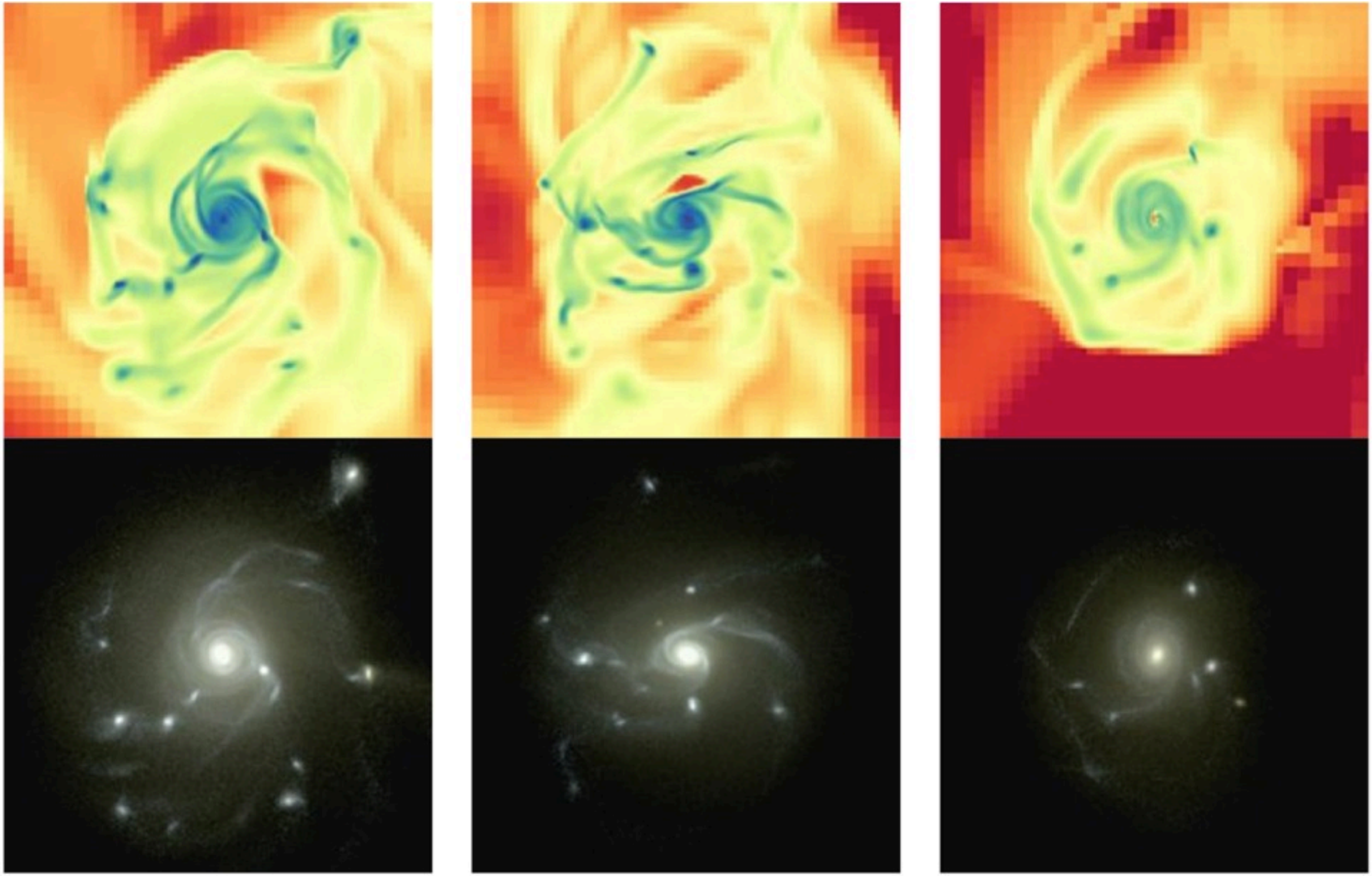
Different hydrodynamical simulation codes are broadly in agreement, albeit with substantial scatter and differences in detail

THE SANTA BARBARA CLUSTER COMPARISON PROJECT

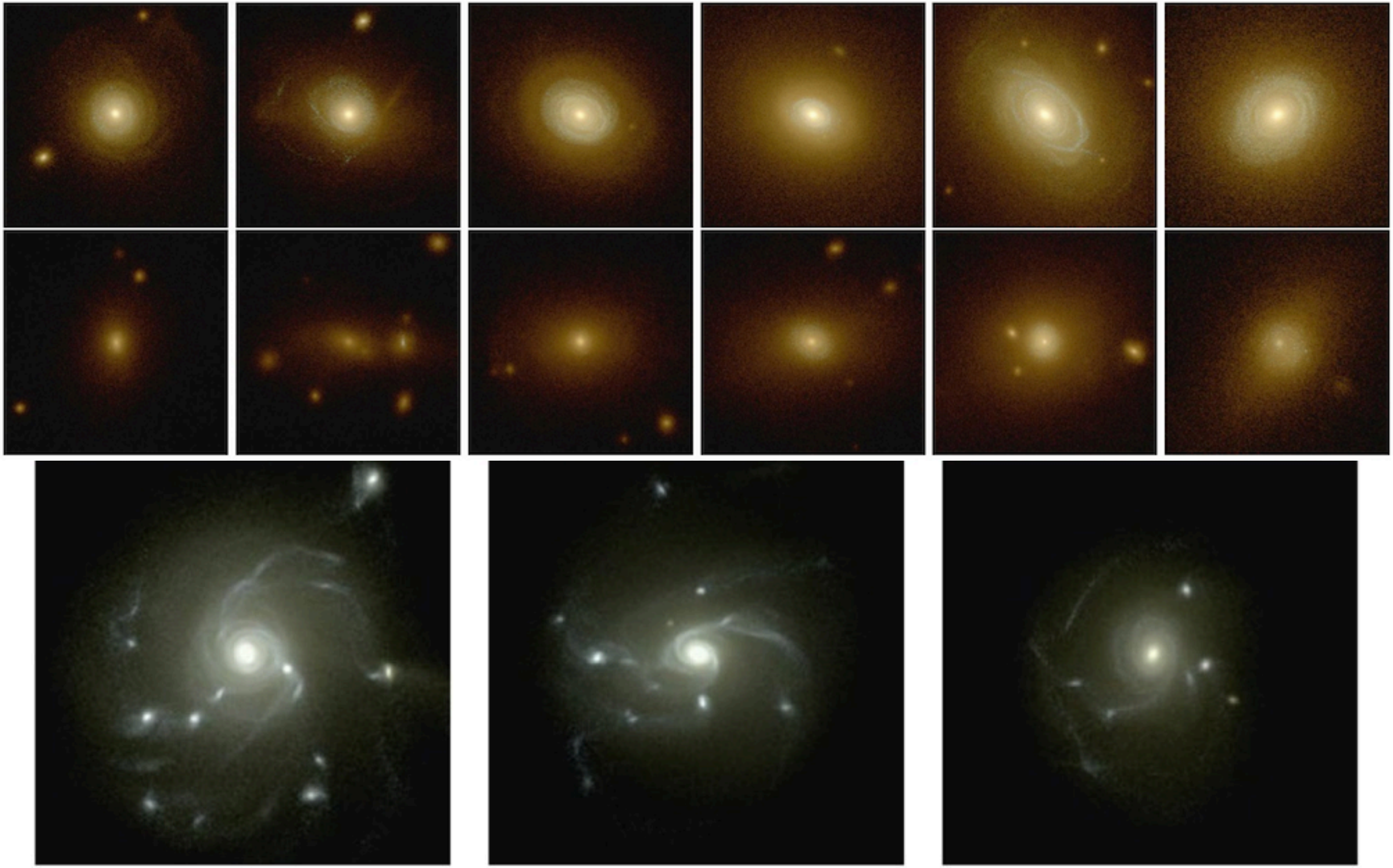
Frenk, White & 23 co-authors (1999)

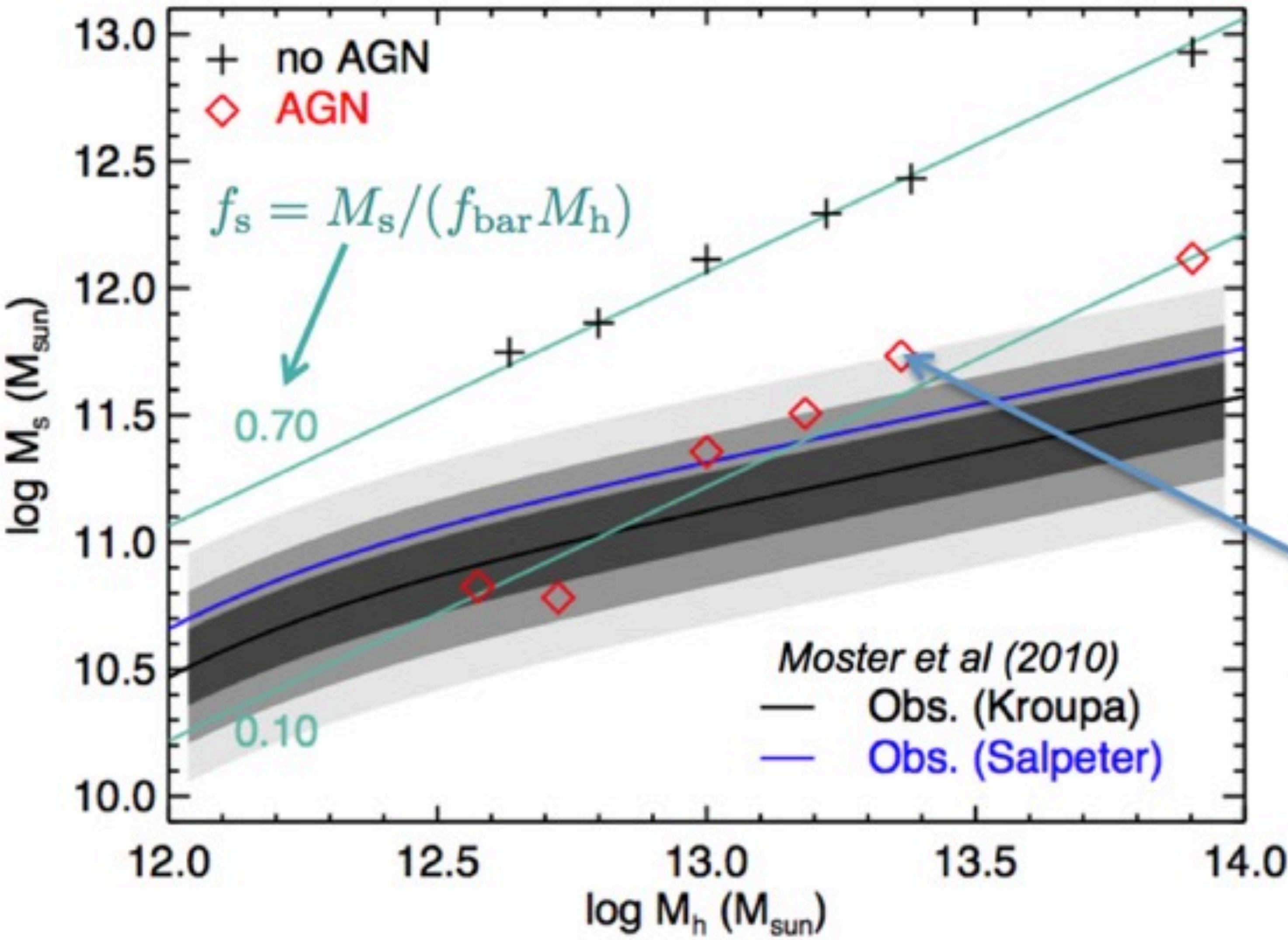


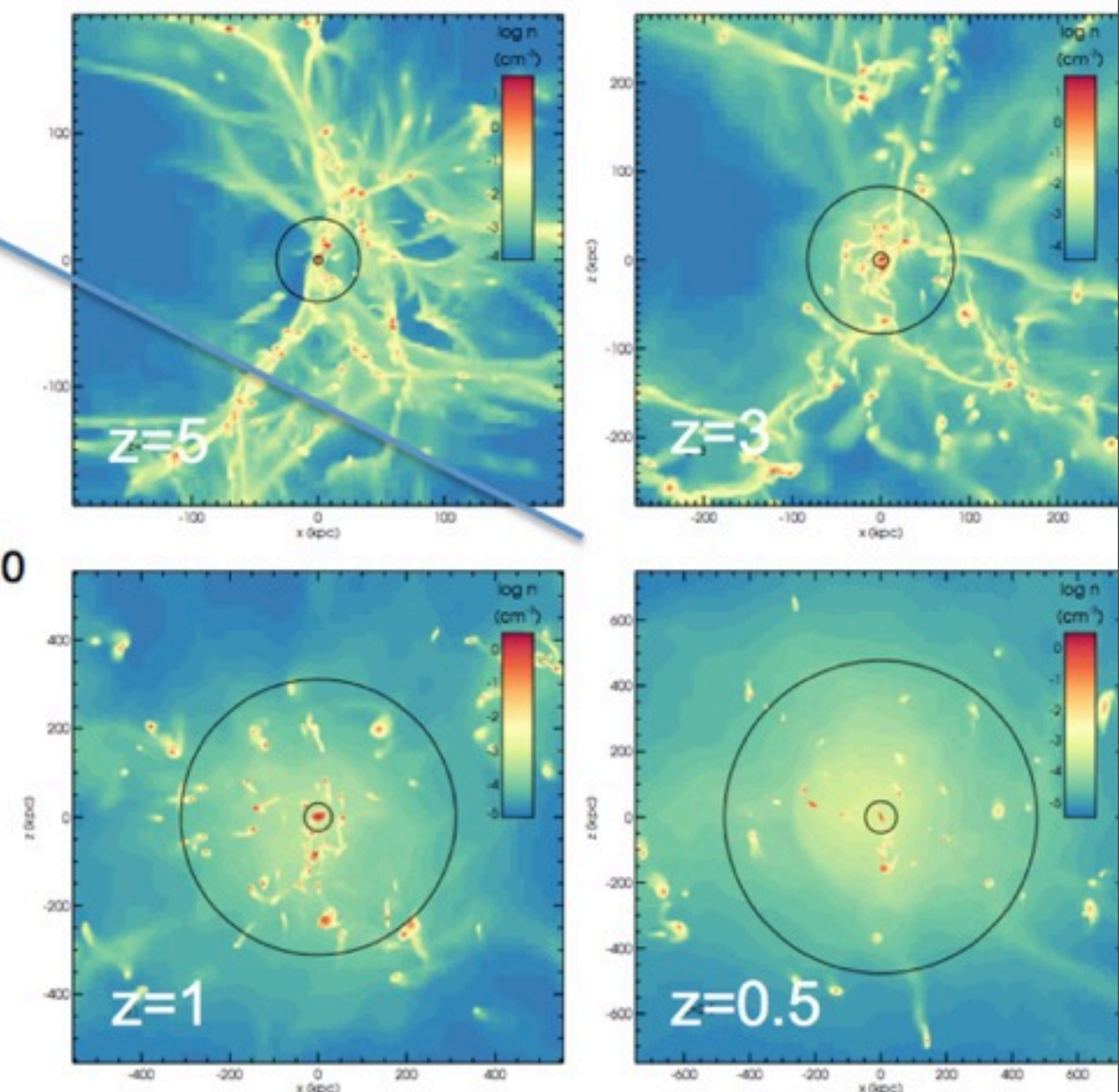
Effect of AGN feedback



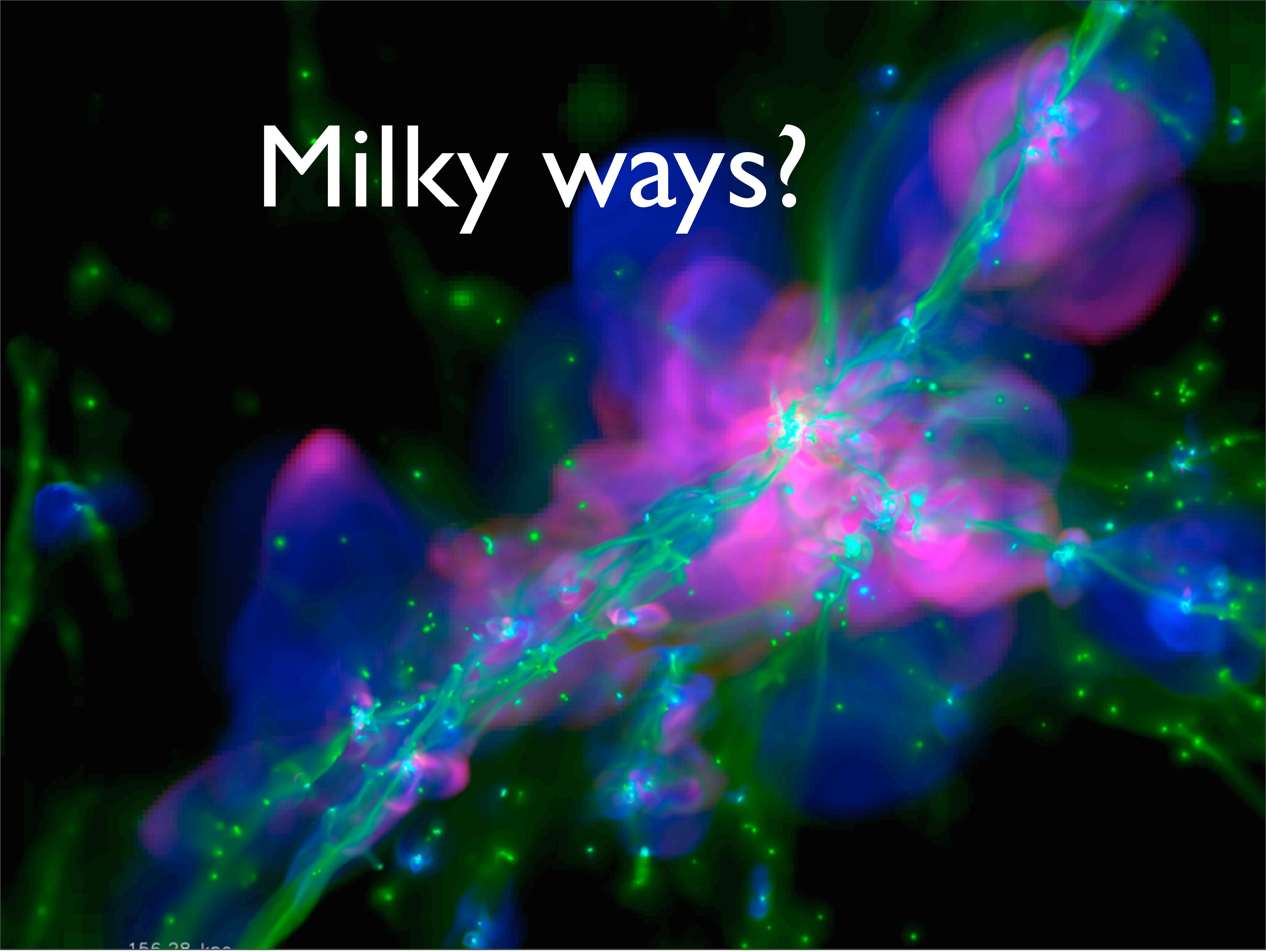
Effect of AGN feedback







Dubois, Gavazzi, Peirani, Silk, 2013


Milky ways?

MW?

The Aquila project contenders

AREPO: moving mesh code (Springel 2010)

Lagrangian mesh points : Galilean invariance

Voronoï tessellation to define interfaces between finite volume elements. Based on the Godunov methodology: Riemann solver + slope limiter.

Feedback models similar to GADGET.

RAMSES: AMR Eulerian code (Teyssier 2002)

Different stellar feedback implementations, all inefficient at large halo masses.

AGN feedback model à la Booth & Schaye 2011

GASOLINE: standard SPH (Wadsley, Stadel & Quinn 2004)

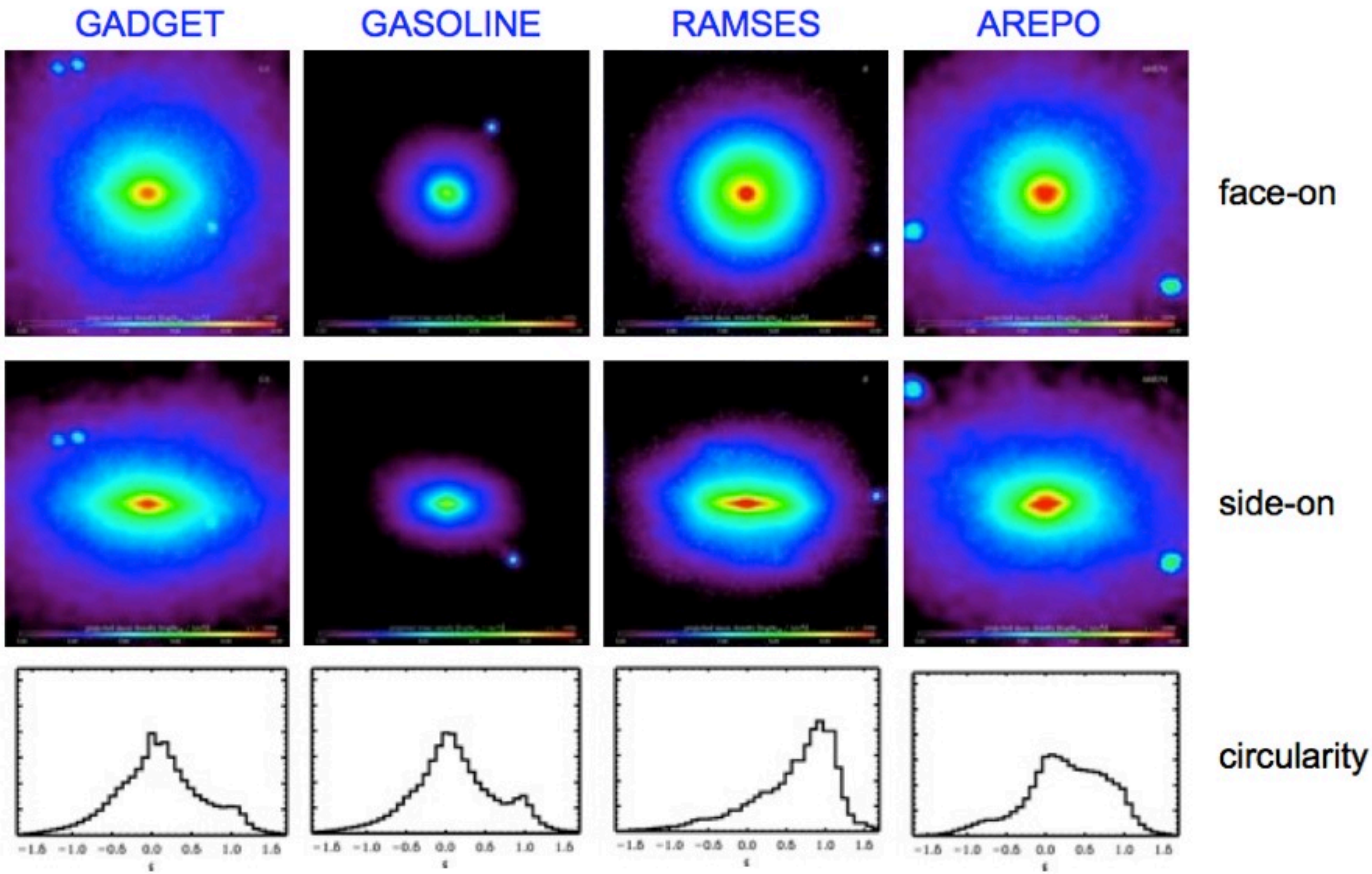
Delayed cooling with blast wave model. Inefficient at large halo masses.

GADGET: standard SPH (Springel 2005)

Many different versions with various feedback recipe.

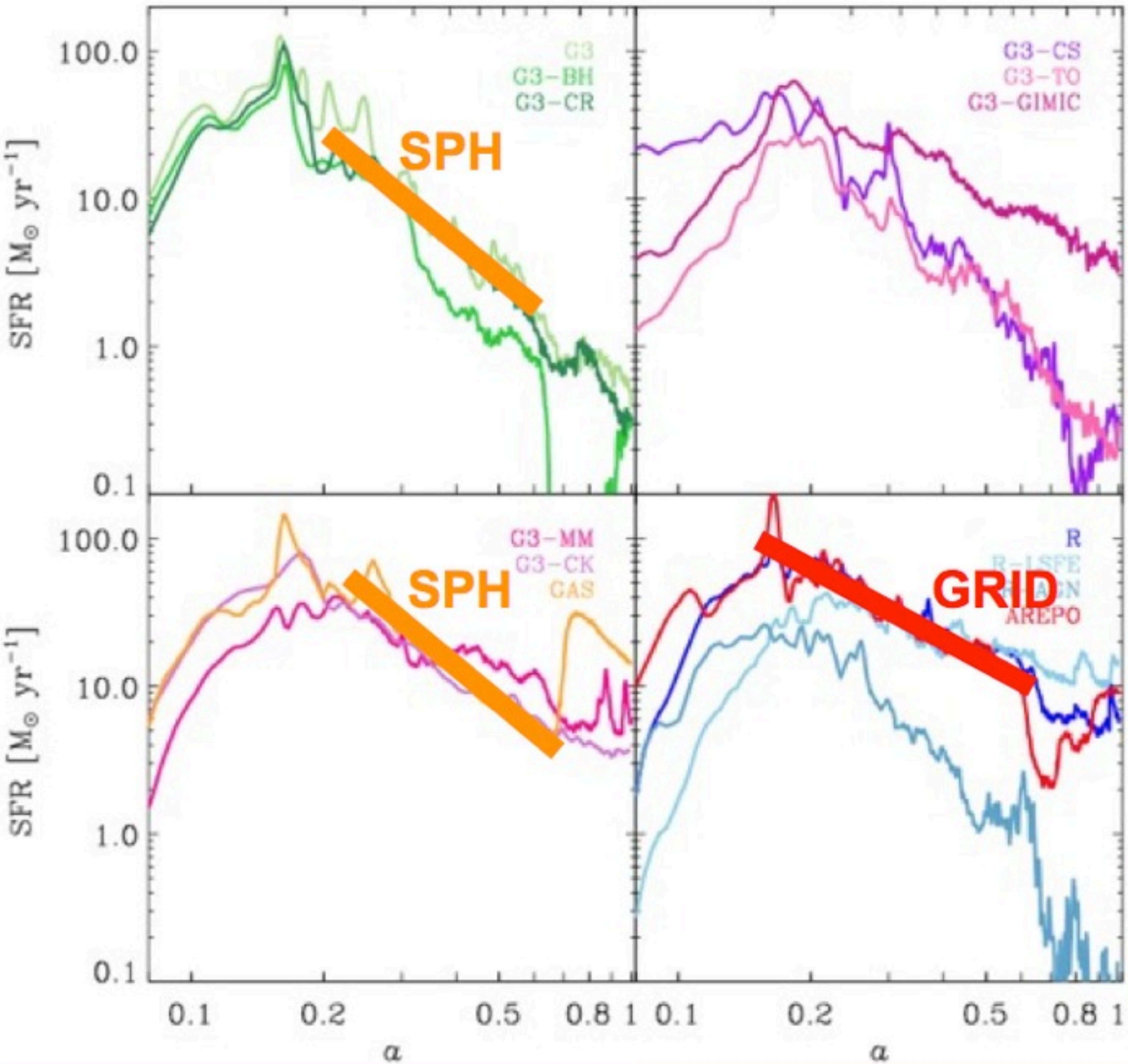
AGN feedback à la Sijacki et al.

Different codes, same physics, different morphologies...

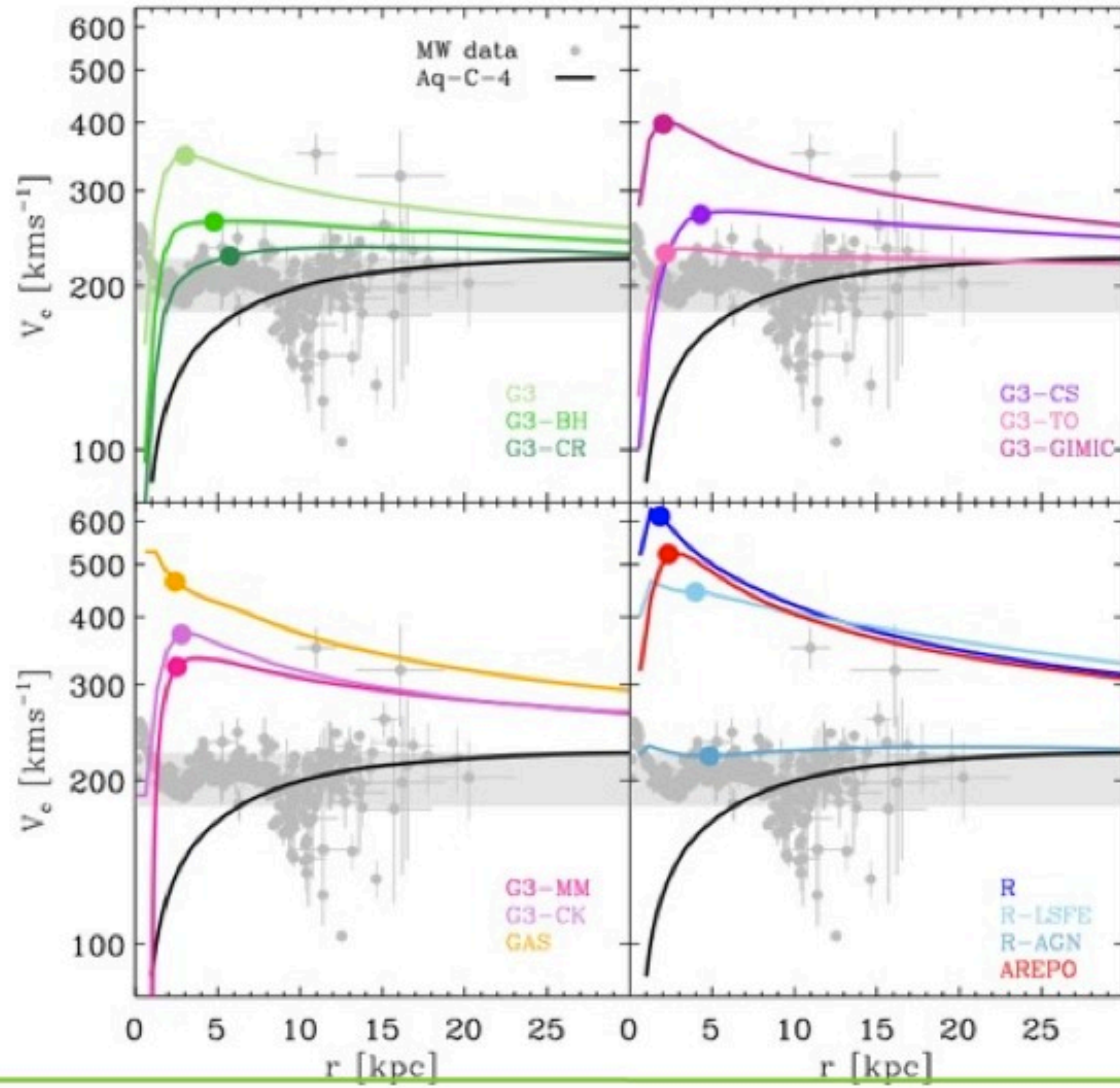


Low resolution runs

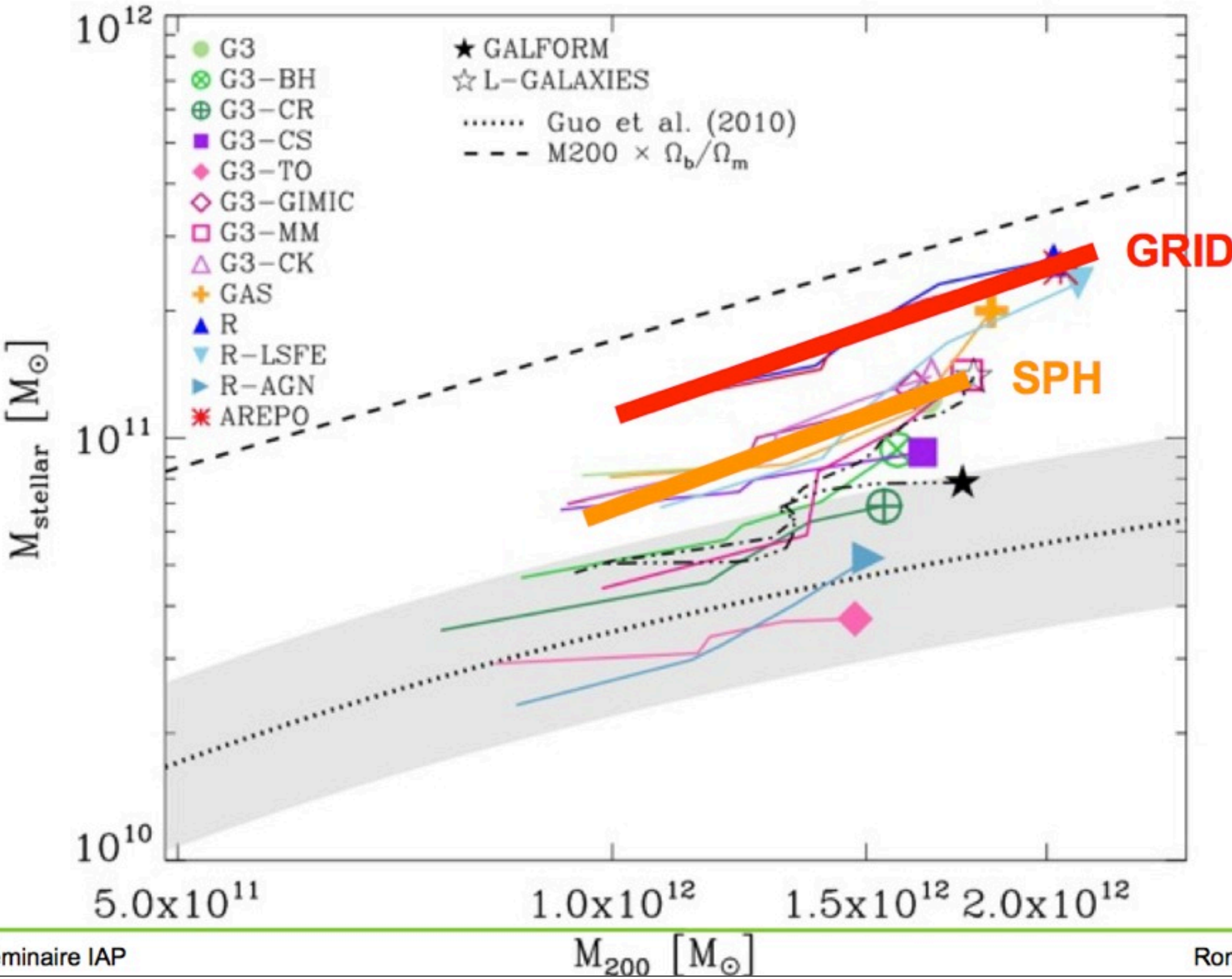
Stronger feedback, earlier star formation...



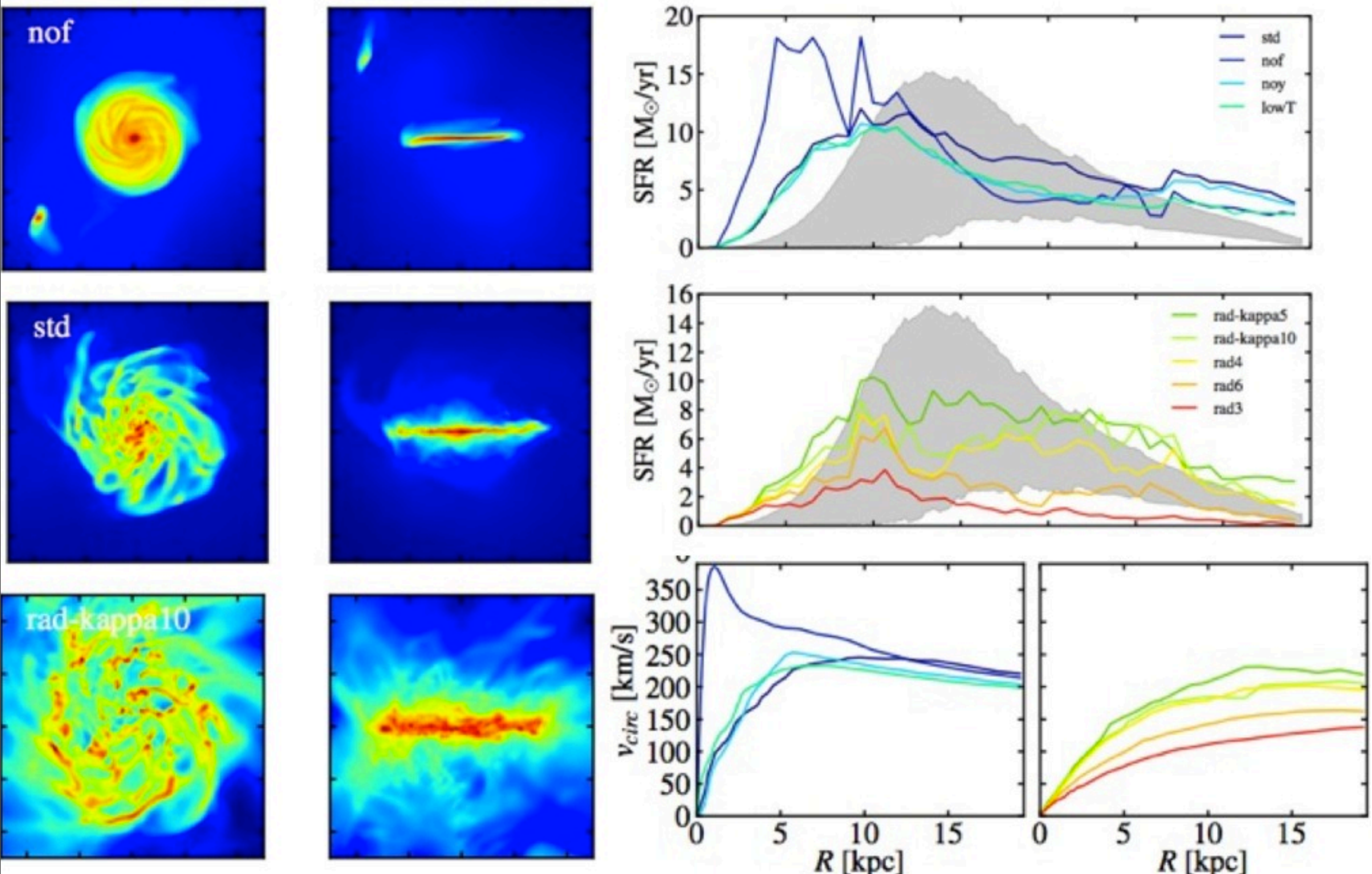
Stronger feedback, flatter rotation curves...



Feedback and SF matter more than code type.

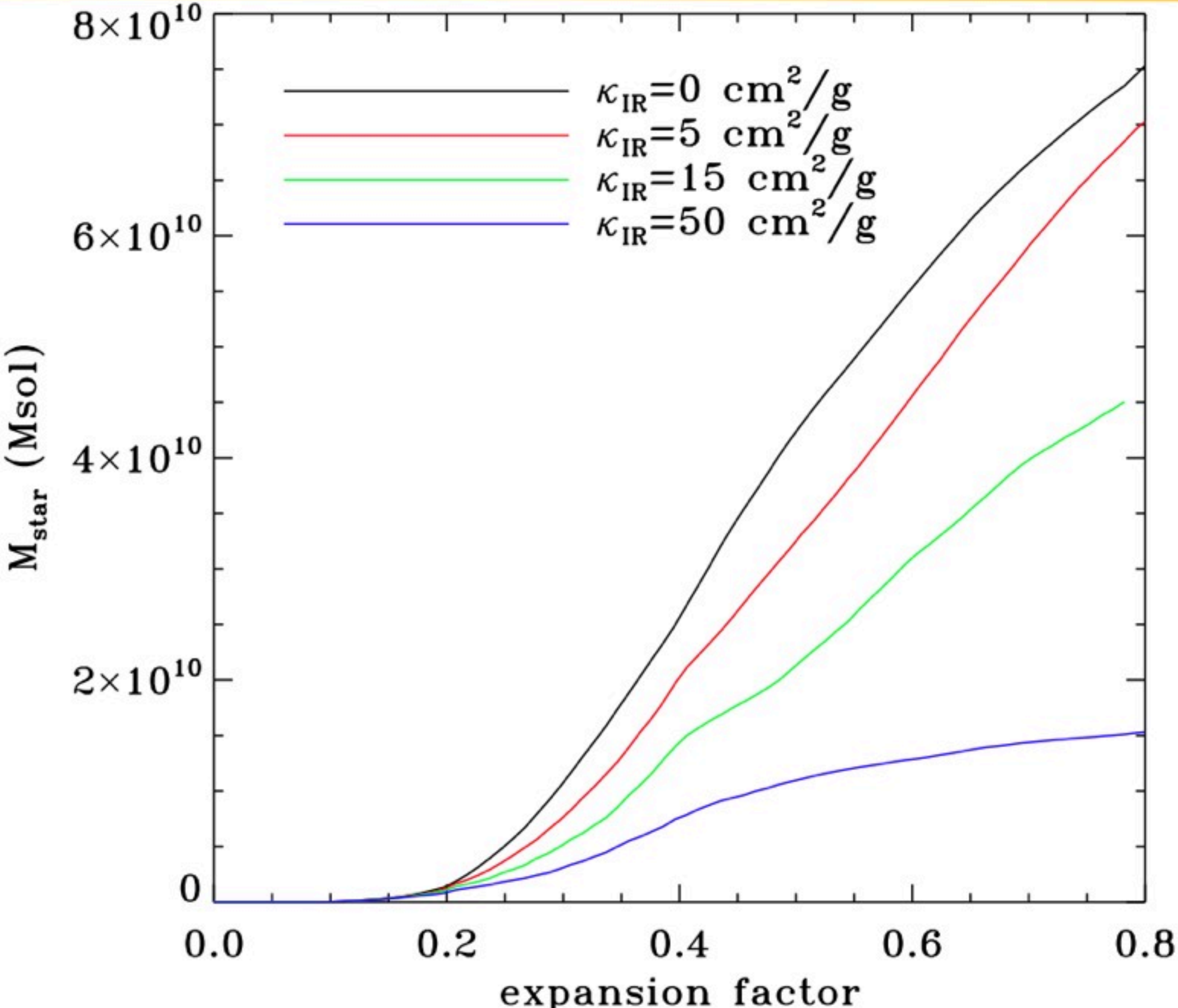


Dwarfs? Momentum-driven radiation feedback



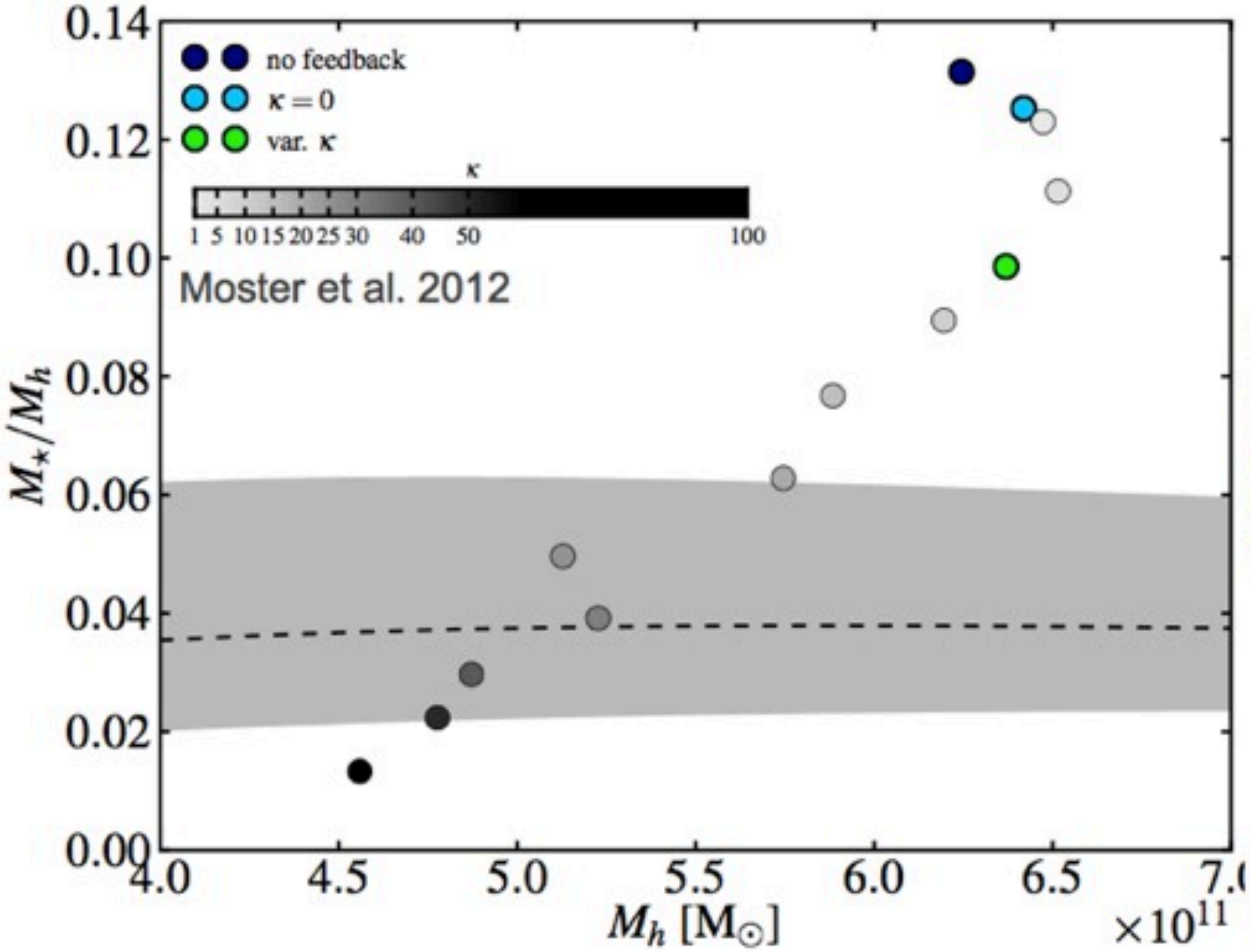
The pb of feedback is local energy deposit

Momentum-driven radiation feedback

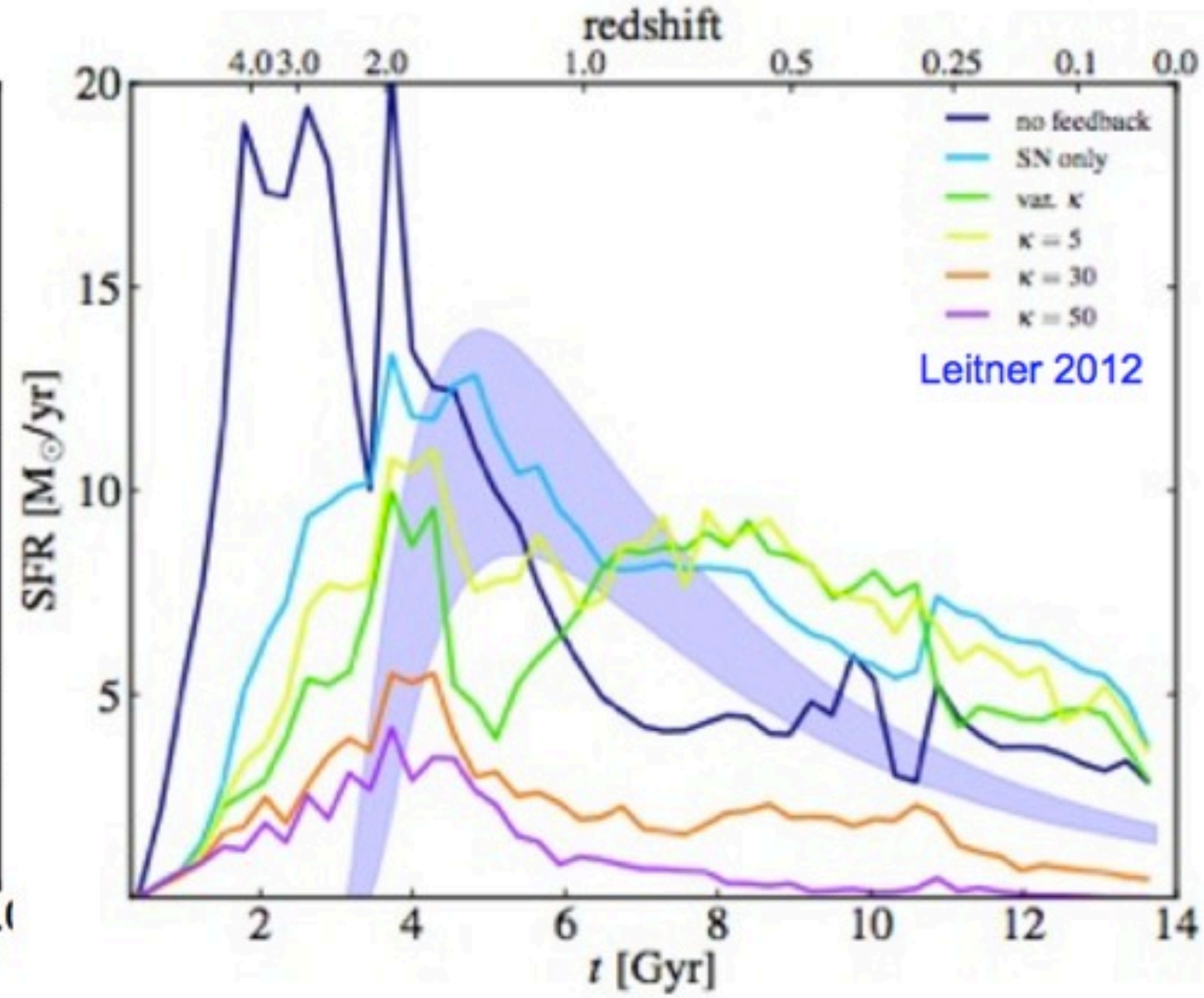


Star formation history

Roskar+13



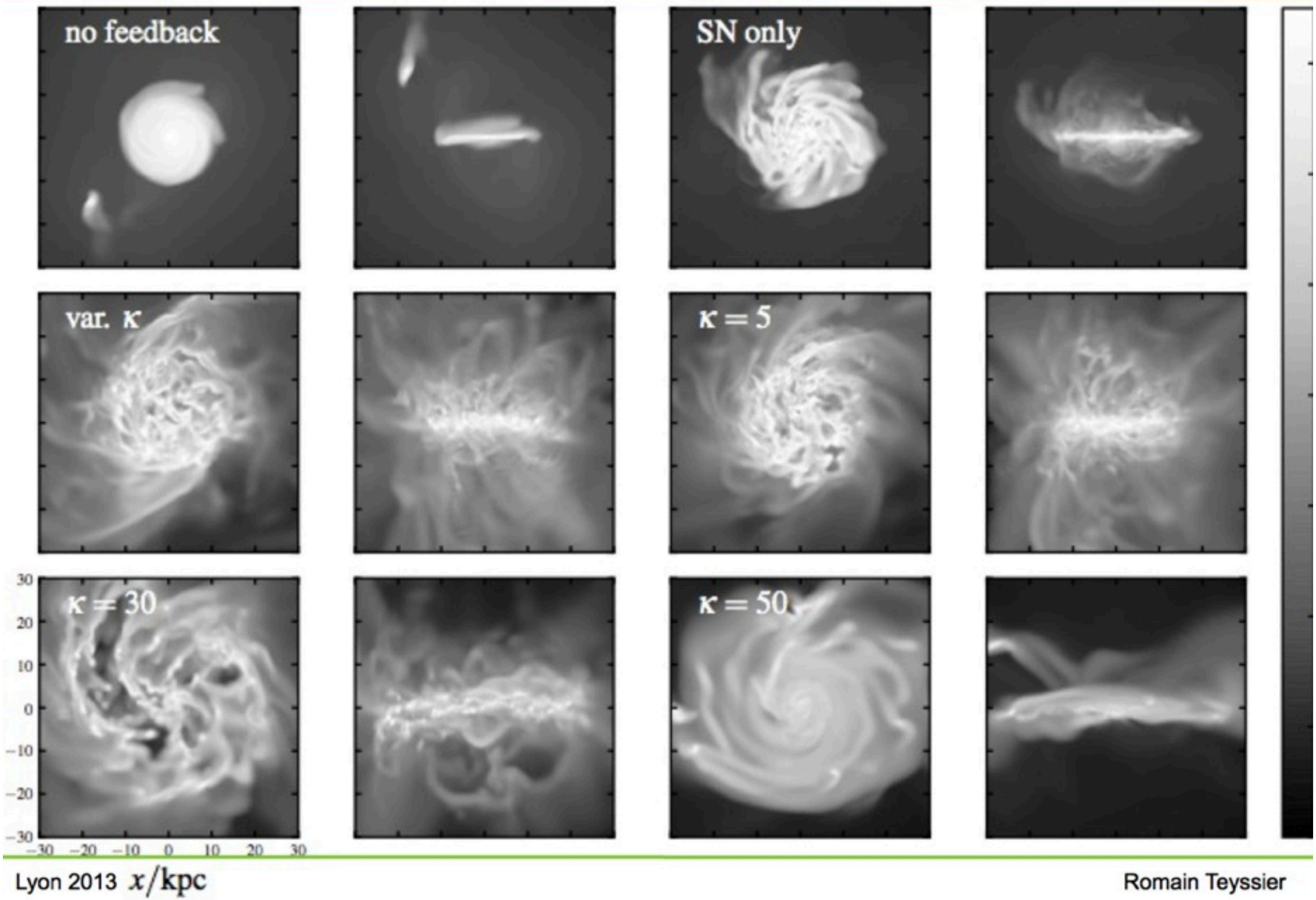
Abundance matching



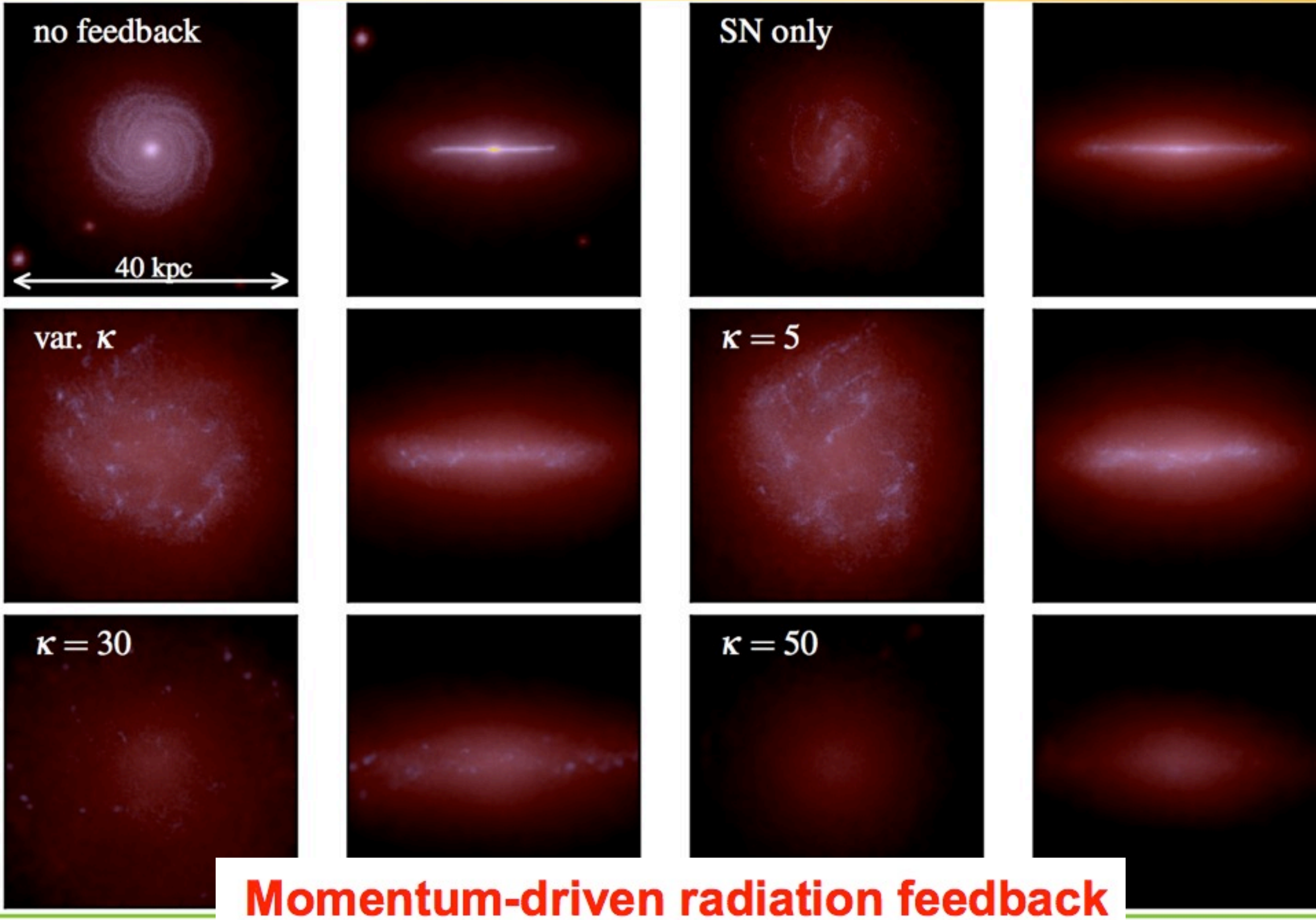
Star formation history

Momentum-driven radiation feedback

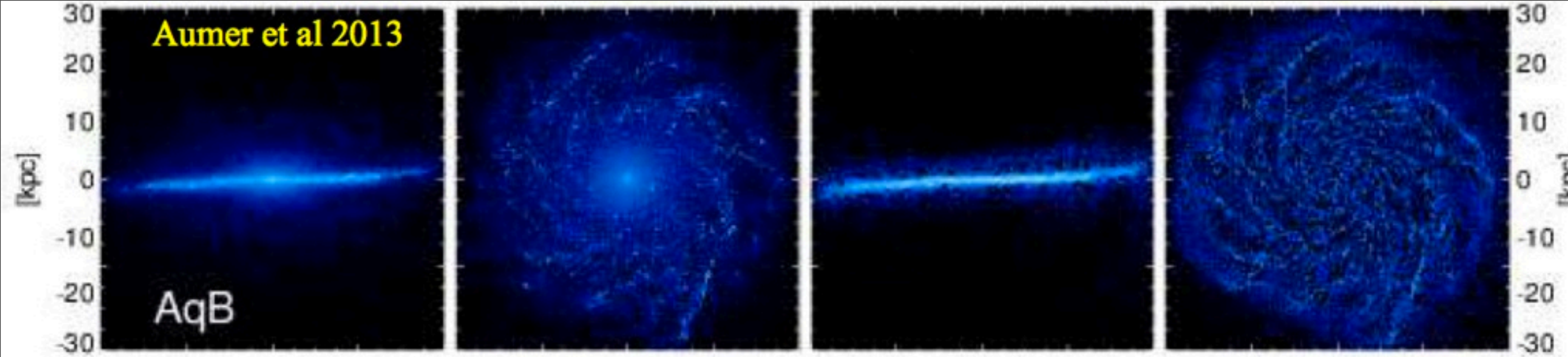
Final gas distribution: from fountains to winds



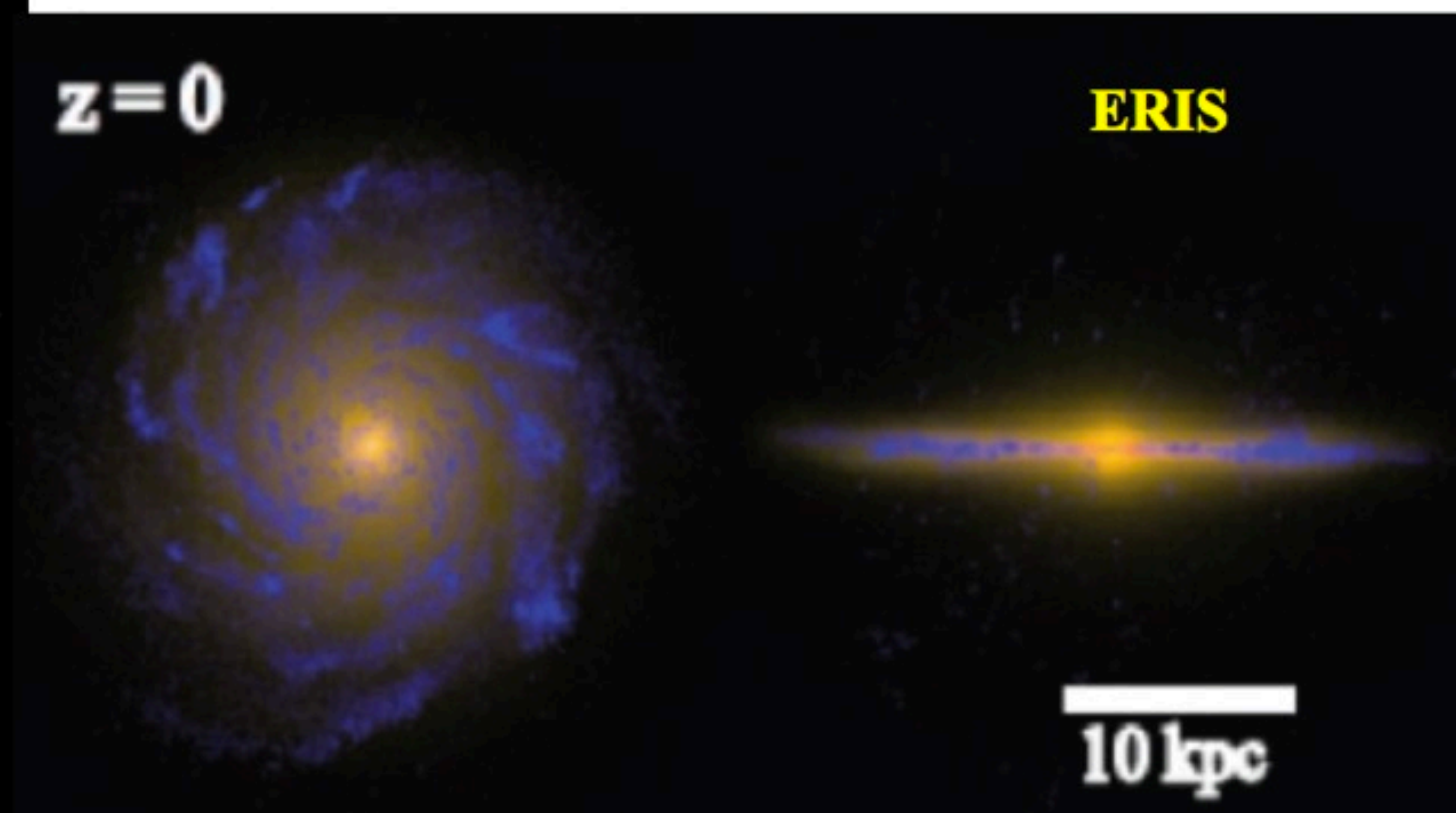
Final stellar distribution: from disks to spheroids



Momentum-driven radiation feedback



Several groups now make viable Milky Ways. They have different, differently implemented and incomplete “subgrid” phenomenology. The agreement is a result of parameter tuning



Guedes et al. 2011, 2012

CONCLUSION

Many interacting physical processes are important and span a very wide range of physical scales

Many cannot be resolved and so must be handled by phenomenological "subgrid" models

These are typically highly simplified, incomplete and uncertain, involving various undetermined parameters

Parameter ***tuning*** may give a good fit to observation but this does **not** necessarily imply **correctness** of model

CONCLUSIONS

- Galaxy formation is still poorly understood in details: even ***one*** point function such as stellar mass in galaxies is a challenge.
- Galaxy formation is highly *nonlinear* and sensitive to sub-grid *recipes*, to *numerical* implementations, and to *cosmology*. These are ***not*** easily separated.
- Feedback effects in a galaxy formation affect the mass power spectrum at ~ percent level even at λ ~ 10 Mpc : "precision" cosmology??

Why?

PROS

- properly account for scale coupling/ anisotropy
- allow for visualisation of the effect of complex processes
- decide quantitatively which non-linear process dominates
- make (large) virtual data sets/ surveys;
- validate inverse methods;
- build realistic estimators/ model biases;
- calibrate new instrument:

  how well can we measure things from

  a given *incomplete* survey?
- estimate error bars/covariance matrices;
- validate perturbation theory

CONS

- Most players present a very skewed view of success/failure
- can be Garbage In Garbage Out
- Misleading because *too* convincing compared to thought experiments
- Sometimes, domain of scientific interest of zero measure
- Chaotic solution possibly driven by algorithmic limitation
- Sociologic bias towards runaway: code validation sporadic
- A lot of work !

  * write a code
  * validate the code
  * run the simulations : big mock data (@ IAP ~ PB)
  * validate the simulation
  * produce virtual observables
  * write the estimator
  * validate the estimator
  * explore domain of relevance * study biasses

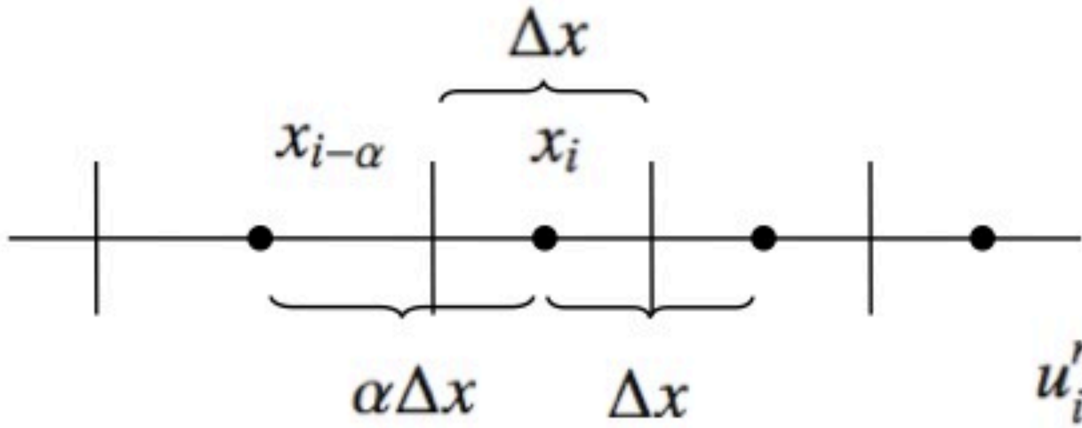
Hockney, R.W. and Eastwood, J.W. 1988, "Computer Simulation Using Particles", Taylor & Francis
Simulations of Structure Formation in the Universe" Bertschinger, E. 1998, ARA&A, 36, 599

http://www.ics.uzh.ch/~teyssier/Teaching.html
http://www.astro.iag.usp.br/~xiiieaa/talks/springel-1.pdf

http://arxiv.org/pdf/astro-ph/0411730v1.pdf
http://www.scholarpedia.org/article/N-body_simulations_(gravitational)

http://horizon-simulation.org
http://www.cosmicorigin.org
http://illustris-project.org
http://projet-horizon.fr
http://icc.dur.ac.uk/Eagle/

The AMR catastrophe



Assume a and C>0.

$$u_{i+1/2}^{n+1/2} = u_i^n + (1-C)\frac{\Delta x}{2}\left(\frac{\partial u}{\partial x}\right)_i$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a\frac{u_{i+1/2}^{n+1/2} - u_{i-1/2}^{n+1/2}}{\Delta x} = 0$$

$$u_{i-1/2}^{n+1/2} = u_{i-\alpha}^n + (2\alpha - 1 - C)\frac{\Delta x}{2}\left(\frac{\partial u}{\partial x}\right)_{i-1}$$

First order scheme: $$\left(\frac{\partial u}{\partial t}\right) + \alpha a\left(\frac{\partial u}{\partial x}\right) = a\frac{\Delta x}{2}(\alpha^2 - C)\left(\frac{\partial^2 u}{\partial x^2}\right) + O(\Delta t^2, \Delta x^2)$$

Second order scheme: $$\left(\frac{\partial u}{\partial t}\right) + a\left(\frac{\partial u}{\partial x}\right) = a\frac{\Delta x}{2}(\alpha - C)(1-\alpha)\left(\frac{\partial^2 u}{\partial x^2}\right) + O(\Delta t^2, \Delta x^2)$$

At level boundary, we loose one order of accuracy in the modified equation.

First order scheme: the AMR extension is *not consistent* at level boundary.

Second order scheme: for α=1.5, AMR is *unstable* at level boundary.

Solutions: 1- refine gradients, 2- enforce first order, 3- add artificial diffusion