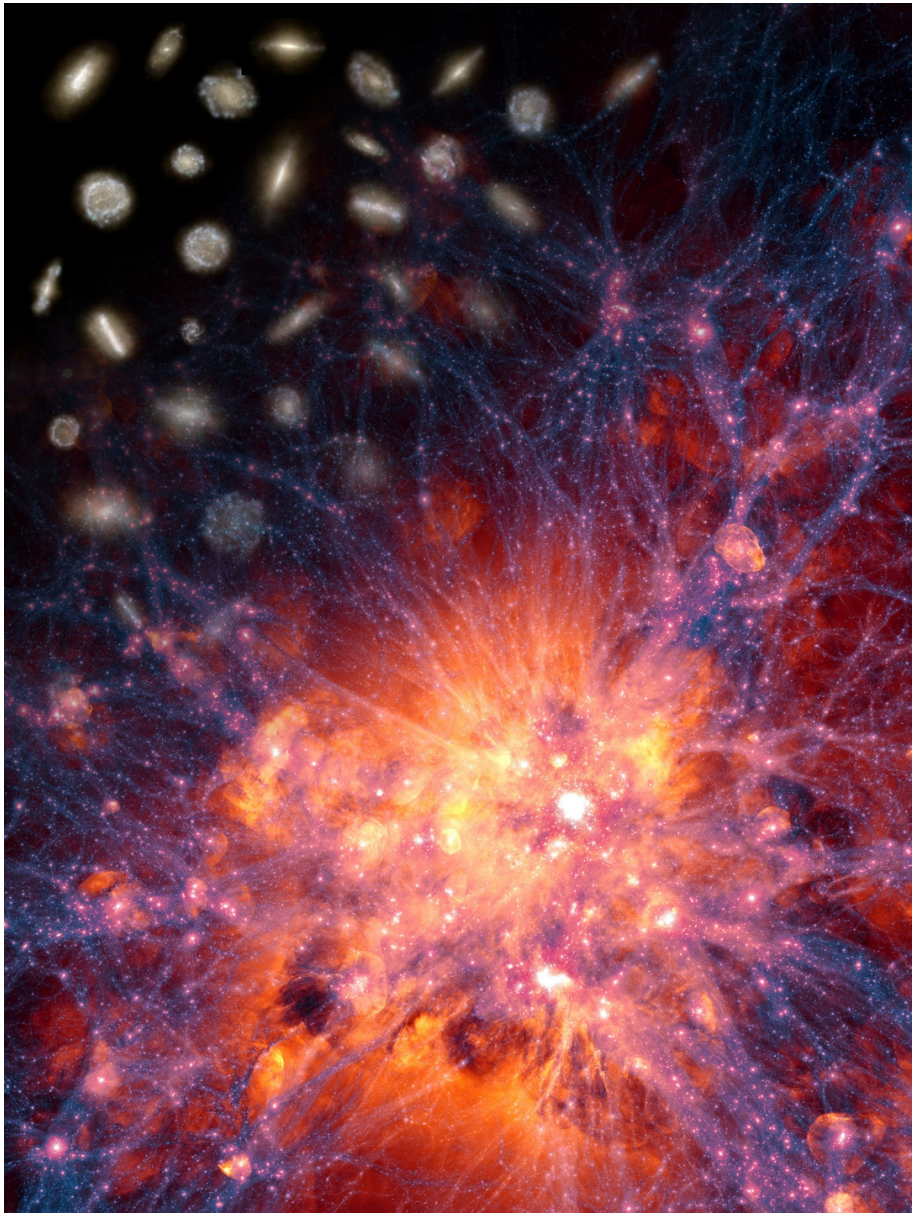
Exascale simulations of the magnetic universe (EXAMAG)



Prof. Dr. Volker Springel

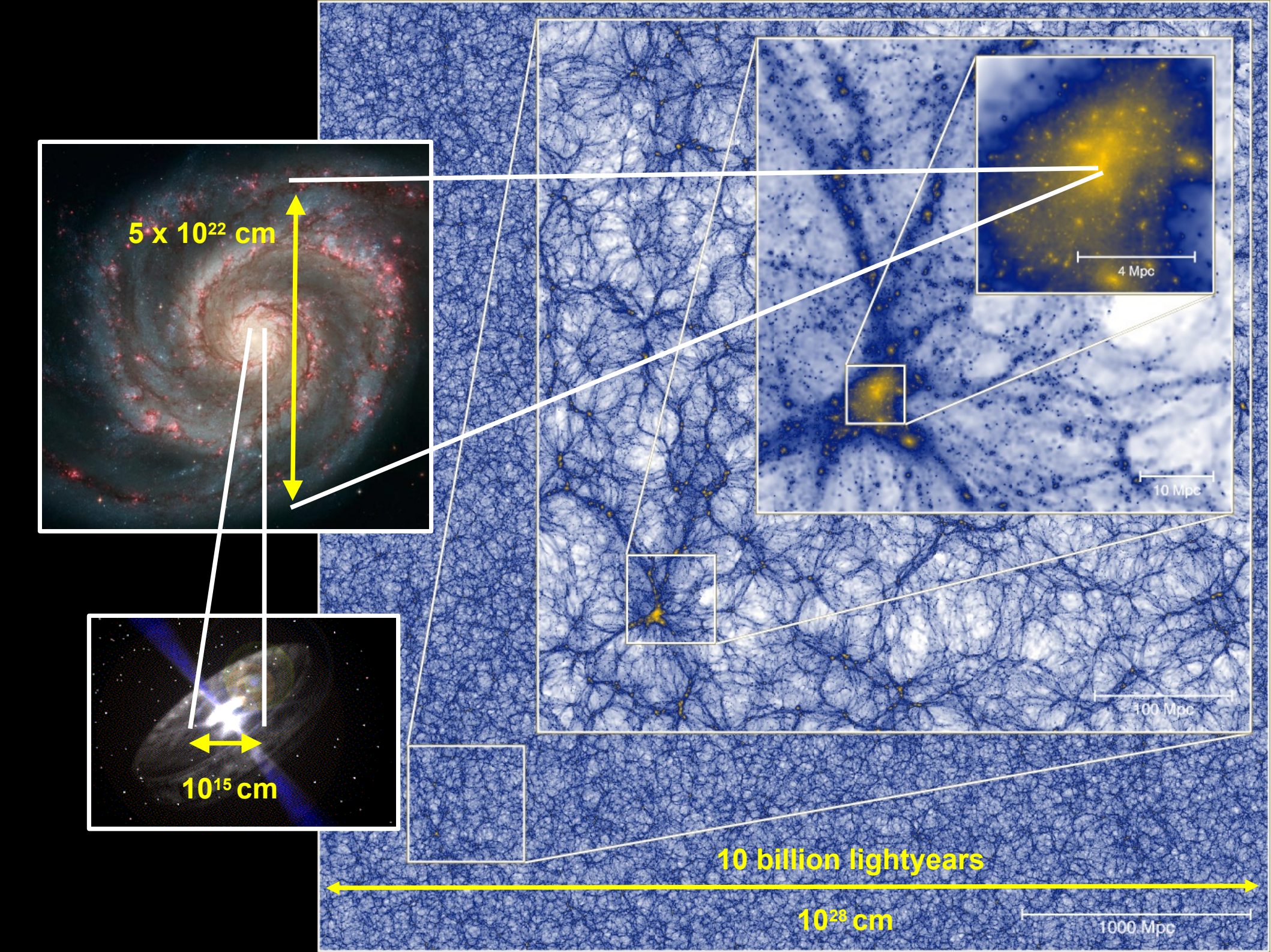
Other EXAMAG PIs:

Prof. Dr. Christian Klingenberg (Würzburg)

Prof. Dr. Naoki Yoshida (Tokyo)

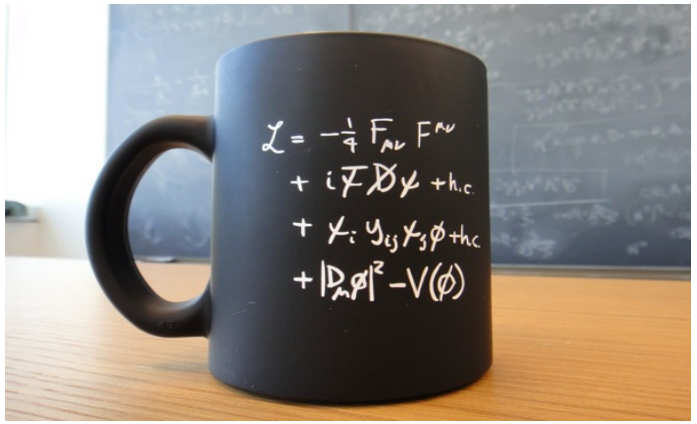
Prof. Dr. Philippe Helluy (Strasbourg)

- **Project motivation**
- **Some recent science results**
- **Some technical developments**


5 x 10^22 cm
10^15 cm
4 Mpc
10 Mpc
100 Mpc
1000 Mpc
10 billion lightyears
10^28 cm

Much of astrophysics is described through systems of **Partial Differential Equations (PDEs)**

UNDERSTANDING THE PHYSICS REQUIRES SOLVING THESE EQUATIONS



- Euler/Navier-Stokes equations
- Collisionless dynamics
- Maxwell's equations
- Radiative transfer
- General relativity

hyperbolic conservation laws of fluid dynamics

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \mathbf{v}) = 0$$

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla(\rho \mathbf{v}\mathbf{v}^T + P) = \nabla \mathbf{\Pi}$$

$$\frac{\partial}{\partial t}(\rho e) + \nabla[(\rho e + P)\mathbf{v}] = \nabla(\mathbf{\Pi}\mathbf{v})$$

Poisson-Vlasov system

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \mathbf{x}} \cdot \mathbf{v} + \frac{\partial f}{\partial \mathbf{v}} \cdot \left(-\frac{\partial \Phi}{\partial \mathbf{x}} \right) = 0$$

$$\nabla^2 \Phi(\mathbf{x}, t) = 4\pi G \int f(\mathbf{x}, \mathbf{v}, t)\, \mathrm{d}\mathbf{v}$$

Main goals of the EXAMAG Project: **Software for exascale science realized by a team of astrophysicists and mathematicians**

Improve hydro discretizations (code accuracy & efficiency)

- Complete high-order discontinuous Galerkin methods on static and moving meshes
- Formulate improved MHD treatments
- Improve robustness for large timesteps with new positivity preserving schemes

Implement new types of solvers (physics capabilities)

- Anisotropic transport of cosmic rays & heat
- Primordial chemistry network for first star simulations
- Fast multipole method for better gravity performance

Enable use of exascale machines (code performance & scaling)

- Multi-threading in all code parts
- Implement GPU and many-core support
- Prepare for fault-tolerant calculations (MPI-3)
- Implement new hierarchical Hamiltonian time-stepping

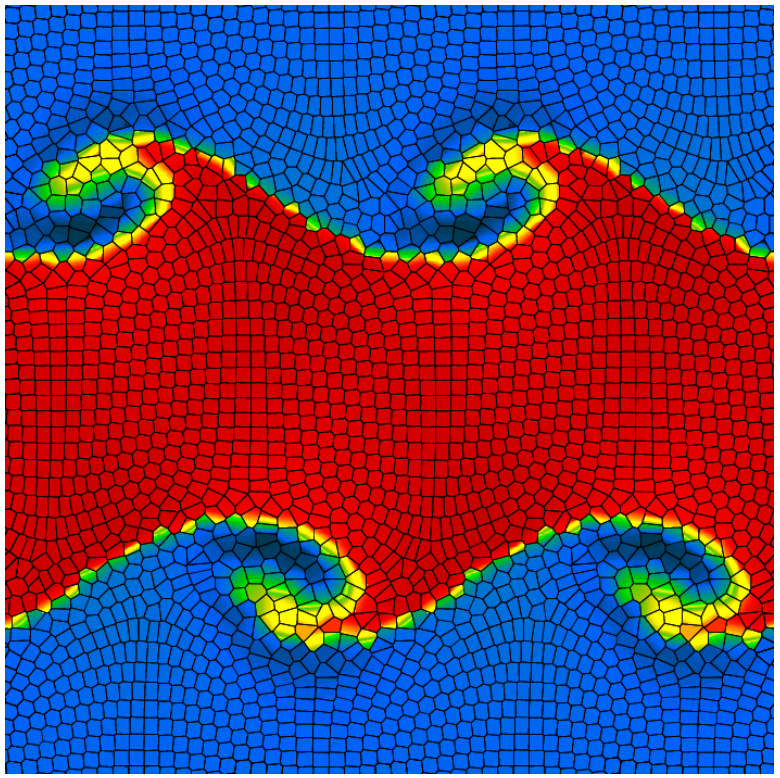
Apply codes at the leading edge (scientific exploitation)

- Push towards up initio calculations of the formation of Milky Way like galaxies
- Carry out state-of-the art simulations of cosmic structure formation that account for magnetic field and associated physics
- Do simulations of the first stars in the universe

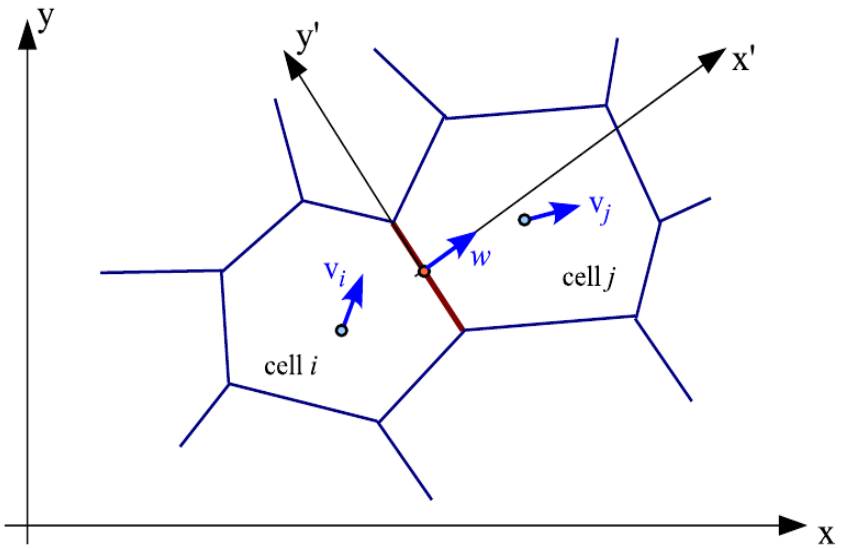
The **moving-mesh hydrodynamics AREPO** is ideally matched to cosmology

PRINCIPAL ADVANTAGES

- Low numerical viscosity, very low advection errors
- Full adaptivity and manifest Galilean invariance
- Makes larger timesteps possible in supersonic flows
- Crucial accuracy improvement over SPH technique



Sketch of flux calculation



The motion of the mesh generators uniquely determines the motion of all cell boundaries

State left of cell face $\begin{pmatrix} \rho_L \\ \mathbf{v}_L \\ P_L \end{pmatrix}$ **State right of cell face** $\begin{pmatrix} \rho_R \\ \mathbf{v}_R \\ P_R \end{pmatrix}$

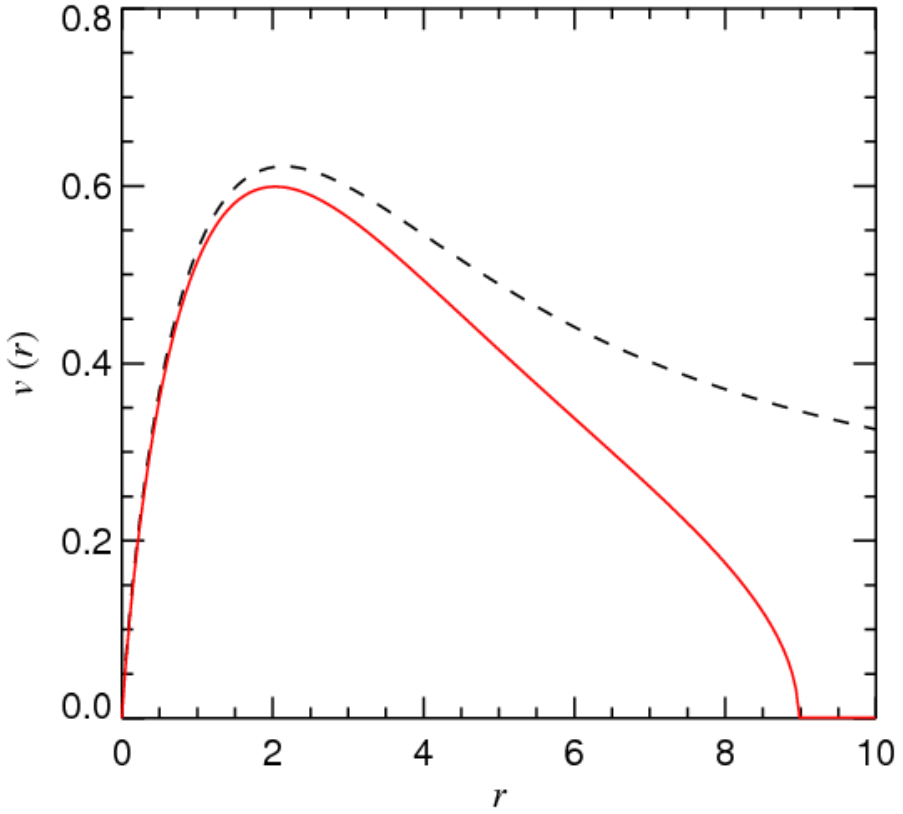
Riemann solver
(in frame of cell face) $\rightarrow \begin{pmatrix} \rho \\ \mathbf{v} \\ P \end{pmatrix} \rightarrow \mathbf{F}(\mathbf{U})$

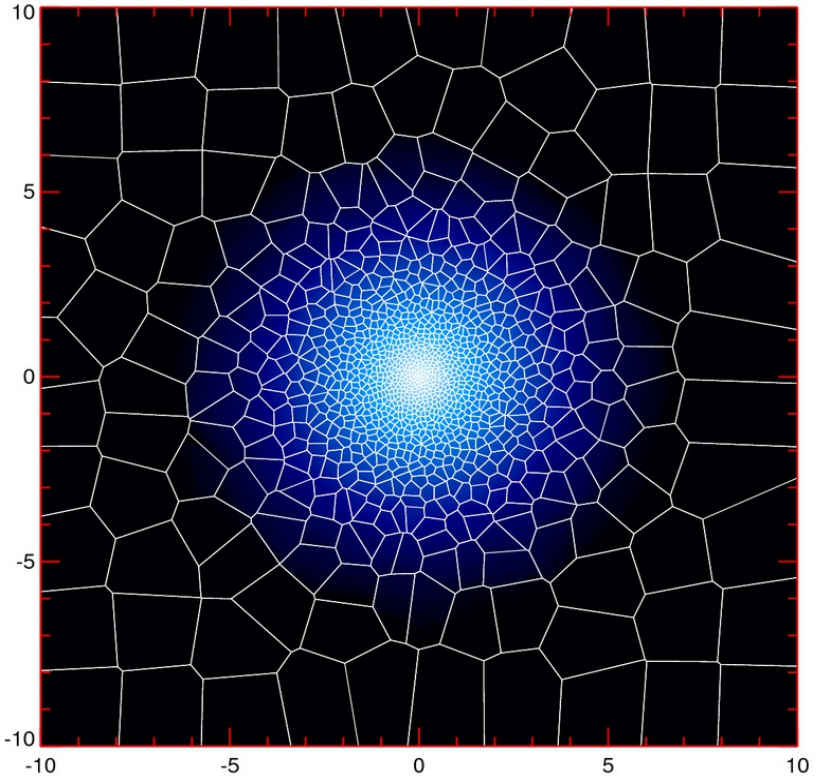
A differentially rotating gaseous disk with strong shear can be simulated well with the moving mesh code

MODEL FOR A CENTRIFUGALLY SUPPORTED, THIN DISK

$$\Sigma(r) = \Sigma_0 \exp(-r/h)$$

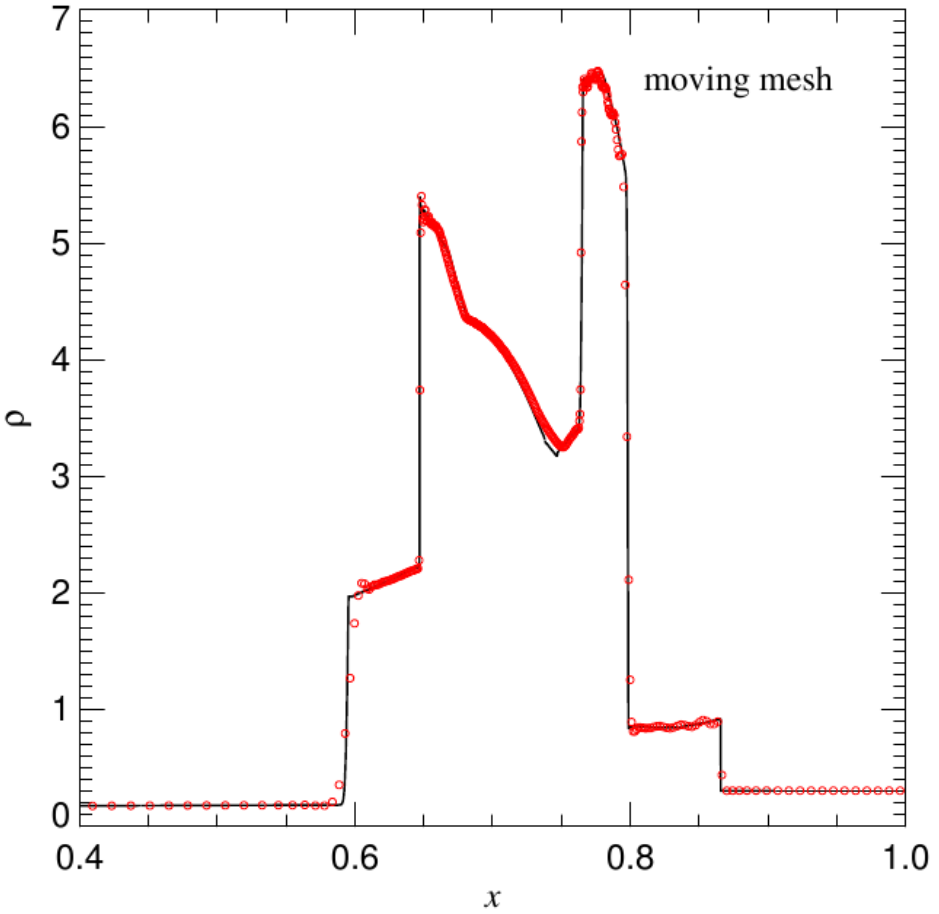
$$v_c^2(r) \equiv r\frac{\partial \Phi}{\partial r} = 2\frac{Gm}{h}y^2\left[I_0(y)K_0(y) - I_1(y)K_1(y)\right]$$

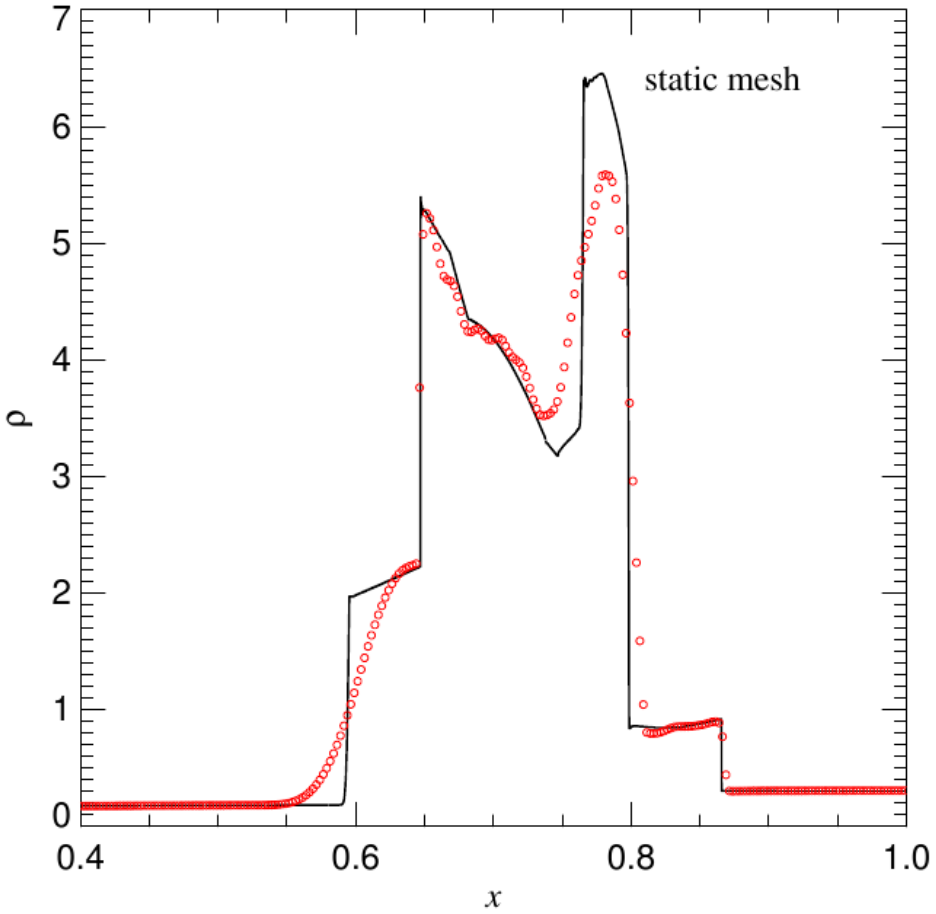




The moving-mesh code deals well will problems that involve complicated shock interactions

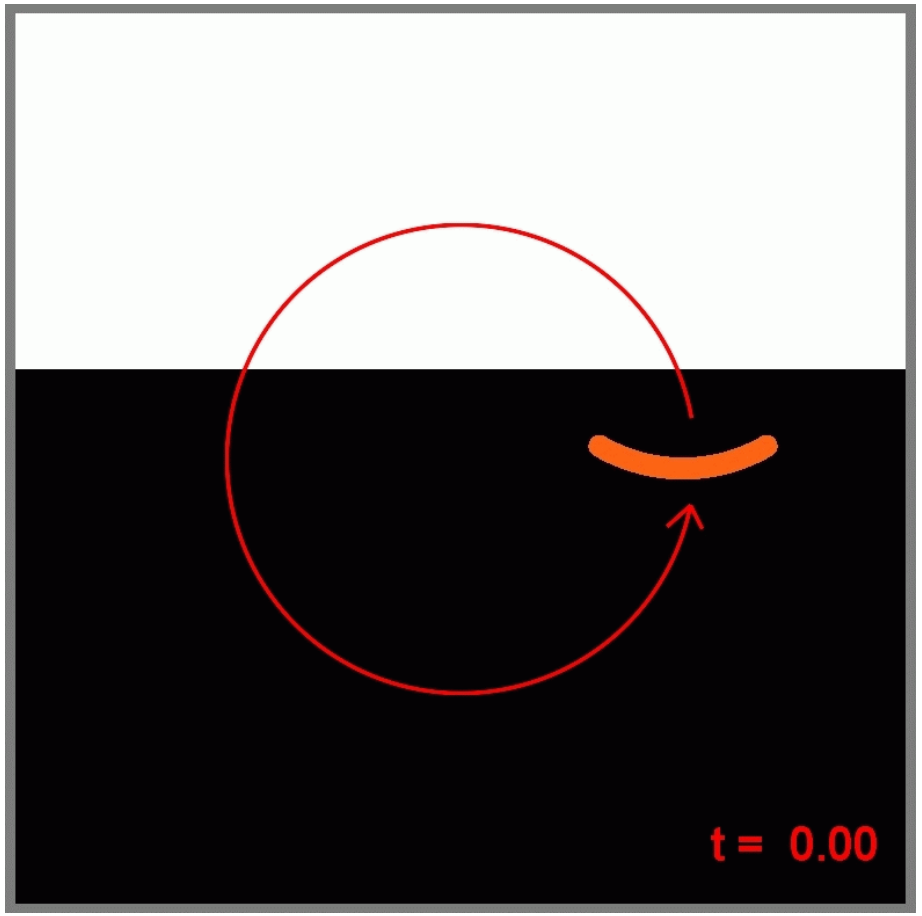
WOODWARD & COLELLA'S INTERACTING DOUBLE BLAST PROBLEM

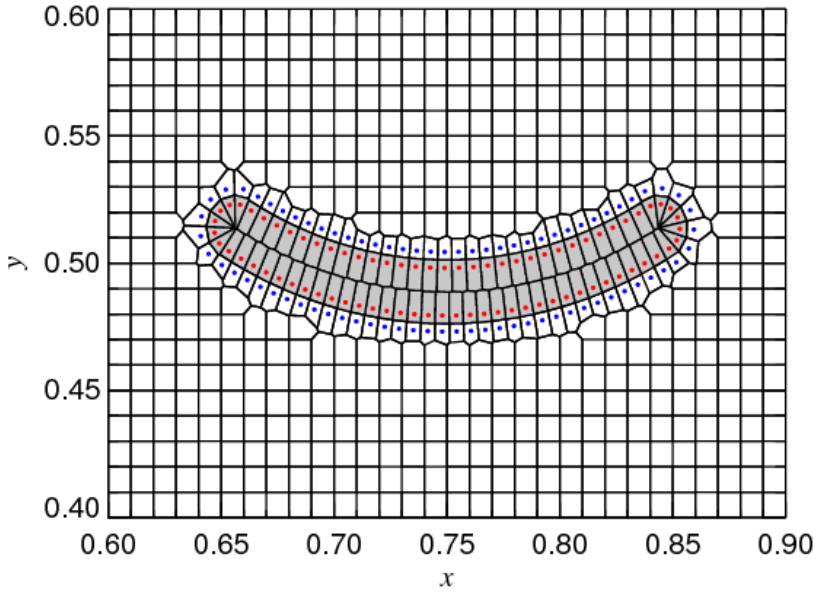


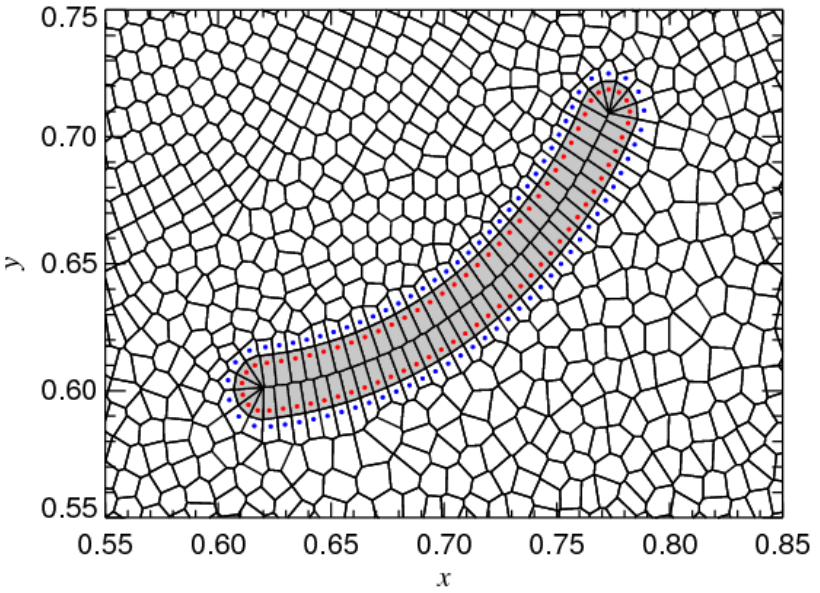


The moving-mesh approach can also be used to realize arbitrarily shaped, moving boundaries

STIRRING A COFFEE MUG

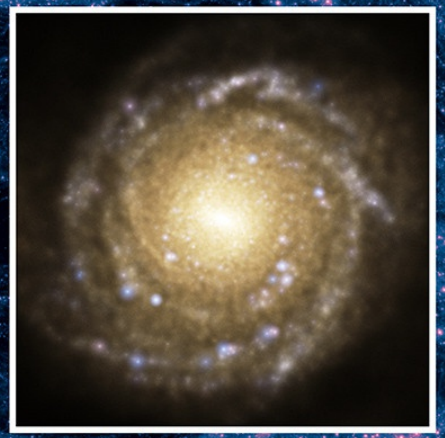


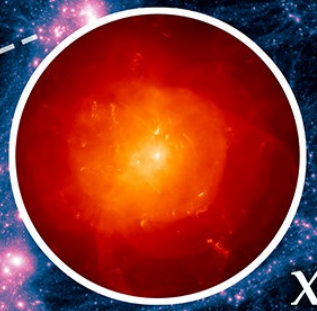


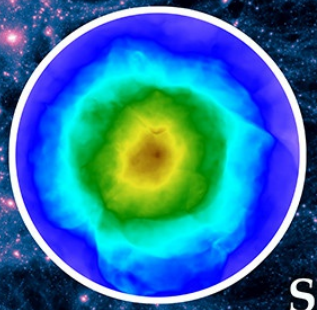


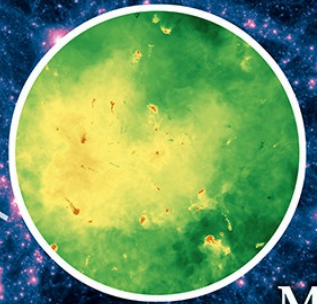
The Illustris Simulation

M. Vogelsberger S. Genel V. Springel P. Torrey D. Sijacki D. Xu G. Snyder S. Bird D. Nelson L. Hernquist







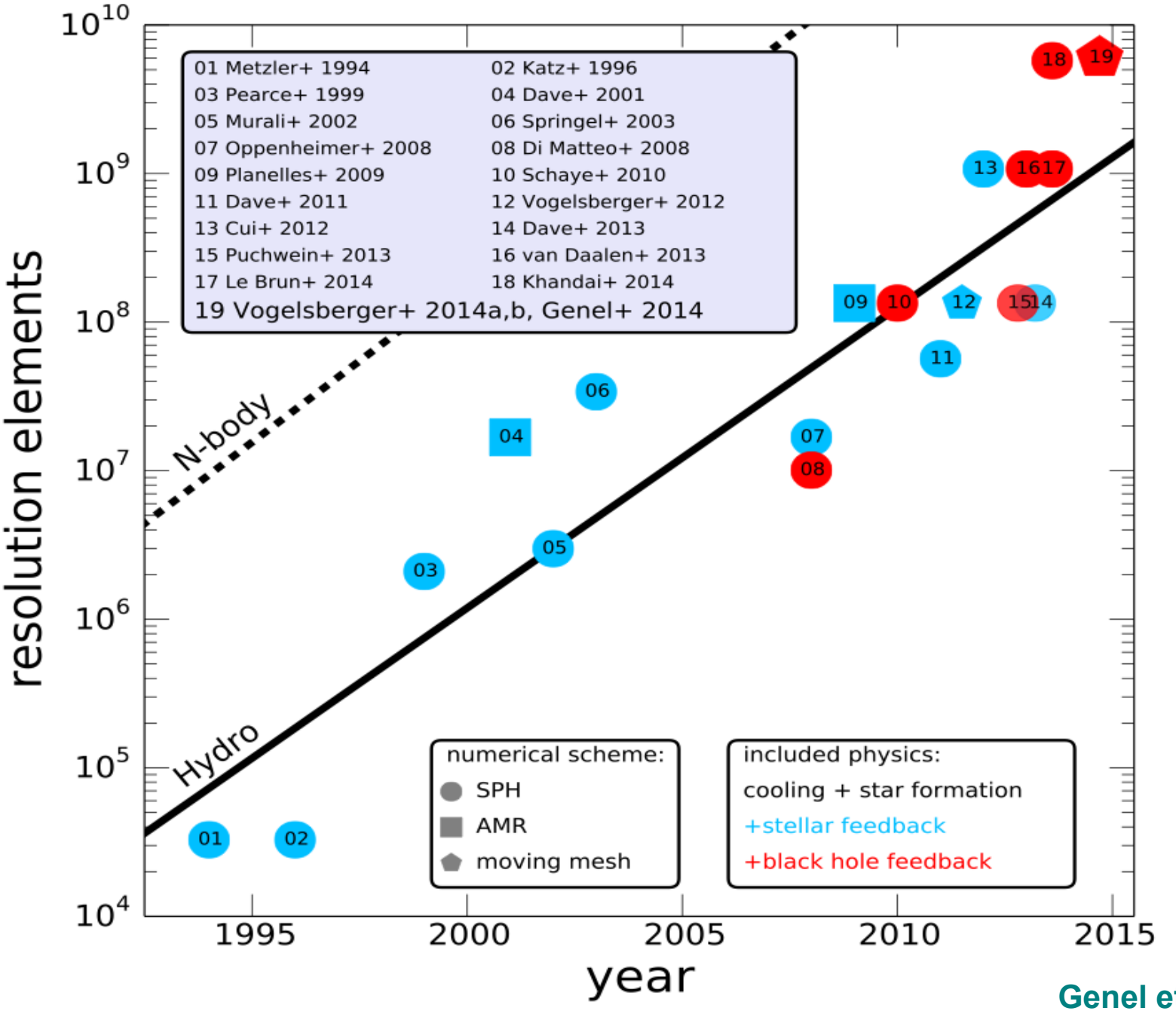


Dark Matter Density

Gas Density

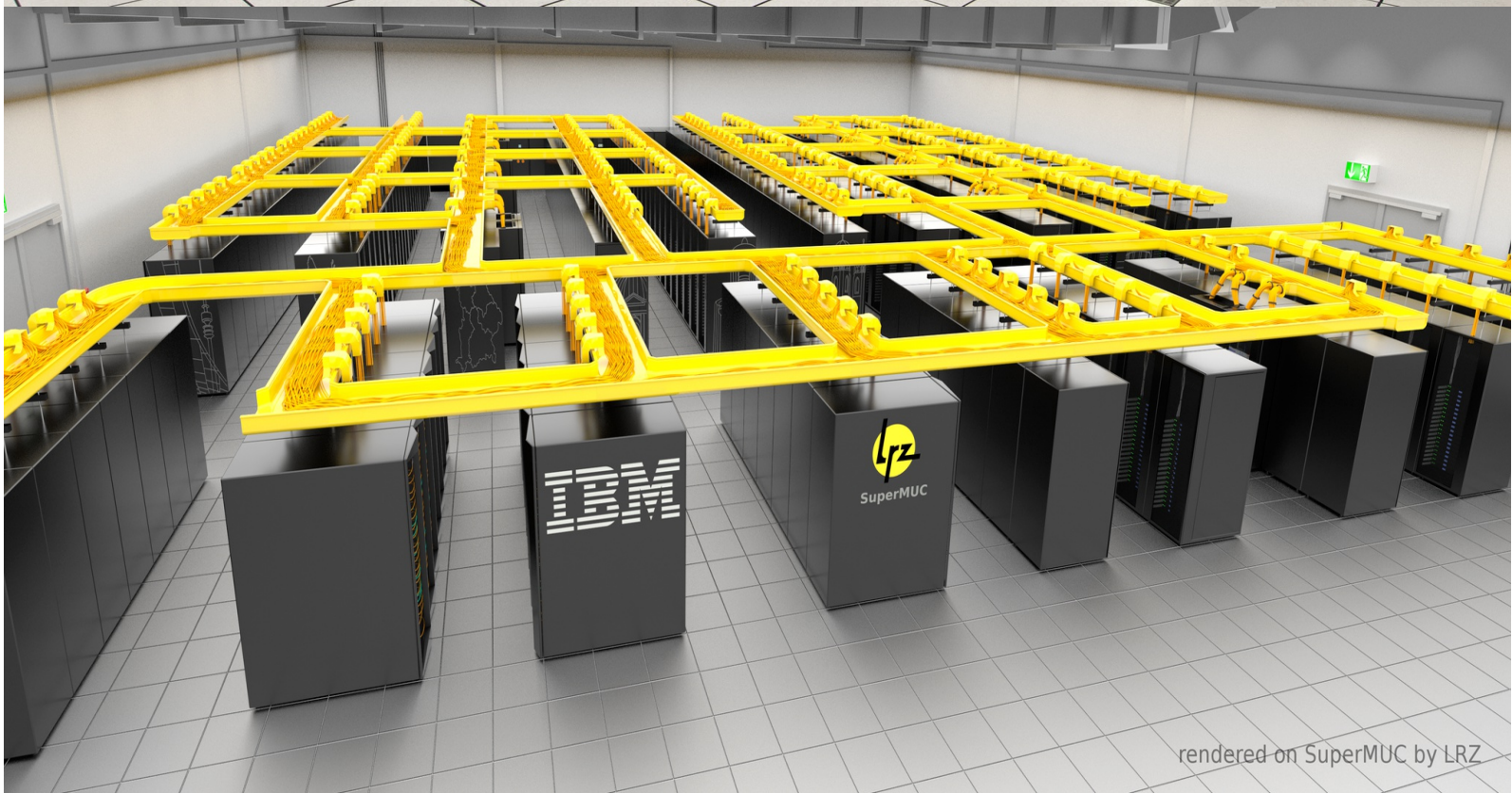
Hydrodynamical simulation sizes as a function of publication date

SIMULATIONS EVOLVED TO Z = 0 WITH COOLING AND STAR FORMATION



Genel et al. (2014)

Illustris was executed on CURIE (France) and SuperMUC (Germany)

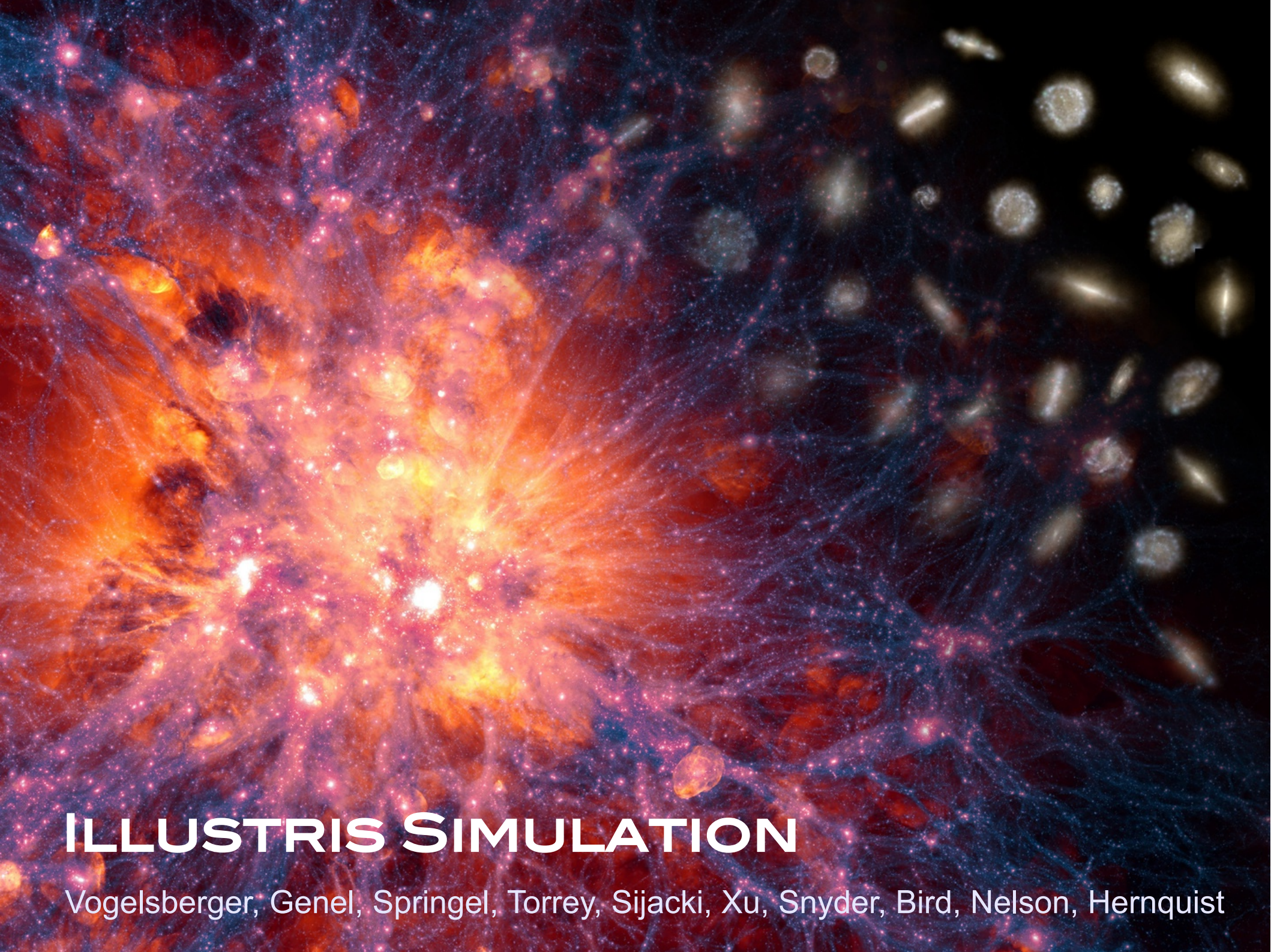


rendered on SuperMUC by LRZ

GCS
Gauss Centre for Supercomputing

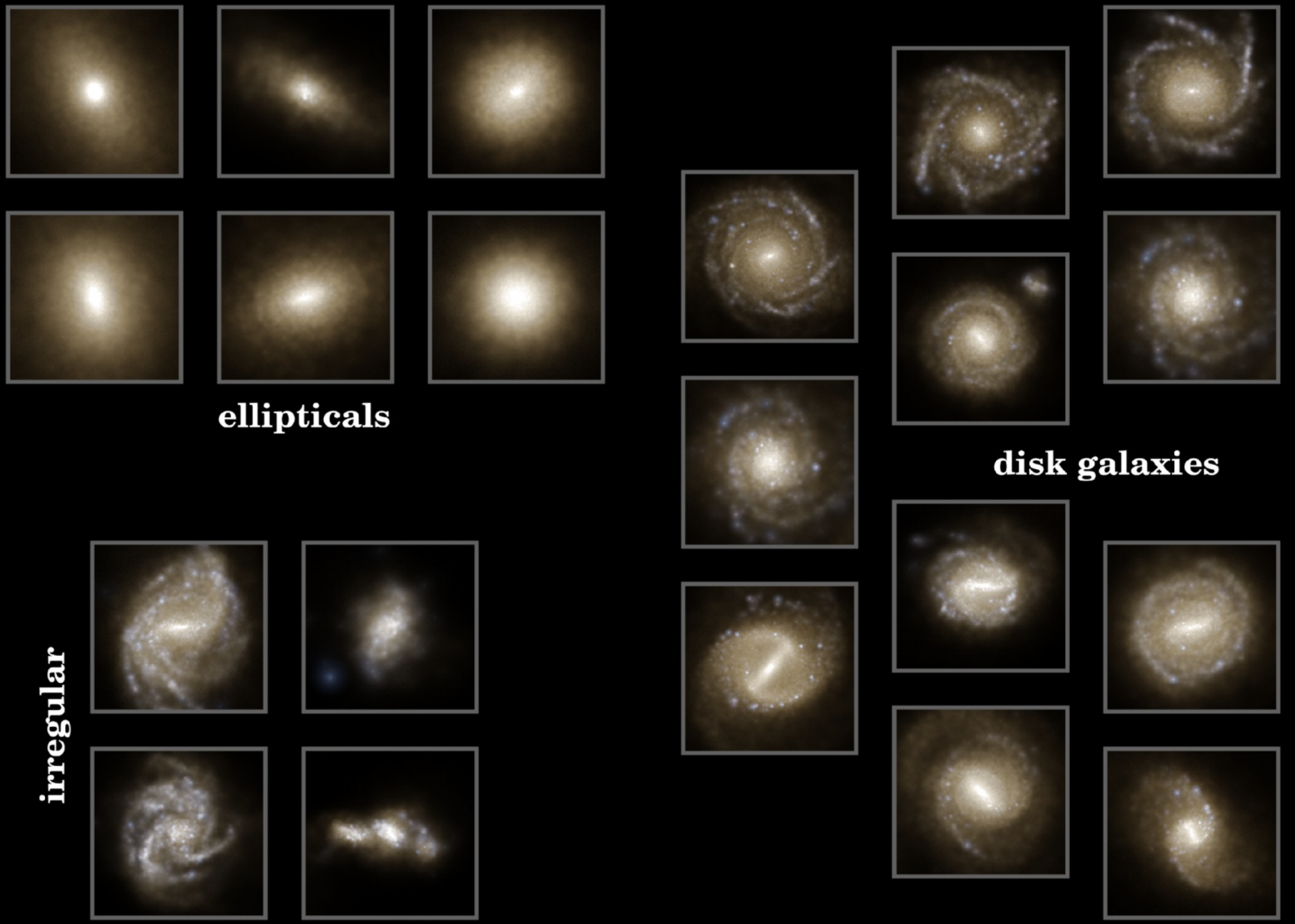
PRACE

XSEDE
Extreme Science and Engineering Discovery Environment


Illustris Simulation
Vogelsberger, Genel, Springel, Torrey, Sijacki, Xu, Snyder, Bird, Nelson, Hernquist

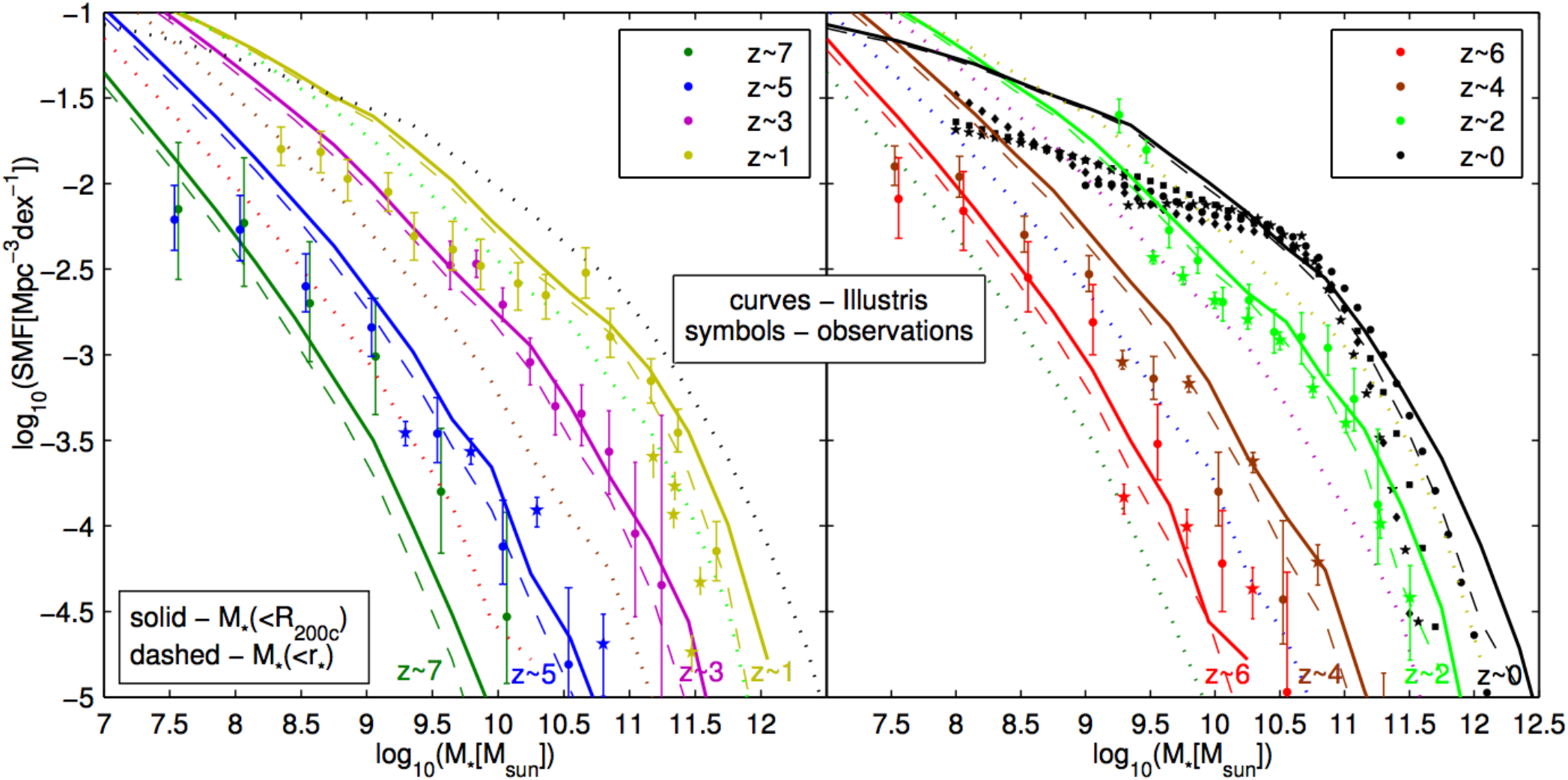
The Illustris simulation reproduces the morphological mix of galaxies

SIMULATED HUBBLE TUNING FORK DIAGRAM



The stellar mass functions match observations at high redshift well

STELLAR MASS FUNCTIONS OF ILLUSTRIS COMPARED TO HIGH-Z OBSERVATIONS



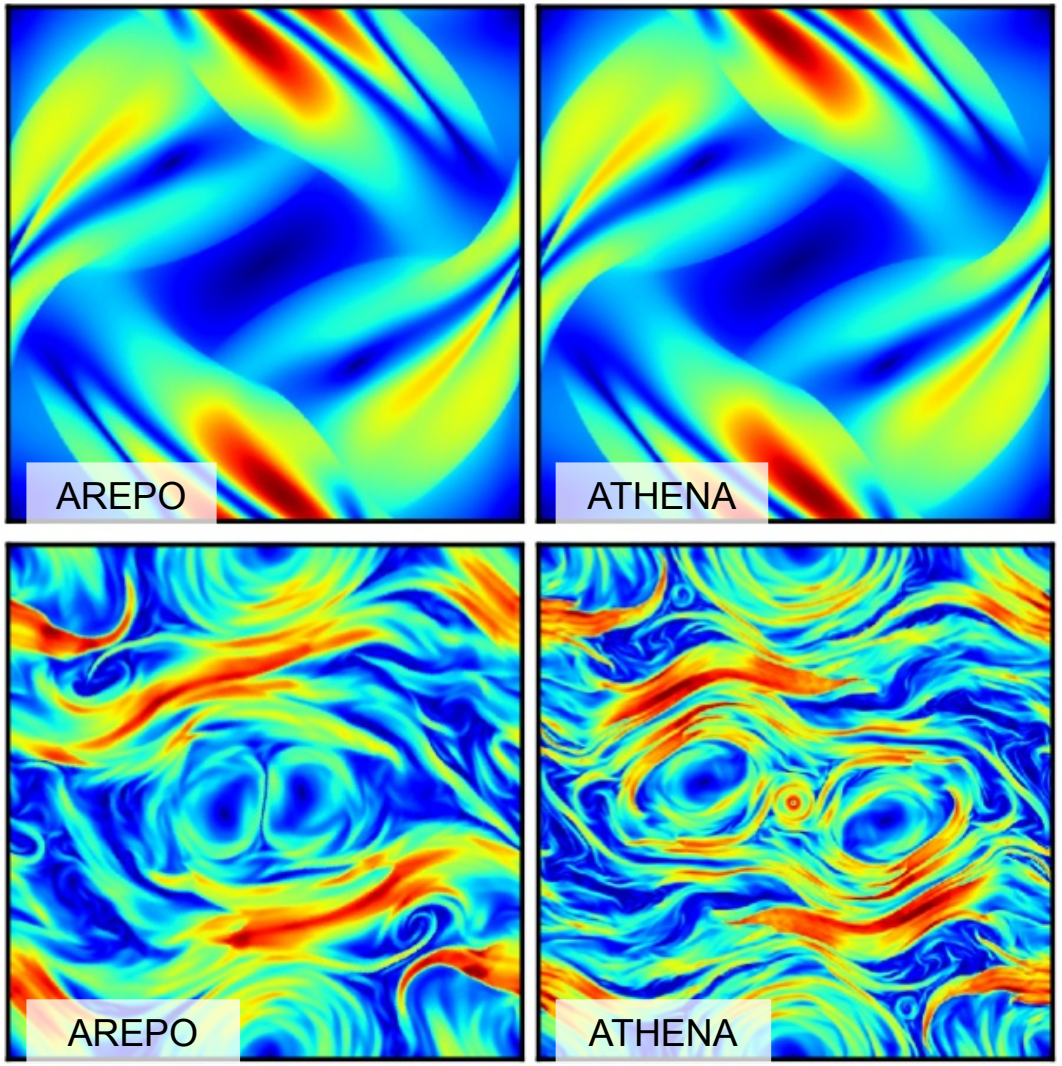
Genel et al. (2014)

We have an ideal MHD implementation in AREPO that seems to work well

EQUATIONS AND SOME TESTS

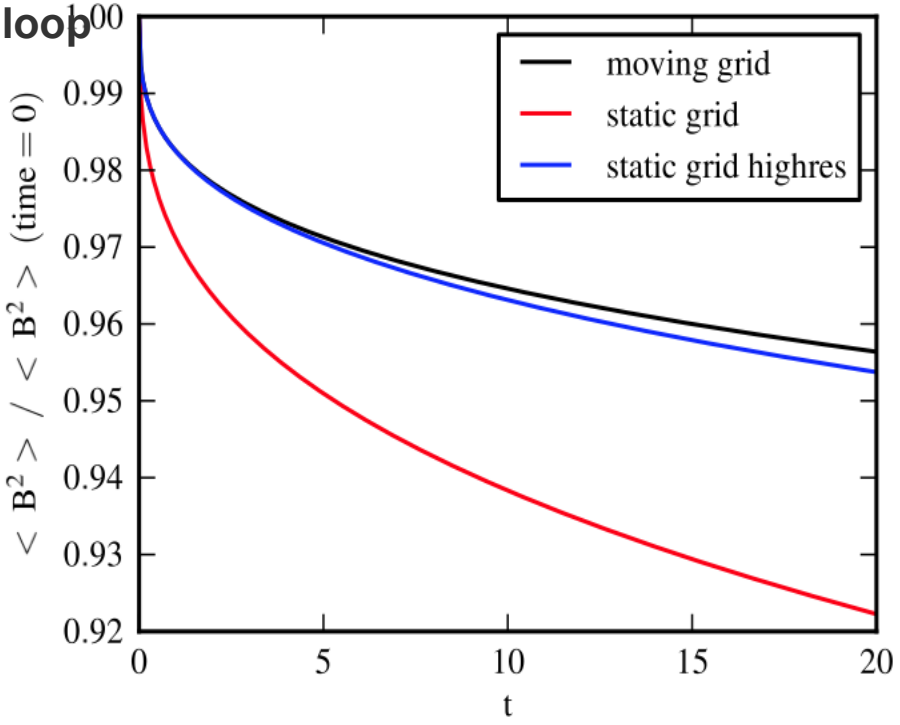
$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho\mathbf{v} \\ \rho e \\ \mathbf{B} \\ \psi \end{pmatrix} \qquad \mathbf{F}(\mathbf{U}) = \begin{pmatrix} \rho\mathbf{v} \\ \rho\mathbf{v}\mathbf{v}^T + p - \mathbf{B}\mathbf{B}^T \\ \rho e\mathbf{v} + p\mathbf{v} - \mathbf{B}\,(\mathbf{v}\cdot\mathbf{B}) \\ \mathbf{B}\mathbf{v}^T - \mathbf{v}\mathbf{B}^T + \psi I \\ c_h^2\mathbf{B} \end{pmatrix}$$

Orszag-Tang vortex test



- 8-wave Powell scheme for divergence cleaning
- Approximate HLLD Riemann solver

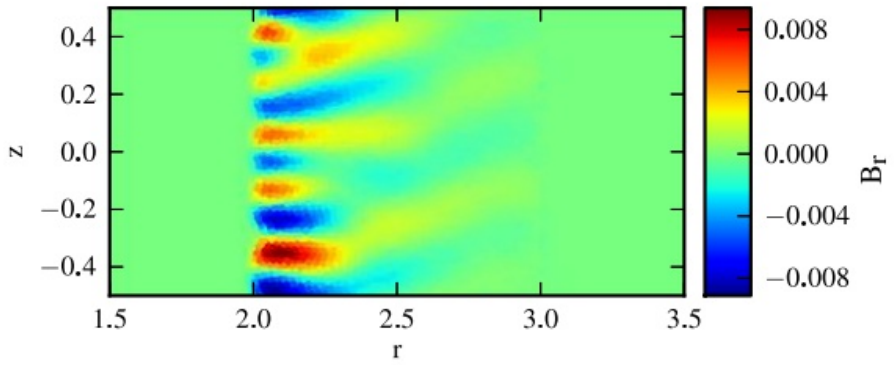
Loss of magnetic energy in moving field loop

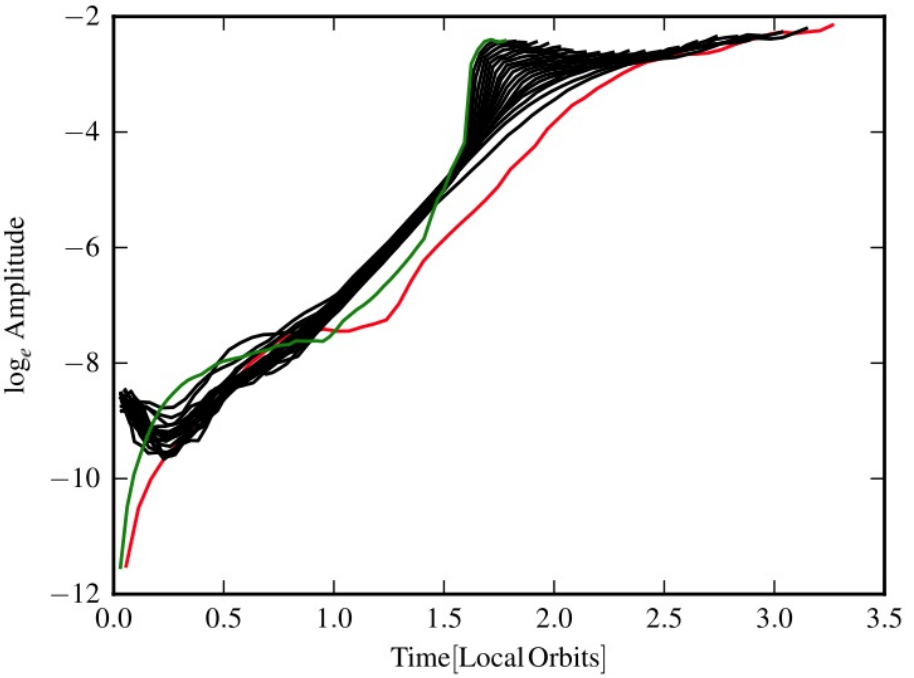


The MHD implemention gives the correct growth rate of the MRI

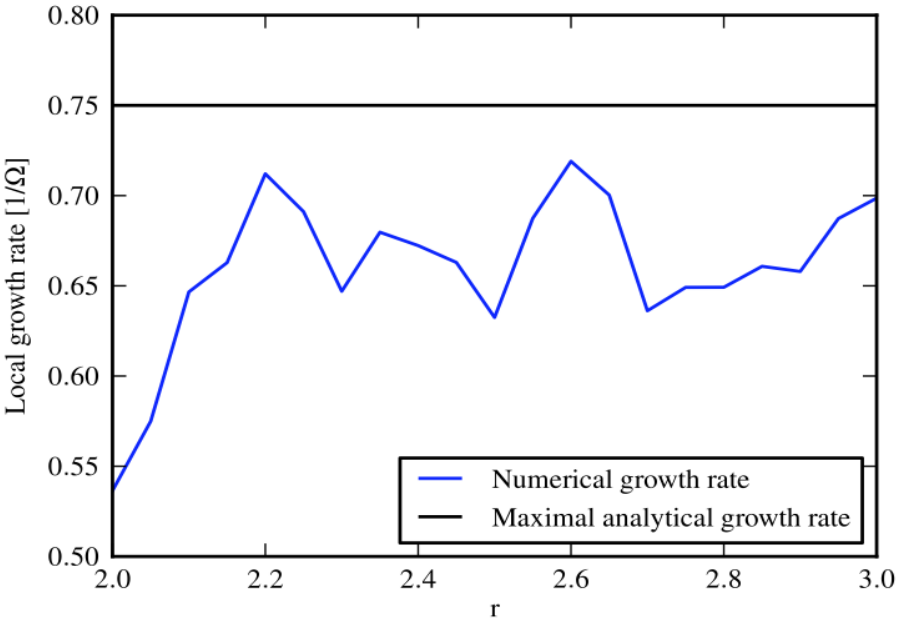
MAGNETO-ROTATIONAL INSTABILITY SIMULATED WITH AREPO

Magneto-rotational instability in 3D



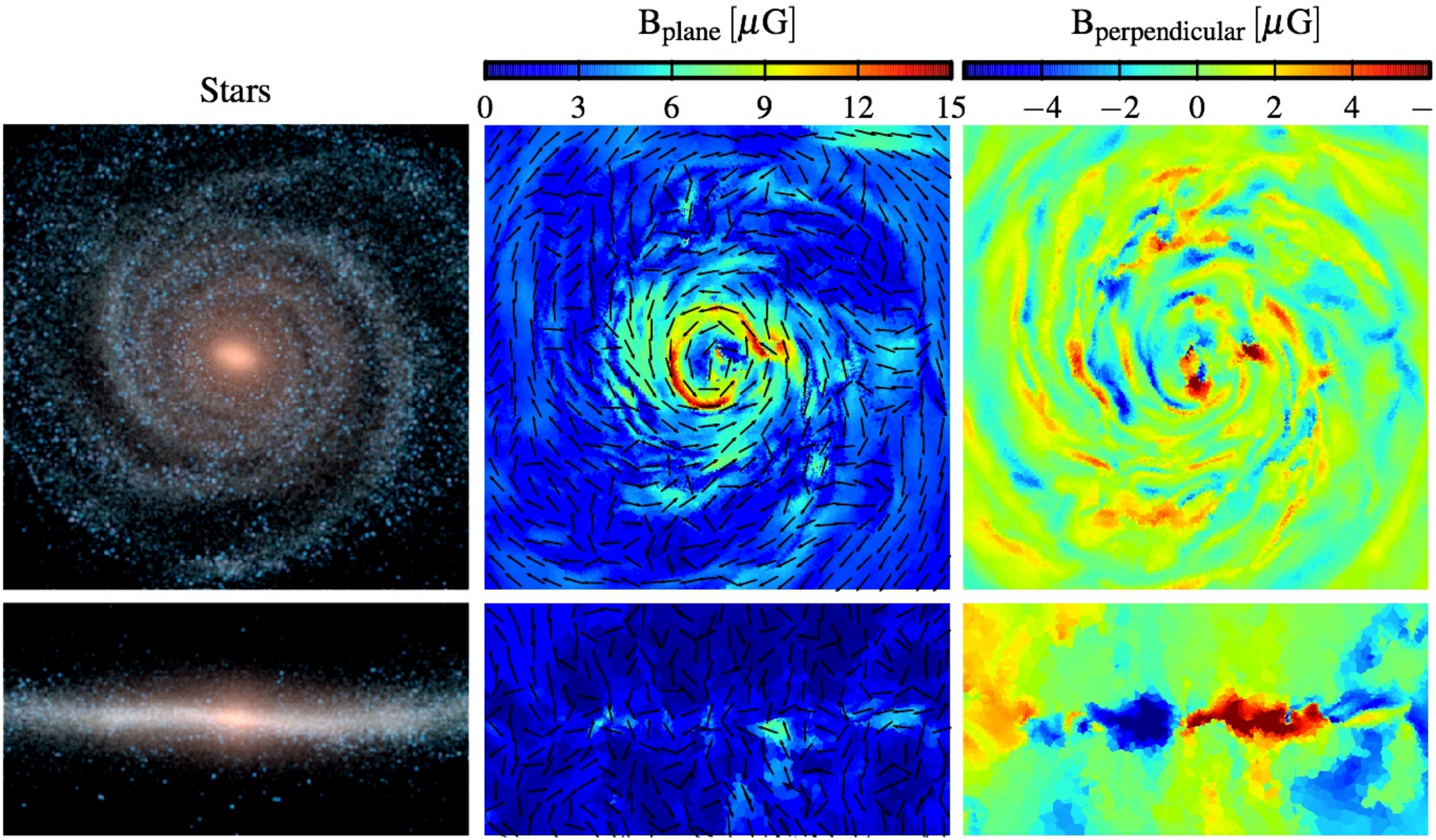


→ **we get the correct linear growth rate**



With the MHD implemention in AREPO, we now produce realistic disk galaxies

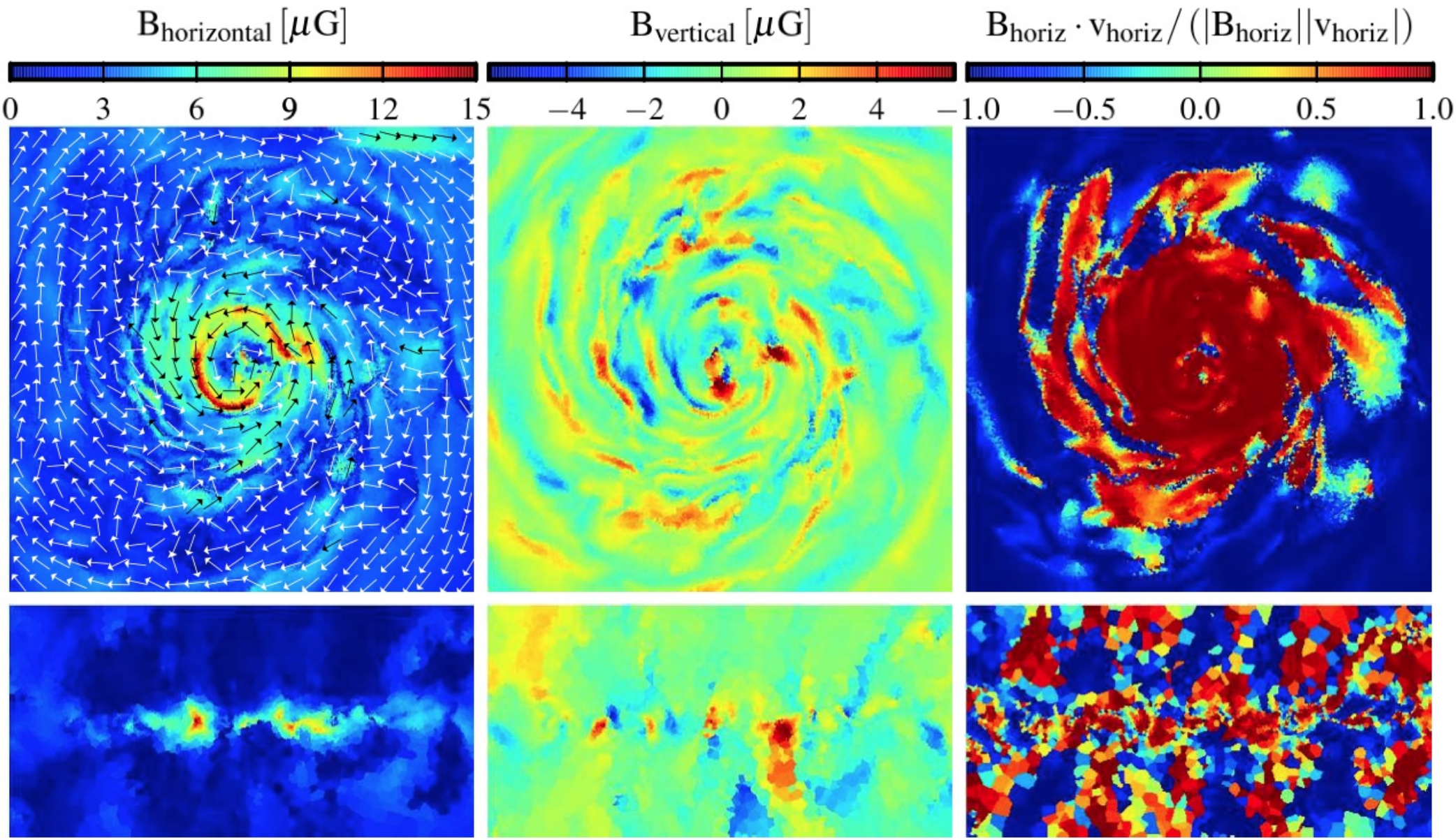
PROJECTED FACE-ON AND EDGE-ON MAPS OF A MILKY-WAY LIKE GALAXY



Pakmor et al. (2014)

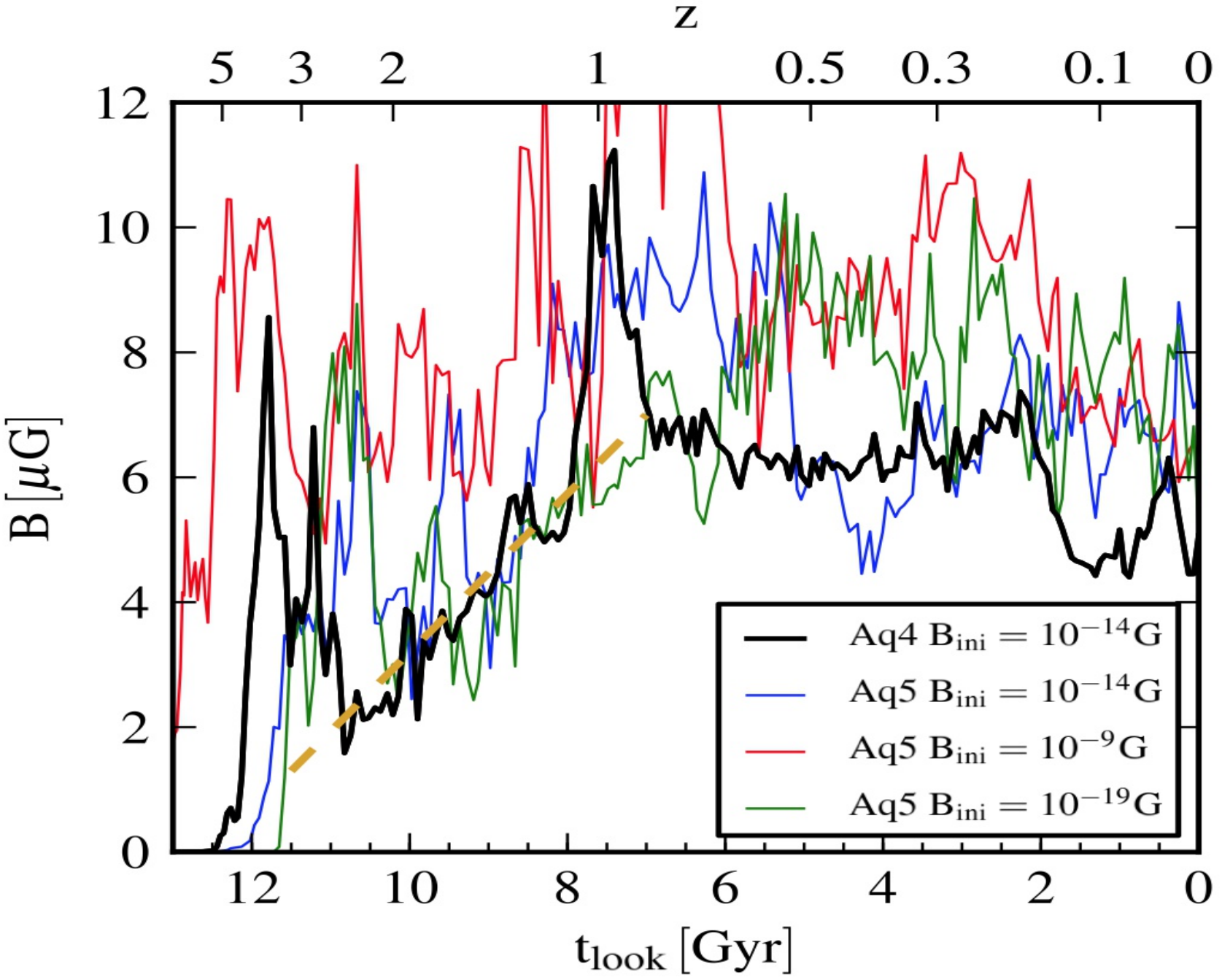
The predicted present-day B-field is largely toroidal

MAGNETIC FIELD IN THE DISK AT REDSHIFT Z=0



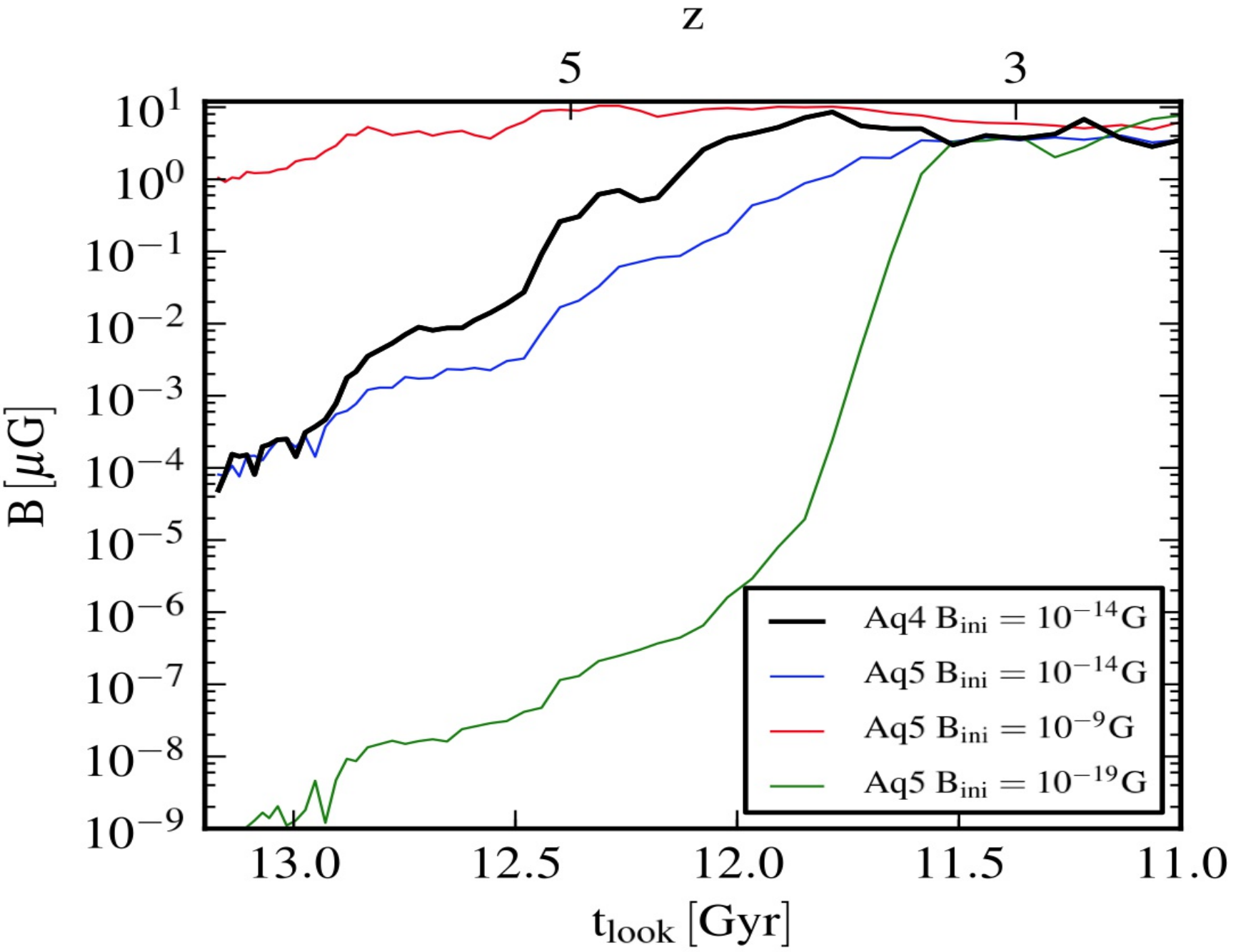
The amplification of the B-field proceeds in different phases

EVOLUTION OF THE VOLUME-WEIGHTED RMS B-FIELD STRENGTH



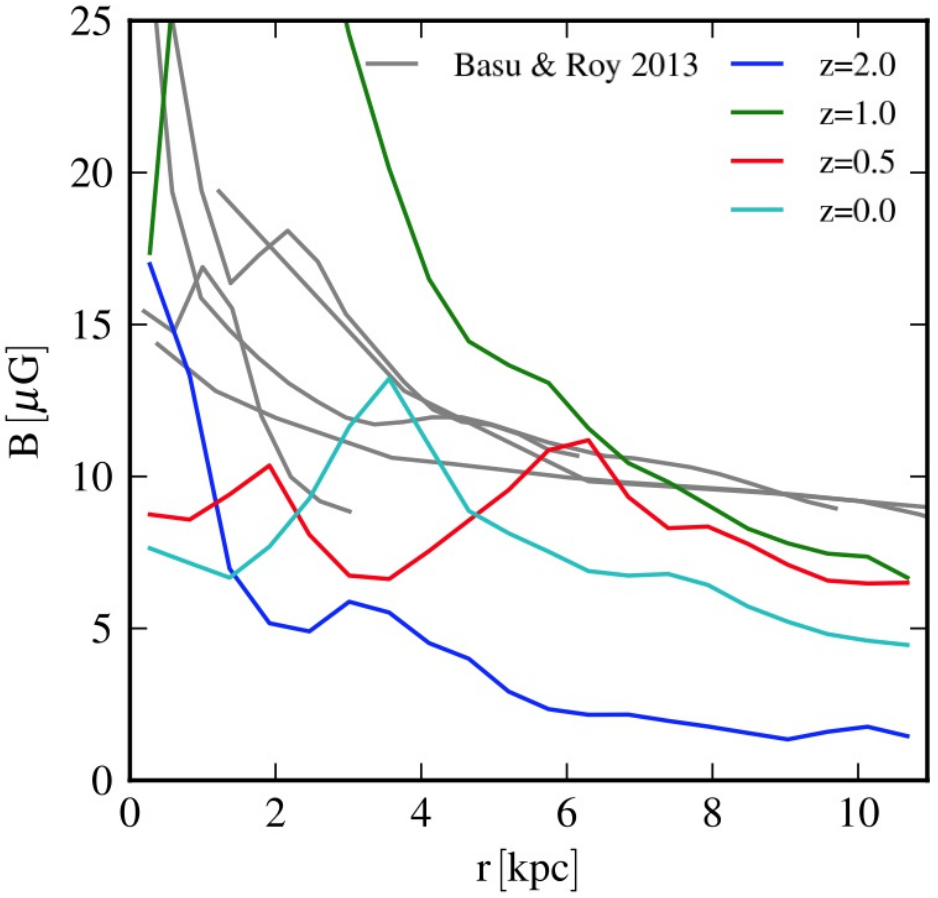
The small-scale dynamo is active at very high redshift

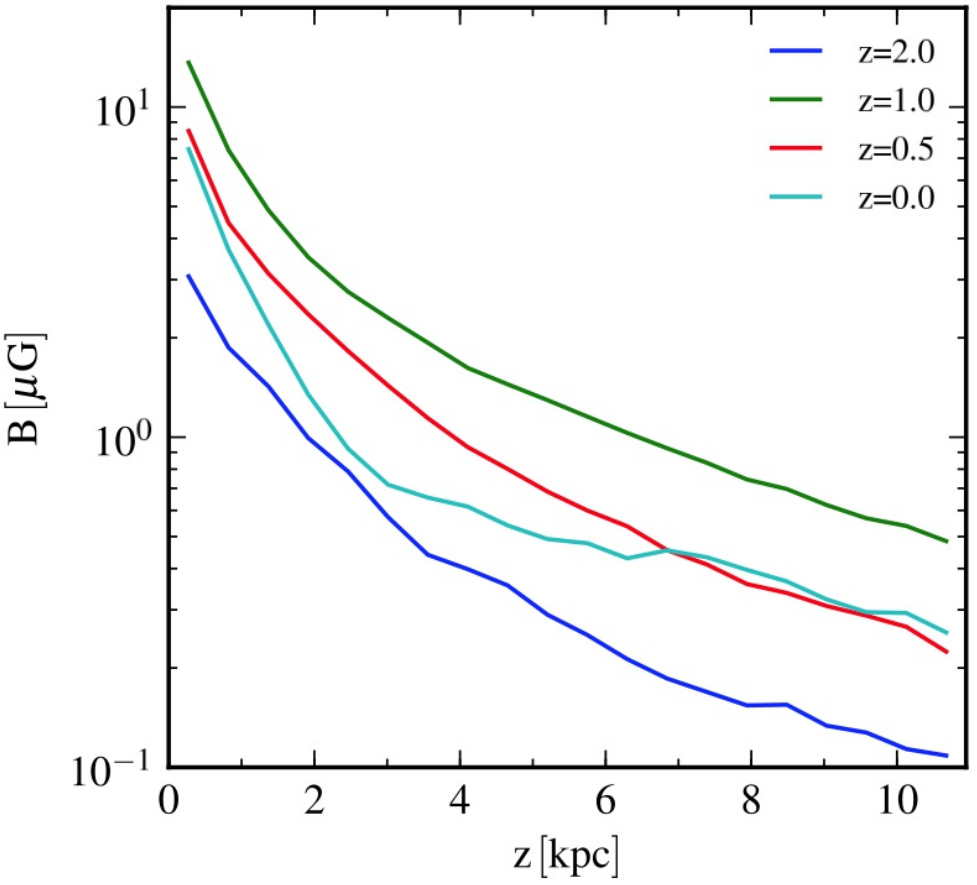
EVOLUTION OF THE VOLUME-WEIGHTED RMS B-FIELD STRENGTH FOR DIFFERENT SEED FIELDS



The predicted magnetic field strength agrees quite well with observations

PROFILES OF MAGNETIC FIELD STRENGTH IN SIMULATIONS AND OBSERVATIONS



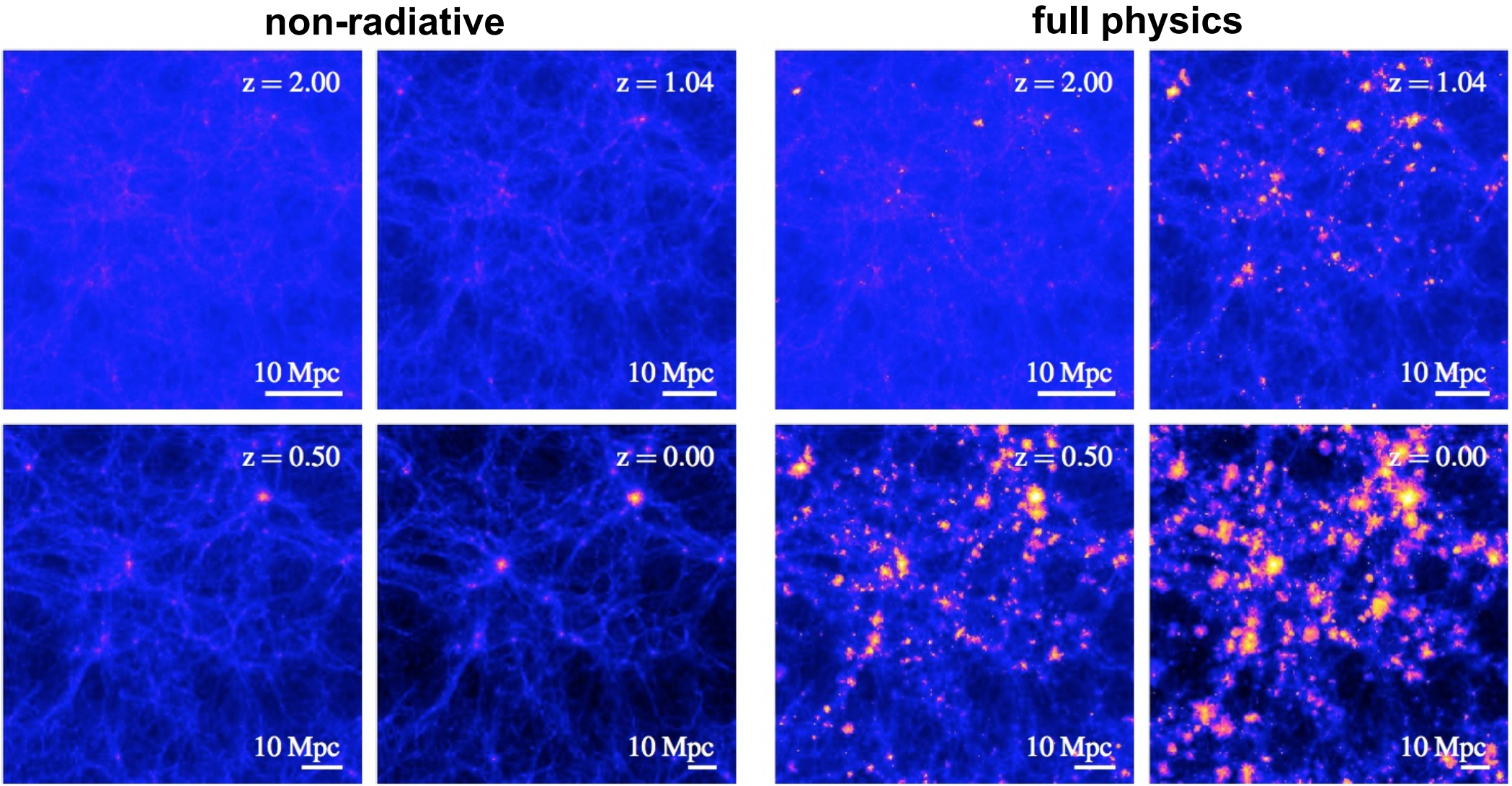


The magnetic field amplification in halos is drastically different in simulations with full feedback physics

$100\ h^{-1}\mathrm{Mpc}$

2×512^3

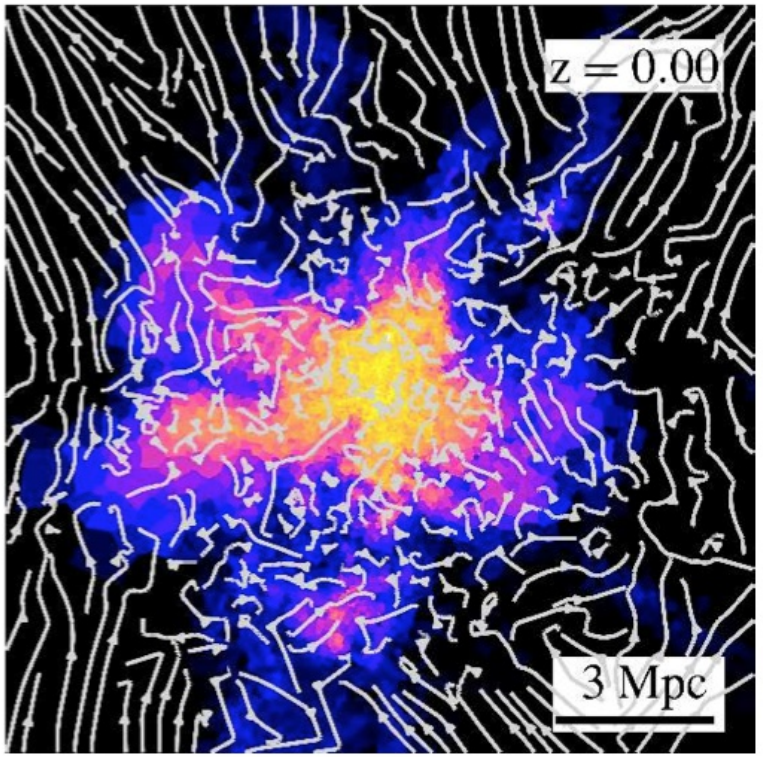
MASS-WEIGHTED PROJECTIONS OF THE B-FIELD INTENSITY

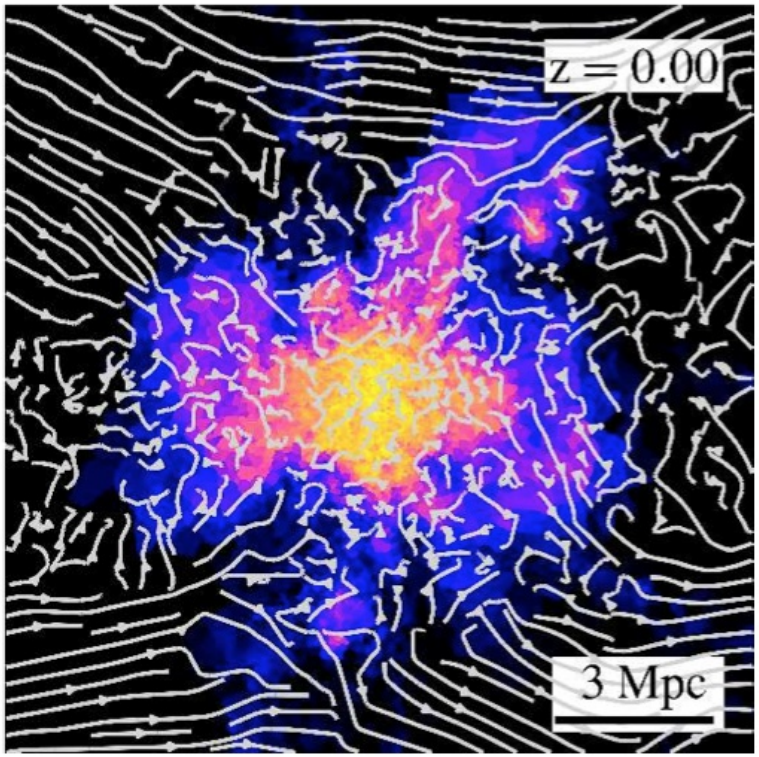


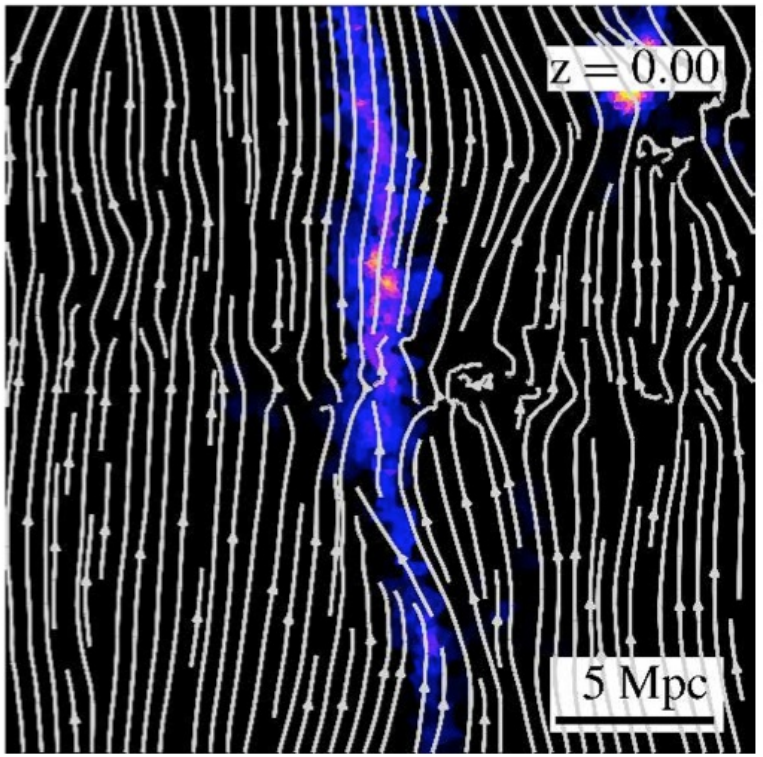
Marinacci et al. (2015)

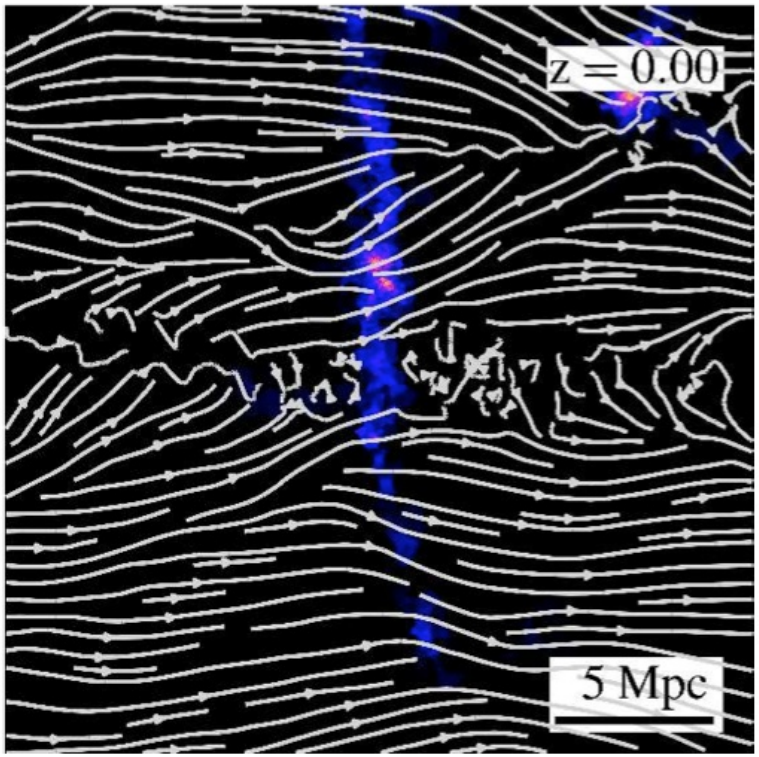
In filaments, memory of the initial field geometry is still kept, and this affects also the amplification

FIELD DISTRIBUTION IN TWO IDENTICAL SIMULATIONS WHERE THE INITIAL ORIENTATION OF THE B-FIELD WAS CHANGED



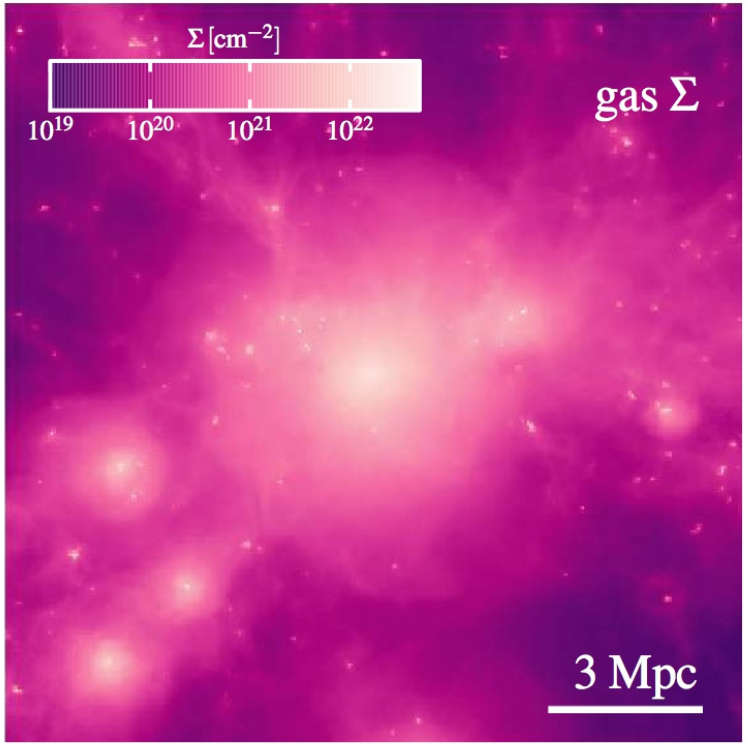


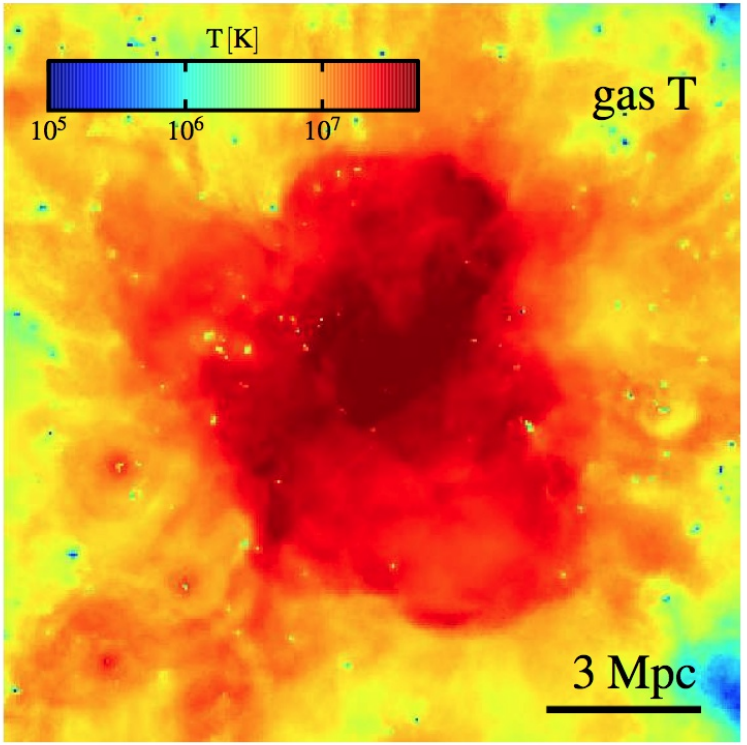


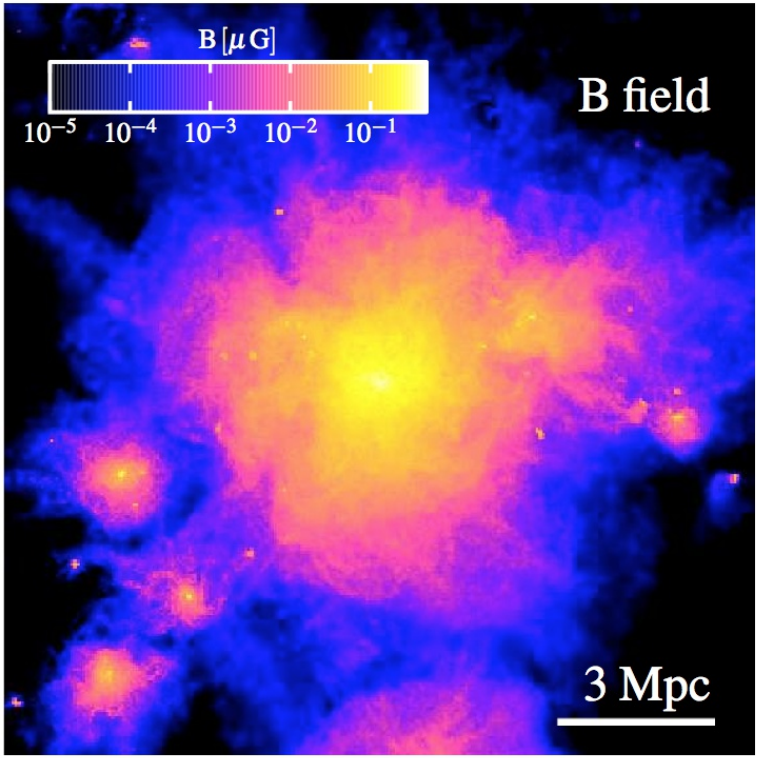


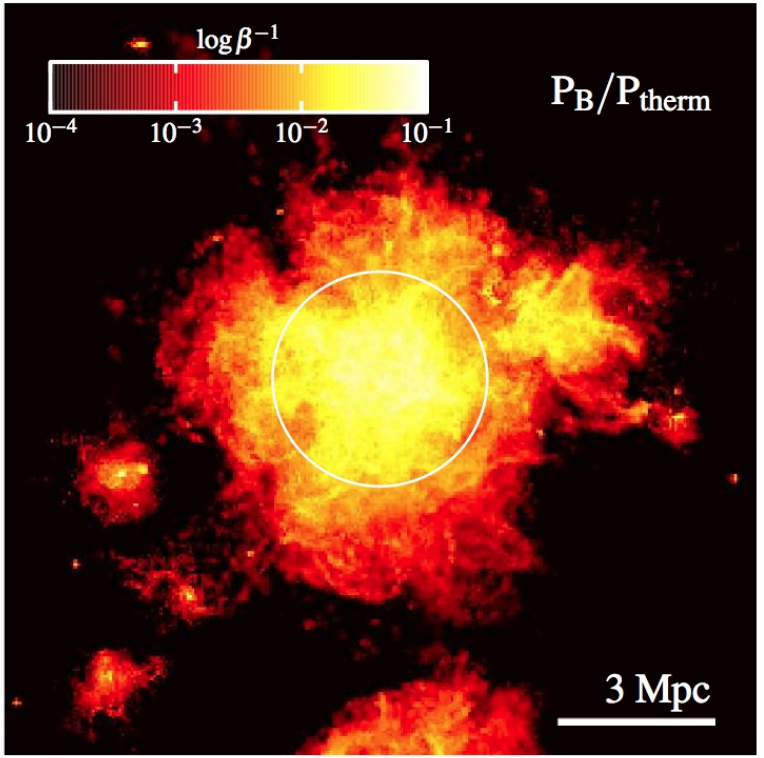
The B-field inside halos is dynamically unimportant except at the very center

MAPS OF DIFFERENT GAS PROPERTIES AROUND A TYPICAL MASSIVE HALO





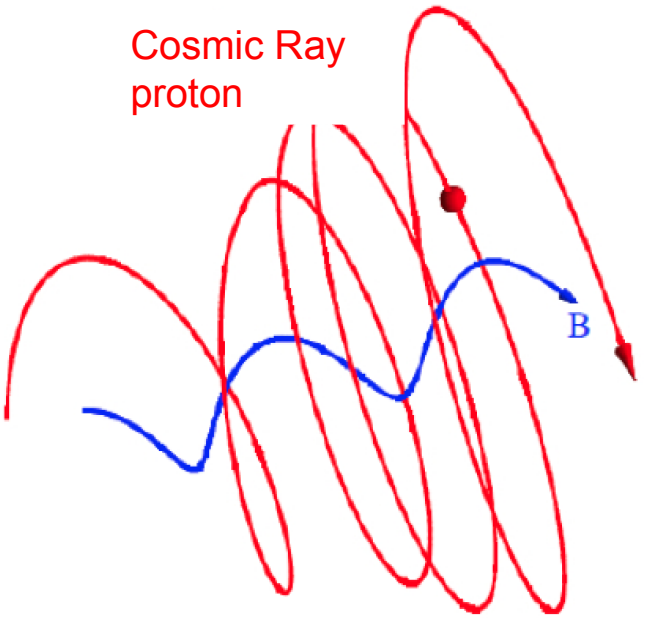




Cosmic ray dynamics is coupled to magnetic fields

INTERACTIONS OF COSMIC RAYS AND MAGNETIC FIELDS

Cosmic rays scatter on magnetic fields – this lets them exert a pressure on the thermal gas, and diffuse relative to its rest frame.



Streaming instability:

- CRs can in principle move rapidly along field lines (with c), which acts to reduce any gradient in their number density.
- but if $c_s > v_A$, CR excite Alfven waves (streaming instability)
- scattering off this wave field in turn limits the CR bulk speed to a much smaller, effective streaming speed v_{str}
- streaming speed: $\mathbf{v}_{\rm str} = -v_{\rm str} \dfrac{\nabla P_{\rm cr}}{|\nabla P_{\rm cr}|}$ $\quad v_{\rm str} = \lambda \max(c_S, v_A)$ $\quad \lambda \sim 1$

The CR transport complicates fluids dynamics considerable

COSMIC RAY DYNAMICS WITHOUT SOURCE AND SINK TERMS

$$\frac{\partial n_{\rm cr}}{\partial t} = -\nabla \cdot [(\mathbf{v}_{\rm gas} + \mathbf{v}_{\rm str}) n_{\rm cr}] + \nabla \cdot (\mathbf{K} \nabla\, n_{\rm cr})$$

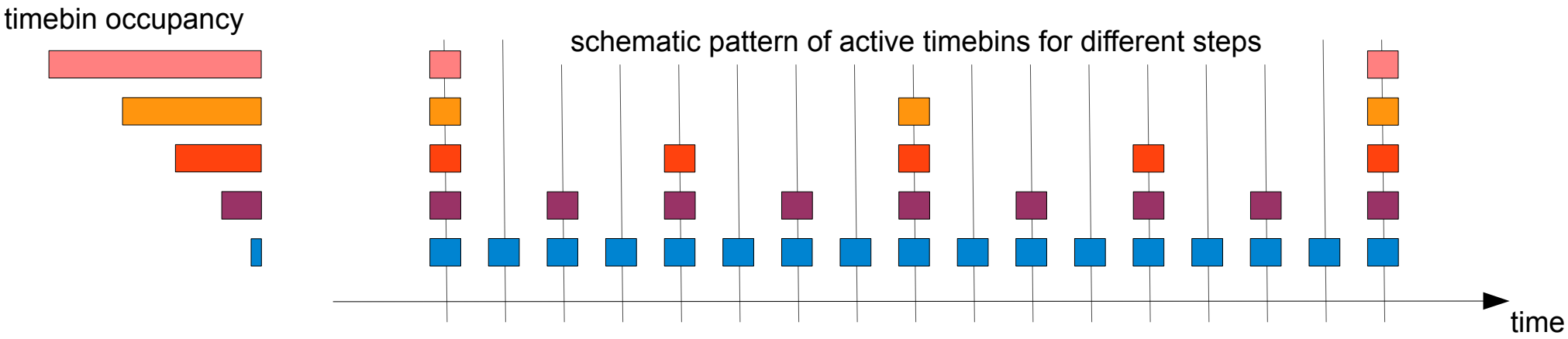
$$\frac{\partial \epsilon_{\rm cr}}{\partial t} = (\mathbf{v}_{\rm gas} + \mathbf{v}_{\rm str}) \cdot \nabla P_{\rm cr} - \nabla \cdot [(\mathbf{v}_{\rm gas} + \mathbf{v}_{\rm str})(\epsilon_{\rm cr} + P_{\rm cr})] + \nabla \cdot (\mathbf{K} \nabla\, \epsilon_{\rm cr})$$

cosmic ray streaming not negligible in typical ISM conditions

diffusion should be small for a plasma with $P_{\rm B} \sim P_{\rm th}$, so may well be negligible

Nevertheless, the streaming term has simply been forgotten in several recent works in the literature.

Execution times of different levels of the timestep hierarchy in Illustris




```
Sync-Point 912913, Time: 0.999995, Redshift: 4.62727e-06, Systemstep: 2.31361e-06, Dloga: 2.31363e-06
Occupied timebins: non-cells     cells       dt                  cumulative A D    avg-time  cpu-frac
    bin=16      4866563102  4542638866     0.000592288851      11907084302   *      319.98     16.0%
    bin=15      1029558638   496930277     0.000296144425       2497882334          162.70      8.1%
    bin=14       456190725   185824857     0.000148072213        971393419          128.60     12.9%
    bin=13       216201669    42568324     0.000074036106        329377837           65.53     13.1%
    bin=12        64651120     2745964     0.000037018053         70607844           28.49     11.4%
    bin=11         3004109      186565     0.000018509027          3210760           10.45      8.4%
    bin=10              99       18602     0.000009254513            20086            2.91      4.7%
 X  bin= 9              23        1236     0.000004627257             1385 <          2.75      8.8%
 X  bin= 8               4         122     0.000002313628              126            2.62     16.8%
               ------------------------
Total active:           27        1358    Sum:       1385
```

A hierarchical Hamiltonian split has been implemented in AREPO to achieve a clean separation of timescales

AVOIDING OVERHEADS IN THE TAIL OF THE TIMESTEP DISTRIBUTION

Recall second-order symplectic integration: $H = H_1 + H_2$

$$E(H, \Delta t) \simeq E\left(H_1, \frac{\Delta t}{2}\right) \circ E(H_2, \Delta t) \circ E\left(H_1, \frac{\Delta t}{2}\right)$$

For a Hamiltonian system P of particles, define a split into a slow system S (Δt), and a fast system F (Δt/2)

$$H = H_{\rm kin} + H_{\rm pot} \qquad \mathrm{P} = \mathrm{S} + \mathrm{F}$$

We can now write the system as:

$$H = H^{\rm S}_{\rm kin} + H^{\rm S}_{\rm pot} + H^{\rm F}_{\rm kin} + H^{\rm F}_{\rm pot} + H^{\rm FS}_{\rm pot}$$

$$H = H^{\rm S} + H^{\rm F} + H^{\rm FS}_{\rm pot}$$

And define a time-integration operator as:

$$E(H, \Delta t) \simeq E\left(H^{\rm FS}_{\rm pot}, \frac{\Delta t}{2}\right) \circ E\left(H^{\rm F}, \frac{\Delta t}{2}\right) \circ E(H^{\rm S}, \Delta t) \circ E\left(H^{\rm F}, \frac{\Delta t}{2}\right) \circ E\left(H^{\rm FS}_{\rm pot}, \frac{\Delta t}{2}\right)$$

Expressed as kick and drift operators, this becomes:

$$E(H, \Delta t) \simeq K^{\rm F}_{\rm S}\left(\frac{\Delta t}{2}\right) K^{\rm S}_{\rm F}\left(\frac{\Delta t}{2}\right) K^{\rm F}_{\rm F}\left(\frac{\Delta t}{4}\right) D_{\rm F}\left(\frac{\Delta t}{2}\right) K^{\rm F}_{\rm F}\left(\frac{\Delta t}{4}\right) K^{\rm S}_{\rm S}\left(\frac{\Delta t}{2}\right) D_{\rm S}\left(\Delta t\right) K^{\rm S}_{\rm S}\left(\frac{\Delta t}{2}\right) \cdots$$

commutes with D_F and can be moved

This can be simplified into:

$$E(H, \Delta t) \simeq K^{\rm P}_{\rm P}\left(\frac{\Delta t}{2}\right) K^{\rm F}_{\rm F}\left(-\frac{\Delta t}{4}\right) D_{\rm F}\left(\frac{\Delta t}{2}\right) K^{\rm F}_{\rm F}\left(\frac{\Delta t}{4}\right) D_{\rm S}\left(\Delta t\right) \cdots$$

Notes:

- Can be applied hierarchically
- Momentum conserving despite individual timesteps

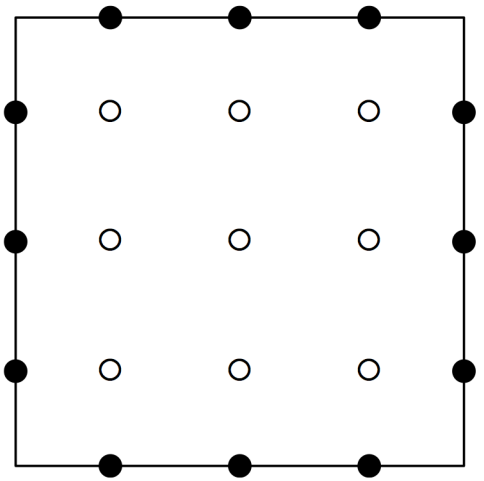
We have developed a new Discontinuous Galerkin (DG) code combined with AMR for the cosmological hydrodynamical equations

BASIC DISCONTINUOUS GALERKIN EQUATIONS

Schaal, Springel, Klingenberg et al. (2015)

$$\frac{\partial}{\partial t} u + \vec{\nabla} \vec{F}(u) = 0$$

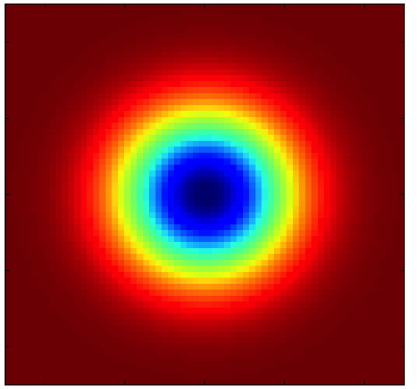
$$\frac{\partial}{\partial t} \underbrace{\int_K u \, \phi_j \, \mathrm{d}V}_{|K| w_j} + \oint_{\partial K} \phi_j \vec{F}(u) \vec{n} \, \mathrm{d}S - \int_K \vec{F}(u) \vec{\nabla} \phi_j \, \mathrm{d}V = 0$$

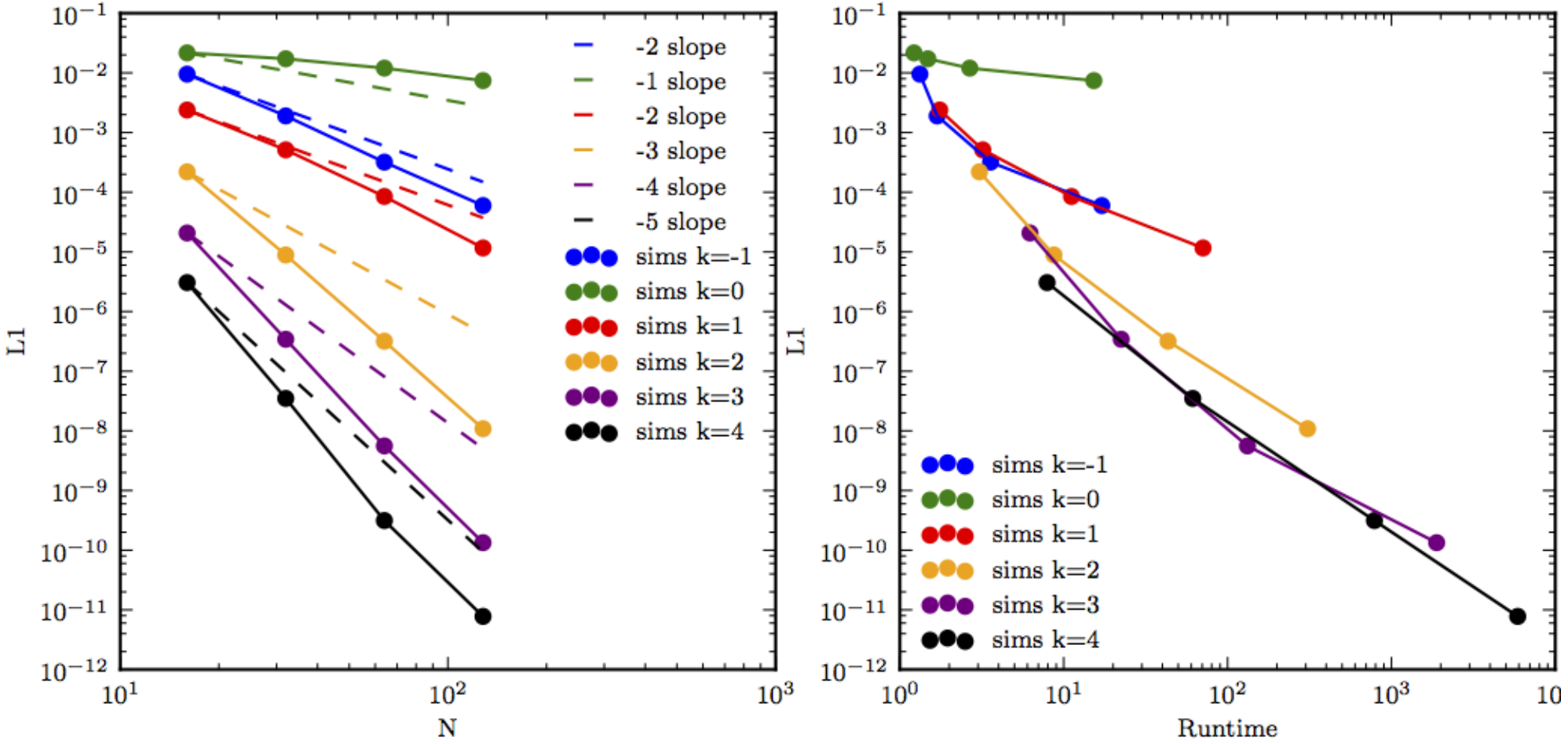


Gaussian quadrature

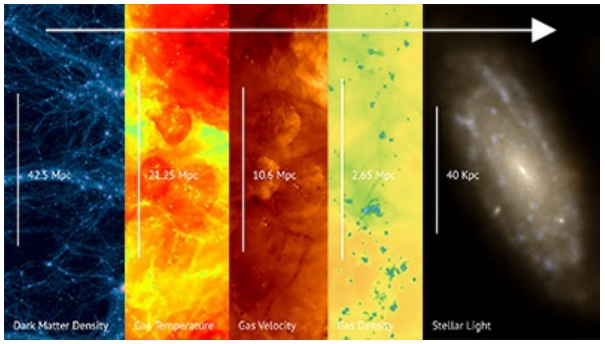
The DG code TENET shows a promising accuracy and efficiency gain compared to the default finite volume scheme

CONVERGENCE RATES AT DIFFERENT ORDER FOR A STATIONARY ISENTROPIC VORTEX





Summary points



- **Simulations of cosmic structure formation are one of the most powerful tools in astrophysics.** New numerical methods are needed to fully exploit current and upcoming HPC systems.

- **Hydrodynamical simulations of galaxy formation start to be successful.** Morphology and stellar mass function come out right for the first time. Also, we are able to successfully follow the build-up of the magnetic field in Milky Way sized galaxies.

- Cosmological hydrodynamic simulations are computationally extremely demanding. **The multi-scale physics can presently be addressed only for a small range, and more adaptive integration methods need to be developed.**