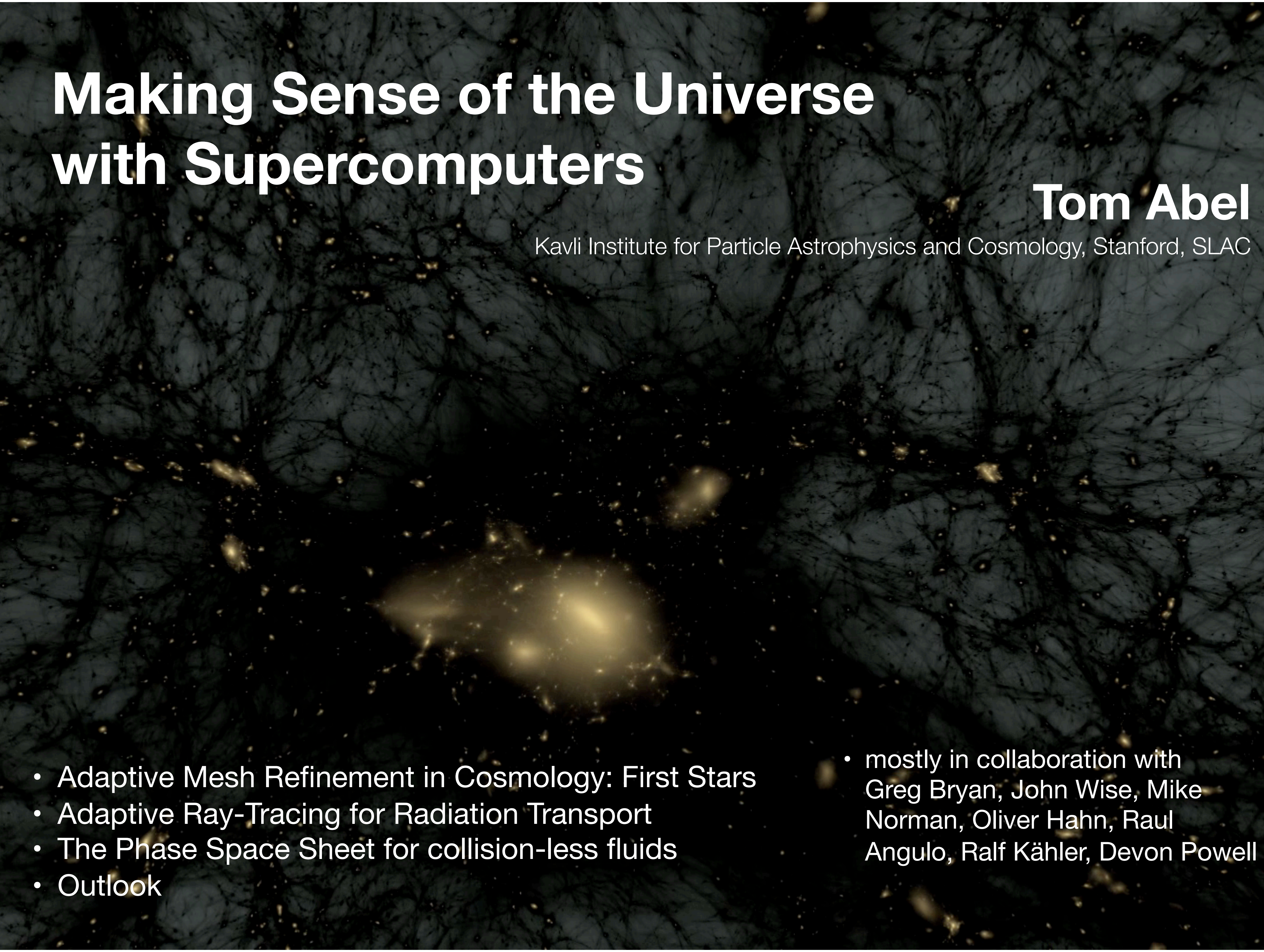


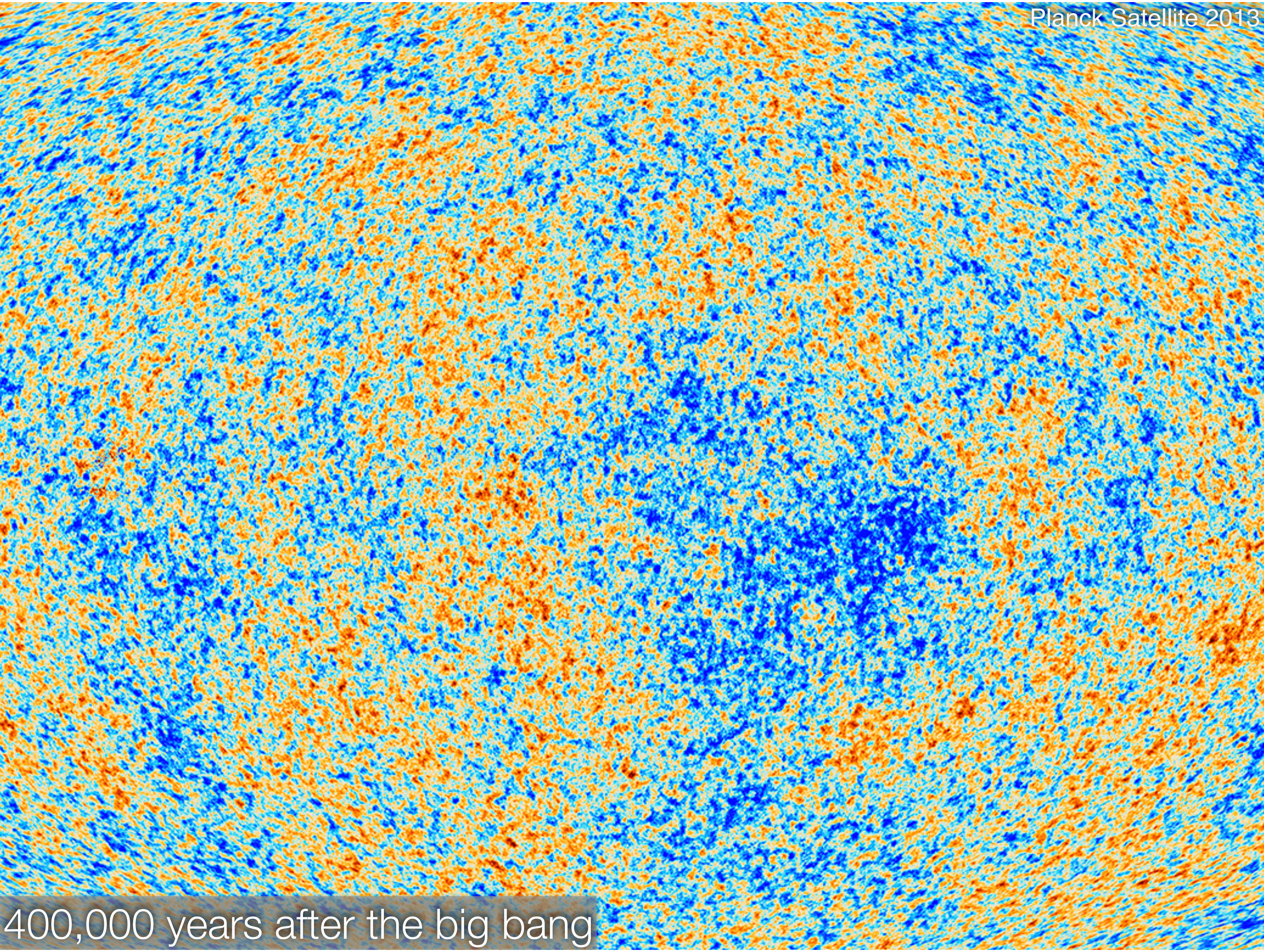
Making Sense of the Universe with Supercomputers

Tom Abel

Kavli Institute for Particle Astrophysics and Cosmology, Stanford, SLAC

- Adaptive Mesh Refinement in Cosmology: First Stars
- Adaptive Ray-Tracing for Radiation Transport
- The Phase Space Sheet for collision-less fluids
- Outlook

- mostly in collaboration with Greg Bryan, John Wise, Mike Norman, Oliver Hahn, Raul Angulo, Ralf Kähler, Devon Powell



Planck Satellite 2013

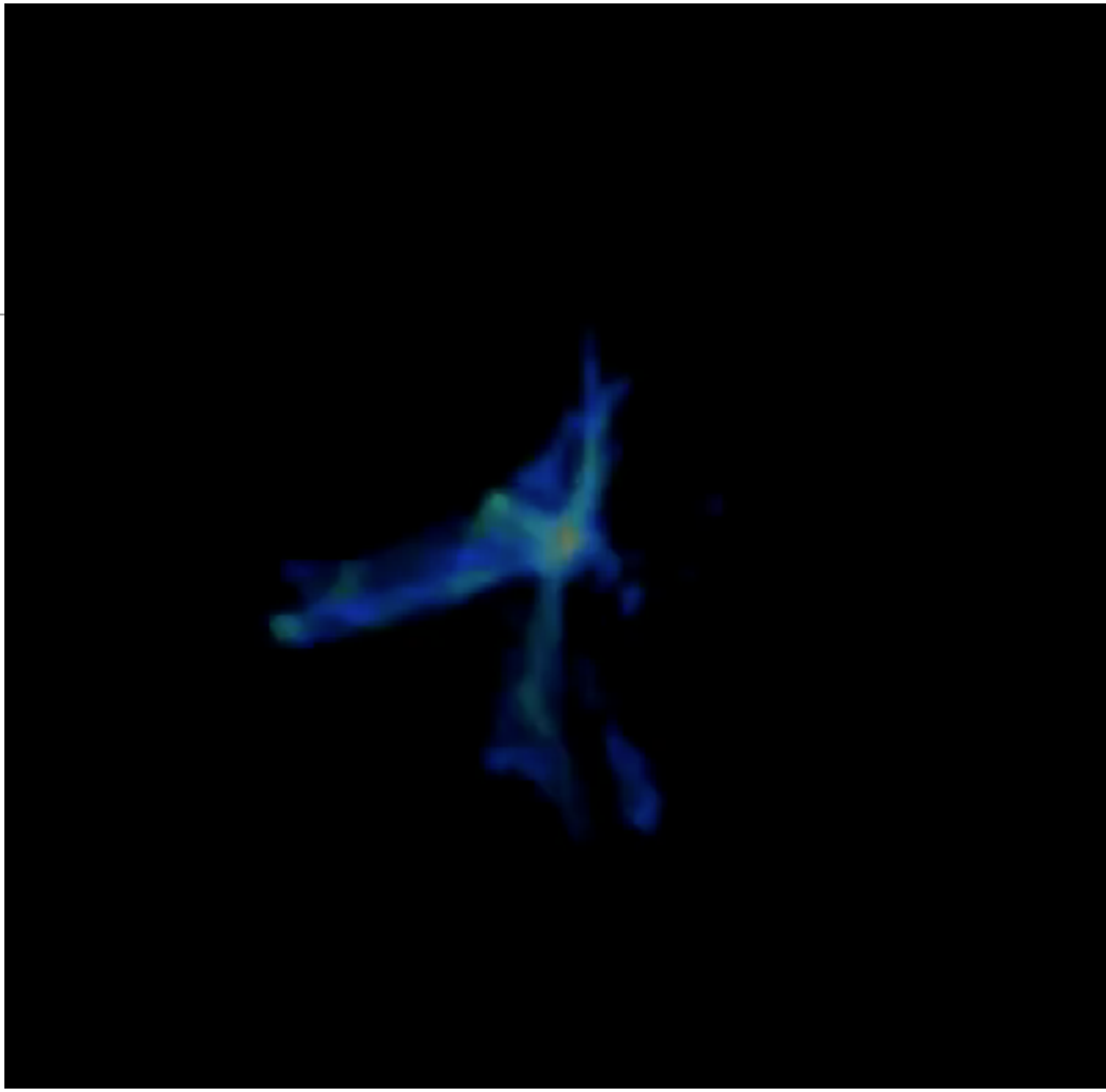
400,000 years after the big bang

Universe at 400,000 years

- Temperature 3000K, fluctuations 1 part in 100,000
- Density 300 per cm^3, fluctuations 1 part in 1,000
- Hydrogen 76% & Helium 24%.
  Ion fraction: 2 part in 100,000
- Dark Matter about 6 times more than baryons
- **No observations between 400,000 and 800 million years of the universe! So called Dark Ages.**

First Things in the Universe

Physics problem:



Ralf Kähler & Tom Abel for PBS Origins. Aired Dec 04

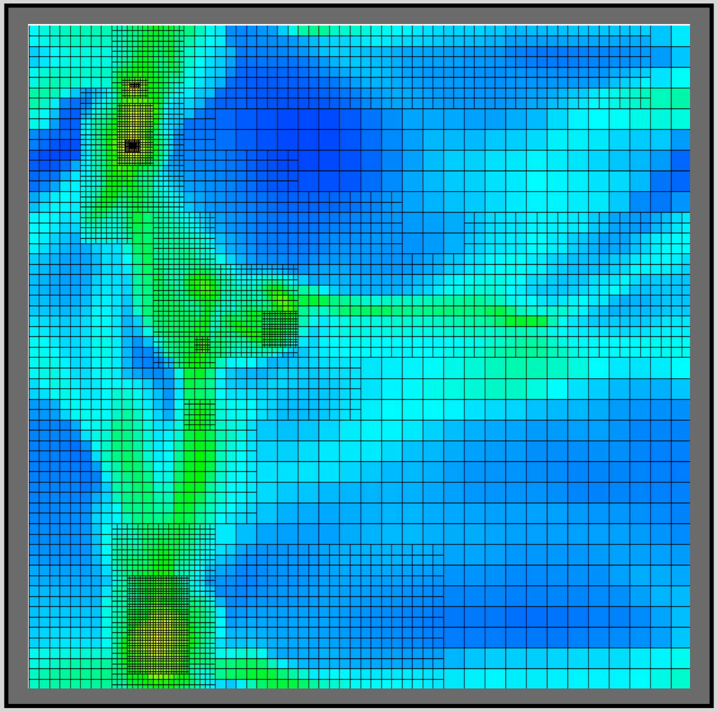
- Initial Conditions measured
- Constituents, Density Fluctuations, Thermal History
- Physics: Gravity: DM & Gas, HD, Chemistry, Radiative Cooling, Radiation Transport, Cosmic Rays, Dust drift & cooling, Supernovae, Stellar evolution, etc.
- Transition from Linear to Non-Linear:
  - Using patched based structured adaptive (space & time) mesh refinement
  - Use a computer!

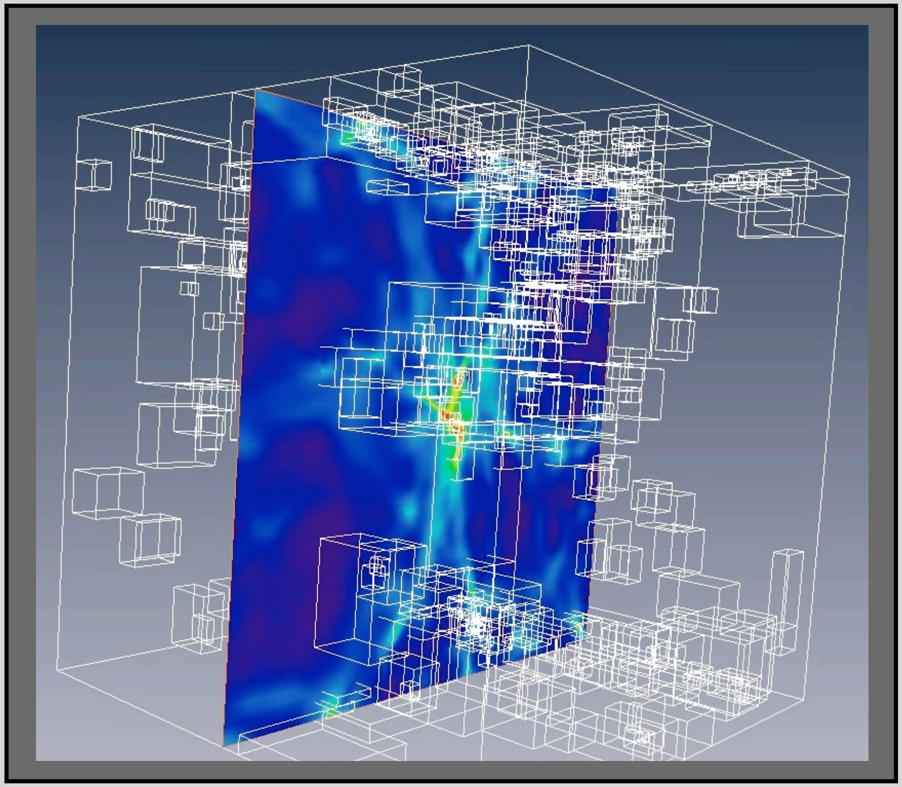
$$\frac{R_\odot}{R_{\mathrm{Milky Way}}} \approx 10^{-12}$$

$$\frac{P_{\odot,\mathrm{Kepler}}}{t_{\mathrm{Hubble}}(z=30)} \approx 10^{-12}$$

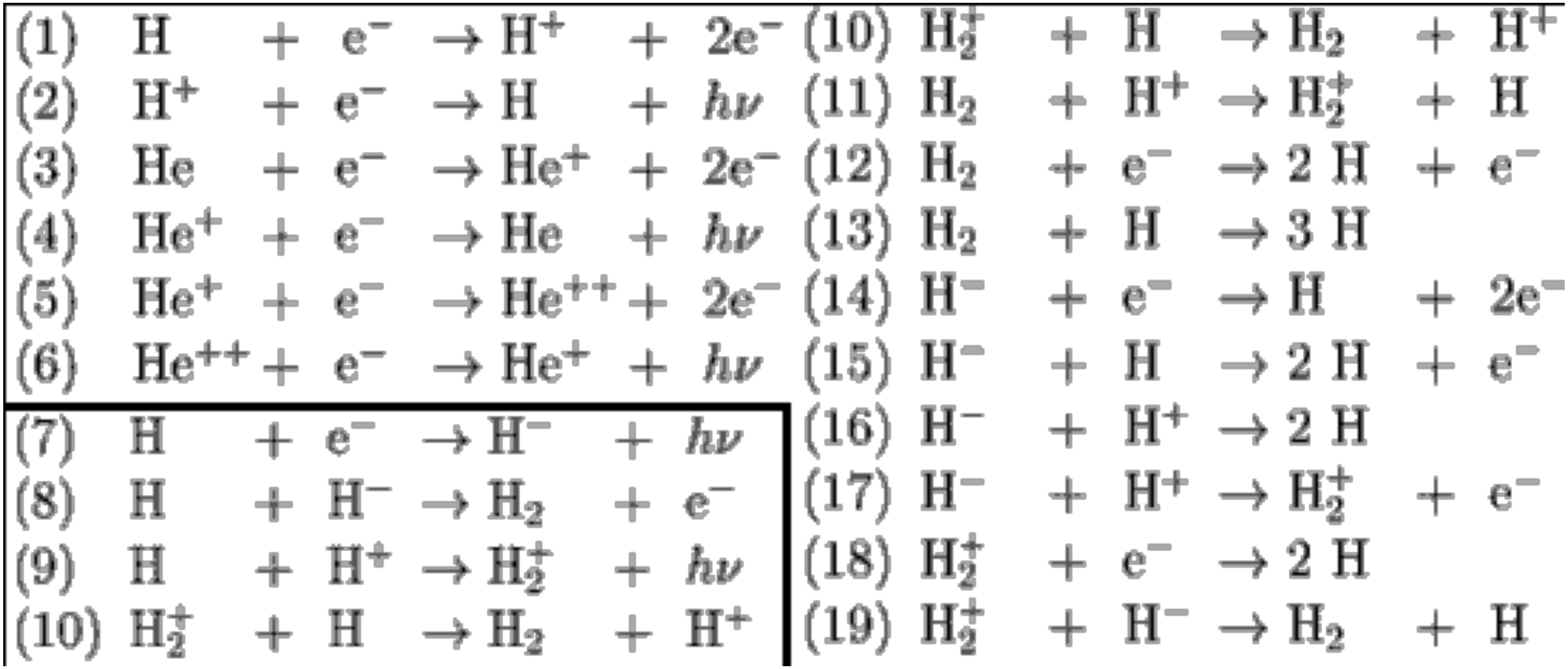
Adaptive Mesh Refinement

- **Enzo:** Bryan and Norman 1997-
  Bryan, Abel & Norman 2002;
  O'Shea et al 2004; Abel, Wise & Bryan 2006, Bryan et al. 2014
  - Gravity, DM, Gas, Chemistry, Radiation, star formation & feedback, MHD, Cosmic Rays
  - > 300,000 lines of code in C++ and F77
  - Cosmological Radiation Hydrodynamics adapting in space and time
  - Dynamic range up to 1e15 using up to 128 bit precision coordinates in space and time
  - Has been run with up to millions of grid patches
  - Dynamically load balanced parallel with MPI
  - **www.enzo-project.org**





Primordial Gas Chemistry



(1) $\mathrm{H} + e^- \rightarrow \mathrm{H}^+ + 2e^-$

(2) $\mathrm{H}^+ + e^- \rightarrow \mathrm{H} + h\nu$

(3) $\mathrm{He} + e^- \rightarrow \mathrm{He}^+ + 2e^-$

(4) $\mathrm{He}^+ + e^- \rightarrow \mathrm{He} + h\nu$

(5) $\mathrm{He}^+ + e^- \rightarrow \mathrm{He}^{++} + 2e^-$

(6) $\mathrm{He}^{++} + e^- \rightarrow \mathrm{He}^+ + h\nu$

(7) $\mathrm{H} + e^- \rightarrow \mathrm{H}^- + h\nu$

(8) $\mathrm{H} + \mathrm{H}^- \rightarrow \mathrm{H}_2 + e^-$

(9) $\mathrm{H} + \mathrm{H}^+ \rightarrow \mathrm{H}_2^+ + h\nu$

(10) $\mathrm{H}_2^+ + \mathrm{H} \rightarrow \mathrm{H}_2 + \mathrm{H}^+$

(10) $\mathrm{H}_2^+ + \mathrm{H} \rightarrow \mathrm{H}_2 + \mathrm{H}^+$

(11) $\mathrm{H}_2 + \mathrm{H}^+ \rightarrow \mathrm{H}_2^+ + \mathrm{H}$

(12) $\mathrm{H}_2 + e^- \rightarrow 2\,\mathrm{H} + e^-$

(13) $\mathrm{H}_2 + \mathrm{H} \rightarrow 3\,\mathrm{H}$

(14) $\mathrm{H}^- + e^- \rightarrow \mathrm{H} + 2e^-$

(15) $\mathrm{H}^- + \mathrm{H} \rightarrow 2\,\mathrm{H} + e^-$

(16) $\mathrm{H}^- + \mathrm{H}^+ \rightarrow 2\,\mathrm{H}$

(17) $\mathrm{H}^- + \mathrm{H}^+ \rightarrow \mathrm{H}_2^+ + e^-$

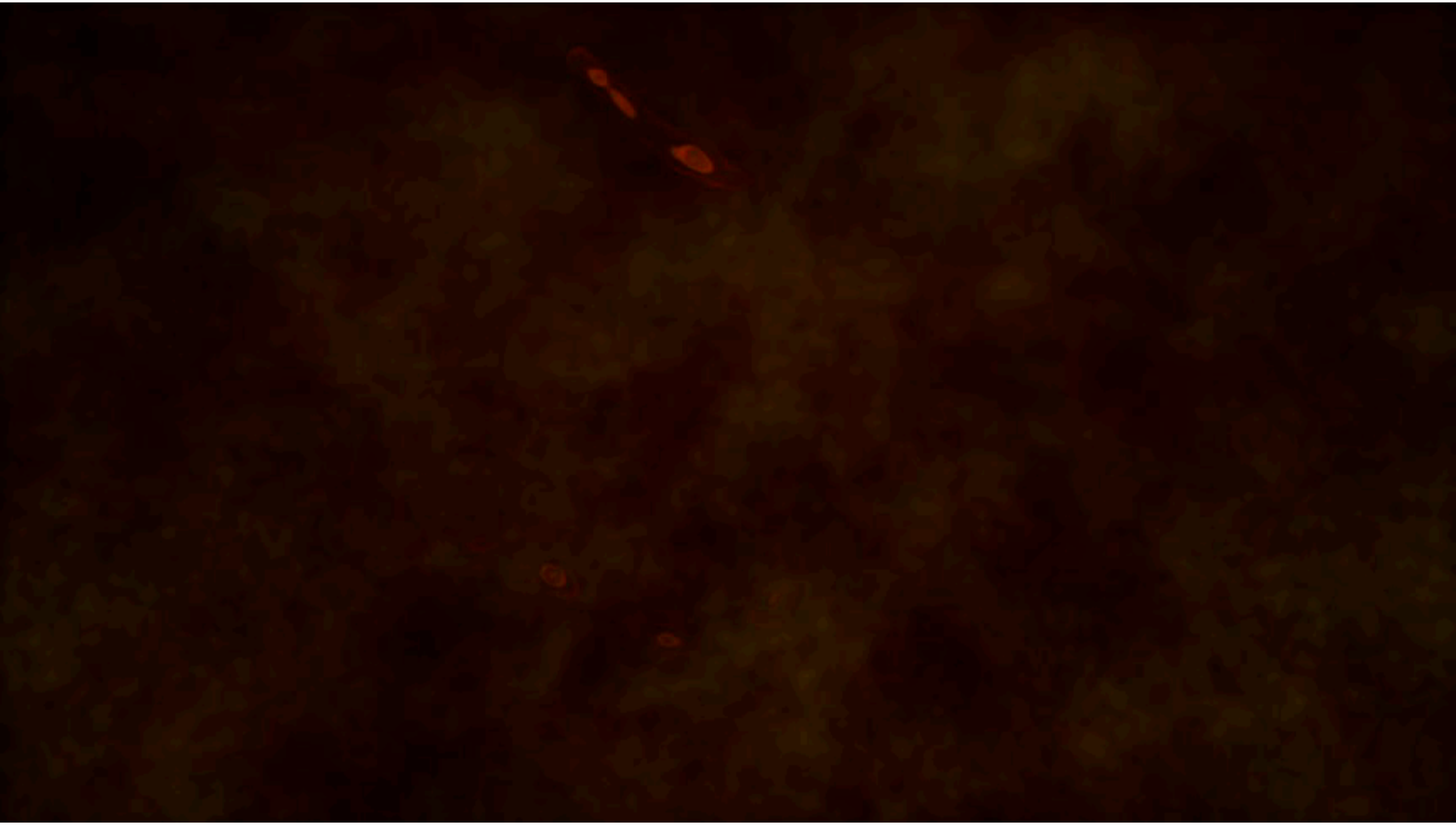
(18) $\mathrm{H}_2^+ + e^- \rightarrow 2\,\mathrm{H}$

(19) $\mathrm{H}_2^+ + \mathrm{H}^- \rightarrow \mathrm{H}_2 + \mathrm{H}$

- Reaction 8 is much faster than reaction 7.
- I.e. (7) will continue as long as free electrons are available -> H2 formation timescale = recombination timescale
- However, $k_7 \propto T^{0.88}$ hence adiabatic contraction important. Requires sufficiently high virial temperatures and so introduces a temperature (mass) scale based on chemistry

$$T_{vir}^{Chem} \approx 10^3\,\mathrm{K}$$

Making a proto-star

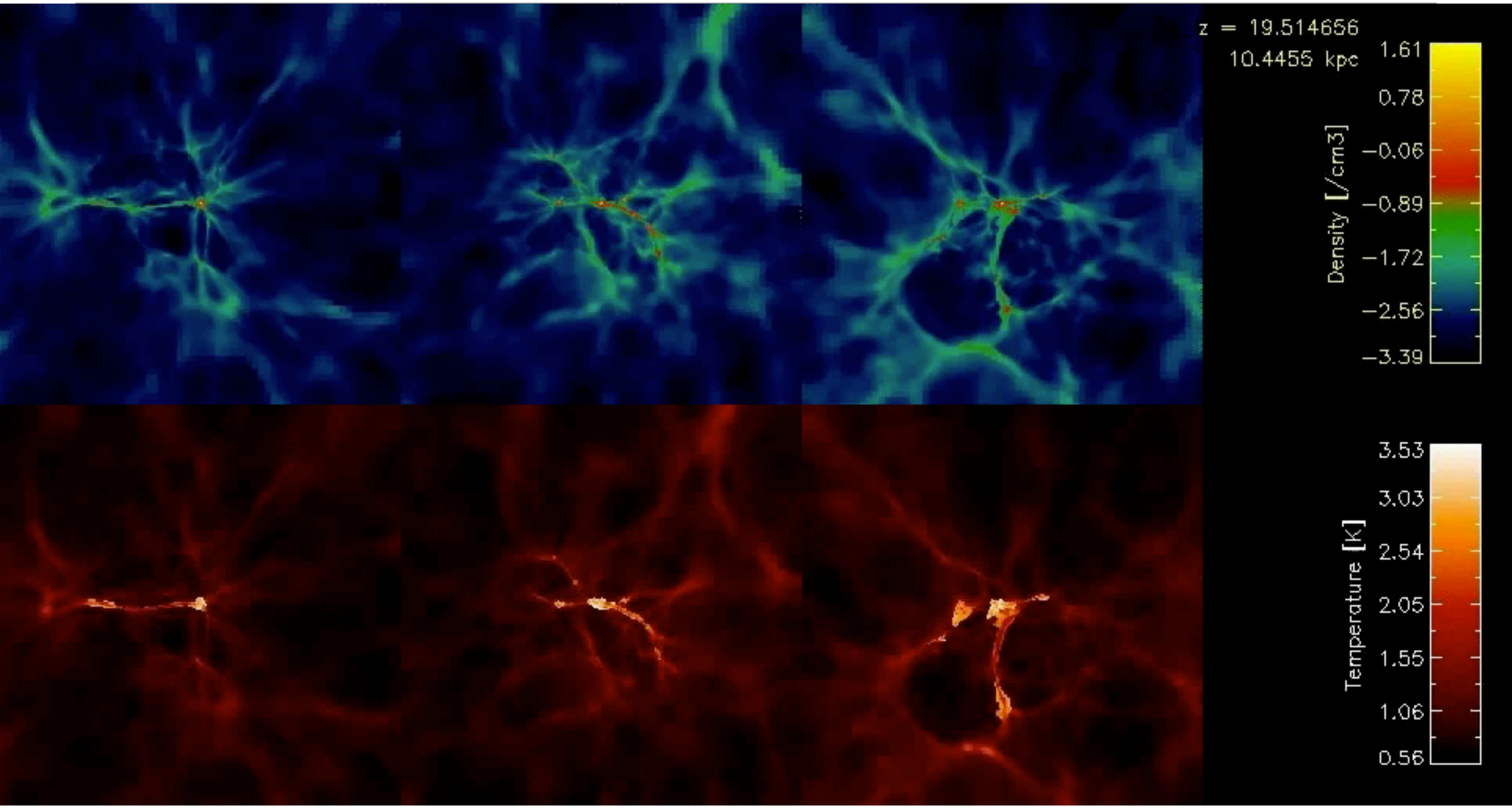


Simulation: Tom Abel (KIPAC/Stanford), Greg Bryan (Columbia), Mike Norman (UCSD)
Viz: Ralf Kähler (AEI, ZIB, KIPAC), Bob Patterson, Stuart Levy, Donna Cox (NCSA), Tom Abel

Zoom in

Dynamic range ~1e12.
> 30 levels of refinement
tens of thousands of grid patches
dynamically load balanced
MPI. 16 processors enough

Typically 3 solar mass dm particles
> 8 cells per local Jeans Length
non-equilibrium chemistry
RT effects above 1e12 cm^{-3}



Turk & Abel 2007

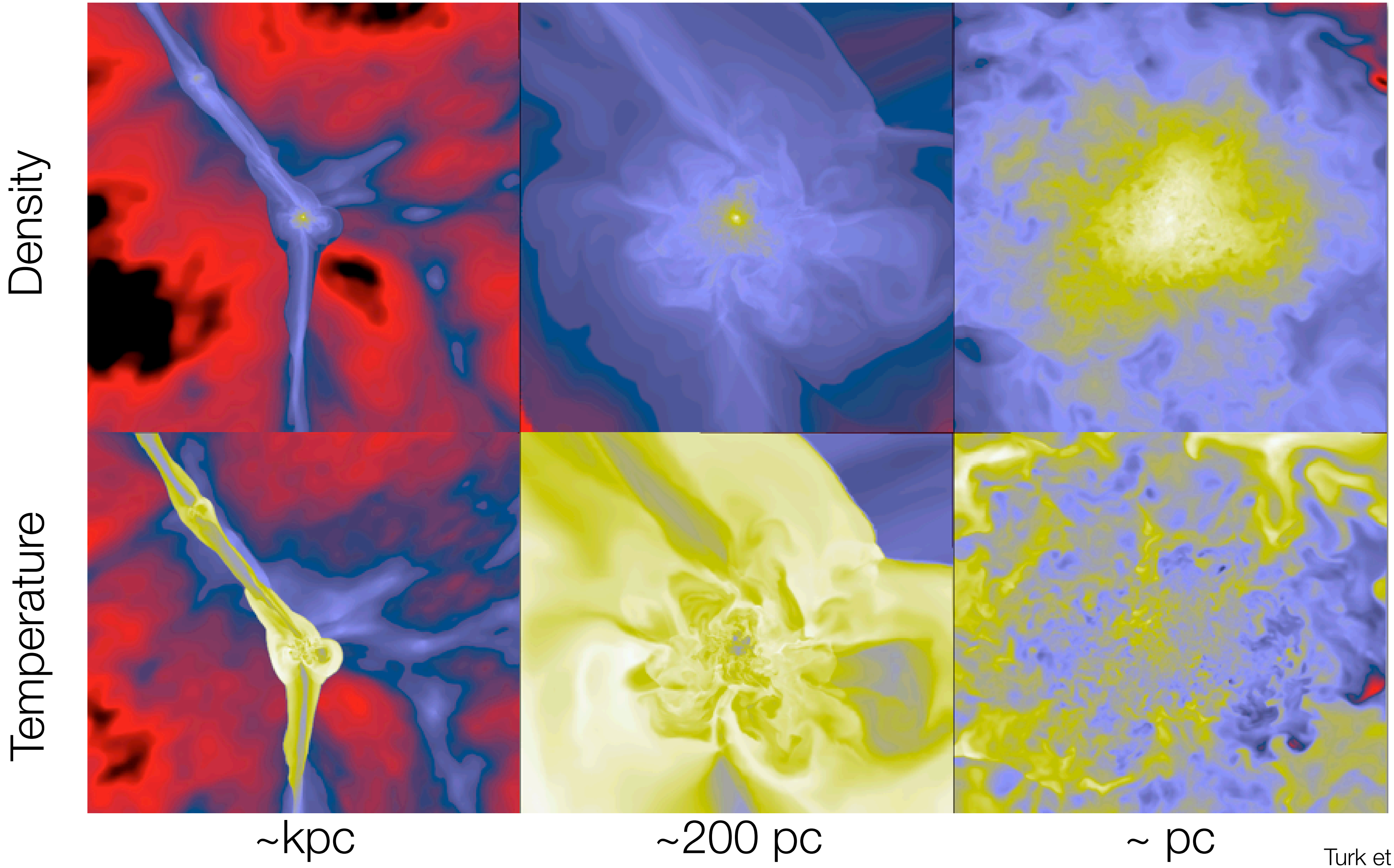
Note disks within disks which happens routinely in turbulent collapses!

Formation of the very first stars very well suited to ab initio modeling

Can only increase effective Reynolds number with super-computing

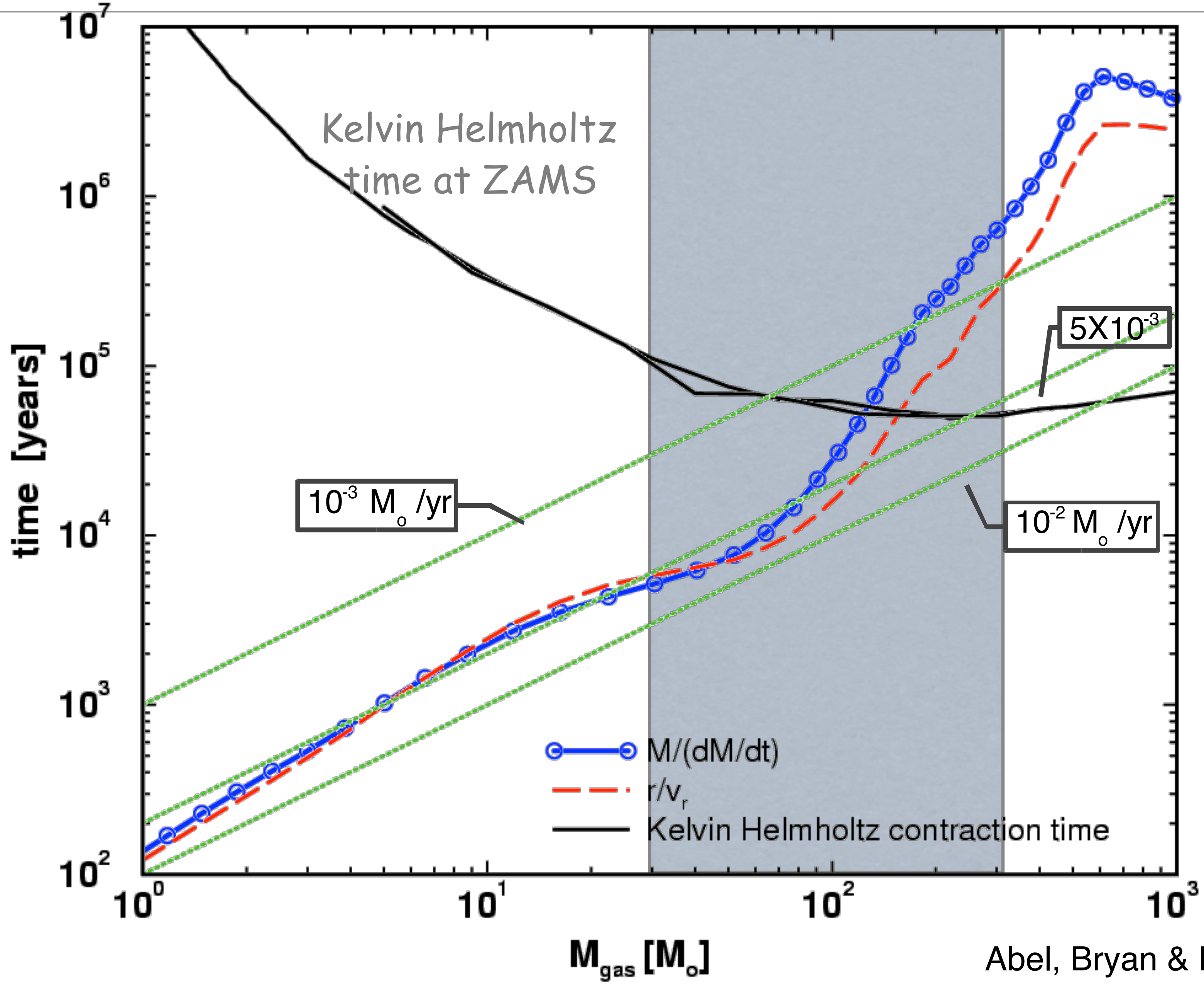
Average properties such as mass and temperature profiles converge reasonably well.

Amount of turbulence, vorticity and magnetic field generated less so.



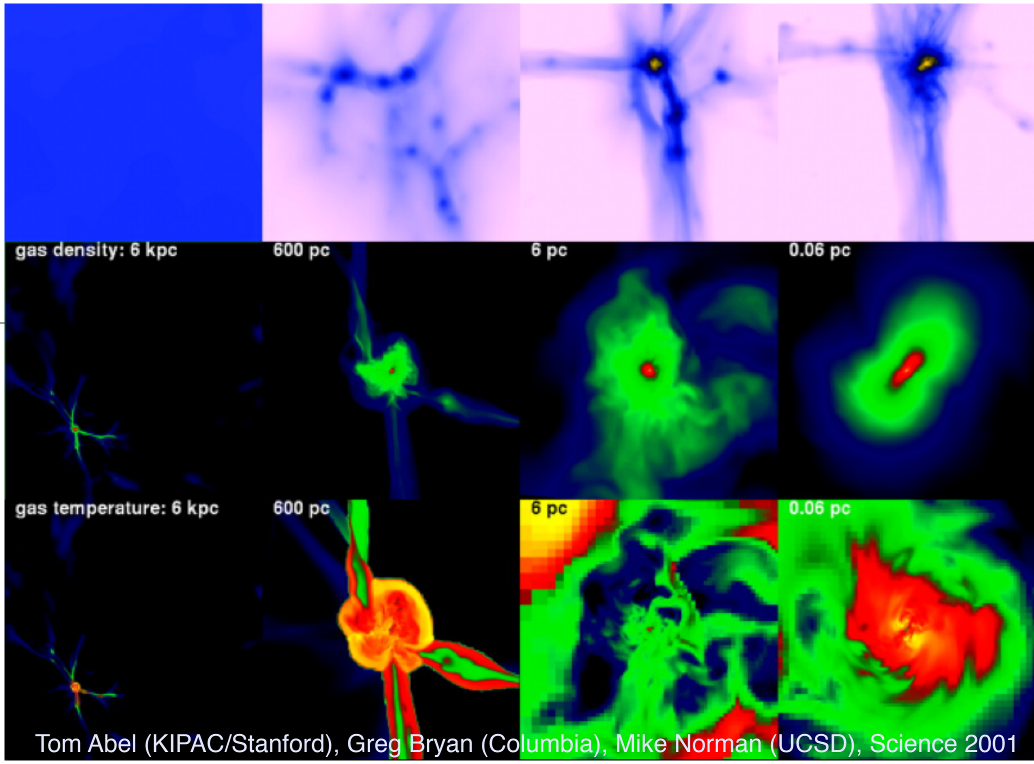
Turk et al, ongoing

Mass Scales?



Abel, Bryan & Norman 2002

Recap



Tom Abel (KIPAC/Stanford), Greg Bryan (Columbia), Mike Norman (UCSD), Science 2001

First Stars are isolated and very massive

- Theoretical uncertainty: 30 - 300 solar mass

Many simulations with three different numerical techniques and a large range of numerical resolutions have converged to this result. Some of these calculations capture 20 orders of magnitude in density!

Non-equilibrium chemistry & cooling, three body H2 formation, chemical heating, H2 line transfer, collision induced emission and its transport, and sufficient resolution to capture chemo-thermal and gravitational instabilities.
Stable results against variations on all so far test dark matter variations, as well as strong soft UV backgrounds.

cosmological: Abel et al 1998; Abel, Bryan & Norman 2000, 2002; O’Shea et al 2006; Yoshida et al 2006; Gao et al 2006
idealized spheres: Haiman et al 1997; Nishi & Susa 1998; Bromm et al 1999,2000,2002; Ripamonti & Abel 2004

CALIFORNIA NEBULA, NGC1499
500 pc = 1,500 light years away
30 pc long
Xi Persei, منكب mankib, Shoulder of Pleiades:
O7.5III
330,000 solar luminosities
~40 solar masses, Teff=3.7e4K

3D Cosmological Radiation Hydrodynamics

Focus on point sources

Early methods: Abel, Norman & Madau 1999 ApJ; Abel & Wandelt 2002, MNRAS; Variable Eddington tensors: Gnedin & Abel 2001, NewA

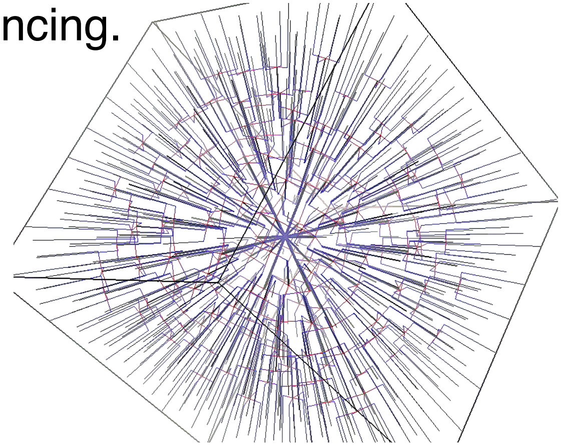
Abel, Wise & Bryan 06, MNRAS. Keeps time dependence of transfer equation using photon package concept from Monte Carlo techniques, yet not using any random numbers.

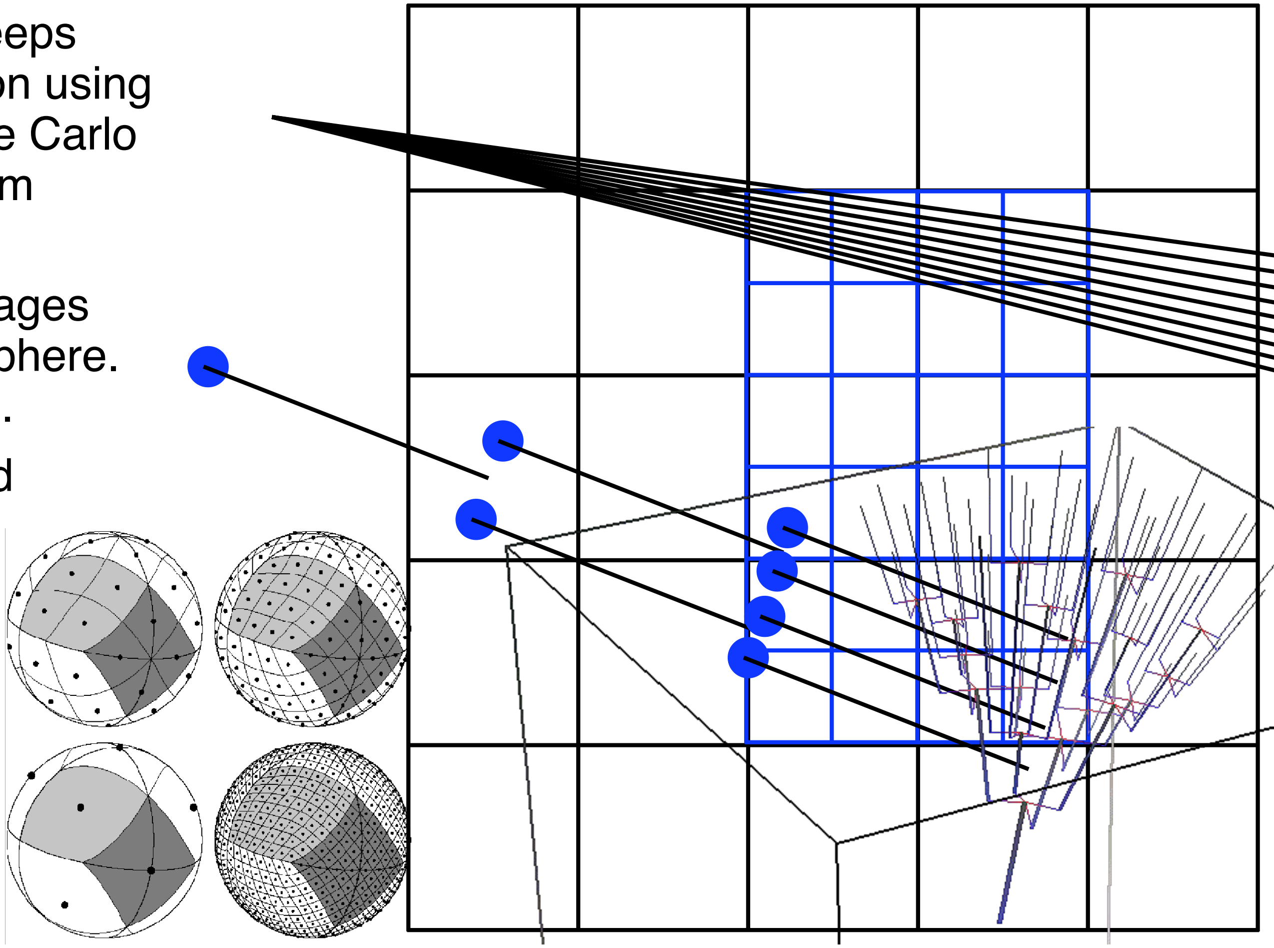
Adaptive ray-tracing of PhotonPackages using HEALPIX pixelization of the sphere. Photon conserving at any resolution.

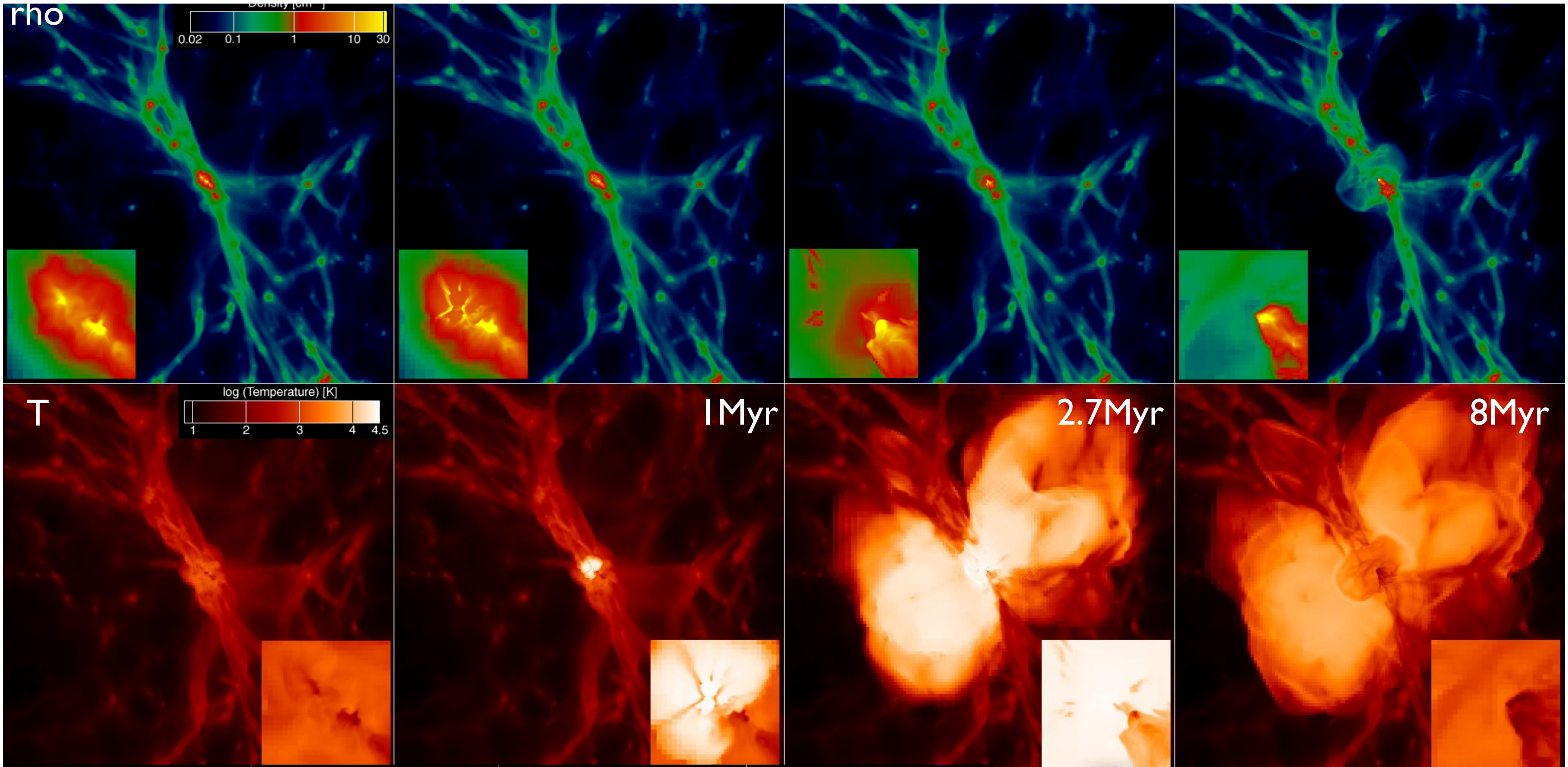
Parallel using MPI and dynamic load balancing.

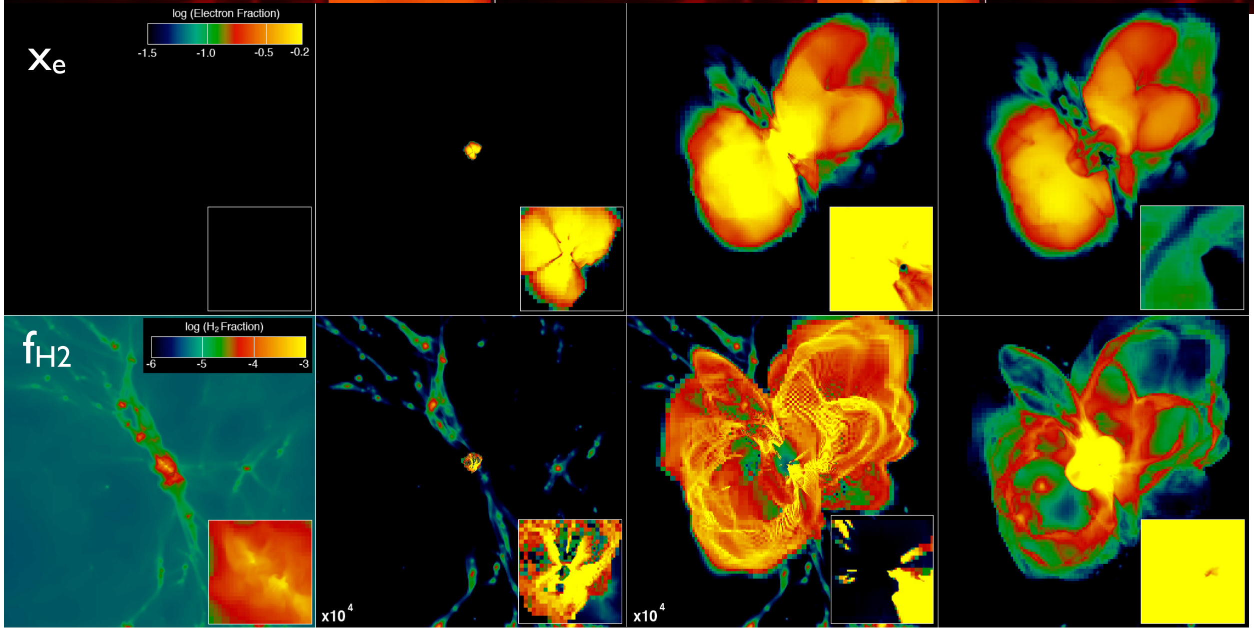
$$\frac{1}{c}\frac{\partial I_\nu}{\partial t}+\frac{\partial I_\nu}{\partial r}=-\kappa I_\nu$$

Transfer done along adaptive rays
Case B recombination



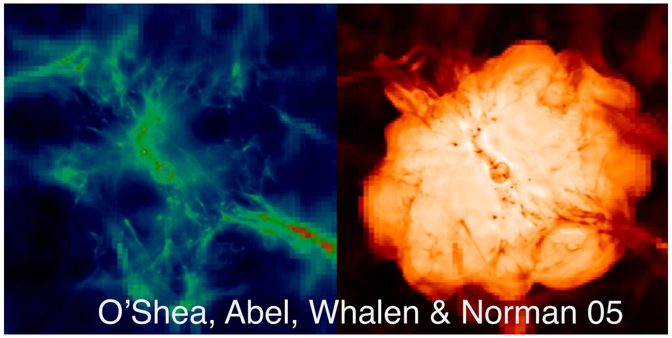






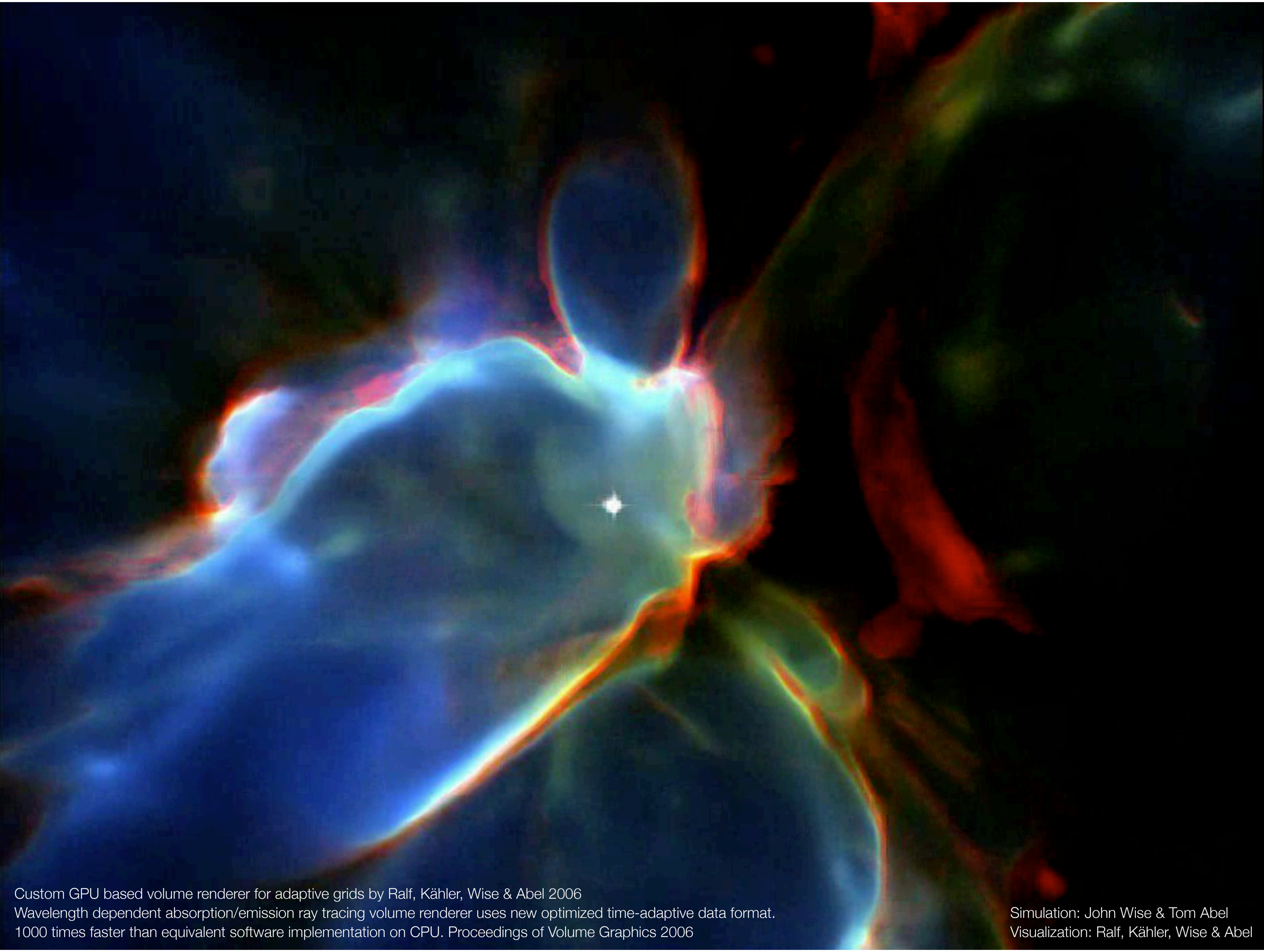
150pc ↔ 3kpc, 1/4 box

Redshift ~20



O'Shea, Abel, Whalen & Norman 05

Abel, Wise & Bryan 07 ApJL

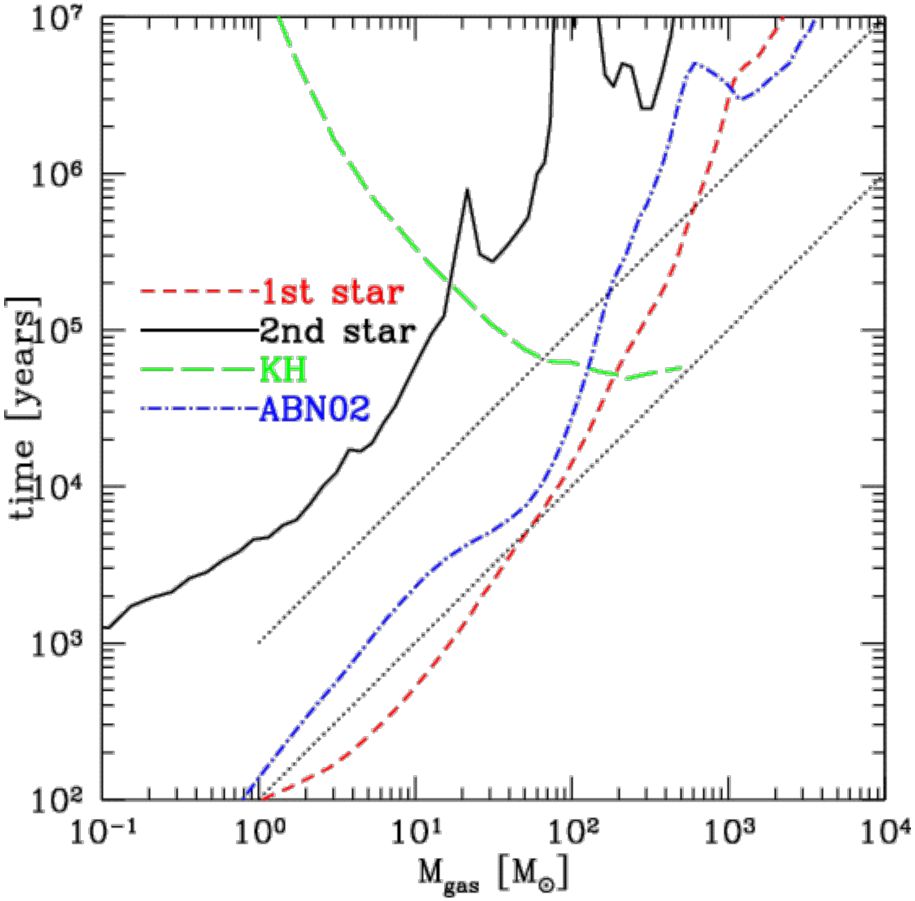


Custom GPU based volume renderer for adaptive grids by Ralf, Kähler, Wise & Abel 2006
Wavelength dependent absorption/emission ray tracing volume renderer uses new optimized time-adaptive data format.
1000 times faster than equivalent software implementation on CPU. Proceedings of Volume Graphics 2006

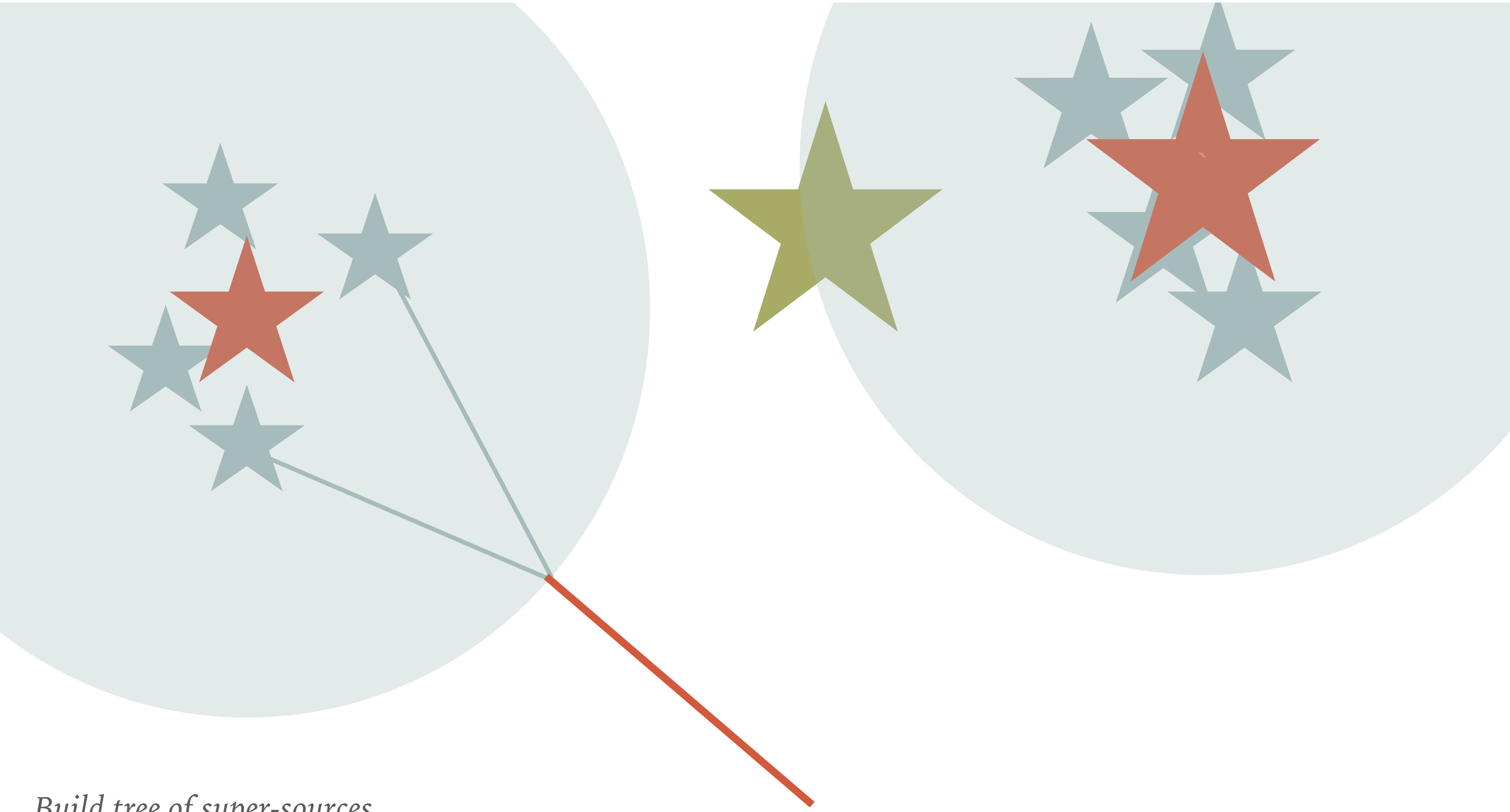
Simulation: John Wise & Tom Abel
Visualization: Ralf, Kähler, Wise & Abel

Feedback changes initial conditions for next generation of stars and their stellar masses.

- Input on small scales ...
- Formation of early disks more common?
- Caveat: Small numbers of simulations so far
- Mass range: 10-100 in second generation of metal free stars? This second generation may be much more abundant.



O’Shea, Abel, Whalen & Norman 2005
Yoshida et al 2006



Build tree of super-sources

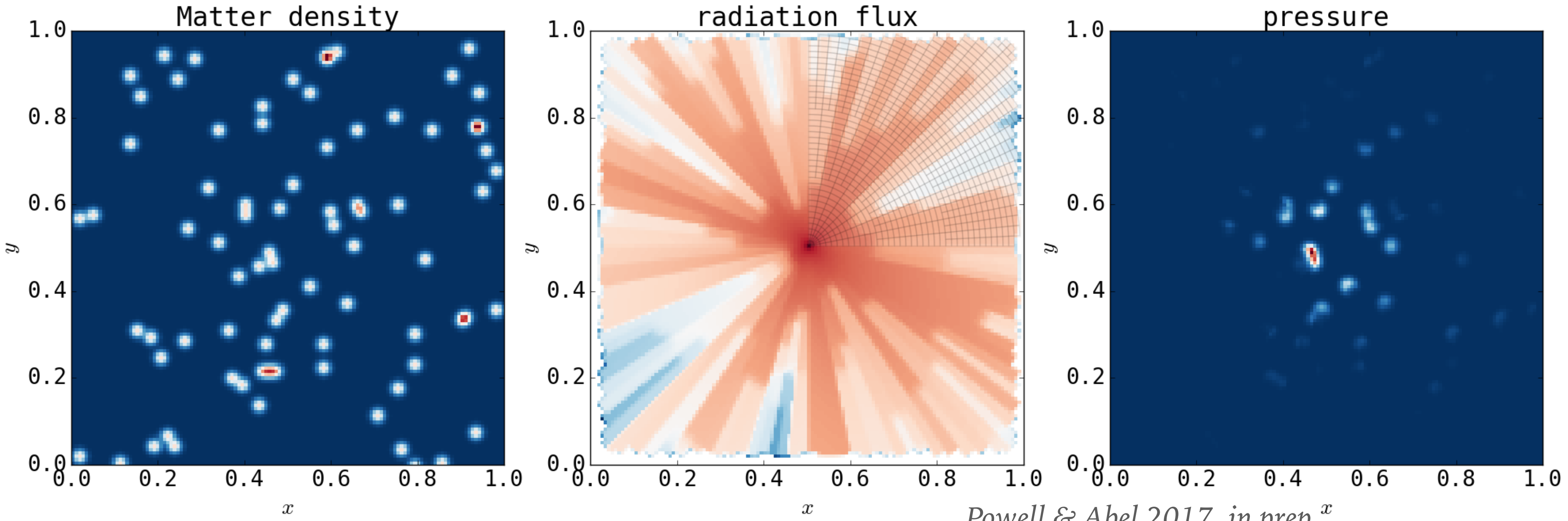
Rays halt at a fix radius from their associated super source (one level up in tree)

Rays check whether they are in the same pixel on the sphere of the SS

If they are they can combine and the added new ray intensity now travels radially from SS

BEAM TRACING

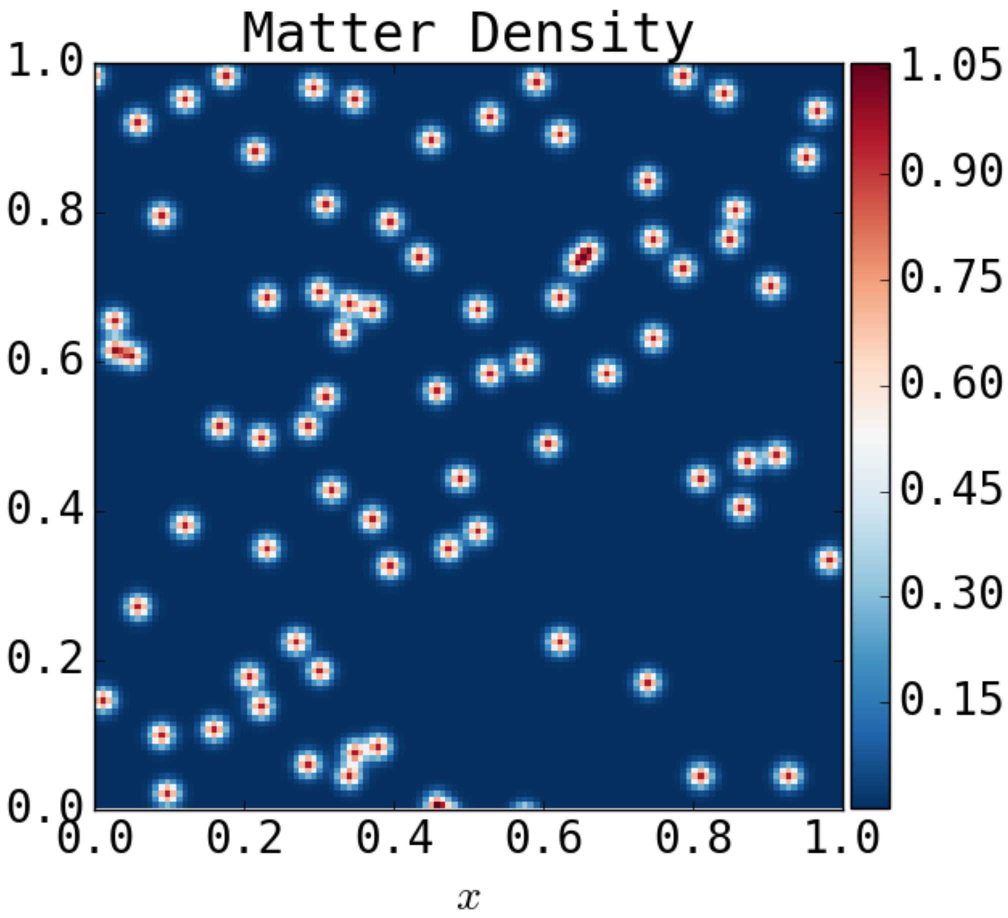
- Instead of tracing single one dimensional trace entire beam through volume.
  - Improve accuracy for same number of rays
  - Have much fewer rays for same accuracy. -> Less communication and more floating point ops.

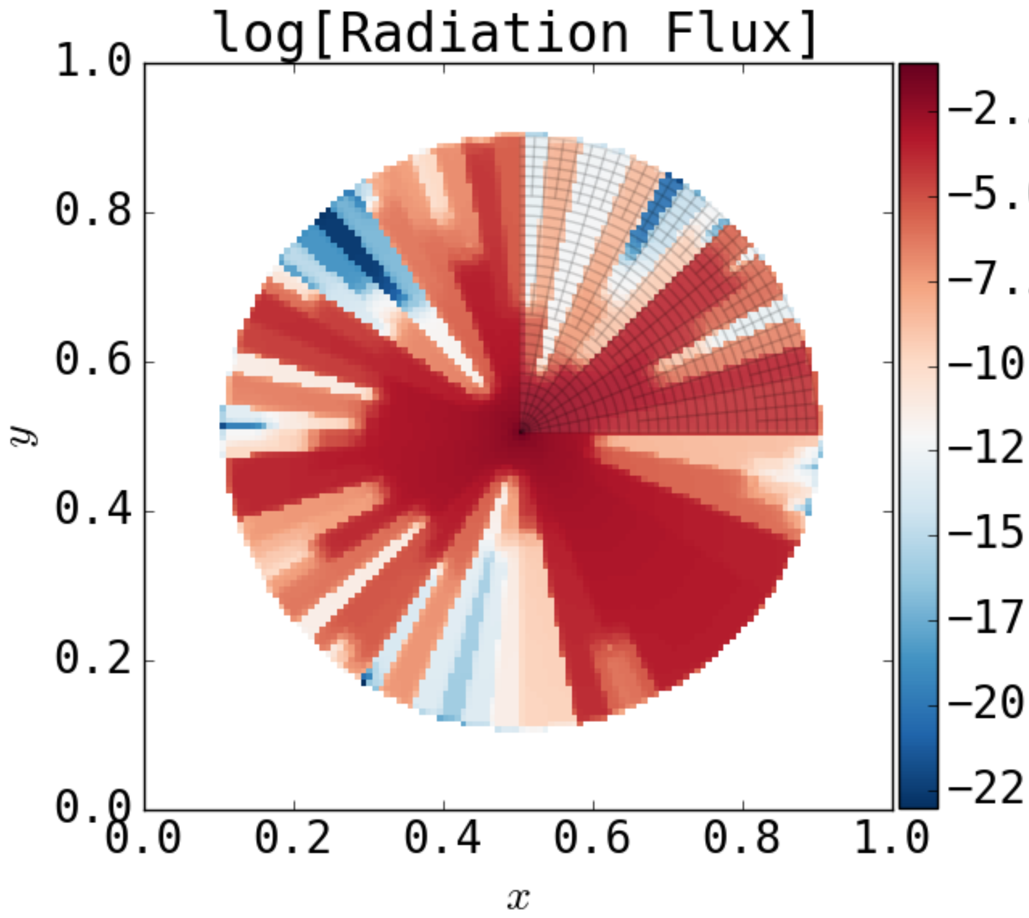


Powell & Abel 2017, in prep.^{x}

BEAM TRACING

- Coarse. Beam < 4 dx

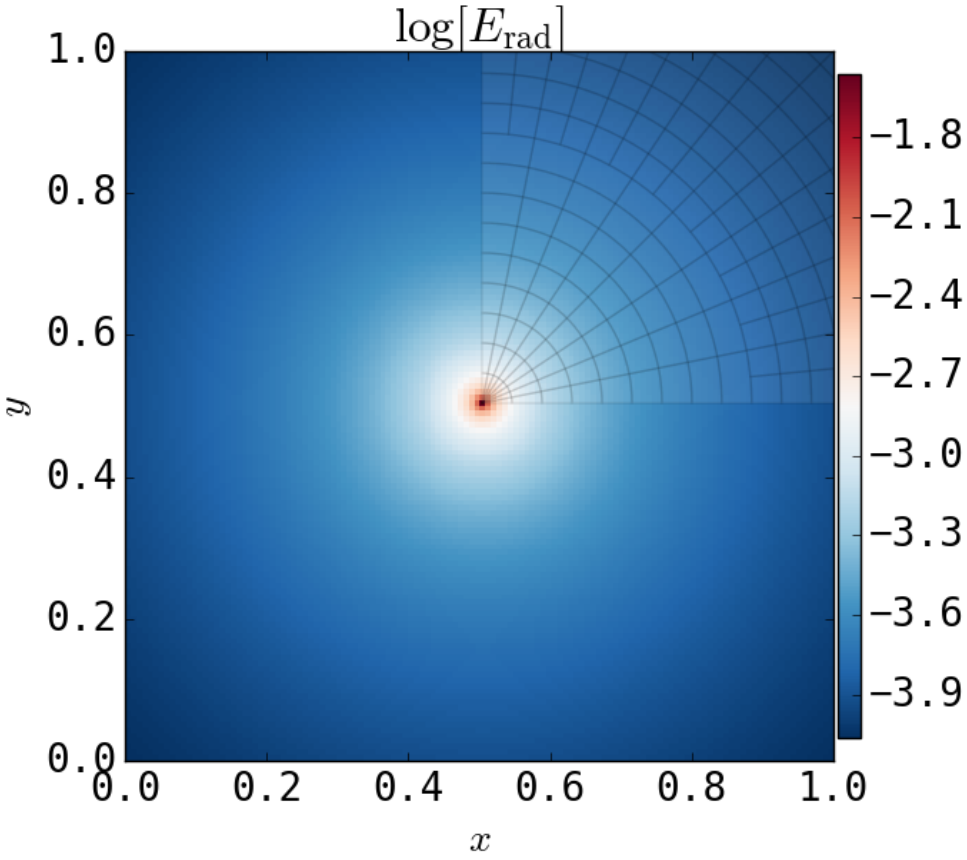


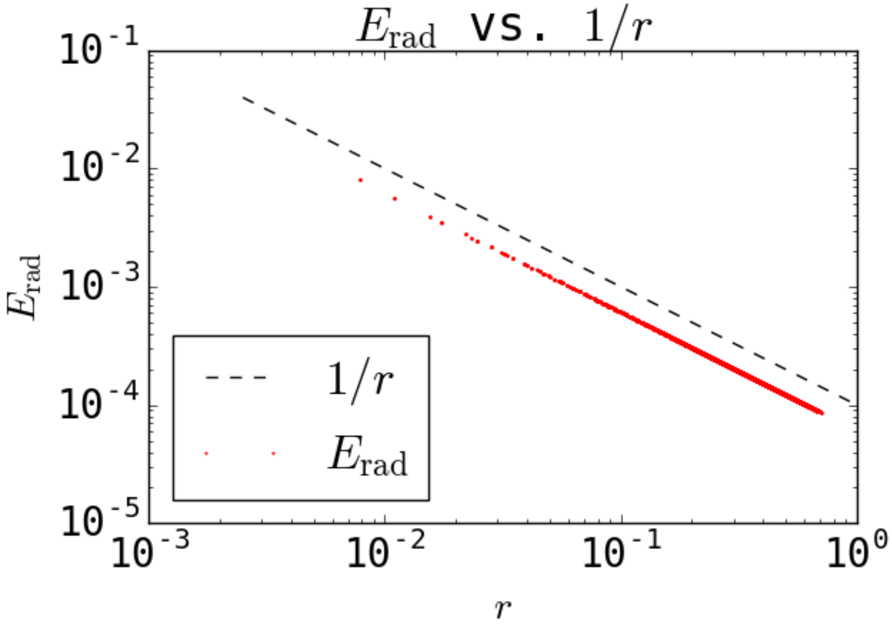


Powell & Abel 2017, in prep.

EXACT RADIAL DEPENDENCE

- Perfect symmetry

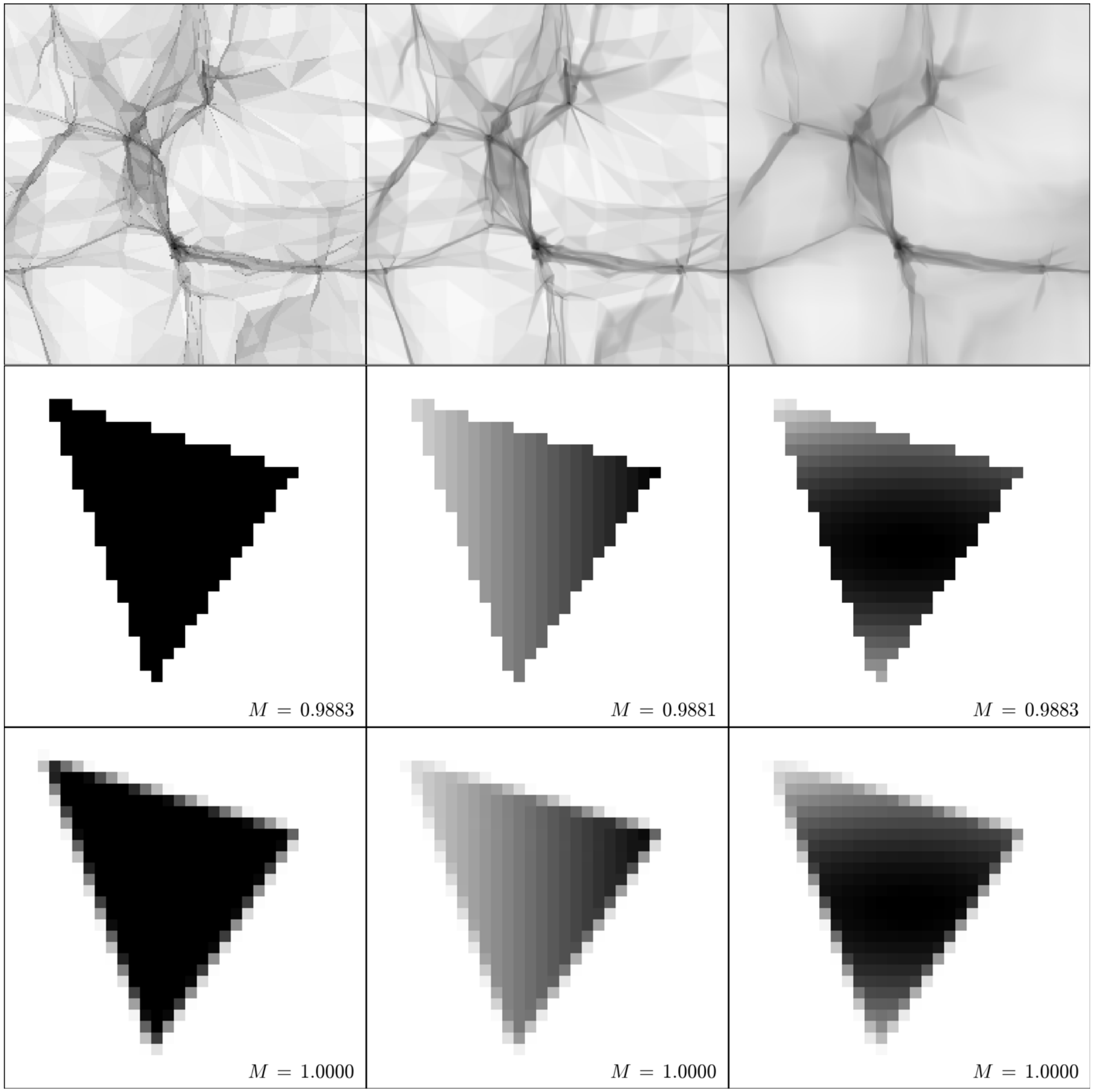




Powell & Abel 2017, in prep.

EXACT OVERLAP INTEGRALS. USEFUL BLACK BOX?

- To write new cosmology and plasma codes exploiting cold three dimensional manifolds in 6D phase space one needs to learn how to calculate overlap integrals of Polyhedra.
- This leads to exact and robust **remeshing** techniques which likely much more generally useful.
- Developed in N-dimensions with N-th order polynomial functions
- Started to use these ideas to do beam tracing for radiation transport.
- Enables waterbags in higher dimensions.
- New hydro methods?

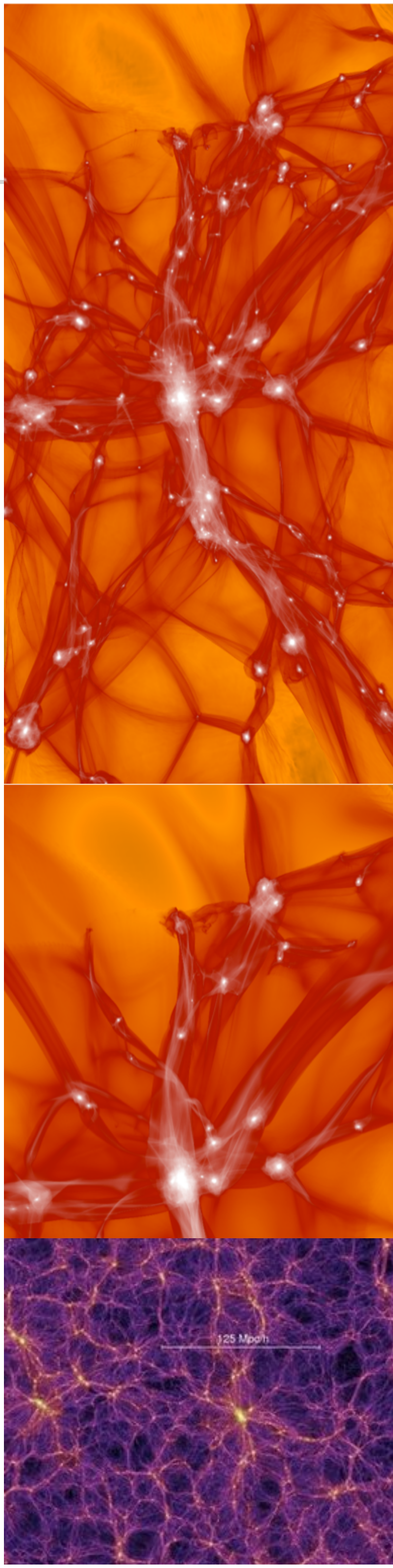


Powell & Abel 2016, J. Comp. Phys.

Surprising Life

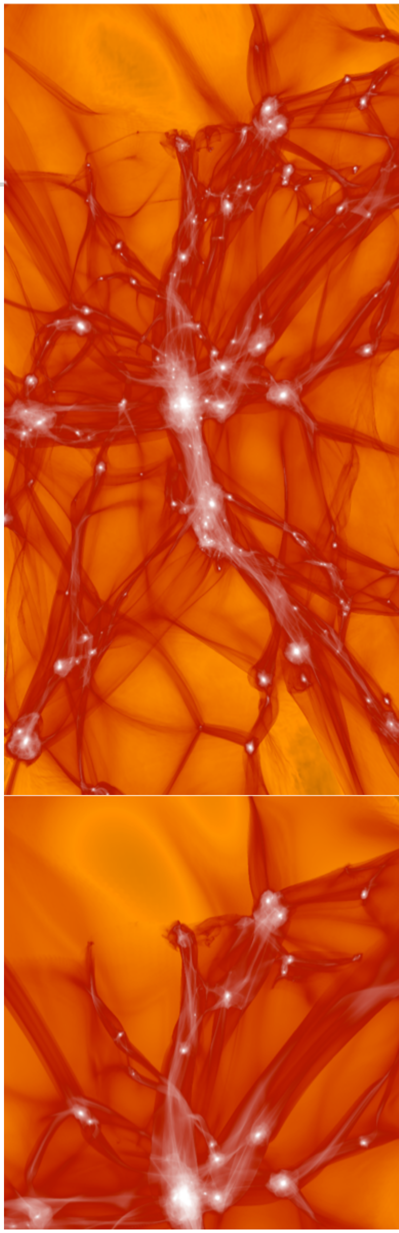
- No three dimensional stellar evolution calculations but much poorly constrained relevant physics
    - Angular momentum transport
    - Mixing from core, mixing into the atmosphere?
    - Stellar winds, as well as episodic mass loss?
    - Magnetic dynamo? Guaranteed seed field of ~ 4×10^{-10} Gauss from recombination.
- Can do:
    - Proto-stars (1st & 2nd generation)
    - HII regions (HeII & HeIII regions)
    - Metal enrichment & potential GRB remnants
    - Beginning of Cosmic Reionization
- Relevant mass range : 1) 30 - 300 solar mass and 2) 10 - 100 solar mass

Cosmological N-body simulations



- Used to make predictions about the distribution of dark matter in the Universe
- Key results
    - Galaxies are arranged in cosmic web of voids/sheets/filaments/halos
    - Universal spherical Dark Matter density profile (NFW) [not understood from analytical arguments]
    - Predicted mass functions of halos and their clustering and velocity statistics
- Primary tool to study observational consequences of LCDM
    - initial conditions: warm vs cold DM, Gaussian vs non-Gaussian
    - sensitivity on global cosmological parameters such as the total matter content and amount of dark energy, etc.
    - Gravitational Lensing signatures

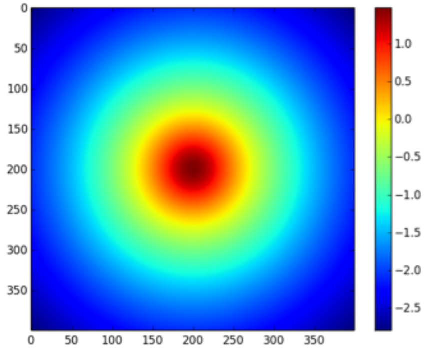
Cosmological N-body simulations

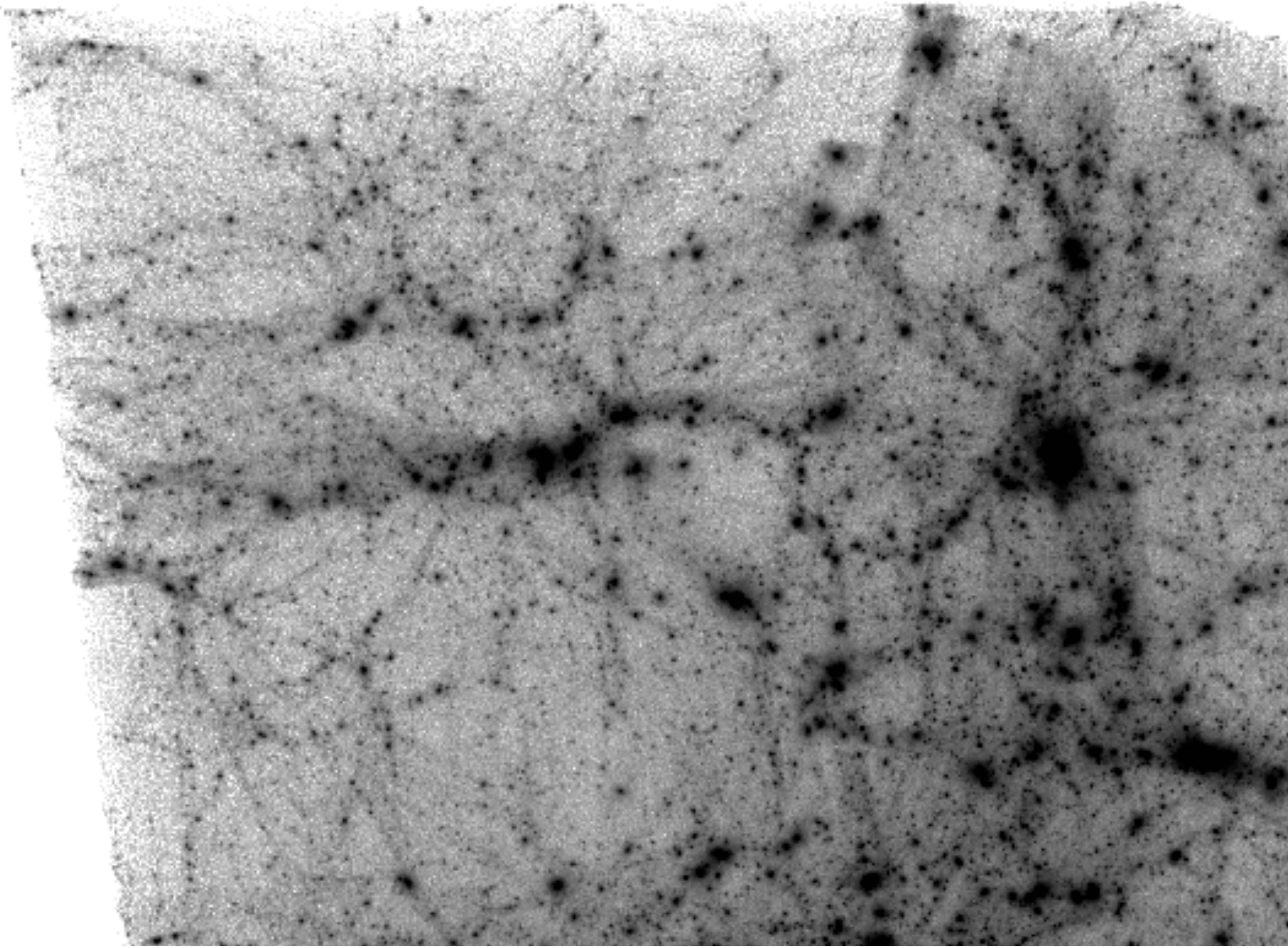


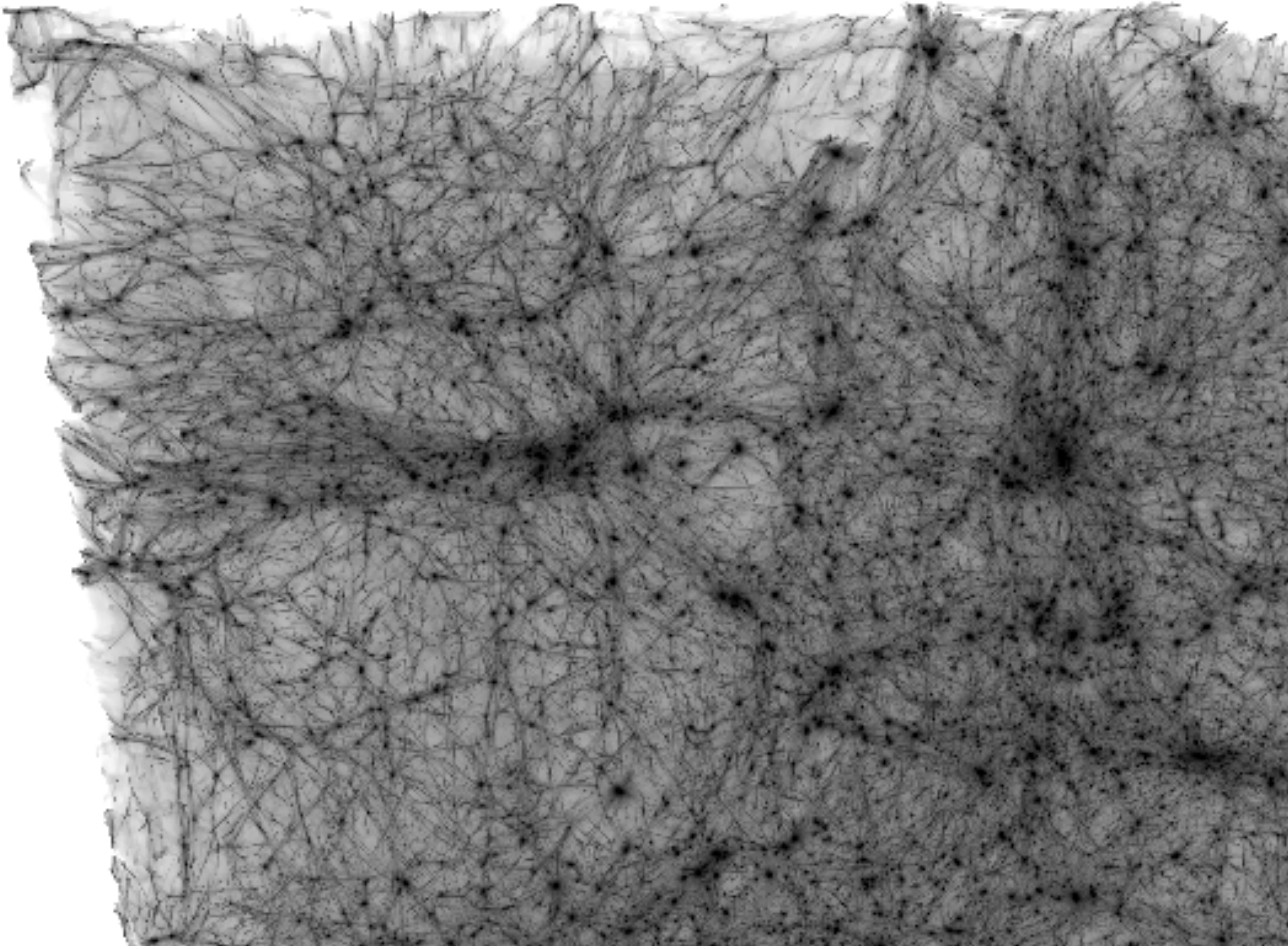
$$\dot{\mathbf{x}} = \mathbf{v}(t) \qquad \dot{\mathbf{v}}_{\mathbf{i}} = -\sum_{i\neq j}^{N} G m_i m_j \frac{(\mathbf{x_j} - \mathbf{x_i})}{|\mathbf{x_j} - \mathbf{x_i}|^3}$$

- All modern cosmological simulation codes only differ in how they accelerate the computation of the sum over all particles to obtain the net force
- End result are simply the positions and velocities of all particles
- Softening of forces (add epsilon^2 in denominator) avoids singularities.
- Limit N goes to infinity must give correct answer, right?
- Plummer

$$\dot{\mathbf{v}}_i = -\sum_{i\neq j}^{N} G\, m_i\, m_j \frac{(\mathbf{x}_j - \mathbf{x}_i)}{\left(|\mathbf{x}_j - \mathbf{x}_i|^2 + \epsilon^2\right)^{3/2}}$$







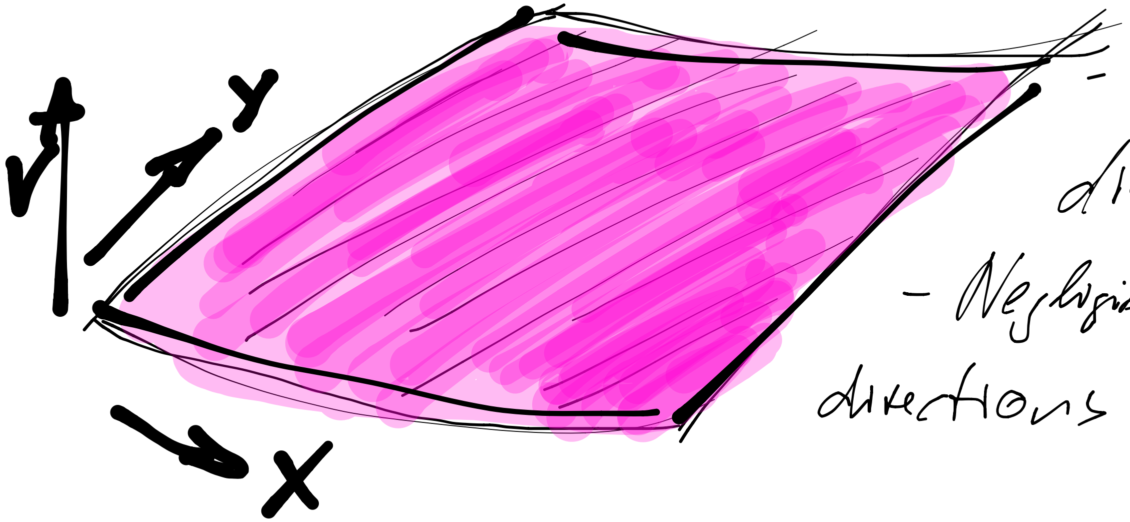
The Dark Matter Sheet?

COOL WIMPS

Dark Matter is commonly hypothesized to originate within seconds after the BIG BANG. If it were moving relativistically today, galaxies and other structures would not exist. We speak of **COLD DARK MATTER**.

Working HYPOTHESIS:

- Weakly interacting massive particle (say ≈ 100 GeV).
- Very cold. Even keV particles would only have ~ $\frac{m}{s}$ speeds today.



- Almost perfectly uniformly distributed initially.
- Negligible extent along velocity directions in phase space.

The Dark Matter Sheet ?

Fluid

OF DARK MATTER PARTICLES IN THE MILKY WAY :

$$N_{DM} \approx 10^{67}\left(\frac{100GeV}{m_{DM}}\right) \gg \text{\# OF STARS IN THE UNIVERSE}$$

$$\gg \text{\# OF PARTICLES THAT FIT ON A COMPUTER}$$

USING ALL THE COMPUTERS IN THE WORLD : $\lesssim 10^{17}$ particles

SOLVE VLASOV-POISSON SYSTEM INSTEAD.

$$\frac{\partial f}{\partial t} + \vec{v}\cdot\nabla_x f + \vec{a}\cdot\vec{\nabla}_v f = 0$$

$$\vec{a} = -\vec{\nabla}\phi$$

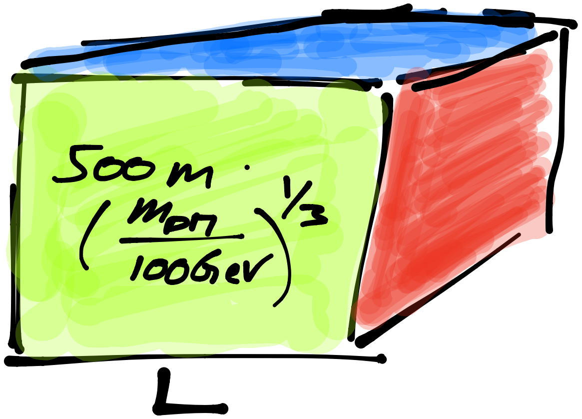
$$\nabla^2\phi = 4\pi G\rho$$

f: distribution function IN PHASE SPACE

ϕ: potential

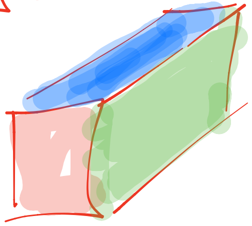
FOR PHASE SPACE ELEMENT TO CONTAIN 10^6 PARTICLES @ MEAN DENSITY IT HAS TO BE LARGER THAN

$$L \sim 500m\left(\frac{m_{DM}}{100GeV}\right)^{1/3}$$



The Dark Matter Sheet ?

3D MANIFOLD MOVING IN SIX DIMENSIONAL PHASE SPACE



Phase space volume is conserved

$$\Delta V \cdot (\Delta v)^3 = \text{const}$$

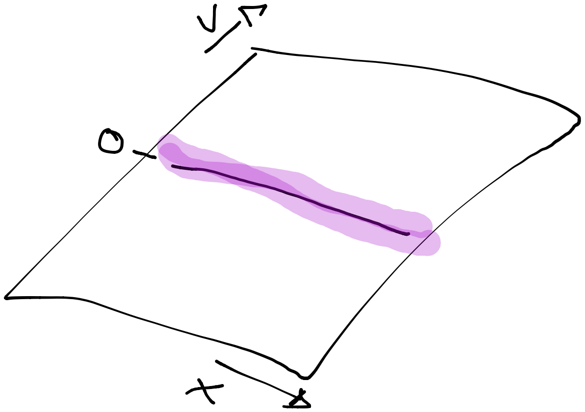
spatial volume   volume in velocity space

redshift when $E \simeq 100\,\text{GeV}$: 1eV @ $z \sim 1000$

100 GeV @ $z \sim 10^{14}$

Matter density dropped by a factor $\sim 10^{42}$ since then.

→ YES. VERY COLD.



Tiny initial peculiar velocities

⇒ distribution function $f(\vec{x},\vec{v}) = f_0\ \delta(\vec{v})$

is single valued at every $\vec{x}$ DIRAC DELTA

GRAVITY:

TOTAL MASS DENSITY

POISSON EQUATION : $\nabla^2\phi = 4\pi G \rho$

CONTINUUM DESCRIPTION

$$\vec{F}/m = -\nabla\phi$$

VLASOV EQUATION $\frac{\partial f}{\partial t} + v\nabla_x f - \nabla\phi\nabla_v f = 0$

FOR N → ∞ ↕ IDENTICAL

N POINT MASSES : $\vec{a}_j = -\sum_{i\neq j} \frac{G m_i}{|\vec{x}_j-\vec{x}_i|^2+\varepsilon^2} \frac{(\vec{x}_j-\vec{x}_i)}{|\vec{x}_j-\vec{x}_i|}$

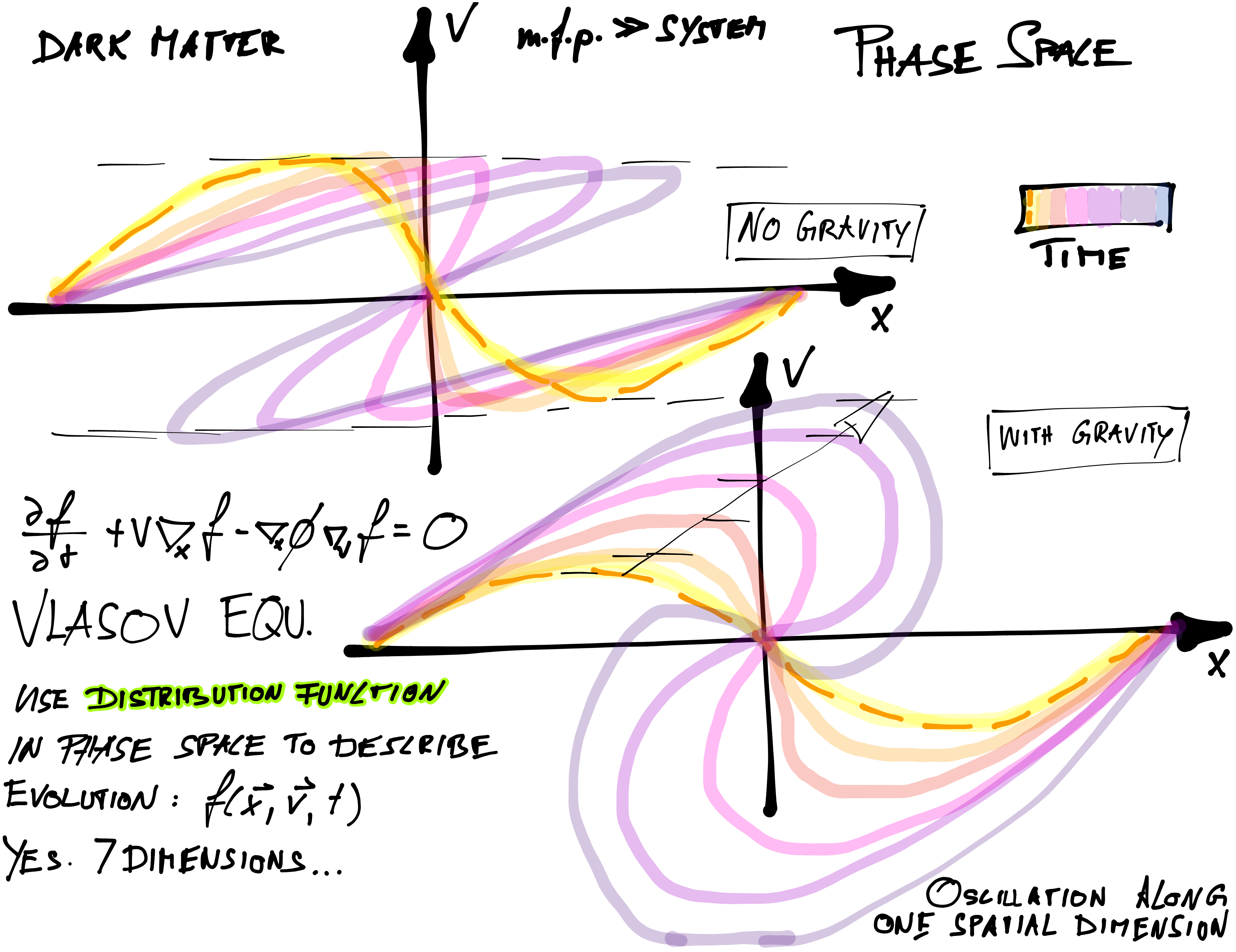
PARTICLE PICTURE

Particle "advection": $\frac{\partial \vec{x}_j}{\partial t} = \vec{v}$; $\frac{\partial \vec{v}_j}{\partial t} = \vec{a}_j$

DARK MATTER

m.f.p. >> SYSTEM

PHASE SPACE



$$\frac{\partial f}{\partial t} + v\nabla_x f - \nabla_x \phi \nabla_v f = 0$$

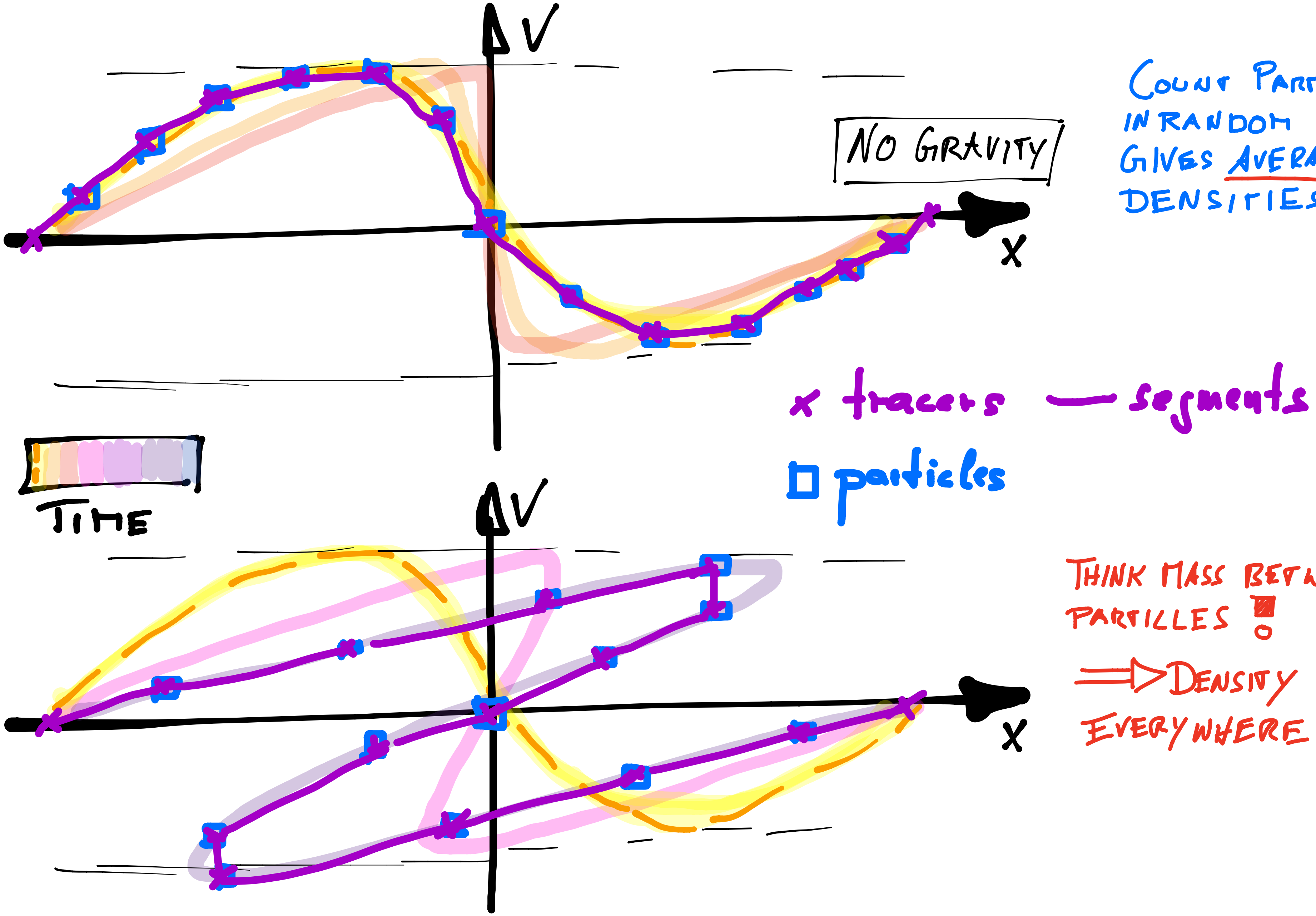
VLASOV EQU.

USE **DISTRIBUTION FUNCTION** IN PHASE SPACE TO DESCRIBE EVOLUTION : $f(\vec{x}, \vec{v}, t)$

YES. 7 DIMENSIONS...

OSCILLATION ALONG ONE SPATIAL DIMENSION

DISCRETIZE DARK MATTER DISTRIBUTION: Mass or Volume?



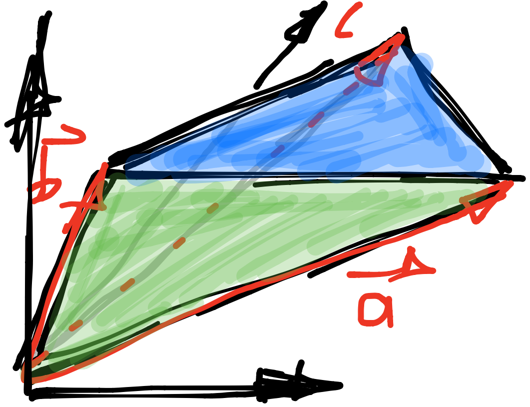
COUNT PARTICLES IN RANDOM VOLUMES GIVES AVERAGE DENSITIES

THINK MASS BETWEEN PARTICLES !

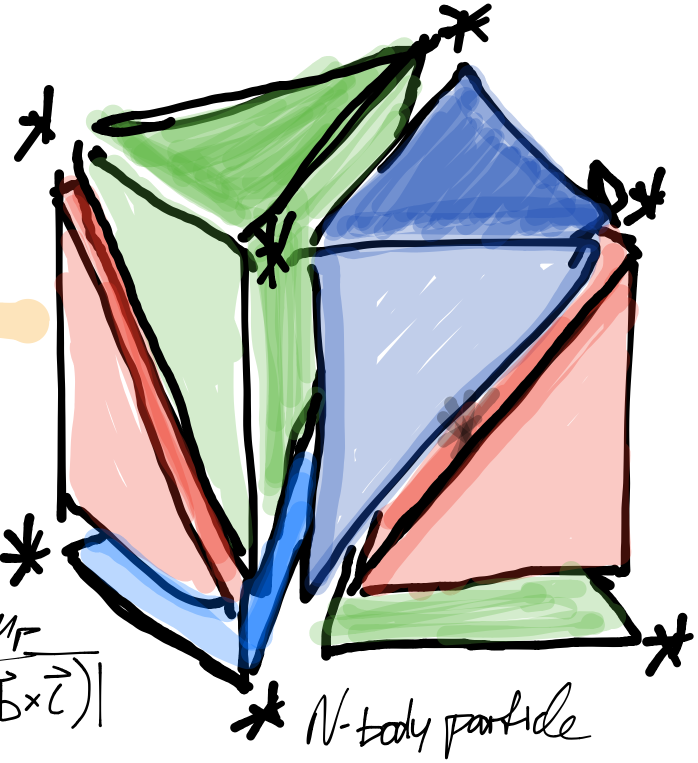
⟹ DENSITY KNOWN EVERYWHERE !

TESSELATE 3D MANIFOLD & TRACK IN 6D PHASE SPACE

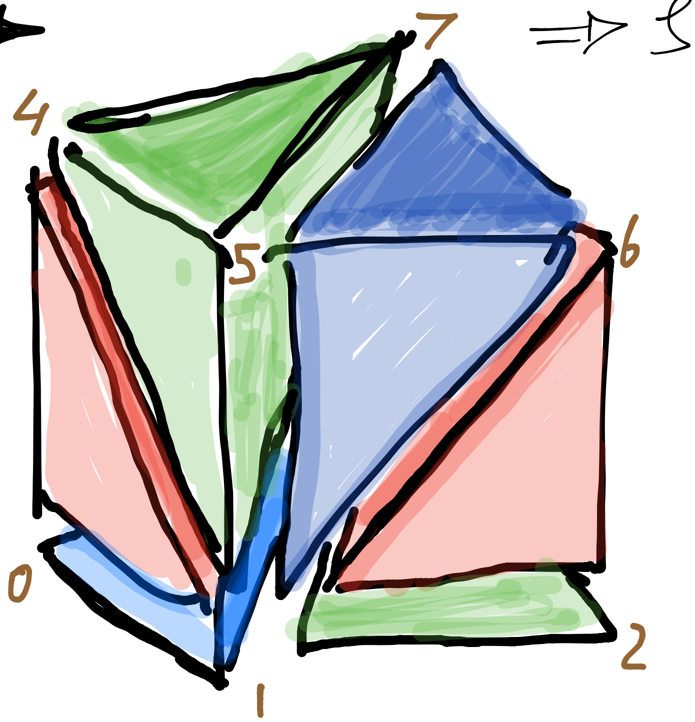
- NATURAL TESSELATION SPLITS CUBE INTO 6 EQUAL SIZED TETRAHEDRA
- mass per tetrahedron = 1/6 of DM particle mass.



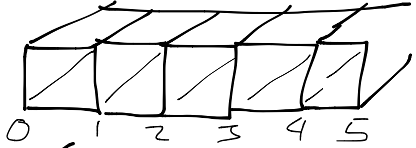
$$V = \frac{|\vec{a}\cdot(\vec{b}\times\vec{c})|}{6}$$



$$\Rightarrow \rho = \frac{m_p}{6V} = \frac{m_p}{|\vec{a}\cdot(\vec{b}\times\vec{c})|}$$

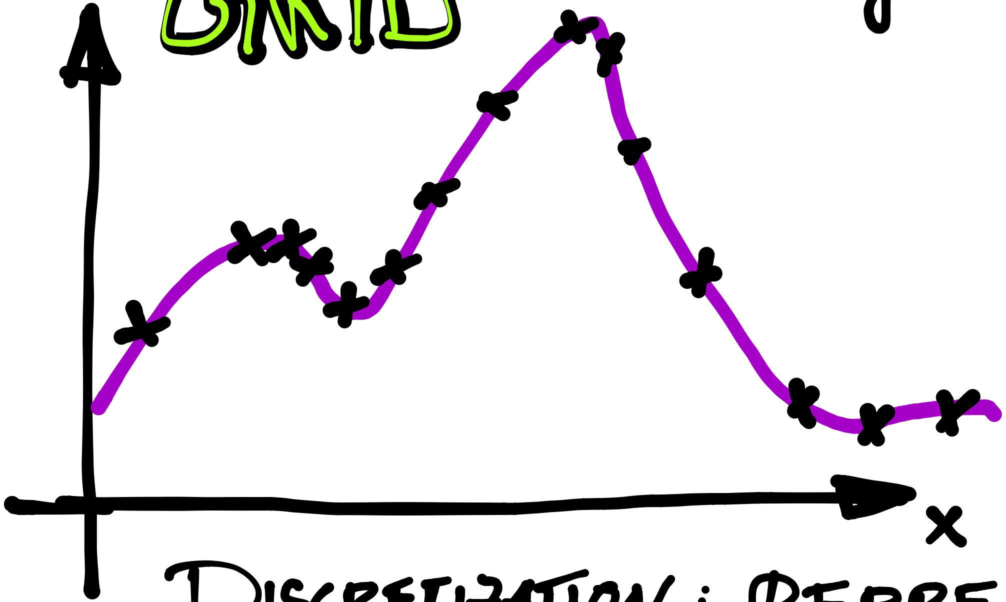


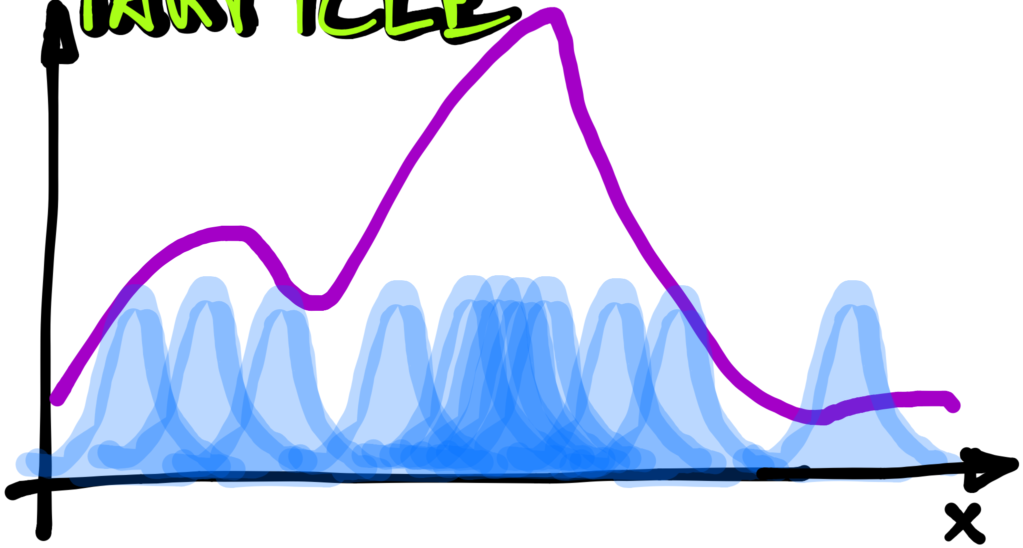
- Number the edges of the cube
- think of lattice
- Looping over



The initial cartesian (LAGRANGIAN lattice generates the 6N tetrahedra.

GRID e.g. PARTICLE





DISCRETIZATION: REPRESENT CONTIUUM SOLUTION WITH FINITE NUMBER OF ELEMENTS

("COMPRESSION")

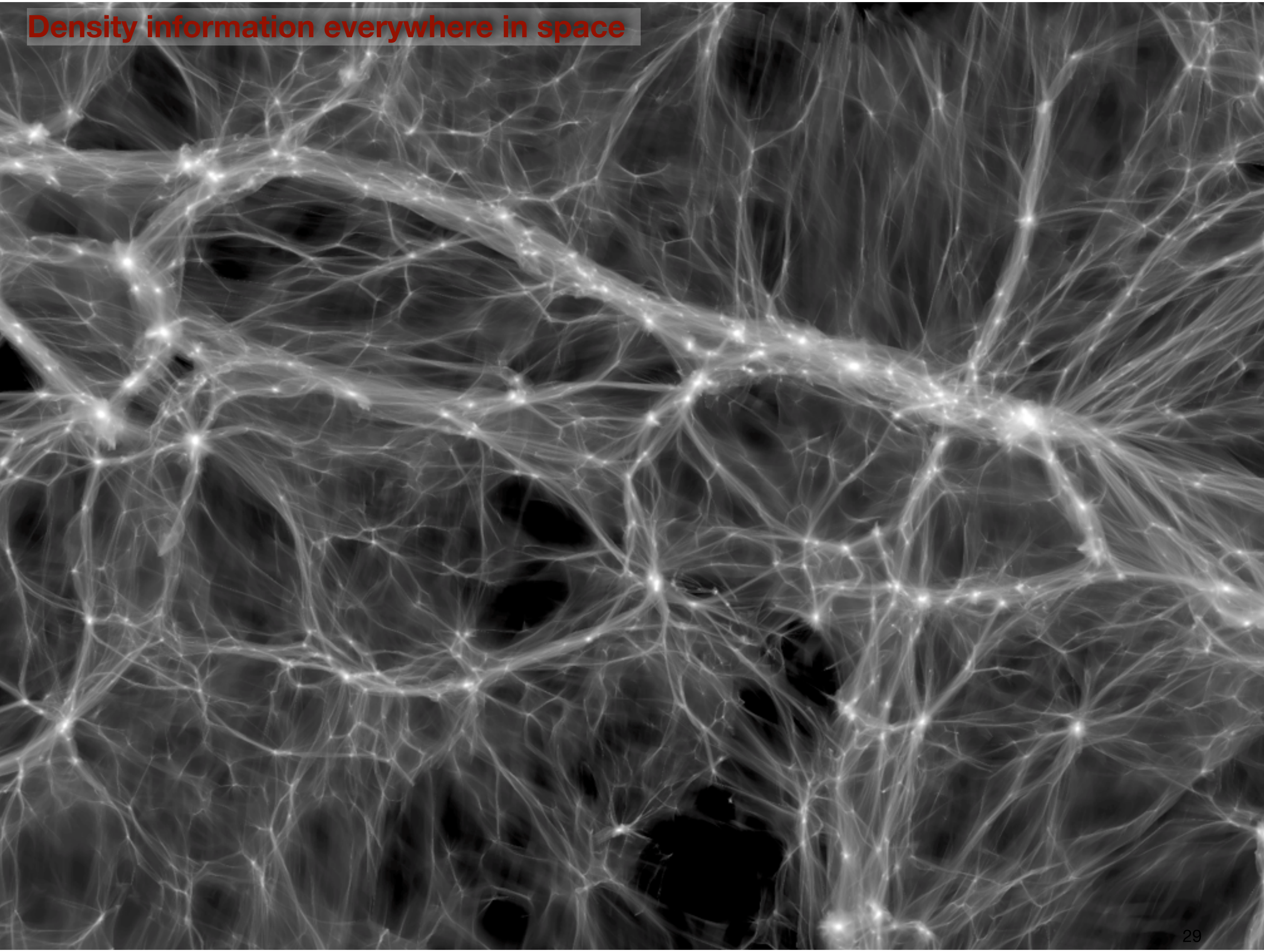
uniform, adaptive, moving, structured, unstructured, tetrahedral, cartesian, cylindrical

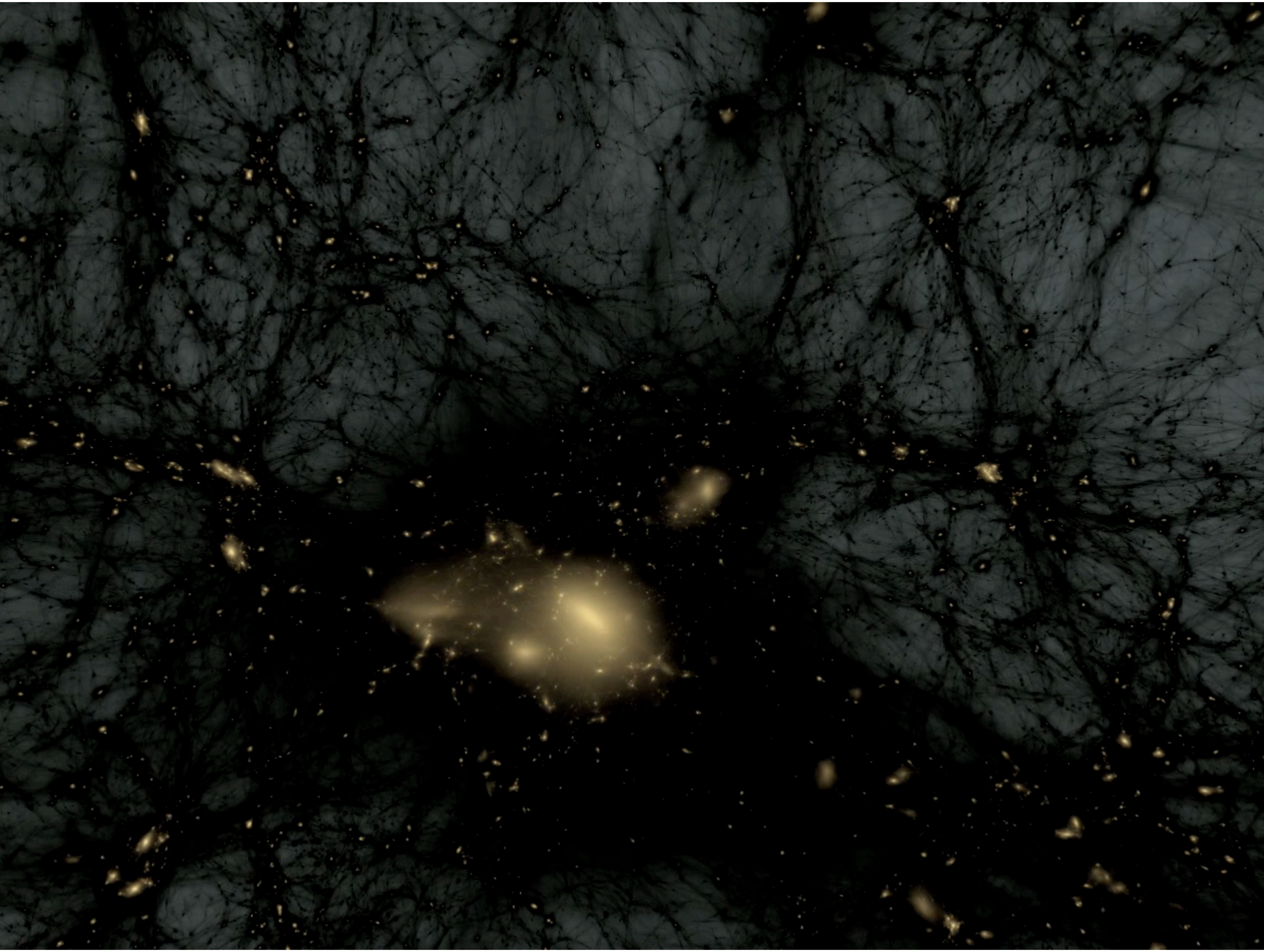
MESH

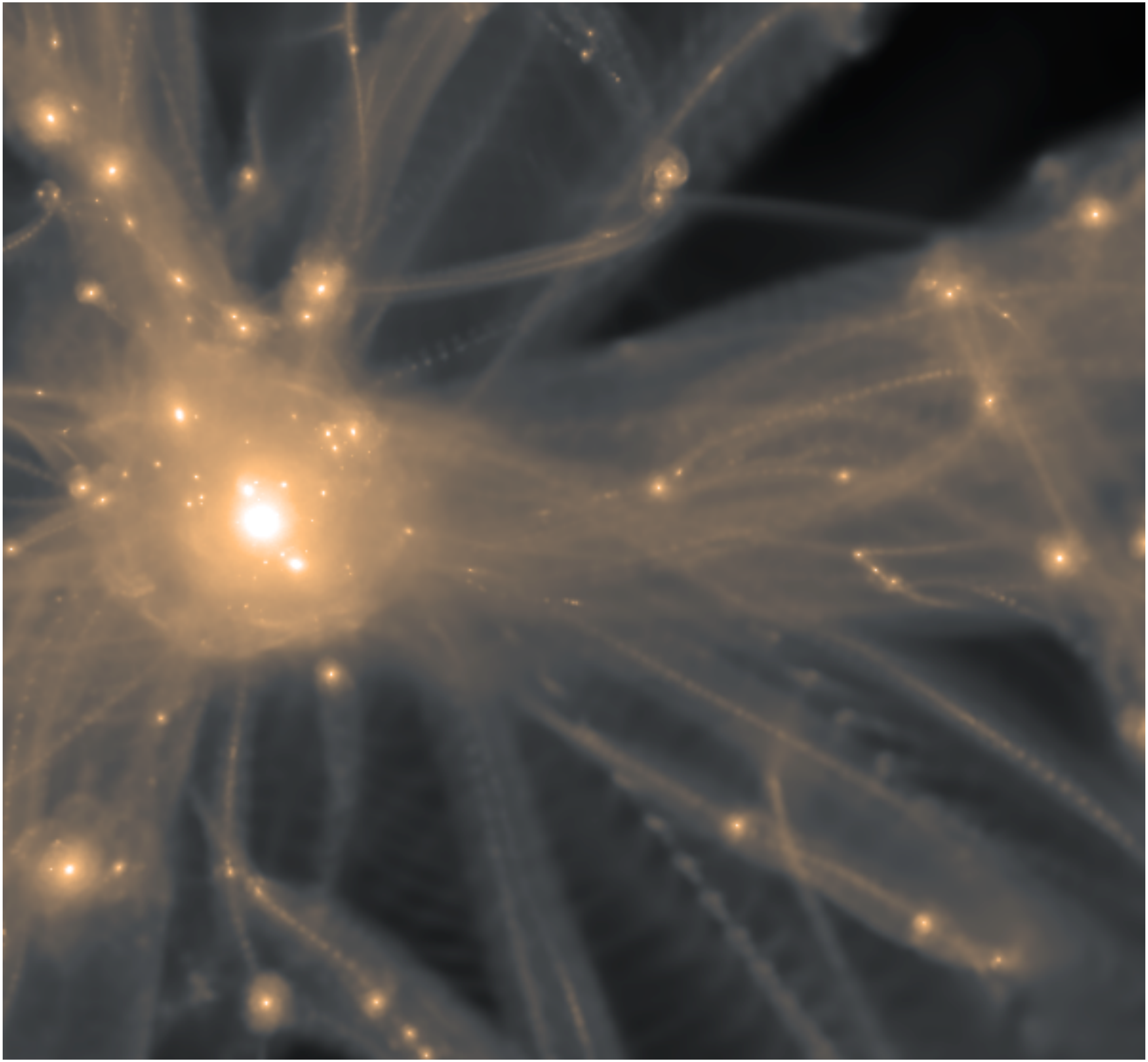
fixed, adaptive, high order, assymmetric, ...

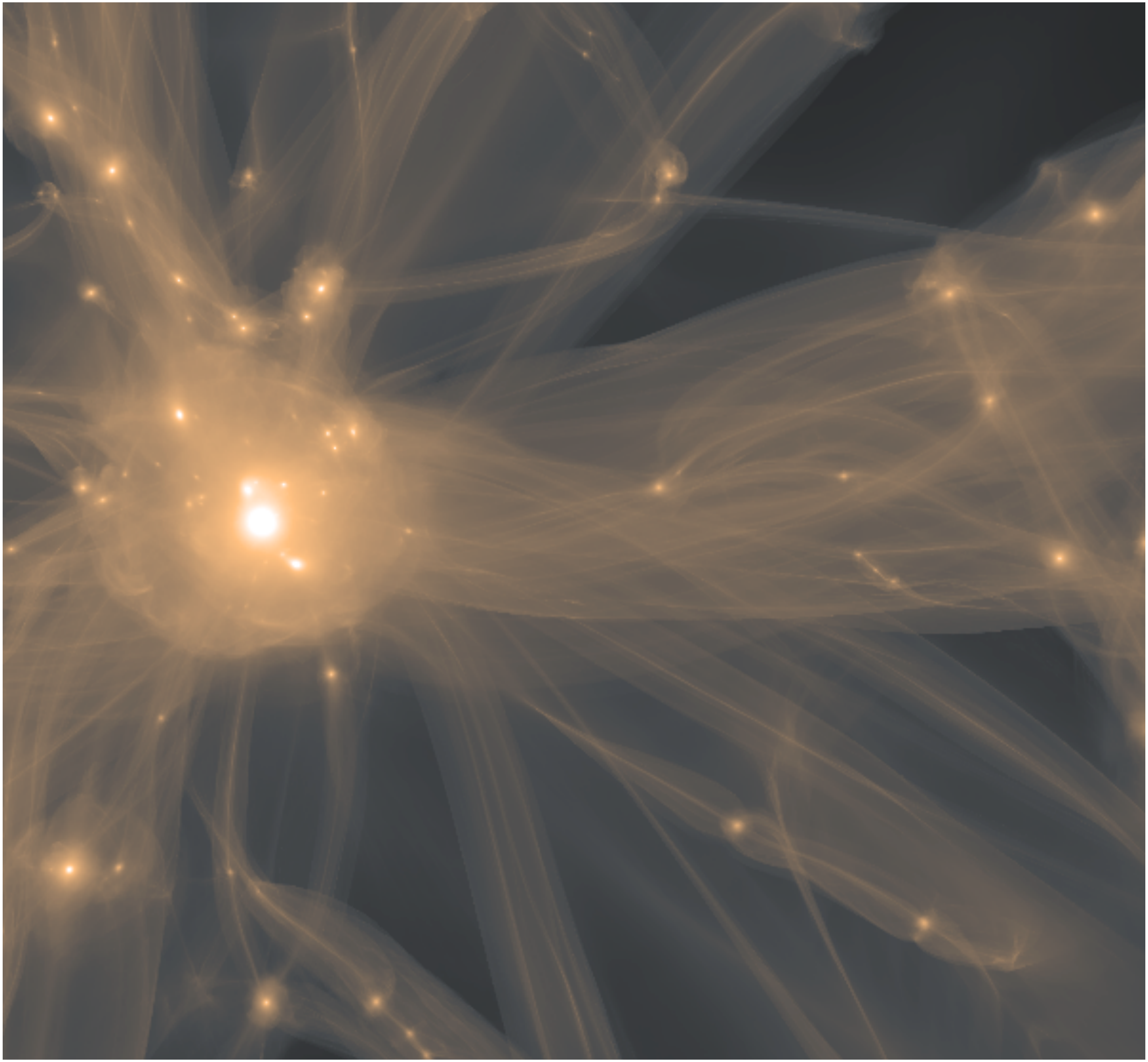
KERNEL

Density information everywhere in space



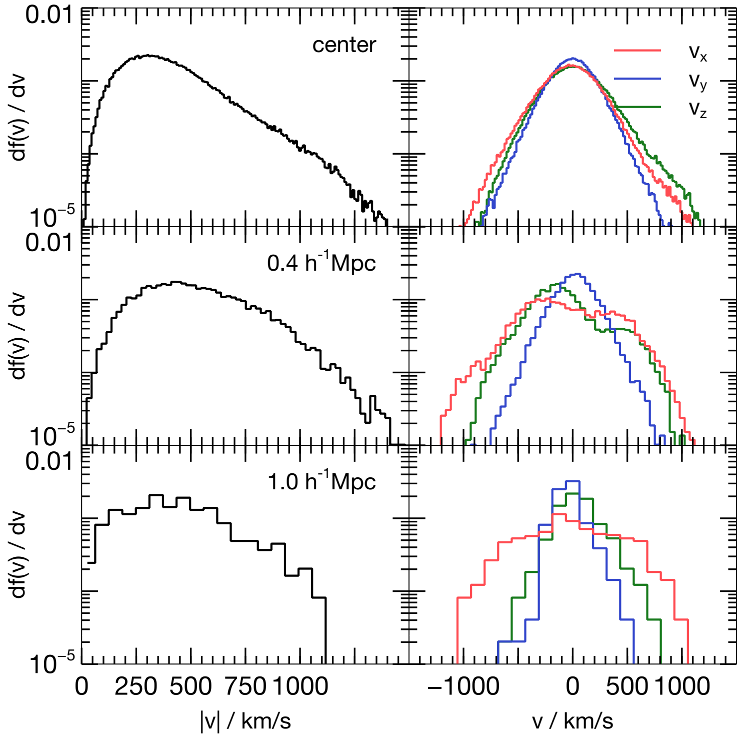


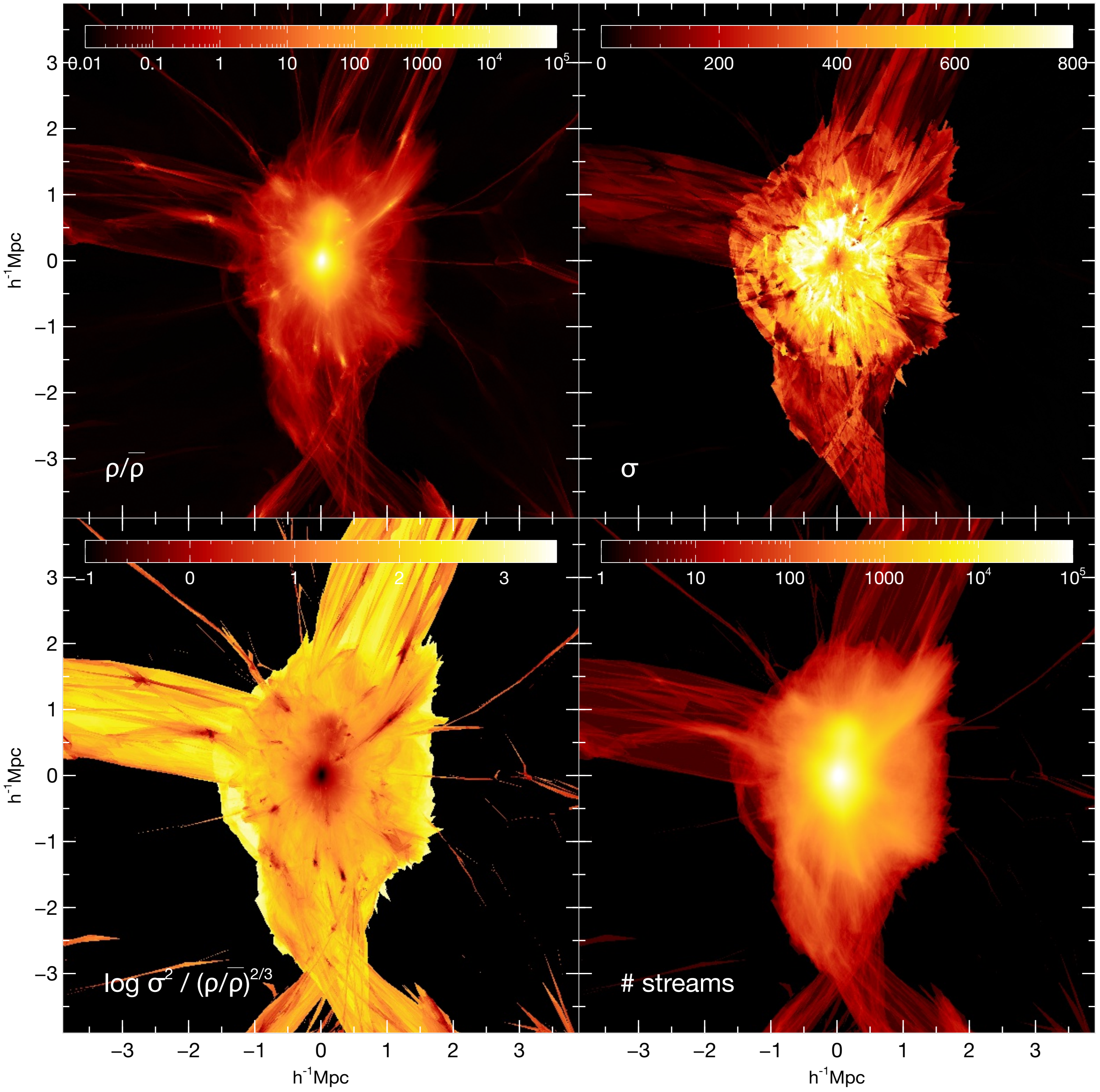




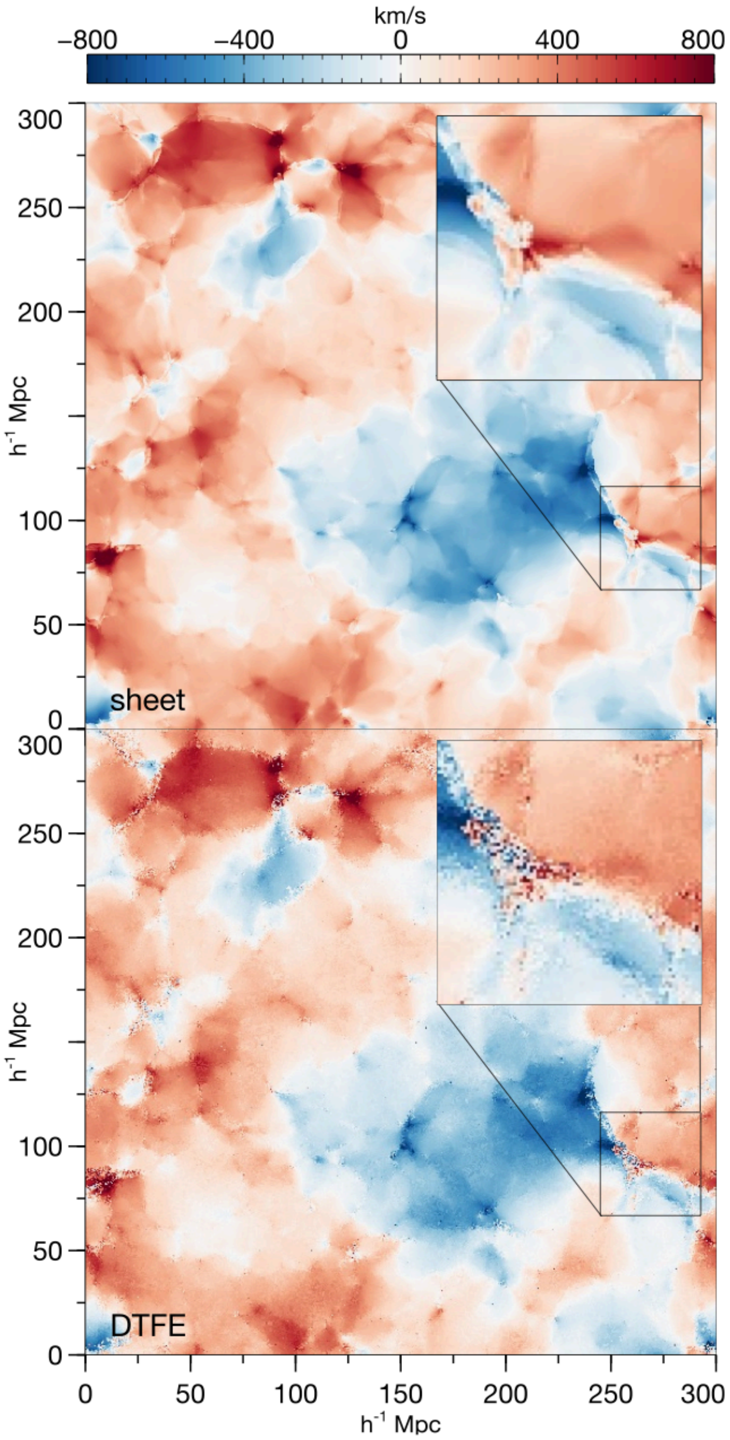
All microphysical phase space information available

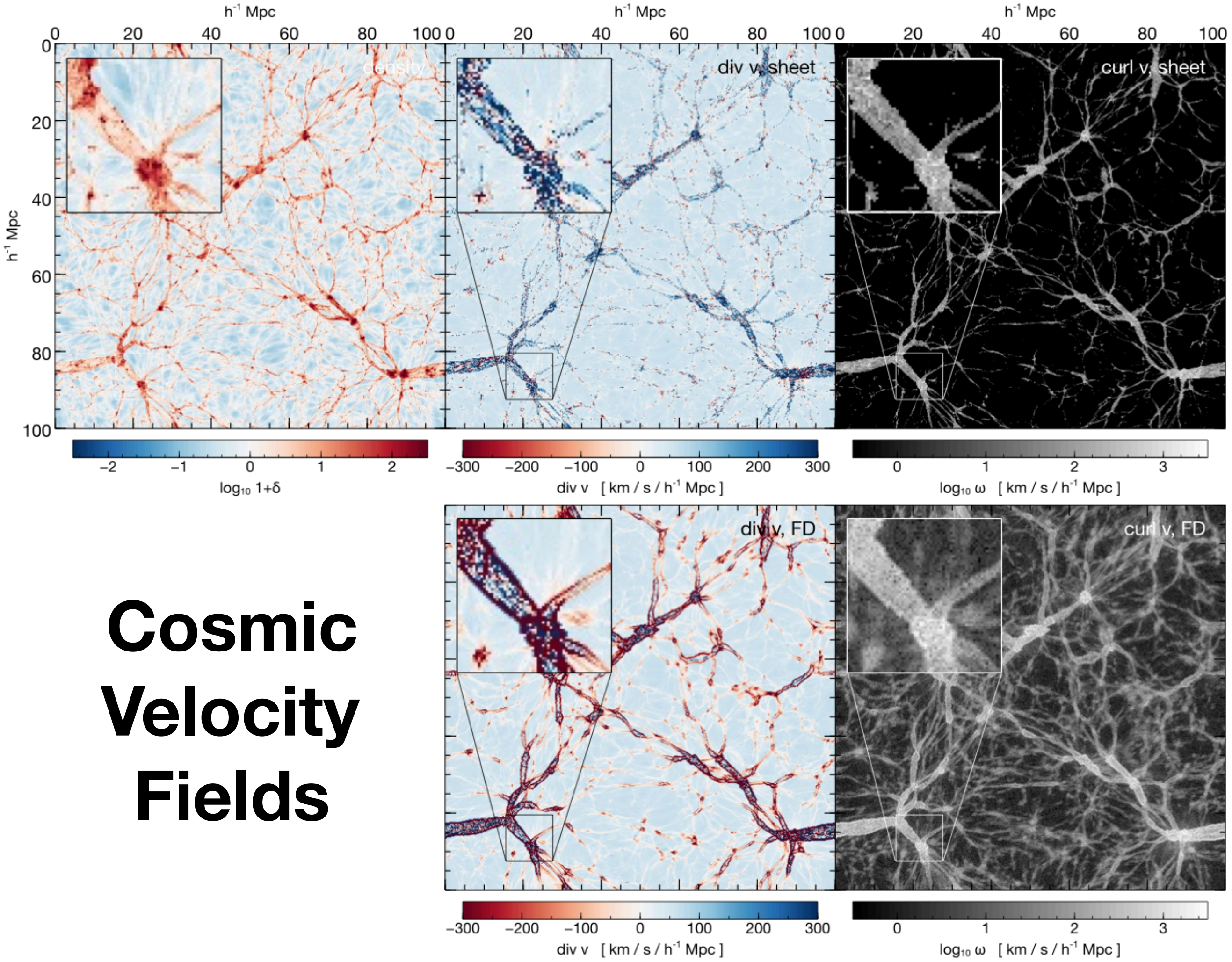
can probe
fine-grained
phase space
structure.

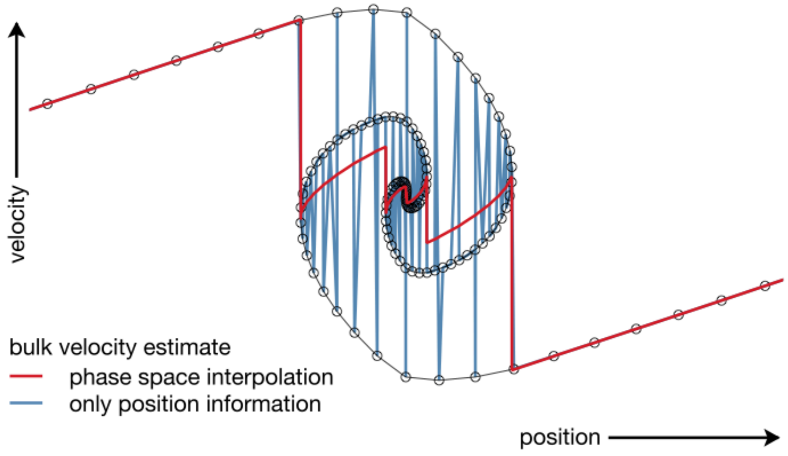




Cosmic Velocity Fields







N-body

Quadrilaterals + refinement

Quadrilaterals

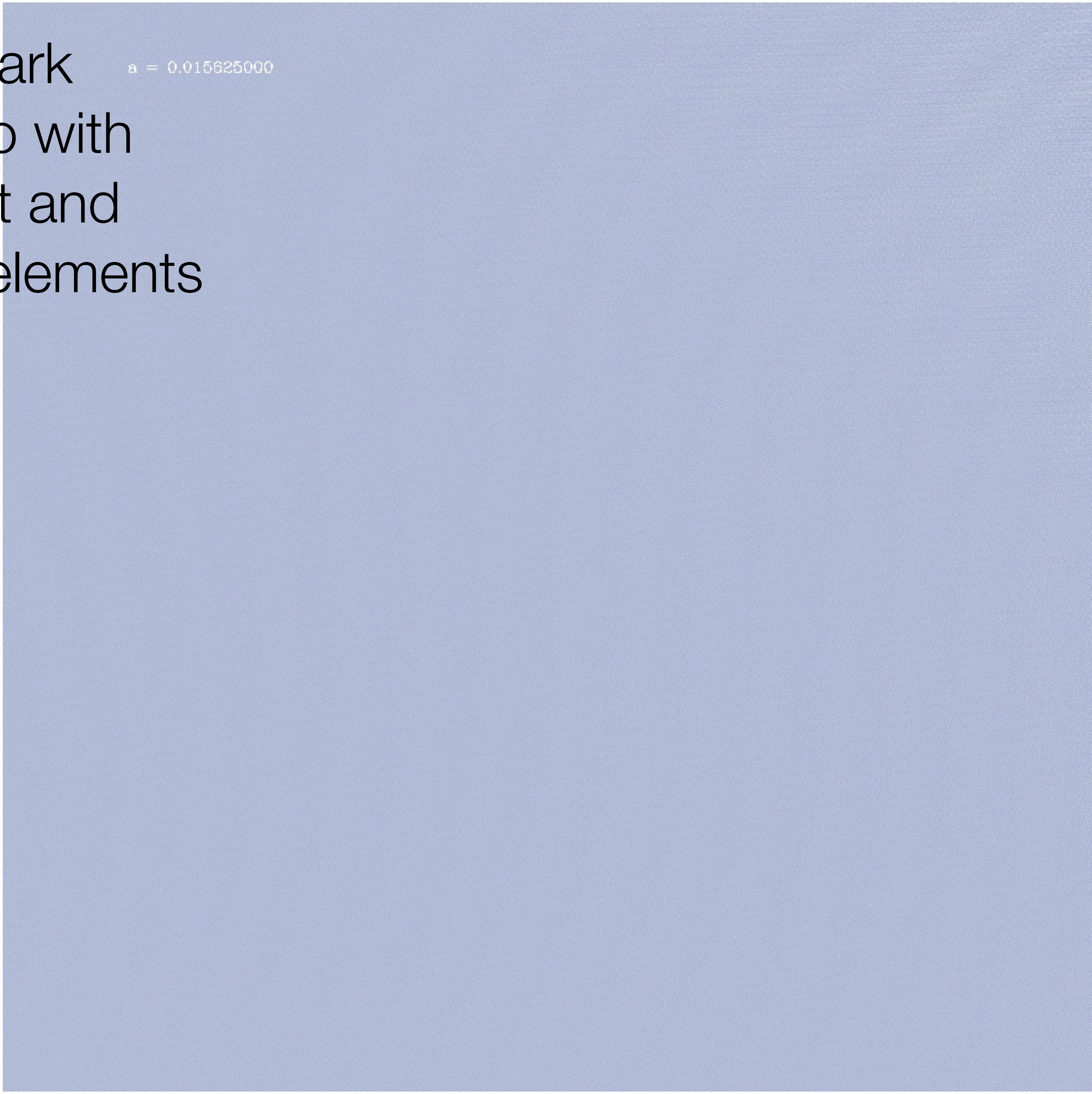
Linear tets + refinement

Linear tets

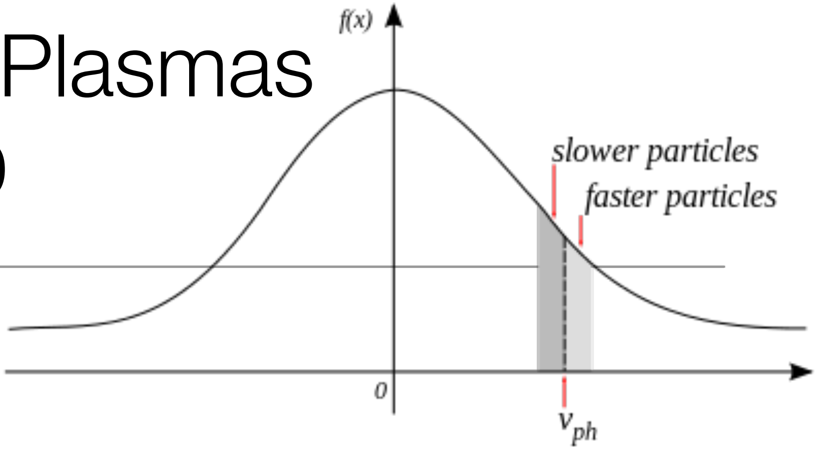
Enormous accuracy gains with higher order interpolation schemes.
Shown here in the test case of a cube evolving in a static potential.

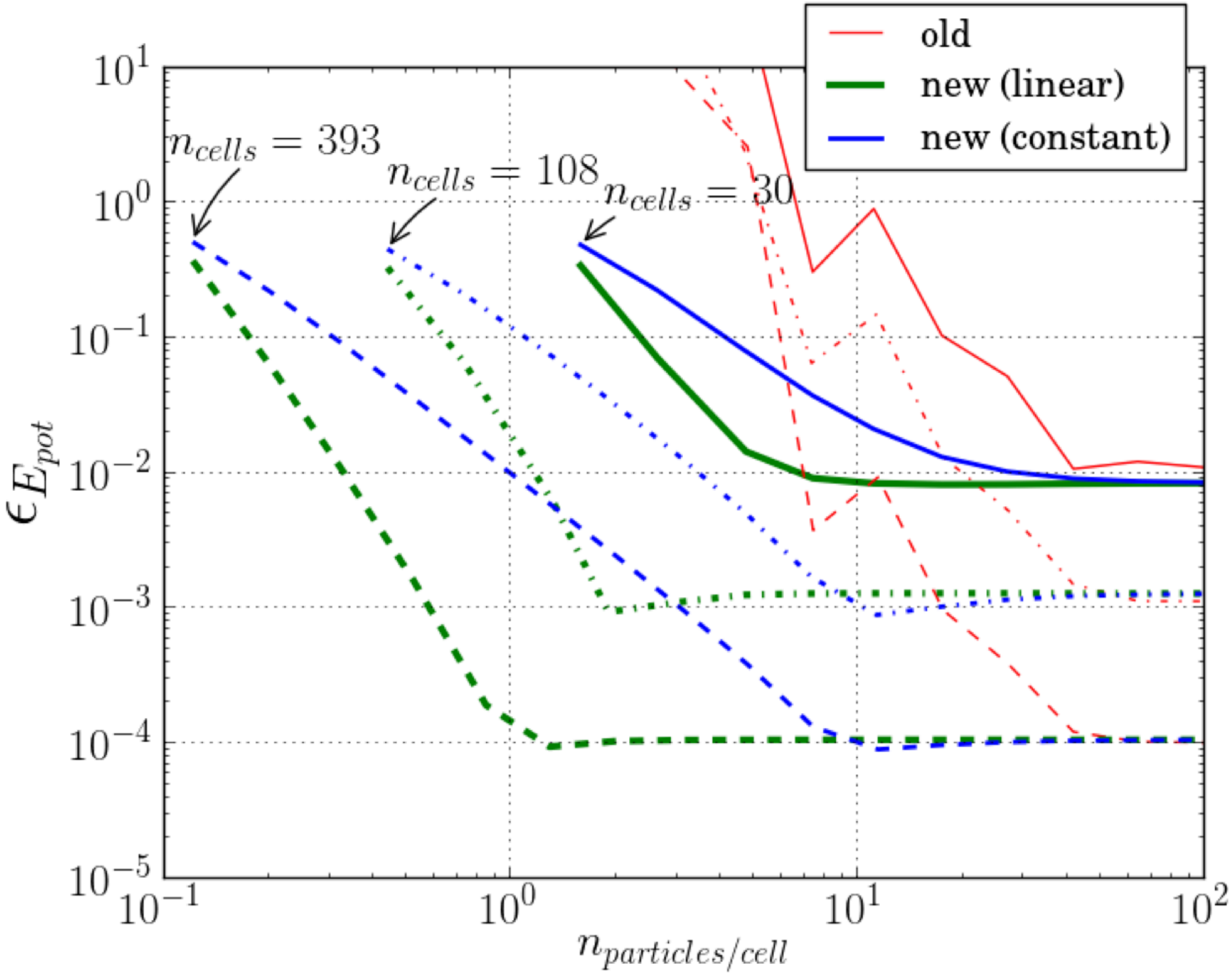
Hahn & Angulo 2015, MNRAS
Angulo et al. in prep.

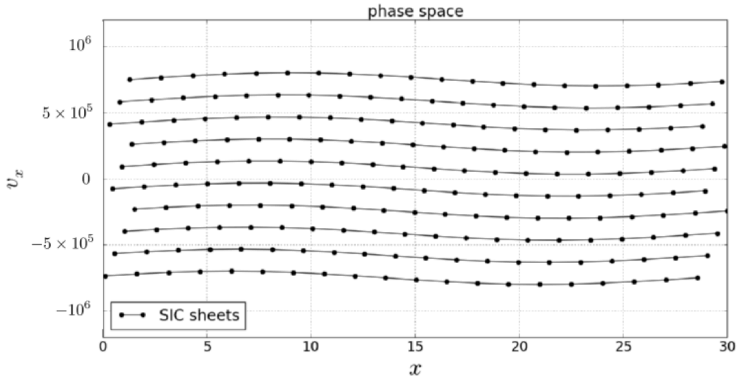
Warm dark matter halo with refinement and higher order elements



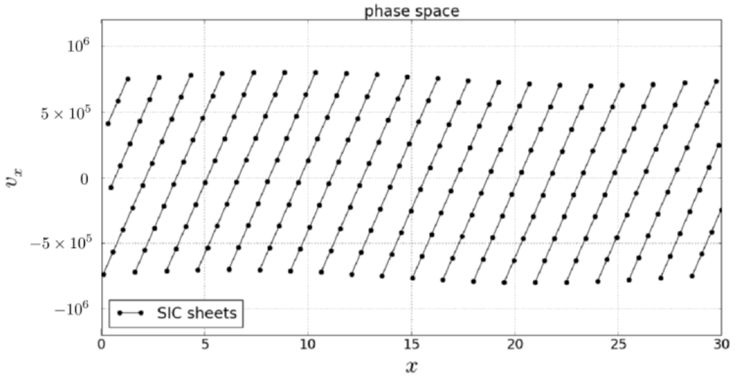
Also applicable to Collision-less Plasmas
Example: Landau Damping in1D







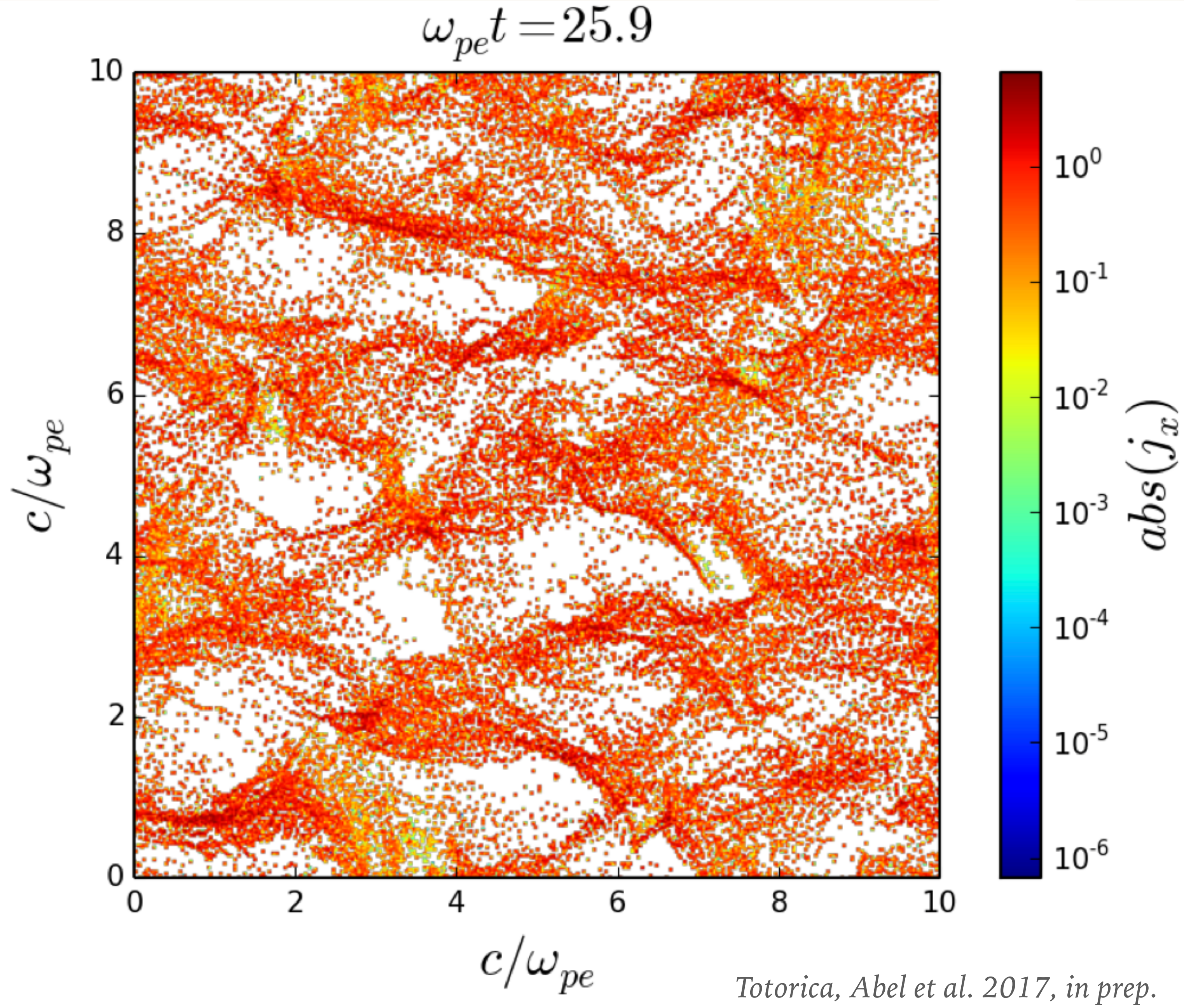
(a) horizontal streams



(b) vertical streams

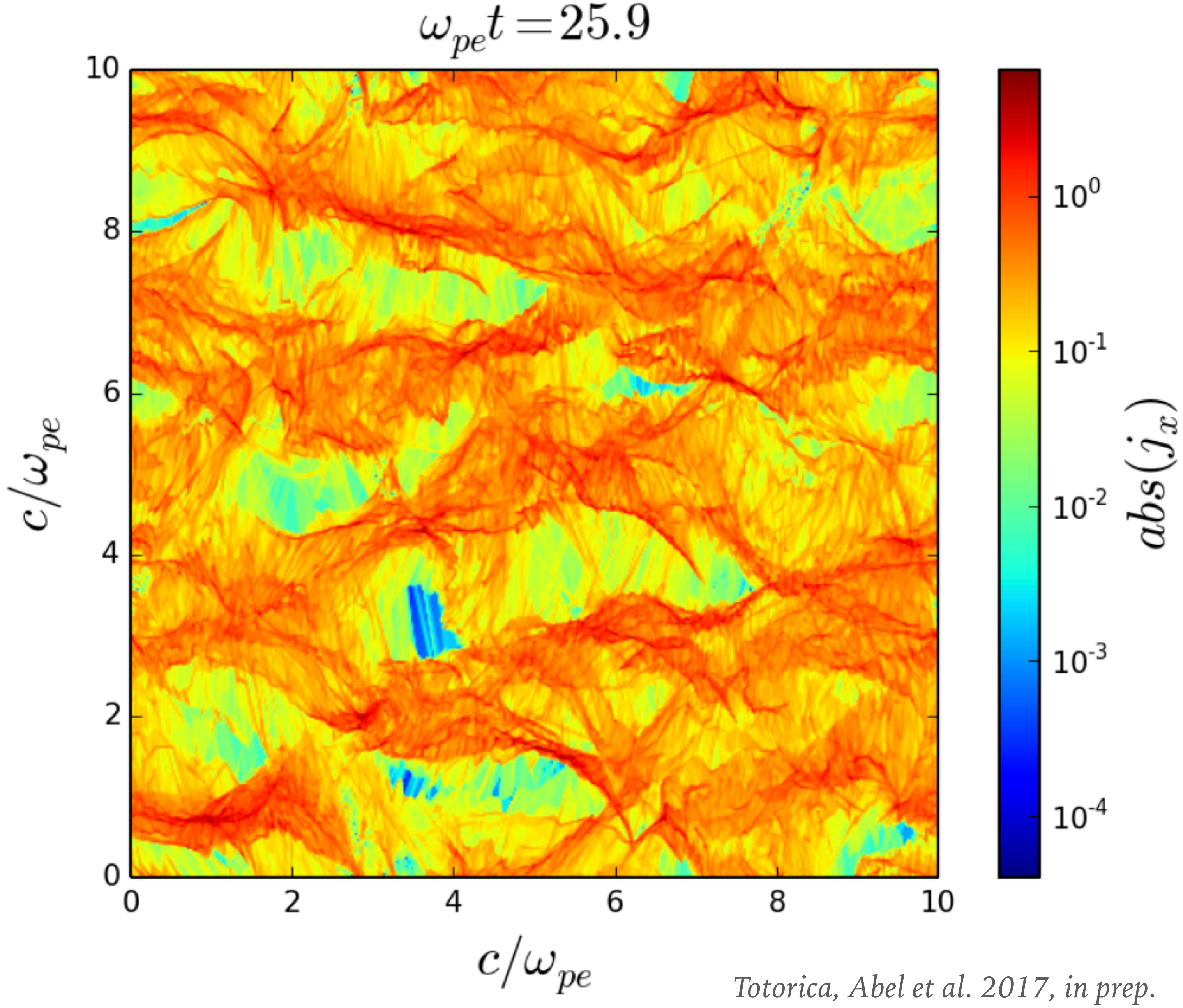
Kates-Harbeck, Totorica, Zrake & Abel 2015, JCompPhys

abs(j_x) with log norm color scale
CIC 16X Resolution



Totorica, Abel et al. 2017, in prep.

abs(j_x) with log norm color scale
Triangles 16X Resolution

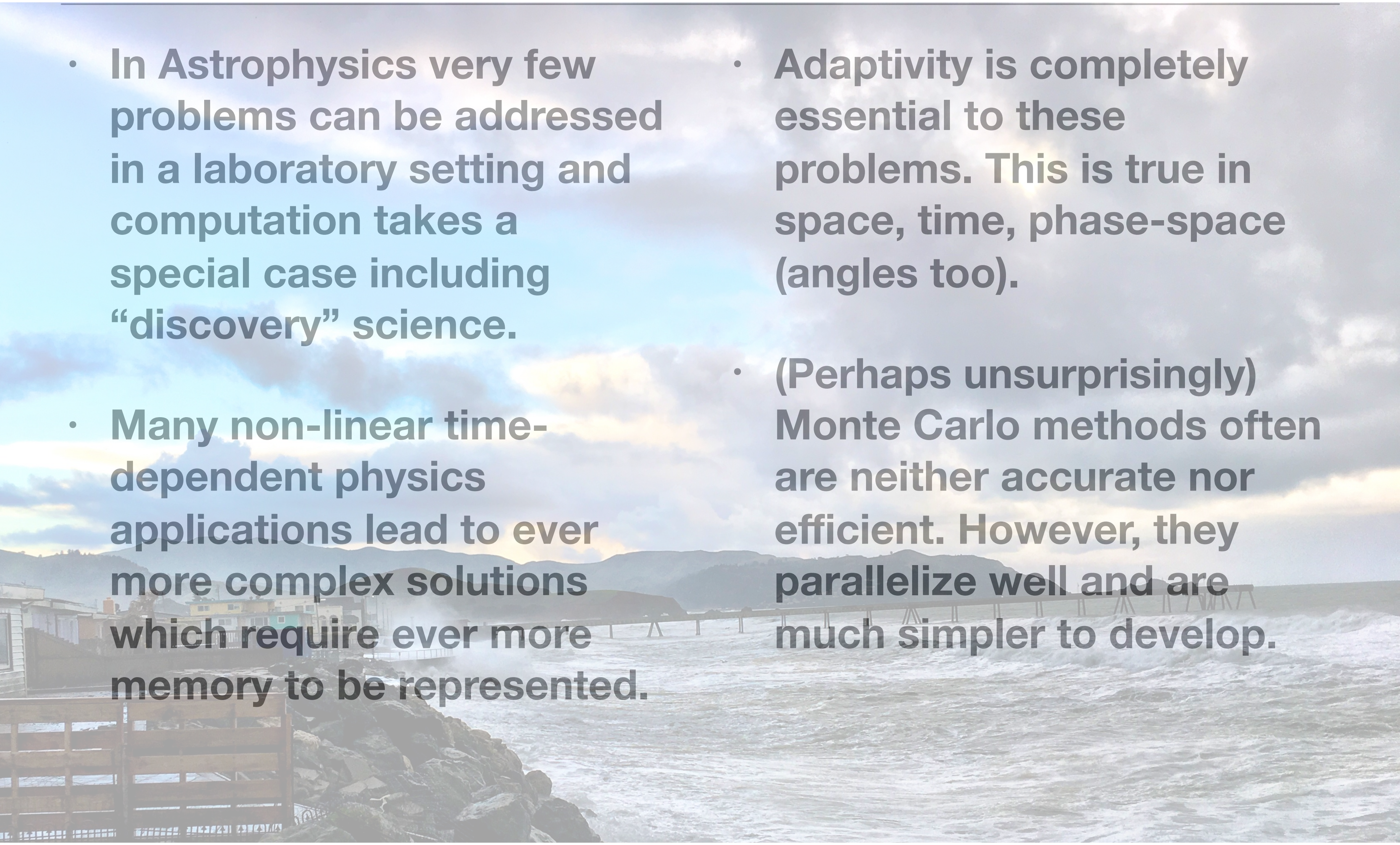


Totorica, Abel et al. 2017, in prep.

Lagrangian Tessellation: What’s it good for?

- Analyzing N-body sims, including web classification, velocity dispersion, profiles, resolution study (Abel, Hahn, Kaehler 2012)
- DM visualization (Kaehler, Hahn, Abel 2012)
- Better Numerical Methods (Hahn, Abel & Kaehler 2013, Hahn, Angulo & Abel 2014-)
- Finally reliable WDM mass functions below the cutoff scale (Angulo, Hahn, Abel 2013)
- Gravitational Lensing predictions (Angulo, Chen, Hilbert & Abel 2014)
- Cosmic Velocity fields (Hahn, Angulo, Abel 2014)
- The SIC method for Plasma simulations (Vlasov/Poisson) (Kates-Harbeck, Totorica, Zrake & Abel 2015, JCompPhys)
- Exact overlap integrals of Polyhedra (Powell & Abel 2015 JCompPhys)
- Void profiles, Wojtak, Powell, Abel 2016 ArXive : 1602.08541
- Totorica, et. al. Weibel instabilities, shocks, particle acceleration in PIC simulations in prep.
- your application here …

Final Remarks



- In Astrophysics very few problems can be addressed in a laboratory setting and computation takes a special case including “discovery” science.
- Many non-linear time-dependent physics applications lead to ever more complex solutions which require ever more memory to be represented.
- Adaptivity is completely essential to these problems. This is true in space, time, phase-space (angles too).
- (Perhaps unsurprisingly) Monte Carlo methods often are neither accurate nor efficient. However, they parallelize well and are much simpler to develop.