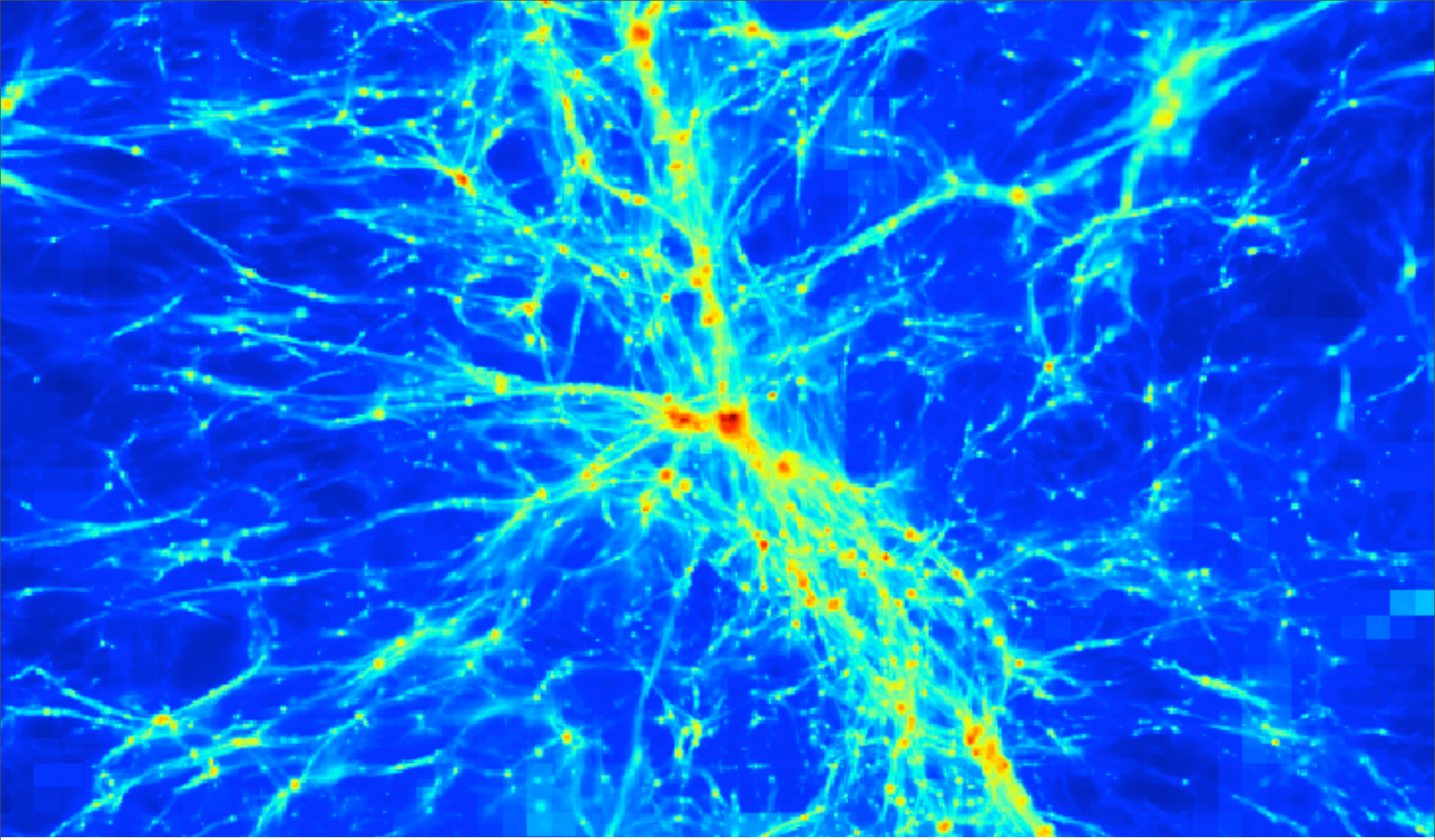


Cosmology Simulations with Enzo

John Wise (Georgia Tech)
Enzo Workshop
北海道大学 – 17 May 2012

Outline

Based on the simulation setup of
Abel, Wise, & Bryan (2007), *The HII Region of a Primordial Star*

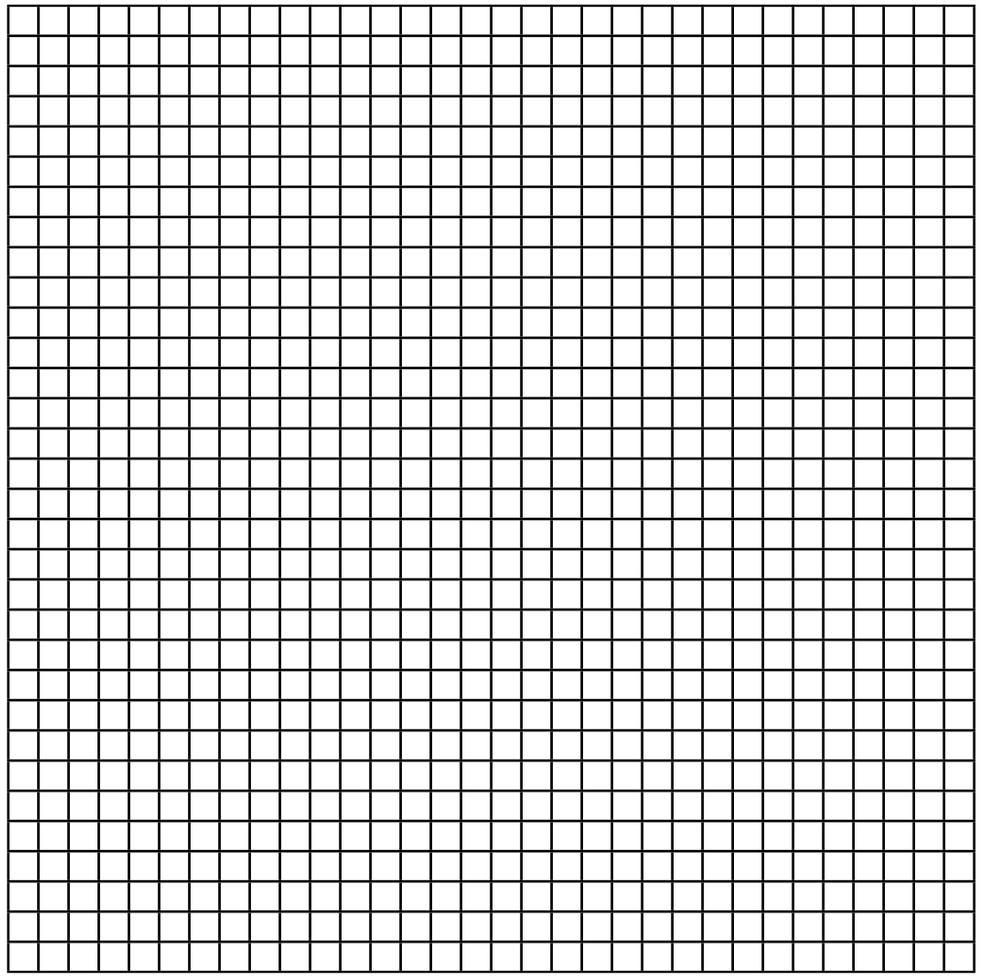
- Introduction to unigrid cosmology simulations
- Introduction to nested grid cosmology simulations
- Using different non-equilibrium chemistry models
- Including Population III star formation and feedback

Unigrid Initial Conditions

- Two programs are provided to generate cosmology initial conditions: **inits** (src/inits) or **mpgrafic** (src/mpgrafic)
- This tutorial will cover how to set up initial conditions with **mpgrafic**.
- 7 initial condition files in HDF5 file format
  - Baryon Density: 1 x N x N x N
  - (x,y,z) Baryon Velocity: 1 x N x N x N
  - (x,y,z) Particle Velocity: 1 x N x N x N

Unigrid Initial Conditions with *mpgrafic*

- MPI parallel version of Bertschinger's grafic (Prunet et al. 2008; RAMSES)
- Adapted to write data format suitable for enzo (parallel HDF5)
- Calculates nested grid simulations by brute force
  - Create the data for the entire box at the finest resolution, then de-resolve the volume outside the nested grids.



Unigrid Initial Conditions with *mpgrafic*

- MPI parallel version of Bertschinger's grafic (Prunet et al. 2008; RAMSES)
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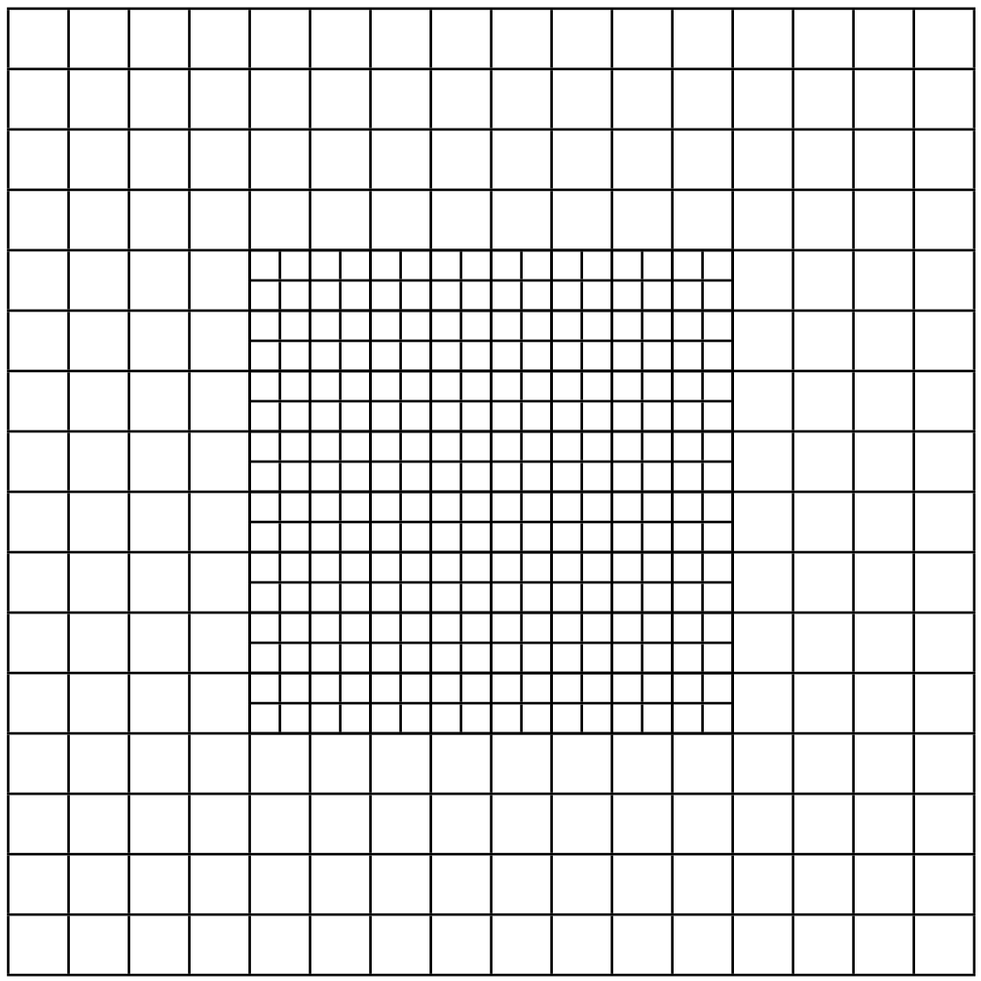

Unigrid Initial Conditions with *mpgrafic*

- **Requirements:**

  - **Parallel HDF5**

```
./configure --enable-parallel --enable-fortran
make install
```

  - **FFTW 2.x with MPI support (float and double support)**

```
./configure --enable-mpi --enable-type-prefix
make install
make clean
./configure --enable-mpi --enable-type-prefix \
  --enable-float
make install
```

Unigrid Initial Conditions with *mpgrafic*

- Configure mpgrafic and degraf. No need to make; the script will make it later.

Terminal — 80×25 — ⌘4

```
mpgrafic-0.2% ls
Makefile.am   autom4te.cache   conf.ranger_intel   configure      missing
Makefile.in   conf.discover    conf.ranger_pgi     configure.ac   src
TODO          conf.kraken      conf.red            depcomp
aclocal.m4    conf.mac         config.h.in         install-sh
mpgrafic-0.2% cat conf.mac
#!/bin/sh
./configure \
    CFLAGS="" \
    FCFLAGS="" \
    LDFLAGS="-bind_at_load" \
    FC=mpif90 \
    CC=mpicc \
    --enable-enzo \
    --enable-double \
    --enable-onedim \
    --with-hdf=/usr/local/hdf5/1.8.3p

mpgrafic-0.2%
```

One velocity field per file.

If not set, 3-velocities are stored in one file. Problems with HDF5 in >2048^3 datasets.

Initial Conditions Parameters

- Cosmology Parameters: box size, Hubble constant, mass-energy fractions (Ω_Λ, Ω_m, Ω_b). *Note: initial redshift will be determined automatically*

- Power spectrum parameters: power spectrum type, σ_8, random seed

    - Using the same random seed with different grid dimensions will result in the same realization

        - Using the same random seed with a different box size will result in a very similar result.

- Grid parameters: resolution

- See http://enzo-project.org/doc/user_guide/CosmologicalInitialConditions.html#using-mpgrafic for more details

Initial Conditions Parameters – Grid parameters

`src/mpgrafic/make_ic.py`

```
#-------------------- PARAMETERS ------------------
#enzo          = True                # On for Enzo ICs
nprocs         = 16                  # Number of processors
boxsize        = 17.831669               # Boxsize in comoving Mpc (not Mpc/h)
resolution     = 512                 # Topgrid resolution
n_levels       = 0                  # Number of nested grids
inner_width    = 0.4375              # If using nested grids, width of finest grid
buffer_cells   = 4                   # Number of cells between refined grids
seed           = 200905130           # Random seed (MUST be 9-digits)
name           = "LAE512"

center = [0.5, 0.5, 0.5]             # Center of interest (no shift = 0.5,0.5,0.5)
#center = [0.7717, 0.0405, 0.3435]   # Center of interest (no shift = 0.5,0.5,0.5)
LargeScaleCorrection = False         # If using noise from a low-resolution run
LargeScaleFile = "200902187_64.dat" # That noise file
OneDimPerFile = True                 # Write one dimension per file

#------------------- COSMOLOGY PARAMETERS -------------------
omega_m      = 0.279                 # Omega matter
omega_v      = 0.721                 # Omega lambda
```

Initial Conditions Parameters – Grid parameters

src/mpgrafic/make_ic.py

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omega_m      = 0.279                 # Omega matter
omega_v      = 0.721                 # Omega lambda
```

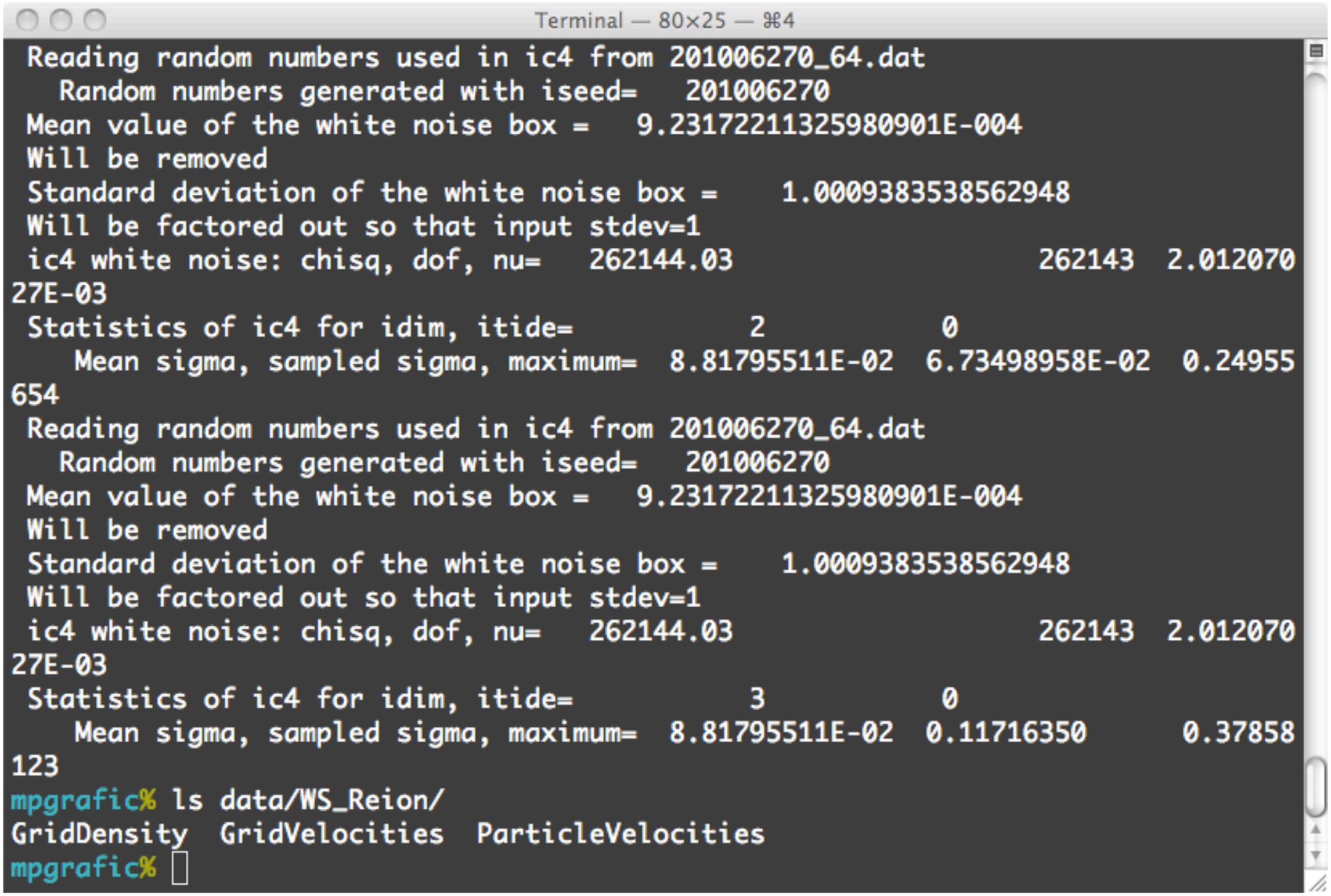
Initial Conditions Parameters – Power spectrum parameters

```
#-------------------- COSMOLOGY PARAMETERS -------------------
omega_m      = 0.279                 # Omega matter
omega_v      = 0.721                 # Omega lambda
omega_b      = 0.0462                # Omega baryon
h0           = 70.1                  # Hubble constant
sigma8       = 0.817                 # sigma_8
n_plawslope = 0.960                  # Slope of power spectrum
```

src/mpgrafic/make_ic.py

Create the initial conditions!

- `python make_ic.py`



Initial redshift

- grafic determines the initial redshift by the density fluctuation amplitude.
- The default is 0.1.
- Smaller sigma → Higher redshift.
  - Tip: Don’t go to an extremely low amplitude. Enzo’s gravity solver doesn’t work well with small perturbations in the particles.
- Unfortunately, it doesn’t report the initial redshift.

Set up *Enzo* parameter file

- See `run/Cosmology/Hydro/AMRCosmology/AMRCosmology.enzo`

Terminal — 85×49 — ⌘4

```
#
# AMR PROBLEM DEFINITION FILE: Cosmology Simulation (amr version)
#
#  define problem
#
ProblemType                = 30      // cosmology simulation
TopGridRank                = 3
TopGridDimensions          = 16 16 16
SelfGravity                = 1       // gravity on
TopGridGravityBoundary     = 0       // Periodic BC for gravity
LeftFaceBoundaryCondition  = 3 3 3   // same for fluid
RightFaceBoundaryCondition = 3 3 3
#
#  problem parameters
#
CosmologySimulationOmegaBaryonNow       = 0.04
CosmologySimulationOmegaCDMNow          = 0.26
CosmologySimulationDensityName          = GridDensity
CosmologySimulationVelocity1Name        = GridVelocities
```

Set up *Enzo* parameter file

with *mpgrafic*, must modify these parameters to be

```
LeftFaceBoundaryCondition  = 3 3 3   // same for fluid
RightFaceBoundaryCondition = 3 3 3
#
#  problem parameters
#
CosmologySimulationOmegaBaryonNow       = 0.04
CosmologySimulationOmegaCDMNow          = 0.26
CosmologySimulationDensityName          = GridDensity
CosmologySimulationVelocity1Name        = GridVelocities
CosmologySimulationVelocity2Name        = GridVelocities
CosmologySimulationVelocity3Name        = GridVelocities
CosmologySimulationParticlePositionName = ParticlePositions
CosmologySimulationParticleVelocityName = ParticleVelocities
#
#  define cosmology parameters
#
ComovingCoordinates         = 1       // Expansion ON
CosmologyOmegaMatterNow     = 0.3
CosmologyOmegaLambdaNow     = 0.7
CosmologyHubbleConstantNow = 0.5      // in 100 km/s/Mpc
CosmologyComovingBoxSize    = 16.0    // in Mpc/h
CosmologyMaxExpansionRate   = 0.015   // maximum allowed delta(a)/a
CosmologyInitialRedshift    = 30      //
CosmologyFinalRedshift      = 0       //
GravitationalConstant       = 1       // this must be true for cosmology
#
#  set I/O and stop/start parameters
#
StopCycle                   = 1000          // stop after this many cycles
```

Set up *Enzo* parameter file

```
LeftFaceBoundaryCondition  = 3 3 3   // same for fluid
RightFaceBoundaryCondition = 3 3 3
#
#  problem parameters
#
#
#  problem parameters
#
CosmologySimulationOmegaBaryonNow       = 0.04
CosmologySimulationOmegaCDMNow          = 0.26
CosmologySimulationDensityName          = GridDensity
CosmologySimulationVelocity1Name        = GridVelocities_x
CosmologySimulationVelocity2Name        = GridVelocities_y
CosmologySimulationVelocity3Name        = GridVelocities_z
#CosmologySimulationParticlePositionName = ParticlePositions
CosmologySimulationParticleVelocity1Name = ParticleVelocities_x
CosmologySimulationParticleVelocity2Name = ParticleVelocities_y
CosmologySimulationParticleVelocity1Name = ParticleVelocities_z
CosmologySimulationCalculatePositions    = 1
CosmologyInitialRedshift    = 30      //
CosmologyFinalRedshift      = 0       //
GravitationalConstant       = 1       // this must be true for cosmology
#
#  set I/O and stop/start parameters
#
StopCycle                   = 1000          // stop after this many cycles
```

with *mpgrafic*, must modify these parameters to be

Run the simulation

- Move parameter file and initial conditions into the same directory

- Run enzo!

```
AMRCosmology% ./enzo.exe AMRCosmology.enzo
```

Nested Grid Cosmology Simulations

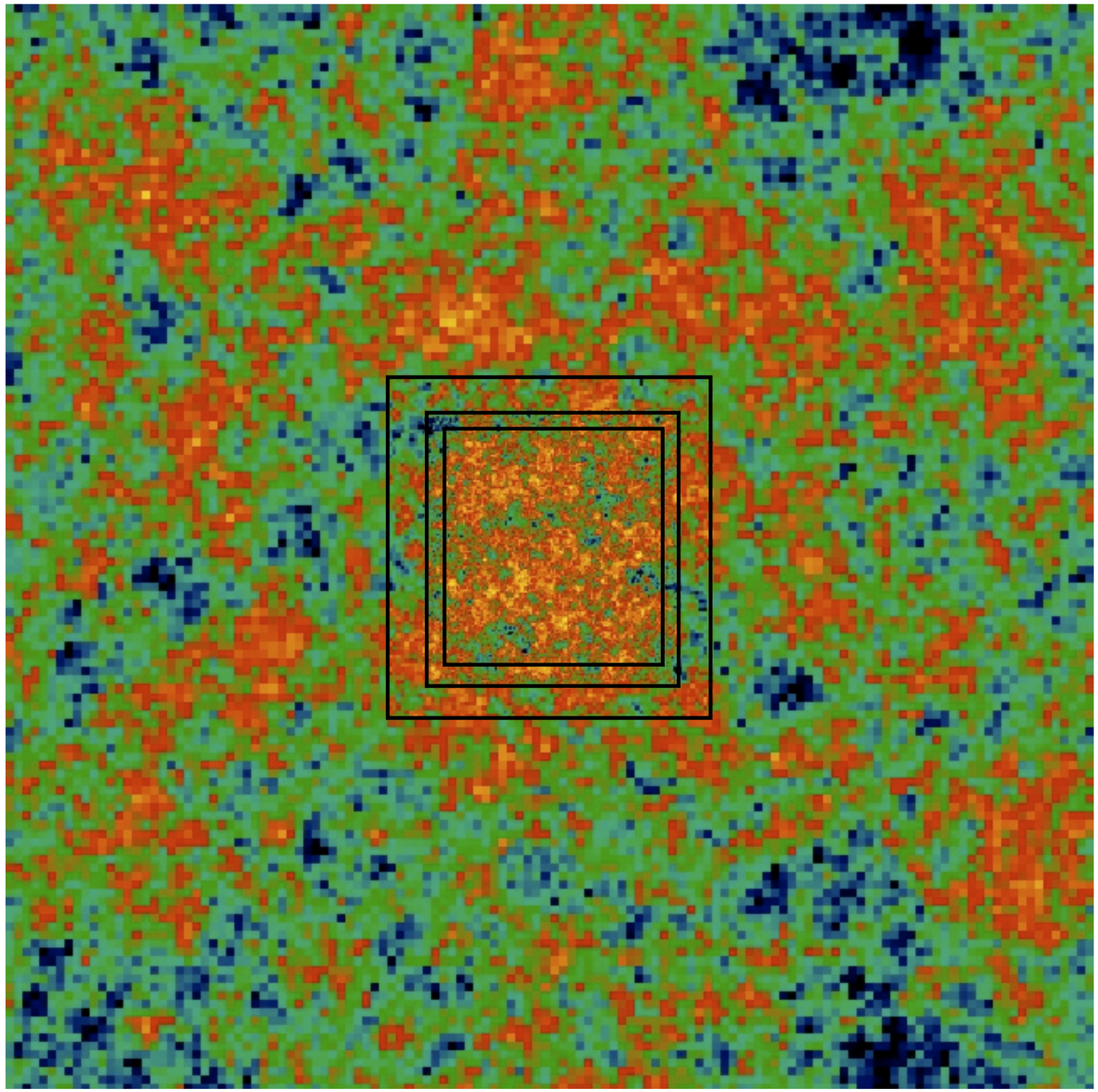
aka Zoom-in calculations

1. *n*-Body Simulation

2. Locate region of interest, e.g. most massive halo

3. Generate nested grid initial conditions

4. Run simulation!



n-body Simulation

- Usually run at the same resolution as the production level-0 resolution
- Create initial conditions with *inits* or *mpgrafic*
- Key parameters

```
#
CosmologySimulationOmegaBaryonNow       = 0.0
CosmologySimulationOmegaCDMNow          = 0.266
#CosmologySimulationInitialTemperature  = 200
#CosmologySimulationDensityName         = GridDensity
#CosmologySimulationVelocity1Name       = GridVelocities
#CosmologySimulationVelocity2Name       = GridVelocities
#CosmologySimulationVelocity3Name       = GridVelocities
CosmologySimulationParticlePositionName = ParticlePositions
CosmologySimulationParticleVelocityName = ParticleVelocities
CosmologySimulationCalculatePositions   = 0
CosmologySimulationNumberOfInitialGrids = 1
```

```
InlineHaloFinder = 1
HaloFinderCycleSkip = 0
```

```
RefineBy                = 2   // refinement factor
#CellFlaggingMethod     = 2 4 6  // use baryon mass for refinement
CellFlaggingMethod      = 4   // use DM mass for refinement
MinimumEfficiency       = 0.4  // fraction efficiency
```

Terminal — 80×30 — ⌘3

```
# Time      = 15.921139
# Redshift = 12.802003
# Number of halos = 83
#
# Column 1.  Center of mass (x)
# Column 2.  Center of mass (y)
# Column 3.  Center of mass (z)
# Column 4.  Halo number
# Column 5.  Number of particles
# Column 6.  Halo mass [solar masses]
# Column 7.  Virial mass [solar masses]
# Column 8.  Stellar mass [solar masses]
# Column 9.  Virial radius (r200) [kpc]
# Column 10. Mean x-velocity [km/s]
# Column 11. Mean y-velocity [km/s]
# Column 12. Mean z-velocity [km/s]
# Column 13. Velocity dispersion [km/s]
# Column 14. Mean x-angular momentum [Mpc * km/s]
# Column 15. Mean y-angular momentum [Mpc * km/s]
# Column 16. Mean z-angular momentum [Mpc * km/s]
# Column 17. Spin parameter
#
# datavar lines are for partiview.  Ignore them if you're not partiview.
#
datavar 0 halo_number
datavar 1 number_of_particles
datavar 2 halo_mass
datavar 3 virial_mass
datavar 4 stellar_mass
groups_00137.dat lines 1-29/122 4%
```

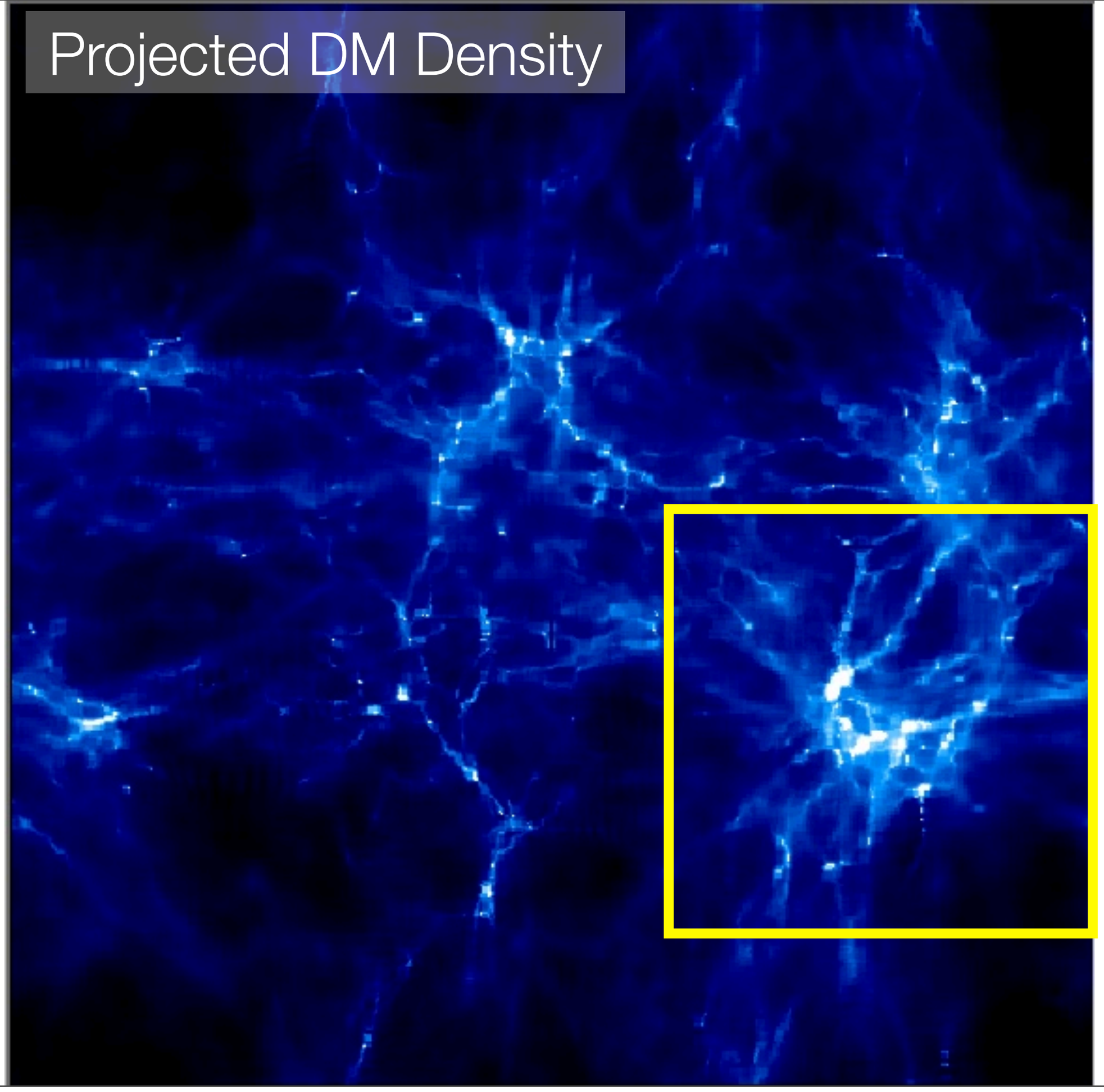
Terminal — 80×30 — ⌘3

```
datavar 0 halo_number
datavar 1 number_of_particles
datavar 2 halo_mass
datavar 3 virial_mass
datavar 4 stellar_mass
datavar 5 virial_radius
datavar 6 x_velocity
datavar 7 y_velocity
datavar 8 z_velocity
datavar 9 velocity_dispersion
datavar 10 x_angular_momentum
datavar 11 y_angular_momentum
datavar 12 z_angular_momentum
datavar 13 spin
```

Position

Mass

```
 0.76364088   0.29754913   0.37248853             0          2060    571700.88
 447925.16             0   0.11323795   0.84548277  -0.41380891    1.0349354
5.341588 2.408008e-05 3.4065459e-05 -6.1198812e-06   0.11691254
 0.46177065   0.61586523    0.6905852             1          1390    385758.56
 372992.47             0   0.10630372    2.0898418   0.23426482    -1.659736    4
.6082692 5.5966311e-06 1.264129e-05 -3.7420041e-06  0.041144241
 0.84373128   0.67770523   0.27474043             2           415     115172.2
 70213.453             0  0.060892154  -0.90891731  -0.64614326    2.0012767    2
.8843138 2.717258e-06 -1.8763769e-06 -7.576411e-06  0.078942753
 0.51242203   0.62618536   0.67746228             3           372    103238.98
 95745.844             0  0.067207284  -0.48392525   0.49669054   -2.3942778    2
.9666159 7.2602943e-06 3.2799553e-06 -2.7749318e-06  0.060778547
 0.77068067   0.30860633   0.33854923             4           330         91583
 81314.617             0   0.06338729   -1.6947181  -0.76077771    3.8264091    2
groups_00137.dat lines 25-44/122 11%
```


Projected DM Density

Nested Grid Initial Conditions with *mpgrafic*

```
#
CosmologySimulationOmegaBaryonNow       = 0.0
CosmologySimulationOmegaCDMNow          = 0.266
#CosmologySimulationInitialTemperature   = 200
#CosmologySimulationDensityName          = GridDensity
#CosmologySimulationVelocity1Name        = GridVelocities
#CosmologySimulationVelocity2Name        = GridVelocities
#CosmologySimulationVelocity3Name        = GridVelocities
CosmologySimulationParticlePositionName = ParticlePositions
CosmologySimulationParticleVelocityName = ParticleVelocities
CosmologySimulationCalculatePositions   = 1
CosmologySimulationNumberOfInitialGrids = 1
```

Set to one when using with mpgrafic.

Moves the particle position calculation into enzo.

Not necessary to run `ring` for large simulations!

make_ic.py: Parameters

```
#-------------------- PARAMETERS --------------------
#enzo          = True                 # On for Enzo ICs
nprocs         = 16                   # Number of processors
boxsize        = 17.831669                # Boxsize in comoving Mpc (not Mpc/h)
resolution     = 512                  # Topgrid resolution
n_levels       = 2                  # Number of nested grids
inner_width    = 0.4375               # If using nested grids, width of finest grid
buffer_cells   = 2                  # Number of cells between refined grids
seed           = 200905130            # Random seed (MUST be 9-digits)
name           = "LAE512"

center = [0.5, 0.5, 0.5]           # Center of interest (no shift = 0.5,0.5,0.5)
#center = [0.7717, 0.0405, 0.3435]   # Center of interest (no shift = 0.5,0.5,0.5)
LargeScaleCorrection = False       # If using noise from a low-resolution run
LargeScaleFile = "200902187_64.dat" # That noise file
OneDimPerFile = True               # Write one dimension per file

#-------------------- COSMOLOGY PARAMETERS --------------------
omega_m      = 0.279               # Omega matter
omega_v      = 0.721               # Omega lambda
omega_b      = 0.0462              # Omega baryon
h0           = 70.1                # Hubble constant
sigma8       = 0.817               # sigma_8
n_plawslope = 0.960                # Slope of power spectrum
```

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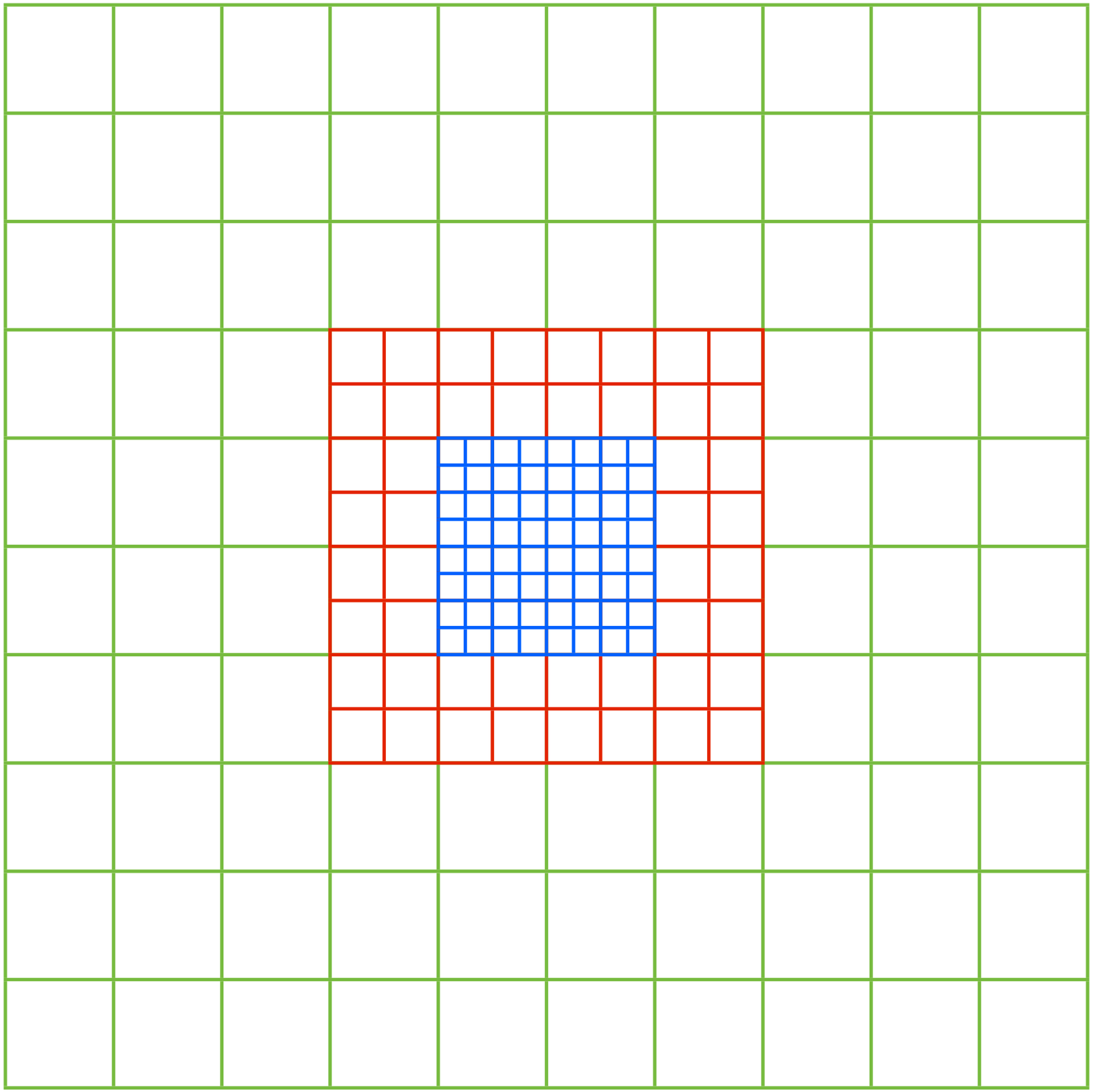
```

buffer_cells = 2



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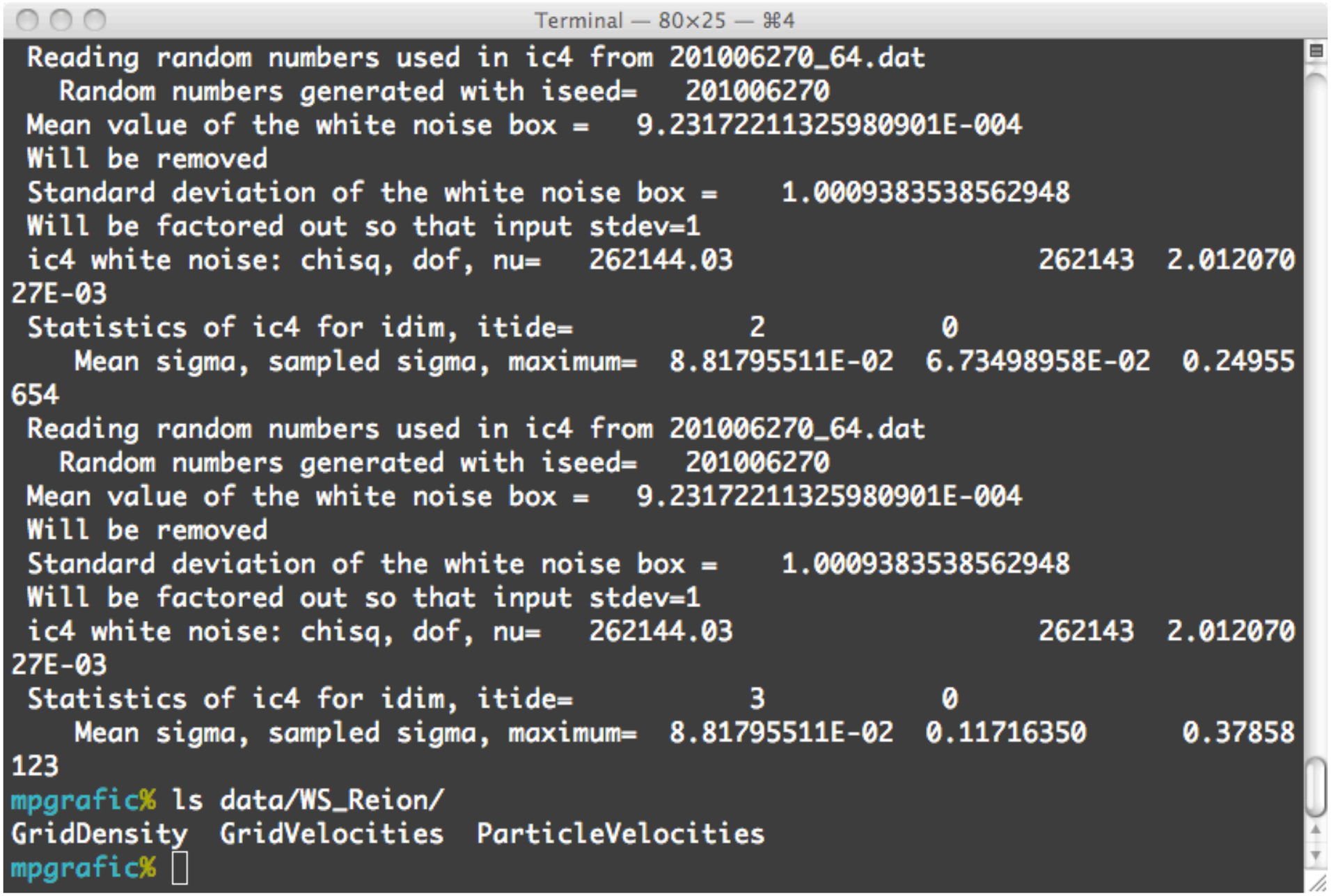
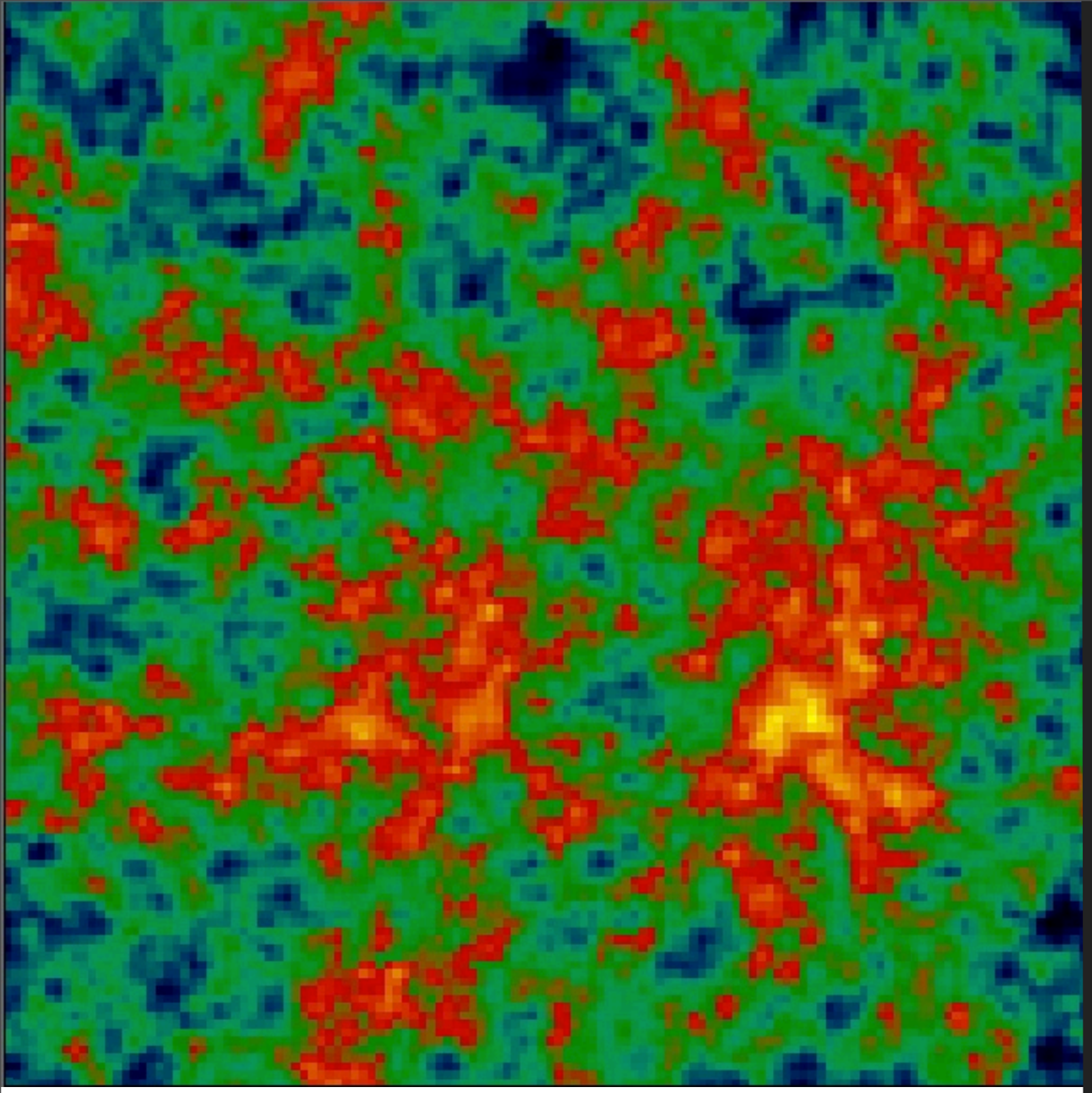
```

Nested Grid Initial Conditions with *mpgrafic*

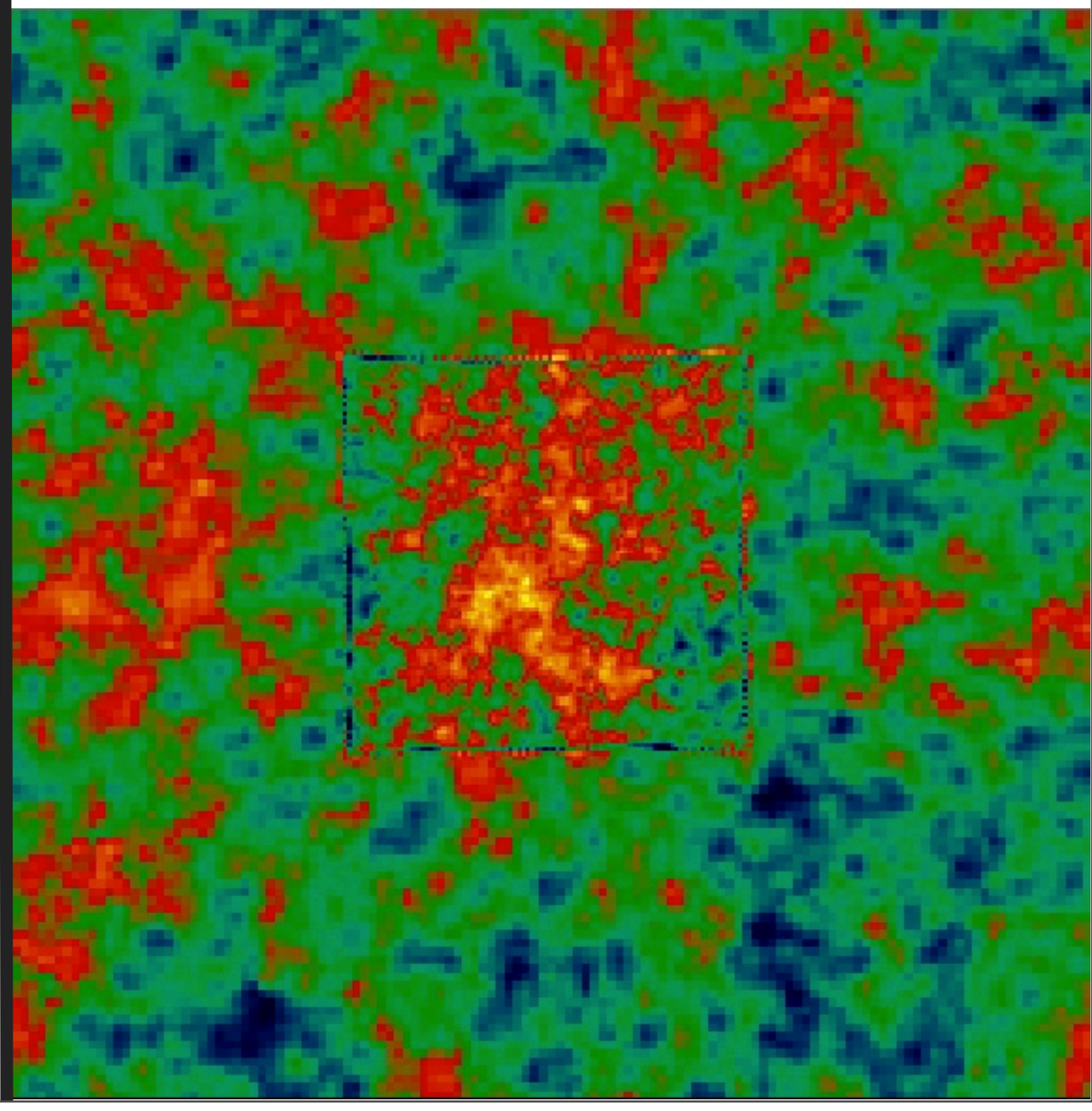
- `python make_ic.py`





Unigrid
Smoothed DM Density Slice

1 Nested Grid



Setting up the Nested Grid Parameter File

```
#
#  problem parameters
#
CosmologySimulationOmegaBaryonNow       = 0.0449
CosmologySimulationOmegaCDMNow          = 0.2211
#CosmologySimulationInitialTemperature   = 300
CosmologySimulationDensityName          = GridDensity
CosmologySimulationVelocity1Name        = GridVelocities
CosmologySimulationVelocity2Name        = GridVelocities
CosmologySimulationVelocity3Name        = GridVelocities
CosmologySimulationParticleVelocityName = ParticleVelocities
CosmologySimulationParticlePositionName = ParticlePositions
CosmologySimulationCalculatePositions   = 0
CosmologySimulationNumberOfInitialGrids = 2
CosmologySimulationGridDimension[1] =     96 96 96
CosmologySimulationGridLeftEdge[1] =  0.3125 0.3125 0.3125
CosmologySimulationGridRightEdge[1] = 0.6875 0.6875 0.6875
CosmologySimulationGridLevel[1]     = 1

RefineRegionAutoAdjust = 1
RefineRegionLeftEdge  = 0.3125 0.3125 0.3125
RefineRegionRightEdge = 0.6875 0.6875 0.6875
```

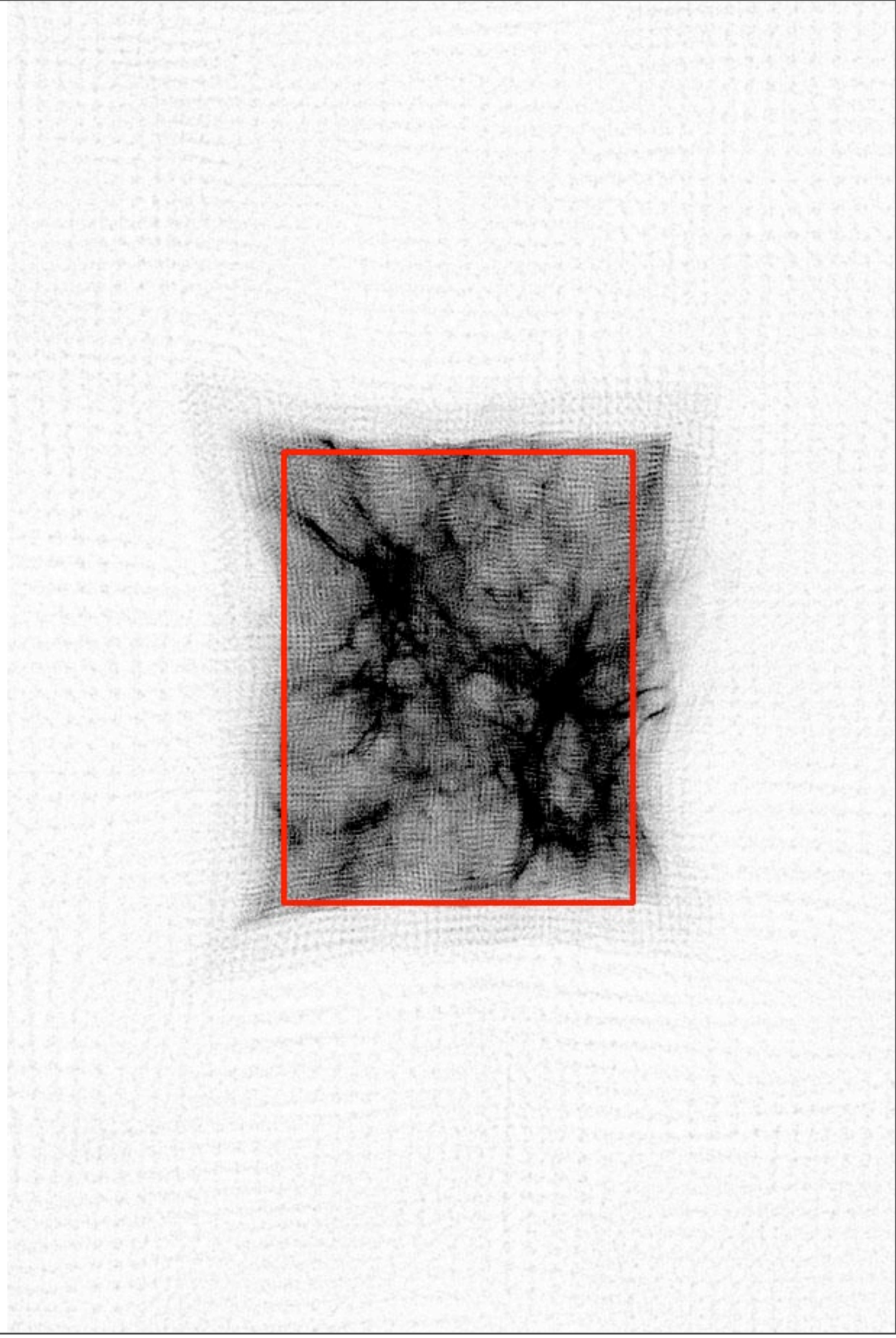
Nested Grid Dimensions and Boundaries

Should equal or be smaller than the finest nested grid

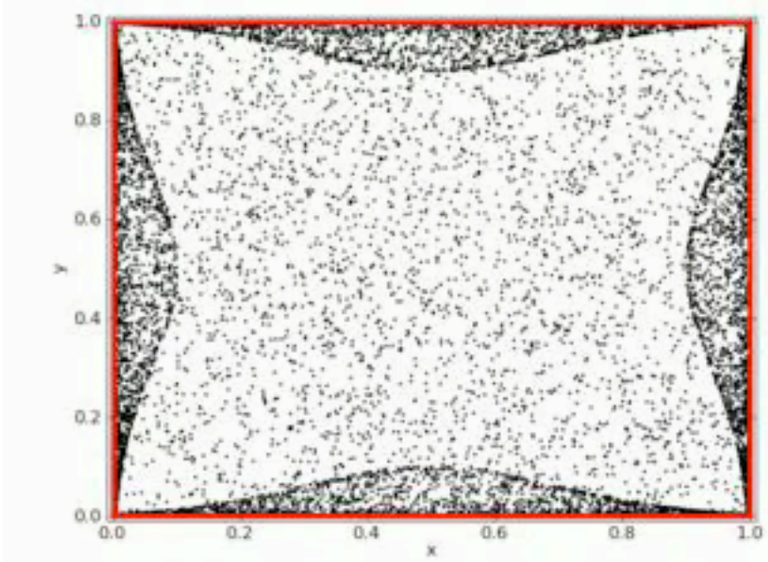
Auto-adjusting refine region

- Automatically changes the refine region to only include high-resolution particles.

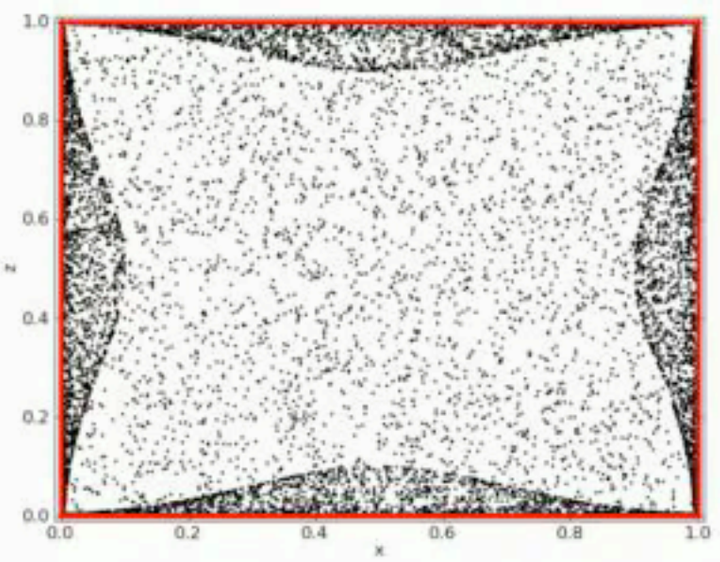
- Particles from low-resolution initial regions might dominate the potential in halos and cause artificial collapse.



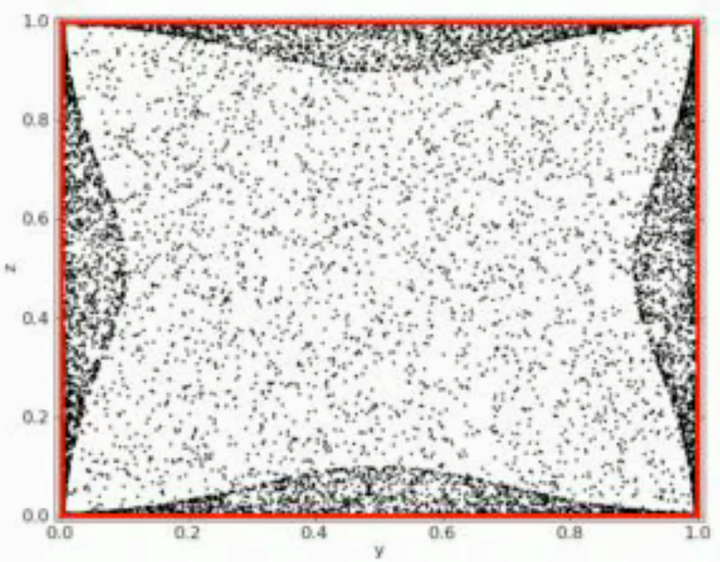
Auto-adjusting refine region



x-y



x-z



y-z

Displaying low-resolution particles inside refine region

Overdensity criteria

- **Very important:** Must divide the baryon and DM mass refinement criteria by a factor of 8^n, where n := maximum initial level
- e.g. Refine on an overdensity of 3 with 2 initial grids → 3.0/64 = 0.046875
- If not done, the hierarchy will remain under-resolved, compared with the desired results.

```
#
#  set grid refinement parameters
#
StaticHierarchy           = 0    // dynamic hierarchy
MaximumRefinementLevel    = 8
MaximumGravityRefinementLevel    = 8
MaximumParticleRefinementLevel   = 8
RefineBy                  = 2    // refinement factor
CellFlaggingMethod        = 2 4 6   // use baryon mass for refinement
#CellFlaggingMethod        = 4    // use DM mass for refinement
MinimumEfficiency         = 0.3  // fraction efficiency
MinimumOverDensityForRefinement = 0.5 0.5 // times the initial density refers to top g
rid: divide by 8 for each additional level
MinimumMassForRefinementLevelExponent = -0.2 0.0
```

Different chemistry and cooling models

- **MultiSpecies == 0:** Equation of state with an adiabatic index ϒ
    - **RadiativeCooling == 1:** Cooling from a tabulated cooling curve (copy input/cool_rates.in to working directory)

Non-equilibrium chemistry

- **MultiSpecies == 1:** 6-species (H, H^+, He, He^+, He^{++}, e^-)
- **MultiSpecies == 2:** 9-species (H, H^+, He, He^+, He^{++}, e^-, H^-, H_2, H_2^+); i.e. +molecular hydrogen cooling
- **MultiSpecies == 3:** 12-species (H, H^+, He, He^+, He^{++}, e^-, H^-, H_2, H_2^+, D, D^+, HD); +HD cooling

Different chemistry and cooling models

- **MetalCooling == 1:** Tabulated cooling table from Glover & Jappsen (2007) & Sutherland & Dopita (1993) – input/metal_cool.dat.
  - $T < 10^4$ K: fine-structure metal-line cooling
  - $T > 10^4$ K: collisional ionization equilibrium
- **MetalCooling == 2:** Explicitly calculated metal cooling rates (Cen)
- **MetalCooling == 3:** Tabulated cooling table from CLOUDY (Smith et al. 2008)

Let's set up Abel, Wise, & Bryan (2007)

on conival: `cp -r ~guest12/AWB07/ .`

```
#
#  problem parameters
#
CosmologySimulationOmegaBaryonNow       = 0.0441
CosmologySimulationOmegaCDMNow          = 0.2139
#CosmologySimulationInitialTemperature   = 300
CosmologySimulationDensityName          = GridDensity
CosmologySimulationVelocity1Name        = GridVelocities
CosmologySimulationVelocity2Name        = GridVelocities
CosmologySimulationVelocity3Name        = GridVelocities
CosmologySimulationParticleVelocityName = ParticleVelocities
CosmologySimulationParticlePositionName = ParticlePositions
CosmologySimulationCalculatePositions   = 0
CosmologySimulationNumberOfInitialGrids = 2
CosmologySimulationGridDimension[1] =     96 96 96
CosmologySimulationGridLeftEdge[1] =  0.3125 0.3125 0.3125
CosmologySimulationGridRightEdge[1] = 0.6875 0.6875 0.6875
CosmologySimulationGridLevel[1]     = 1
```

Let's set up Abel, Wise, & Bryan (2007)

```
#
#  set hydro parameters
#
Gamma                      = 1.6667
PPMDiffusionParameter      = 0       // diffusion off
DualEnergyFormalism        = 1       // use total & internal energy
InterpolationMethod        = 1     // SecondOrderA
FluxCorrection             = 1
ConservativeInterpolation = 1
CourantSafetyNumber        = 0.5
ParticleCourantSafetyNumber = 0.8
RadiativeCooling                = 1
MultiSpecies                    = 2
UseMinimumPressureSupport       = 0
RefineByJeansLengthSafetyFactor  = 16.0
```

H, He, H_2 non-equilibrium chemistry

Resolve local Jeans length by 16 cells

Let's set up Abel, Wise, & Bryan (2007)

```
#
#  set grid refinement parameters
#
StaticHierarchy           = 0    // dynamic hierarchy
MaximumRefinementLevel    = 8
MaximumGravityRefinementLevel    = 8
MaximumParticleRefinementLevel   = 8
RefineBy                  = 2    // refinement factor
CellFlaggingMethod        = 2 4 6   // u
#CellFlaggingMethod        = 4    // use DM mass for refinement
MinimumEfficiency         = 0.3  // fraction efficiency
MinimumOverDensityForRefinement = 0.5 0.5 // times the initial density refers to top grid
: divide by 8 for each additional level
MinimumMassForRefinementLevelExponent = -0.2 0.0
```

Maximum AMR level

Refine by baryon, DM, and Jeans lengths

Let's set up Abel, Wise, & Bryan (2007)

```
#
# Star formation parameters
#
StarParticleCreation = 8
StarParticleFeedback = 8
PopIIIStarMass       = 100
PopIIIOverDensityThreshold = 5e5
#
# Radiative transfer parameters
#
RadiativeTransfer = 1
RadiativeTransferHydrogenOnly = 1
RadiativeTransferAdaptiveTimestep = 1
#
# Halo finder parameters (run every output)
#
InlineHaloFinder                = 1
HaloFinderCycleSkip             = 0
```

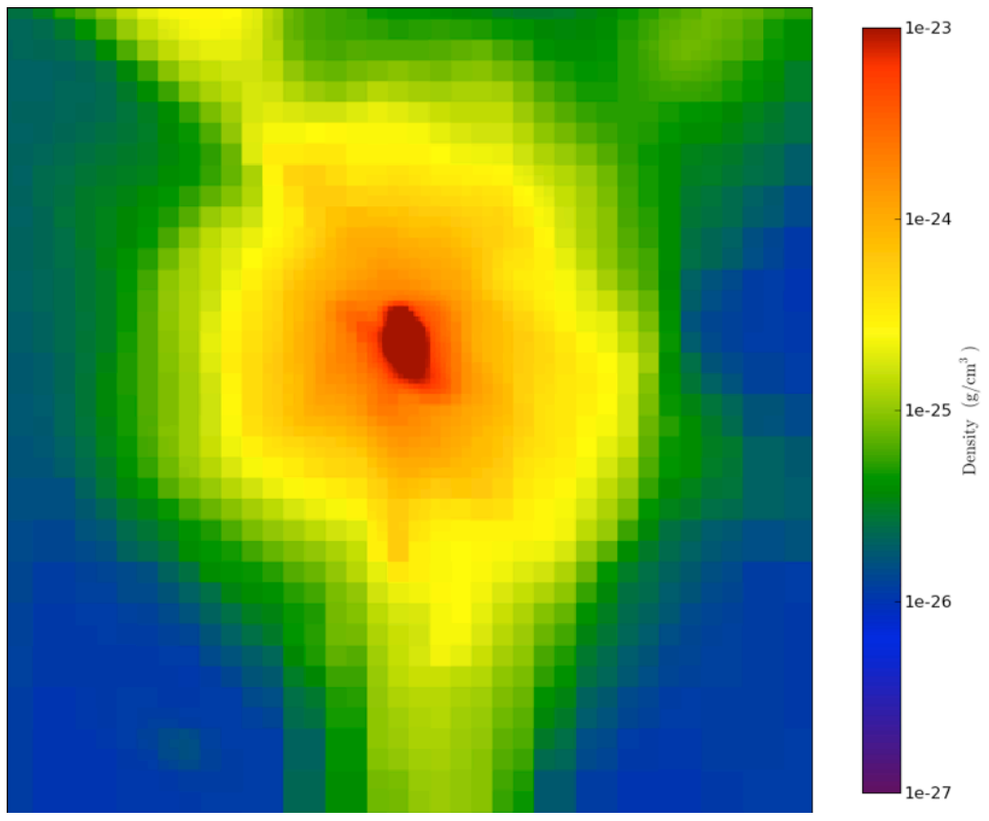
- Pop III star formation
- Create 100 solar mass stars
- At a 5 x 10^5 overdensity (plus other criteria), create stars

Turn on radiative transfer for hydrogen

For convenience, turn on halo finder

2 more parameters for **large** nested grid runs

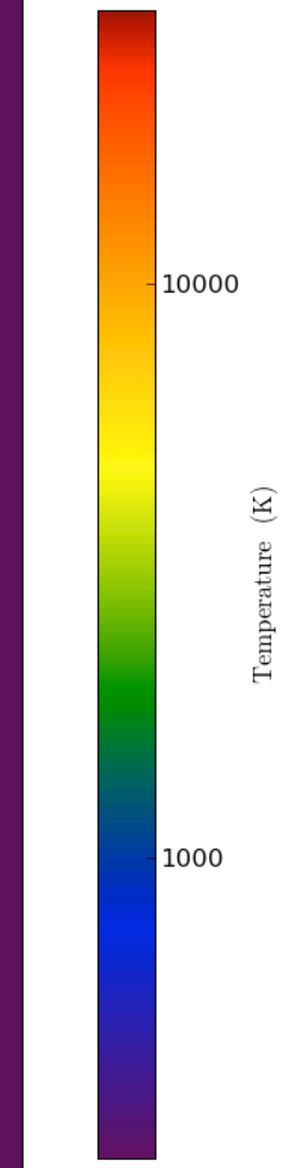
- i.e. >256^3 nested grids
- `ParallelRootGridIO = 1`: Root grids are tiled before I/O, and each processor reads/writes their own tile
- `PartitionNestedGrids = 1`: Same thing as above but for nested grids

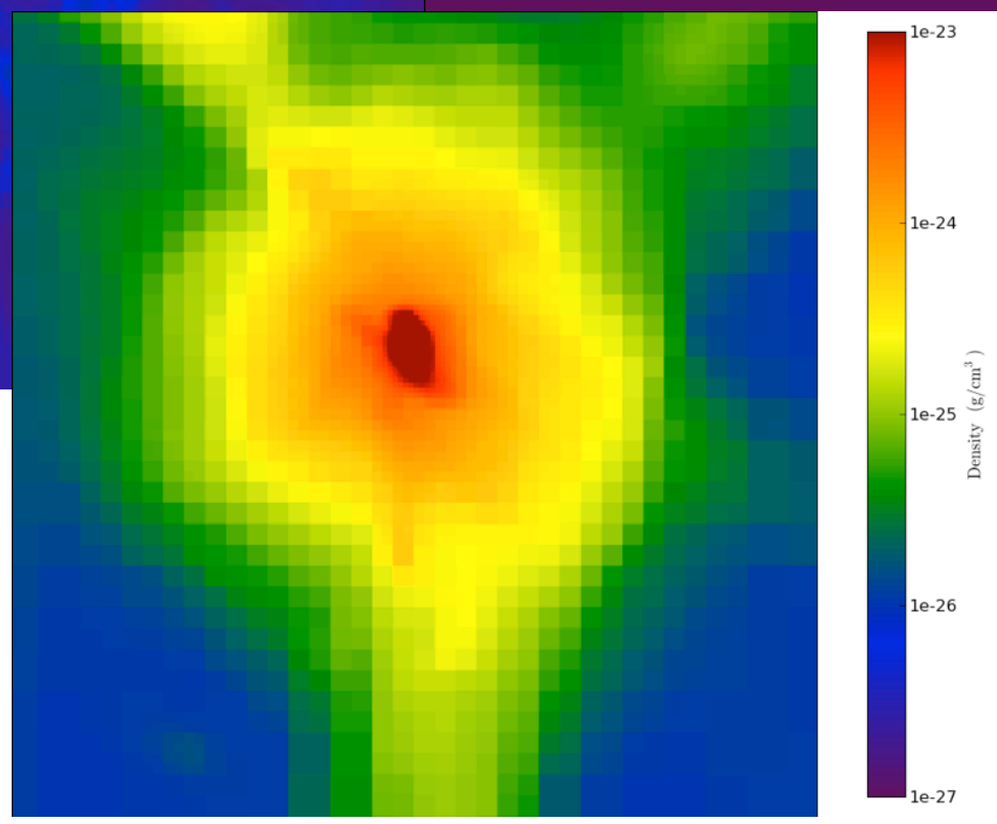


Projected Density (300 pc)

Projected Density (10 kpc)

Projected Temperature





Projected Density (300 pc)

Summary

You should now know **how to:**

- Create cosmological unigrid and nested grid initial conditions with *mpgrafic.* For more, see
  - http://enzo-project.org/doc/user_guide/CosmologicalInitialConditions.html#using-mpgrafic
- Run cosmological nested grid runs (n-Body and n-Body + gas)
- Use radiative cooling (with cooling curves) and non-equilibrium chemistry
- Use Population III star particles with ray-tracing for radiation feedback