Enzo Lectures Mike Norman, Matt Turk Laboratory for Computational Astrophysics UC San Diego

	Morning	Afternoon
Mon.	Introduction to Enzo	
Tue.	 Setting Up and Running Enzo Enzo Projects 	Introduction to YT
Wed.	Enzo Algorithms	Lab session
Thu.	Applications to First Stars, First Galaxies, and Reionization	Lab session
Fri.	What's New in Enzo 2.0?	Q & A

radiative transfer

Ionization + magnetic fields

New Features in Enzo 2.0

Feature	Authors
physics	
star particle class	John Wise, Ji-hoon Kim
adaptive ray tracing radiative transfer	John Wise, Tom Abel
flux limited diffusion radiative transfer	Dan Reynolds
Runge-Kutta2 MHD	Tom Abel, Peng Wang
CUDA MHD	Tom Abel, Peng Wang
high-density primordial chemistry	Matt Turk
CLOUDY cooling	Britton Smith
sink particles	John Wise, Peng Wang, Tom Abel

New Features in Enzo 2.0

Feature	Authors
numerics	
particle splitting	Ji–hoon Kim
shearing box boundary conditions	Tom Abel, Fen Zhao
inline Friends-Of-Friends	John Wise
mpgraphic initial conditions	John Wise
non-blocking communication	John Wise, Greg Bryan
AMR checkpoint dumps	Matt Turk
r16 Positioning	Matt Turk
Python embedding	Matt Turk
LCA-perf	James Bordner
New Streaming Format	John Wise, Tom Abel

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Stopping Parameters Initialization Parameters I/O Parameters Hierarchy Control Parameters Hydrodynamic Parameters Cosmology Parameters Gravity Parameters Particle Parameters Parameters for Additional Physics Test Problem Parameters Shock Tube (1: unigrid and AMR) Wave Pool (2) Shock Pool (3: unigrid 2D, AMR 2D and unigrid 3D) Double Mach Reflection (4) Shock in a Box (5) Zeldovich Pancake (20) Pressureless Collapse (21) Adiabatic Expansion (22) Test Gravity (23) Spherical Infall (24) Test Gravity: Sphere (25) Gravity Equilibrium Test (26) Collapse Test (27) Cosmology Simulation (30) Supernova Restart Simulation (40) Other External Parameters Other Internal Parameters Parameters to be Described

V1.5

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Stopping Parameters Initialization Parameters Simulation Identifiers and UUIDs I/O Parameters Streaming Data Format Hierarchy Control Parameters Hydrodynamic Parameters Magnetohydrodynamic Parameters Cosmology Parameters Gravity Parameters Particle Parameters Parameters for Additional Physics Cloudy Cooling Inline Halo Finding Inline Python Star Formation and Feedback Parameters Normal Star Formation Population III Star Formation Jeans Resolved Star Formation Massive Black Hole Particle Formation Background Radiation Parameters Minimum Pressure Support Parameters Radiative Transfer (Ray Tracing) Parameters Radiative Transfer (FLD) Parameters Radiative Transfer (FLD) Implicit Solver Parameters Radiative Transfer (FLD) Split Solver Parameters Massive Black Hole Physics Parameters Accretion Physics Feedback Physics Test Problem Parameters Shock Tube (1: unigrid and AMR) Wave Pool (2) Shock Pool (3: unigrid 2D, AMR 2D and unigrid 3D)

I. Radiative Transfer with Ray Tracing II. Radiating "Star" Particles

John Wise (Princeton) Enzo Workshop UCSD – 29 Jun 2010



Cosmological Radiative Transfer Equation

$$I_{\nu} \equiv I(\nu, \mathbf{x}, \Omega, t)$$

 $\begin{array}{l} n := normal vector \\ a := scale factor \\ \bar{a} := a/a_{em} \\ H := Hubble factor \\ v := frequency \end{array}$

$$\frac{1}{c} \frac{\partial I_{\nu}}{\partial t} + \frac{\hat{n} \cdot \nabla I_{\nu}}{\bar{a}} - \frac{H}{c} \left(\nu \frac{\partial I_{\nu}}{\partial \nu} - 3I_{\nu} \right) = -\kappa_{\nu} I_{\nu} + j_{\nu}$$

Cosmological Radiative Transfer Equation

n := normal vector a := scale factor $\bar{a} := a/a_{em}$



 $I_{\nu} \equiv I(\nu, \mathbf{x}, \Omega, t)$

Simplifications – "Local" Approximation

- 1. Short timesteps ($\bar{a} = 1$)
- 2. Ignore cosmological redshift and dilution (may become important >50 Mpc)



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Simplifications – "Local" Approximation

- 1. Short timesteps ($\bar{a} = 1$)
- 2. Ignore cosmological redshift and dilution (may become important >50 Mpc)



RT Equation along a Ray

- Consider point sources of radiation
- Initially, the radiation flux is split equally among all rays.

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



• P := photon flux in the ray

Abel & Wandelt (2002)



Abel & Wandelt (2002)



- Ray directions and splitting based on HEALPix (Gorski et al. 2005)
- Rays are split into 4 child rays when the solid angle is large compared to the cell face area
- Well-suited for AMR
- Fully coupled to the chemistry and energy solvers in Enzo, i.e. radiation hydrodynamics!



Abel & Wandelt (2002)

- Each ray is mono-chromatic
- Hydrogen ionizing (E > 13.6 eV)
- Helium singly ionizing (E > 24.6 eV)
- Helium doubly ionizing (E > 54.4 eV)

• X-rays

- hydrogen ionizations
- secondary ionizations
- helium ionizations
- reduced photo-heating
- H₂ dissociating (Lyman-Werner)



Time for an **example**!

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Terminal - 80×25 - #3

52weeks-of-code% cd doc/examples/RadiationTransport/ RadiationTransport% ls PhotonShadowing PhotonTest PhotonTestAMR RadiationTransport% cd PhotonTest PhotonTest% ls PhotonTest.enzo PhotonTest%

> Cosmological RT Codes Comparison Iliev et al. (2006)

Test 1

Source at the origin Uniform density field No hydrodynamics Isothermal Mono-chromatic spectrum (13.6 eV)



Tuesday, 29 June 2010

$\odot \odot \odot$	Terminal — 80	×25 — #3			
File Edit Options Buffers	Tools Help				
RadiativeTransferRaysPerCell = 5.1 RadiativeTransferInitialHEALPixLevel = 3 RadiativeTransferHIIRestrictedTimestep = 1		Minimum rays res	per cell, i.e. angular olution		
RadiativeTransferAdaptiveTimestep = 1 RadiativeTransferHydrogenOnly = 1					
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HydroMethod = DualEnergyFormalism = :	-1 // no hydro 1)			
TopGridGravityBoundary LeftFaceBoundaryCondition RightFaceBoundaryCondition	= 0 = 3 3 3 / = 3 3 3	// same for fluid			
StaticHierarchy MaximumRefinementLevel RefineBy CellFlaggingMethod	= 1 // N = 0 // u = 2 // r = 2 // u	lo AMR ise up to levels refinement factor ise baryon mass for	refinement		
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-uu-:F1 PhotonTest.enzo 22% L21 Hg-13	374 (Fundamental)			

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HydroMethod = -1 // no hydro DualEnergyFormalism = 1	If set to 0, uses hydro timestep on the finest level.			
TopGridGravityBoundary = 0 LeftFaceBoundaryCondition = 3 3 3 // same for fluid RightFaceBoundaryCondition = 3 3 3				
StaticHierarchy= 1// No AMaximumRefinementLevel= 0// useRefineBy= 2// refiCellFlaggingMethod= 2// use	MR up to levels inement factor baryon mass for refinement			
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ComovingCoordinates = DensityUnits = 1.673e-27 TimeUnits = 3.1557e13 / LengthUnits = 2.03676e22	= 0 // 1e-3 c // Myr // 6.6 kpc	:m^-3	Determines timestep by restricting HI fraction change to 5%. Not stable for big runs (yet).
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Tuesday, 29 June 2010

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PhotonTestNumberOfSources	= 1		Number of point sources
PhotonTestSourceType[0] PhotonTestSourcePosition[0]	= 1 = 1e-3 1e-	3 1e-3	For future use.
<pre>PhotonTestSourceLuminosity[0 PhotonTestSourceLifeTime[0] PhotonTestSourceEnergyBins[0 #PhotonTestSourceEnergy[0] = PhotonTestSourceEnergy[0] =</pre>] = 5e48 = 1e10] = 1 23.2686 13.60001	// phot	con number flux [#/s]
PhotonTestNumberOfSpheres	= 0		
<pre> "#PhotonTestSphereType[0] #PhotonTestSphereRadius[0] #PhotonTestSphereDensity[0] #PhotonTestSphereTemperature #PhotonTestSphereCoreRadius[#PhotonTestSpherePosition[0]</pre>	= 1 = 0.5 = 2. [0] = 1.e3 [0] = 0.05 = 0.5 0.	5 0.5	
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-uu-:F1 PhotonTest.enzo	68% L62	Hg-1374 ((Fundamental)

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PhotonTestNumberOfSpheres	= 0		
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-uu-:F1 PhotonTest.enzo	68% L62	Hg-1374 ((Fundamental)

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File Edit Options Buffers Tools Help	
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<pre>PhotonTestSourceEnergyBins[0] = 1 #PhotonTestSourceEnergy[0] = 23 2686</pre>	Total photon luminosity (ph/sec)
PhotonTestSourceEnergy[0] = 13.60001	
PhotonTestNumberOfSpheres = 0	
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-uu-:F1 PhotonTest.enzo 68% L62 Hg-137	4 (Fundamental)

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File Edit Options Buffers Tools Help)	
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-uu-:F1 PhotonTest.enzo 68% L6	62 Hg-1374 ((Fundamental)

● ○ ○ Terminal - 80×25 - ₩3		
File Edit Options Buffers Tools Help		
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-uu-:F1 PhotonTest.enzo 68% L62 Hg-1374	(Fundamental)	



Electron_F raction

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PhotonTest% ls ... PhotonShadowing PhotonTest PhotonTestAMR PhotonTest% cd ../PhotonTestAMR/ PhotonTestAMR% ls PhotonTestAMR.enzo PhotonTestAMR%

> Cosmological RT Codes Comparison II Iliev et al. (2009)

Test 6 (with AMR)

Source at the origin 1/r² density profile Hydrodynamics Blackbody spectrum (10⁵ K)







Bot L60

Hg-1382

(Fundamental)

Tuesday, 29 June 2010

-uu-:---F1

PhotonTestAMR.enzo



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File Edit Options Buffers Tools	C++ Help	
PhotonTestNumberOfSources =	1	
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<pre>PhotonTestOmegaBaryonNow = 1.0 PhotonTestInitialTemperature = 8 PhotonTestInitialFractionHII =</pre>	0 3000 0.99	
PhotonTestNumberOfSpheres =	= 1	1
-uu-:F1 PhotonTest.enzo 49	9% L41 (C++/l Abbrev)	
$\odot \odot \odot$	Terminal — 80×25 — #3	
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File Edit Options Buffers Tools	C++ Help	
PhotonTestNumberOfSources =	1	How do I have
PhotonTestRefineAtStart =	1	>1 energy group?
PhotonTestNumberOfSources PhotonTestSourceType[0]	= 1 = 1	
PhotonTestSourcePosition[0] PhotonTestSourceLuminosity[0] PhotonTestSourceLifeTime[0] PhotonTestSourceCreationTime[0] PhotonTestSourceRampTime[0] PhotonTestSourceEnergyBins[0] PhotonTestSourceSED[0]	$= 0.001 \ 0.5 \ 0.5$ = 2.99186e+51 = 1e+10 = 0 = 0 = 4 = 0.277 \ 0.335 \ 0.2 \ 0.1	Example: 10 ⁵ K blackbody in 4 energy groups
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	0.00		~
PhotonTestNumberOfSpheres	= 1		
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<pre>PhotonTestSourceLifeTime[0] =</pre>	1e+10
<pre>PhotonTestSourceCreationTime[0] =</pre>	Ø 4 energy groups
PhotonTestSourceRampTime[0] =	0
<pre>PhotonTestSourceEnergyBins[0] =</pre>	4
PhotonTestSourceSED[0] =	0.277 0.335 0.2 0.188
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Radiative "Star" Particles

Complex behavior encouraged!

Star particle overview

- Two types of star particles: (1) Normal and (2) Radiative
- Normal star particles are similar to DM particles but have particle attributes
 - Creation time
 - Dynamical time (or lifetime)
 - Metallicity
- Normal star particles only interact with local grid cells.
- Feedback is accomplished through energy injection

Star class

• To mirror nature better, star particles needed more flexibility.



- The class is an **additional layer** on top of the normal star particle, so it is included in the gravity solver and refinement criteria.
- Main advantage: greater interactivity between the stars and grid
 - Able to change cells on multiple grids and levels

Feedback spheres



Star class

- Different types of feedback modes (all operate in spheres of any radius)
 - Star formation instantaneous accretion
 - Supernova feedback thermal energy injection
 - Strömgren sphere radial profile taken from Whalen et al. (2004)
 - Color field Marks sphere with a color

Star class

- Can represent a single star, star cluster, black hole, neutron star, etc.
- Can grow from a pre-determined accretion rate "future".
- Easy to merge.

```
if (Star1->Mergable(Star2)) {
   Star1 += Star2;
   Star2->DisableParticle(LevelArray);
}
```

 Doesn't necessarily creates radiation. This is determined in Star_IsARadiationSource.C.

http://lca.ucsd.edu/projects/enzo/wiki/Tutorials/StarParticleClass



http://lca.ucsd.edu/projects/enzo/wiki/Tutorials/StarParticleClass



Radiative Star Particles

- Population III stars method 3. Represent single Pop III stars. Luminosity, lifetime, and endpoint determined from PopIIIStarMass
- "Star cluster" particles method 5. Represents a star cluster or galaxy (depending on resolution).
- In Enzo 2.0, multiple star formation routines may be used.
 - Specified in a bitwise fashion.
 - Method $3 \rightarrow 2^3 = 8$
 - Method 4 \rightarrow 2⁴ = 16
 - Method 3 & 5 \rightarrow 2³ + 2⁵ = 40
- **Black hole particles** PopIIIBlackHoles = 1

	Ferminal — 80×25 — #3
StarClusterUseMetalField	= 1
StarClusterMinDynamicalTime	= 1e+07 Metal enrichment
StarClusterIonizingLuminosity	= 3e+46
StarClusterHeliumIonization	= 0
StarClusterSNEnergy	= 2.4e+48
StarClusterSNRadius	= 10
StarClusterFormEfficiency	= 0.07
StarClusterMinimumMass	= 1000
StarClusterCombineRadius	= 10
StarClusterRegionLeftEdge	= 0.000000 0.000000 0.000000
StarClusterRegionRightEdge	= 1.000000 1.000000 1.000000
PopIIIStarMass	= 170
PopIIIBlackHoles	= 0
PopIIIBHLuminosityEfficiency	= 0.100000
PopIII0verDensityThreshold	= 1e+06
PopIIIH2CriticalFraction	= 0.0005
PopIIIMetalCriticalFraction	= 2.2e-06
PopIIISupernovaRadius	= 50
PopIIISupernovaUseColour	= 1
PopIIISupernovaMustRefine	= 1
PopIIISupernovaMustRefineResolutio	on = 32
PopIIIColorDensityThreshold	= 1e+06
PopIIIColorMass	= 1e+06
DD0004/output_0004 lines 326-349/4	51 76%

●	erminal — 80×25 — #3
StarClusterUseMetalField	
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StarClusterIonizingLuminosity	= 3e+46 Minimum type of a star forming
StarClusterHeliumIonization	$= 0$ $molecular eloud (bigber \rightarrow lower$
StarClusterSNEnergy	= 2.4e+48
StarClusterSNRadius	= 10 dens. & more massive). In years,
StarClusterFormEfficiency	= 0.07
StarClusterMinimumMass	= 1000
StarClusterCombineRadius	= 10
StarClusterRegionLeftEdge	= 0.000000 0.000000 0.000000
StarClusterRegionRightEdge	= 1.000000 1.000000 1.000000
PopIIIStarMass	= 170
PopIIIBlackHoles	= 0
PopIIIBHLuminosityEfficiency	= 0.100000
PopIII0verDensityThreshold	= 1e+06
PopIIIH2CriticalFraction	= 0.0005
PopIIIMetalCriticalFraction	= 2.2e-06
PopIIISupernovaRadius	= 50
PopIIISupernovaUseColour	= 1
PopIIISupernovaMustRefine	= 1
PopIIISupernovaMustRefineResolution	n = 32
PopIIIColorDensityThreshold	= 1e+06
PopIIIColorMass	= 1e+06
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StarClusterUseMetalField	= 3	1		Actal aprichment
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StarClusterHeliumIonization	= (0	molecula	ar cloud (higher → lower
StarClusterSNEnergy	=	2.4e+48	dens & r	more massive) In vears
StarClusterSNRadius	= 3	10		nore massive). In years .
StarClusterFormEfficiency	= (0.07	Ionizir	ng photons / sec / M $_{\odot}$
StarClusterMinimumMass	= 3	1000		
StarClusterCombineRadius	=	10		
StarClusterRegionLeftEdge	= (0.000000	0.000000	0.00000
StarClusterRegionRightEdge	=	1.000000	1.000000 :	1.000000
PopIIIStarMass	=	170		
PopIIIBlackHoles	=	0		
PopIIIBHLuminosityEfficiency	=	0.100000		
PopIII0verDensityThreshold	=	1e+06		
PopIIIH2CriticalFraction	=	0.0005		
PopIIIMetalCriticalFraction	=	2.2e-06		
PopIIISupernovaRadius	=	50		
PopIIISupernovaUseColour	=	1		
PopIIISupernovaMustRefine	=	1		
PopIIISupernovaMustRefineResolution	on =	32		
PopIIIColorDensityThreshold	=	1e+06		
PopIIIColorMass	=	1e+06		
DD0004/output_0004 lines 326-349/	451 76%			

\odot	Terminal —	80×25 — #3	
StarClusterUseMetalField	=	1	Matal apriabre ant
StarClusterMinDynamicalTime	=	1e+07	Metal enrichment
StarClusterIonizingLuminosity	=	3e+46	Minimum t _{etm} of a star-forming
StarClusterHeliumIonization	=	0	molecular cloud (bigher \rightarrow lower
StarClusterSNEnergy	=	2.4e+48	done & moro massivo) In voars
StarClusterSNRadius	=	10	uens. a more massive). In years.
StarClusterFormEfficiency	=	0.07	Ionizing photons / sec / M_{\odot}
StarClusterMinimumMass	=	1000	
StarClusterCombineRadius	=	10	Use helium ionizing photons
StarClusterRegionLeftEdge	=	0.000000	0.000000 0.000000
StarClusterRegionRightEdge	=	1.000000	1.000000 1.000000
PopIIIStarMass	=	170	
PopIIIBlackHoles	=	0	
PopIIIBHLuminosityEfficiency	=	0.100000	
PopIII0verDensityThreshold	=	1e+06	
PopIIIH2CriticalFraction	=	0.0005	
PopIIIMetalCriticalFraction	=	2.2e-06	
PopIIISupernovaRadius	=	50	
PopIIISupernovaUseColour	=	1	
PopIIISupernovaMustRefine	=	1	
PopIIISupernovaMustRefineResolutio	on =	32	
PopIIIColorDensityThreshold	=	1e+06	
PopIIIColorMass	=	1e+06	
DD0004/output_0004 lines 326-349/4	451 76%		

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	erminal — 80×25 — ೫3	
StarClusterUseMetalField	= 1	Metal enrichment
StarClusterMinDynamicalitme		
StarClusterionizingLuminosity	= 30+40	Minimum t _{dyn} of a star-forming
StarClusterHellumIonization	= 0	molecular cloud (higher \rightarrow lower
StarClusterSNEnergy	= 2.4e+48	dens. & more massive). In vears .
StarClusterSNRadius	= 10	
StarClusterFormEfficiency	= 0.07	lonizing photons / sec / M_{\odot}
StarClusterMinimumMass	= 1000	
StarClusterCombineRadius	= 10	Use helium ionizing photons
StarClusterRegionLeftEdge	= 0.000000 (
StarClusterRegionRightEdge	= 1.0000001	SN energy – erg / M₀
PopIIIStarMass	= 170	
PopIIIBlackHoles	= 0	
PopIIIBHLuminosityEfficiency	= 0.100000	
PopIII0verDensityThreshold	= 1e+06	
PopIIIH2CriticalFraction	= 0.0005	
PopIIIMetalCriticalFraction	= 2.2e-06	
PopIIISupernovaRadius	= 50	
PopIIISupernovaUseColour	= 1	
PopIIISupernovaMustRefine	= 1	
PopIIISupernovaMustRefineResolution	n = 32	
PopIIIColorDensityThreshold	= 1e+06	
PopIIIColorMass	= 1e+06	
DD0004/output_0004 lines 326-349/4	51 76%	

Tuesday, 29 June 2010

$\odot \odot \odot$	Terminal — 80×25 — #3
StarClusterUseMetalField StarClusterMinDynamicalTime	 = 1 = 1e+07 Metal enrichment
StarClusterIonizingLuminosity StarClusterHeliumIonization StarClusterSNEnergy StarClusterSNRadius	= $3e+46$ = 0 = $2.4e+48$ = 10 Minimum t_{dyn} of a star-forming molecular cloud (higher \rightarrow lower dens. & more massive). In years .
StarClusterFormEfficiency	= 0.07 Ionizing photons / sec / M _☉
StarClusterCombineRadius	= 1000 = 10 Use helium ionizing photons
StarClusterRegionLeftEdge StarClusterRegionRightEdge	= 0.000000 (* 1444444 A tatatatata = 1.000000 1 SN energy – erg / M₀
PopIIIStarMass PopIIIBlackHoles PopIIIBHLuminosityEfficiency PopIIIOverDensityThreshold	 = 170 = 0 = 0.1000000 = 10±06 Radius (pc) to inject SN feedback thermal energy. In the code, minimum of 3.5 cell widths.
PopIIIH2CriticalFraction PopIIIMetalCriticalFraction PopIIISupernovaRadius	= 0.0005 = 2.2e-06 = 50
PopIIISupernovaUseColour PopIIISupernovaMustRefine	= 1 = 1
PoplilSupernovaMustRefineResoluti	on = 32
PopIIIColorDensityThreshold PopIIIColorMass DD0004/output_0004 lines 326-349/	= 1e+06 = 1e+06 451 76%

Tuesday, 29 June 2010

$\odot \odot \odot$	Terminal — 80×25 — ೫3	
StarClusterUseMetalField StarClusterMinDynamicalTime	= 1 = 1e+07	Metal enrichment
StarClusterIonizingLuminosity StarClusterHeliumIonization StarClusterSNEnergy StarClusterSNRadius	= 3e+46 = 0 = 2.4e+48 = 10	Minimum t _{dyn} of a star-forming molecular cloud (higher → lower dens. & more massive). In years .
StarClusterFormEfficiency	= 0.07	lonizing photons / sec / M_{\odot}
StarClusterMinimumMass StarClusterCombineRadius	= 1000 = 10	Use helium ionizing photons
StarClusterRegionLeftEdge StarClusterRegionRightEdge	= 0.000000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	SN energy – erg / M_{\odot}
PopIIIStarMass PopIIIBlackHoles PopIIIBHLuminosityEfficiency PopIIIOverDensityThreshold	= 170 = 0 = 0.100000 = 1e+06	Radius (pc) to inject SN feedback thermal energy. In the code, minimum of 3.5 cell widths.
PopIIIH2CriticalFraction PopIIIMetalCriticalFraction PopIIISupernovaRadius	= 0.0005 = 2.2e-06 = 50 - 1	Star formation efficiency. This fraction of the cold gas mass is converted into a star.
PopIIISupernovaMustRefine PopIIISupernovaMustRefineResoluti	= 1 on = 32	
PopIIIColorDensityThreshold PopIIIColorMass DD0004/output_0004 lines 326-349/4	= 1e+06 = 1e+06 451 76%	

$\odot \odot \odot$	Terminal — 80×25 — %3	
StarClusterUseMetalField StarClusterMinDynamicalTime	= 1 = 1e+07	Metal enrichment
StarClusterIonizingLuminosity StarClusterHeliumIonization StarClusterSNEnergy StarClusterSNRadius	= 3e+46 = 0 = 2.4e+48 = 10	Minimum t _{dyn} of a star-forming molecular cloud (higher → lower dens. & more massive). In years .
StarClusterFormEfficiency	= 0.07	Ionizing photons / sec / M_{\odot}
StarClusterMinimumMass StarClusterCombineRadius	= 1000 = 10	Use helium ionizing photons
StarClusterRegionLeftEdge StarClusterRegionRightEdge	= 0.00000000 = 1.000000000000000000000000000000000000	SN energy – erg / M₀
PopIIIStarMass PopIIIBlackHoles PopIIIBHLuminosityEfficiency PopIIIOverDensityThreshold	= 170 = 0 = 0.100000 = 1e+06	Radius (pc) to inject SN feedback thermal energy. In the code, minimum of 3.5 cell widths.
PopIIIH2CriticalFraction PopIIIMetalCriticalFraction PopIIISupernovaRadius PopIIISupernovallseColour	= 0.0005 = 2.2e-06 = 50 = 1	Star formation efficiency. This fraction of the cold gas mass is converted into a star.
PopIIISupernovaMustRefine	= 1	Star cluster minimum mass (M₀)
PopIIISupernovaMustRefineResoluti	on = 32	
PopIIIColorDensityThreshold PopIIIColorMass DD0004/output_0004 lines 326-349/	= 1e+06 = 1e+06 451 76%	

000	Terminal — 80×25 — ೫3	
StarClusterUseMetalField StarClusterMinDynamicalTime	= 1 = 1e+07	Metal enrichment
StarClusterIonizingLuminosity StarClusterHeliumIonization StarClusterSNEnergy StarClusterSNRadius	= 3e+46 = 0 = 2.4e+48 = 10	Minimum t _{dyn} of a star-forming molecular cloud (higher → lower dens. & more massive). In years .
StarClusterFormEfficiency	= 0.07	lonizing photons / sec / M_{\odot}
StarClusterCombineRadius	= 1000	Use helium ionizing photons
StarClusterRegionLeftEdge StarClusterRegionRightEdge	= 0.000000 (= 1.000000 1	SN energy – erg / M₀
PopIIIStarMass PopIIIBlackHoles PopIIIBHLuminosityEfficiency PopIIIOverDensityThreshold	= 170 = 0 = 0.100000 = 1e+06	Radius (pc) to inject SN feedback thermal energy. In the code, minimum of 3.5 cell widths.
PopIIIH2CriticalFraction PopIIIMetalCriticalFraction PopIIISupernovaRadius PopIIISupernovallseColour	= 0.0005 = 2.2e-06 = 50 = 1	Star formation efficiency. This fraction of the cold gas mass is converted into a star.
PopIIISupernovaMustRefine	= 1	Star cluster minimum mass (M₀)
PopIIISupernovaMustRefineResolutio	on = 32 = 1e+06	Radius (pc) to combine stars when first created
PopIIIColorMass DD0004/output_0004 lines 326-349/4	= 1e+06 451 76%	

\odot	Terminal — 80×25 — #3
StarClusterUseMetalField	= 1
StarClusterMinDynamicalTime	= 1e+07 Stellar mass in M _☉ (constant)
StarClusterIonizingLuminosity	= 3e+46
StarClusterHeliumIonization	= 0
StarClusterSNEnergy	= 2.4e+48
StarClusterSNRadius	= 10
StarClusterFormEfficiency	= 0.07
StarClusterMinimumMass	= 1000
StarClusterCombineRadius	= 10
StarClusterRegionLeftEdge	= 0.000000 0.000000 0.000000
StarClusterRegionRightEdge	= 1.000000 1.000000 1.000000
PopIIIStarMass	= 170
PopIIIBlackHoles	= 0
PopIIIBHLuminosityEfficiency	= 0.100000
PopIII0verDensityThreshold	= 1e+06
PopIIIH2CriticalFraction	= 0.0005
PopIIIMetalCriticalFraction	= 2.2e-06
PopIIISupernovaRadius	= 50
PopIIISupernovaUseColour	= 1
PopIIISupernovaMustRefine	= 1
PopIIISupernovaMustRefineResoluti	on = 32
PopIIIColorDensityThreshold	= 1e+06
PopIIIColorMass	= 1e+06
DD0004/output_0004 lines 326-349/	451 76%

O Term Term	minal — 80×25 — 第3
StarClusterUseMetalField	= 1
StarClusterMinDynamicalTime	= 1e+07 Stellar mass in M _☉ (constant)
StarClusterIonizingLuminosity	= 3e+46
StarClusterHeliumIonization	$= 0$ $< 1/0 M_{\odot}$ and $> 260 M_{\odot}$ stars
StarClusterSNEnergy	= 2.4e+48
StarClusterSNRadius	= 10
StarClusterFormEfficiency	= 0.07
StarClusterMinimumMass	= 1000
StarClusterCombineRadius	= 10
StarClusterRegionLeftEdge	= 0.000000 0.000000 0.000000
StarClusterRegionRightEdge	= 1.000000 1.000000 1.000000
PopIIIStarMass	= 170
PopIIIBlackHoles	= 0
PopIIIBHLuminosityEfficiency	= 0.100000
PopIII0verDensityThreshold	= 1e+06
PopIIIH2CriticalFraction	= 0.0005
PopIIIMetalCriticalFraction	= 2.2e-06
PopIIISupernovaRadius	= 50
PopIIISupernovaUseColour	= 1
PopIIISupernovaMustRefine	= 1
PopIIISupernovaMustRefineResolution	= 32
PopIIIColorDensityThreshold	= 1e+06
PopIIIColorMass	= 1e+06
DD0004/output_0004 lines 326-349/451	1 76%

	Terminal — 80×25 — Ж3
StarClusterUseMetalField	= 1 Stellar mass in M _o (constant)
StarClusterMinDynamicallime	= 1e+07
StarClusterIonizingLuminosity	= 3e+46 Use radiative BH particles when
StarClusterHeliumIonization	= 0 <140 M _o and >260 M _o stars
StarClusterSNEnergy	= 2.4e+48
StarClusterSNRadius	= 10 $L_{BH} = f * dM_{BH}/dt * c^2$
StarClusterFormEfficiency	= 0.07
StarClusterMinimumMass	= 1000
StarClusterCombineRadius	= 10
StarClusterRegionLeftEdge	= 0.000000 0.000000 0.000000
StarClusterRegionRightEdge	= 1.000000 1.000000 1.000000
PopIIIStarMass	= 170
PopIIIBlackHoles	= 0
PopIIIBHLuminosityEfficiency	= 0.100000
PopIII0verDensityThreshold	= 1e+06
PopIIIH2CriticalFraction	= 0.0005
PopIIIMetalCriticalFraction	= 2.2e-06
PopIIISupernovaRadius	= 50
PopIIISupernovaUseColour	= 1
PopIIISupernovaMustRefine	= 1
PopIIISupernovaMustRefineResolution	on = 32
PopIIIColorDensityThreshold	= 1e+06
PopIIIColorMass	= 1e+06
DD0004/output_0004 lines 326-349/45	51 76%

$\odot \odot \odot$	Terminal — 80×25 — %3	
StarClusterUseMetalField StarClusterMinDynamicalTime	= 1 = 1e+07	Stellar mass in M₀ (constant)
StarClusterIonizingLuminosity StarClusterHeliumIonization StarClusterSNEneray	= 3e+46 = 0 = 2.4e+48	Use radiative BH particles when <140 M₀ and >260 M₀ stars
StarClusterSNRadius StarClusterFormEfficiency	= 10 = 0.07	L _{BH} = f * dM _{BH} /dt * c ²
StarClusterMinimumMass StarClusterCombineRadius StarClusterRegionLeftEdge	$= 1000 \\ = 10 \\ = 0.000000 $	Overdensity to form StarCluster and Pop III star particles (pegative value for units of cm ⁻³)
StarClusterRegionRightEdge PopIIIStarMass	= 1.000000 1 = 170	
PopIIIBlackHoles PopIIIBHLuminosityEfficiency PopIIIOverDensityThreshold	= 0 = 0.100000 = 1e+06	
PopIIIH2CriticalFraction PopIIIMetalCriticalFraction PopIIISuperpoveRadius	= 0.0005 = 2.2e-06 - 50	
PopIIISupernovaUseColour PopIIISupernovaUseColour	= 30 = 1 = 1	
PopIIISupernovaMustRefineResolutio	on = 32	
PopIIIColorDensityThreshold PopIIIColorMass DD0004/output 0004 lines 326-349/4	= 1e+06 = 1e+06 451 76%	
DD0004/output_0004 lines 326-349/4	451 76%	

$\odot \odot \odot$	Terminal — 80×25 — #3
StarClusterUseMetalField	 = 1 Stellar mass in M_☉ (constant)
StarClusterIonizingLuminosity	= 3e+46
StarClusterHeliumIonization	$= \emptyset$ Use radiative BH particles when $<140 \text{ M}_{\odot} \text{ and } >260 \text{ M}_{\odot} \text{ stars}$
StarClusterSNEnergy	= 2.4e+48
StarClusterSNRadius	= 10 $L_{BH} = f * dM_{BH}/dt * c^2$
StarClusterFormEfficiency	= 0.07 - 1000 Overdensity to form StarCluster
StarClusterCombineRadius	= 10 and Pop III star particles
StarClusterRegionLeftEdge	= 0.000000 (negative value for units of cm ⁻³)
StarClusterRegionRightEdge	= 1.000000 1 Managana 1 Managana
PopIIIStarMass	= 170 Minimum H ₂ fraction to form
PopIIIBlackHoles	
PoplilBHLuminosityEfficiency	= 0.100000
PopIIIOverbensity incessora PopIIIH2Critical Fraction	= 10+00 = 0 0005
PopIIIMetalCriticalFraction	= 2.2e-06
PopIIISupernovaRadius	= 50
PopIIISupernovaUseColour	= 1
PopIIISupernovaMustRefine	= 1
PopIIISupernovaMustRefineResoluti	.on = 32
PopIIIColorDensityThreshold	= 1e+06
PopIIIColorMass	= 1e+06
DD0004/output_0004 lines 326-349/	[′] 451 76%

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StarClusterUseMetalField StarClusterMinDynamicalTime	 = 1 Stellar mass in M_☉ (constant)
StarClusterIonizingLuminosity StarClusterHeliumIonization	= $3e+46$ = 0 <140 M _o and >260 M _o stars
StarClusterSNEnergy StarClusterSNRadius StarClusterFormEfficiency	= 2.4e+48 = 10 = 0.07 L _{BH} = f * dM _{BH} /dt * c ²
StarClusterMinimumMass StarClusterCombineRadius StarClusterRegionLeftEdge	 = 1000 = 10 = 0.0000000 (Overdensity to form StarCluster and Pop III star particles (negative value for units of cm⁻³)
StarClusterRegionRightEdge PopIIIStarMass	= 1.000000 1 $= 170$ $= 170$ $= 170$ $= 170$ $= 170$ $= 170$ $= 170$ $= 170$ $= 170$ $= 170$ $= 170$ $= 170$ $= 170$ $= 170$ $= 170$ $= 170$ $= 170$
PopIIIBLackHoles PopIIIBHLuminosityEfficiency PopIIIOverDensitvThreshold	 = 0 = 0.100000 = 1e+06 Maximum metallicity (in absolute, not solar, fractions) of Pop III stars
PopIIIH2CriticalFraction PopIIIMetalCriticalFraction	= 0.0005 = 2.2e-06
PopIIISupernovaRadius PopIIISupernovaUseColour	= 50 = 1
PopIIISupernovaMustRefine PopIIISupernovaMustRefineResolutio	= 1 on $= 32$
PopIIIColorDensityThreshold PopIIIColorMass DD0004/output_0004 lines 326-349/4	= 1e+06 = 1e+06 -51 76%

● ○ ○ T	Terminal — 80×25 — #3
StarClusterUseMetalField StarClusterMinDynamicalTime	 = 1 Stellar mass in M_☉ (constant)
StarClusterIonizingLuminosity StarClusterHeliumIonization	= $3e+46$ = 0 = $140 M_{\odot}$ and >260 M _{\odot} stars
StarClusterSNEnergy StarClusterSNRadius StarClusterFormEfficiency	= 2.4e+48 = 10 = 0.07 LBH = f * dMBH/dt * c ²
StarClusterMinimumMass StarClusterCombineRadius StarClusterRegionLeftEdge	 = 1000 = 10 = 0.0000000 (Overdensity to form StarCluster and Pop III star particles (negative value for units of cm⁻³)
StarClusterRegionRightEdge PopIIIStarMass	= 1.000000
PopIIIBLackHoles PopIIIBHLuminosityEfficiency PopIIIOverDensityThreshold	 = 0 = 0.100000 = 1e+06 Maximum metallicity (in absolute, not solar, fractions) of Pop III stars
PopIIIH2CriticalFraction PopIIIMetalCriticalFraction	 = 0.0005 = 2.2e-06 Radius (pc) to inject SN energy
PopIIISupernovaRadius PopIIISupernovaUseColour PopIIISupernovaMustRefine	= 50 = 1 = 1
PopIIISupernovaMustRefineResolutio	on = 32
PopIIIColorDensityThreshold PopIIIColorMass DD0004/output_0004 lines 326-349/4	= 1e+06 = 1e+06 +51 76%

$\odot \odot \odot$	Terminal — 80×25 — %3	
StarClusterUseMetalField StarClusterMinDynamicalTime	= 1 = 1e+07	Stellar mass in M₀ (constant)
StarClusterIonizingLuminosity StarClusterHeliumIonization	= 3e+46 = 0 = 2.40.49	Use radiative BH particles when <140 M₀ and >260 M₀ stars
StarClusterSNEnergy StarClusterSNRadius StarClusterFormEfficiency	= 2.4e+40 = 10 = 0.07	L _{BH} = f * dM _{BH} /dt * c ²
StarClusterMinimumMass StarClusterCombineRadius StarClusterRegionLeftEdge	$= 1000 \\ = 10 \\ = 0.000000 ($	Overdensity to form StarCluster and Pop III star particles (negative value for units of cm ⁻³)
StarClusterRegionRightEdge PopIIIStarMass	= 1.000000 1 = 170	Minimum H ₂ fraction to form
PopIIIBlackHoles PopIIIBHLuminosityEfficiency PopIIIOverDensityThreshold	= 0 = 0.100000 = 1e+06	Maximum metallicity (in absolute, not solar, fractions) of Pop III stars
PopIIIH2CriticalFraction PopIIIMetalCriticalFraction	= 0.0005 = 2.2e-06	Radius (pc) to inject SN energy
PopIIISupernovaRadius PopIIISupernovaUseColour	= 50 = 1	Use a color (metal) field in SN feedback
PopIIISupernovaMustRefine PopIIISupernovaMustRefineResoluti	= 1 on = 32	
PopIIIColorDensityThreshold PopIIIColorMass DD0004/output_0004 lines 326-349/4	= 1e+06 = 1e+06 451 76%	

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000	Terminal — 80×25 — ೫3	
StarClusterUseMetalField StarClusterMinDvnamicalTime	= 1 = 1e+07	Stellar mass in M_{\odot} (constant)
StarClusterIonizingLuminosity StarClusterHeliumIonization	= 3e+46 = 0	Use radiative BH particles when <140 M₀ and >260 M₀ stars
StarClusterSNEnergy StarClusterSNRadius StarClusterFormEfficiency	= 2.4e+48 = 10 = 0.07	L _{BH} = f * dM _{BH} /dt * c ²
StarClusterMinimumMass StarClusterCombineRadius StarClusterRegionLeftEdge	$= 1000 \\ = 10 \\ = 0.000000 ($	Overdensity to form StarCluster and Pop III star particles (negative value for units of cm ⁻³)
StarClusterRegionRightEdge PopIIIStarMass	= 1.000000 1 = 170	Minimum H ₂ fraction to form
PopIIIBLACKHOLES PopIIIBHLuminosityEfficiency PopIIIOverDensityThreshold	= 0 = 0.100000 = 1e+06	Maximum metallicity (in absolute, not solar, fractions) of Pop III stars
PopIIIH2CriticalFraction PopIIIMetalCriticalFraction	= 0.0005 = 2.2e-06	Radius (pc) to inject SN energy
PopIIISupernovaRadius PopIIISupernovaUseColour	= 50 = 1	Use a color (metal) field in SN feedback
PopIIISupernovaMustRefine PopIIISupernovaMustRefineResolutio	= 1 on = 32	Use at your own risk. Pre-refines region before supernova.
PopIIIColorDensityThreshold PopIIIColorMass DD0004/output_0004 lines 326-349/4	= 1e+06 = 1e+06 451 76%	





Let's put them **together**.



Toy Reionization Simulation

- 30 Mpc, 64³ resolution
- AMR with 8 levels
- Maximal spatial resolution of 1.8 comoving kpc
- 4 x 10 $^9~M_{\odot}$ DM mass resolution
- Hydrogen ionization only
- Star cluster particles with metal enrichment
- Stop at z = 6





No full reionization because of mass resolution (i.e. we miss all of the low-luminosity dwarfs)

Create your own star particle type

1. In macros_and_parameters.h, add your particle type macro.



- 2. Add a "star_maker" to Grid_StarParticleHandler.C or create your own routine that adds particles to the grid (e.g., only done in a restart).
 - Assign the new particles a particle type = -NEW_PARTICLE_TYPE, which tells the Star class routines to create a new Star object from this particle. It will be changed into a positive number when the Star object is created.

Create your own star particle type

3. Add your new star particle type to the **if**-statement in Grid_FindNewStarParticles.C

```
for (i = 0; i < NumberOfParticles; i++)
    if (ParticleType[i] == -PARTICLE_TYPE_SINGLE_STAR ||
        ParticleType[i] == -PARTICLE_TYPE_BLACK_HOLE ||
        ParticleType[i] == -PARTICLE_TYPE_CLUSTER ||
        ParticleType[i] == -PARTICLE_TYPE_COLOR_STAR) {</pre>
```

4. Add a case-statement to Star_SetFeedbackFlag

```
case PopIII:
    if (this->type < 0) // birth
        this->FeedbackFlag = FORMATION;
    else if (Time > this->BirthTime + this->LifeTime) // endpoint
    if (this->Mass >= PISNLowerMass && this->Mass <= PISNUpperMass)
        this->FeedbackFlag = SUPERNOVA;
    else
        this->FeedbackFlag = NO_FEEDBACK; // BH formation
    else // main sequence
        this->FeedbackFlag = NO_FEEDBACK;
    break;
```
3. Add your new star particle type to the **if**-statement in Grid_FindNewStarParticles.C

for (i = 0; i < NumberOfParticles; i++)
 if (ParticleType[i] == -PARTICLE_TYPE_SINGLE_STAR ||
 ParticleType[i] == -PARTICLE_TYPE_BLACK_HOLE ||
 ParticleType[i] == -PARTICLE_TYPE_CLUSTER ||
 ParticleType[i] == -PARTICLE_TYPE_COLOR_STAR) {</pre>

4. Add a case-statement to Star_SetFeedbackFlag

case BlackHole: this->FeedbackFlag = NO_FEEDBACK; break;

5. If adding a feedback sphere, you can customize your own sphere in

Star_CalculateFeedbackParameters.C

case SUPERNOVA: // pair-instability SNe	
Radius = PopIIISupernovaRadius * pc / LengthUnits;	
Radius = max(Radius, 3.5*StarLevelCellWidth);	
EjectaVolume = 4.0/3.0 * 3.14159 * pow(PopIIISupernovaRadius*pc, 3);	
<pre>EjectaDensity = Mass * Msun / EjectaVolume / DensityUnits;</pre>	
HeliumCoreMass = (13./24.) * (Mass - 20);	
SNEnergy = (5.0 + 1.304 * (HeliumCoreMass - 64)) * 1e51;	
<pre>EjectaMetalDensity = HeliumCoreMass * Msun / EjectaVolume / DensityUnits;</pre>	
<pre>EjectaThermalEnergy = SNEnergy / (Mass * Msun) / VelocityUnits / VelocityUnits;</pre>	

Grid_AddFeedbackSphere.C.

if (cstar->FeedbackFlag == SUPERNOVA ||
 cstar->FeedbackFlag == CONT_SUPERNOVA) {

6. Add a case-statement to Star_ActivateNewStar.C



7. If you don't want your new star particle type to be radiating (i.e. only add feedback spheres), add an additional logic check in Star_IsARadiationSource.C.



Summary

- Run non-cosmological radiative hydrodynamics problems.
- New Star class
- New "star cluster" and Population III star particles.
- Run cosmological simulations with radiation transport from dynamically created star particles
- Create your own radiating "star" particle type.

Self-consistent Cosmological Radiation Hydrodynamics/Ionization

- implicit flux limited diffusion solver
- coupled to ionization kinetics and gas energy equation
- only for unigrid in 2.0 (AMR not supported yet)
- requires hypre library from LLNL



Self-consistent Cosmological Radiation Hydrodynamics/Ionization Reynolds, Hayes, Paschos & MN (2009)

- Goal
 - Create a parallel scalable solver that couples cosmological hydrodynamics, radiation transport, chemical ionization, and gas photoheating selfconsistently



Cosmological Radiative Transfer Equation



Spatial gradients WRT coordinates comoving with expanding universe

Flux-Limited Diffusion Radiation Transfer

We approximate the radiative flux as a function of the energy density gradient,

 $\mathbf{F}_{\boldsymbol{\nu}} = -D \, \nabla E_{\boldsymbol{\nu}},$

where $D: \Omega \to \mathbb{R}^{3\times 3}$ is the flux-limiter*, $D = D(e, E_{\nu}, \nabla E_{\nu})$.

With this approximation, the radiation energy equation becomes

$$\partial_t E_{\nu} + \frac{1}{a} \nabla \cdot (E_{\nu} \mathbf{v}_b) - \frac{1}{a^2} \nabla \cdot (D \nabla E_{\nu}) - \frac{1}{ca^3} \left(\nabla (D \nabla E_{\nu}) \right) \cdot (\nabla \mathbf{v}_b) \\ = \nu \frac{\dot{a}}{a} \partial_{\nu} E_{\nu} - 3 \frac{\dot{a}}{a} E_{\nu} + 4\pi \eta_{\nu} - ck_{\nu} E_{\nu}.$$

$$\partial_t E_v + \frac{1}{a} \nabla \cdot (E_v \upsilon_b) = \frac{1}{a^2} \nabla \cdot (D \nabla E_v) + \frac{\dot{a}}{a} (v \partial_v E_v - 3E_v) + 4\pi \eta_v - c\kappa_v E_v$$

Reduces to standard equation setting a=1

Spectral Modeling: 1-group Approximation

$$E_{\nu}(\mathbf{x}, t, \nu) = \tilde{E}(\mathbf{x}, t) \chi_{E}(\nu)$$

$$\chi_{E}(v) = \begin{cases} \delta(v - v_{0}) & monochromatic \\ B_{v}(T) & blackbody \\ \chi_{0}(v / v_{0})^{\alpha} & powerlaw \end{cases}$$

Comoving radiation energy density

$$\begin{split} E(\mathbf{x},t) &= \int_{\nu_0}^{\infty} E_{\nu}(\mathbf{x},t,\nu) d\nu = \tilde{E}(\mathbf{x},t) \int_{\nu_0}^{\infty} \chi_E(\nu) d\nu.\\ \partial_t E + \frac{1}{a} \nabla \cdot (E\nu_b) &= \frac{1}{a^2} \nabla \cdot (D\nabla E) + m \frac{\dot{a}}{a} E + 4\pi \eta - c\kappa E \end{split}$$

Why use FLD?

- Invented by my thesis adviser Jim Wilson
- Simple and easy (no formal solution needed)
- Correct behavior in limiting regimes
- Causal propagation of radiation energy
- I am interested in large volumes and many sources, where diffuse radiation backgrounds dominate local effects (i.e., shadows)
- SPD matrix → efficient solution methods
- Extenstion to VTEF with analytic EFs straightforward

System of Equations

$$\partial_t \rho_b + \frac{1}{a} \mathbf{v}_b \cdot \nabla \rho_b = -\frac{1}{a} \rho_b \nabla \cdot \mathbf{v}_b, \tag{1}$$

$$\partial_t \mathbf{v}_b + \frac{1}{a} \left(\mathbf{v}_b \cdot \nabla \right) \mathbf{v}_b = -\frac{\dot{a}}{a} \mathbf{v}_b - \frac{1}{a\rho_b} \nabla p - \frac{1}{a} \nabla \phi, \tag{2}$$

$$\partial_t e + \frac{1}{a} \mathbf{v}_b \cdot \nabla e = -\frac{2\dot{a}}{a} e - \frac{1}{a\rho_b} \nabla \cdot (p\mathbf{v}_b) - \frac{1}{a} \mathbf{v}_b \cdot \nabla \phi + G - \Lambda \quad (3)$$

$$\partial_t \mathbf{n}_i + \frac{1}{a} \nabla \cdot (\mathbf{n}_i \mathbf{v}_b) = \alpha_{i,j} \mathbf{n}_e \mathbf{n}_j - \mathbf{n}_i \Gamma_i^{ph}, \qquad i = 1, \dots, N_s \tag{4}$$

$$\partial_t E + \frac{1}{a} \nabla \cdot (E \mathbf{v}_b) = \nabla \cdot (D \nabla E) - m \frac{\dot{a}}{a} E + 4\pi \eta - c\kappa E.$$
(5)

$$\nabla^2 \phi = \frac{4\pi g}{a} (\rho_b + \rho_{dm} - \langle \rho \rangle), \tag{6}$$

$$e = \frac{p}{\rho_b(\gamma - 1)} + \frac{1}{2} |\mathbf{v}_b|^2,$$
(7)

$$\Gamma_i^{ph} = \int_{\nu_i}^{\infty} c \,\sigma_{\mathbf{n}_i}(\nu) \,\frac{E_{\nu}}{h\nu} \,d\nu$$

Operator Splitting

let

 $e = e_h + e_c$

where

- e_h is gas energy due to hydrodynamic motions
- e_c is energy correction due to coupling with radiation/ionization

Gas energy equation

$$\partial_t (e_h + e_c) + \frac{1}{a} \mathbf{v}_b \cdot \nabla (e_h + e_c) =$$

$$- \frac{2\dot{a}}{a} (e_h + e_c) - \frac{1}{a\rho_b} \nabla \cdot (p\mathbf{v}_b) - \frac{1}{a} \mathbf{v}_b \cdot \nabla \phi + G - \Lambda.$$
(13)

Explicit hydrodynamics

$$\partial_t \rho_b + \frac{1}{a} \mathbf{v}_b \cdot \nabla \rho_b = -\frac{1}{a} \rho_b \nabla \cdot \mathbf{v}_b, \tag{14}$$

$$\partial_t \mathbf{v}_b + \frac{1}{a} \left(\mathbf{v}_b \cdot \nabla \right) \mathbf{v}_b = -\frac{\dot{a}}{a} \mathbf{v}_b - \frac{1}{a\rho_b} \nabla p - \frac{1}{a} \nabla \phi, \tag{15}$$

$$\partial_t e_h + \frac{1}{a} \mathbf{v}_b \cdot \nabla e_h = -\frac{2\dot{a}}{a} e_h - \frac{1}{a\rho_b} \nabla \cdot (p\mathbf{v}_b) - \frac{1}{a} \mathbf{v}_b \cdot \nabla \phi \tag{16}$$

$$\partial_t \mathbf{n}_i + \frac{1}{a} \nabla \cdot (\mathbf{n}_i \mathbf{v}_b) = 0, \tag{17}$$

$$\partial_t E + \frac{1}{a} \nabla \cdot (E \mathbf{v}_b) = 0, \tag{18}$$

This is what ENZO already does

Implicit Coupled System

non-equilibrium multispecies model

$$\partial_t e_c = -\frac{2\dot{a}}{a}e_c + G - \Lambda, \tag{19}$$

$$\partial_t \mathbf{n}_i = \alpha_{i,j} \mathbf{n}_e \mathbf{n}_j - \mathbf{n}_i \Gamma_i^{ph}, \tag{20}$$

$$\partial_t E = \nabla \cdot (D\nabla E) - m \frac{a}{a} E + 4\pi\eta - c\kappa E, \qquad (21)$$

• LTE (2 temperature) model

$$\partial_t e_c = -\frac{2\dot{a}}{a}e_c + G - \Lambda,\tag{19}$$

$$\partial_t E = \nabla \cdot (D\nabla E) - m \frac{\dot{a}}{a} E + 4\pi\eta - c\kappa E, \qquad (21)$$

Temporal Discretization

Generalized Crank-Nicholson (theta scheme)

$$e_c^{n+1} + \Delta t \theta \mathcal{L}_e^{n+1} = e_c^n + \Delta t (\theta - 1) \mathcal{L}_e^n, \tag{22}$$

$$\mathbf{n}_{i}^{n+1} + \Delta t \theta \mathcal{L}_{\mathbf{n}_{i}}^{n+1} = \mathbf{n}_{i}^{n} + \Delta t (\theta - 1) \mathcal{L}_{\mathbf{n}_{i}}^{n}, \tag{23}$$

$$E^{n+1} + \Delta t\theta \left[\mathcal{D}_E^{n+1} + \mathcal{L}_E^{n+1} \right] = E^n + \Delta t(\theta - 1) \left[\mathcal{D}_E^n + \mathcal{L}_E^n \right].$$
(24)

$$\mathcal{D}_E = \mathcal{D}_E(E, \mathbf{n}_i) \equiv -\nabla \cdot (D\nabla E), \qquad (25)$$

and we have defined the local "reaction" operators as

$$\mathcal{L}_e = \mathcal{L}_e(e_c, E, \mathbf{n}_i) \equiv \frac{2\dot{a}}{a}e_c - G + \Lambda$$
(26)

$$\mathcal{L}_{\mathbf{n}_{i}} = \mathcal{L}_{\mathbf{n}_{i}}\left(\mathbf{n}_{i}, e_{c}, E\right) \equiv \mathbf{n}_{i}\Gamma_{i}^{ph} - \alpha_{i,j}\mathbf{n}_{e}\mathbf{n}_{j}$$
(27)

$$\mathcal{L}_E = \mathcal{L}_E \left(E, e_c, \mathbf{n}_i \right) \equiv m \frac{a}{a} E - 4\pi \eta + ckE.$$
(28)

Multigrid-Preconditioned Conjugate Gradient

• The primary difficulty in solving these systems lies in the Schur complement system

$$(D - LM^{-1}U) x_E = b_E - LM^{-1}b_M$$

- Due to the diffusion approximation, and the spatial locality of *M* and *L*, this matrix is symmetric and positive definite.
- SPD systems are often solved using the *conjugate-gradient* method; a robust, low-memory Krylov iterative solver. Unfortunately, CG convergence rates depend on the eigenvalues of the matrix, which here spread rapidly with mesh refinement, resulting in slower convergence as the mesh is refined.
- We therefore *precondition* the CG solver, i.e. $Ax = b \rightarrow (P^{-1}AP^{-1})(Px) = P^{-1}b$, where the symmetric operator P^{-1} comes from a *geometric multigrid* (MG) solver.
- MG methods, while less robust, exhibit convergence rates that are independent of the matrix spectrum, resulting in near optimal log-linear algorithm complexity, and scalability to thousands of processors.
- This MG-CG combination results in a robust, scalable solver for the inner Schur systems.

HYPRE solver library, LLNL



		Configuration ●○○○○○		
Build	Configurat	tion		

• To use any FLD solver module, Enzo <u>must</u> be configured with:

۲	gmake	photon-yes	[enables all radiation solvers]
۲	gmake	hypre-yes	[enables HYPRE solver interface]
۹	gmake	use-mpi-yes	[enables MPI]

- Moreover, the machine Makefile must specify how to include and link with an available HYPRE library (version $\geq 2.4.0b$).
- If you must compile HYPRE yourself, use the configuration option --with-no-global-partition for runs using over 1000 tasks.
- Optional/recommended Enzo configuration options include:
 - gmake emissivity-yes [enables coupling with star-maker]
 - gmake precision-64 [the solvers prefer double precision]

		Configuration ○●○○○○		
Start	up Paramet	ers		

The main problem parameter file must have the following parameters:

- RadiativeTransferFLD [0] this must be 2.
- ImplicitProblem [0] use 3 for gFLDSplit, 1 for gFLDProblem.
- ProblemType [0] FLD-based solvers use values in the 400's.
- RadHydroParamfile [NULL] the filename containing all FLD-specific solver parameters (next slide).
- RadiativeTransferOpticallyThinH2 [1] this must be 0.
- RadiationFieldType [0] can be any value *except* 10 or 11.
- RadiativeTransferFLDCallOnLevel [0] must currently be 0.

- RadiativeTransfer [0] this must be be 0.
- RadiativeCooling [0] must currently be 0.

The following parameters control various aspects of gFLDSplit:

- RadHydroESpectrum [1] form for radiation spectrum $\chi_E(\nu)$:
 - -1. is monochromatic at $h\nu = 13.6$ eV,
 - 0. is power law,
 - 1. is $T = 10^5$ blackbody.
- RadHydroChemistry [1] controls whether to use n_{HI} (1 yes, 0 no)
- RadHydroHFraction [1] controls the fraction of baryonic matter comprised of Hydrogen (RadHydroHFraction $\in [0, 1]$).
- RadHydroModel [1] determines which model for radiation-matter coupling we wish to use:
 - 1. Chemistry-dependent model with case B recombination coeff.
 - 4. Same as model 1, with an isothermal gas energy.
 - 10. Local thermodynamic equilibrium model (no n_{HI}).



- RadHydroMaxDt $[10^{20}]$ sets Δt_{max} in scaled time units.
- RadHydroMinDt [0] sets Δt_{\min} in scaled time units.
- RadHydroInitDt $[10^{20}]$ sets the initial Δt_E in scaled time units.
- RadHydroDtNorm [2] sets p in computing the time error estimate.
- RadHydroDtRadFac, RadHydroDtGasFac, RadHydroDtChemFac $[10^{20}]$ the values of $\tau_{i,tol}$ in computing Δt_E , Δt_e and Δt_{HI} .
- RadiationScaling, EnergyCorrectionScaling, ChemistryScaling [1.0] – the scaling factors s_E , s_e and s_n .
- RadHydroTheta [1.0] the $\partial_t E$ discretization parameter, θ .
- RadHydroSolTolerance $[10^{-8}]$ linear solver tolerance δ .

	Configuration ○○○○●○		
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FLD Solver Parameters – continued

- RadiationBoundaryX0Faces, RadiationBoundaryX1Faces, RadiationBoundaryX2Faces [0 0] - BC types at each face:
 - 0. periodic (must match on both faces in a given direction)
 - 1. Dirichlet
 - 2. Neumann
- EnergyOpacityCO-EnergyOpacityC2 [1, 1, 0] the opacity-defining constants C_0 - C_2 for the LTE model.
- RadHydroMaxMGIters [50] max number of MG-CG iterations.
- RadHydroMGRelaxType [1] the MG relaxation method:
 - 0. Jacobi
 - 1. Weighted Jacobi
 - 2. Red/Black Gauss-Seidel (symmetric)
 - 3. Red/Black Gauss-Seidel (nonsymmetric)
- RadHydroMGPreRelax [1] number of pre-relaxation MG sweeps.
- RadHydroMGPostRelax [1] number of post-relaxation MG sweeps.

		Configuration ○○○○○●		
Custo	omization			

To set up a new FLD problem:

- Allocate a baryon field with FieldType set to RadiationFreq0.
- Set η(x, t) by either:
 - Edit gFLDSplit_RadiationSource.src90 or gFLDProblem_RadiationSource.src90,
 - Fill in the baryon field EmissivityO, and edit logic in gFLDSplit_Evolve.C or gFLDProblem_Evolve.C to use that field (emulate logic for StarMakerEmissivityField).
- Edit gFLDSplit_Initialize.C or gFLDProblem_Initialize.C to call the problem initializer and set BCs.
- All other requirements for setting up a new ProblemType in Enzo are like normal (InitializeNew.C, problem initialization files, etc.).

[on Triton: /home/enzo-1/IlievEtA15]

Dynamic ionization test of an initially-neutral hydrogen region:

- Box size L = 15 kpc; Run time $T_f = 500$ Myr.
- ${\cal T}=10^5$ blackbody spectrum, at rate $\dot{N}_\gamma=5\cdot 10^{48}$ photon/s.
- Initial conditions: $n = 10^{-3} \text{ cm}^{-3}$, T = 100 K, $E = 10^{-30} \frac{\text{erg}}{\text{cm}^3}$.

No available analytical solution, but:

• Front transitions from R- to D-type as it reaches Strömgren radius,

$$r_{I}^{R} = r_{S} \left[1 - e^{-t\alpha_{B}(T_{i})n_{H}} \right]^{1/3}, \qquad r_{I}^{D} = r_{S} \left[1 + (7c_{s}t)/(4r_{S}) \right]^{4/7},$$

• Eventually stalls at $r_f = r_S \left(\frac{2T_i}{T_e}\right)^{2/3}$, where T_i and T_e are the temperatures behind and ahead of the l-front.

[Whalen & Norman, ApJS, 2006; Iliev et al., MNRAS, 2009]

 Model
 Solution Approach
 Configuration
 Non-Cosmological Problems
 Cosmological Problems
 Cosmological Problems
 End

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 Hydrodynamic Radiative Ionization Results



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[in enzo-2.0: run/RadiationTransportFLD/SG_q5z4_sp] Repeat of previous test, but in a cosmologically expanding universe, with a static, isothermal gas, using a monochromatic radiation spectrum.

Four tests:

<i>q</i> 0	zi	L _i [kpc]	$\rho_{b,i} [g cm^{-3}]$	H ₀	Ω_m	ΩΛ	Ω_b
0.5	4	80	1.18e-28	0.5	1.0	0	0.2
0.05	4	60	2.35e-28	1.0	0.1	0	0.1
0.5	10	36	1.18e-28	0.5	1.0	0	0.2
0.05	10	27	2.35e-28	1.0	0.1	0	0.1

Analytical solution given by

$$\begin{split} r_{I}(t) &= r_{S,i} \left(\lambda e^{-\tau(t)} \int_{1}^{a(t)} e^{\tau(b)} [1 - 2q_{0} + 2q_{0}(1 + z_{i})/b]^{-1/2} \mathrm{d}b \right)^{1/3}, \\ \tau(a) &= \lambda \left[F(a) - F(1) \right] \left[6q_{0}^{2}(1 + z_{i})^{2} \right]^{-1}, \qquad \lambda = \frac{\alpha_{B} n_{H,i}}{H_{0}(1 + z_{i})}, \\ F(a) &= \left[2 - 4q_{0} - 2q_{0} \frac{1 + z_{i}}{a} \right] \left[1 - 2q_{0} + 2q_{0} \frac{1 + z_{i}}{a} \right]^{1/2}. \end{split}$$

[Shapiro & Giroux, ApJ, 1987]



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[in enzo-2.0: run/RadiationTransportFLD/CosmologyFLD_RT]

Geoffrey So has constructed an interface to StarMaker to seed $\eta(\mathbf{x}, t)$:

- Requires Enzo configuration with EMISSIVITY enabled,
- Adds StarMakerEmissivityField=1 to main parameter file,
- The interface fills the EmissivityO baryon field based on emission from star particles; the FLD modules copy this field into $\eta(\mathbf{x}, t)$.
- Utilizes identical startup machinery as typical cosmology runs, via CosmologySimulationInitialize.C [ProblemType 30], with additional input file options to enable the FLD solver module.



Model Solution Approach Configuration Non-Cosmological Problems Cosmological Problems End 00000 00000 00 00 000 00 Summary of Current Results

The gFLDSplit and gFLDProblem solver modules implement a grey, field-based, flux-limited diffusion radiation approximation for unigrid runs:

- Implicit MG-CG solvers enable scalable solution on many thousands of cores, *independently* of the number of ionization sources.
- Accurately solves couplings between radiation, ionization and gas energy, due to implicit formulation and coupled solvers.
- Split and implicit formulations allow for tradeoffs between robustness/efficiency and accuracy.

However, this approximation has its shortcomings:

- Single radiation field allows full absorption by hydrogen, even though higher-frequency radiation should pass through.
- Though better than simpler approximations, grey approach cannot accurately handle multi-species problems (hence H-only restriction).
- Currently limited to unigrid Enzo simulations.