Methods

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Physics

Illustris and AREPO

Illustris dataset[10, 19] uses the AREPO solver, which evolves the fluid quantities according to the "hyperbolic conservation laws of ideal hydrodynamics:"[15]

State vector	$\mathbf{U} = \begin{pmatrix} \rho \\ \rho\mathbf{v} \\ \rho E \end{pmatrix}$
Flux	$\mathbf{F}(\mathbf{U}) = \begin{pmatrix} \rho\mathbf{v} \\ \rho\mathbf{v}\mathbf{v}^T + P \\ (\rho E + P)\mathbf{v} \end{pmatrix}$
RHS	$\mathbf{W} = \begin{pmatrix} 0 \\ -\frac{\dot{a}}{a}\rho\mathbf{v} - \frac{\rho}{a^2}\boldsymbol{\nabla}\phi \\ -2\frac{\dot{a}}{a\rho E} - \frac{\rho\mathbf{v}}{a^2}\boldsymbol{\nabla}\phi \end{pmatrix}$
Evolution with time	$\frac{\partial\mathbf{U}}{\partial t} + \frac{1}{a}\boldsymbol{\nabla}\cdot\mathbf{F} = \mathbf{W}$
Equation of state	$P = (\gamma - 1)u$
Energy	$E = u + \frac{1}{2}\rho v^2$
Gravitational potential	$\boldsymbol{\nabla}^2\phi = \frac{4\pi G}{a}\rho_{\text{total}} - \rho_0$

where ρ is the density field, ρ_0 is the mean density field, $\mathbf{v}$ is the velocity vector field, P is the pressure field, u is the internal energy field, a is the cosmological expansion constant, G is the gravitational constant, and γ is the ratio of specific heats, on an unstructured, moving, Voronoi tessellation mesh [15]. AREPO is second order in space and second order in time, due to hierarchical adaptive time-stepping [10].

AREPO uses Godunov's method in a MUSCL-Hancock scheme to solve these equations [15]. The MUSCL-Hancock scheme is "a slope-limited piece-wise linear reconstruction step within each cell, a first-order prediction step for the evolution over half a time-step, and finally a Riemann solver to estimate the time-averaged inter-cell fluxes for the time-step"[8, 9]. Note that since the mesh is not cartesian, AREPO cannot employ operator splitting [18].

AREPO uses Tree-PM (particle mesh) approach for computing self-gravity. Long-range forces are calculated using the Fourier particle-mesh method while short-range forces are computed with a hierarchical tree algorithm [10].

The Illustris simulation further use Monte Carlo tracer particle scheme described in [6].

The Illustris initial conditions are set by running CAMB [14] using parameters found in the Wilkinson Anisotropy probe [7] or RECFAST [13] (see Table 1).

Ω_m	0.2726
Ω_Λ	0.7274
Ω_b	0.0456
σ_8	0.809
n_s	0.963
H_0	100 h km / sec Mpc
h	0.704
$T(z = 157)$	245 K

Table 1: Initial conditions for CAMB.

Enzo

Enzo [11, 2] solves the magneto-hydrodynamics problem, in contrast to Illustris/AREPO which ignore magnetism. Enzo evolves the "equations of ideal magnetohydrodynamics (MHD) including gravity, in a coordinate systems co-moving with the cosmological expansion:"

State vector	$\mathbf{U} = \begin{pmatrix} \rho \\ \rho\mathbf{v} \\ \rho E \end{pmatrix}$
Flux	$\mathbf{F}(\mathbf{U}) = \begin{pmatrix} \rho\mathbf{v} \\ \rho\mathbf{v}\mathbf{v}^T + P + \frac{B^2}{2a} - \frac{\mathbf{B}\mathbf{B}}{a} \\ (\rho E + P + \frac{B^2}{2a})\mathbf{v} - \frac{1}{a}\mathbf{B}(\mathbf{B}\cdot\mathbf{v}) \end{pmatrix}$
RHS	$\mathbf{W} = \begin{pmatrix} 0 \\ -\frac{\dot{a}}{a}\rho\mathbf{v} - \frac{1}{a}\rho\boldsymbol{\nabla}\phi \\ -\frac{\dot{a}}{a}\left(2u - E - \frac{B^2}{2a}\right) - \frac{\rho}{a}\mathbf{v}\dot{\boldsymbol{\nabla}}\phi - \Lambda + \Gamma + \frac{1}{a^2}\boldsymbol{\nabla}\cdot\mathbf{F}_{\text{cond}} \end{pmatrix}$
Evolution with time	$\frac{\partial\mathbf{U}}{\partial t} + \frac{1}{a}\boldsymbol{\nabla}\cdot\mathbf{F} = \mathbf{W}$
Equation of state	$P = (\gamma - 1)u$
Energy	$E = u + \frac{1}{2}\rho\mathbf{v}^2 + \frac{B^2}{2a}$
Maxwell's Equations	$\frac{\partial\mathbf{B}}{\partial t} - \frac{1}{a}\boldsymbol{\nabla}\times(\mathbf{v}\times\mathbf{B}) = 0$
Gravitational potential	$\boldsymbol{\nabla}^2\phi = \frac{4\pi G}{a}\rho_{\text{total}} - \rho_0$

where the variables are the same as in Illustris, but with magnetic vector field $\mathbf{B}$, radiative cooling Λ, radiative heating Γ, and thermal heat conduction $\mathbf{F}_{\text{cond}}$. However, the situation I am simulating lacks a magnetic field anyway, so the extra magnetic capabilities won't matter. These equations are simulated on a structured grid with adaptive mesh refinement [2]. Enzo takes adaptive timesteps. The order of accuracy depends on the spatial solver used in Enzo.

For a spatial solver, Enzo can use:

1. the hydrodynamic-only piecewise parabolic method (PPM) [3, 1],
2. the MUSCL-like Godunov scheme [8, 9],
3. a constrained transport (CT) staggered MHD scheme [4],
4. the second-order finite difference hydro-dynamics method described in ZEUS [16, 17]

Enzo uses cloud-in-cell (CIC) at half-time steps and the Fourier method to compute the gravitational field.

Enzo can also simulate Lagrangian "trace particles" using kick-drift-kick update.

Applicability

I am mostly not deciding which class of solvers to use, because I am wanting to reuse the neural network in [12] trained on Illustris data. Thus I am bound by the choices that Schaurecker et al. made in [12] and Nelson et al. in [10, 19]. One in particular, Schaurecker chose to simulate dark-matter only. This is a coarser understanding of the universe, but it will be easier to process in a neural network.

Software

Last time, I had difficulty installing the code on the campus cluster. I was getting errors indicating the linker could not find libiverbs, despite it being referenced by the MPICH code I was trying to compile. This doesn't make sense because I activated the `module` for MPICH, which should have brought all of the relevant libraries into the linker's path, but I guess not.

I decided to use the Spack package manager[5] instead of installing Enzo from source. There is already a package for Enzo[1], so Spack knows what libraries Enzo depends on and how to build them on supported platforms. There is no need to look up each dependency individually, download it, learn how to compile it, compile it, add it to the system path, and change the configuration file of other programs to find it. One can reproduce this work by:

```
$ # See https://spack.readthedocs.io/en/latest/getting_started.html#shell-support
$ # Download Spack
$ git clone -c feature.manyFiles=true https://github.com/spack/spack.git

$ # Activate Spack's environment to add it to the path.
$ # See the documentation for other shells.
$ . spack/share/spack/setup-env.sh
$ echo '. spack/share/spack/setup-env.sh' >> .bashrc

$ # Now we actually install Enzo.
$ spack install enzo
$ # This build takes 20 minutes, because Spack has to bootstrap itself
$ # and then build Enzo's dependencies from source.
$ spack load enzo
$ enzo_dir=$(dirname $(dirname $(which enzo)))

$ # Now I will run Enzo on a test problem.
$ # I will use the Sedov Blast problem, because I know what to expect.
$ rm -rf $HOME/data
$ mkdir $HOME/data
$ enzo -d $enzo_dir/run/Hydro/Hydro-2D/SedovBlast/SedovBlast.enzo
```

[1] The package can be found at https://spack.readthedocs.io/en/latest/package_list.html#enzo.

```
$ # Now that I know this invocation works on a single node, I will try it in SLURM.
$ rm -rf $HOME/data
$ mkdir $HOME/data
$ sbatch \
  --time=0-00:08:00           --chdir=$HOME/data          \
  --ntasks=1                  --cpus-per-task=1           \
  --job-name=test             --partition=eng-instruction \
  --output=$HOME/data/stdout  --error=$HOME/data/stderr   \
  --wrap="mpirun enzo -d $enzo_dir/run/Hydro/Hydro-2D/SedovBlast/SedovBlast.enzo"
$ # Wait for the job to finish
$ watch --differences --interval 2 -- squeue --user $USER
$ # Check the status
$ tail stderr
...
Successful run, exiting.

$ # Visualize the data
$ pip install yt h5py
$ yt plot DD0001/sb_0001
$ yt plot DD0007/sb_0007
$ # View the data in data/frames/sb_000{1,7}_Slice_z_density.png
```

You should see figures similar to those in Figure 1.

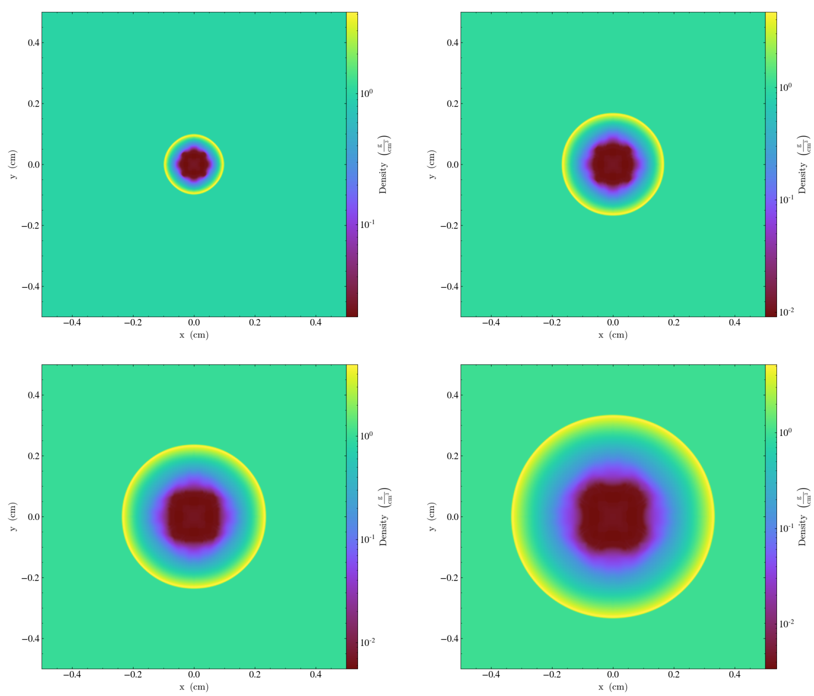

Figure 1: A Sedov blast at 0.01, 0.03, 0.06, and 0.12 seconds after detonation.

References

[1] Greg L. Bryan et al. "A piecewise parabolic method for cosmological hydrodynamics". In: *Computer Physics Communications* 89 (Aug. 1, 1995). ADS Bibcode: 1995CoPhC..89..149B, pp. 149–168. ISSN: 0010-4655. DOI: 10.1016/0010-4655(94)00191-4. URL: https://ui.adsabs.harvard.edu/abs/1995CoPhC..89..149B (visited on 04/11/2022).

[2] Greg L. Bryan et al. "Enzo: An Adaptive Mesh Refinement Code for Astrophysics". In: *The Astrophysical Journal Supplement Series* 211.2 (Mar. 2014). Publisher: American Astronomical Society, p. 19. ISSN: 0067-0049. DOI: 10.1088/0067-0049/211/2/19. URL: https://doi.org/10.1088/0067-0049/211/2/19 (visited on 04/11/2022).

[3] P. Colella and Paul R. Woodward. "The Piecewise Parabolic Method (PPM) for Gas-Dynamical Simulations". In: *Journal of Computational Physics* 54 (Sept. 1, 1984). ADS Bibcode: 1984JCoPh..54..174C, pp. 174–201. ISSN: 0021-9991. DOI: 10.1016/0021-9991(84)90143-8. URL: https://ui.adsabs.harvard.edu/abs/1984JCoPh..54..174C (visited on 04/11/2022).

[4] David C. Collins et al. "Cosmological Adaptive Mesh Refinement Magnetohydrodynamics with Enzo". In: *The Astrophysical Journal Supplement Series* 186 (Feb. 1, 2010). ADS Bibcode: 2010ApJS..186..308C, pp. 308–333. ISSN: 0067-0049. DOI: 10.1088/0067-0049/186/2/308. URL: https://ui.adsabs.harvard.edu/abs/2010ApJS..186..308C (visited on 04/11/2022).

[5] Todd Gamblin et al. "The Spack package manager: bringing order to HPC software chaos". In: *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*. SC '15. interest: 50. New York, NY, USA: Association for Computing Machinery, Nov. 15, 2015, pp. 1–12. ISBN: 978-1-4503-3723-6. DOI: 10.1145/2807591.2807623. URL: https://doi.org/10.1145/2807591.2807623 (visited on 04/10/2022).

[6] Shy Genel et al. "Following the flow: tracer particles in astrophysical fluid simulations". In: *Monthly Notices of the Royal Astronomical Society* 435.2 (Oct. 21, 2013), pp. 1426–1442. ISSN: 0035-8711. DOI: 10.1093/mnras/stt1383. URL: https://doi.org/10.1093/mnras/stt1383 (visited on 04/11/2022).

[7] G. Hinshaw et al. "Nine-year Wilkinson Microwave Anisotropy Probe (WMAP) Observations: Cosmological Parameter Results". In: *The Astrophysical Journal Supplement Series* 208 (Oct. 1, 2013). ADS Bibcode: 2013ApJS..208...19H, p. 19. ISSN: 0067-0049. DOI: 10.1088/0067-0049/208/2/19. URL: https://ui.adsabs.harvard.edu/abs/2013ApJS..208...19H (visited on 04/11/2022).

[8] Bram van Leer. “On the Relation Between the Upwind-Differencing Schemes of Godunov, EngquistOsher and Roe”. In: *SIAM Journal on Scientific and Statistical Computing* 5.1 (Mar. 1984). Publisher: Society for Industrial and Applied Mathematics, pp. 1–20. ISSN: 0196-5204. DOI: 10.1137/0905001. URL: https://epubs.siam.org/doi/10.1137/0905001 (visited on 04/11/2022).

[9] Bram van Leer. “Upwind and High-Resolution Methods for Compressible Flow: From Donor Cell to Residual-Distribution Schemes”. In: *16th AIAA Computational Fluid Dynamics Conference*. Session: CFD-8: Thirty Years of CFD II. _eprint: https://arc.aiaa.org/doi/pdf/10.2514/6.2003-3559. American Institute of Aeronautics and Astronautics, June 25, 2012. DOI: 10.2514/6.2003-3559. URL: https://arc.aiaa.org/doi/abs/10.2514/6.2003-3559 (visited on 04/11/2022).

[10] D. Nelson et al. “The illustris simulation: Public data release”. In: *Astronomy and Computing* 13 (Nov. 1, 2015), pp. 12–37. ISSN: 2213-1337. DOI: 10.1016/j.ascom.2015.09.003. URL: https://www.sciencedirect.com/science/article/pii/S2213133715000864 (visited on 04/11/2022).

[11] Brian W. O’Shea et al. “Introducing Enzo, an AMR Cosmology Application”. In: *arXiv e-prints* (Mar. 2004), astro–ph/0403044. URL: https://ui.adsabs.harvard.edu/abs/2004astro.ph..3044O/abstract (visited on 04/11/2022).

[12] David Schaurecker et al. “Super-resolving Dark Matter Halos using Generative Deep Learning”. In: *arXiv:2111.06393 [astro-ph]* (Nov. 11, 2021). arXiv: 2111.06393. URL: http://arxiv.org/abs/2111.06393 (visited on 04/11/2022).

[13] S. Seager, D. D. Sasselov, and D. Scott. “A New Calculation of the Recombination Epoch”. In: *The Astrophysical Journal* 523 (Sept. 1, 1999). ADS Bibcode: 1999ApJ...523L...1S, pp. L1–L5. ISSN: 0004-637X. DOI: 10.1086/312250. URL: https://ui.adsabs.harvard.edu/abs/1999ApJ...523L...1S (visited on 04/11/2022).

[14] Uros Seljak and Matias Zaldarriaga. “A Line-of-Sight Integration Approach to Cosmic Microwave Background Anisotropies”. In: *The Astrophysical Journal* 469 (Oct. 1, 1996). ADS Bibcode: 1996ApJ...469..437S, p. 437. ISSN: 0004-637X. DOI: 10.1086/177793. URL: https://ui.adsabs.harvard.edu/abs/1996ApJ...469..437S (visited on 04/11/2022).

[15] Volker Springel. “E pur si muove: Galilean-invariant cosmological hydrodynamical simulations on a moving mesh”. In: *Monthly Notices of the Royal Astronomical Society* 401.2 (Jan. 11, 2010), pp. 791–851. ISSN: 0035-8711. DOI: 10.1111/j.1365-2966.2009.15715.x. URL: https://doi.org/10.1111/j.1365-2966.2009.15715.x (visited on 04/11/2022).

[16] James M. Stone and Michael L. Norman. "ZEUS-2D: A Radiation Magnetohydrodynamics Code for Astrophysical Flows in Two Space Dimensions. I. The Hydrodynamic Algorithms and Tests". In: *The Astrophysical Journal Supplement Series* 80 (June 1, 1992). ADS Bibcode: 1992ApJS...80..753S, p. 753. ISSN: 0067-0049. DOI: 10.1086/191680. URL: https://ui.adsabs.harvard.edu/abs/1992ApJS...80..753S (visited on 04/11/2022).

[17] James M. Stone and Michael L. Norman. "ZEUS-2D: A Radiation Magnetohydrodynamics Code for Astrophysical Flows in Two Space Dimensions. II. The Magnetohydrodynamic Algorithms and Tests". In: *The Astrophysical Journal Supplement Series* 80 (June 1, 1992). ADS Bibcode: 1992ApJS...80..791S, p. 791. ISSN: 0067-0049. DOI: 10.1086/191681. URL: https://ui.adsabs.harvard.edu/abs/1992ApJS...80..791S (visited on 04/11/2022).

[18] Gilbert Strang. "On the Construction and Comparison of Difference Schemes". In: *SIAM Journal on Numerical Analysis* 5.3 (Sept. 1968). Publisher: Society for Industrial and Applied Mathematics, pp. 506–517. ISSN: 0036-1429. DOI: 10.1137/0705041. URL: https://epubs.siam.org/doi/10.1137/0705041 (visited on 04/11/2022).

[19] Mark Vogelsberger et al. "Introducing the Illustris Project: simulating the coevolution of dark and visible matter in the Universe". In: *Monthly Notices of the Royal Astronomical Society* 444.2 (Oct. 21, 2014), pp. 1518–1547. ISSN: 0035-8711. DOI: 10.1093/mnras/stu1536. URL: https://doi.org/10.1093/mnras/stu1536 (visited on 04/11/2022).