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Nyx: A Massively Parallel AMR Code for Computational Cosmology

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Summary

Nyx is a highly parallel, adaptive mesh, finite-volume N-body compressible hydrodynamics solver for cosmological simulations. It has been used to simulate different cosmological scenarios with a recent focus on the intergalactic medium and Lyman alpha forest. Together, Nyx, the compressible astrophysical simulation code, Castro (Almgren et al., 2010), and the low Mach number code MAESTROeX (Fan et al., 2019), make up the AMReX-Astrophysics Suite of open-source, adaptive mesh, performance-portable astrophysical simulation codes. Other examples of cosmological simulation research codes include Enzo (Bryan et al., 2014), Enzo-P/Cello (Bordner & Norman, 2018; Norman et al., 2018), RAMSES (Teyssier, 2002), ART (Kravtsov et al., 1997), FLASH (Fryxell et al., 2000), Cholla (Villasenor et al., 2021), as well as Gadget (Springel et al., 2021), Gasoline (Wadsley et al., 2017), Arepo (Weinberger et al., 2020), Gizmo (Hopkins, 2014), and SWIFT (Schaller et al., 2016).

The core hydrodynamics solver in Nyx (Almgren et al., 2013) is based on the directionally unsplit corner transport upwind method of Colella (1990) with piecewise parabolic reconstruction (Colella & Woodward, 1984). In Nyx, we have several modes of coupling the stiff heating-cooling source terms to the hydro. The simplest method is the traditional operator splitting approach, using Strang splitting (Strang, 1968) to achieve second-order accuracy in time. However, this coupling can break down, and we have an alternative to Strang splitting based on spectral deferred corrections (SDC), a method that aims to prevent the hydro and stiff source terms from becoming decoupled. The simplified SDC method uses the CTU PPM hydro together with an iterative scheme to fully couple the source terms and hydro, still to second-order accuracy in time (Zingale et al., 2019).

Nyx has a set of additional physics necessary to model the intergalactic medium using heating-cooling source terms. The code follows the abundance of six species: neutral and ionized hydrogen, neutral, once and twice ionized helium, and free electrons. For these species, all relevant atomic processes - ionization, recombination, and free-free transitions are modeled in the code. Heating and cooling source terms are calculated using a sub-cycled approach in order to avoid running the whole code on a short, cooling timescale. Cosmological reionization is accounted for via a spatially uniform, but time-varying ultraviolet background (UVB) radiation field, inputted to the code as a list of photoionization and photoheating rates that vary with redshift. Nyx also has the capability to model flash reionization as well as inhomogeneous reionization (Oñorbe et al., 2019).

The evolution of baryonic gas is coupled with an N-body treatment of the dark matter in an expanding universe. The mesh-based hydrodynamical baryonic gas evolution is coupled through gravity to the particle-based representation of dark matter. The dark matter particles are moved with a move-kick-drift algorithm (Miniati & Colella, 2007). The Poisson equation

for self-gravity of the baryonic gas and dark matter is solved using the geometric multigrid method. Nyx simulations can optionally model neutrino particle effects and active galactic nuclei feedback.

Nyx is built on the AMReX (Zhang et al., 2019) adaptive mesh refinement (AMR) library and is written in C++. AMR levels are advanced at their own timestep (sub-cycling) and jumps by factors of 2 and 4 are supported between levels. We use MPI to distribute AMR grids across nodes and use logical tiling with OpenMP to divide a grid across threads for multi-core CPU machines (exposing coarse-grained parallelism) or CUDA/HIP/DPC++ to spread the work across GPU threads on GPU-based machines (fine-grained parallelism). All of the core physics can run on GPUs and have been shown to scale well. For performance portability, we use the same source code for both CPUs and GPUs; additionally, we implement our parallel loops in an abstraction layer provided by AMReX. An abstract parallel for loop accepts as arguments a range of indices and the body of the loop to execute for a given index, and the AMReX backend dispatches the work appropriately (e.g., one cell per GPU thread). This strategy is similar to the way the Kokkos (Edwards et al., 2014) and RAJA (Beckingsale et al., 2019) abstraction models provide performance portability in C++.

Statement of Need

While there are a number of cosmological simulation codes, Nyx offers a few unique features. The original motivation for developing Nyx was to build a simulation code based on a modern, well-supported AMR library (BoxLib which evolved to AMReX), using unsplit integration techniques. The large developer community contributing to AMReX helps in Nyx continually gaining optimizations for new architectures and various operating systems.

At present, Nyx is mostly used to model the cosmological evolution of the intergalactic medium (IGM) - a reservoir of low density gas that fills the space between galaxies. Different physical effects, ranging from the nature of dark matter to different reionization scenarios related to the radiation from star-forming galaxies, set the observable properties of IGM, making it a powerful probe of cosmology and astrophysics. But in order to extract scientific insights, confronting observations of the IGM (usually through the Lyman alpha forest) against simulated models is a necessity, and that is where Nyx steps in. Incoming observations, for example, Dark Energy Spectroscopic Instrument (DESI) or high-resolution spectrographs like the one mounted on the Keck telescope, are noticeably reducing the statistical errors of measurements; the community needs tools capable of producing model universes that are of the same or better accuracy as observations. Nyx's scalability allows modeling of representative cosmological volumes, while maintaining the resolution needed to resolve small fluctuations in the intergalactic gas. Nyx includes physics to allow simulations of different cosmological and reionization scenarios, enabling users to produce mock universes for a variety of physically relevant models.

Our main targets are high-performance computer architectures and massively parallel simulations needed for cosmological and astrophysical research. Given these targets, Nyx's computational optimizations focus on large simulations on HPC systems, although smaller simulations can be run on Linux distributions and macOS using AMReX's build system support.

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