RevMexAA (Serie de Conferencias), **9**, 66–71 (2000)

Astrophysical Plasmas: Codes, Models, and Observations (Mexico City, 25-29 October 1999)
Editors: Jane Arthur, Nancy Brickhouse, & José Franco

INTRODUCING ZEUS-MP: A 3D, PARALLEL, MULTIPHYSICS CODE FOR ASTROPHYSICAL FLUID DYNAMICS

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RESUMEN

Describimos ZEUS-MP: un código Multi-Física, Masivamente-Paralelo, Pasa-Mensajes para simulaciones tridimensionales de dinámica de fluidos astrofísicos. ZEUS-MP es la continuación de los códigos ZEUS-2D y ZEUS-3D, desarrollados y diseminados por el Laboratorio de Astrofísica Computacional (`lca.ncsa.uiuc.edu`) del NCSA. La versión V1.0, liberada el 1/1/2000, contiene los siguientes módulos: hidrodinámica ideal, MHD ideal y auto-gravedad. Las próximas versiones tendrán difusión radiativa de flujo limitado, conducción de calor, plasma de dos temperaturas y funciones de enfriamiento y calentamiento. Las ecuaciones covariantes están avanzadas en una malla Euleriana móvil en coordenadas Cartesianas, cilíndricas y polares esféricas. La paralelización es hecha por descomposición del dominio y está implementada en F77 y MPI. El código es portable en un amplio rango de plataformas, desde redes de estaciones de trabajo hasta procesadores de paralelismo masivo. Se presentan algunos resultados de la eficiencia en paralelo junto con una aplicación a formación estelar turbulenta.

ABSTRACT

We describe ZEUS-MP: a Multi-Physics, Massively-Parallel, Message-Passing code for astrophysical fluid dynamics simulations in 3 dimensions. ZEUS-MP is a follow-on to the sequential ZEUS-2D and ZEUS-3D codes developed and disseminated by the Laboratory for Computational Astrophysics (`lca.ncsa.uiuc.edu`) at NCSA. V1.0 released 1/1/2000 includes the following physics modules: ideal hydrodynamics, ideal MHD, and self-gravity. Future releases will include flux-limited radiation diffusion, thermal heat conduction, two-temperature plasma, and heating and cooling functions. The covariant equations are cast on a moving Eulerian grid with Cartesian, cylindrical, and spherical polar coordinates currently supported. Parallelization is done by domain decomposition and implemented in F77 and MPI. The code is portable across a wide range of platforms from networks of workstations to massively parallel processors. Some parallel performance results are presented as well as an application to turbulent star formation.

Key Words: **HYDRODYNAMICS — METHODS: NUMERICAL — MHD**

1. A BRIEF HISTORY OF ZEUS

ZEUS is a family of codes for astrophysical fluid dynamics simulations developed at the Laboratory for Computational Astrophysics (LCA) of the National Center for Supercomputing Applications (NCSA) at the University of Illinois, Urbana-Champaign. The purpose of this paper is to announce the availability of the latest implementation: ZEUS-MP. Version 1.0 released 1/1/2000 is available from the LCA's website `lca.ncsa.uiuc.edu`.

ZEUS has its roots in a 2D Eulerian hydro code developed by M. Norman for simulations of rotating protostellar collapse (Norman, Wilson, & Barton 1980) while he was a student at the Lawrence Livermore

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National Laboratory. The hydrodynamics algorithm, which has changed little in subsequent versions, is based on a simple staggered-grid finite-difference scheme (Norman 1980; Norman & Winkler 1986). Shock waves were captured within a few cells with a von Neumann-Richtmyer type artificial viscosity. A powerful and essential feature of the code, which has been retained in subsequent versions, was that the equations of self-gravitating hydrodynamics were solved on a moving Eulerian grid permitting accurate simulation over a range of scales in the collapsing protostar.

A significant improvement to the hydrodynamics algorithm came with the incorporation of the second order-accurate, monotonic advection scheme (van Leer 1977). This code version, innocuously called A2, was vectorized for the Cray-1 supercomputer at the Max-Planck-Institut für Astrophysik, and extensively applied to the simulation of extragalactic radio jets (Norman et al. 1982).

The first code called ZEUS was developed by David Clarke as a part of his Ph.D. thesis on MHD jets (Clarke 1988; Clarke, Norman, & Burns 1986) under Norman's supervision. One of the principal challenges in numerical MHD simulations is satisfying the zero-divergence constraint on B. In our axisymmetric simulations, this was ensured by evolving the toroidal component of the magnetic vector potential from which divergence-free poloidal field components can be derived, as well as evolving the toroidal magnetic field component directly. Third order-accurate monotonic advection was used for evolving A_ϕ in order to improve the quality of the derived current densities.

The next development was a major rewrite and significant extension of ZEUS by James Stone as a part of his Ph.D. thesis at the University of Illinois. The resulting code, named ZEUS-2D, solves the equations of self-gravitating radiation magnetohydrodynamics in 2D or 2-1/2D. Many new algorithms were developed and incorporated into ZEUS-2D including: (1) a covariant formulation, allowing simulations in various coordinate geometries; (2) a tensor artificial viscosity; (3) a new, more accurate MHD algorithm (MOC-CT) combining the Constrained Transport algorithm (Evans & Hawley 1988) with a Method Of Characteristics treatment for Alfvén waves; and (4) a variable tensor Eddington factor solution for the equations of radiation hydrodynamics. ZEUS-2D's algorithms and tests are described in detail in a series of three papers (Stone & Norman 1992a; Stone & Norman 1992b; Stone, Mihalas, & Norman 1992)(the ZEUS Trilogy).

The MOC-CT algorithm for numerical MHD was specifically designed to be extensible to 3D, and work on a 3D version of ZEUS began in 1989 when David Clarke came to Illinois as Norman's postdoc. Written for the Cray-2 supercomputer, ZEUS-3D physics options included hydrodynamics, MHD, self-gravity, and optically thin radiative cooling. Parallelization was done using Cray Autotasking compiler directives. Novel features of the code included the use of a custom source code pre-processor which handled a variety of source code transformations. Another useful feature of ZEUS-3D was an extensive set of inline graphics and diagnostic routines, as well as the ability to run in 1D and 2D mode.

With a grant from the National Science Foundation in 1992, the LCA was established with the purpose of disseminating ZEUS-2D, ZEUS-3D and the TITAN implicit adaptive-mesh radiation hydrodynamics code (Gehmeyer & Mihalas 1994) to the international community. Currently, there are over 500 registered users of LCA codes in over 30 countries. Some recent applications of ZEUS include planetary nebulae (García-Segura et al. 1999), molecular cloud turbulence (Mac Low 1999), and solar magnetic arcades (Low & Manchester 2000).

Work was begun on ZEUS-MP in the fall of 1996 by Robert Fiedler and subsequently by John Hayes and James Bordner with support from the Department of Energy to explore algorithms for parallel radiation hydrodynamics simulations in 3D.

2. WHY ZEUS-MP?

ZEUS-MP is a portable, parallel rewrite of ZEUS-3D. MP stands for: *Multi-Physics*, *Massively-Parallel*, and *Message-Passing*. 3D simulations are by their nature memory– and compute–intensive. The most powerful computers available today are parallel computers with hundreds to thousands of processors connected into a cluster. While some systems offer a shared memory view to the applications programmer, others, such as Beowulf clusters, do not. Thus, for portability sake we have assumed "shared nothing" and implemented ZEUS-MP as a SPMD (Single Program, Multiple Data) parallel code using the MPI message-passing library to affect interprocessor communication.

Figure 1 shows a block diagram of the major components of ZEUS-MP. ZEUS-MP is composed of an application layer (second row) and a libraries layer (third row), all resting on the MPI message passing library.

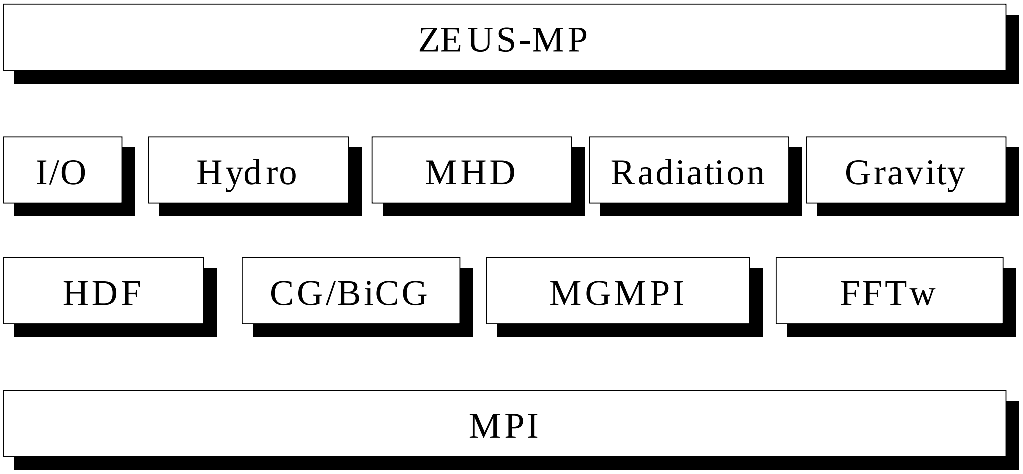

Fig. 1. Block diagram of the ZEUS-MP code.

A brief description follows.

There are four main physics modules: hydro, MHD, radiation transport, and self-gravity. The hydro and MHD modules are time-explicit, and thus require no linear algebra libraries for their solution. The hydro algorithm is a straight-forward 3D extension of the algorithm described in (Stone & Norman 1992a). The MHD algorithm is the MOC-CT algorithm described in (Stone & Norman 1992b) with the modifications described in (Hawley & Stone 1995) for enhanced stability in weakly magnetized, strongly sheared flows. At present, nonideal effects (viscosity, resistivity) are not included, however one can choose between an ideal gamma-law or isothermal equations of state. The radiation transport algorithm implements the time-implicit flux-limited diffusion algorithm of Stone (1994). The radiation and gas energy equations are solved as a coupled, implicit system, resulting in a large, sparse, banded system of linear equations which must be solved within an outer nonlinear Newton iteration. Two linear system solvers are built into ZEUS-MP: a conjugate gradient solver (CG/BiCG) with diagonal preconditioning, and a multigrid solver (MGMPI) (Bordner 2000). Problems involving self-gravity require the solution of the Poisson equation. Two Poisson solvers are built into ZEUS-MP: a Fourier space solver for triply periodic cubic grids, and an elliptic finite difference solver for all other geometries and boundary conditions. The former utilizes the FFTw library developed at MIT, while the latter uses MGMPI.

As in earlier versions of ZEUS, the equations solved by ZEUS-MP are formulated on a covariant, moving Eulerian grid. Problems in Cartesian, cylindrical, and spherical polar coordinates can be run with a variety of boundary conditions and types (periodic, Dirichlet, Neumann). The linear system solvers are designed to handle all cases.

File I/O is done using NCSA's HDF (Hierarchical Data File) standard (Folk et al. 2000), which is a widely adopted portable file format for scientific data.

3. PARALLELISM

ZEUS-MP utilizes *domain decomposition* (Foster 1995) for parallelization, wherein the computational domain is subdivided into a number of equally-sized regions, each of which is assigned to a different processor for execution. Depending upon the problem size and the number of processors targeted, the user can specify a 1D "slab", 2D "pencil", or 3D "block" decomposition. A region is represented in processor memory as arrays of data storing the solution vector for a specific subdomain. The arrays are dimensioned so as to include two layers of buffer zones on each face of the block for the purpose of transferring boundary conditions from neighboring processors. Data transfer between neighboring blocks, as well as collective operations and global reductions

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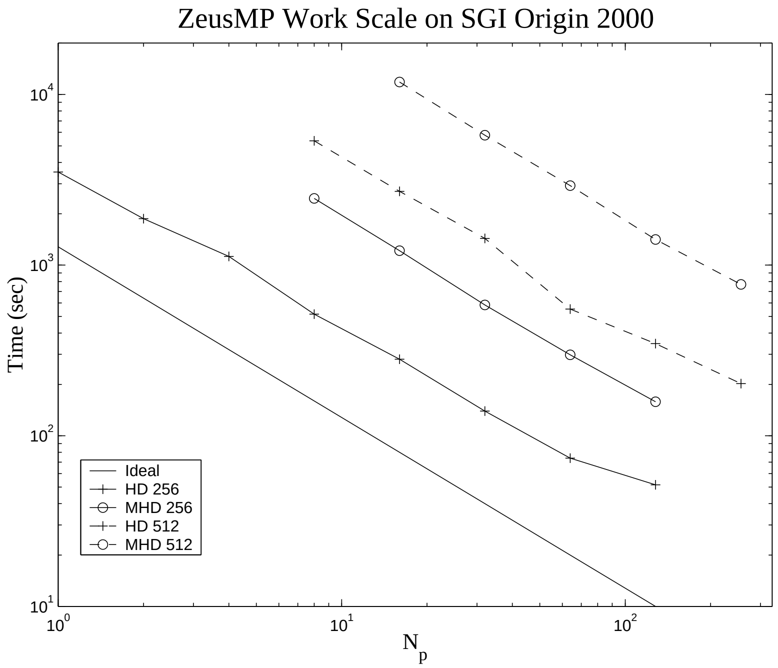

Fig. 2. Execution time for ZEUS-MP parallel benchmarks on the SGI/Cray Origin2000. Curves plot time for 30 timesteps for "fixed work" scaling tests for hydrodynamic and MHD blast tests at 256^3 and 512^3 resolution. The solid line without symbols shows ideal linear speedup. As can be seen, ZEUS-MP achieves near-ideal scaling.

are handled via MPI function calls.

ZEUS-MP performance has been optimized in two ways (Fiedler 1997): (1) single processor performance, using a variety of standard cache optimization techniques; and (2) parallel performance, using asynchronous communication, wherein computation and communication is overlapped. Single-node performance on an MIPS R10000 processor is in the range of 100 MFlop/s. Parallel speedup results depend sensitively on the properties of the network hardware and software on the host computer. A collection of benchmark results can be found on the ZEUS-MP website `zeus.ncsa.uiuc.edu/lca_intro_zeusmp.html`. Figure 2 shows near-ideal scaling on an SGI/Cray Origin2000 for hydrodynamic and MHD tests of size 256^3 and 512^3 on up to 256 processors.

4. SOURCE CODE AVAILABILITY

V1.0 is available now as a downloadable tar file from the ZEUS-MP website. Rudimentary documentation describing how to make the executable and run any of the five test problems is also available online. At present, the radiation module is not included; pending clarification of export restrictions, it will be made available in a later release.

Also available is a new 3D visualization tool called LCA Vision. This can be obtained from the website `zeus.ncsa.uiuc.edu/~miksa/LCAVision1.0.html`. Vision reads HDF files and provides a variety of visualization tools in an easy-to-use, menu-driven interface.

5. SAMPLE APPLICATION

To illustrate ZEUS-MP's capabilities, we present an application to magnetic star formation. The purpose is to understand the competition between turbulent, magnetic, and gravitational stresses in the formation of gravitationally bound cores in a turbulent molecular cloud (Heitsch, Mac Low, & Klessen 2000). In particular, we want to explore whether the critical mass-to-flux ratio (Mouschovias & Spitzer 1976) is a good predictor of gravitational collapse in a cloud driven by turbulence.

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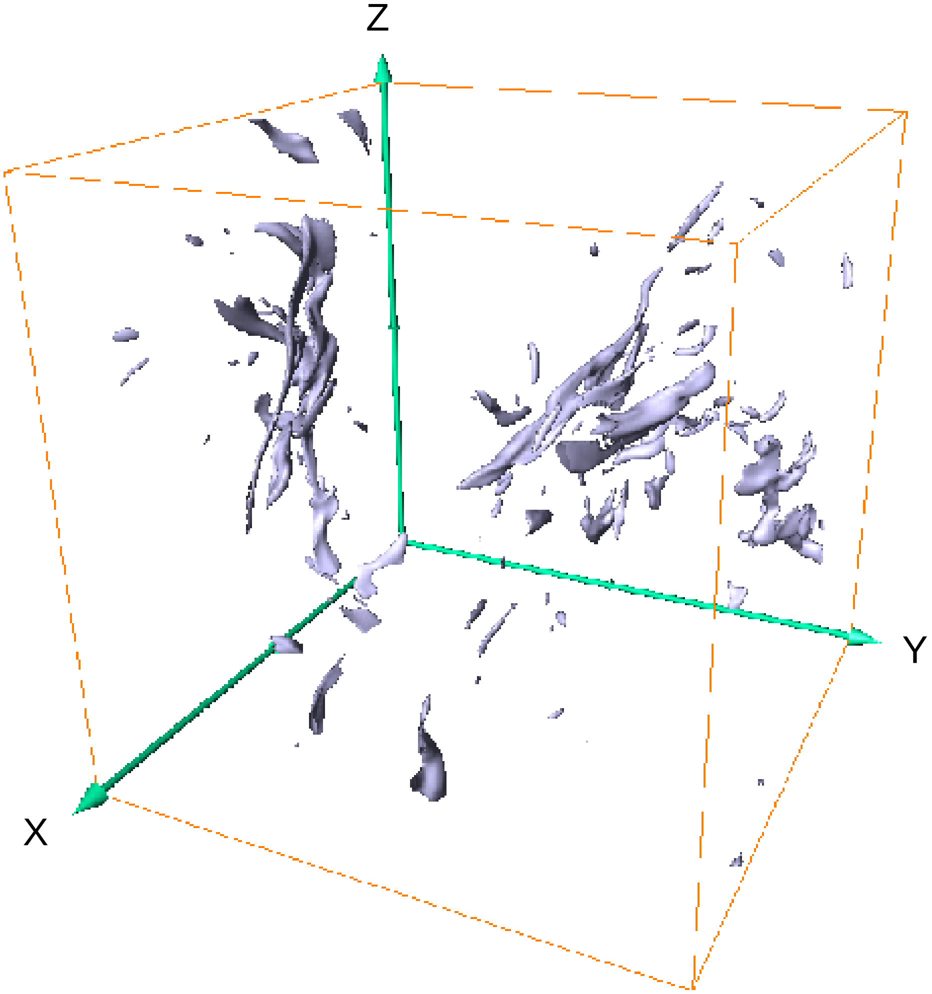

Fig. 3. ZEUS-MP simulation of a turbulent, magnetized, self-gravitating molecular cloud with $M/M_{cr} = 1.1$. An isosurface at 8 times the mean density is shown. The mean magnetic field is parallel to the Z-axis. Gravitational collapse of filamentary clouds is found, despite supersonic ($M = 5$) driving.

The calculation is done in a triply periodic cube with 256^3 cells distributed across 64 processors (4^3 cubic decomposition.) One begins with a uniform density gas filling the box threaded by a uniform magnetic field in the Z-direction. The gas is assumed to be isothermal. A turbulent velocity field is established by driving in Fourier space over a limited range of wavenumbers as described in (Mac Low 1999). A statistical steady state is reached within a few dynamical times, and once it has, gravity is switched on. Thereafter, density peaks formed by colliding gas streams may become gravitationally bound and collapse. The problem is described by a few dimensionless parameters formed by combinations of the gas density, sound speed, magnetic field strength, rms velocity perturbation, and box length,: $n_J = 12$, the number of thermal Jeans' masses in the box; $M/M_{cr} = 1.1$, the ratio of the box mass to the critical mass that can be supported by a static magnetic field; $M_{turb} = 5$, the turbulent Mach number; and k_{drv}=2, the driving wavenumber in units of the inverse box length.

Figure 3 shows isosurfaces of gas density at 1.82 freefall times after gravity was switched on. The isolevel is eight times the initial uniform density. One can see evidence for filamentary and flattened condensations which are both aligned and perpendicular to the mean field direction. Gravitational collapse is already underway, as indicated by high densities in the centers of several filaments. We find, as did Heitsch, Mac Low, & Klessen (2000) using ZEUS-3D, that supersonic turbulence is not able to prevent gravitational collapse from occurring in magnetically supercritical clouds. Simulations at 512^3 grid resolution and beyond are underway to investigate this further.

I gratefully acknowledge my colleagues, past and present, who have materially contributed to ZEUS-MP: Jim Stone and David Clarke for their foundational contributions embodied in ZEUS-2D and ZEUS-3D; Robert Fiedler, who wrote the first hydrodynamics version of ZEUS-MP code and optimized it for cache-based parallel systems; John “radiation cowboy” Hayes, who implemented the implicit radiation diffusion module along with the CG/BiCG linear solver; Mordecai-Mark Mac Low, who ported the HSMOC MHD algorithm from ZEUS-3D, which in turn was incorporated by Byung-Il Jun; Pakshing Li, who developed and tested both Poisson solvers and prepared the V1.0 release; and James Bordner, developer of the MGMPI multigrid solver and patient fixer of what we break. I thank my collaborators Fabian Heitsch, Mordecai Mac Low and Pakshing Li for allowing me to show our unpublished results (Fig. 3). This work has been supported by contracts B324163 and B506131 from the Lawrence Livermore National Laboratory. I would like to thank Frank Graziani of B Division for his continued interest and support.

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