Toward fidelity and scalability in non-vacuum mergers

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Abstract
We study the evolution of two fiducial configurations for binary neutron stars using two different general relativistic hydrodynamics (GRHD), distributed adaptive mesh codes. One code, HAD, has for many years been used to study mergers of compact object binaries, while a new code, MHDuet, has been recently developed with the experience gained with the older one as well as several novel features for scalability improvements. As such, we examine the performance of each, placing particular focus on future requirements for the extraction of gravitational wave signatures of non-vacuum binaries.

Keywords: numerical relativity, binary neutron stars, gravitational waves

(Some figures may appear in colour only in the online journal)

1. Introduction

The merger of a binary neutron star (BNS) system produces a wide range of potentially observable signals and hence provides an ideal event for studying high energy astrophysics through gravitational and electromagnetic waves as well as (for sufficiently close systems) neutrinos. Recently, the very first merger of such a system, GW170817, was observed both by LIGO and conventional telescopes. Much of our understanding of this system arises from comparing these observations with the results of numerical codes simulating such a system. A second binary neutron star event, labeled GW190425, was detected during O3, but only through gravitational waves due to its farther distance from the earth⁵. A large fraction of future BNS

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⁵Though the energy for both types of waves falls off as an inverse square, GW observatories are sensitive to amplitude which falls off more slowly as 1/r. This aspect, combined with the higher efficiency with which the central engine converts mass and binding energy to GW radiation, leads to larger observable distances.
observations will only be detectable gravitationally, which underscores the need for a thorough understanding of ‘golden’ type events—observed through multiple messengers so that this knowledge can be exploited in the rest of them.

Numerical simulations have been providing an ever more detailed description of non-vacuum binaries and observational opportunities, though the complexity of physics involved is such that, while qualitative features are under control (prior to merger), improvements at the quantitative level are still required. In particular, deviations from binary black hole gravitational waveforms only appear at fifth post-Newtonian order. Thus some effects related to the equation of state will require very high signal-to-noise-ratios (SNRs). Moreover, as the signal-to-noise ratio of detectors continues to improve (in current and future 3rd generation detectors), increased accuracy will be expected from theoretically constructed waveforms and their ability to reveal the behavior of dense matter in strongly gravitating and dynamical regimes.

A number of codes capable of evolving a BNS through merger with fully nonlinear general relativity exist (for reviews see references [1, 2]). Such codes generally are written for distribution among a large number of compute nodes and with the ability to refine particular spatial regions for certain times. These implementations are called distributed adaptive mesh refinement (AMR) codes, and one of such codes, Had, has been used extensively by the authors to model compact object mergers (involving black holes, neutron stars and boson stars) within general relativity and extensions to it. A number of efforts are currently underway to improve scalability and take advantage of massive parallel infrastructures. The overarching goal being to improve the study of relevant systems exploiting advances (and related challenges) in hardware. For instance, work is already underway with discontinuous Galerkin methods [3, 4] and early explorations of spectral methods for discontinuous solutions [5]. Other potential improvements have also been explored through possible GPU usage [6], wavelet adaptivity [7], etc. Clearly, there is fertile ground at several levels for considerable gains, though much effort lies ahead to converge to the ideal set of options.

Recently, we have developed a new code that builds on the experience gained with Had but which has a number of important new features and improvements, called MHDuet. Most importantly this code leverages the parallel infrastructure Samrai developed at Lawrence Livermore National Laboratory to enable large scale, high resolution simulations necessary for the GW astrophysics of non-vacuum mergers to firmly move into the quantitative regime. In this work, we compare the results for these two codes for two particular situations to assess relative accuracy of obtained solutions and discuss scalability of the new implementation.

The modeling of neutron stars requires the choice of an equation of state (EOS) that describes certain properties of the fluid constituting the star and serves to close the equations of motion. For this comparison, we consider two particular EOSs: the so-called SLy EOS, which is soft and relatively compressible, and the MS1b EOS, which is by contrast quite stiff. Notice that both of them are compatible with current constraints; the SLy and MS1b EOSs produce non-rotating NSs with maximum masses of 2.06 \( M_\odot \) and 2.76 \( M_\odot \), respectively, consistent with pulsar observations of a 2.01\( M_\odot \) NS [8]. These EOSs have been adopted by various groups, including for example reference [9] in the context of hybridization and reference [10] which discussed errors and convergence. We note that while the MS1b EOS is under some pressure due to EOS inferences from gravitational wave observations [11–13] it nevertheless serves as a useful testbed for our purposes.

2. Setup

We describe briefly here the evolution equations and the numerical schemes employed by the two codes of our comparison. The Einstein equations are written as evolution equations using
the $3 + 1$ decomposition of the CCZ4 formalism \cite{14, 15} with constraint damping parameters $\kappa_z = 0.1$ and $\kappa_c = 1.1$. We also use the standard $1 + \log$ and Gamma-freezing gauge conditions \cite{15} with $\eta = 4/M$, where $M$ is the initial mass of the binary. All these damping parameters are constant in the near zone up to $r = 60$ km (i.e., just beyond the region occupied by the stars) and then decay with $1/r$. The magneto-hydrodynamical (MHD) equations describing the fluid are written as a system of conservation laws \cite{16, 17}, namely

$$ \partial_t U + \partial_k F^k(U) = S(U) \quad (1) $$

where $U$ is the vector of evolved fields and $F^k(U)$ their corresponding fluxes. These fluxes are non-linear but they depend only on the fields themselves and not on their derivatives. Although the full MHD system is implemented in both codes, the studies presented here sets the initial magnetic field to zero.

2.1. Numerical schemes

In both codes the discretization of the continuum equations is performed using the method of lines, which separates the time and space discretizations, on a regular Cartesian grid. The spatial discretization for the evolution of the spacetime fields is performed using fourth-order accurate, spatial difference operators satisfying summation by parts \cite{18}, which are based on Taylor expansions and are therefore suitable for smooth solutions. The high-frequency modes, which can not be accurately resolved by our numerical grids, are damped by applying an artificial Kreiss–Oliger (KO) sixth-order dissipation operator with coefficient $\sigma = 0.1$ to our evolved fields \cite{19} so as not to spoil the convergence order of our fourth-order numerical scheme (rigorously expected in the unigrid case for smooth solutions). A summary of the specific operators can be found in reference \cite{20}.

However, these finite difference operators are not adequate for the spatial discretization of fluxes in genuinely non-linear systems such as GRMHD, which generically develop non-smooth solutions. For that reason, we employ high-resolution-shock-capturing (HRSC) methods \cite{21, 22} to deal with such phenomenology in the hydrodynamical variables. Traditionally, most efforts in general relativistic MHD have been dedicated to the development of HRSC schemes based on finite-volumes, commonly simplified and adapted to finite-difference codes. However, in the last decade there have been several HRSC implementations based directly on finite-difference schemes, which are cheaper than finite-volume ones and can achieve high order accuracy even in multi-dimensions in a straightforward way. In both cases (i.e., finite-volume and finite-difference approaches), the fluxes are discretized by using a conservative scheme, and the semi-discrete system in one dimension can be formally written as

$$ \partial_t U_i = -\frac{1}{\Delta x} \left( F^x_{i+1/2} - F^x_{i-1/2} \right) + S_i $$

where $F^x_{i\pm 1/2}$ are the set of fluxes along the $x$-direction evaluated at the interfaces between two neighboring cells, located at $x_{i\pm 1/2}$. The crucial issue when dealing with shocks is how to approximately solve the Riemann problem, by reconstructing the fluxes at the interfaces such that no spurious oscillations appear in the solutions. The differences between finite-volume and finite-difference approaches arise in the method of computation of these fluxes, and are summarized below in the description of the codes.

An important feature of relativistic fluids is that the evolved or conserved fields are different from the physical or primitive ones appearing in the fluxes and sources. This relation is highly non-linear and the recovery of primitive fields from the conserved ones involves a numerical root solver which is one of the most delicate parts of the code. For this comparison to be
Table 1. Characterization of the two different EOSs used in this work. Each EOS is defined as a piecewise polytrope with $n = 4$ segments and with $K_0\text{[CGS]} = 3.593 \times 10^{13}$ and $\Gamma_0 = 1.356\,92$. Each segment is delineated by a transition density $\rho_i$ expressed in cgs units.

| EOS  | $\Gamma_1$ | $\Gamma_2$ | $\Gamma_3$ | $\log_{10}\rho_0$ | $\log_{10}\rho_1$ | $\log_{10}\rho_2$ |
|------|------------|------------|------------|-------------------|-------------------|-------------------|
| SLy  | 3.005      | 2.988      | 2.851      | 14.165            | 14.7              | 15.0              |
| MS1b | 3.456      | 3.011      | 1.425      | 14.055            | 5.6938           | 14.7              | 15.0              |

meaningful, we have implemented the same algorithm for the recovery, similar to the one presented in [23]. Another delicate issue is how to deal with the regions outside the stars, usually filled with a low density atmosphere. Here too, the two codes are very similar in the way in which floor values and certain energy conditions are enforced on the conserved fields.

The time integration of the resulting semi-discrete equations is performed by using either a 3rd or 4th order Runge–Kutta scheme [24], which ensures the stability and convergence of the solution. We adopt a Courant parameter, defined as the ratio between the timestep and the grid size, such that $\Delta t_l = \lambda_c \Delta x_l$ on each refinement level $l$ to guarantee that the Courant–Friedrichs–Levy (CFL) condition is satisfied.

We next discuss details particular to each of the two codes compared here.

2.1.1. Had. The relativistic hydrodynamics equations are discretized in space by using HRSC method based on finite volumes. In particular, the fields at the interfaces are computed with a piecewise parabolic reconstruction [25], and then the fluxes at the interfaces are obtained from the Harten–Lax–van Leer–Einfeldt flux formula [21, 26]. The time integration is performed with a third order strong-stability-preserving Runge–Kutta [24, 27] with a CFL factor $\lambda_c = 0.25$, such that the total variation is preserved.

To ensure sufficient resolution, we employ AMR via the Had computational infrastructure that provides distributed, Berger–Oliger style AMR [28, 29] with full sub-cycling in time, together with the tapered treatment of artificial boundaries [30]. More details of the Had code can be found in recent studies with it of BNS mergers [23, 31, 32].

2.1.2. MHDuet. The code MHDUET has been automatically generated by using Simflowny [33, 34], an open-source platform to easily implement scientific dynamical models by means of a domain specific language, to run under the Samrai infrastructure [35, 36], which provides parallelization and adaptive mesh refinement. We incorporated a novel AMR boundary treatment that uses an internal dense output interpolator with the information from all the RK sub-steps on the coarse grid to compute accurately the interpolated solution on the fine one [37, 38]. This algorithm (i.e., Berger–Oliger without order reduction) is not only accurate, but also fast and efficient because uses minimal bandwidth when compared with the tapered approach of Had$^6$. Moreover, we have extended the algorithm to allow arbitrary resolution ratios between consecutive AMR grids. The combination of this algorithm with the efficient parallelization provided by Samrai, allows us to scale at least up to 10 K processes in binary black hole simulations even with high order discrete operators [20]. Since a GRMHD code involves higher computational load per grid-point, scaling in the non-vacuum case is further enhanced.

$^6$The tapered approach rigorously ensures no loss of accuracy/convergence—respecting that of the combination of time-integrator and spatial derivative operators—for smooth solutions, though with significant overhead and at a consequent cost in efficiency. The approach in MHDUET ensures 4th order accuracy for smooth solutions.
Table 2. Details of the various simulations presented here. For each simulation, the name of the code used, the name of the EOS characterizing the fluid, the name we use to refer to the simulation, the number of levels, the number of points in each direction for the coarse level, the finest grid spacing achieved, and finally the CFL ratio of the timestep to grid spacing are displayed.

| Code   | EOS    | Name   | # levels | N   | Δx  | Δt/Δx |
|--------|--------|--------|----------|-----|-----|-------|
| HAD    | SLy    | Low (L) | 5        | 81  | 0.37| 0.25  |
| HAD    | SLy    | Medium (M)| 5     | 121 | 0.25| 0.25  |
| HAD    | MS1b   | Low (L) | 5        | 81  | 0.37| 0.25  |
| HAD    | MS1b   | Medium (M)| 5     | 121 | 0.25| 0.25  |
| MHDUET | SLy    | Low (L) | 5        | 154 | 0.208| 0.25 |
| MHDUET | SLy    | Medium (M)| 5     | 154 | 0.208| 0.4  |
| MHDUET | SLy    | High (H) | 5      | 192 | 0.167| 0.4  |
| MHDUET | MS1b   | Low (L) | 5        | 154 | 0.208| 0.4  |
| MHDUET | MS1b   | Medium (M)| 5     | 192 | 0.167| 0.4  |
| MHDUET | MS1b   | High (H) | 5      | 240 | 0.134| 0.4  |

We have also implemented high-order finite-difference HRSC methods to solve the fluid fields, similar to those in [10, 39]. The flux formula used consist of a Lax–Friedrichs splitting [22], which combines the fluxes and the fields at each node $i$ as follows:

$$ F^+_{i} = \frac{1}{2} (F_i + \lambda U_i) $$

where $\lambda$ is the maximum propagation speed of the system in the neighboring points. Then, we reconstruct the fluxes of each interface using the values $\{F^\pm\}$ from the neighboring nodes.

MHDUET already incorporates some commonly used reconstructions, like the weighted-essentially-non-oscillatory (WENO) reconstructions [22, 40] and MP5 [41], as well as other implementations like the FDOC families [42]. For the numerical simulations of binary neutron stars presented below we use MP5, which is our preferred choice for its robustness and ability to preserve sharp profiles.

The time integration is performed with the classical fourth order Runge–Kutta, which has only been shown to preserve the total variation, under certain conditions\(^7\), for values of the Courant factor below $2/3$ in 1D [24]. In these simulations we use $\lambda_c = 0.4$, although we also perform a simulation with $\lambda_c = 0.25$ to illustrate consistency and accuracy of the solutions obtained within this code and also to compare with results obtained using HAD.

2.2. Initial data and EOS

We consider the coalescence of equal mass neutron star binaries in quasi-circular orbit configuration. The initial data is created with LORENE using two different realistic EOSs at zero temperature, fitted as piecewise polytropes [43]. The parameters of these EOSs, commonly known as SLy and MS1b, are summarized in table 1. During the evolution we employ a hybrid EOS, where the zero temperature effects are implemented with the piecewise polytrope, while thermal effects are modeled by an additional pressure contribution given by the ideal gas EOS with $\Gamma = 1.75$ [44]. The total mass $M = 2.677M_\odot$ is the same for the two binaries with

\(^7\)In the way the flux operators are written.
Figure 1. Had evolutions for both EOSs and different resolutions. The GW strain is shown in the top frame, the GW frequency is shown in the middle, and the GW phase is shown at bottom.

different EOSs, as is the initial separation $d = 52.42$ km and the initial angular frequency $\Omega = 1428$ rad s$^{-1}$.

2.3. Analysis

For each of the simulations, we calculate a number of quantities as described here. We compute a retarded time $u$ in terms of the tortoise coordinate $r_*$ as

$$u = t - r_*$$

$$r_* = R + 2M \log \left( \frac{R}{2M} - 1 \right)$$

$$R = r \left( 1 + \frac{M}{2r} \right)^2$$

where $R$ is Schwarzschild radius and $r$ the isotropic radius. In terms of our Cartesian coordinates, the isotropic radius is simply $r^2 = x^2 + y^2 + z^2$.

To analyze the gravitational radiation emitted during the coalescence, we have considered the Newman-Penrose scalar $\Psi_4$. As is customary, we expand $\Psi_4$ in terms of spin-weighted spherical harmonics (with spin weight $s = -2$)

$$r\Psi_4(t, r, \theta, \phi) = \sum_{l,m} \Psi_{lm}^4(t, r) Y_{lm}(\theta, \phi).$$

6
The components $\chi_{lm}(t)$ of the strain (per unit distance) can be computed by integrating $\Psi_4$ twice in time.

For equal-mass binaries, the the $\ell = 2 = m$ mode of the gravitational wave strain dominates over other harmonics by orders of magnitude. We therefore concentrate on this mode, $h_{22}$, and present it as

$$r h_{22} = A e^{-i \omega}$$

in terms of which the gravitational wave angular frequency is defined as

$$\omega_{22} = \frac{d \phi}{dt} = -3 \left( \frac{\dot{h}_{22}}{h_{22}} \right).$$

3. Results

Let us first overview the numerical setup and the results of the numerical simulations. Each binary was evolved within Had at two different resolutions, as shown in table 2. The number of levels and most AMR parameters are identical for both runs, but the higher resolution run adopted a resolution 50% higher than, and a threshold for refinement half that of, the medium resolution run. The total number of levels of refinement for all these runs was five with the finest resolution achieved of $\Delta x = 0.25$ (in code units) = 0.38 km.
As also shown in table 2, the MHDuet runs differed only in their overall resolution, with a 25% increase between consecutive resolutions. These simulations use five refinement levels, achieving a finest resolution $\Delta x = 160$ m.

Results from the Had runs are shown in figure 1. Apparent in the figure, the evolutions agree at early times, but the medium resolution merges a bit earlier than the low resolution for both EOSs.

The MHDuet runs were similar to the Had runs in that the SLy case appears to be closer to the convergent regime than the MS1b case which clearly requires higher resolutions, as shown in figure 2.

A direct comparison of the highest resolution simulation available for each binary and for each code can be found in figure 3. Clearly, the deviations increase as the binary proceeds on their orbits, being more significant for the MS1b EOS. Note though that the MHDuet runs generally have higher resolution than the Had runs.

Because we have four different resolutions for the SLy case with the MHDuet code, we can study in detail how these errors behave. In figure 4 we display in the top panel the waveform for the different resolutions. The middle panel displays the difference in phase between the different resolutions. Clearly, it converges to zero rapidly. The bottom panel shows that, for the lowest resolution triad, it converges roughly to fourth order, while it converges to a faster rate for the highest resolution one. This convergence was measured only with the phase of a radiative signal, but nevertheless such high order convergence is not typically observed in BNS simulations (for references see, e.g. [45, 46]). The high convergence order observed in the wave zone can be attributed to a couple factors that go along with the use of high order methods:
the use of adaptive re-gridding designed to satisfy an error threshold and the fact that the fluid discontinuities are not volume filling.

Assuming a constant convergence factor of 4, we can calculate the Richardson extrapolation of the GW phase. By subtracting this phase from each of phases obtained in our simulations, we get another measure of the phase errors. As we display in figure 5, these errors for such long waveforms is of the order of 1 radian over 12 cycles, although it remain below 0.1 radians for most of the coalescence and it only increases in the last 2–3 orbits.

We can also analyze the various radiative quantities that are extracted on a spherical surface. We extract on three spherical surfaces at the different radii $r = \{350, 450, 600\}$ km, and plot those results for the finest resolution SLy run in figure 6. That these quantities largely agree gives some indication that their extraction is correct. We can make a quantitative statement by extrapolating the waveforms to infinity and subtracting each of the signals obtained on each surface. This measure indicates that the error due to the finite size extraction radii are much smaller than the discretization errors.

To examine the errors associated with our use of a large CFL factor $\lambda_c = 0.4$ (as compared to other work using similar numerical schemes in this community [10, 47] using $\lambda_c \approx 0.25$), we adopt these two values with a low resolution run of the SLy EOS with the MHDUET code and compare the results in figure 7. The phase difference between the two simulations suggests
Figure 5. Phase errors relative to the Richardson extrapolated phase for the MHD\textit{UE}\text{T} SLy case. The differences between the extrapolated phase and the various resolutions are shown. That they decrease with resolution is another indication of convergence.

Figure 6. Results from the three different extraction surfaces for the finest SLy run. The top panel shows the strain and the bottom panel shows the differences between the phase obtained on each surface and the phase obtained by extrapolating to infinite radius with the outermost two surfaces.

A small error until merger, as compared to the phase errors between different resolutions displayed in figure 4. This comparison further suggests that accurate (and efficient) simulations can be performed with the MHD\textit{UE}\text{T} code using such a large CFL factor.
Figure 7. Phase error for the MHD\textsc{uet} SLy low resolution runs with two different CFL ratios. That the phase difference (shown in the bottom panel) is small, compared to figure 4, indicate that the use of a CFL factor of 0.40 is not causing a large error in the solution. The ability to run with a high CFL factor is itself an efficient aspect of the MHD\textsc{uet} code.

Figure 8. Weak scaling test of the MHD\textsc{uet} code on \textsc{stampede2} and \textsc{comet}. This run used fixed meshes with two levels. More recent tests have indicated (see figure 15 of \cite{20}) scaling efficiencies of 80\% extend to at least 10,000 processes.

4. Summary

We have presented binary neutron star simulations using two different EOS to compare two codes implemented in separate computational infrastructures. These codes solve the same
evolution equations for both the Einstein and the MHD equations, and share the numerical schemes for smooth solutions. However, they implement different high-resolution-shock-capturing methods: while Had uses an approach strongly inspired on finite-volume methods, where the fields are reconstructed at the interfaces and a flux-formula is used for calculating the fluxes at such interfaces, MHDuet relies on finite-difference methods, which involve a high order reconstruction of a combination of fluxes and fields (i.e., Lax–Friedrichs flux splitting). Another important difference is the treatment of the AMR boundaries, which is more efficient in MHDuet due to the use of a minimum bandwidth. Finally MHDuet is built using the public infrastructure Samrai, which has been developed for a number years and which can reach the exascale, at least for some choice of problems. For our main purposes, that of compact binary simulations, we have achieved good scaling up to 10000 processes with our high-order schemes (see figure 8 for weak scaling results with up to 1500 processes with the GRMHD code and figure 15 of [20], showing that a GR implementation scales strongly up to a factor of 16 and weakly above 80% at least up to $O(10^3)$ processors).

The results presented here show several features. First, we have shown that the solutions of both codes are consistent and agree up to certain level. A more detailed analysis of one of these cases with MHDuet indicates that the solution roughly converges to fourth order. Richardson extrapolation allows us to estimate the errors in the phase, which remain below 0.2 radians for most of the coalescence for the highest resolution case with $\Delta x = 160$ m and only increases to order unity in the last few orbits.

Another important technical result is that the speed and efficiency of the MHDuet code is better than Had, being able to achieve speeds of $\approx 20 M_{\odot}/$hour when running on 500–1000 processors for the highest resolution simulations of binary neutron stars presented here. This speed is roughly 4 times faster than the one reached by Had, which is moreover running at a resolution $\approx 15\%$ lower in our finest resolution comparison. For instance, on comparable architectures, MHDuet does roughly 70 ms per month running on 500–1000 processors with a minimum resolution of $\Delta x = 0.21$, while Had takes approximately 20 ms per month on 256 processors with even a slightly coarser minimum resolution of $\Delta x = 0.25$.

Of course, much still needs to be added to MHDuet. In particular, the ability to handle tabulated equation of state, an approximate neutrino treatment and resistive magnetohydrodynamics, which are already available in Had. These physics ingredients are gradually being incorporated into MHDuet, and further computational improvements to the code being explored include the use of OpenMP and GPUs. Certainly, results presented here are encouraging for this enterprise.

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