Impact of a Multi-TeraFlop Machine to Gravitational Physics

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(January 19, 2022)

Abstract

A multi-TeraFlop/TeraByte machine will enable the application of the Einstein theory of gravity to realistic astrophysical processes. Without the computational power, the complexity of the Einstein theory restricts most studies based on it to the quasi static/linear near-Newtonian regime of the theory.

The application of the Einstein theory to realistic astrophysical processes is bound to bring deep and far-reaching scientific discoveries, and produce results that will inspire the general public. It is an essential component in developing the new frontier of gravitational wave astronomy – an exciting new window to observe our universe.

The computational requirements of carrying out numerical simulations based on the Einstein theory is discussed with an explicit example, the coalescence of a neutron star binary.

This document is prepared for presentation at the National Computational Science Alliance User Advisory Council Meeting at NSF, June 1998, in support of the funding of a NSF TeraFlop computer.
I. INTRODUCTION - ASTRONOMY OF THE NEXT CENTURY AND GRAVITATIONAL PHYSICS

Two major directions of astronomy in the next century are high energy (x-ray, γ-ray) astronomy and gravitational wave astronomy. The former is driven by observations by x- and γ-ray satellites, e.g., CGRO, AXAF, XTE, HETE II, GLAST [1], current or planned for the next few years. High energy radiation is often emitted in regions of strong gravitational fields, near black holes (BHs) or neutron stars (NSs). One of the biggest mysteries of modern astronomy, γ-ray bursts, is likely to be generated by events involving NSs or BHs. For the full description of strong, dynamic gravitational fields, we need Einstein’s theory of general relativity.

The second major direction, gravitational wave astronomy, involves directly the dynamical nature of spacetime in the Einstein theory of gravity. The tremendous recent interest in this frontier is driven by the gravitational wave observatories presently being built or planned in US, Europe and outer space, e.g., LIGO, VIRGO, GEO600, LISA, LAGOS [2], and the Lunar Outpost Astrophysics Program [3]. The American LIGO and its European counterparts VIRGO and GEO600 are scheduled to be on line in a few years [3], making gravitational wave astronomy a reality. These observatories provide a completely new window on the universe: existing observations are mainly provided by the electromagnetic spectrum, emitted by individual electrons, atoms or molecules, easily absorbed, scattered and dispersed. Gravitational waves are produced by coherent bulk motion of matter and travel nearly unscathed through space, coming to us carrying the information of the strong field regions where they were originally generated. [4] This new window will provide very different information about our universe that is either difficult or impossible to obtain by traditional means.

The numerical determination of the gravitational waveform is crucial for gravitational wave astronomy. Physical information in the data is to be extracted through template matching techniques [5], which presupposes that reliable example waveforms are known. [3]
Gravitational waveforms are important both as probes of the fundamental nature of gravity, and for the unique physical and astronomical information they carry. The information would be difficult to obtain otherwise, ranging from nuclear physics (e.g., the EOS of NSs [5]) to cosmology (e.g., direct determination of the Hubble constant [6]). In most situations, the gravitational waveforms cannot be calculated without full scale general relativistic numerical simulations.

In short, both of these frontiers of astronomy call for numerical simulations based on the Einstein theory of gravity. If astrophysicists are to fully understand the non-linear and dynamical gravitational fields involved in these observational data, detailed modeling taking dynamic general relativity into full account must be carried out.

II. CHALLENGES OF COMPUTATIONAL GENERAL RELATIVISTIC ASTROPHYSICS

The application of the Einstein theory of gravity to realistic astrophysical systems needs computational power in the range of (at least) multi-TeraFlop/TeraByte, and corresponding capabilities in visualization, networking and storage.

- Computational challenges due to the complexity of the physics involved: The Einstein equations are probably the most complex partial differential equations in all of physics, forming a system of dozens of coupled, nonlinear equations, with thousands of terms, of mixed hyperbolic, elliptic, and even undefined types in a general coordinate system. The evolution has elliptic constraints that should be satisfied at all times. In simulations without symmetry, as would be the case for realistic processes, it involves hundreds of 3D arrays, and ten of thousands of operations per grid point per update. Moreover, for simulations of astrophysical processes, we need to integrate numerical relativity with traditional tools of computational astrophysics, including hydrodynamics, nuclear astrophysics, radiation transport and magneto-hydrodynamics, which govern the evolution of the source terms (i.e., the right hand side) of the Einstein equations. This complexity demands massively parallel
computation.

- The object under numerical construction being the spacetime itself presents unique challenges: According to the singularity theorems of general relativity, region of strong gravity often generate spacetime singularities. Due to the need to avoid spacetime singularities and to obtain long term stability in the numerical simulations, sophisticated control of the coordinate system is needed for the construction of a numerical spacetime. This dynamic interplay between the spacetime being constructed and the computational coordinate choice itself (“gauge choice”) is a unique feature of general relativity that makes the numerical simulations much more demanding. Beside extra computational power, advanced visualization tools, preferably real time interactive “window into the oven” visualization, are particularly useful in the numerical construction.

- The multi-scale problem: Astrophysics of strongly gravitating systems inherently involves many length and time scales. The microphysics of the shortest scale (the nuclear force), controls macroscopic dynamics on the stellar scale, such as the formation and collapse of neutron stars (NSs). On the other hand, the stellar scale is at least 10 times less than the wavelength of the gravitational waves emitted, and many orders of magnitude less than the astronomical scales of their accretion disk and jets; these larger scales provide the directly observed signals. Numerical studies of these systems, aiming at direct comparison with observations, fundamentally require the capability of handling a wide range of dynamical time and length scales. While such multi-scale problems can be handled with advanced 3D AMR techniques, it leads to further requirements on computation power and (3D AMR) visualization.

In short, in order to meet the challenges of Computational General Relativistic Astrophysics we need to push not only the frontier of the computation power for number crunching. The visualization requires basically as much computer power as what generates the data. The highly multi-disciplinary nature of the research demands collaborative code development. The large amount of data, visualization needs, and collaborative effort require high performance networking and meta-computing. In the following section we use a specific
sample problem to illustrate the requirements on Flop rate, memory, disk and storage sizes, which in turns determine the base line of visualization and networking requirements. Where we stand at present will also be discussed briefly.

III. NEUTRON STAR COALESCENCE AS AN EXAMPLE ON COMPUTATIONAL REQUIREMENTS

We use the problem of coalescing binary neutron stars to show the computational requirements in general relativistic astrophysics. The reason that the coalescence of neutron stars is a meaningful example is many-fold: It is a significant problem in astrophysics and astronomy; it involves many ingredients in general relativistic astrophysics; and it is a problem attracting much current research effort both nationally and internationally.

- Coalescing neutron star binary systems are common in the Universe, with the well known Hulse-Taylor binary pulsar PSR1913+16 being an example. The coalescence events are expected to be detectable by LIGO, with an observation rate of $29 \text{ yr}^{-1}$ for $h = 0.5$ and $43 \text{ yr}^{-1}$ for $h = 0.8$. [9]

- The physical information in LIGO data is to be extracted through the standard template matching technique [5]. For this we need to determine the waveforms of the gravitational radiation generated by the coalescence events, which can only be obtained through large scale simulations.

- A very enticing reason for studying the coalescence event lies in the fact that observations of such events by gravitational wave observatories may allow us to determine cosmological parameters like $H_0$ and $q_0$, without going through the cosmic distance ladder, and is independent of the optical identification of the source and the evolution of the source rate density with redshift. [7,9]

- Gravitational wave signals from coalescing binaries may reveal important information on the equation of state of dense nuclear matter, including the nuclear compression modulus, the hadronic effective masses, the relative hyperon-nucleon and nucleon-nucleon coupling...
constants, possible kaon condensation and a quark/hadron phase transition.

- Study of coalescing neutron star binaries may also answer other long standing questions in nuclear astrophysics. NSNS binary mergers may eject extremely neutron-rich matter which decompresses, beta-decays and neutron captures, forming the classical r-process. Detailed numerical simulations of the shock heating and mass ejection process are needed.

- Coalescing neutron star binaries are among the most popular candidates of gamma ray bursts. In order to evaluate the feasibility of the model, detailed studies taking the full general relativistic effects are needed to determine the maximum possible energy released, heating and mass ejection in the coalescence process.

A. Minimum Configuration

- Description of the Physical System:
  Two 1.4 solar mass neutron stars in head-on collision falling in from infinity. General relativistic simulation begins when the two stars are $4R$ apart, with $R =$ radius of star. Simulation covers $10ms$ in time for the dynamics of the merging and ringdown phases, and $20R$ in space for resolution and boundary considerations.

- Purposes: Study the general relativistic dynamics of the merging and ringdown phases of head-on collision.

- Grid Setup: Resolution=25 gridpoints/$R$, Total Grid Size = $500^3 = 10^8$

- Memory Requirement: 180 GBytes

- Floating Point Operations:
  Flops/gridpt/time step = $10^4$ (With only weak coordinate control)
  Total number of time steps = $10^4$
  Total flops = $10^{16}$
  Run time = 3 hours (With 1 TeraFlops sustained)

- Disk:
Run time disk size = 800 GBytes  (Output 10 functions with 1/100 sampling)

Storage = 8 TeraBytes    (with 10 runs for comparison studies)

• Present Status:

Code for carrying out this simulation is currently available. A code constructed for the NASA Neutron Star Grand Challenge Project which is capable of solving the full Einstein equations coupled to general relativistic hydrodynamics has recently been released. [15] This code has been tested on a 1024 node T3E-1200 (provided for the neutron star project for performance tests, though not available for production runs), achieving 142GFLOps and linear scaling up to 1024 nodes. A summary of the test results are given below. (The NSF Black Hole Grand Challenge Project is also constructing massively parallel code for solving the Einstein equations, see [14] for present status.)

**Code tested:** NASA Neutron Star Grand Challenge GR3D Einstein Spacetime (ADM) coupled to MAHC HYPERBOLIC_HYDRO (code tested with the released version, without special tuning for this 1024 node machine.)

**Date tested:** May 10, 1998

|                      | 32 bit  | 64 bit |
|----------------------|---------|--------|
| Grid Size per Processor | 84x84x84 | 66x66x66 |
| Processor topology    | 8 x 8 x 16 | 8 x 8 x 16 |
| Total Grid Size       | 644 x 644 x 1284 | 500 x 500 x 996 |
| Single Proc MFlop/sec | 144.35   | 118.33 |
| Aggregate GFlop/sec    | 142.2    | 115.8 |
| Scaling efficiency     | 96.2%    | 95.6% |

**B. Medium Configuration**

• Description of Physical System:
Two 1.4 solar mass neutron stars in inspiral coalescence. Full general relativistic simulation begins when stars enter the last 8 orbits. Simulation covers 60\(ms\) in time and 22\(R\) in space.

- Purposes:

  Study the general relativistic inspiral dynamics beginning with the 3PN breakpoint. This enables reliable initial data to be set. Study the effects of the angular momentum and gravitational radiation backreaction on shock heating in the merger phase.

- Grid Setup: Resolution=50 gridpoints/\(R\), Total Grid Size = 10\(^9\)

- Memory Requirement: 1.8\(T\)\(Bytes\)

- Floating Point Operations:

  Flops/gridpt/time step = 10\(^4\) \hspace{1em} (With only weak coordinate control)

  Total number of time steps = 10\(^5\)

  Total flops = 10\(^{18}\)

  Run time = 300 hours \hspace{1em} (With 1 TeraFlops sustained)

- Disk:

  Run time disk size = 20 TBytes \hspace{1em} (Output 10 functions with 1/400 sampling)

  Storage = 100 TeraBytes (with 5 runs for comparison studies)

- Visualization: Need parallel visualization engine.

- Present Status:

  Code basically ready for pilot studies. Tests of the effects of the implementation of weak coordinate control to be performed.

**C. Preferred Configuration**

- Description of Physical System:

  Two 1.4 solar mass neutron stars in inspiral coalescence. Full general relativistic simulation begins when stars enter the last 8 orbits. Simulation covers 60\(ms\) in time and 40\(R\) in space (one wavelength for gravitational wave with period 1ms).
• Purposes: Study the same system with strong coordinate control and more reliable wave-
from extraction.

• Grid Setup:
  Resolution=50 gridpoints/R, Total Grid Size = 10^{10}

• Memory Requirement: 18TBytes

• Floating Point Operations:
  Flops/gridpt/time step = 10^5    (With strong coordinate control)
  Total number of time steps = 10^5
  Total flops = 10^{20}
  Run time = 3,000 hours    (With 10 TeraFlops sustained)

• Disk:
  Run time disk size = 200 TBytes    (Output 10 functions with 1/400 sampling)
  Storage = 1000 TeraBytes
  (with 5 runs for comparison studies, template preparation not included)

• Need to push the frontiers on computation, storage, visualization, and networking.

• Present Status:
  Code basically ready for pilot studies. Efficient control the coordinate system to be
investigated.

IV. ACKNOWLEDGEMENTS

I thank S. Finn, K. Blackburn, M. Miller, L. Smarr, B. Sugar, M. Tobias, J. Towns, C.
Will, and J. York for useful input in preparing this document.

The general relativistic astrophysics code "GR3D" discussed in Sec. 4 is developed by
the NCSA-Potsdam-Wash U numerical relativity collaboration, with support from the NSF
Gravitational Physics Program Grant No. Phy-96-00507, NASA HPCC/ESS Grand Chal-
lenge Applications Grant No. NCCS5-153, NSF NRAC Allocation Grant no. MCA93S025,
and the Albert Einstein Institute.
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