Selected Problems in Numerical Relativity

by

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Abstract

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On September 14th, 2015 LIGO detected gravitational waves from a merging binary black hole. Just under two years later, LIGO detected gravitational waves from merging neutron stars in coincidence with detections of a gamma ray burst and kilonova. Many more detections of this kind are expected in the future. There are several problems that are facing the numerical relativity community now that binary neutron stars have been detected by LIGO. To date, there is no code that can simulate binary neutron stars with all of the microphysics known, the complexity and computing power required is just too high. Secondly, there are very few large sets of simulations of merging binary neutron stars with even some of the microphysics included. Having such sets would allow us to analyze the relationship between optical, neutrino and gravitational emissions and the parameters of the binaries. This thesis aims at making progress towards solutions of both these problems. In Chapter 1 of this thesis, we introduce the main concepts to understand the rest of the text. In Chapter 2, we describe a new code we developed to tackle difficult initial data problems in numerical relativity and we show tests of this solver on a problem mimicking Neutron stars with phase transitions and also on multi-black-hole initial data. The future aim of this code will be to solve for binary neutron star initial data with all of the microphysics we can throw at it. In Chapter 3, we describe a large set of binary neutron star simulations we ran using the SpEC code and a state of the art neutrino transport scheme. We study the matter and

neutrino emission of these merger simulations across different realistic equations of state and different mass ratios. Finally, in the last chapter we conclude our work and describe ongoing efforts to extend the work done in this thesis.

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Chapter 1

Introduction

The initial proposals for gravitational wave detectors using laser interferometry were formulated in the 1980s. The scientific justification was based on detecting the inspiral and merger of compact-object binaries. Since then, the LIGO (LIGO et al. (2018)), Virgo (Acernese et al. (2015)), and GEO600 (Affeldt et al. (2014)) detectors have been developed and operated as a network from 2005 to 2010. No detections were made during this initial stage of sensitivity. Alongside the early-2000 interferometer development, numerical simulations of the Einstein equations were beginning to gather ground. In 2000, the first binary neutron star merger was simulated (Shibata & Uryū (2000)), five years later the first binary black hole merger was simulated (Pretorius (2005)) and finally in 2006 the first binary neutron star - black hole simulations were performed (Shibata & Taniguchi (2011)). A variety of numerical relativity groups started forming at this time all around the globe, the Caltech-Cornell-CITA group (SXS; black-holes.org), the Kyoto group (Nagakura et al. (2014)), the RIT group (CCRG; ccrg.rit.edu), to name but a few. These groups started building banks of simulated waveforms to aid in the parameter estimation studies that were expected to follow from the first detections. On September 9th, 2015, in a very unexpected event during a testing run, LIGO detected the gravitational wave from two coalescing 30-$M_\odot$ black holes (Abbott et al. (2016)). Since this day, there have been multiple binary black

hole waveform detections (LIGO et al. (2018)). More recently however, LIGO made a landmark detection, GW170817 (Abbott et al. (2017)). GW170817 coincided with the detection of a gamma ray burst, GRB 170817A, implying that the source contained matter, which was later substantiated by a series of observations that followed across the electromagnetic spectrum (Villar et al. (2017)). The inferred masses of the bodies and the variety of electromagnetic observations are consistent with the source being a neutron star binary.

With these detections, and the awarding of the Nobel prize to three LIGO members, the gravitational era of astronomy has been born. Much more is expected in the future, with the upcoming earth-based detectors KAGRA (Somiya (2012)) and LIGO-India (**?**), there will be a worldwide detector network capable of precise source localization. Furthermore, they are already planning third generation earth-based detectors such as the Einstein Telescope (Punturo et al. (2010)) and space based detectors such as LISA (**?**). With more and more detectors, both space-based and earth-based, we will be able to gather data from the full frequency spectrum of gravitational waves coming towards us.

Even though numerical relativity has matured greatly since the major developments of the early 2000's, there is still a lot more that needs to be done. The biggest problems today in numerical relativity are the simulation of compact object binaries with matter and the simulation of supernovae, both requiring a great amount of microphysics, multi-scale grids, large sets of complex non-linear PDES, fast supercomputers and modern numerical techniques. With the coming of the exascale age of supercomputing there is an increasingly realistic chance of simulating these systems with all the known microphysics. This thesis aims to make progress in two distinct areas of numerical relativity. 1) Improve the computational techniques used solve the Einstein field equations so that more realistic microphysics may be introduced into the simulations as computing power reaches exascale and beyond. 2) Further probe the parameter

space of binary neutron star simulations with one the most state of the art numerical relativity codes to help understand the emission properties of these LIGO sources for the next generation of detections. Chapter 1 of this thesis will address the former problem, Chapter 2 will address the latter. Finally, the remaining portion of this introductory chapter will briefly describe the physics and computational techniques needed to understand the main text.

1.0.1   Solving the Einstein Field Equations on a Supercomputer

In their usual form, space and time are treated on an equal footing in the Einstein equations. From the perspective of performing a numerical evolution however, we need to reformulate the problem as initial value problem where we have a set of initial gravitational and matter data at some time t, and a set of evolution equations which we can use to get the updated data at some other time. To do this, we make the ansatz that space-time can be treated as a time sequence of spatial hypersurfaces. With this ansatz, the space-time metric $g_{\mu\nu}$ can be decomposed into

$$ds^2 = g_{\mu\nu}dx^\mu dx^\nu = -\alpha^2 dt^2 + \gamma_{ij}(dx^i + \beta^i dt)(dx^j + \beta^j dt), \qquad (1.1)$$

where the spatial metric γ_{ij} is a function of the spatial coordinates x^i and t and α is the lapse function that measures proper time between neighboring hypersurfaces along their timelike unit normals n^μ and β^i is the shift vector that determines how coordinate labels move between each hypersurface. This is known as the 3+1 decomposition of the metric (Arnowitt et al. (2008)).

Now we need to decompose the Einstein field equations into a set of evolution and constraint equations involving the quantities β^i, α and γ_{ij}. To do this, we introduce the projection operator $\perp^\alpha_\beta = \delta^\alpha_\beta + n^\alpha n_\beta$, which can be easily proven to project the space-time components orthogonal to n^μ out of any space-time vector.

The three possible projections of the EFEs: $n^\mu n^\nu G_{\mu\nu} = 8\pi n^\mu n^\nu T_{\mu\nu}$, $n^\mu \perp^\nu_\delta G_{\mu\nu} = 8\pi n^\mu \perp^\nu_\delta T_{\mu\nu}$, $\perp^\mu_\rho \perp^\nu_\delta G_{\mu\nu} = 8\pi \perp^\mu_\rho \perp^\nu_\delta T_{\mu\nu}$ lead to the three York/ADM 3+1 equations respectively:

$$0 = R + K^2 - K^{mn}K_{mn} - 16\pi\rho, \tag{1.2}$$

$$0 = D_i K - D_m K^m_i + 8\pi j_i, \tag{1.3}$$

$$\partial_t K_{ij} = \beta^m \partial_m K_{ij} + K_{mj}\partial_i\beta^m + K_{im}\partial_j\beta^m - D_i D_j \alpha \tag{1.4}$$

$$+ \alpha(R_{ij} + KK_{ij} - 2K_{im}K^m_j) + 4\pi\alpha[(S - \rho)\gamma_{ij} - 2S_{ij}], \tag{1.5}$$

where $K_{ij} = \beta^m \partial_m \gamma_{ij} + \gamma_{mj}\partial_i\beta^m + \gamma_{im}\partial_j\beta^m - \partial_t \gamma_{ij}$, is called the extrinsic curvature and it measures the rate at which the hypersurface deforms as it is carried forward along a normal (Baumgarte & Shapiro (2010)). We also relabelled the projections of the stress tensor by $\rho = T_{\mu\nu}n^\mu n^\nu$, $j_\alpha = - \perp^\nu_\alpha T_{\mu\nu}n^\nu$, $S_{\alpha\beta} = \perp^\mu_\alpha \perp^\nu_\beta T_{\mu\nu}$ and $S = \gamma^{\mu\nu}S_{\mu\nu}$, while R_{ij} and R denote the Ricci tensor and scalar associated with γ_{ij}.

The 3+1 equations are a set of 10 equations, or 3 tensor equations. The 1st equation is known as the Hamiltonian constraint equation. The second tensor equation is called the momentum constraint equation and is composed of three equations. In total, these four elliptic constraint equations play a similar role as the equations $\nabla \cdot \vec{E} = 4\pi\rho$ and $\nabla \cdot \vec{B} = 0$ which constrain the initial $\vec{E}$ and $\vec{B}$ fields in Maxwell's equations. The constraint equations must be solved prior to evolving the initial data and are usually called the **initial data equations**. The last set of six equations are the evolution equations. As they stand, the 3+1 equations still need to be manipulated a bit in order to discretize and solve them on a computer. For the set of evolution equations, the most used schemes are BSSN, Z4 and the Generalized Harmonic Decomposition (although the Generalized Harmonic decomposition doesn't start from the ADM equations, see Chapter 2 for more details) which each manipulate the evolution equations into a slightly different well-posed hyperbolic system. For the initial data equations, the most used schemes are conformal tranverse traceless (CTT), conformal-thin sandwich

(CTS) and the extended-conformal thin-sandwich (XCTS) frameworks (Pfeiffer & York Jr. (2005); Alcubierre (2012); Sopuerta (2015)).

Alongside the field-equations, the matter equations must be solved. These come from the local conservation equations $\nabla_\mu T^{\mu\nu} = 0$ (this changes for the case of radiation-hydrodynamics, see Chapter 2). For Neutron-star matter, a perfect-fluid tensor and an irrotational velocity distribution are usually assumed and are coupled with some choice of equation of state (EOS). For black-holes, we set $\rho = j_\alpha = S_{\alpha\beta} = 0$ because there is only vacuum space. On top of the matter-equations, the equations of neutrino transport must be solved, we will look at this in detail in Chapter 2.

To extract the gravitational waveform, the Weyl scalar ψ_4, which represents the outgoing transverse radiation, is extracted at a large radius away from the simulated binary system (the "wave-zone"). The energy, linear momentum, and angular momentum of the gravitational wave are computed by integrating the ψ_4 scalar in time (Kyutoku et al. (2015)).

For a more in-depth review, see (Sperhake (2014)), (Faber & Rasio (2012)) and (Shibata & Taniguchi (2011)) for BBH, NSNS and NSBH systems respectively. In the next section we discuss problems that are currently plaguing solvers for the initial data equations and then in the subsequent section we discuss new numerical methods that we plan to use to fix these problems.

1.1 Current problems with Einstein Initial Data solvers

In simulations there are two current approaches to modeling neutron stars with temperature-dependent realistic EOSs in binaries. The first is to use nuclear-theory-based EOSs in tabulated form and to interpolate as required during the simulation. Since this can be computationally expensive, the more common approach is to use n piece-wise polytropes with a polytropic thermal correction (Deaton et al. (2013)),

(Kyutoku (2013)), (Bauswein et al. (2014)), (Kyutoku et al. (2015)). The cold piece-wise polytropic part is defined as follows,

$$P_{cold} = K_i \rho^{\Gamma_i}, \quad \epsilon_{cold} = \epsilon_i + \frac{K_i \rho^{\Gamma_i - 1}}{\Gamma_i - 1}, \tag{1.6}$$

where P, ρ, ϵ and K are the pressure, rest-mass density, specific internal energy and the polytropic constant, respectively, with i denoting the $i - th$ polytropic piece. It was found that four polytropic pieces ($n = 4$) will approximate most EOSs of cold neutron matter to good accuracy (Read (2008)). To include thermal effects when using piecewise polytropes, one splits up the pressure $P = P_{cold} + P_{th}$ and internal energy $\epsilon = \epsilon_{cold} + \epsilon_{th}$ and assumes an ideal gas relationship $P_{th} = \rho \epsilon_{th}(\Gamma_{th} - 1)$ where the ideal gas index Γ_{th} is constant for all ρ and ϵ and usually set to 2 (Bauswein et al. (2010)),(Takami et al. (2014)).

The majority of NS binary simulations to date, which includes the initial data solves, use smooth analytic EOSs such as the unrealistic $\Gamma = 2$ polytrope and stars with low compactness ($C = M_{NS}/R_{NS} \approx .1$) (Faber & Rasio (2012)). The main issue with solving the Einstein equations and matter equations with realistic EOSs in tabulated or piecewise-analytic form are that they are not smooth due to the multiple phase transitions and the non-analytic behavior or very steep slopes at the surface of the NS. For example, if we consider the LS220 EOS at low temperature and electron fraction Lattimer & Swesty (1991), near the NS center the EOS can be approximated by a stiff $\Gamma \approx 7/2$ polytrope and then at slightly lower densities ($\approx 10^{14} g/cm^3$) the EOS begins to soften with $\Gamma \approx 1/2$ and then at even lower densities, the EOS asymptotically approaches the adiabatic index of a relativistic Fermi gas, $\Gamma \approx 4/3$. In certain coordinates, these changes can happen very close to the neutron star surface and are difficult to resolve (Deaton et al. (2013)). Furthermore, initial data solves for BNS and NSBH binaries have traditionally used multi-domain spectral finite element methods such as the SpEC elliptic solver Spells (Pfeiffer et al. (2003)) and LORENE

(Gourgoulhon et al. (2001)). Spectral methods have the nice feature of exponential convergence when the underlying problem is smooth. However, when the problem is non-smooth such as is the case when we consider tabulated EOSs or piecewise-analytic EOS fits (e.g. piecewise-polytropes), spectral methods show poor convergence due to Gibbs phenomenon. Unnatural schemes such as inserting subdomains by hand around the non-analytic parts are used to get converging solutions (Deaton et al. (2013)).

Finally, for currently unknown reasons, Spells (Pfeiffer et al. (2003)) doesn't converge for high compactness NS initial-data without multiple extra corrective iteration schemes and even then, it cannot converge to high accuracy data when the binary objects are very close in separation (Henriksson et al. (2014)). This lack of convergence could be due to mathematical non-uniqueness in solutions of the XCTS formulation of the constraint equations (Cordero-Carrión et al. (2009)), but (Henriksson et al. (2014)) hints at the possibility that the compactness can be pushed far beyond previous simulations by using refined iteration schemes. The goal of the SpECTRE elliptic solver will be to alleviate these issues by using more powerful, flexible techniques that scale well. In the next section we discuss a new powerful numerical technique.

1.2   New numerical methods for solving the Einstein Initial Data Equations

The most common methods used in Numerical Relativity to solve the evolution or initial data equations are finite difference, finite volume methods and spectral methods. We can understand all three methods by examining the following general elliptic PDE:

$$R(\bar{u}) = 0. \tag{1.7}$$

Here R is some partial differential operator, usually called the residual, that

operates on the solution u which could be composed of several fields we are solving for (e.g. the four fields in the initial data equations). Each of the different discretization methods used in numerical relativity demand in a different way, that the discrete version of Eqn. 1.7 be zero. In the finite difference method we demand that $R(u)$ is zero at each of the grid points and then we Taylor expand the differential operators and represent the solution as a single number at each grid point. In finite volume methods we demand that the integral of the residual over an element (usually called a "cell") of a mesh is zero in each of the elements and we represent the solution as a single number per cell (the average of the solution over that cell). In the spectral element method we break up the domain into a set of elements with simple topologies and expand the solution over a set of basis functions and we demand that the residual is L_2-orthogonal to these basis functions. That is, on each subdomain we demand

$$\int R(\bar{u})\psi_j \mathrm{d}x = 0 \quad \forall \psi_j, \tag{1.8}$$

which is just another way of setting the residual to be zero.

Recently a new method has been gathering ground. Discontinuous Galerkin (DG) methods (Hesthaven & Warburton (2008); Kidder et al. (2016)) combine the power of spectral methods in smooth regions with the shock-handling features of finite volume methods in discontinuous regions. To do this, DG methods represent the solution on each element as an expansion over a set of basis functions with the residual satisfying Eqn. 1.8. To couple the solution between elements, DG methods use flux terms between neighboring elements which penalize deviation of the solution at the interface. These flux terms allow DG methods to borrow the discontinuity handling techniques of the finite volume method. With these features, DG can obtain exponential convergence even when the solution is not smooth over the entire grid (see Chapter 2 for more details). On top of this, DG methods have the following nice features

1. hp-adaptivity: In DG methods there are two types of refinement, you can increase

the number of basis functions (p-refinement), or you can split an element of the mesh into smaller elements (h-refinement). In smooth regions, p-refinement is preferred and in non-smooth regions h-refinement is preferred. The combination of these two types of refinement (hp-refinement) can lead to rapid convergence of the solution.

2. Minimal communication: Since each element only needs the nearest-neighbour face data to compute the penalty flux terms, the amount of ghost data needed to be transferred between processors is minimal.

3. Easy Boundary handling: Boundary elements can be treated just like interior elements with the boundary conditions being applied through the penalty terms in the flux. This makes algorithms like Multigrid much easier to implement, since no special treatment is required for boundary elements.

4. Easy geometry handling: Unlike finite-difference methods which require special finite difference stencils for the boundaries of curved domains, DG methods can be applied as is to any type of domain, without any significant changes.

1.2.1 Binary Neutron Star Simulations

Neutron stars are amongst the most compact and extreme objects known in the universe and are believed to be born from the result of massive stars going supernova. Neutron stars have cores with densities exceeding far beyond that of the nucleus and since similar conditions are unreachable on earth, neutron stars provide an exceptional testing ground for nuclear physics. In particular, the merger of two neutron stars provides us with an unique opportunity to study the high density region of the equation of state (EOS). Furthermore, as confirmed by GW170817, NS mergers are progenitors for short Gamma ray bursts (sGRBs) and the heavy neutron-rich elements in the universe, whose synthesis in the fast moving neutron-star ejecta produces the

optical and near-infrared EM counterparts that accompany the gravitational wave signal.

It is expected that with the increasing sensitivity of gravitational wave interferometers multiple detections of merging BNSs will be made in the next years (LIGO et al. (2018)). Therefore it will be crucial to study the properties of these fascinating systems in order to extract information from the data. While an analytical approach in general relativity is possible for the stage in which the two bodies are distant and in the post-merger ringdown stage where the remnant loses its hair, numerical computation of the field equations is required for the last few orbits of the inspiral and the merger. Thus it is imperative to have fully generalitivistic simulations of BNS mergers and NSBH mergers in order to maximize the science potential of the next era of detections.

The fully general-relativistic simulation of BNS mergers has now been possible for more than 19 years (Shibata & Uryū (2000)). However, despite continuous developments, current codes have not yet reached the accuracy required to model the gravitational wave signal and the electronmagnetic counterparts at the level required to extract as much information as possible from future detections (See (Barkett et al. (2015))). Furthermore, most codes do not take into account all of the microphysics relevant to the evolution of the post-merger remnant, including a hot nuclear-theory based equation of state, a neutrino transport scheme accounting for both neutrino-matter and neutrino-neutrino interactions, and the evolution of the magnetic fields with enough resolution to resolve the growth of magneto-hydrodynamics instabilities (Foucart et al. (2015a)). That being said, slowly but surely, different levels of micro-physics are being added to the codes. The first papers that studied fully general relativistic BNS simulations including the effects of neutrinos were (Neilsen et al. (2014); Palenzuela et al. (2015)) with a simple leakage scheme and (Sekiguchi et al. (2015)) with a more complex M1 neutrino transport scheme. Both the leakage scheme and M1 transport scheme are approximate methods to deal with neutrinos which are preferred because

solving the 7-dimensional Boltzmann transport equation for the neutrino distribution during a BNS simulation is currently numerically intractable. For a review of leakage and the M1 transport scheme see (Foucart et al. (2015b)). These BNS simulations with neutrino cooling and neutrino transport have focused mainly on equal mass systems with $M_{ns} = 1.35M_\odot$. Collectively these papers find that the ejected mass is only substantial enough to explain the total mass of r-process heavy elements in our galaxy for r-process nucleo-synthesis in the case of a softer equation of state (e.g., more compact stars). The first paper on BNS mergers with neutrino interactions using the SpEC code looked at $1.2M_\odot$ equal mass systems and compared a simple leakage cooling neutrino scheme with the more complicated gray M1 neutrino transport scheme, finding that the more realistic transport scheme had a significant affect on the disk composition and the outflows, producing more neutron rich material that could possibly seed r-process element creation. (Radice et al. (2016)) examined the effects of eccentricity and neutrino cooling on the matter outflows and remnant disk of a LS220 equal mass binary, finding that both had significant effects, with the absence of a neutrino scheme leading to matter outflows a factor of 2 off. Finally, only very recently have there been studies examining the effects on matter outflows due to mass asymmetry in the initial binaries, with both (Lehner et al. (2016)) and (Sekiguchi et al. (2016)) finding that mass asymmetry can affect the neutron-richness and total ejecta for both soft and stiff equations of state.

Chapter 2

hp-Adaptive Discontinuous Galerkin Solver for Multi-Black Hole Puncture Initial Data

2.1 Chapter Overview

The material in this chapter is based on "hp-Adaptive Discontinuous Galerkin Solver for Multi-Black Hole Puncture Initial Data" by Trevor Vincent, Harald Pfeiffer, Nils Fischer submitted to Phys. Rev. D.

Chapter 3

Unequal Mass Binary Neutron Star Simulations with M1 Neutrino Transport: Ejecta and Neutrino Emission

3.1   Chapter Overview

The material in this chapter is based on "Unequal Mass Binary Neutron Star Simulations with M1 Neutrino Transport:
Ejecta and Neutrino Emission" by Trevor Vincent, Francois Foucart, Roland Haas, Matthew Duez, Lawrence Kidder, Harald Pfeiffer, Mark Scheel submitted to Phys. Rev. D.

Chapter 4

Conclusions & Future Work

4.1 Conclusions

It is an exciting time in gravitational-wave astrophysics and numerical relativity. With the first detection of gravitational waves from a a binary neutron star and the coincident detection of electromagnetic counterparts across the EM spectrum, a lot can be discovered about these extreme systems. With many more detections on the horizon, we will need to be prepared on the theoretical side. To help with the ongoing theoretical effort of properly modelling binary compact object systems and their emissions, this thesis has attempted to make progress along two different directions.

Firstly, we have sought to improve the numerical techniques used to solve the partial differential equations that arise in binary neutron star simulations. To this effect, Chapter 2 presented a completely new scheme based on discontinuous Galerkin methods, and we tested it to solve for constant density star initial data, which contains phase transitions similar to that in neutron stars and we also tested it on multi-black hole puncture initial data, which contains multiple non-smooth points. All tests showed promising results. Currently, work is being done to extend this code by Nils Fischer and Prof. Harald Pfeiffer at the Albert Einstein Institute (AEI) in Potsdam, Germany by porting it into the task based parallel code SpECTRE (Kidder et al. (2016)),

which is currently being developed at Cornell, Caltech and AEI to solve hyperbolic problems in numerical relativity on future exascale supercomputers using a task-based parallelism framework. The final goal will be to run our implementation on binary neutron star initial data with realistic microphysics and solve down to accuracies previously unobtainable.

Secondly, we wanted to increase the knowledge-base surrounding emissions from BNS mergers and their connection to binary parameters. Chapter 3 presented 12 state-of-art general relativistic radiation-hydrodynamics simulations of binary neutron star mergers with varying realistic EOS and mass-ratios. With these simulations we established that previous results using different codes were qualitatively correct, even though our neutrino schemes (amongst other things) were not identical. Talk is under way to use these simulations for new studies. Firstly, the subset of simulations which collapsed to a black hole were not evolved past this point and it would be interesting to see what emissions arose afterwards and to study the properties and evolution of the resulting accretion disks, which have been shown to produce a significant amount of ejecta when MHD is introduced (Fernandez et al. (2019)). Secondly, we initially ran each simulation with tracer particles that followed the fluid flow, but stopped this because it was slowing down the code too much to get a report out on time for this thesis. Tracer particles would allow us to better study the properties of the ejecta, by not only tracing out the fluid worldlines of the ejecta, but also by using the tracer data to seed light-curve simulations and nuclear reaction networks. All of this was done for neutron star - black-hole binaries in (Fernández et al. (2016)) by some of our collaborators. In terms of other source parameters, We also neglected in our study the eccentricity of the binary and the spins of the neutron stars, which can produce significantly more ejecta. In the future, the addition of magneto-hydrodynamics, eccentricity, spins and more realistic neutrino transport schemes will definitely be on the agenda.

In conclusion, while this thesis has helped push us closer to the goal of simulating and understanding binary neutron star mergers, a great deal of work still needs to be done. The next few decades should be a very interesting period for both numerical relativity and gravitational wave astrophysics, so stay tuned.

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