

Binary (Neutron Star) Initial Data: Theory

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Einstein Toolkit Summer School 2021

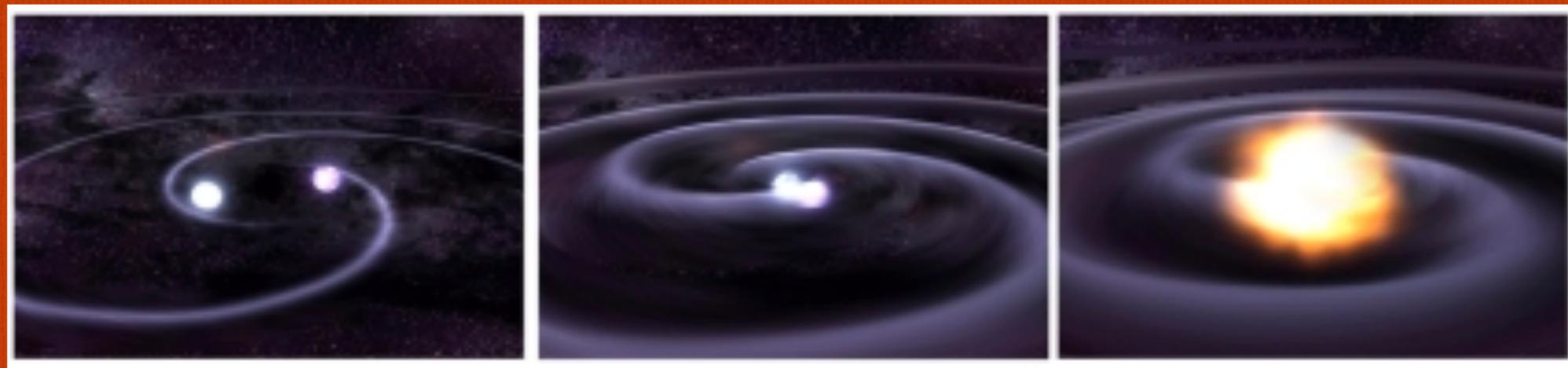


Overview

- Quasi-equilibrium formalisms**
- Binary Black Hole initial data**
- Binary Neutron Star initial data**
- Code implementations**

Why initial data?

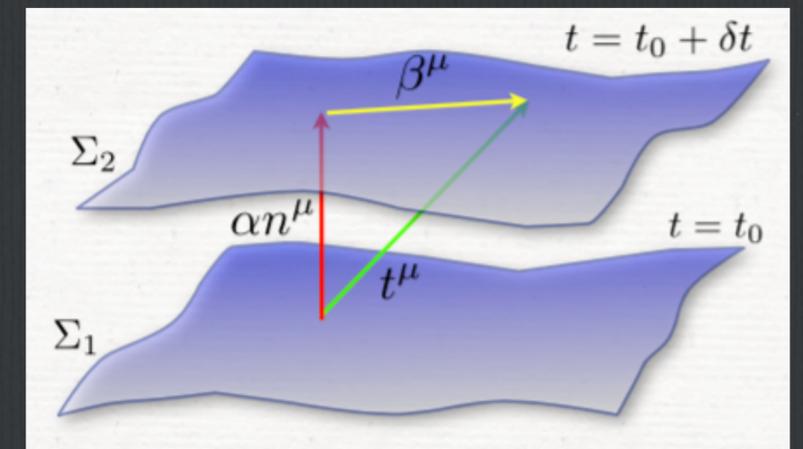
- GR is a second-order hyperbolic evolution scheme, so in order to evolve a spacetime in specified volume of spacetime, we need:
 - Initial data — this is the configuration and its first time derivatives at $T=0$
 - Boundary conditions — this is a topic unto itself
- Initial data problems are typically posed as ELLIPTIC equations — these require different techniques, domain discretizations, etc.
 - Often NOT parallelized, or even parallelizable
 - If the problem requires a supercomputer, you are probably doing it wrong



Source: NASA

Review: 3+1 formalism

- We foliate the spacetime into slices at different times
- Each slice has an **intrinsic 3-metric**
- The extrinsic curvature describes the evolution of one slice to the next
- The **lapse function** and **shift vector** describe the evolution of the coordinates that we choose.



Source: Gourgoulhon

$$ds^2 = -(\alpha^2 - \beta_i \beta^i) dt^2 - 2\beta_i dt dx^i + \gamma_{ij} dx^i dx^j$$

Constraints and beyond

- Initial data must satisfy the Hamiltonian and momentum constraints
 - These constraints should be preserved by the evolution scheme
 - In E+M, the divergence-free nature of the magnetic field plays the same role
- These constraints DO NOT specify our initial data: we also need:
 - Matter/gravitational sources — BH, NS, disks, etc.
 - EM fields
 - Some rule that establishes their quasi-equilibrium configurations and dynamics
- Ideally, we should be able to model any physical effect we want

$\nabla \cdot \mathbf{B} = 0$
$\nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t}$

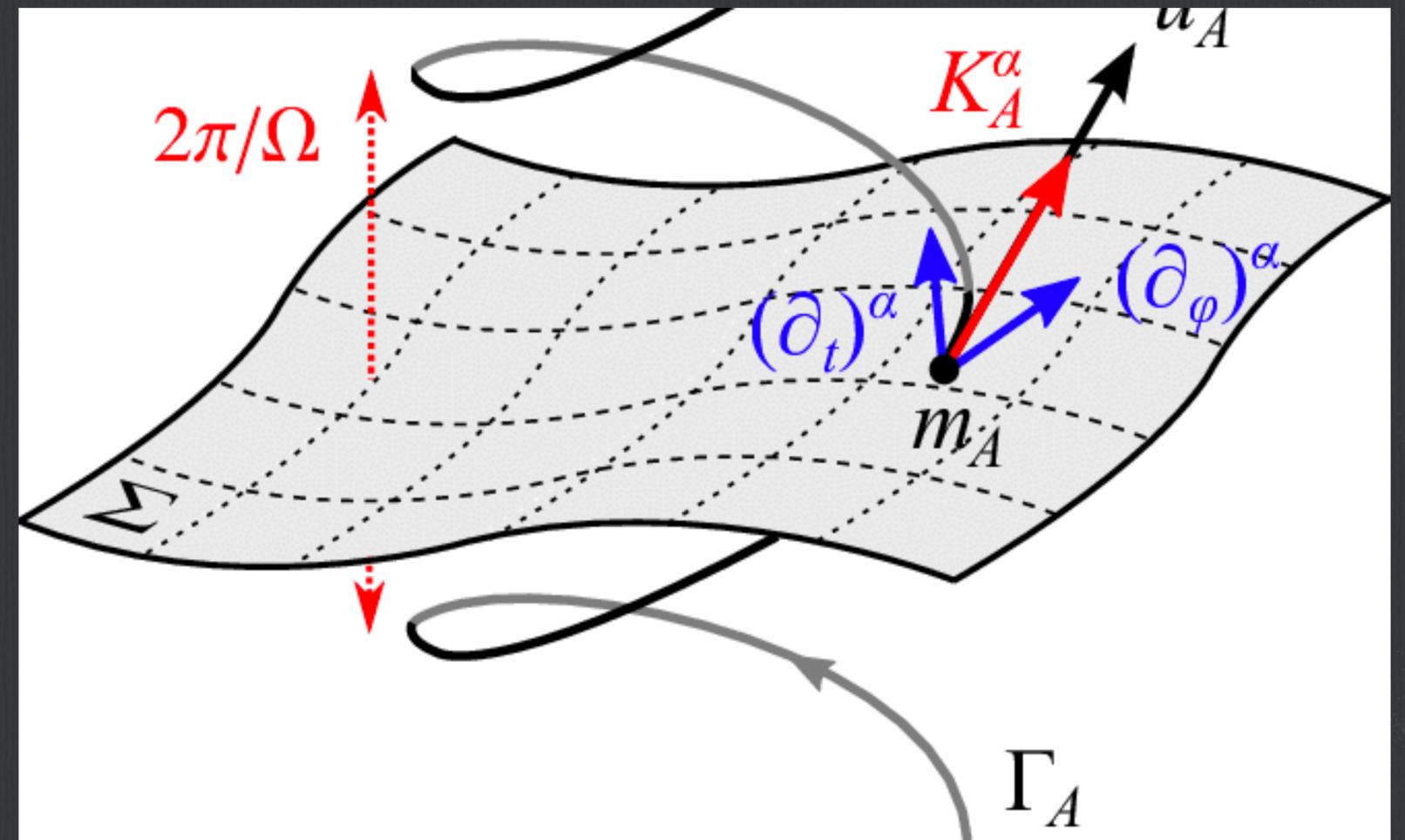
Source: Wikipedia



Source: AAS/John Rowe

Helical Killing vectors

- A Killing vector is defined such that the metric is invariant as we move along it (zero Lie derivative)
- For a helical Killing vector with time and azimuthal components, we find the metric advances in azimuth as time moves forward
- This gives a circular orbit (good!) but leaves out the GW content of the spacetime



Source: Le Tiec

Conformal metrics

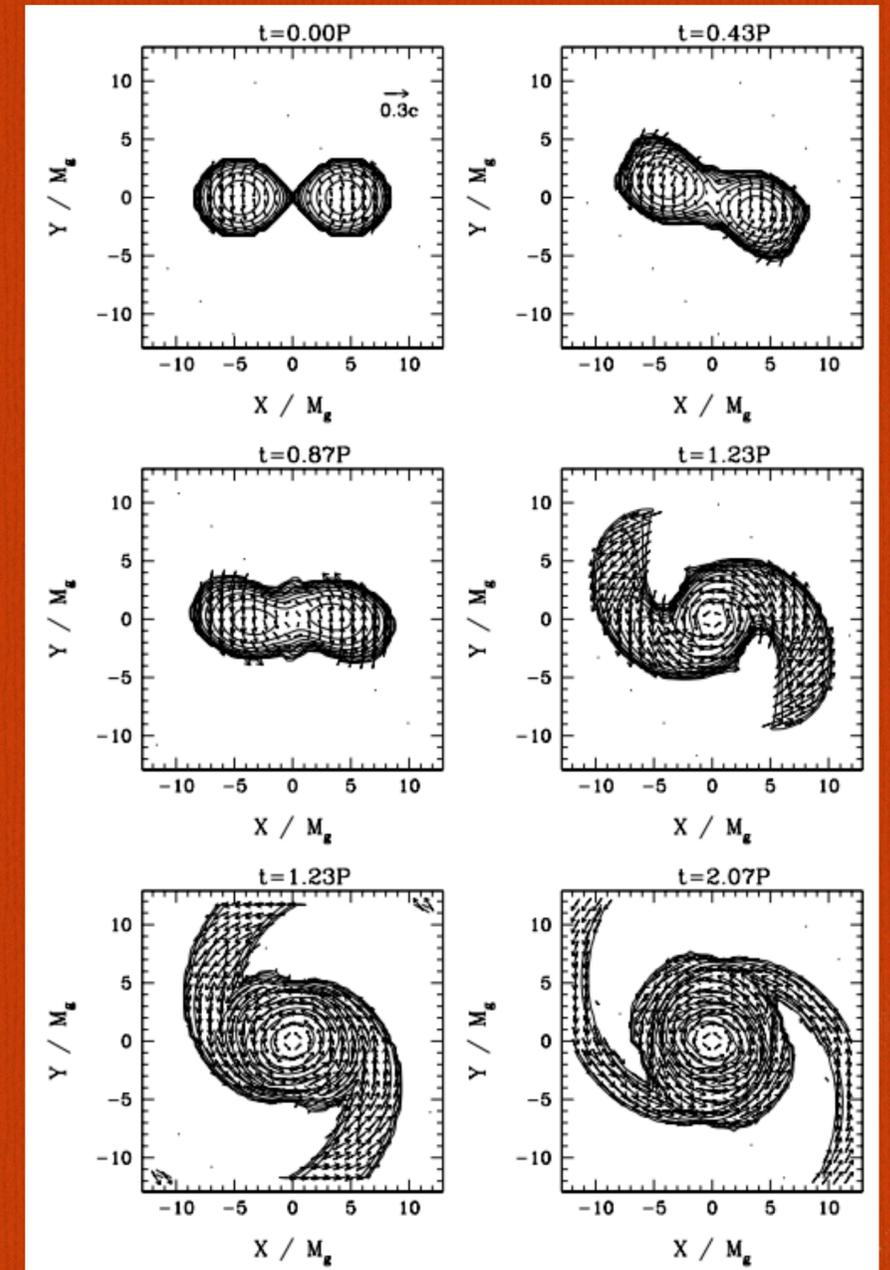
- In practice, nearly all initial data schemes use a CONFORMAL decomposition of the spacetime metric

$$\gamma_{ij} = \psi^4 \bar{\gamma}_{ij}; \quad \det \bar{\gamma}_{ij} = 1$$

- The Conformal Transverse Traceless (CTT) approach (York 1979) requires us to specify two components of the spatial metric, and their two time derivatives, and uses the constraint equations to determine all other quantities
 - Bowen-York initial data for BHs are constructed using the CTT method
- The Conformal Thin Sandwich (CTS) approach (York 1999) assumes some behavior for the metric on neighboring time slices, essentially specifying the time evolution of the metric - often, this is set to zero.
 - This is definitely the standard approach for Neutron Star initial data and quasi-equilibrium configurations.

First problem: Binary BHs

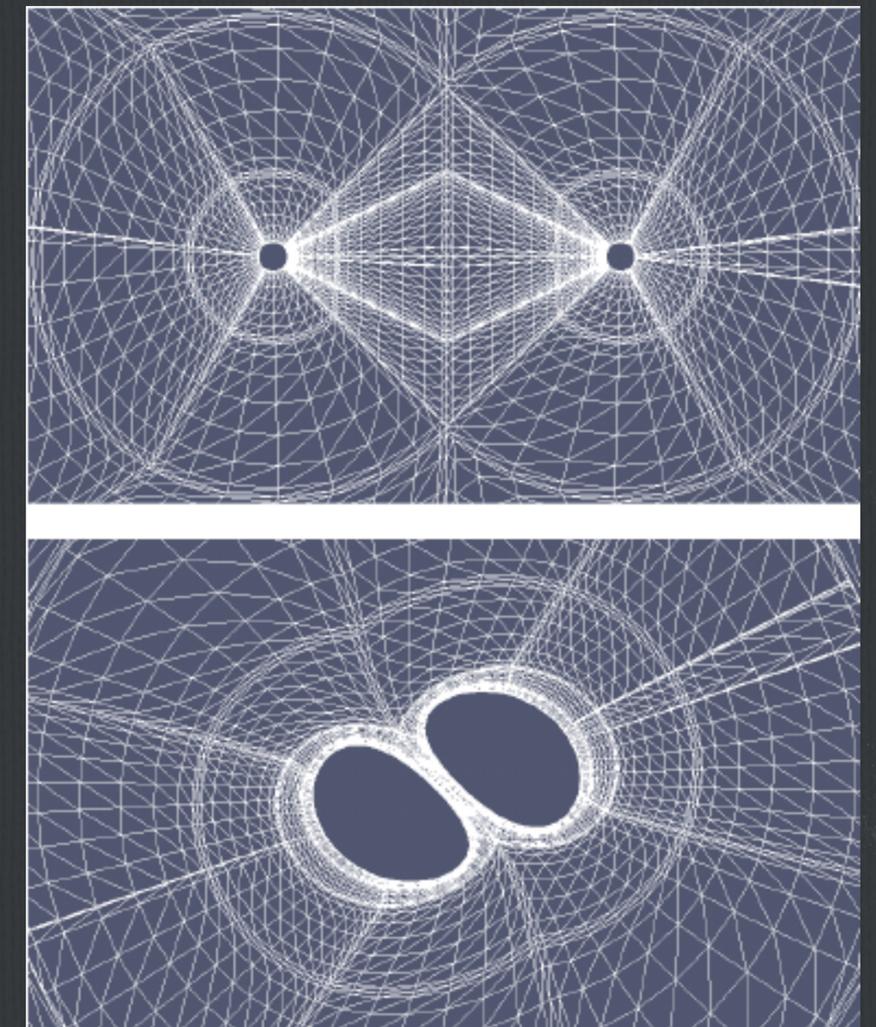
- Before getting to NS, it is helpful to consider BH first:
 - They are “vacuum sources” with no extended matter
 - They have fewer parameters we need to describe: mass, spin, momentum
 - We have many good models to describe them (individually) in detail
- The history is a bit complicated with full GR simulations — the first ones were actually BNS (Shibata and Uryu 2000), then BBH (Pretorius 2005; Campanelli et al. 2005; Baker et al. 2005), then an explosion of all binary types.
- Routines for BBH and BNS initial data — TwoPunctures and Lorene in particular — predate the Einstein Toolkit



Source: Shibata and Uryu (200)

Choices: Punctures vs. Excision

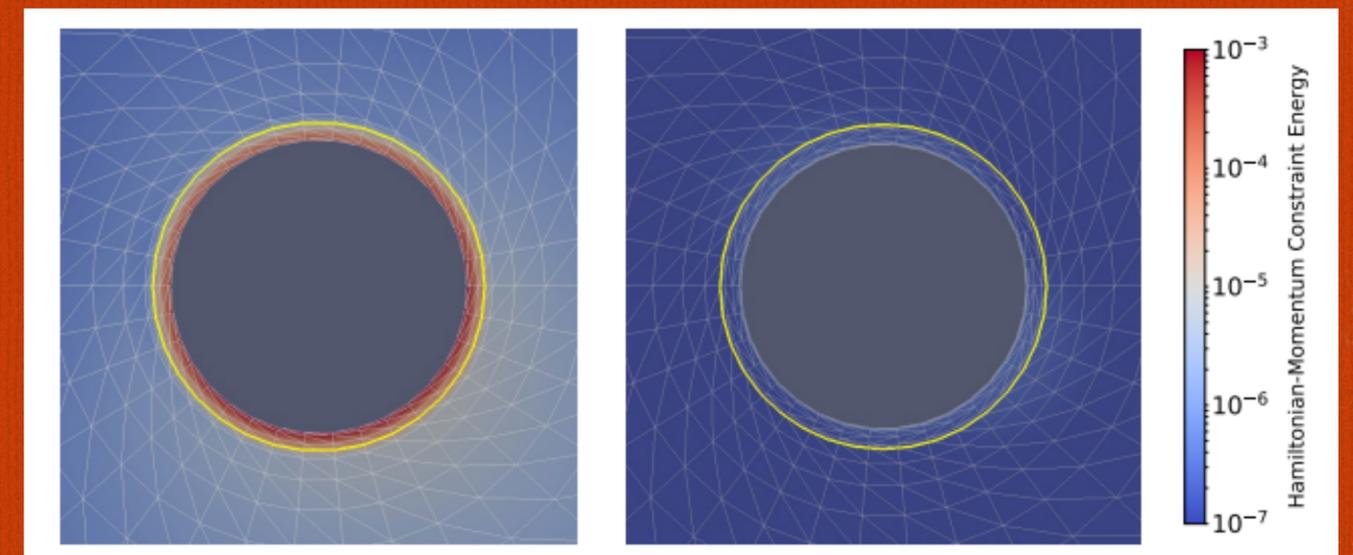
- Black holes have two potential kinds of singularity
 - Coordinate singularities like in the Schwarzschild metric — these resolve just fine in different coordinates
 - Physical singularities — these are unavoidable, and trouble for numerical schemes!
- Something in the metric is going to be infinite near the BH center, and you can't just be clever and set " $1/\psi = 1/\infty = 0$ ", since it won't be smooth there. You have two choices, basically
 - Excision: "cut out" a region around the BH center and impose boundary conditions there. Make sure the excision surface is **INSIDE** the horizon
 - Punctures: Choose coordinates with a point like singularity, and if you'd like, modify the fields somewhere inside the horizon
- In both cases, we will rely on causality to hide our numerical errors



Source: Hemberger et al (2012)

Excision: Boundary Conditions

- This is more commonly used in generalized harmonic gauge evolution calculations
- In an excision calculation, boundary conditions must be applied to a missing region somewhere inside the horizon. Some examples of commonly used treatments (including in Lorene):
- Cook and Pfeiffer (2005): CTS; assume that outgoing null rays have zero expansion and shear, apparent horizon at fixed coordinates initially
- Caudill et al. 2006: Add in quasi-local measures of spins at the horizons
- Varma et al (2018): “Negative expansion” boundary conditions



Source: Varma et al. (2018)

Bowen-York solutions

- We assume a conformally flat metric and maximal slicing (the trace of the extrinsic curvature is zero).

- The extrinsic curvature is given in terms of a vector potential V :

$$K_{ij} = \psi^{-2} \left(V_{j,i} + V_{i,j} - \frac{2}{3} \delta_{ij} \operatorname{div} V \right)$$

- The momentum constraint has solutions for given momenta P_i and spins S_i :

$$V = \sum_{n=1}^{N_p} \left(-\frac{7}{4|\mathbf{x}_n|} P_n - \frac{\mathbf{x}_n \cdot P_n}{4|\mathbf{x}_n|^3} \mathbf{x}_n + \frac{1}{|\mathbf{x}_n|^3} \mathbf{x}_n \times S_n \right)$$

- The Hamiltonian constraint gives us our conformal factor

$$\Delta\psi + \frac{1}{8} \psi^5 K_{ij} K^{ij} = 0,$$

- Note that this is NOT equivalent to a Kerr black hole — Kerr BHs are NOT conformally flat!

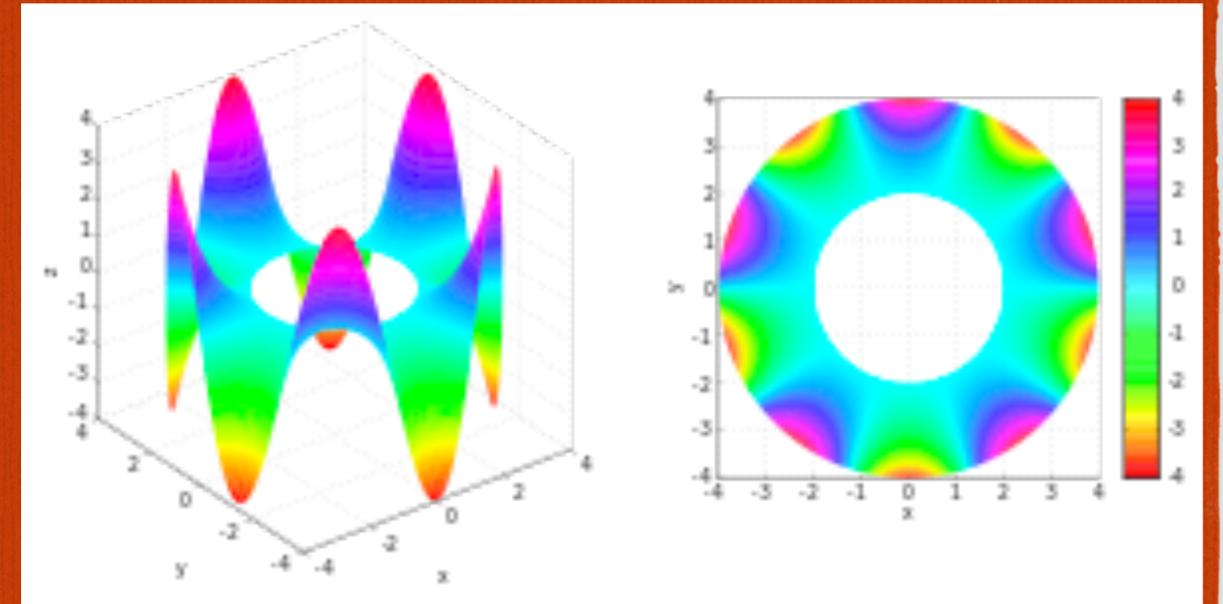
Source: Ansorg et al. (2004)

Punctures: Choosing the parameters

- Use TwoPunctures (Ansorg et al. 2004) or similar to generate conformal factor and extrinsic curvature
- You need to choose the masses, momenta, and spins
 - Logarithmic terms are present in the weak-field expansion, esp. for systems with net linear momentum
- Specify a lapse and shift of your choice — you don't get these from a CTT formalism
- Be prepared for your system to evolve and “ringdown” — your solutions include both spinning BHs plus gravitational radiation required to “flatten” the metric
- There are spin limits for moving punctures — about $a/M = 0.93$ or so

Elliptic equation solvers

- Elliptic equations basically all behave something like Poisson/Laplace equations
 - In GR, they are often more stable than you might expect — relativistic corrections tend to always make gravity stronger
- Interesting problems are almost always NOT smooth somewhere
 - BH: Singularity/horizon
 - NS: Surface of the star, any transition regions inside
- The geometry is not well-suited for Cartesian-based codes
- Much work has going into clever numerical techniques for these equations



Source: Wikipedia

Why not 3-d Cartesian grids?

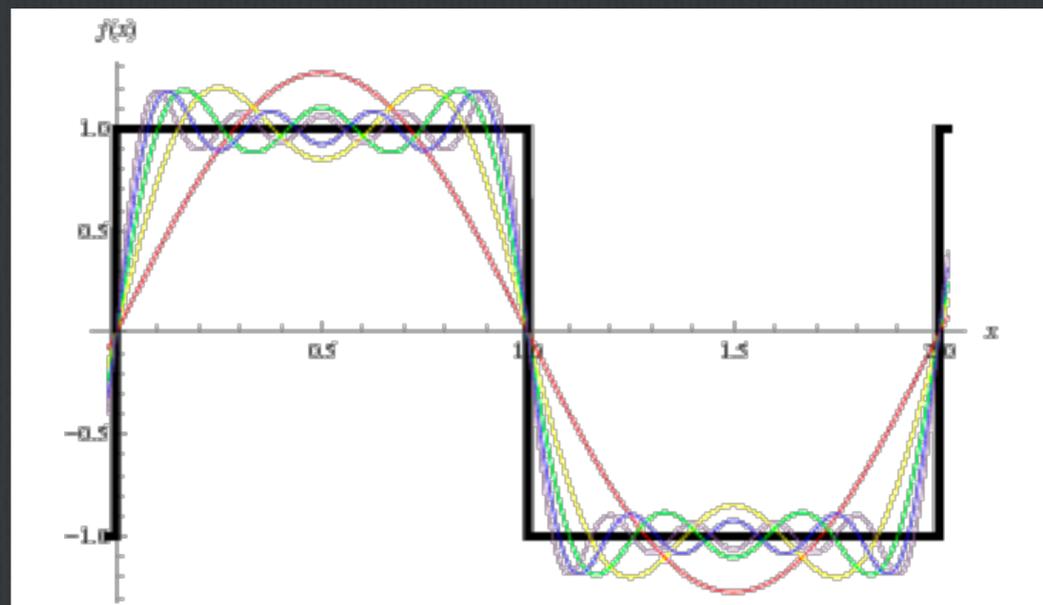
- 3-d Cartesian grids are used widely in Numerical Relativity, why not initial data?
- Boundary conditions matter, and are difficult to get right at finite distances
- Singularities/NS surfaces are present inside the domain — lack of smoothness typically limits accuracy
- Mesh-refinement solvers are something of a programming nightmare
- Mode decompositions in Cartesian coordinates don't match well with the underlying physics
- Turns a desktop computing problem into a supercomputing problem!

Spectral Methods

- Spectral solvers are the workhorses of initial data software
- Coordinates are generally adapted to the problem at hand — either spherical or “spheroidal” in nature
- Spectral methods, which expand a function in a set of modes and coefficients, generally yield exponential convergence when being used to model smooth functions, and power-law convergence for non-smooth functions
 - It is extremely difficult to “supercompute” your way to high accuracy with spectral methods — worker smarter inevitably beats working harder eventually
- Fourier and spherical harmonic decompositions are familiar examples, Chebyshev polynomial fitting widely used, etc.
- Choosing the coordinates and domain structure is often the hardest task

Choosing Coordinates

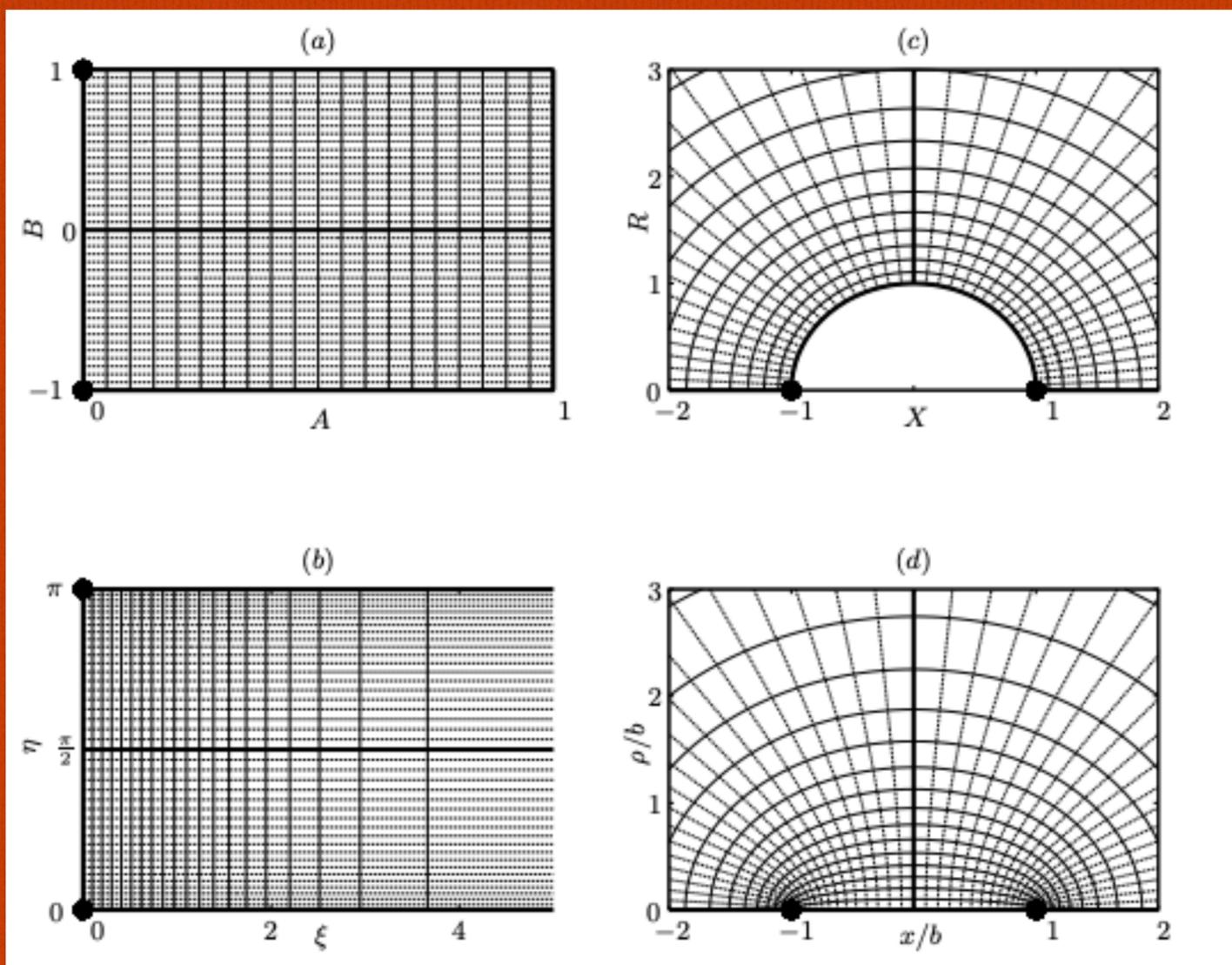
- **Black Holes:** We have either a (puncture) point-like discontinuity, or a spherical surface in the interior of our domain
- **Neutron stars:** we have a spheroidal boundary where quantities are not infinitely differentiable
- **In each case, we want to choose our coordinate scheme very carefully to make sure we don't induce Gibbs' phenomenon:**



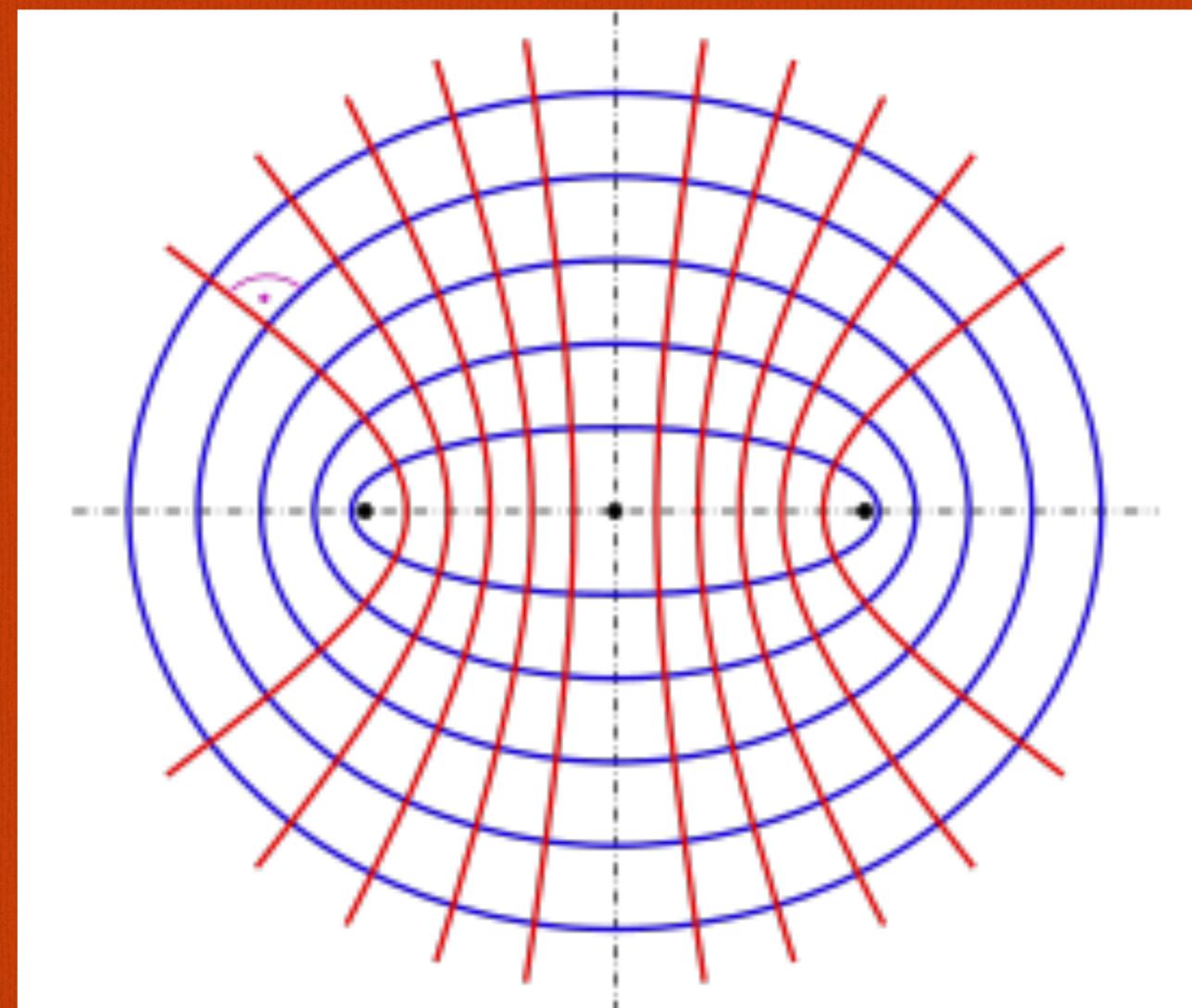
Source: Mathworld

- **For continuous functions, Gibbs' phenomenon causes slow convergence of coefficients — you need more of them, and the result is less accurate**

TwoPunctures: Single domain spectral methods



Source: Ansorg et al. (2004)



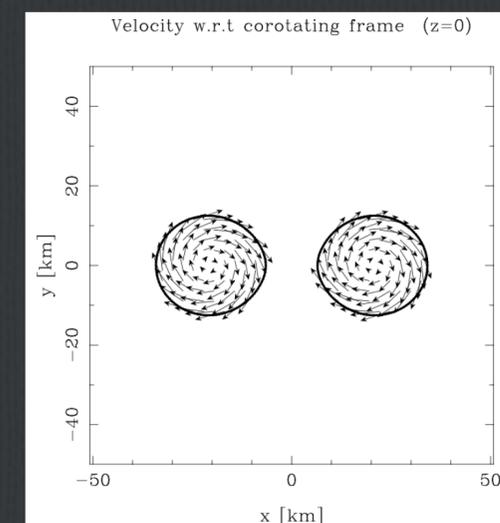
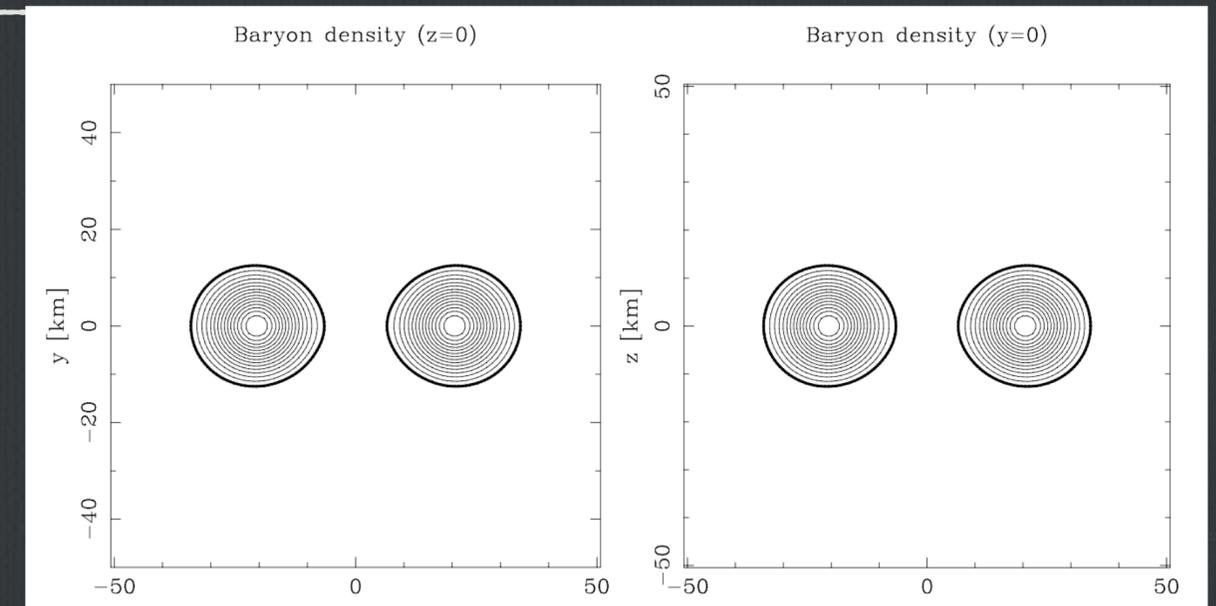
Source: Wikipedia

TwoPunctures: Single domain spectral methods

- The code uses modified confocal elliptical/hyperbolic coordinates, for which the Laplacian operator is still diagonal
- The quasi-radial direction is “compactified” to run from 0 to 1 in the A-variable while covering infinite distances
- Allows for Chebysev expansion in the A-variable (quasi-radius) and the B-variable (quasi-latitude), and Fourier decomposition in the azimuthal direction
- In practice, the solver uses a preconditioned bi-conjugate gradient stabilized method
- Convergence isn't quite spectral for binaries, but can achieve sixth-order

Neutron stars: numerical challenges

- Neutron stars have:
 - Matter in an extended configuration, which means we have to deal with the stress-energy source terms in the constraint equations
 - A pressure and enthalpy that depend on the local density (and potentially more?)
 - We will try to avoid dealing with temperatures, which are generally assumed to be “cold”
 - A tidally extended surface at which many physical quantities have non-differentiable (but generally continuous?) behavior
 - We are ignoring “tidal lags” that can develop over time, esp. when binaries separations get smaller
 - We won't even discuss the formation of cusps on the surfaces of NS
 - EM fields that thread through them
 - Spins that, while slow, are almost certainly not zero



Source: Gourgoulhon et al. (2002)

Matter source terms

- The presence of matter acts on a source term for both the Hamiltonian and momentum constraints, often combined with the maximal slicing condition to yield 5 linked elliptic equations:

$$\begin{aligned}\Delta\Psi + \frac{1}{8}\hat{A}_{ij}\hat{A}^{ij}\Psi^{-7} + 2\pi\tilde{E}\Psi^{-3} &= 0 \\ \Delta\beta^i + \frac{1}{3}\mathcal{D}^i\mathcal{D}_j\beta^j - (L\beta)^{ij}\mathcal{D}_j\ln\tilde{N} &= 16\pi\tilde{N}\tilde{p}^i \\ \Delta(\tilde{N}\Psi^7) - (\tilde{N}\Psi^7) \left[\frac{7}{8}\hat{A}_{ij}\hat{A}^{ij}\Psi^{-8} + 2\pi(\tilde{E} + 2\tilde{S})\Psi^{-4} \right] &= 0,\end{aligned}$$

Source: Gourgoulhon et al. (2007)

$$\underline{\Delta}\nu = 4\pi A^2(E + S) + A^2 K_{ij}K^{ij} - \bar{\nabla}_{i\nu}\bar{\nabla}^i\beta,$$

$$\underline{\Delta}\beta = 4\pi A^2 S + \frac{3}{4}A^2 K_{ij}K^{ij} - \frac{1}{2}(\bar{\nabla}_{i\nu}\bar{\nabla}^i\nu + \bar{\nabla}_i\beta\bar{\nabla}^i\beta)$$

$$\underline{\Delta}N^i + \frac{1}{3}\bar{\nabla}^i(\bar{\nabla}_j N^j) = -16\pi N A^2(E + p)U^i + 2N A^2 K^{ij}\bar{\nabla}_j(3\beta - 4\nu)$$

Source: Gourgoulhon et al. (2002)

- The source terms also include curvature terms and potentially other field terms, depending on the variable set
- We generally need both the total mass-energy and the pressure from the stress-energy tensor for the lapse and conformal vector, as well as the velocity field for the shift vector
- The equations are linked and non-linear, but “well-behaved” — most elliptic solvers using relaxation should be stable

Surface effects: Gibbs phenomenon

- Note that the source terms are in general continuous but not differentiable at the surface of the NS. If this occurs in the interior of a domain, the field terms will be twice differentiable, but we will never achieve spectral convergence.
- This in general will require deformation of coordinates to achieve higher accuracy — the domain around the NS becomes spheroidal, rather than spherical.
- There is a price to pay: such changes are very difficult to perform in a conformal way, and we will have to deal with more general elliptic operators, not diagonal ones
- NS initial data often have to stop once cusps form at the inner edge of a NS, or even close to it, because the mappings induce problems

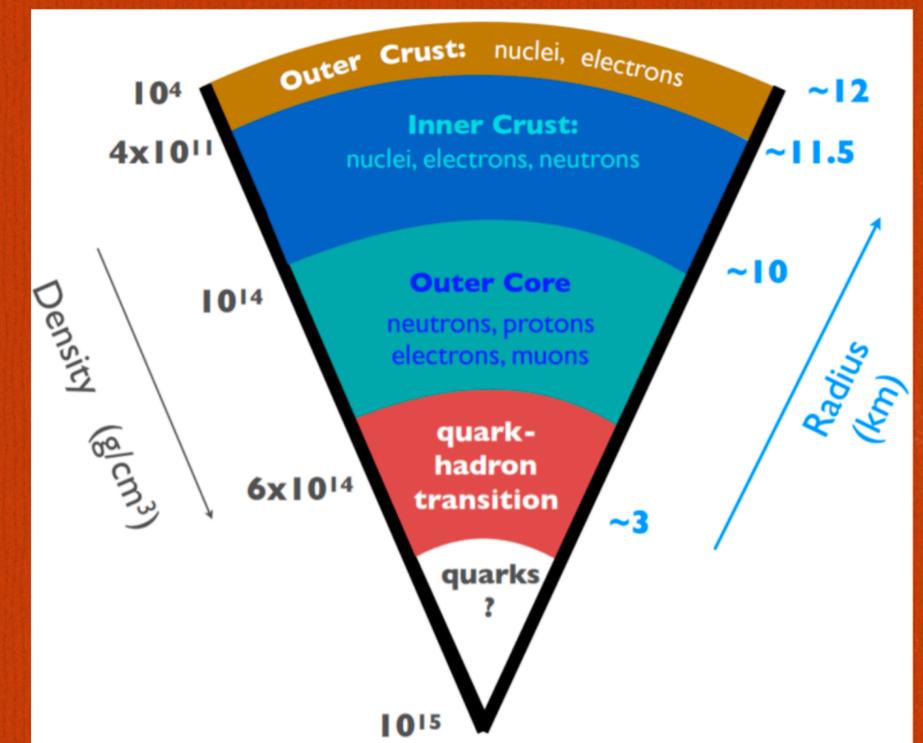
Equations of state

- The equation of state for the NS fluid links the density, internal energy, enthalpy, and pressure, though in practice we can use the laws of thermodynamics to constrain things somewhat:
- Notice we are basically ignoring temperatures — prior to merger, a NS will have had millions of years to settle down, without any obvious sources of recent heating
 - Even if there was a presumed relationship between temperature and density, it can be folded into the EOS
- No one really knows what the true nuclear matter EOS is, so we usually just come up with models, with varying degrees of (over)precision
- NS crusts are largely ignored to the extent they are not fluid in nature

$$\frac{\nabla p}{e + p} = \frac{1}{h} \nabla h ,$$

$$h := \frac{e + p}{m_B n} ,$$

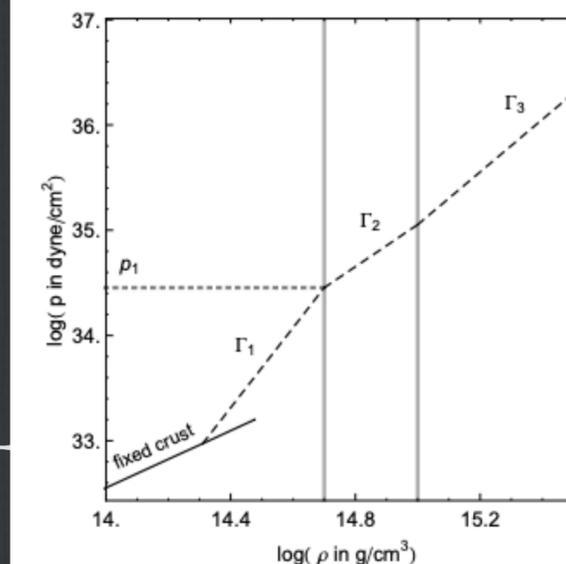
Source: Gourgoulhon et al. (2002)



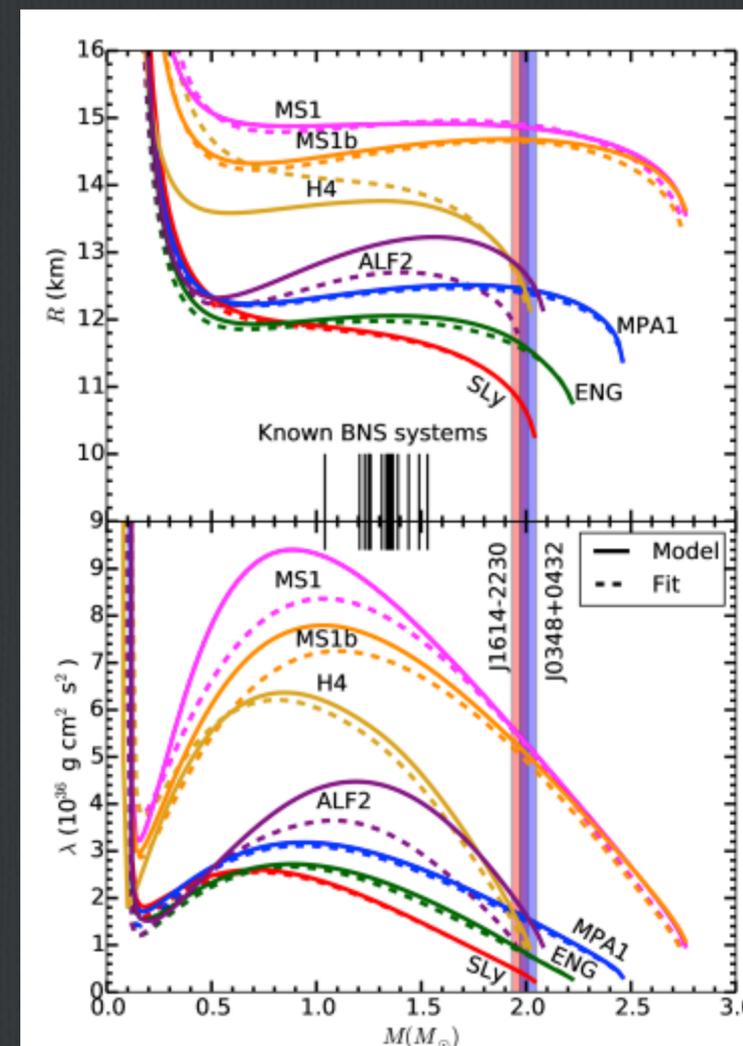
Source: 3G Science white paper

EOS Models

- Polytropes are wonderfully simple, but probably not correct:
- Tabulated EOS models contain too much information, and we need to slice for a given constant temperature, or at least $T(\rho)$ model
- Piecewise polytropes can be simpler to approximate tabulated models
- Accuracy is often good enough to capture qualitative behavior
- Sharp edges are probably less than ideal



Sources: Read et al. (2009); Lackey et al. (2015)



Enthalpy, and velocity

- For a quasi-equilibrium configuration, we can relate the enthalpy to the field values and the local velocity field in order to determine the NS structure:

$$hN \frac{\Gamma}{\Gamma_0} = \text{const} .$$

- For a corotating configuration, this is relatively simple. For an irrotational configuration, it is more complicated:

$$\zeta H \Delta \Psi_0 + \left[(1 - \zeta H) \bar{\nabla}^i H + \zeta H \bar{\nabla}^i \beta \right] \bar{\nabla}_i \Psi_0 = (W^i - W_0^i) \bar{\nabla}_i H + \zeta H \left(W_0^i \bar{\nabla}_i (H - \beta) + \frac{W^i}{\Gamma_n} \bar{\nabla}_i \Gamma_n \right) .$$

Source: Gourgoulhon et al. (2002)

- Here, Psi is the velocity potential — note that an “irrotational” neutron star has vanishing vorticity, rather than solid-body rotation
- We can change the central enthalpy of a NS to change its total mass

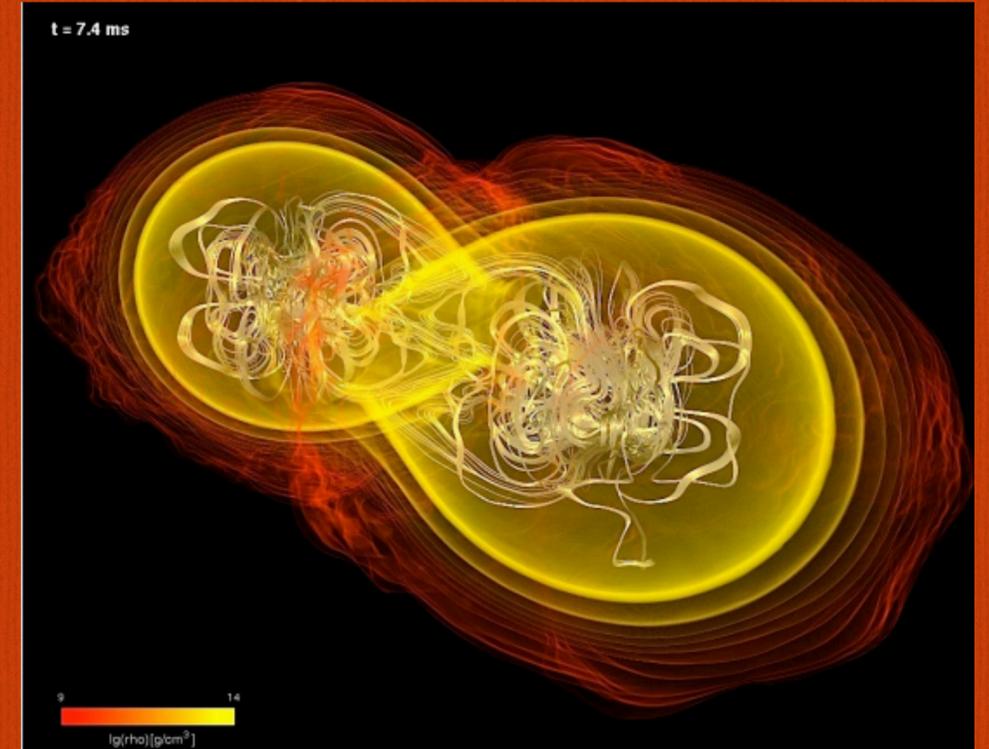
NS spins: corotating vs. irrotational

- NS are expected to be nearly irrotational in the inertial frame
 - NS spin fast! But the orbital angular velocity immediately prior to merger is also very fast!
- Corotating and irrotational models have been widely used throughout the field, particularly the latter in recent years
- Arbitrary spins are possible! See the works by Tichy and collaborators — a nice review of the “Constant Rotational Velocity” formulation can be found in Tichy, arXiv:1610.03805:

$$h\underline{u} = \underline{p} = d\phi + \underline{w},$$

$$w^i = \epsilon^{ijk} \omega^j (x^k - x_{C^*}^k)$$

Magnetic fields

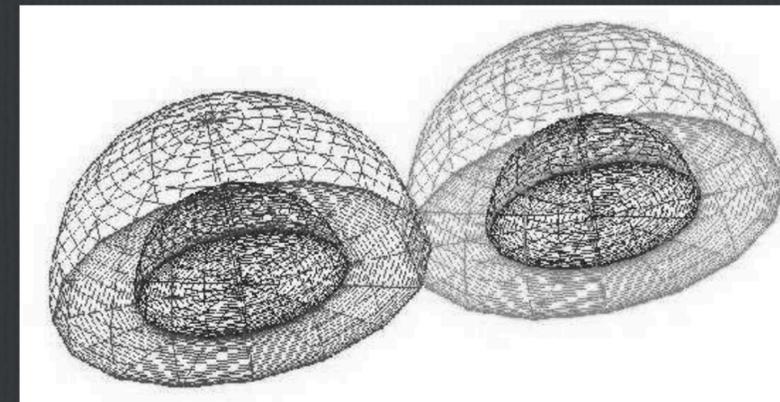


Source: Koppitz and Rezzolla

- Magnetic fields typically won't affect the stress-energy tensor significantly prior to merger — one has to compare the magnetic pressure to the fluid pressure
- They can be added onto an existing initial data model in a post hoc way, e.g., Kawamura et al. (2017):
$$A_\phi \equiv \varpi^2 A_b \max(p - p_{\text{cut}}, 0)^{n_s}$$
- Initial data for more generic magnetic field configurations can be generated for SINGLE neutron stars, see e.g., Uryu et al. (2019)

Lorene: Multi-domain spectral methods

- Lorene (<http://lorene.obspm.fr>) has long been a publicly available code for constructing quasi-equilibrium binary initial data configurations
- It uses a multi domain spectral methods approach:



- Each star is surrounded by a set of spheroidal domains, filling all of space — every point in space has different coordinates relative to both of the domains
- Fields are split into two components, each of which is centered on a different star

$$\underline{\Delta}\nu_{\langle a \rangle} = 4\pi A^2 (E_{\langle a \rangle} + S_{\langle a \rangle}) + Q_{\langle a \rangle} + Q_{\langle b \rightarrow a \rangle} - \bar{\nabla}_i \nu_{\langle a \rangle} \left[\bar{\nabla}^i \beta_{\langle a \rangle} + (\bar{\nabla}^i \beta)_{\langle b \rightarrow a \rangle} \right]$$

$$\nu = \nu_{\langle 1 \rangle} + \nu_{\langle 2 \rangle} = \nu_{\langle 1 \rangle} + \nu_{\langle 2 \rightarrow 1 \rangle} = \nu_{\langle 1 \rightarrow 2 \rangle} + \nu_{\langle 2 \rangle} ,$$

$$\beta = \beta_{\langle 1 \rangle} + \beta_{\langle 2 \rangle} = \beta_{\langle 1 \rangle} + \beta_{\langle 2 \rightarrow 1 \rangle} = \beta_{\langle 1 \rightarrow 2 \rangle} + \beta_{\langle 2 \rangle} ,$$

$$N^i = N_{\langle 1 \rangle}^i + N_{\langle 2 \rangle}^i = N_{\langle 1 \rangle}^i + N_{\langle 2 \rightarrow 1 \rangle}^i = N_{\langle 1 \rightarrow 2 \rangle}^i + N_{\langle 2 \rangle}^i$$

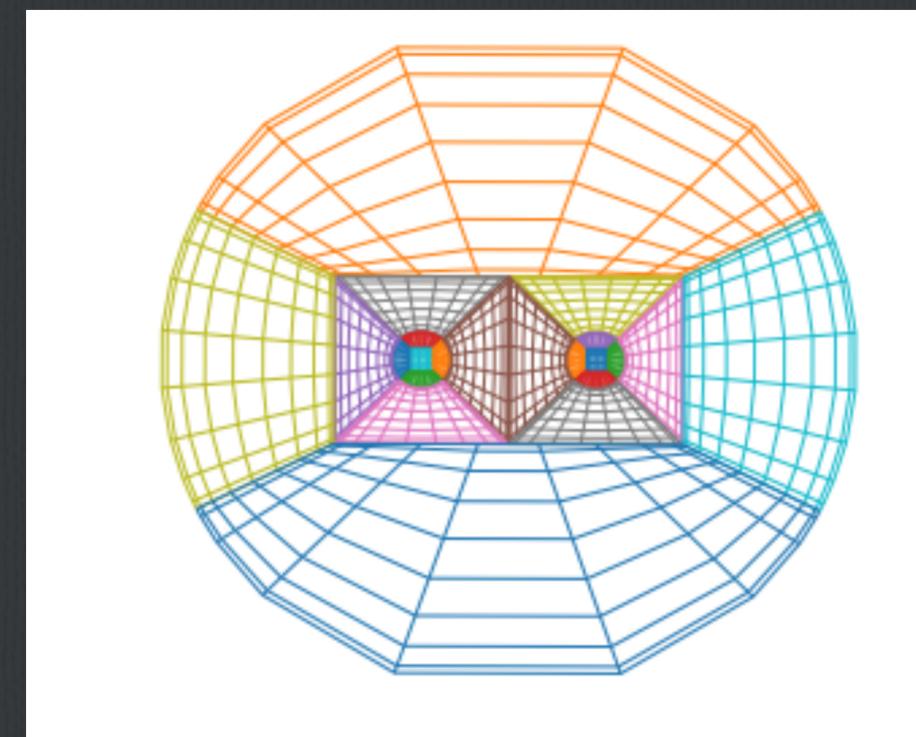
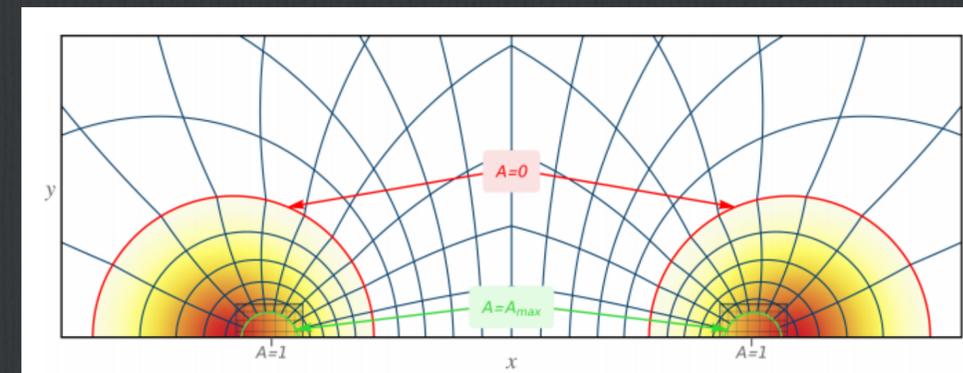
Source: Gourgoulhon et al. (2002)

Lorene: Workflow of a relaxation step

- Determine angular velocity and system rotation axis — this is a root-finder, which doesn't relax well!**
- Establish the velocity potential and the enthalpy**
- Adapt the shape of the inner domain to the stellar surface**
- Solve for the field configurations**
- After a certain number of steps, adapt the central enthalpy to yield the proper baryon mass**

Other code implementations

- COCAL: Uryu et al. — Multiple patches, Green's functions techniques
- SGRID: Tichy et al. — Multiple patches, arbitrary spins
- SPELLS: Foucart et al. — used by the SXS collaboration
- Kadath: PUBLIC spectral code, many different coordinate schemes: <https://kadath.obspm.fr/>
- It would help if more codes were public...



Source: Tichy et al.

RIT Binary Neutron Star Initial Data Library

- We have a public repository of Lorene-based data, along with all required input files, code patch instructions and documentation for users to generate their own data
- <https://ccrg.rit.edu/content/data/bns-initial-data>
- The project has been led by RIT PhD student Tanmayee Gupte, with assistance from former undergraduates Grace Fiasco (now Montana St. U.) and Trung Ha (now U. North Texas).

On these pages, you will find the RIT Binary Neutron Star Initial Data Library. These data we constructed using [Lorene](#), a public, open-source code consisting of C++ classes that solves systems of elliptic partial differential equations, particularly those that arise in general relativity. Lorene uses a multi-domain spectral method in which each component of a binary is placed in its own set of space-filling, nested spherical domains used when evaluating the equations. All fields are broken into two components, one centered on each star, and final quantities are then calculated via spectral expansion of both components at desired locations in space. Using this method, the code can compute the initial configuration of pre-coalescing BNS systems in quasi-equilibrium.

Summary

- Elliptic solvers work very differently than hyperbolic evolution schemes
- Some physics, particularly EOS, are easy to implement
- Some physics, particularly spins or magnetic fields, are more complicated because formulating and solving a quasi-equilibrium set of equations is challenging
- Lorene remains the most commonly used public solver at present
- Multipatch approaches may be more accurate in the long run, because they handle surface effects the most naturally