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CENTRE *for*
THEORETICAL
SCIENCES

TATA INSTITUTE OF FUNDAMENTAL RESEARCH



SIMULATING EXTREME SPACETIMES

Black holes, neutron stars, and beyond...

Challenges in Computational Astrophysics with Black Holes

Prayush Kumar

International Center for Theoretical Sciences

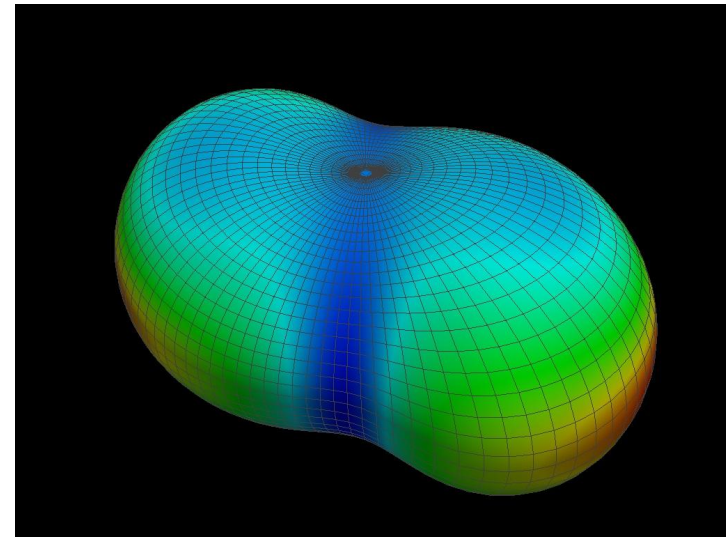
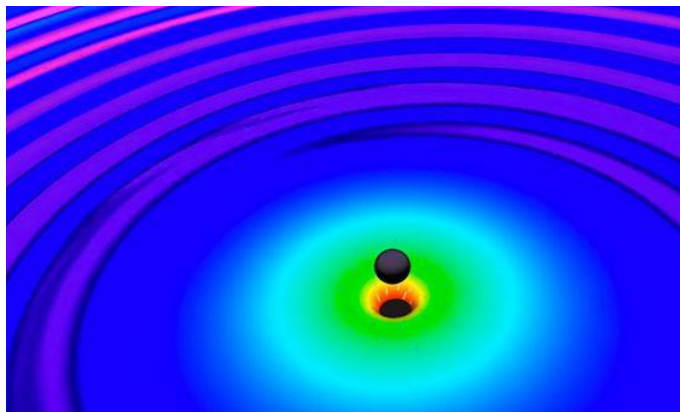
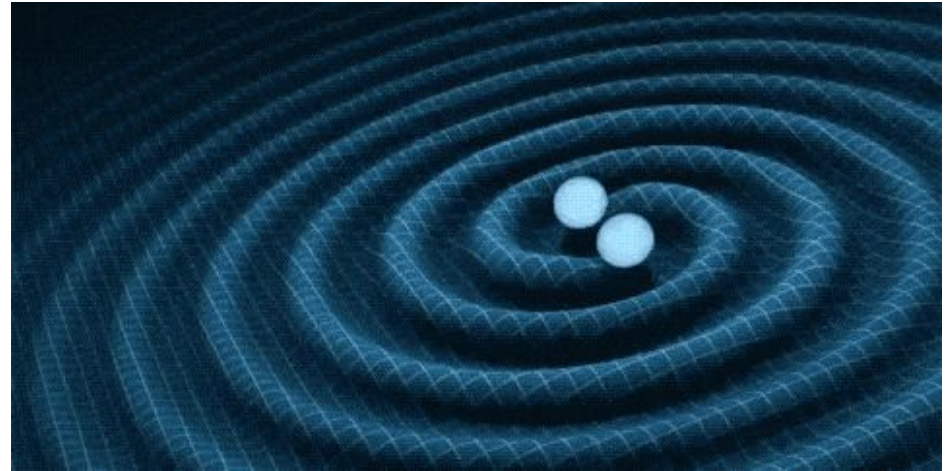
NUMERICAL AND ANALYTICAL RELATIVITY (NAR-2024)

*Department of Applied Sciences, Indian Institute of Information Technology
Allahabad*

March 21, 2024

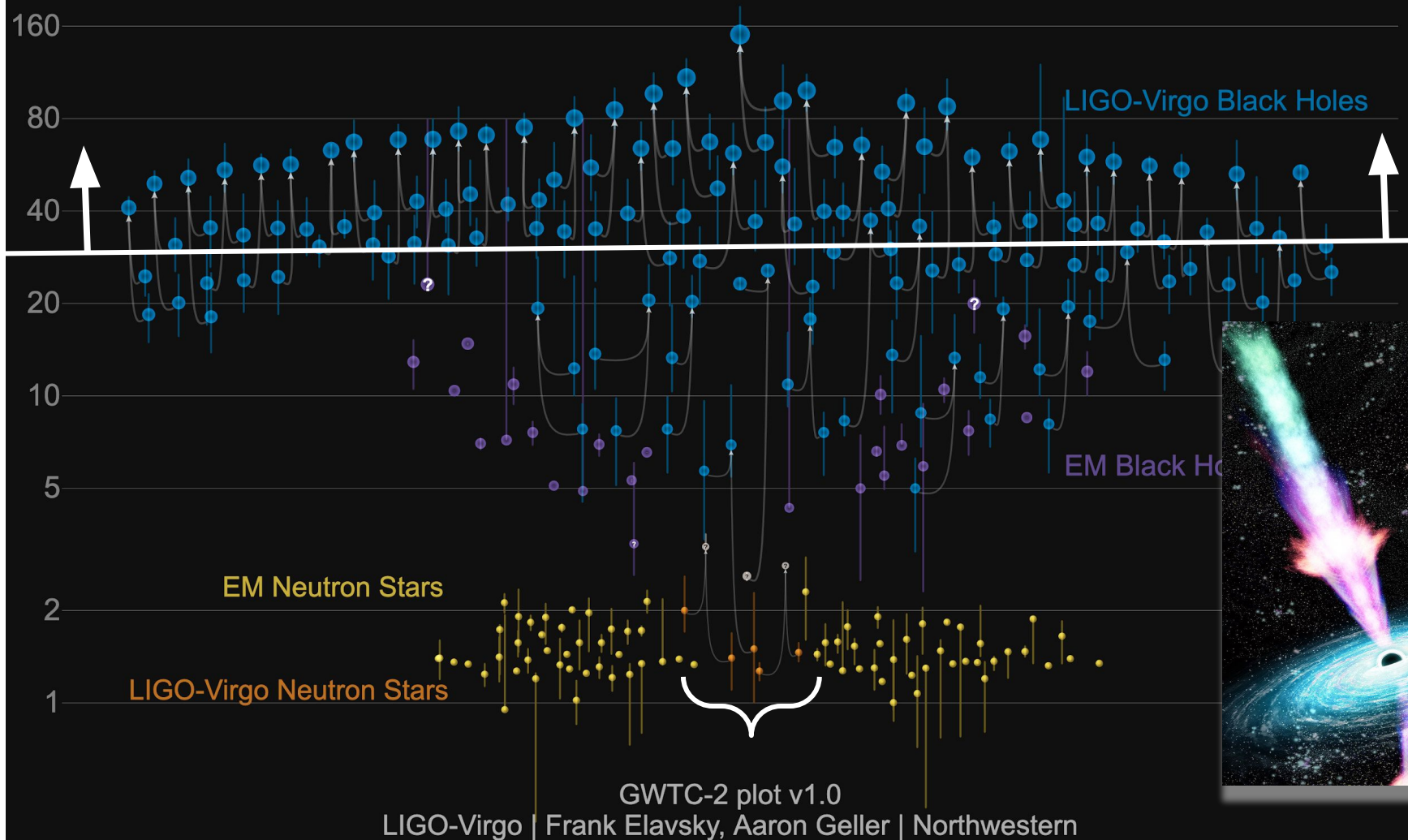
Black Hole *Binaries* emit Gravitational Waves

- Orbiting systems of stars evolve into binary black holes. They emit gravitational waves and lose orbital energy.
- Orbits keeps tightening till the black holes collide. Remnant is also a black hole.
- Remnant black hole is very distorted at birth. It emits gravitational waves and settles down to a quiescent state.



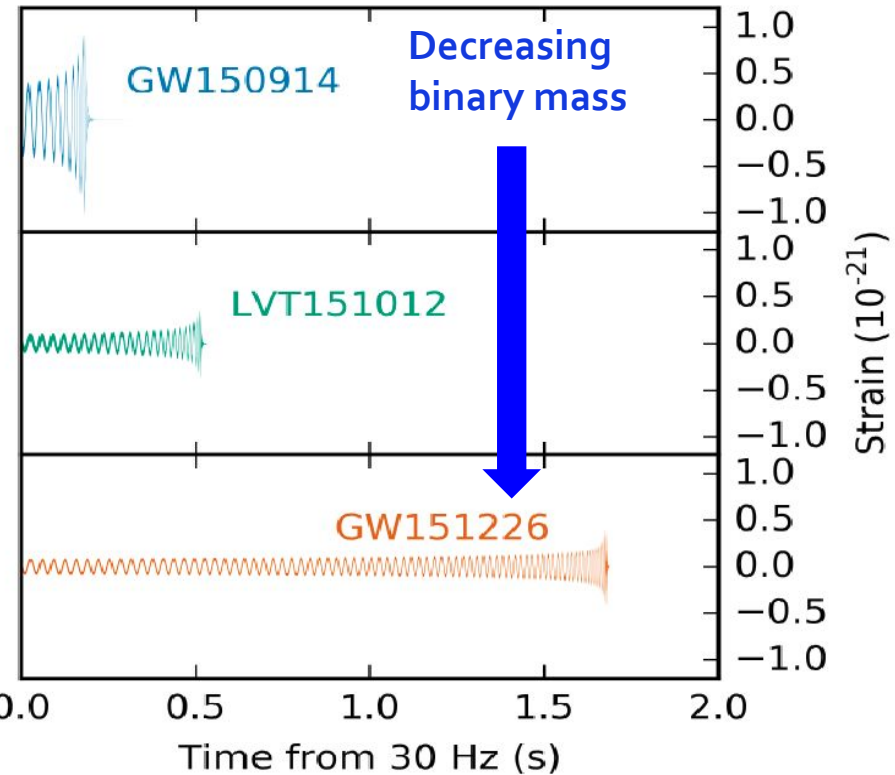
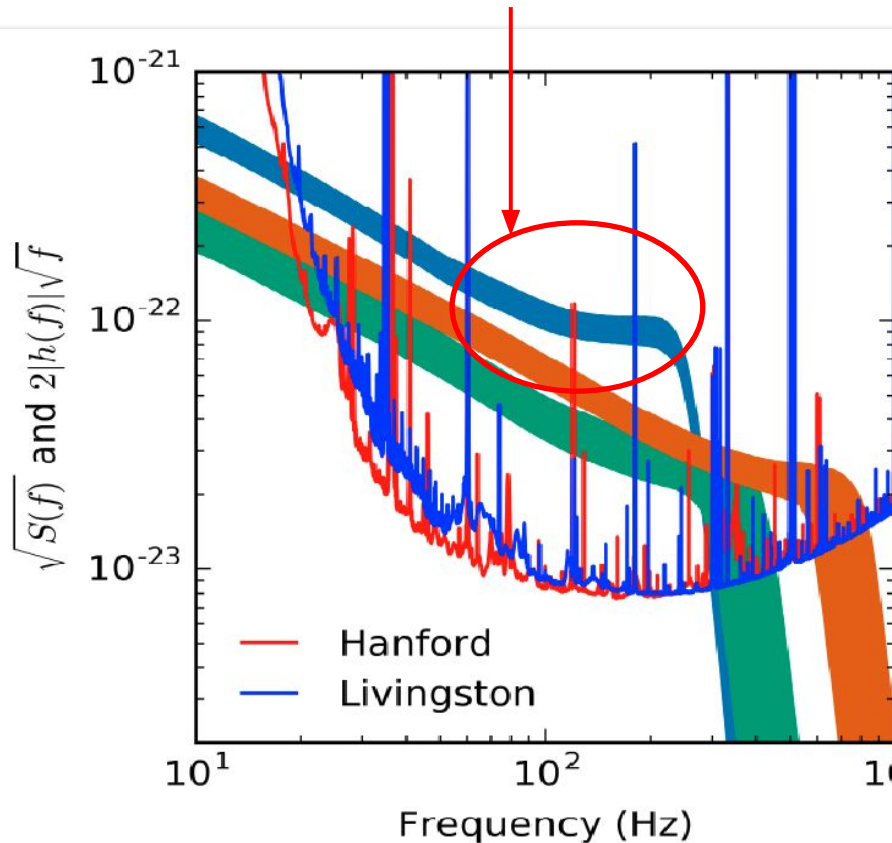
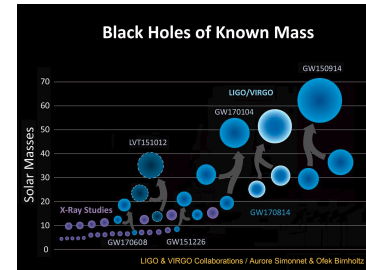
GW Observations with LIGO

Masses in the Stellar Graveyard *in Solar Masses*



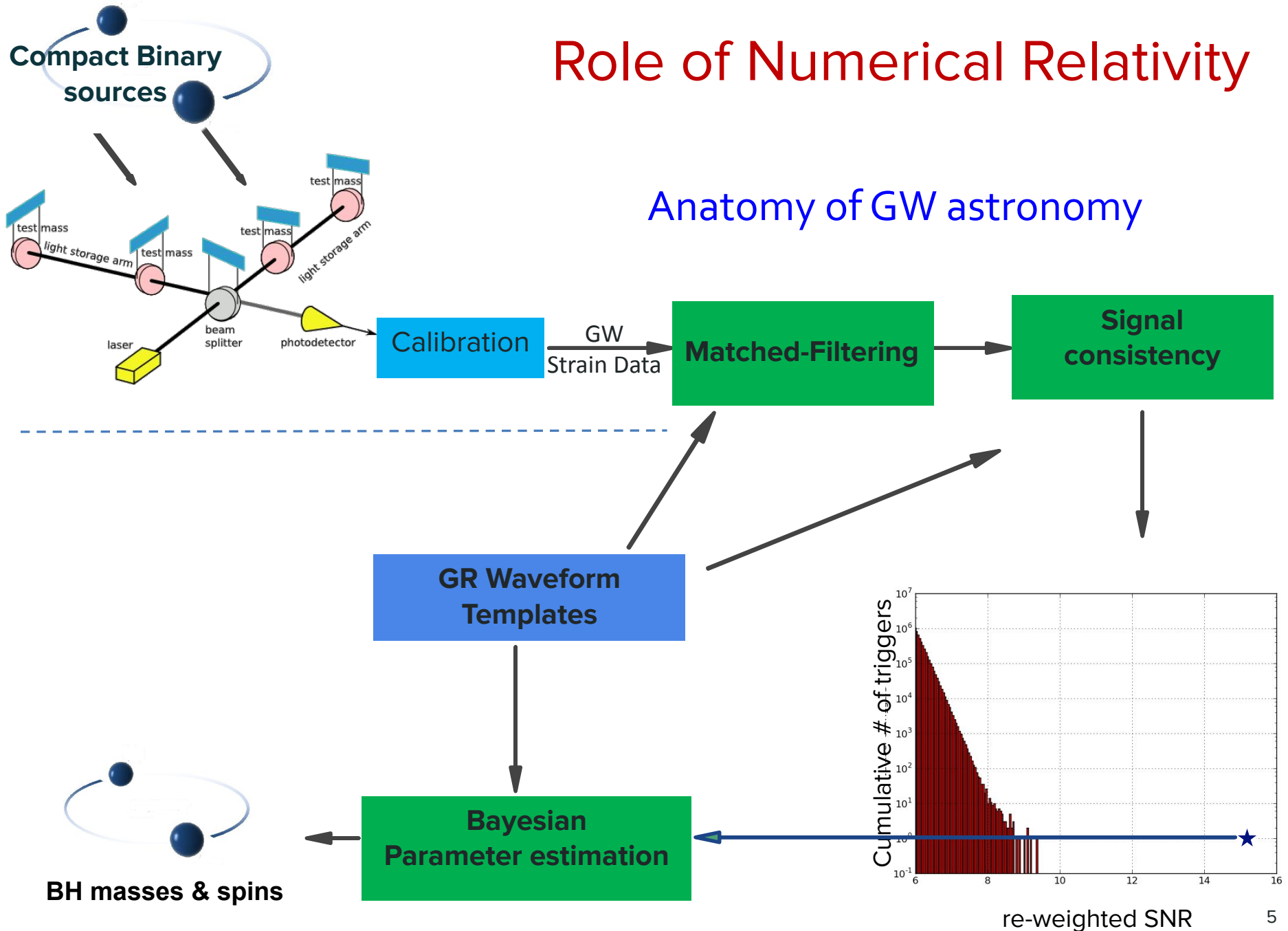
GW observations: these black holes are heavy!

Massive binaries \rightarrow Strong-field non-linear GR dynamics observable!

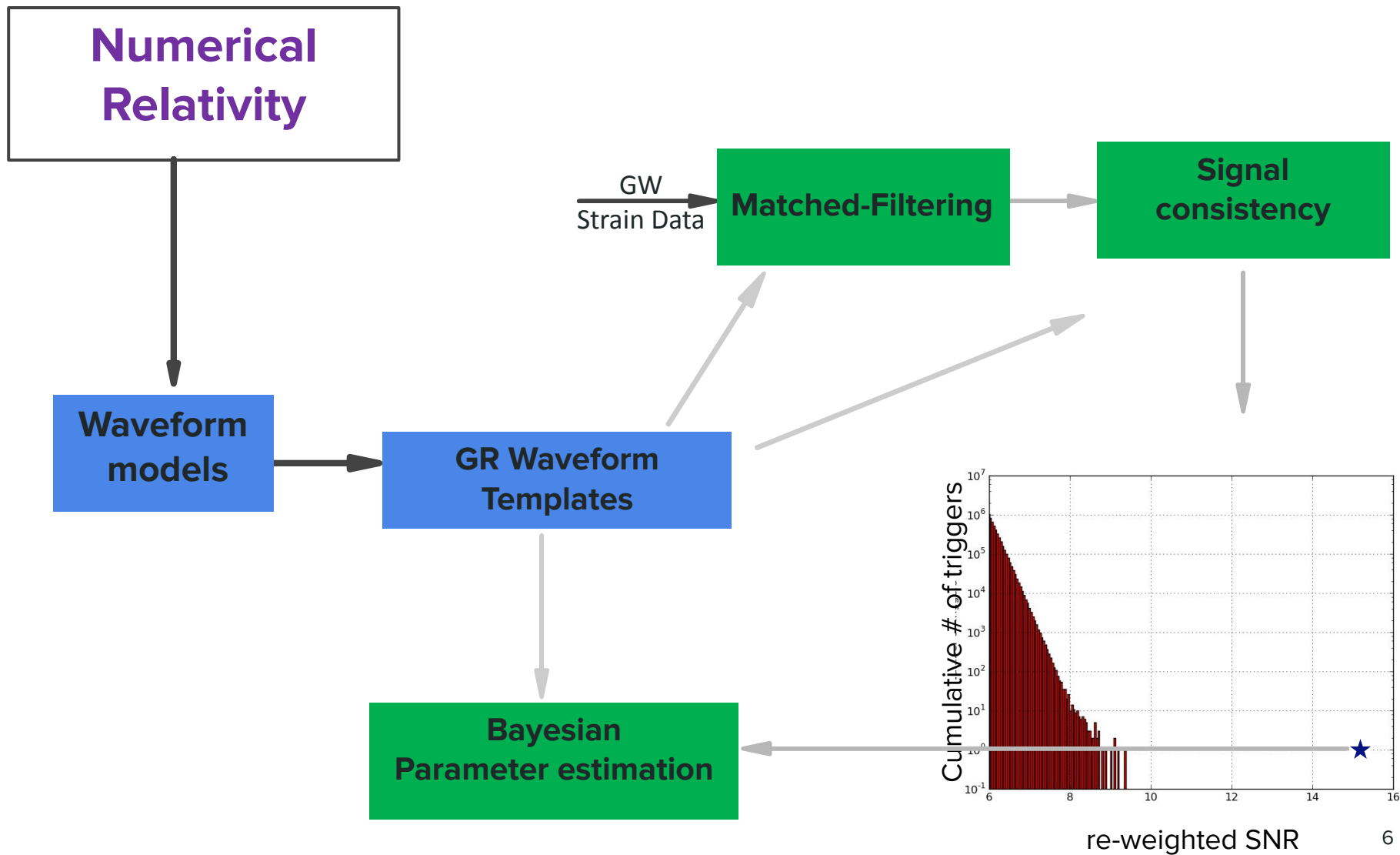


Role of Numerical Relativity

Anatomy of GW astronomy



Role of Numerical Relativity

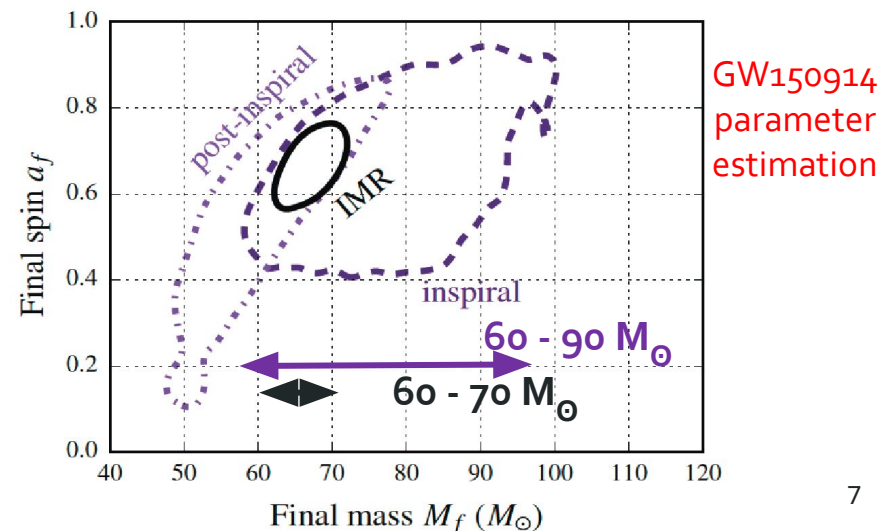
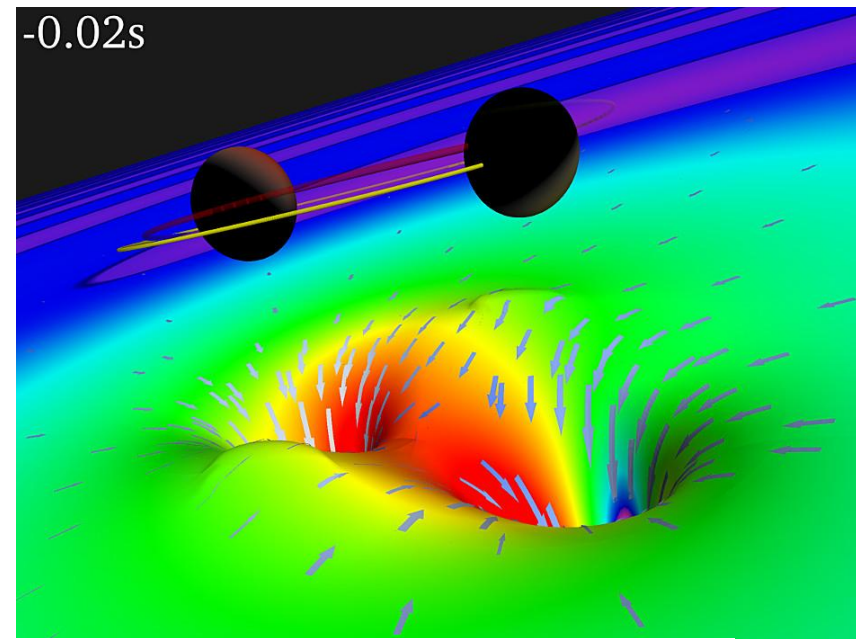


Numerical simulations are *necessary* for BBH science

For BBH, last ~ 10 orbits, merger and ringdown, can only be computed with full numerical solutions of Einstein's equations.

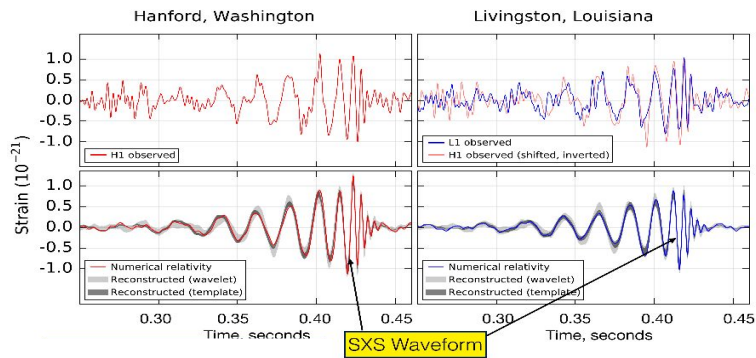
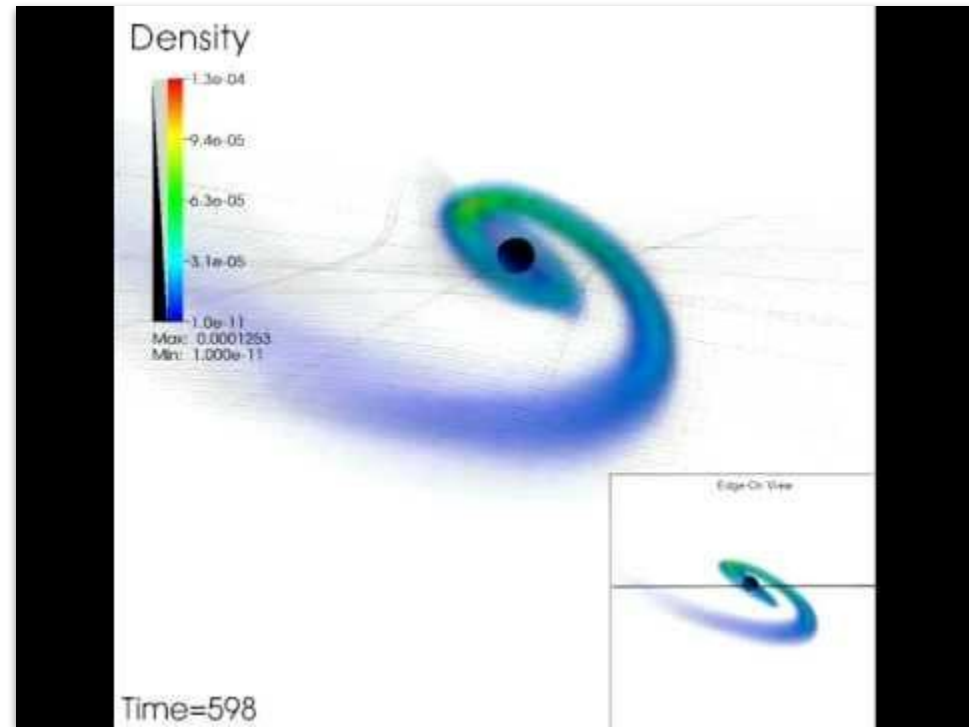
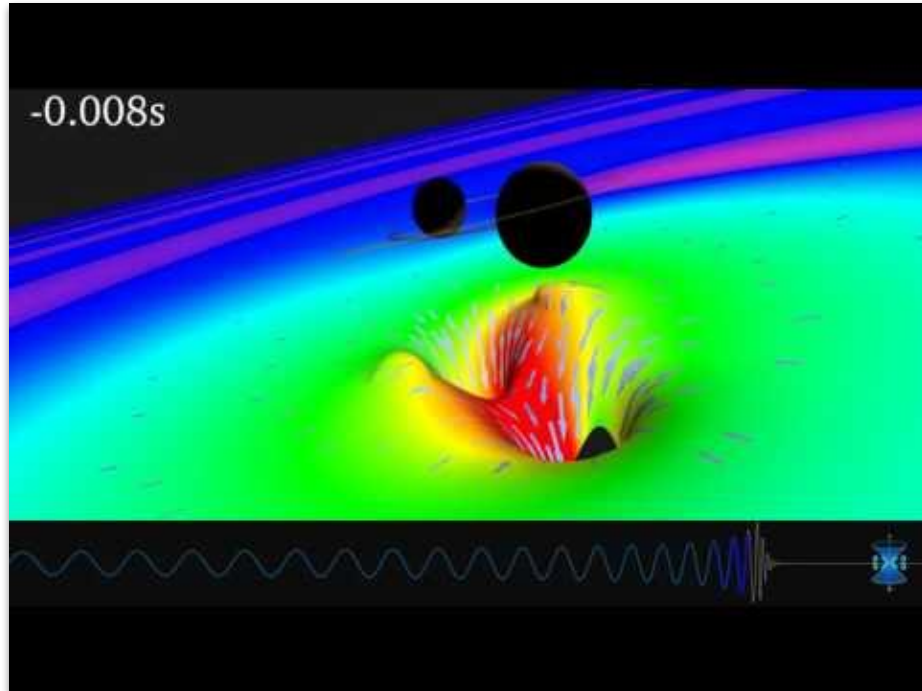
Without Numerical Relativity:

- GW events like GW150914, GW151226, GW170104 - would have had much lower significance ("probable" vs "confident" detection)
- If GW150914's source merged 25% further away, it would not even have been detected in Livingston
- We would only very approximately determine black hole characteristics from the GW signal \longrightarrow
- We could not have tested GR



Simulating Binary Black Hole Coalescence

Black holes and Neutron stars



GR and Einstein's Equations

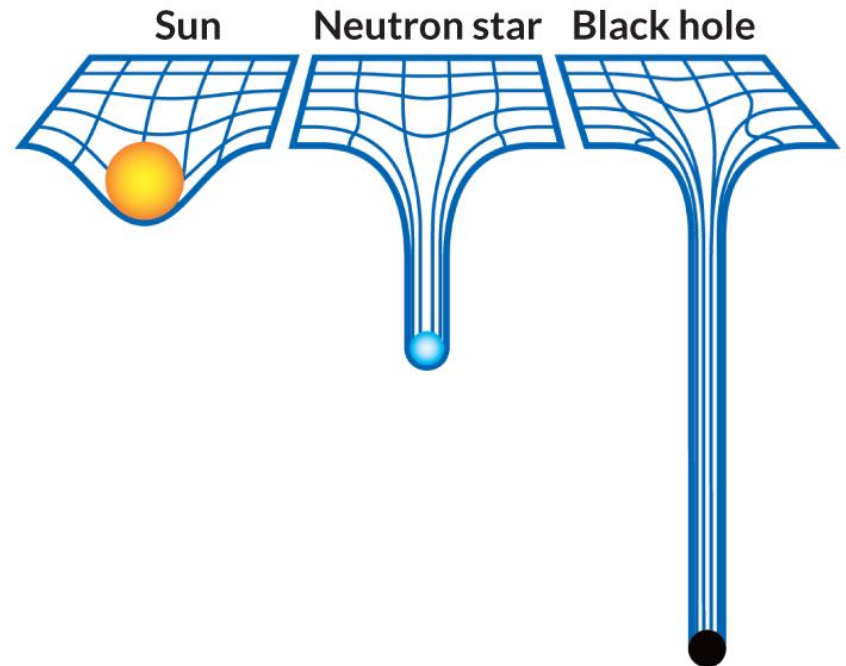
- Newtonian gravity:
Flat Space-time

$$\vec{\nabla}^2 \Phi = 4\pi G \rho \quad \vec{a} = -\vec{\nabla} \Phi$$

- Einsteinian gravity:

(i) **Curved space-time**

(ii) Geometry represented by the space-time **metric** $g_{ab}(\vec{x}, t)$, $a, b = \{x, y, z, t\}$.
Metric is determined by solving Einstein Field Equations



GR and Einstein's Equations

- (ii) Geometry represented by the space-time metric $g_{ab}(\vec{x}, t)$, $a, b = \{x, y, z, t\}$.
Metric is determined by solving Einstein Field Equations:

$$R_{ab}[g_{ab}(\vec{x}, t)] = 0, \quad a, b = 0, \dots, 3$$

$$R_{ab} = \sum_{d=0}^3 \partial_d \Gamma_{ab}^d - \sum_{d=0}^3 \partial_b \Gamma_{da}^d + \sum_{c,d=0}^3 \Gamma_{cd}^c \Gamma_{ab}^d - \sum_{c,d=0}^3 \Gamma_{bc}^d \Gamma_{da}^c$$

$$\Gamma_{bc}^a = \sum_{d=1}^4 (g_{ad})^{-1} (\partial_b g_{db} + \partial_c g_{bd} - \partial_d g_{bc})$$

The Two-Body Problem in Geometrostatics

SUSAN G. HAHN

International Business Machines Corporation, New York, New York

AND

RICHARD W. LINDQUIST

100 kFlops*

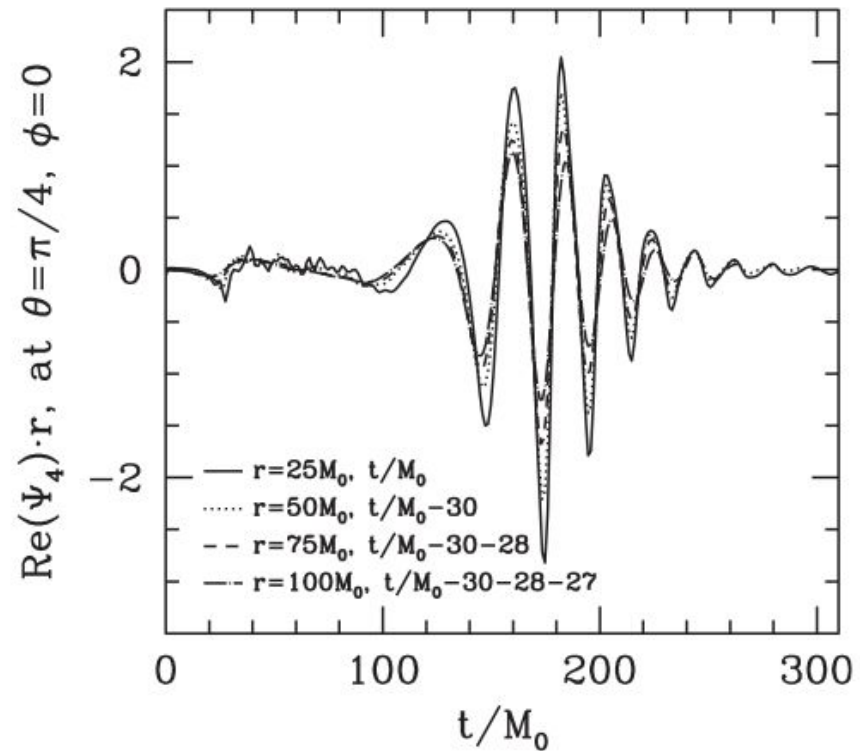
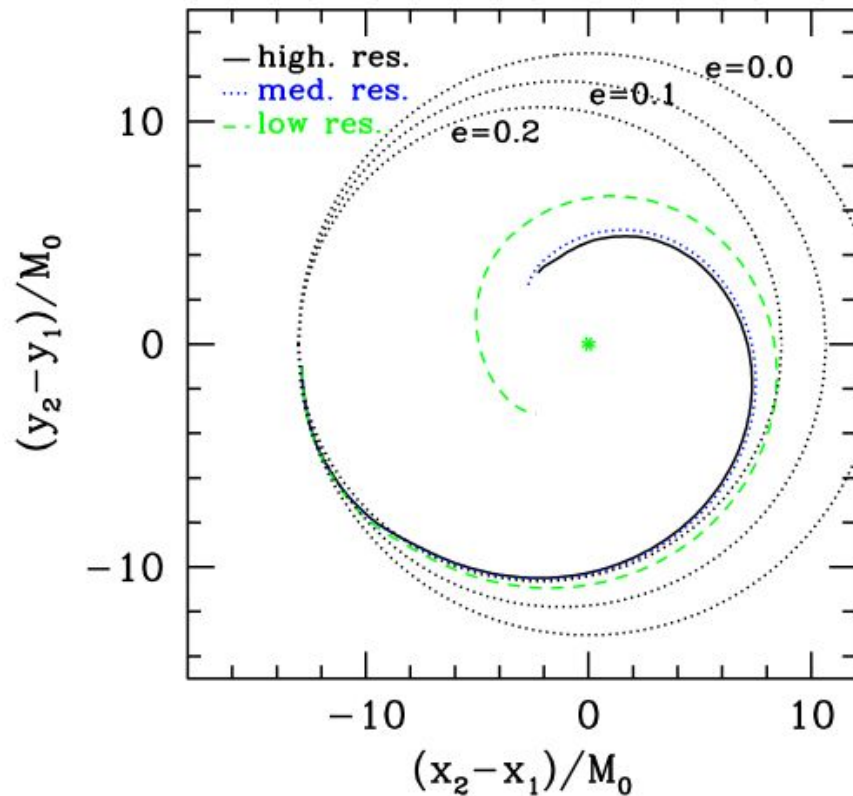
The numerical calculations were carried out on an IBM 7090 electronic computer. The parameters a and μ_0 were both set equal to unity; the mesh lengths were assigned the values $h_1 = 0.02$, $h_2 = \pi/150 \approx 0.021$, yielding a 51 × 151 mesh. The calculations of all unknown functions, including a great number of input-output operations and some built-in checking procedures, took approximately four minutes per time step. Different check routines indicated that results close to the point $\mu = 0$, $\eta = 0$ lost accuracy fairly quickly. Since these would, in the long run, influence meshpoints further away, the computations were stopped after the 50th time step, when the total time elapsed was approximately 1.8. Some of the results are shown in Table I.

Evolution of Binary Black-Hole Spacetimes

Frans Pretorius^{1,2,*}

¹Theoretical Astrophysics, California Institute of Technology, Pasadena, California 91125, USA

²Department of Physics, University of Alberta, Edmonton, AB T6G 2J1 Canada

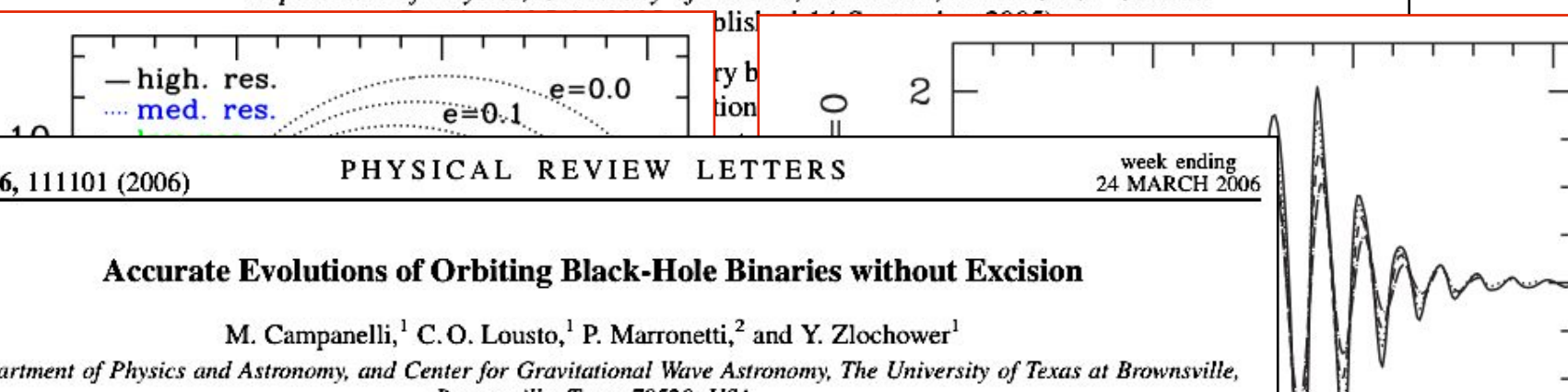


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Accurate Evolutions of Orbiting Black-Hole Binaries without Excision

M. Campanelli,¹ C. O. Lousto,¹ P. Marronetti,² and Y. Zlochower¹

¹*Department of Physics and Astronomy, and Center for Gravitational Wave Astronomy, The University of Texas at Brownsville, Brownsville, Texas 78520, USA*

²*Depart*

Gravitational-Wave Extraction from an Inspiring Configuration of Merging Black Holes

John G. Baker,¹ Joan Centrella,¹ Dae-II Choi,^{1,2} Michael Koppitz,¹ and James van Meter¹

¹*Gravitational Astrophysics Laboratory, NASA Goddard Space Flight Center, 8800 Greenbelt Road, Greenbelt, Maryland 20771, USA*

²*Universities Space Research Association, 10211 Wincopin Circle, Suite 500, Columbia, Maryland 21044, USA*

(Received 15 November 2005; published 22 March 2006)

We present new ideas for evolving black holes through a computational grid without excision, which enable accurate and stable evolutions of binary black hole systems with the accurate determination of gravitational waveforms directly from the wave zone region. Rather than excising the black hole interiors, our approach follows the “puncture” treatment of black holes, but utilizing a new gauge condition which allows the black holes to move successfully through the computational domain. We apply these techniques to an inspiraling binary, modeling the radiation generated during the final plunge and ringdown. We demonstrate convergence of the waveforms and good conservation of mass-energy, with just over 3% of the system’s mass converted to gravitational radiation.

We present a r
corotating shift.
factor. This sys
equations, when
and remains non
use this techniqu
regime. We show
and angular mon
Lazarus approach

Solving Einstein Equations: 3+1 split

- Goal: Space-time metric g_{ab} satisfying

$$R_{ab}[g_{ab}] = 0$$

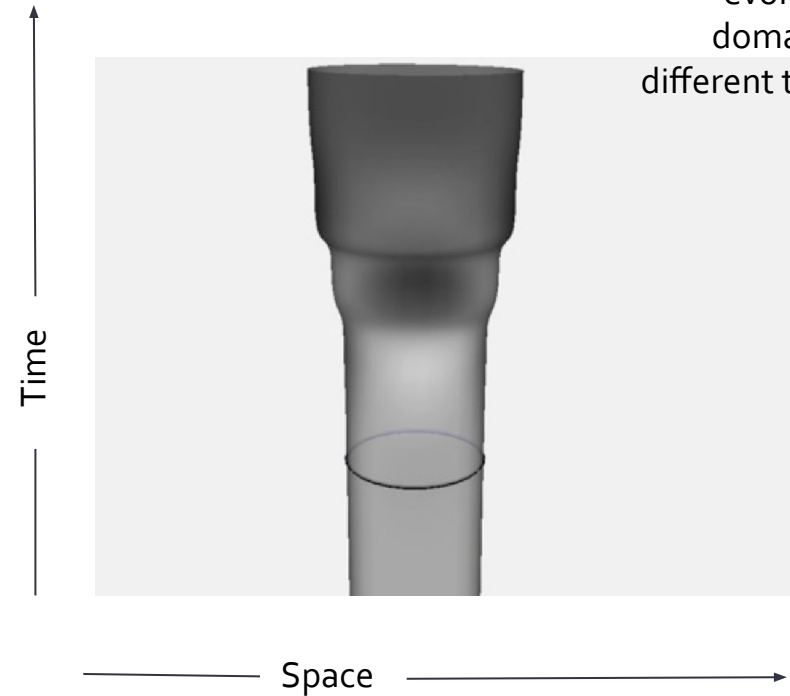
- Split space-time into space *and* time

Evolution equations

$$\partial_t g_{ij} = \dots$$
$$\partial_t K_{ij} = \dots$$

Constraints

$$R[g_{ij}] + K^2 - K_{ij}K^{ij} = 0$$
$$\nabla_j (K^{ij} - g^{ij}K) = 0$$



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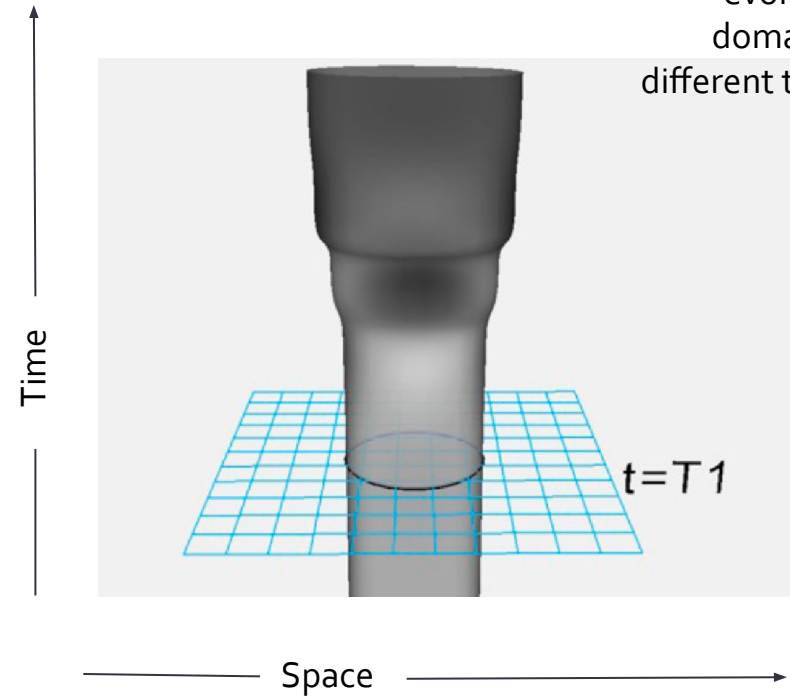
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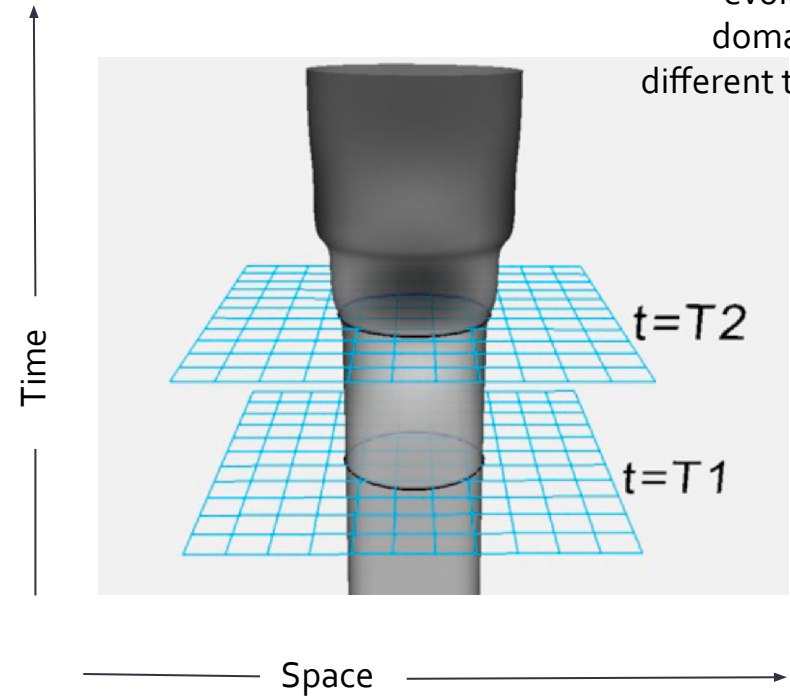
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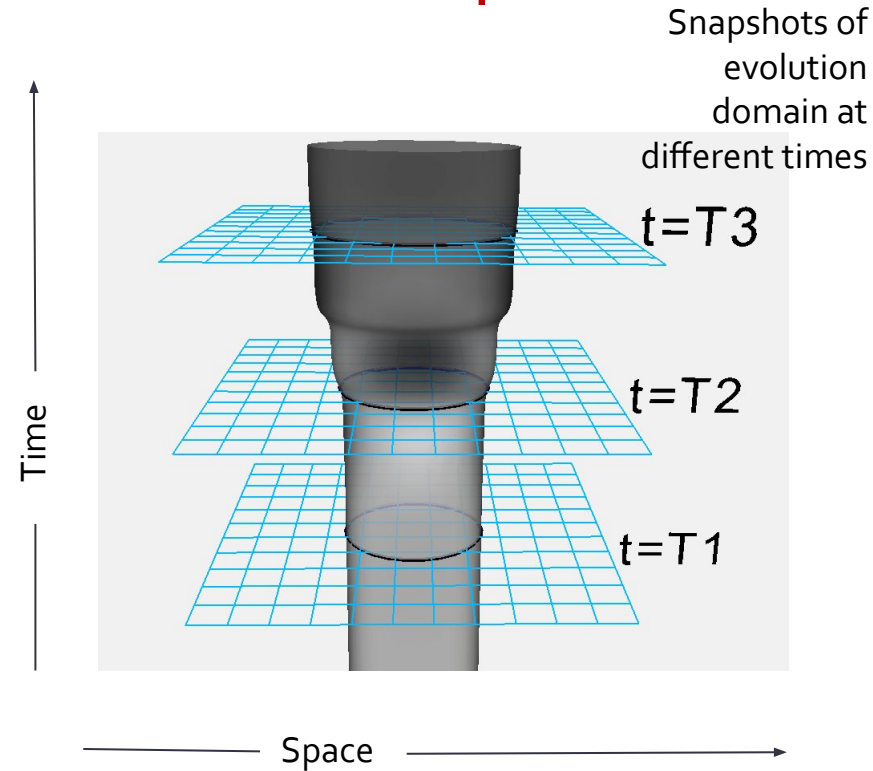
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Maxwell's equations

$$\partial_t \vec{E} = \nabla \times \vec{B}$$
$$\partial_t \vec{B} = -\nabla \times \vec{E}$$
$$\nabla \cdot \vec{E} = 0$$
$$\nabla \cdot \vec{B} = 0$$

What makes it challenging:

Multiple length/time scales, Courant limit, Accuracy required

1. Multiple length scales:

- Size of BH ~ $O(1M)$
- Separation ~ $O(10M)$
- Wavelength $\lambda_{\text{GW}} \sim O(100M)$
- Wave extraction ~ **several** λ_{GW}
- GW flux, that drives the inspiral, is small:

$$\dot{E}/E \sim 10^{-5}$$

What makes it challenging:

Multiple length/time scales, Courant limit, Accuracy required

1. Multiple length/time scales (BH size $\sim O(1)$; $\lambda_{\text{GW}} \sim O(100)$, Outer bdry $\sim O(1000)$)
2. Which coordinates to use (for a spacetime one doesn't know yet)?
3. Putting Black holes (singularity) on a grid
4. Einstein constraints grew exponentially: for many ~~years~~ decades
5. Resolving shocks (discontinuities)
6. Computational Challenges:
 - 20–50 variables
 - Global timestep too small
 - Computing efficiency
7. High accuracy required by LIGO:
 - Absolute phase error $\ll 1$ rad / 20+ orbits

What makes it challenging:

Multiple length/time scales, Courant limit, Accuracy required

1. Multiple length scales
2. Which coordinates to use (for a spacetime one doesn't know yet)?
3. Putting Black holes (singularity) on a grid
4. Einstein constraints $C = 0$: for many years, $\partial_t C \sim C$
5. Resolving shocks (discontinuities)
6. Computational Challenges
7. High accuracy required by LIGO

But, in vacuum, solutions are smooth \Rightarrow Spectral methods

Spectral Einstein Code (SpEC*)

Goal: Solve Einstein's equations to enable robust gravitational-wave science

In development since 2002

650,000 lines, 130 publications



Brief timeline of developments:

2005, Pretorius:

First BBH merger

2006, Goddard group & UBT group: BBH mergers with different formulation

2007, BBH mergers with SpEC code: Now leading code to provide waveforms for LIGO

SpEC: (non-local) Spectral discretization

Evolution quantities are smoothly varying.

- Expand them in basis-functions, solve for coefficients

$$u(x, t) = \sum_{k=1}^N \tilde{u}(t)_k \Phi_k(x)$$

- Compute derivatives *exactly*

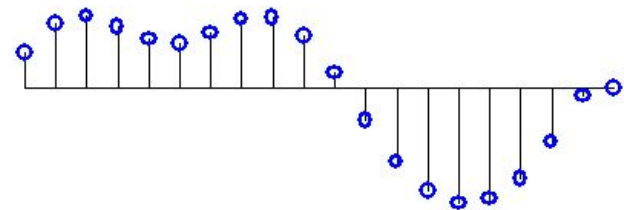
$$u'(x, t) = \sum_{k=1}^N \tilde{u}(t)_k \Phi'_k(x)$$

- Compute nonlinearities in physical space

Spectral



Finite differences



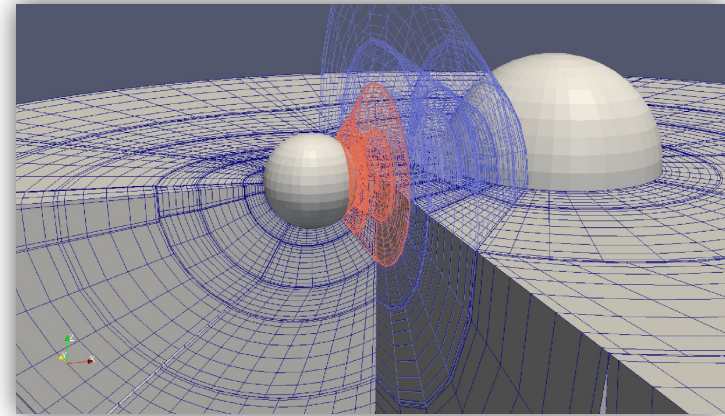
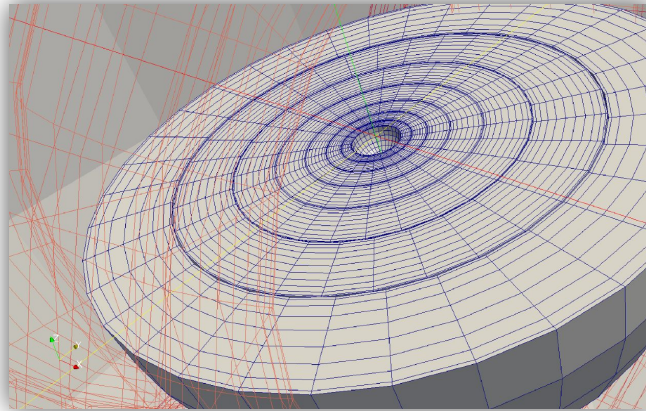
Domain decomposition

I1: Chebyshev
polynomials

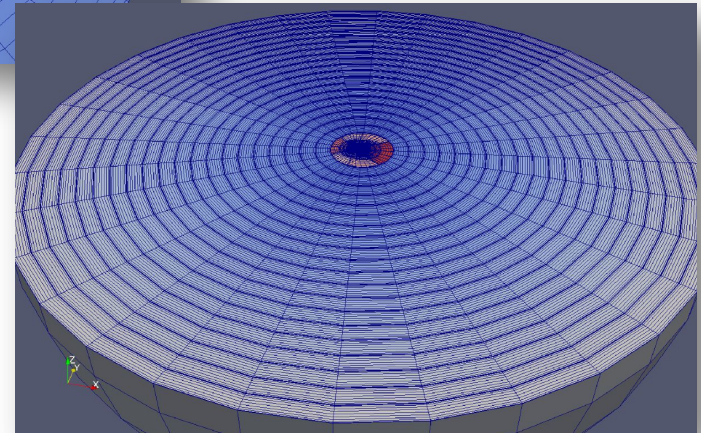
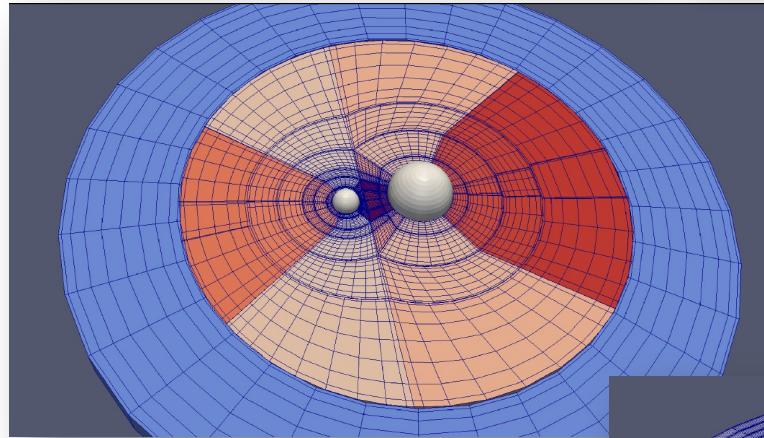
S1: Fourier

S2: ScalarYlm

B2: One-sided Jacobi
polynomials.



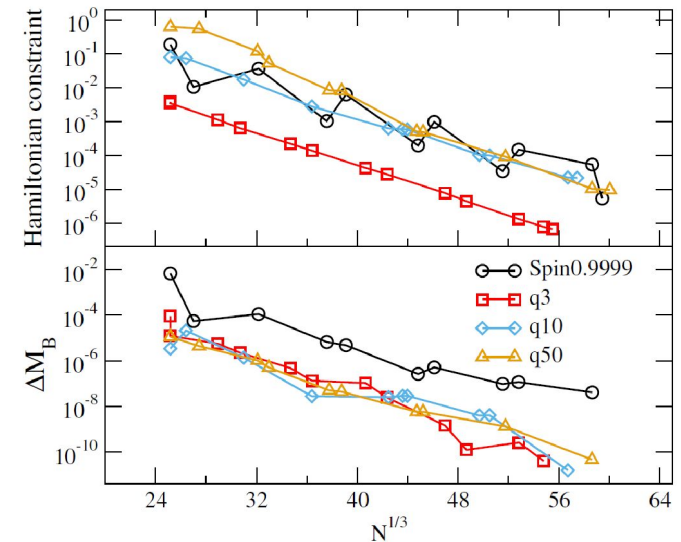
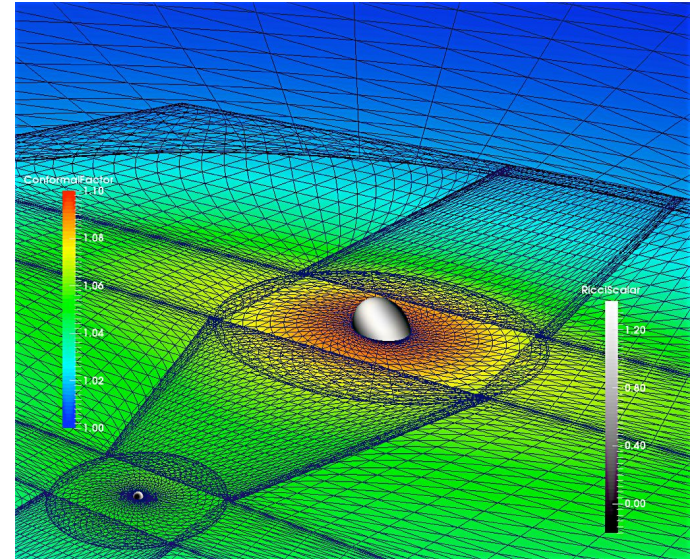
- Local resolution
controllable
dynamically
- **MPI**
parallelization by
sub-domain



Length scale
↓

Initial data: Solve Einstein constraint equations

- Need $\{K_{ij}, g_{ij}\}$ that satisfy Einstein constraints
- Conformal formulation of constraints. Free data provided for $\{\text{conformal 3-metric}, K, \text{ and their } \partial_t\}$
- Solve constraints for $u^\delta = \{\psi, N, N^k\}$. Boundary conditions for u^δ , on S^A & S^B & ∂D , give desired physics: BH spins and orbital properties.
- Second-order coupled Elliptic PDEs



Initial data: Solve Einstein constraint equations

Newton Raphson for elliptic equations

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- Second-order coupled Elliptic PDEs :

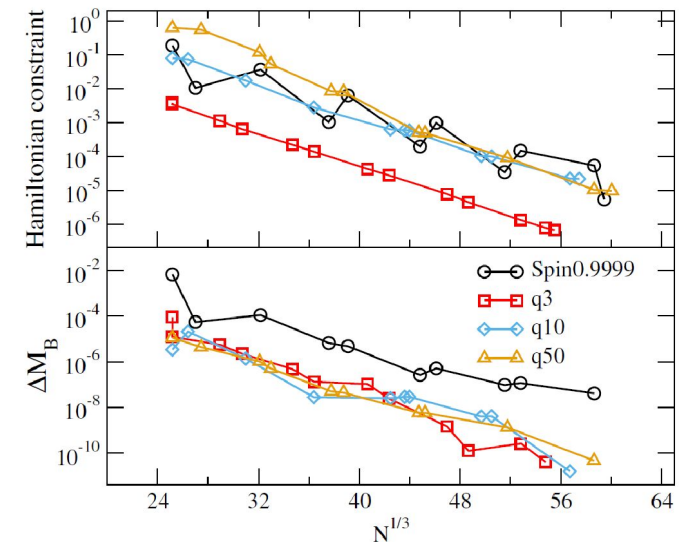
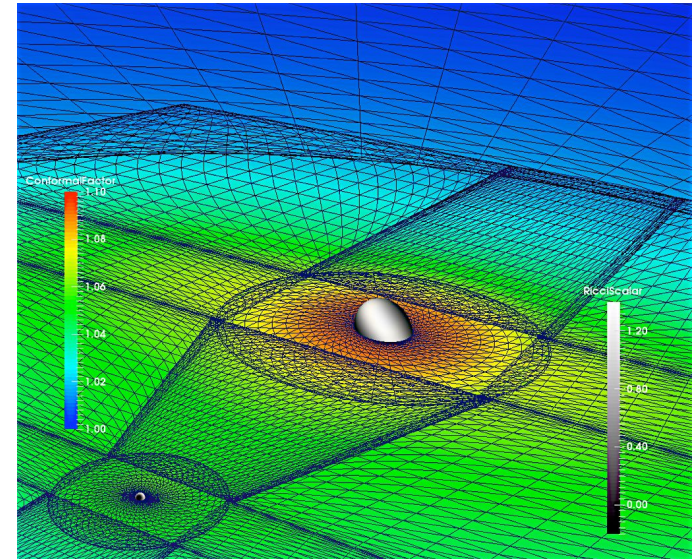
$$\mathcal{S}[\underline{u}(\vec{x})] = 0$$

- Expand on spectral bases in each sub-domain:

$$\underline{u}(\vec{x}) = \sum_i \tilde{u}_i \Phi_i(\vec{x})$$

- Linearize \mathcal{S} and solve with Newton-Raphson

- Adaptive refinement of grid for high mass-ratios



Evolution: First-order system

We evolve a first order representation of Einstein evolution equations:

$$\partial_t u^\alpha + A_\beta^{k\alpha} \partial_k u^\beta = F^\alpha$$

$$u^\alpha = \{g_{ab}, \Pi_{ab} = -t^c \partial_c g_{ab}, \Phi_{iab} = \partial_i g_{ab}\}$$

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Principal parts:

$$\partial_t g_{ab} - N^k \partial_k g_{ab} \simeq 0,$$

$$\partial_t \Pi_{ab} - N^k \partial_k \Pi_{ab} + N \psi^{ki} \partial_k \Phi_{iab} \simeq 0,$$

$$\partial_t \Phi_{iab} - N^k \partial_k \Phi_{iab} + N \partial_i \Pi_{ab} \simeq 0.$$

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Subject to constraints:

$$C_a = C_{iab} = 0$$

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Subject to constraints:

$$C_a = C_{iab} = 0$$

... which can grow exponentially!

$$\partial_t C \propto C$$

Constraint Damping: Example

An illustrative example :
scalar wave in flat spacetime

$$\partial_\mu \partial^\mu \psi = 0$$

First-order form:

$$\left\{ \begin{array}{l} \partial_t \psi + \Pi = 0, \\ \partial_t \Pi + \partial^i \Phi_i = 0, \\ \partial_t \Phi_i + \partial_i \Pi = 0. \end{array} \right.$$

Constraint:

$$C_i = \partial_i \psi - \Phi_i = 0$$

Constraint evolution:

$$\partial_t C_i = 0$$

Constraint Damping: Example

An illustrative example :
scalar wave in flat spacetime

$$\partial_\mu \partial^\mu \psi = 0$$

Modified first-order form:

$$\left\{ \begin{array}{l} \partial_t \psi + \Pi = 0, \\ \partial_t \Pi + \partial^i \Phi_i = 0, \\ \partial_t \Phi_i + \partial_i \Pi = \gamma_2 C_i \end{array} \right.$$

Constraint violations exponentially
damped:

$$\partial_t C_i = -\gamma_2 C_i \implies C_i(t) = C_i(0) e^{-\gamma_2 t}$$

Constraint Damping: Einstein Equations

With damping terms, evolution equations expanded:

Modified first-order form:

$$\partial_t \psi_{ab} - (1 + \gamma_1) N^k \partial_k \psi_{ab} = -N \Pi_{ab} - \gamma_1 N^i \Phi_{iab},$$

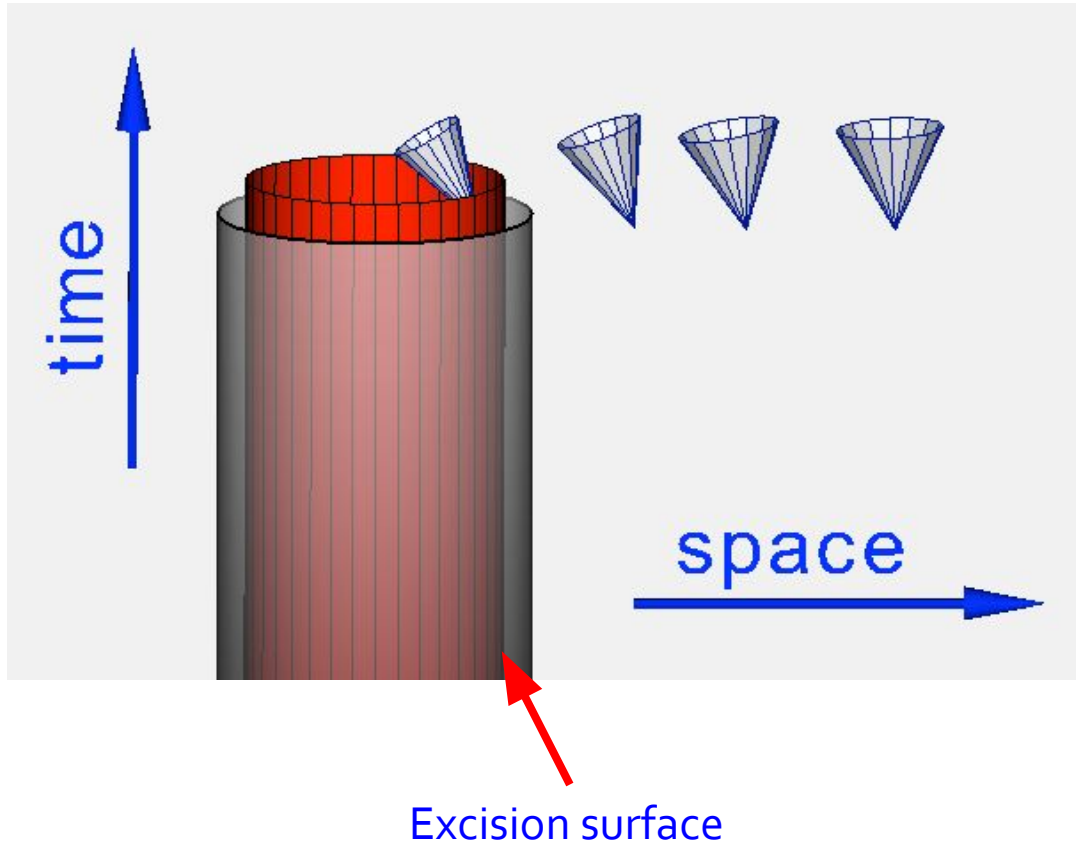
$$\begin{aligned} \partial_t \Pi_{ab} - N^k \partial_k \Pi_{ab} + N \psi^{ki} \partial_k \Phi_{iab} - \gamma_1 \gamma_2 N^k \partial_k g_{ab} \\ = 2N g^{cd} (\psi^{ij} \Phi_{ica} \Phi_{jdb} - \Pi_{ca} \Pi_{db} - g^{ef} \Gamma_{ace} \Gamma_{bdf}) \\ - 2N \nabla_{(a} H_{b)} - N t^c t^d \Pi_{cd} \Pi_{ab} - N t^c \Pi_{ci} \psi^{ij} \Phi_{jab} \\ + N \gamma_0 [2\delta_{(a}^c t_{b)} - g_{ab} t^c] (H_c + \Gamma_c) - \gamma_1 \gamma_2 N^i \Phi_{iab}, \end{aligned}$$

$$\begin{aligned} \partial_t \Phi_{iab} - N^k \partial_k \Phi_{iab} + N \partial_i \Pi_{ab} - N \gamma_2 \partial_i g_{ab} \\ = \frac{1}{2} N t^c t^d \Phi_{icd} \Pi_{ab} + N \psi^{jk} t^c \Phi_{ijc} \Phi_{kab} - N \gamma_2 \Phi_{iab}. \end{aligned}$$

Constraint violations exponentially damped!

$$\begin{aligned} C_a (= \Gamma_a + H_a) &\propto e^{-\gamma_0 t} \\ C_{iab} (= \partial_i g_{ab} - \Phi_{iab}) &\propto e^{-\gamma_2 t} \end{aligned}$$

Singularity treatment: excision

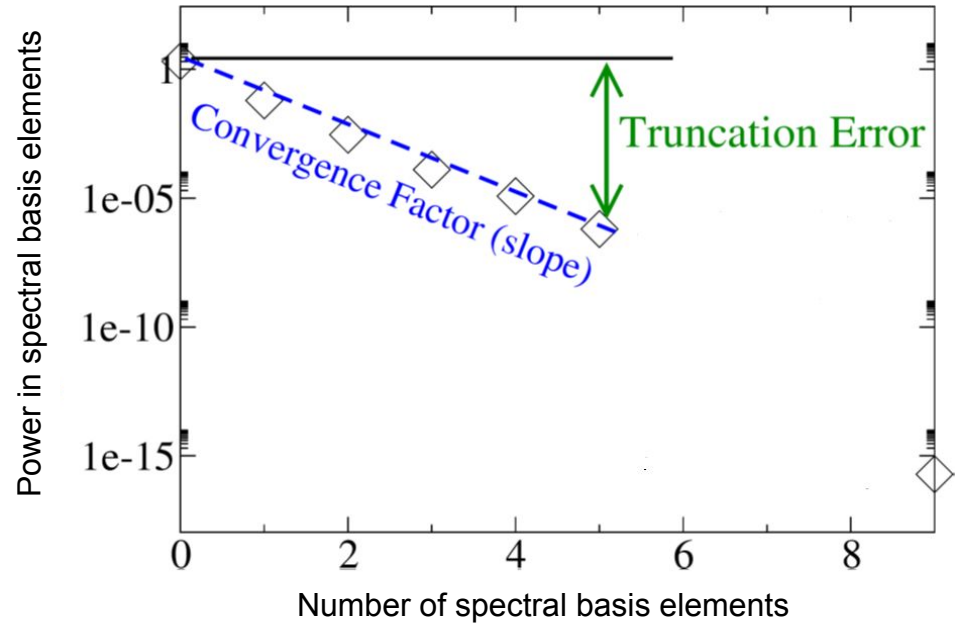


- Formulation of field equations is causal
- No boundary conditions required
- The excision boundary must track the shape and motion of the horizon

Robustness: Adaptive Mesh Refinement

Truncation error (or spectral basis representation error) is the primary accuracy diagnostic

Can be specified and thresholded on in a spacetime dependent manner

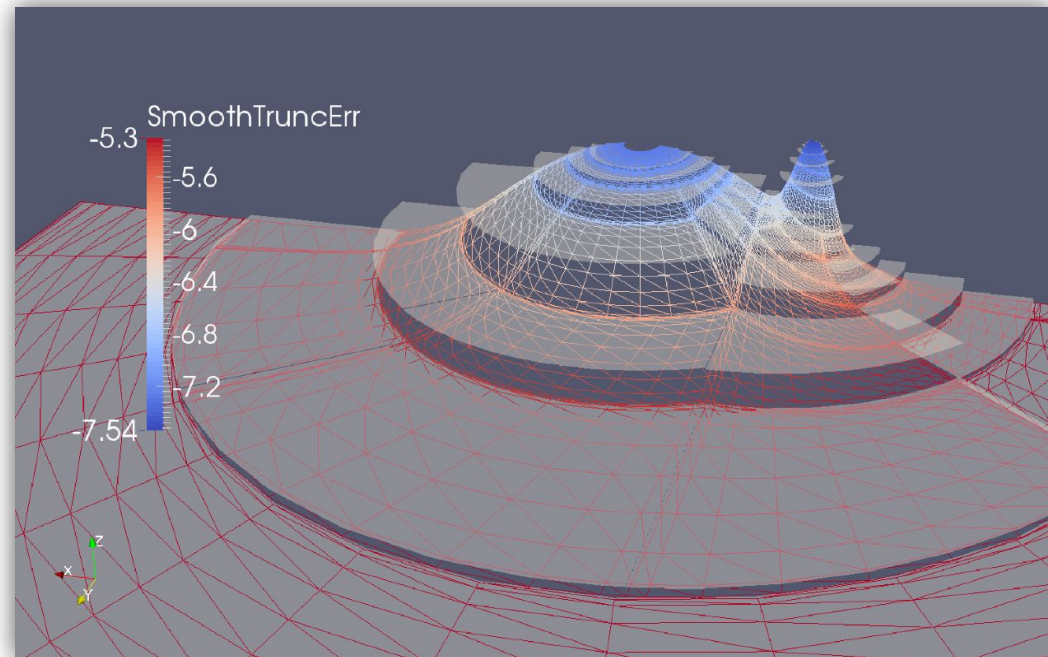
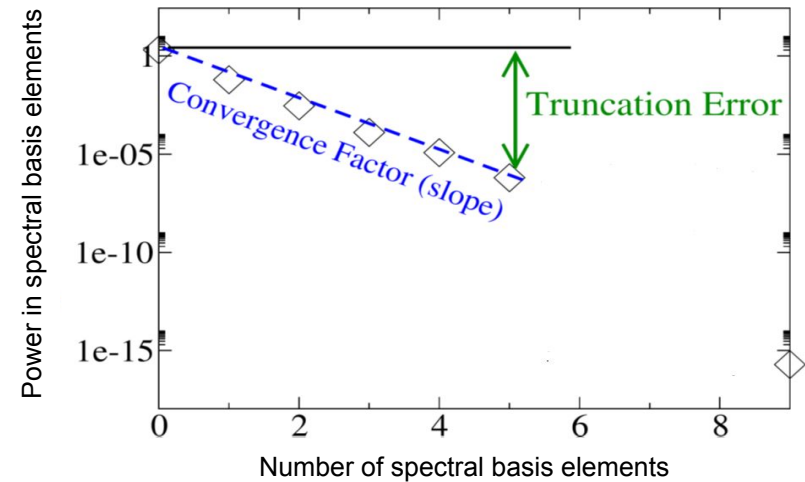


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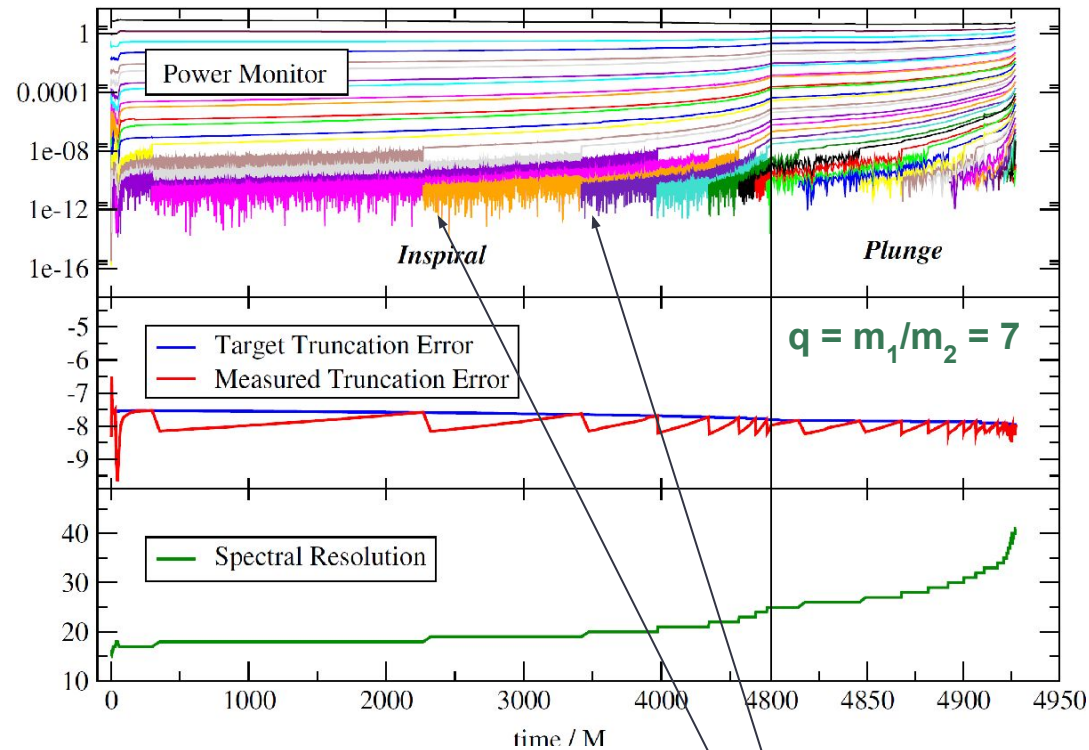
Numerical/Grid resolution is controlled through truncation error. We can get desired resolution in physically more interesting regions, without increasing it in the large wave-zone.



Robustness: Adaptive Mesh Refinement

Based on truncation error:

Type I: Collocation points added, domain structure unchanged



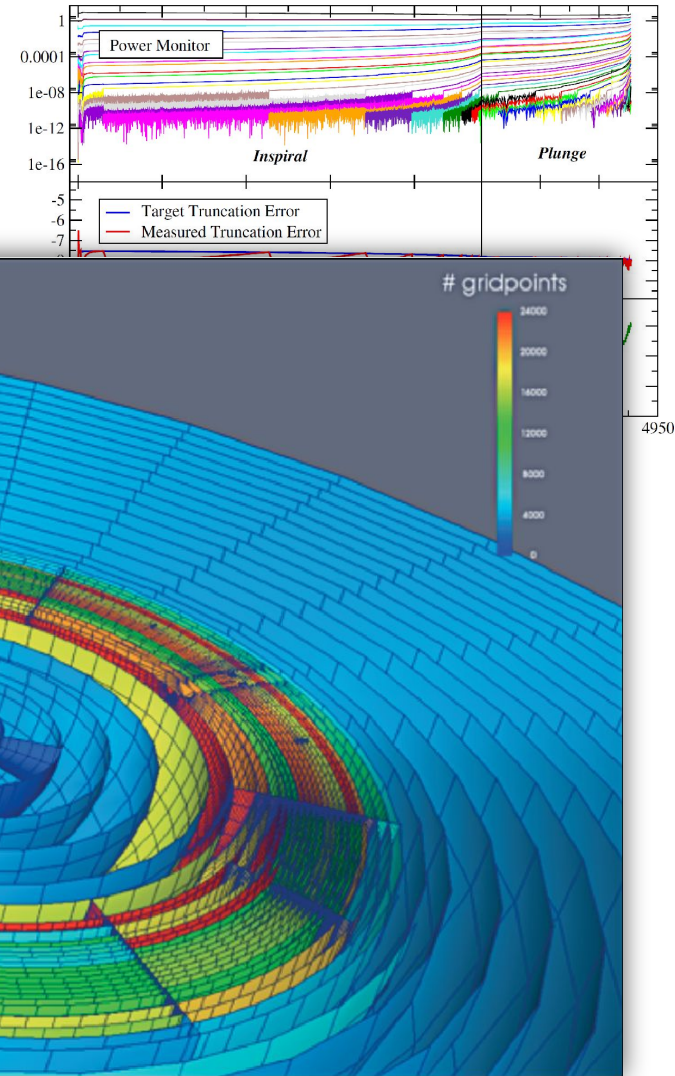
Add a spectral basis element when:
truncation error > target

Robustness: Adaptive Mesh Refinement

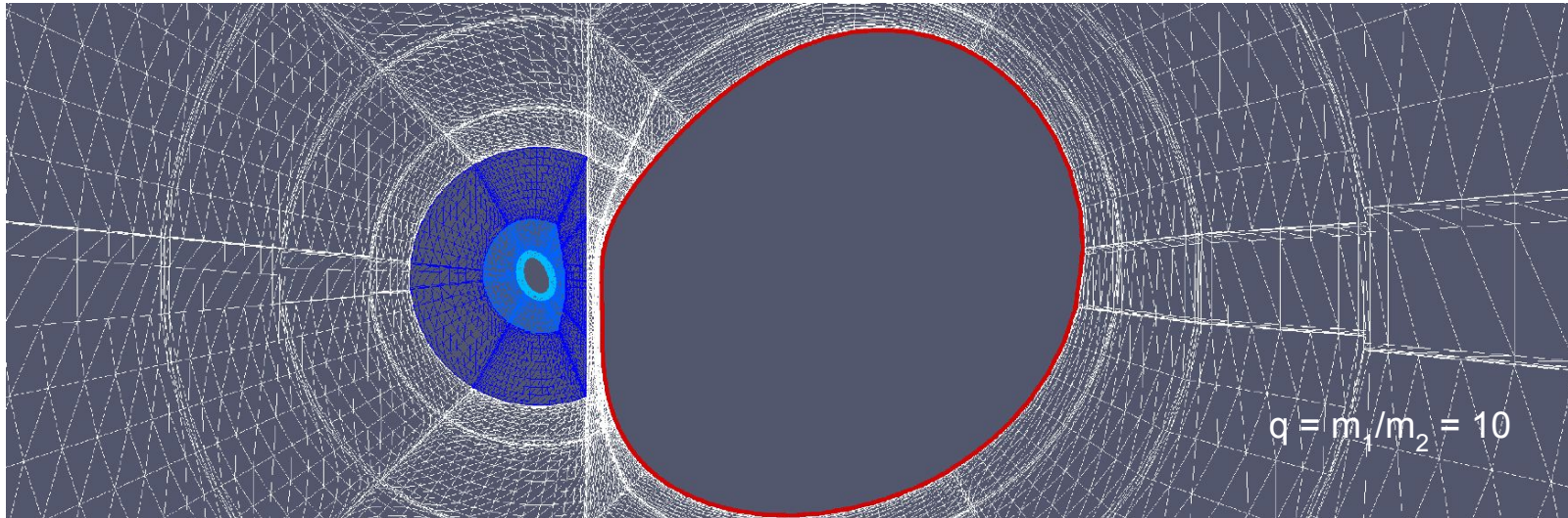
Based on truncation error:

Type I: Collocation points added, domain structure unchanged

Type II: Sub-domain boundaries re-drawn. Splitting or Merging of subdomains.



Robustness: Control Systems



- Compute (apparent) horizons often
- Sub-domains smoothly deformed to track the horizons' shape and position :
- Feedback-loop control of the coefficients : R_{lm}

$$r_H = \sum_{l,m} R_{lm} Y^{lm}(\theta, \phi)$$

What made it challenging:

Multiple length/time scales, Courant limit, Accuracy required

1. Multiple length/time scales
2. Which coordinates to use (for a spacetime one doesn't know yet)?
3. Putting Black holes (singularity) on a grid
4. Einstein constraints grew exponentially
5. Resolving shocks (discontinuities)
6. Computational Challenges
7. High accuracy required by LIGO

What still makes it challenging

1. Multiple length/time scales
2. ~~Which coordinates to use (for a spacetime one doesn't know yet)?~~
3. ~~Putting Black holes (singularity) on a grid~~
4. ~~Einstein constraints grew exponentially~~
5. Resolving shocks (discontinuities)
6. Computational Challenges
7. High accuracy required by LIGO



Spectral Einstein
Code (SpEC)

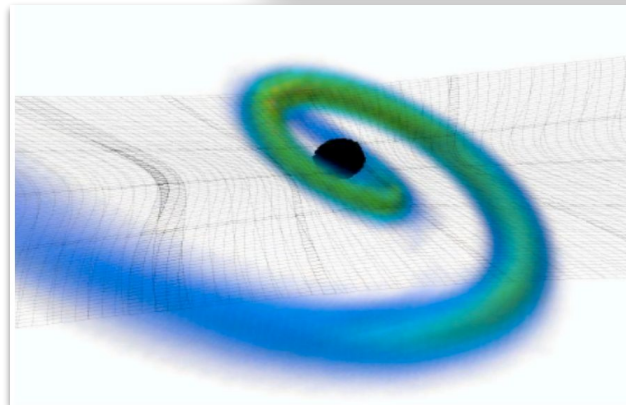
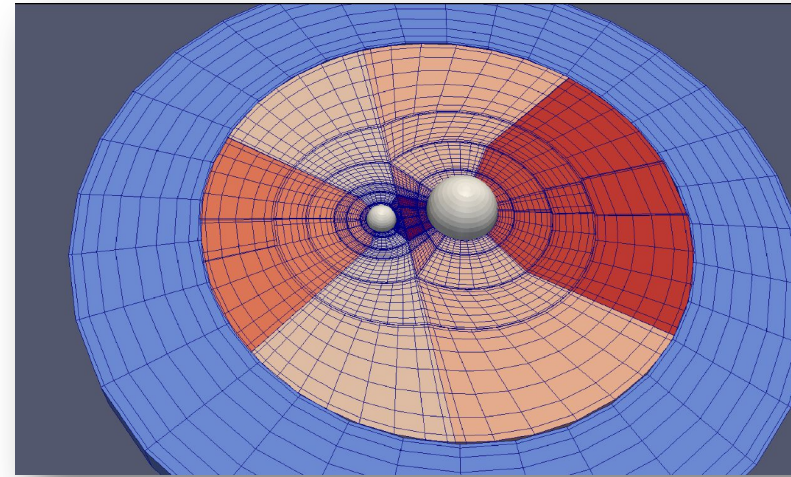


SIMULATING EXTREME SPACETIMES
Black holes, neutron stars, and beyond...



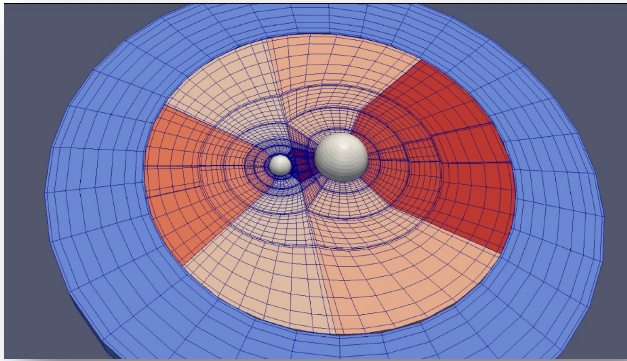
What still makes it challenging

1. Multiple length/time scales
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4. ~~Einstein constraints grew exponentially~~
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6. Computational Challenges
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Back to the drawing board

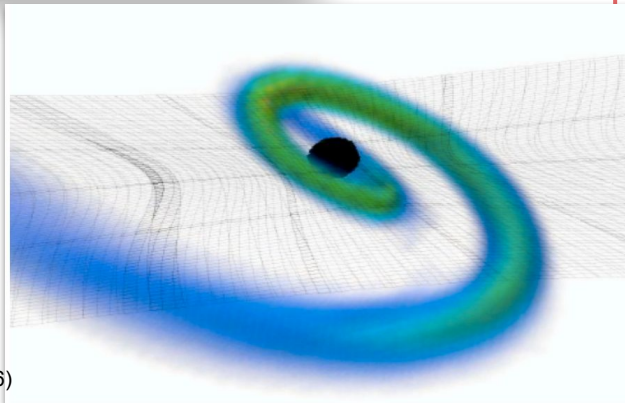
1. Multiple scales
2. Computational Challenges
3. Shocks
4. High accuracy



1. Discretization scheme that:
 - a. is local at high order
 - b. can handle discontinuities
 - c. amenable to inhomogeneous grid

1. Parallelization scheme that can scale, and use all computing available

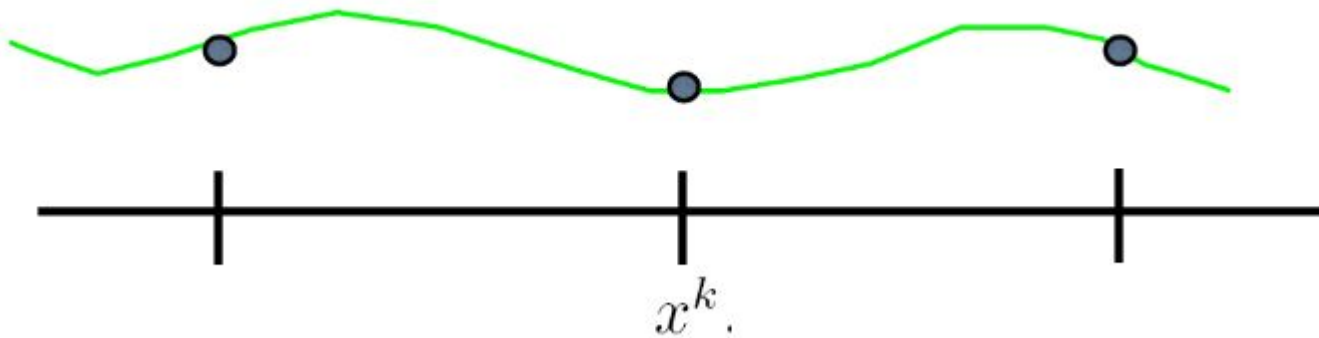
1. Local time-stepping to handle multiple time scales



Discretization: Finite Difference Methods

- Domain is a **set of collocation points**
- Solution represented **locally as a polynomial**
- Derivatives require stencils

Local at low-order	↑
Local at high-order	↓
Handle discontinuities	↑
Inhomogeneous grids	↑



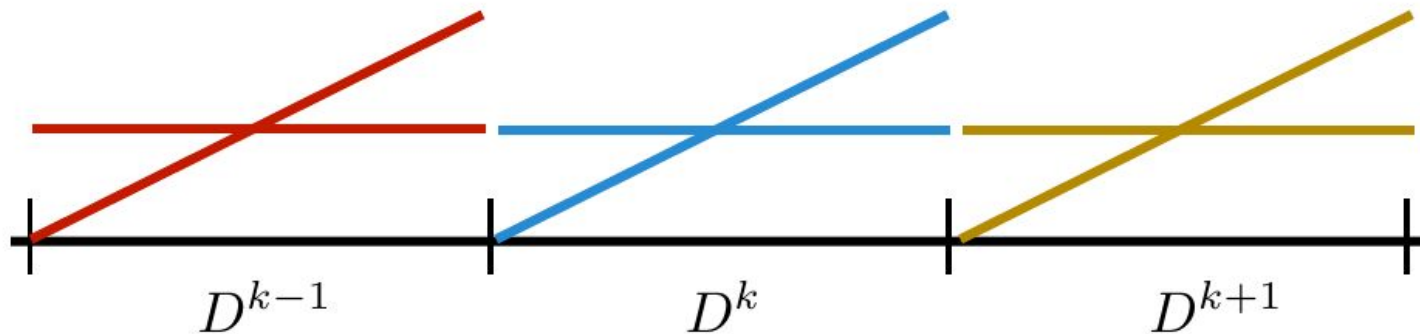
Discretization: Spectral Methods

- Solution expanded on a **local basis**



SIMULATING EXTREME SPACETIMES
Black holes, neutron stars, and beyond...

Spectral Einstein Code (SpEC)



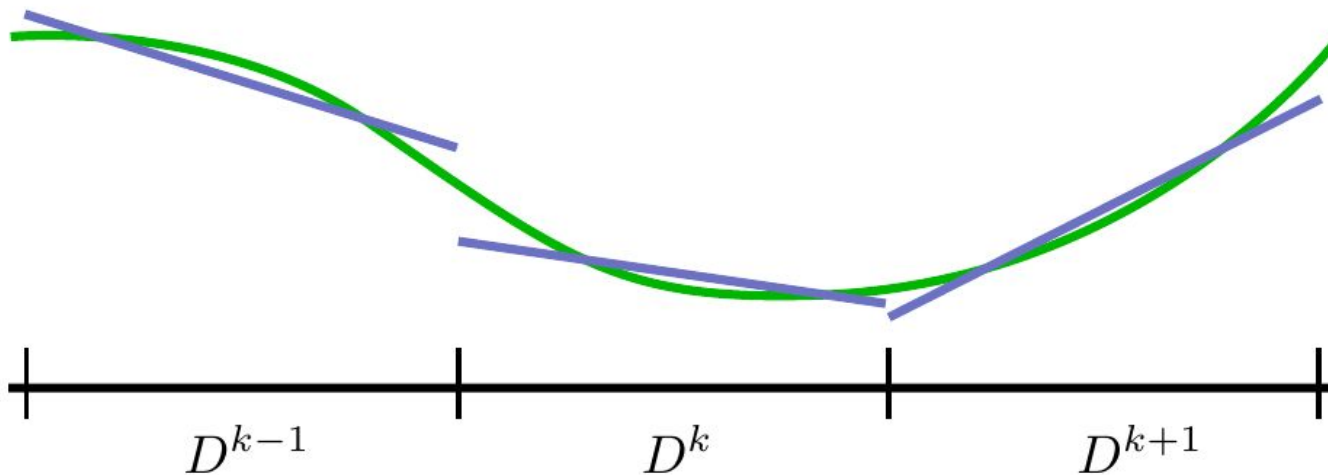
Discretization: Spectral Methods

- Solution expanded on a **local basis**
- Local high order \Rightarrow **exponential convergence in smooth regions**



SIMULATING EXTREME SPACETIMES
Black holes, neutron stars, and beyond...

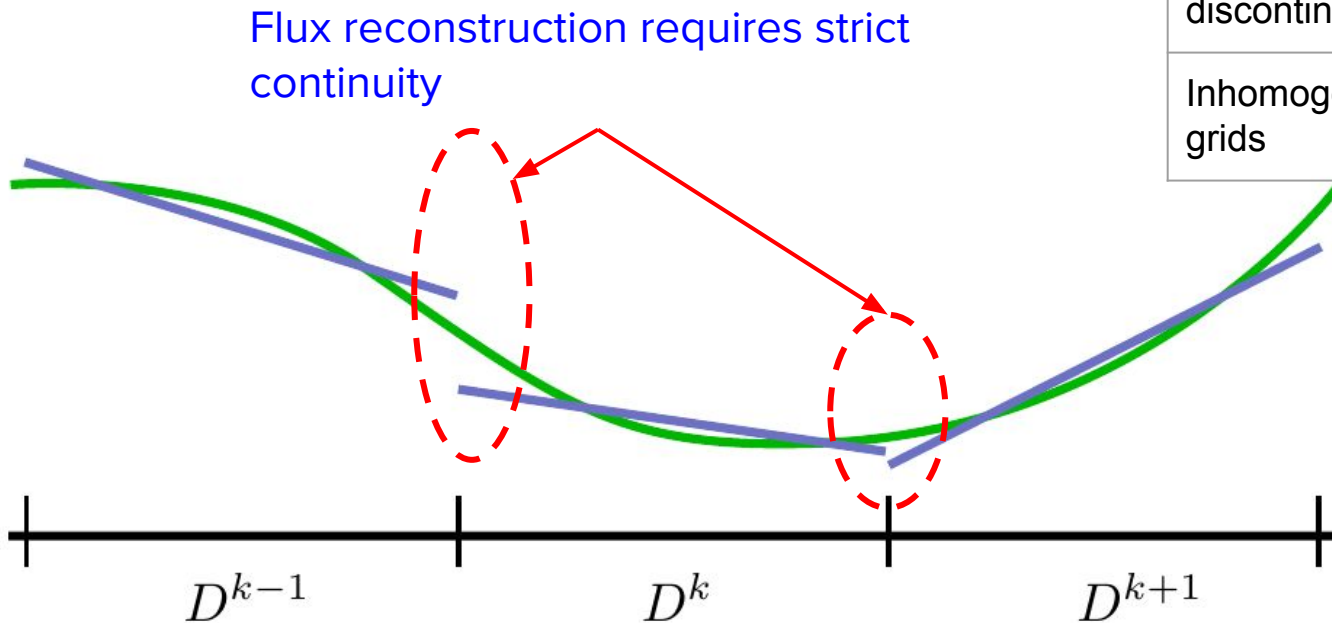
Spectral Einstein Code (SpEC)



Discretization: Spectral Methods

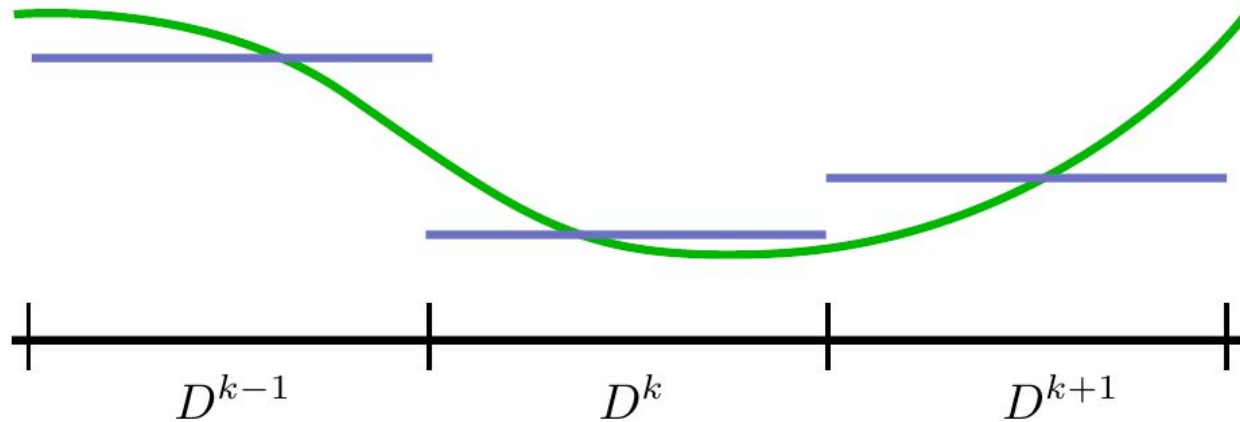
- Solution expanded on a **local basis**
- Local high order \Rightarrow **exponential convergence in smooth regions**
- ... **but flux cannot handle discontinuities / shocks**

Local at low-order	↑
Local at high-order	↑
Handle discontinuities	↓
Inhomogeneous grids	↑



Discretization: Finite Volume Methods

- Solution represented by **cell averages**

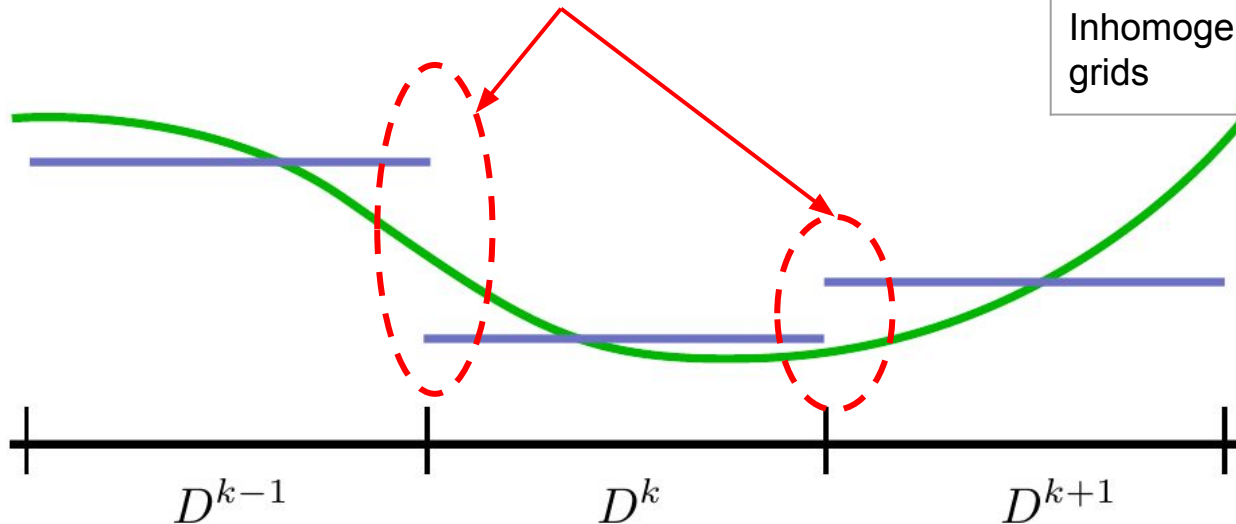


Discretization: Finite Volume Methods

- Solution represented by **cell averages**
- Flux reconstruction can handle shocks
- ... **but high order requires wide stencils** (as in FD)

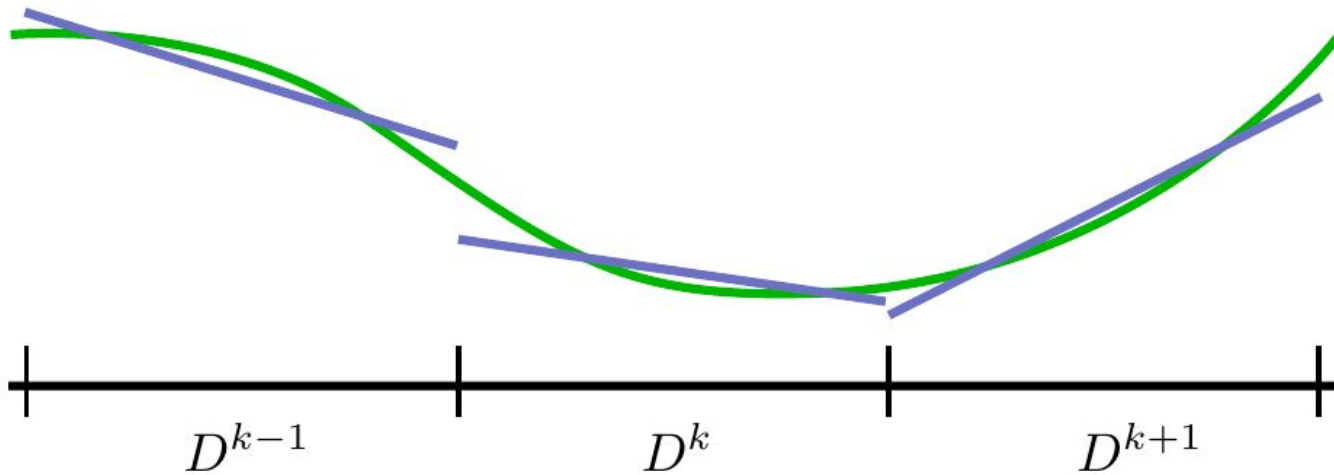
Local at low-order	↑
Local at high-order	↓
Handle discontinuities	↑
Inhomogeneous grids	↑

Flux reconstruction needed



Discretization: Discontinuous Galerkin (DG)

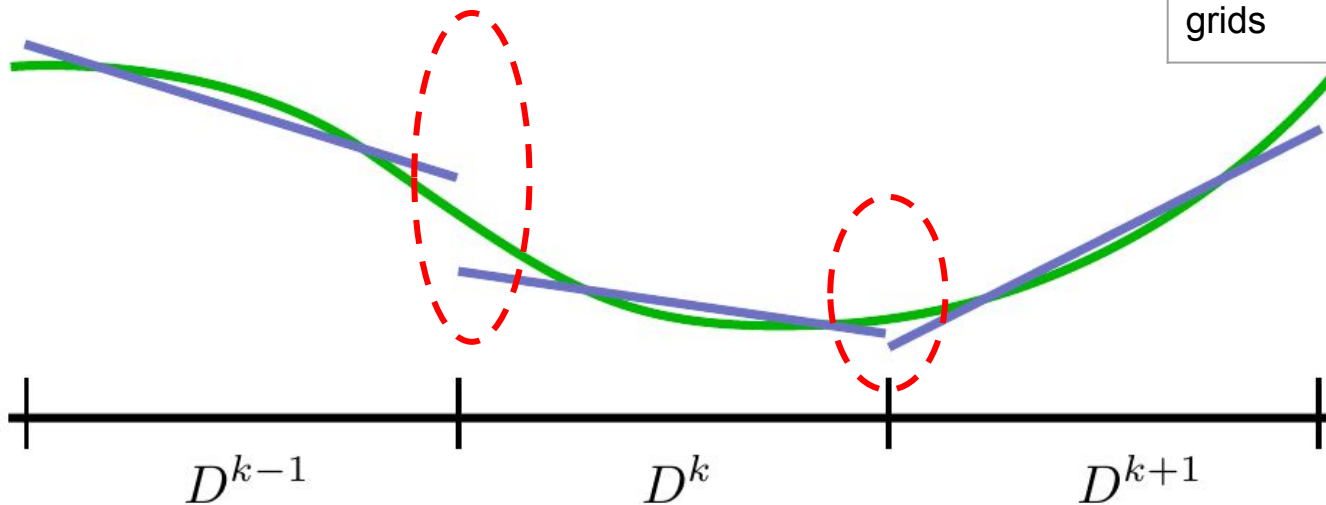
- Solution expanded on a **local basis**



Discretization: Discontinuous Galerkin (DG)

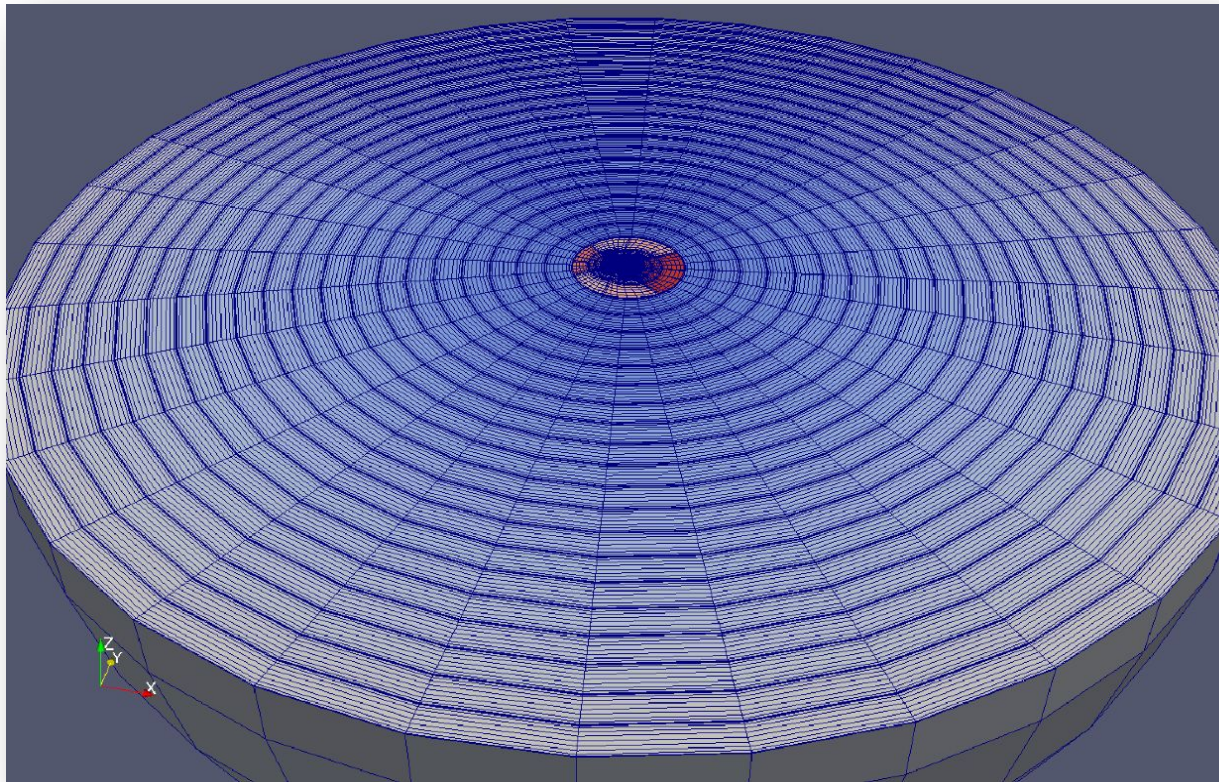
- Solution expanded on a **local basis**
- Exponential convergence in smooth regions
- ... **and formulation allows “arbitrary” fluxes** \Rightarrow **can handle shocks!**

Local at low-order	↑
Local at high-order	↑
Handle discontinuities	↑
Inhomogeneous grids	↑



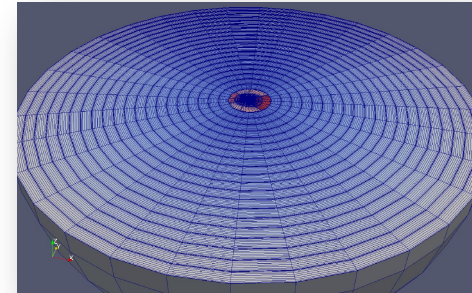
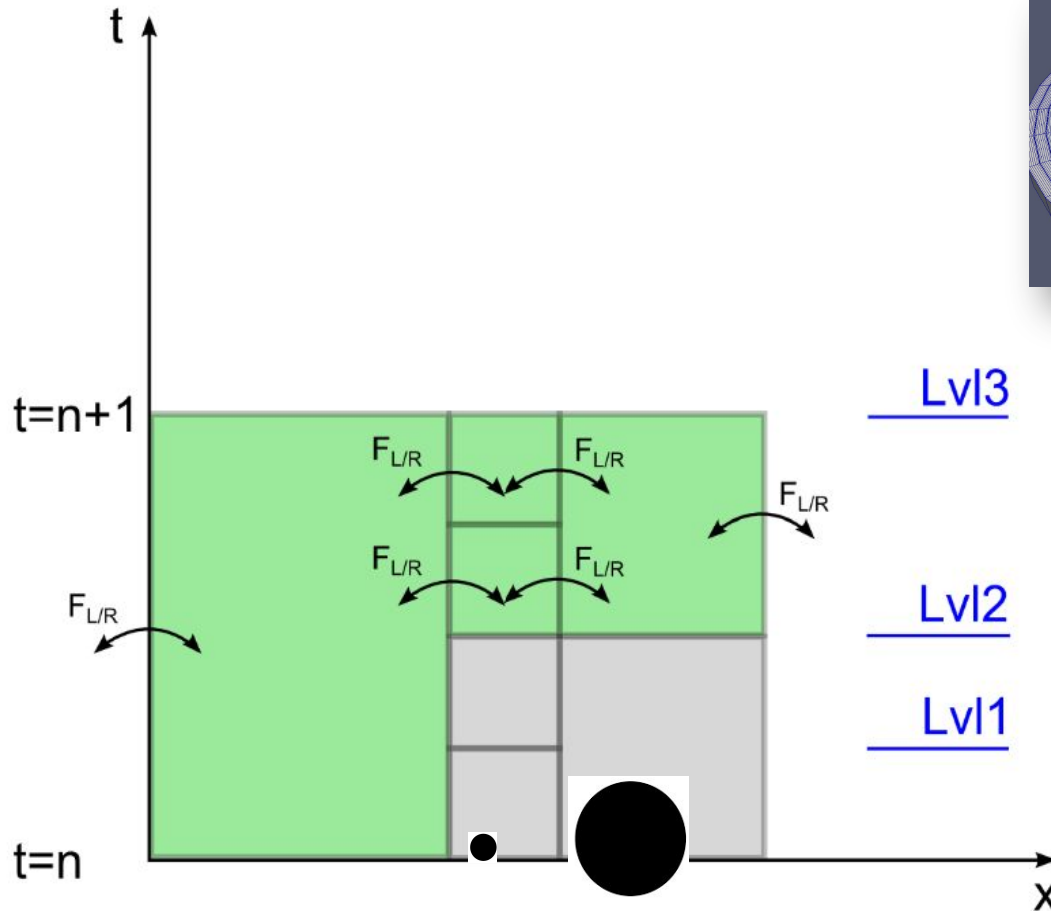
Local time-stepping

- Evolve the solution in time depending on the local needs
- No wastage of computing due to one corner with high-frequency activity

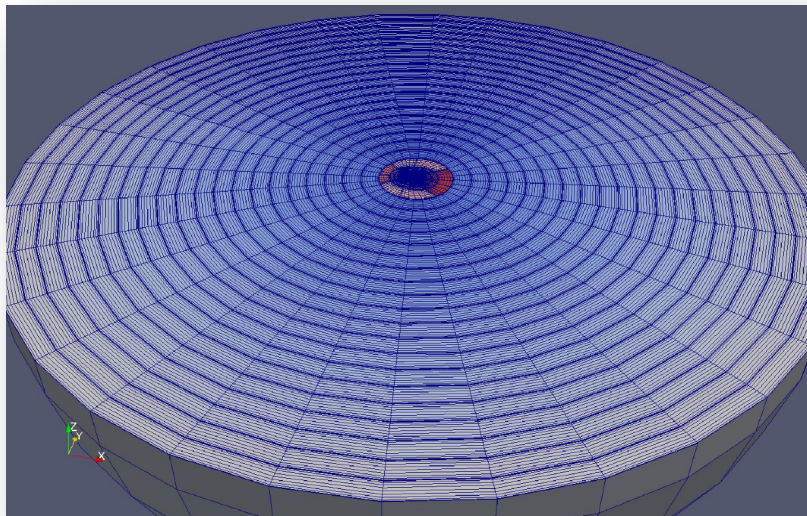
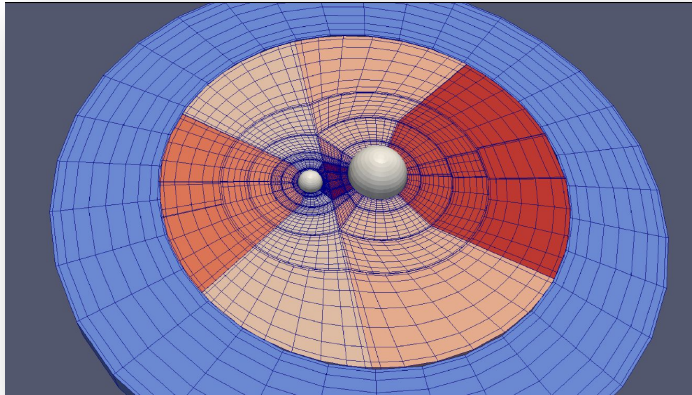


Local time-stepping

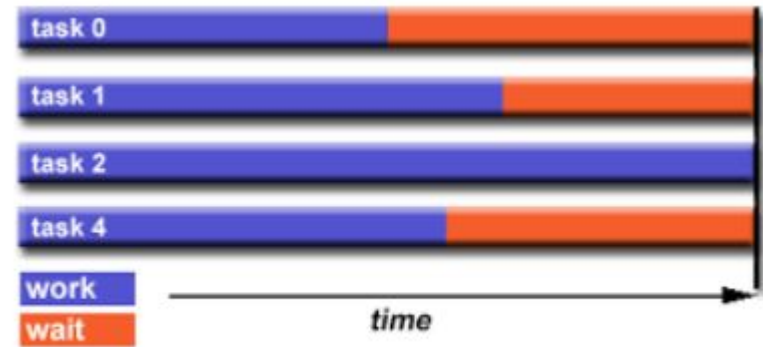
- Evolve the solution in time depending on the local needs
- No wastage of computing due to one corner with high-frequency activity



Parallelization scheme: MPI Domain based



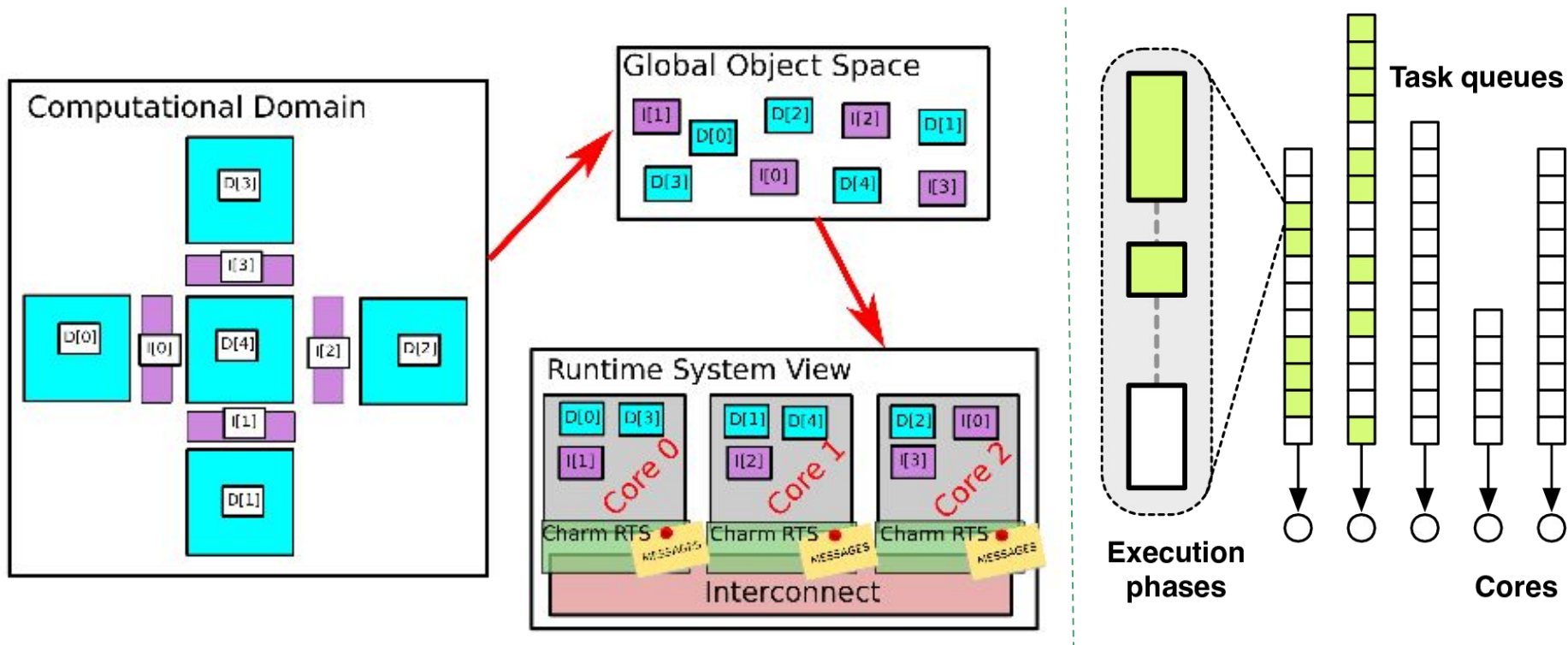
- Allocate one domain element per core
- Use MPI



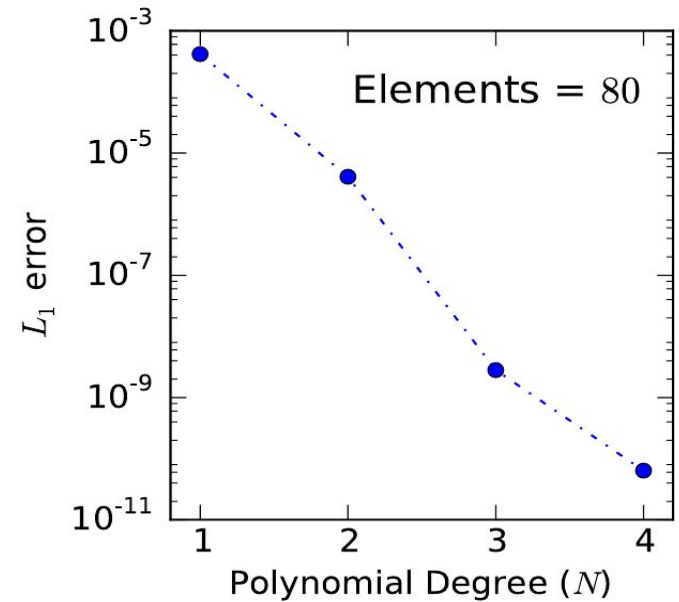
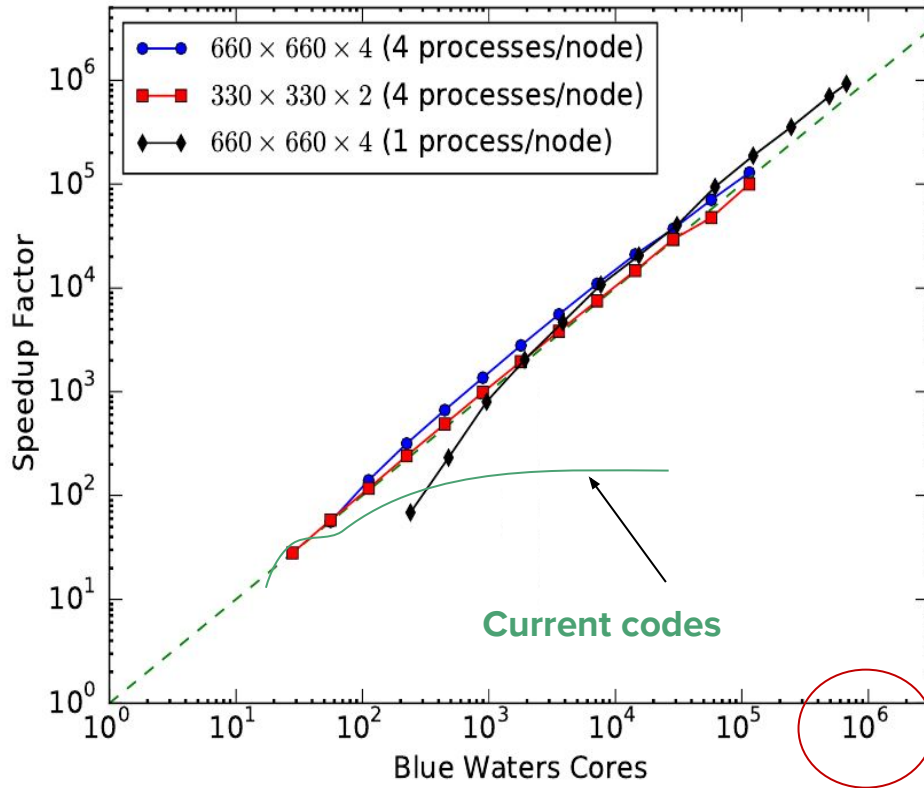
⇒ ...terrible terrible idea for systems with length scales that span several orders of magnitude!

Parallelization scheme: Task-based

- Divide computation by tasks, not physical domain
- Make communication of data between elements also a task
- Communication-cost hidden behind computation

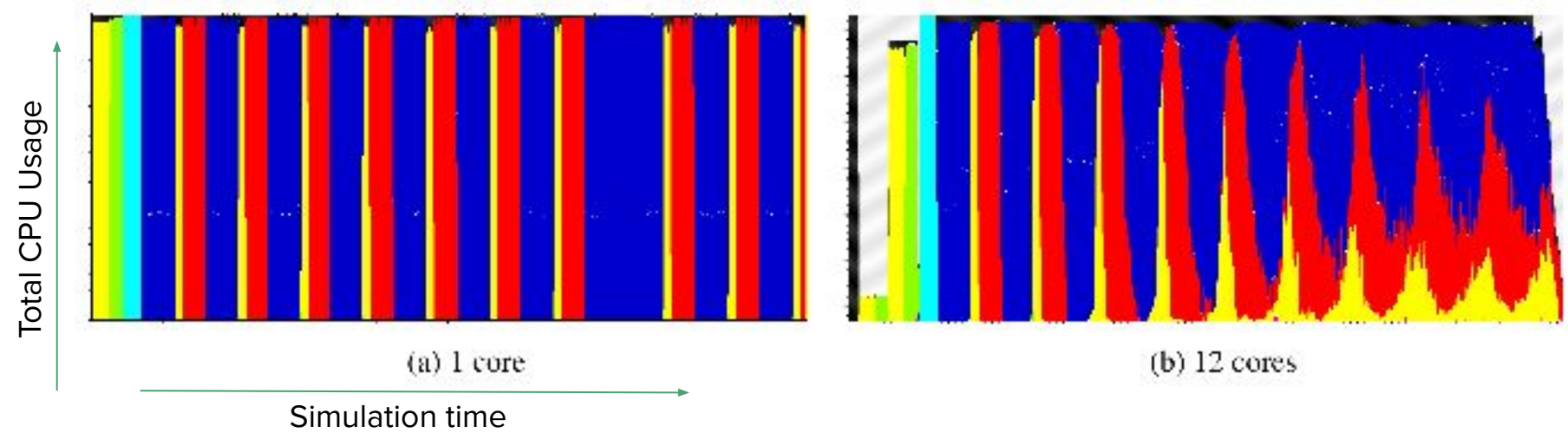


SpECTRE: scaling

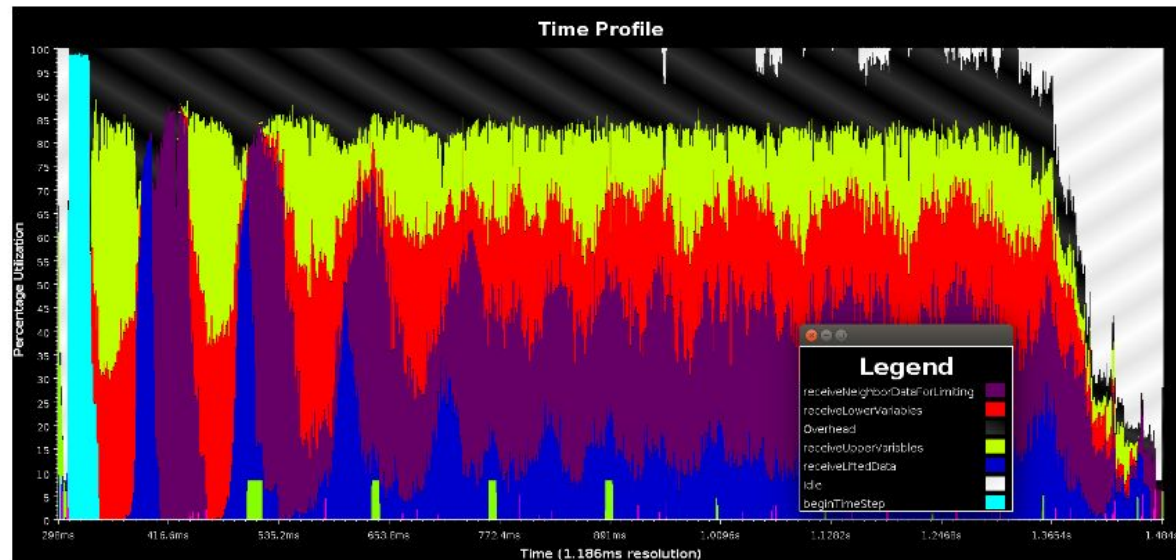
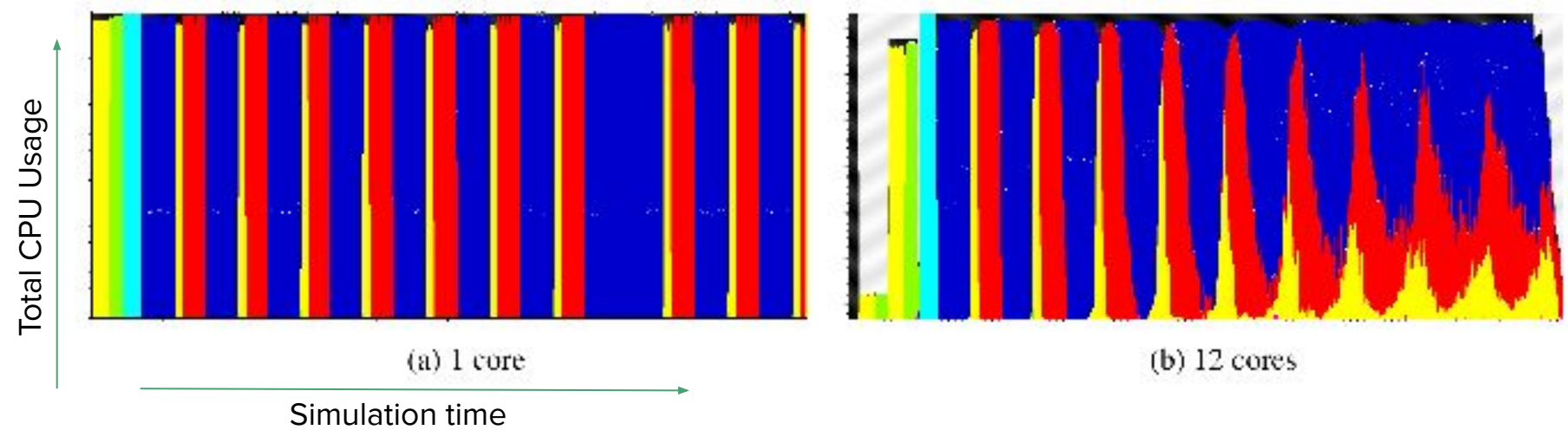


- SpECTRE aims to **combine the high-order accuracy of spectral methods with the local nature of finite-volume/element methods**
- **Future proof:** Computing efficiently scales to $\sim 600,000$ cores. Future proof: exascale computing!

SpECTRE: parallelism



SpECTRE: parallelism



Red/Yellow: data to interfaces (hides RHS vol.)
 Blue: fluxes to elements
 Cyan: setup

Purple: slope limiting
 Black: Charm++

White: idle

Summary

1. **Spectre** is a radically forward-looking computational (astro)physics code that adopts cutting-edge computing paradigms:

- DG-FEM discretization**
- Local time-stepping**
- Task-based parallelism**

1. **TBP will enable exascale computing**

2. **Einstein/MHD equations implemented**

3. **Boundary treatment nearly complete**

1. **Need control systems!**

1. **Spectre is open-source!**

<https://github.com/sxs-collaboration/spectre>

sxs-collaboration / spectre

Unwatch 15 Unstar 73 Fork

<> Code Issues 307 Pull requests 60 Discussions Actions Projects 7 Security Insights

develop 3 branches 2 tags Go to file Add file Code

sxs-bot Prepare release 2020.01.11 f291da7 1 minute ago 6,760 commits

.github	Upload and download release notes so they can be reviewed	5 days ago
.travis	Update Charm to v6.10.2	5 months ago
cmake	Merge pull request #2741 from wthrowel/clang_optimizer	3 days ago
containers	Build charm++ with O2 in container	7 days ago
docs	Merge pull request #2738 from nilsleiffischer/fix_release_on_protecte...	3 days ago
external	Make finding Python in build system more robust	20 days ago
src	Merge pull request #2740 from fmahebert/cleanup_coord_maps	2 days ago
support	Update libxsmm on ocean to 1.16.1	3 days ago
tests	Merge pull request #2700 from nilsdeppe/boundary_correction_random	yesterday
tools	Prevent TODO comments in CI	5 days ago
.clang-format	Fix clang-format style with older and newer versions	14 months ago
.clang-tidy	Add clang-tidy config file	last month
.gitignore	Add configuration files to quick-start new users with VSCode	last month
.style.yapf	Add yapf style file for formatting python code	12 months ago
.travis.yml	Update Charm to v6.10.2	5 months ago
CMakeLists.txt	Fix version strings that had leading zeros stripped	20 days ago
LICENSE.txt	Update copyright year to 2020	12 months ago
Metadata.yaml	Prepare release 2020.01.11	1 minute ago
README.md	Prepare release 2020.01.11	1 minute ago

About

SpECTRE is a code for multi-scale, multi-physics problems in astrophysics and gravitational physics.

[spectre-code.org/](#)

Readme

View license

Releases 2

Release 2020.01.11 (Latest) 1 minute ago

+ 1 release

Packages

No packages published

Contributors 29

+ 18 contributors

Languages

C++ 94.2% CMake 2.6% Python 2.6% Shell 0.6%

README.md

license MIT c++ 17 Tests failing coverage 56% codecov 99% release v2020.01.11 DOI 10.5281/zenodo.4421023

What is SpECTRE?

SpECTRE is an open-source code for multi-scale, multi-physics problems in astrophysics and gravitational physics. In

Thank You for Listening!

Questions?

