Numerical Relativity Simulations of Merging Binaries:

Key Insights, Challenges, and Prospects for the Future

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compact-binaries.org

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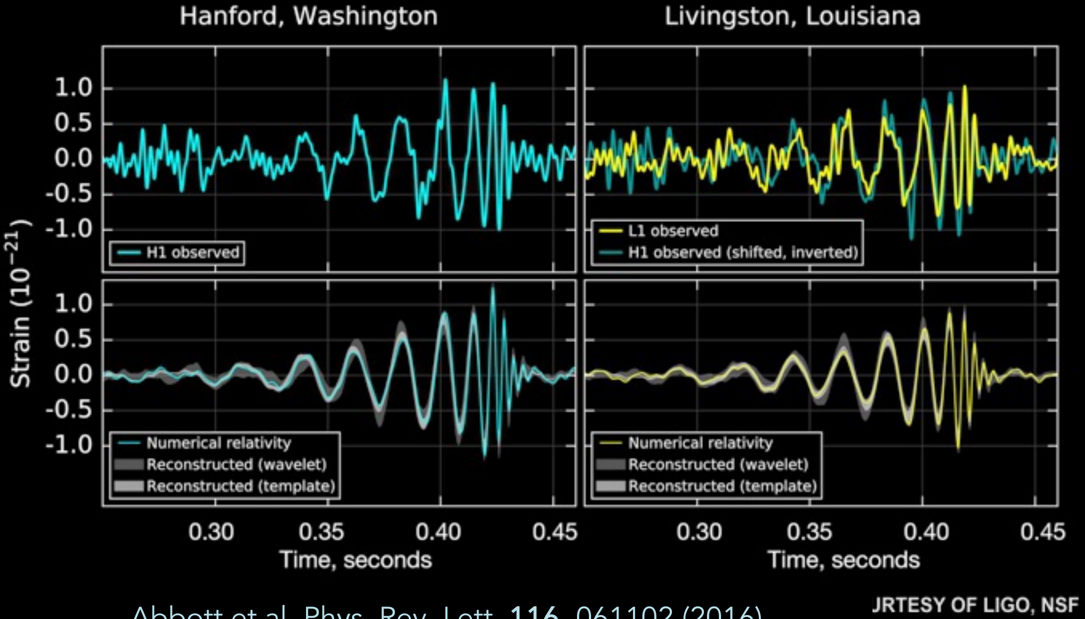
The role of NR in the first observation of GWs from a Binary Black Hole (BBH) merger

NR has been historically tied to gravitational-wave (GW) observations.

The serendipitous case of GW150914



Abbott et al, Phys. Rev. Lett. **116**, 061102 (2016)

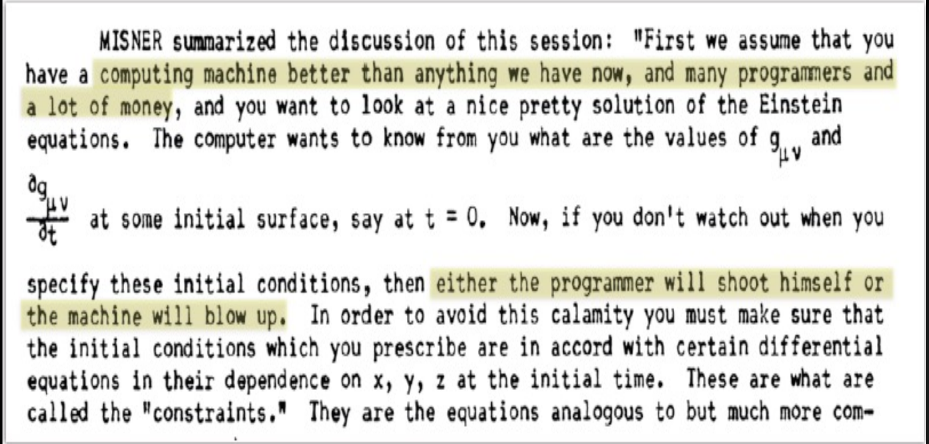
"I have bet these numerical relativists that gravitational waves will be detected from black-hole collisions before their computations are sophisticated enough to simulate them. I expect to win … but hope to lose, because the simulation results are crucial to interpreting the observed waves."

K.S. Thorne, in R.H. Price, ed., *The Future of Spacetime* (W.W. Norton, New York, 2002).

``I heaved a sigh of relief; perhaps I would actually lose my bet!"

K.S. Thorne, LIGO and Gravitational Waves, III: Nobel Lecture, December 8, 2017.

There a lot of History in NR...



MISNER summarized the discussion of this session: "First we assume that you have a computing machine better than anything we have now, and many programmers and a lot of money, and you want to look at a nice pretty solution of the Einstein equations. The computer wants to know from you what are the values of $g_{\mu\nu}$ and $\frac{\partial g_{\mu\nu}}{\partial t}$ at some initial surface, say at $t = 0$. Now, if you don't watch out when you specify these initial conditions, then either the programmer will shoot himself or the machine will blow up. In order to avoid this calamity you must make sure that the initial conditions which you prescribe are in accord with certain differential equations in their dependence on x, y, z at the initial time. These are what are called the "constraints." They are the equations analogous to but much more com-

Charlie Misner (1957)

GR 1: Conference on the role of gravitation in physics
University of North Carolina, Chapel Hill [January 18-23, 1957]

``I heaved a sigh of relief; perhaps I would actually lose my bet!"

K.S. Thorne, LIGO and Gravitational Waves, III: Nobel Lecture, December 8, 2017.

It took more than four decades for numerical relativity (NR) to solve on solving the BBH problem …

Then in 2005 there were breakthroughs

Pretorius 2005, Baker+2006, Campanelli+ 2006

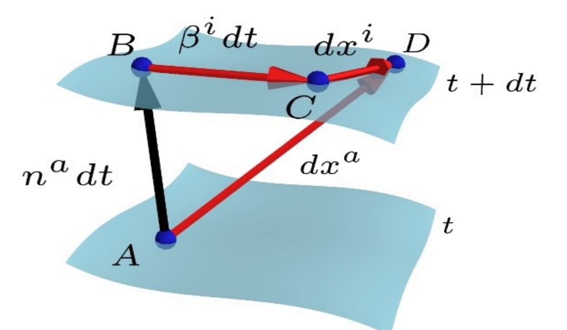
and codes didn't blow-up anymore …

Kip Thorne (2017)

NR Codes Today

Most of them uses:

- The 3+1 formulation (Choquet-Bruhat 1956, Arnowitt+1959, Shibata+1987, 1995, Baumgarte+1999)
- The moving puncture gauge (Baker+ & Campanelli+ 2005)



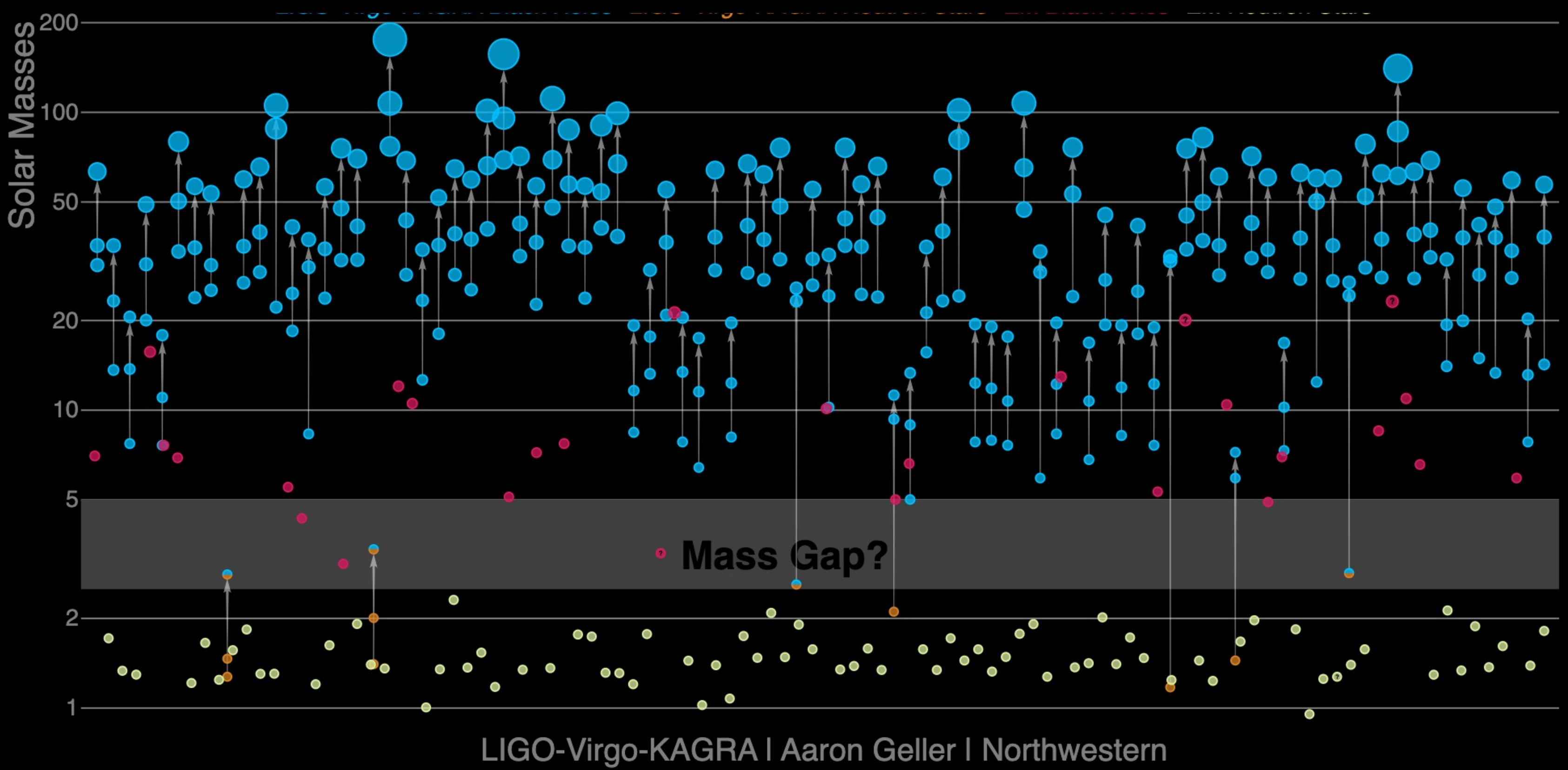
Baumgarte, NASEM Webinar 2019

Code	Open Source	Catalog	Formulation	Hydro	Beyond GR
AMSS-NCKU [43–46]	Yes	No	BSSN/Z4c	No	Yes
BAM [47–49]	No	[18]	BSSN/Z4c	Yes	No
BAMPS [50, 51]	No	No	GHG	Yes	No
COFFEE[52, 53]	Yes	No	GCFE	No	Yes
Dendro-GR [54–56]	Yes	No	BSSN/CCZ4	No	Yes
Einstein Toolkit [57, 58]	Yes	No	BSSN/Z4c	Yes	Yes
*Canuda [59–62]	Yes	No	BSSN	No	Yes
*IllinoisGRMHD [63]	Yes	No	BSSN	Yes	No
*LazEv [37, 64]	No	[65–68]	BSSN+CCZ4	No	No
*Lean [69, 70]	Partially	No	BSSN	No	Yes
*MAYA [71]	No	[71]	BSSN	No	Yes
*NRPy+ [72]	Yes	No	BSSN	Yes	No
*SphericalNR [73, 74]	No	No	spherical BSSN	Yes	No
*THC [75–77]	Yes	[18]	BSSN/Z4c	Yes	No
ExaHyPE [78]	Yes	No	CCZ4	Yes	No
FIL[79]	No	No	BSSN/Z4c/CCZ4	Yes	No
FUKA [80, 81]	Yes	No	XCTS	Yes	No
GR-Athena++ [82]	Yes	No	Z4c	Yes	No
GRChombo [83–85]	Yes	No	BSSN+CCZ4	No	Yes
HAD [86–88]	No	No	CCZ4	Yes	Yes
Illinois GRMHD [89, 90]	No	Yes	BSSN	Yes	No
MANGA/NRPy+ [91]	Partially	No	BSSN	Yes	No
MHDuet [92, 93]	No	No	CCZ4	Yes	Yes
SACRA-MPI [94]	No		BSSN+Z4c	Yes	No
SpEC [95, 96]	No	[96, 97]	GHG	Yes	Yes
SpECTRE [98, 99]	Yes	No	GHG	Yes	No
SPHINCS_BSSN [100]		No	BSSN	SPH	No

Foucart++ snowmass arXiv:2203.08139

LIGO/Virgo Compact Binary Mergers Today!

Today, NR simulations are routinely used to model compact binary mergers with black holes (BH) and neutron stars (NS), and there are a lot of them!



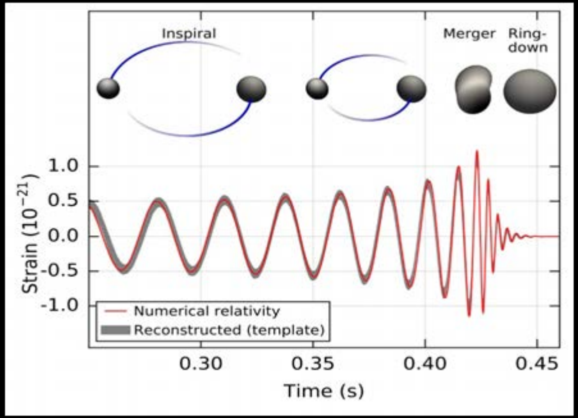
Status of NR Calculations of BBH Waveforms

- GW waveform models are essential to infer source parameters such as masses, BHs effective spins, distance, NSs radius and EoS of matter, etc.

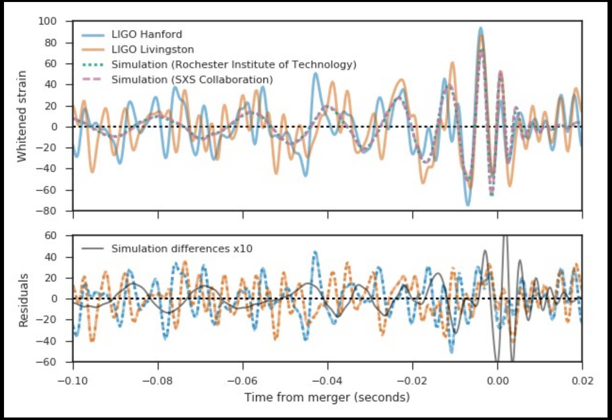
- NR calculations are used to build PN+NR hybridized and phenomenological models, and to calibrate EoB models. Surrogate models are interpolated from NR simulations. Similarly, tidal deformation models are used to extract information from BNS signals.

- Direct NR simulations are also used to build GW templates.
  - ➢ See for example, RIFT: Rapid inference via Iterative FiTting, Lange & O'Shaughenessy (RIT/UTA)

- Today, there are thousands of such NR calculations and templates for a variety masses spins, eccentricity and waveforms lengths, but they are mostly focused on BBH mergers.

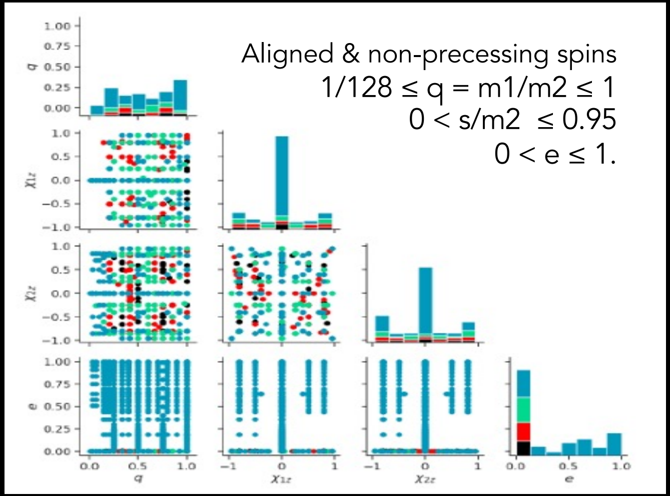


NR waveform modeling GW150914



RIT NR waveform of GW170104 (precessing spinning BBH) 10 x better than residuals.

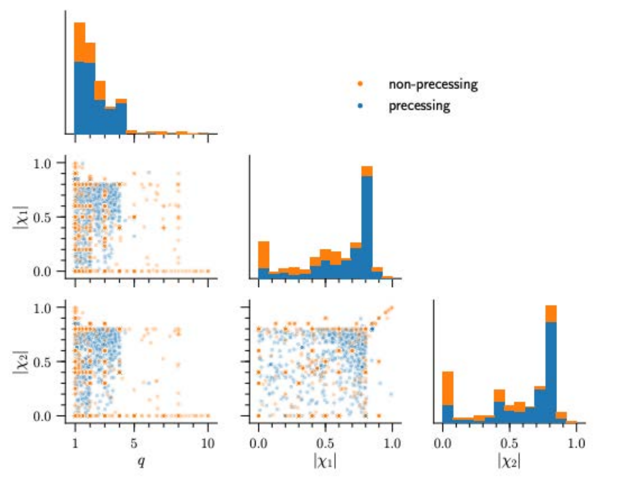
NR Waveform Catalogs for BBH



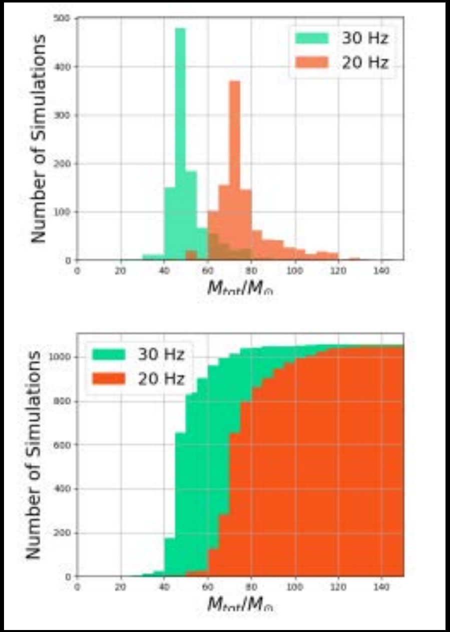
RIT waveform catalogs, ~2000+ waveforms - Healy+2017,2019,2020,2022

- BBH with q~150:1 and 1000:1 (12 orbits) – Healy &Lousto+2022.
- Set of 600+ eccentric BBH (GW190521 with highly eccentric merger (e~0.69; 90% credible level) V. Gayathri ++. Nature Astron. (2022).

The SXS catalog, 2000+ waveforms, including surrogates with 20 orbits - Mroue+2013, Boyle++ 2019



With all catalogs, very high spins remain challenging, especially with unequal masses, and very high mass ratios remain challenging!

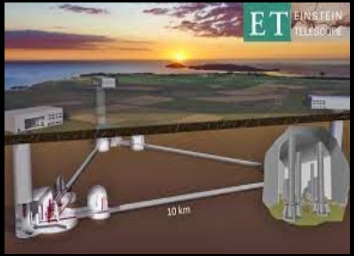


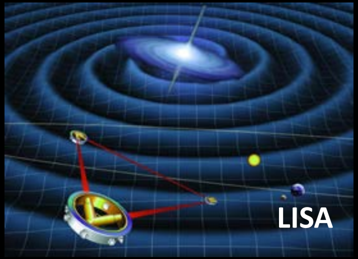
Healy+2022

Still too few waveforms at 20Hz and lower …

Future GW Observations

In the 2030s, observations from 3G detectors and LISA will allow us to do precision GW astronomy, SNR ~ O(1000) or greater.

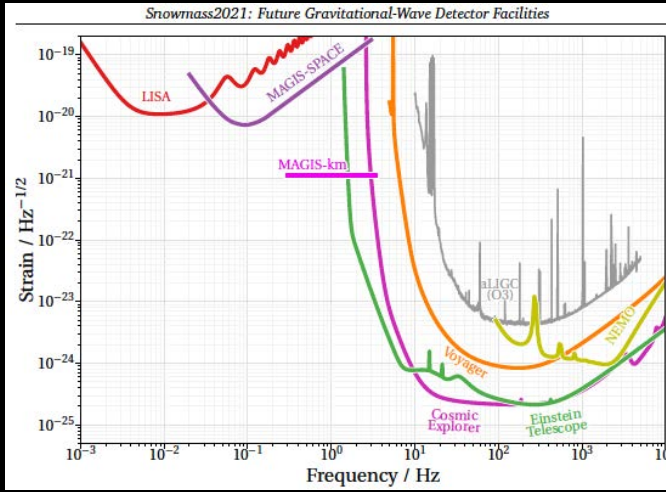




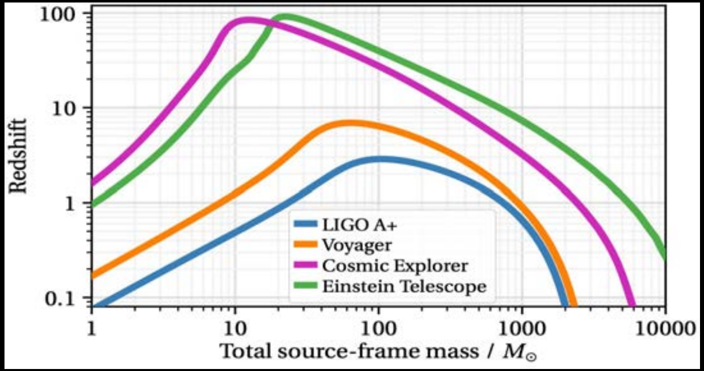
They will allow us to observe BHs and NSs across cosmic time!

We will then completely nail down their astrophysical origin and history, and their relation to the surrounding environment; e.g. multi-spectrum GW combining 3G + LISA – e.g. Vitale+2018, Sesana 2016, Breivik+2016, Rodriguez+2017;

We will be able to study the physics of extreme dense matter; e.g. NS nuclear physics, and do precision test of GR.

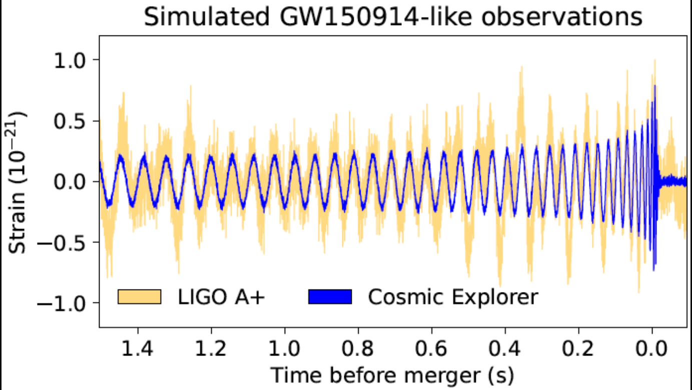


Ballmer++ snowmass arXiv:2203.08228

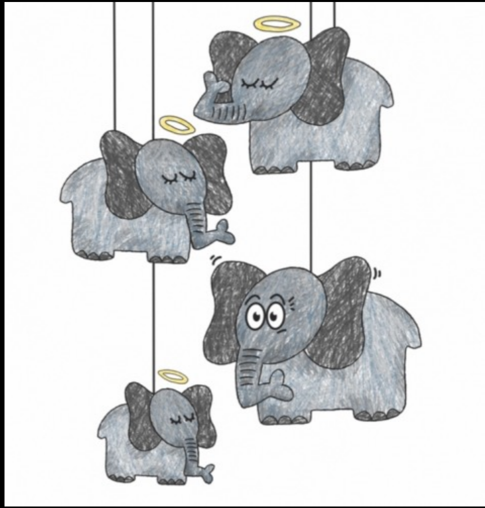


Ready for Next-Generation GW Science?

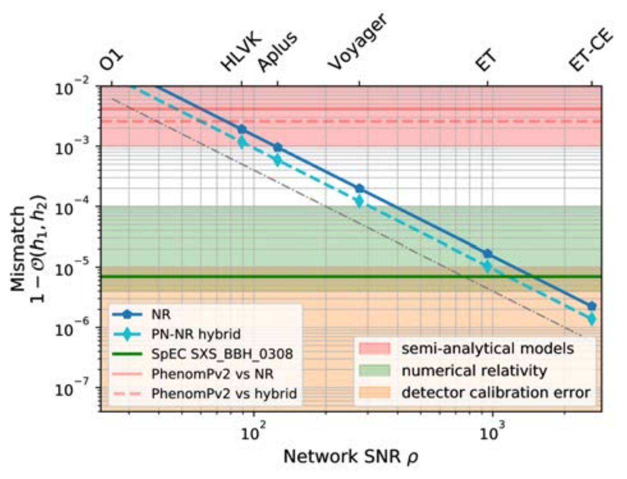
Waveform accuracy, length and parameter space coverage need to improve for future GW observations with 3G detectors and LISA - Puerrer and Haster, 2020, Ferguson++, 2021



Foucart++ snowmass arXiv:2203.08139



Elephants in the Room (Broadway North ...)



Puerrer and Haster, 2020

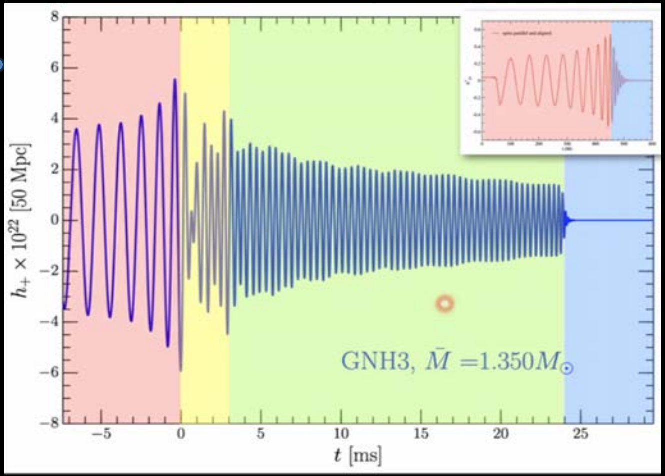
- Errors in current NR BBH waveforms need to be decreased by an order of magnitude and errors in semi-analytical waveform models need to be decreased by three orders of magnitude.
- GWs from merging BBH in 3G detectors and LISA will be in band for longer periods of time which will require much longer NR waveforms.
- For BNS, analytical models (via tidal deformations) and NR waveforms (~10 ms), limited accuracy, physics, parameters, etc …

BNS waveforms tell a complex story…

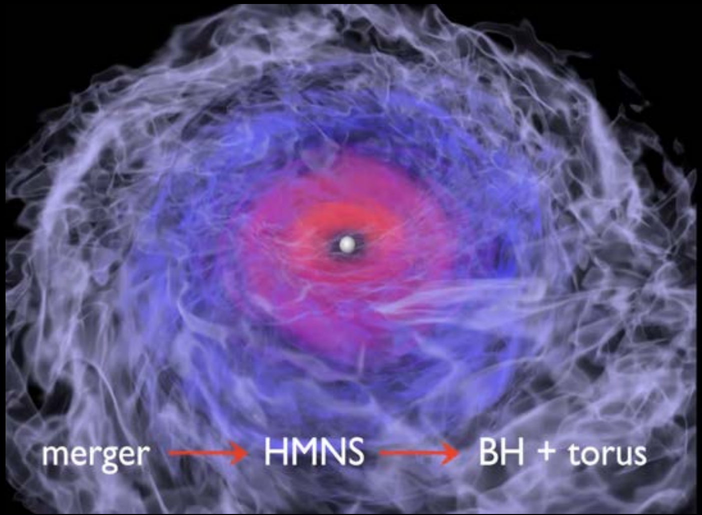
- For black holes the process is very simple:
  - ➢ BH + BH → BH + GWs

- For BNS, the merger leads to an hyper-massive neutron star (HMNS), i.e. a metastable equilibrium:
  - ➢ NS + NS → HMNS + debris/ejecta + … → BH + disk + jet … → BH + GWs

- Hence, BNS waveforms differ in the merger and postmerger phases due to:
  - ➢ ×total mass (prompt vs delayed collapse to a BH remnant)
  - ➢ ×mass asymmetries and merger debris (HMNS and disk)
  - ➢ ×soft/stiff Equation of State (EoS) of nuclear matter …
  - ➢ ×⍰⍰neutrinos can cool the debris and disk, influence outflows …
  - ➢ magnetic fields can grow very large quickly due Kelvin-Helmholtz instability (KHI) and affect HMNS's lifetime and jet and kilonowvae!



Rezzola + 2016

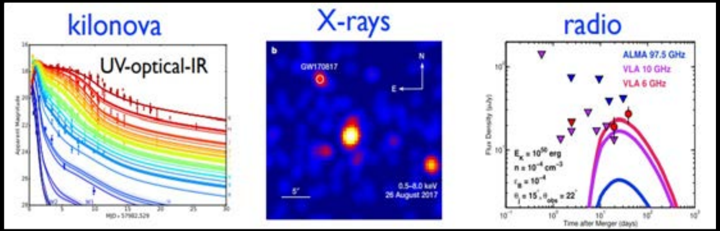


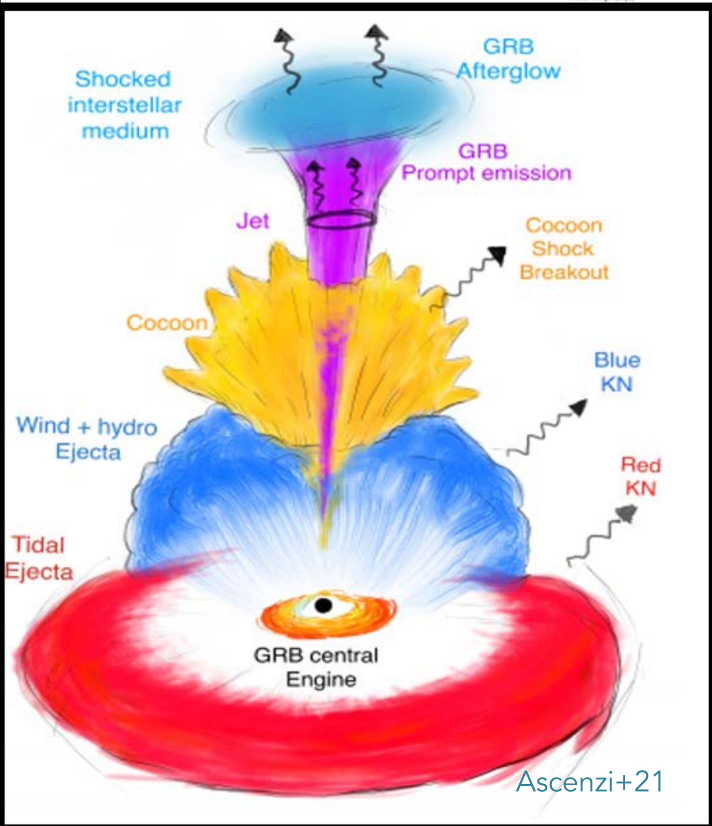
Firework from GW170817…

- The 2017 BNS merger signed the beginning of multi-messenger astronomy (MMA), but it also left us with important open questions:
  - ➢ What is the central engine of a short GRB?
  - ➢ And what is the origin of the blue kilonovae signal?

  - ➢ What is the nature of the remnant and what is the EoS?
  - ➢ How is the jet launched?
  - ➢ What is the magnetic field amplification and topology?
  - ➢ How much mass is ejected? What role neutrinos play?

- **We need GRMHD simulations of the merger and post-merger phases for self-consistent and quantitative models of ejection and their EM signature!**





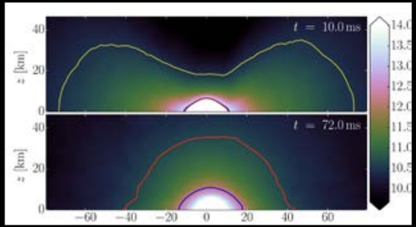
Ascenzi+21

How to launch a jet …

- Prompt collapse to a BH + disk can produce a jet after ~10 ms – e.g. Kiuchi+2015, Ruiz+2016 …

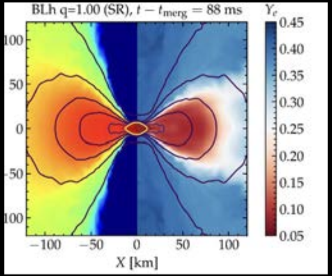
- Growing evidence that long-lived HMNS/magnetar remnants can produce collimated outflows and blue kilonova.

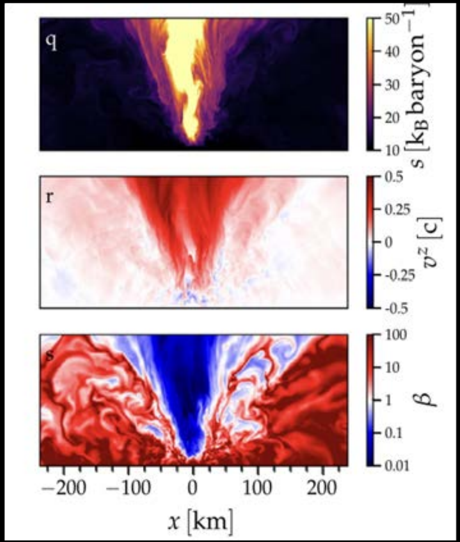
- This requires both MHD + neutrinos!



HD + neutrinos, no magnetic field: - Radice 2018, Nedora 2019, etc

MHD but no neutrinos: Ciolfi 2019, 2020, Kalinani+ in prep

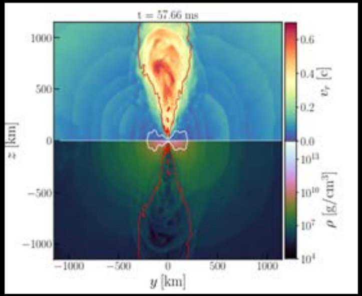




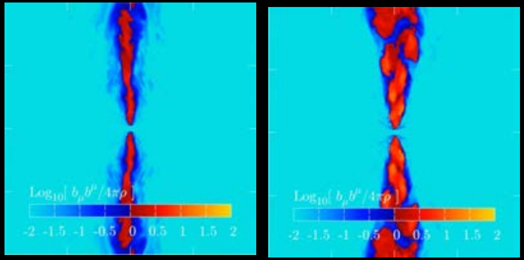
First simulations in full MHD + neutrinos - Moesta 2020, Curtis 2022 (jet before collapse but starting from large magnetic field …)

However, how to power a sGRB jet still an open question …

Need to sustain this to ~1s to get the needed large Lorentz factor …



MHD + Neutrinos + EoS: collimated outflow at ~10 ms, magnetic field + non-linear spiral wave amplification generate blue kilonova – Combi+2023

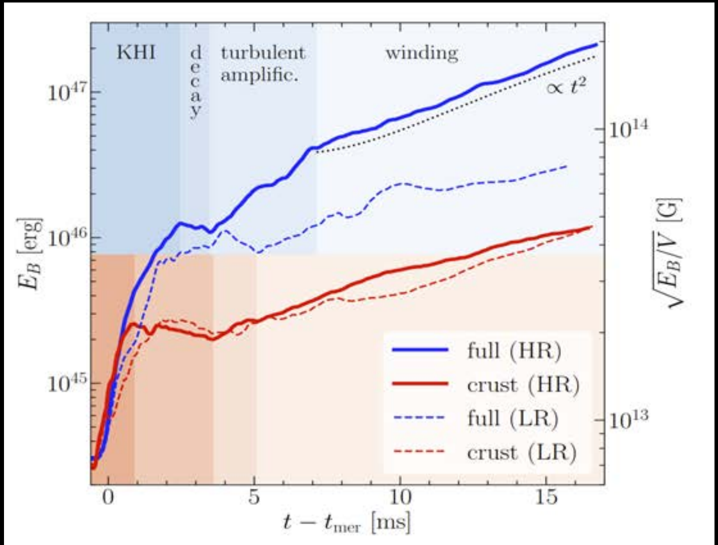


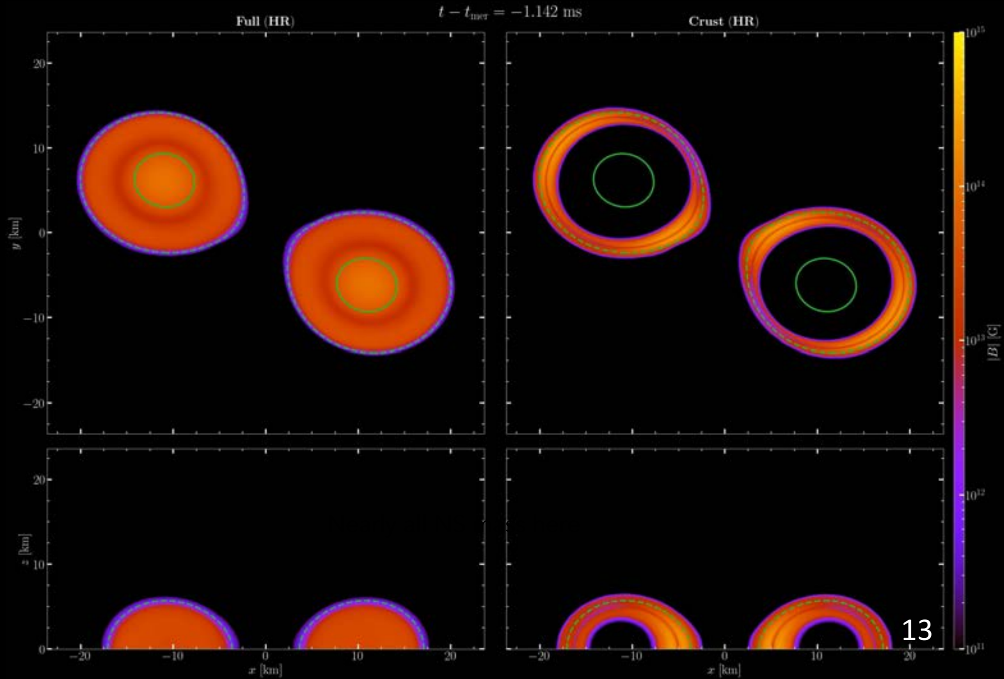
MHD +Neutrinos +EoS: collimated outflow up to 150ms, blue kilonova with resolution for **KHI** (12.5m) amplification! – Kiuchi+2023

The full enchilada is needed!

- Magnetic field amplification via the Kelvin-Helmholtz instability (KHI) can be obtained in the first ~10 ms, with sufficient resolution – Kiuchi+2015,2018

- KHI requires the physics of deep NS interior - Chabanov, in prep 2023
  - ❖ Loss of strongly magnetized matter at the surface!





A Multi-Physics Challenge

We solve NR fully coupled with MHD fluids, EoS, radiation and microphysics eqs

Gravity
Newtonian/Post-Newtonian (PN) or General Relativity (GR)

Magnetohydrodynamics (MHD)
Gas/plasma dynamics

Nuclear and Neutrino Physics
Nuclear EOS, nuclear reactions & ν interactions

Boltzmann Transport Theory
Radiation Transport (RT) and/or Neutrino Transport (NT)

$$R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = 8\pi T_{\mu\nu}\,, \text{ (Einstein equations)}$$

$$\nabla_\mu T^{\mu\nu} = 0\,, \quad \text{(cons. energy/momentum)}$$

$$\nabla_\mu (\rho u^\mu) = 0\,, \quad \text{(cons. rest mass)}$$

$$p = p(\rho, \epsilon, Y_e, \ldots)\,, \quad \text{(equation of state)}$$

$$\nabla_\nu F^{\mu\nu} = I^\mu\,, \qquad \nabla_\nu^* F^{\mu\nu} = 0\,, \quad \text{(Maxwell equations)}$$

$$\nabla_\mu T^{\mu\nu}_{\text{rad}} = S^\nu\,, \quad \text{(radiative losses)}$$

$$T_{\mu\nu} = T^{\text{fluid}}_{\mu\nu} + T^{\text{EM}}_{\mu\nu} + T^{\text{rad}}_{\mu\nu} + \ldots \quad \text{(energy} - \text{momentum tensor)}$$

(F, Padova)

Next Generation NR Codes

Current NR codes only scale to thousand of cores due to communication bottlenecks, but new techniques promise to enable scaling to millions of cores for exascale supercomputers.

- Improve the accuracy of numerical methods
  - higher order schemes in FD, FV and/or FE
  - discontinuous galerkin (DG) methods for exponential accuracy with resolution – e.g. Deppe+2021
- Improve the efficiency of codes
  - Exascale infrastructure & efficient AMR using both CPUs & GPUs – e.g Shankar + 2022
  - Task based parallelism to minimize global synchronizations and load imbalances – e.g. Daszuta+2021
  - Wavelet adaptive multiresolution representation (WAMR) – e.g. Fernando+2019
- Taking advantage of curvilinear grids with filtering techniques for time stepping – Mewes+2018 &2019, Ji+2023

NSF's Frontera system @ TACC: 38.7 petaflops, 8008 nodes (56 CPUs/node, intel Xeon processors)

DOE's Frontier system @ OLCF: 1.102 exaflops, 9,472 AMD CPUs (606,208 cores) + Radeon Instinct 37,888 GPUs (8,335,360 cores)

BNS simulations are challenging …

- Hydrodynamics simulations, using realistic tabulated EoS and approximate neutrino transport schemes can now deliver reasonably good physics (e.g. waveforms) in ~10 ms …

- Hence, magnetic fields are crucial to the evolution of BNS mergers and their post-merger remnants. This requires a lot of small-scale physics over a sustained range of time!

- Post-merger remnants likely produce collimated relativistic outflows (jets) that are currently believed to be the source of short-hard gamma-ray bursts (SGRBs).

- The growth of large-scale magnetic fields from small –scale instabilities needed for this is not sufficiently resolved, even in simulations that do not include neutrinos.

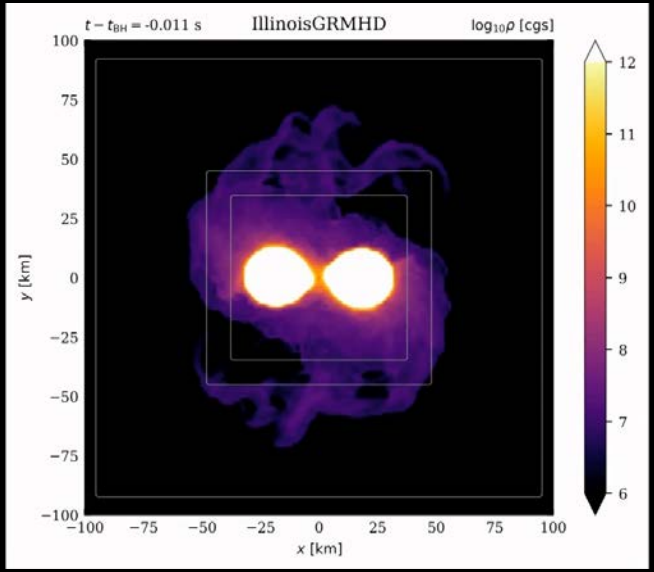
    - ❖ affordable NR simulations can resolve up to the scale of 50-100 meters, and must start with large dipolar magnetic fields ($\gtrsim 10^{15}$ G), and can run for up to ~100ms …

- Even if we can reach the key resolution how do we sustain it up to few seconds after the onset of the merger?

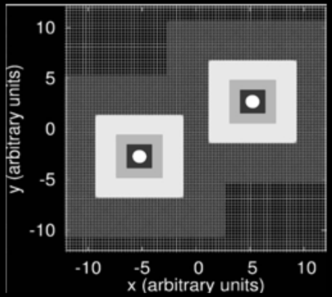
Riccardo Ciolfi (INAF, Padova)

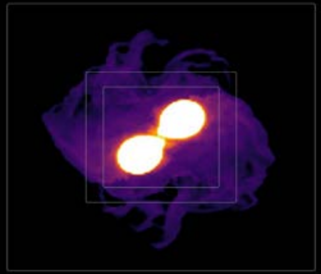
A code hand-off strategy

Divide problem according to physical characteristics; use different codes and grids for different regimes, and develop self-consistent "hand-off" techniques among them!

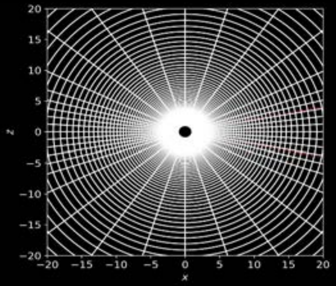


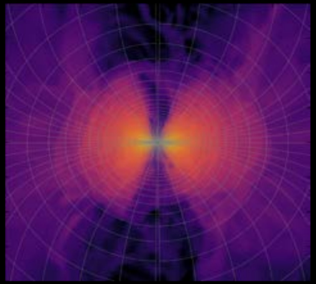
Merger, dynamical ejecta



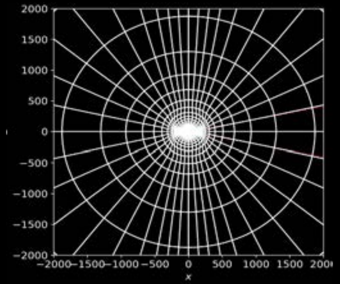


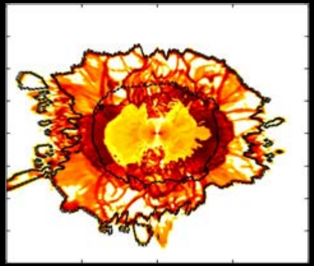
Accretion, MRI, various winds, BZ mechanism





Jet propagation and break-out, ejecta expansion





Enabling long-term, highly accurate and coordinate-optimized simulations of BNS post-mergers!

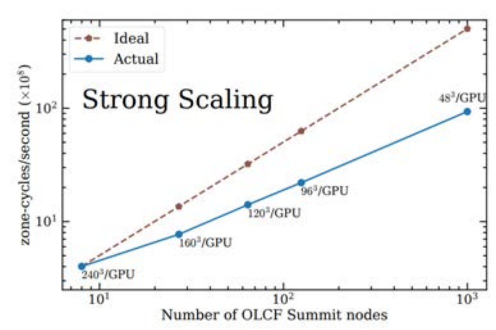
TCAN-BNS collaboration
(compact-binaries.org)
NASA TCAN17-0018 80NSSC18K1488

Harnessing the power of GPUs

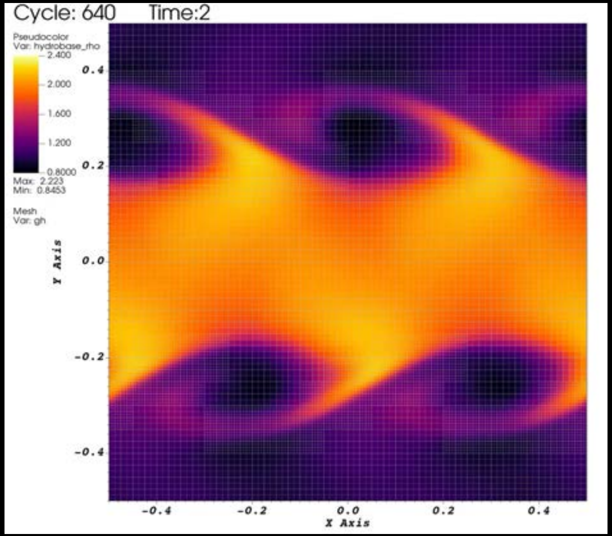
- New open-source AMR drivers promise to scale on thousands of CPUs and GPUs

  - ❖ **AMRex/CarpetX** is a new driver for the Einstein Toolits, based on the AMReX framework – Brandt, Hass, Schnetter ++

- Next generation GRMHD codes that can perform simulations 2-10x faster; ~20-40 times more simulations with same allocation
  - ❖ GRaM-X, Magnetic field (B) - Shankar + 2022
  - ❖ AsterX - Kalinani+ 2023 in prep



GRaM-X: Shankar + 2022



AsterX: KHI (Kalinani + 2023)

Will be the key for achieving the needed accuracy for magnetic field growth, radiation, neutrinos physics treatments …

BNS simulations in the next decade …

Realistic high-resolution GRMHD simulations using advanced neutrino transport schemes over the seconds time scales are needed to follow the evolution of a post-merger remnants. This remains an extremely difficult problem to solve for years to come.

- Neutrino transport now use leakage, moments (e.g. M0 or M1) and Monte-Carlo methods (e.g. Foucart 2021 for a review) can be used to answer some physics questions more or less reliably …

- The 6d Boltzmann's equations of radiation transport has only been tried for radiation in non-dynamical GR (e.g. Davis+2023) so far, and in principle can be generalized to neutrinos coupled to MHD and GR …

    - ❖ For neutrinos, some processes such as neutrino oscillations, pair annihilation, inelastic scattering, and potentially direct and modified URCA processes also need to be included.
    - ❖ For photons, realistic frequency-dependent opacities and non-LTE effects are still missing …

- Large-Eddy-Simulations (LES) and subgrid models can be used to quantitatively model MRI-driven turbulence in BNS mergers over longer periods – e.g. Palenzuela+2022.

- Use ML methods or physics-informed neural networks (PINNs)? e.g. refine inversion operator from LES, speed-up contoprim methods (Radice+2022), refine optical depth and temperatures maps in MC …

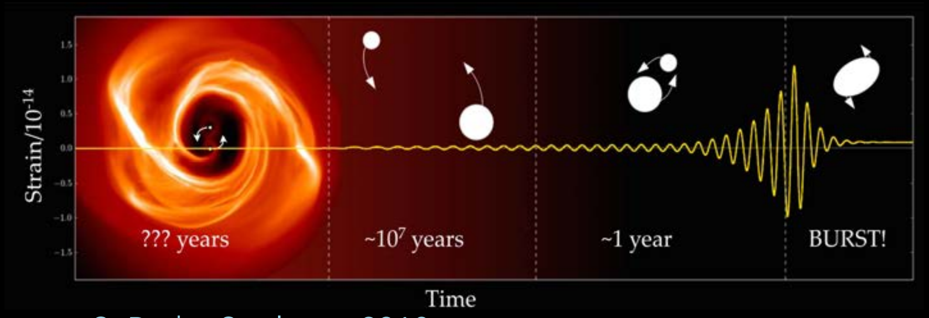
Supermassive Binary Black Hole Mergers

- Supermassive black hole binaries (SMBBH) should form from post-galaxy-mergers; once into the AGN core they should accrete hot gas and emit powerful radio jets …

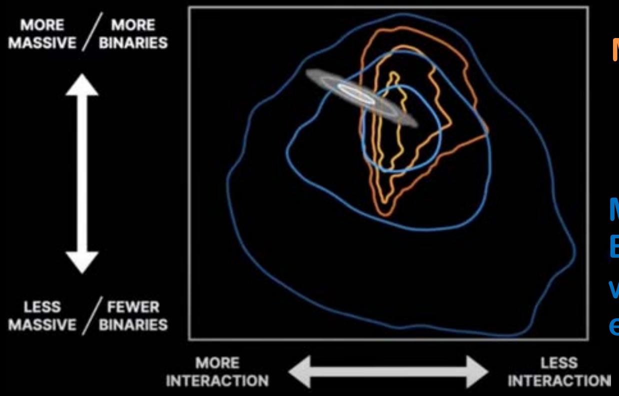
- Stellar dynamical friction, torques from gas, is expected to bring the pair to sub-pc scales - Begelman, Blandford & Rees 1980; no ``last parsec problem" Milosavljevic & Merritt, 2003

- Then GW should do the rest, making SMBBH primary targets for LISA and PTA campaigns
- Multimessenger (MMA) sources, e.g. EM signatures help localize GW events in the sky

Did the GW background from PTA observations come from SMBBH?

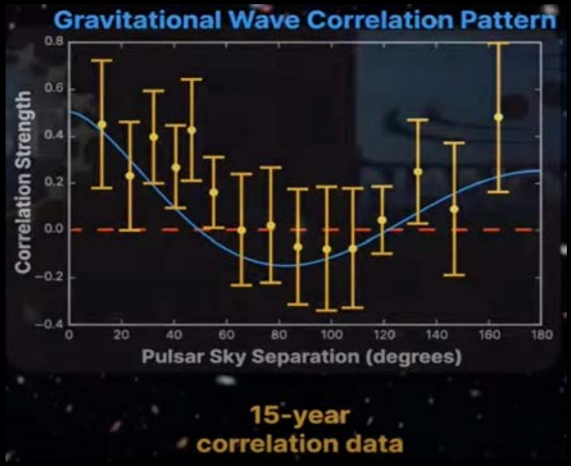


S. Burke-Spolaor +2018



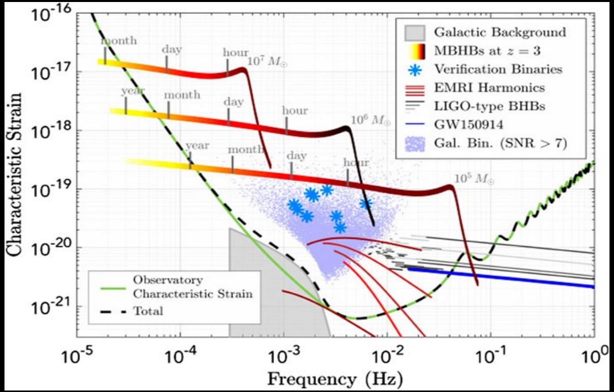
Model with isolated BBH

Model where BBH interact with their environments



Very good news for LISA (maybe)!

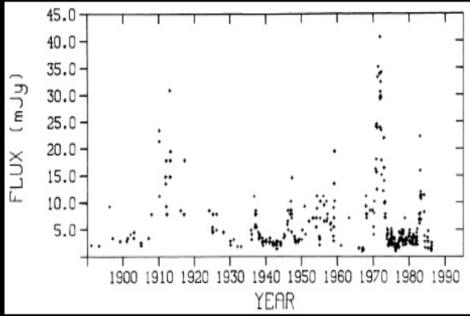
LISA's detection rate ~ 1 SMBBH merger per year within z < 1



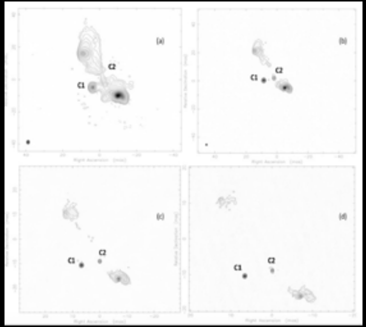
LISA sensitity curve - Sesana+2021

Distinguishing SMBBH from single AGN …

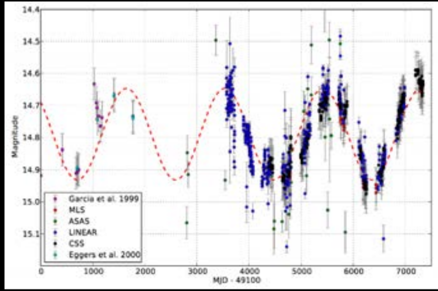
Identification of sub-pc SMBHBs has been challenging, but new sources will be uncovered through continued long term monitoring and new surveys and observatories:



Periodic flares; OJ287 (Valtonen et al. 1988)

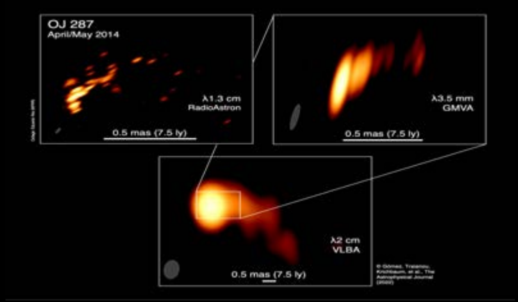


Direct Imaging of double nuclei (radio); 0402+379 - Bansal+2017, 12 years of multi-frequency VLBI observations

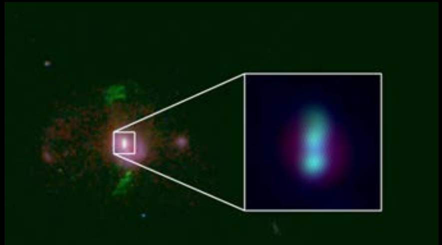


Sinusoidal light curves: PG1302-102 (Graham et al. 2015)

e.g. JWST and LSST might uncover "many" binary-AGN in the haystack!



New polarimetric space VLBI observations of OJ 287



Optical HST image; SDSS J1010+1413, Goulding+ ApJL 2019;

- Hundreds of EM-distinguishable binary-AGN from galaxy evolution models at z~1; in the PTA range - Krolik+2019
- Important for understanding galaxy evolution models!

What Simulations can tell us?

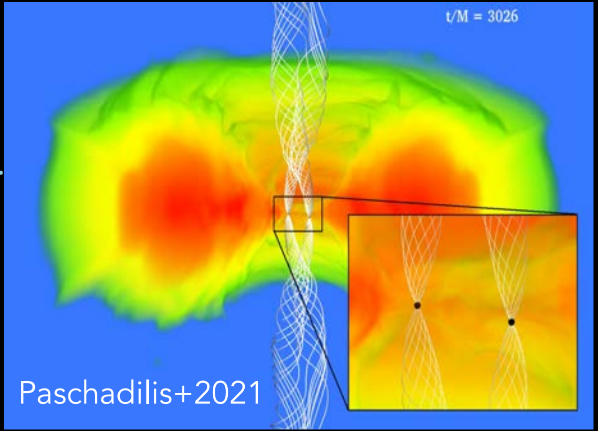
- Key questions: How much gas is present at merger? Is there a decoupling regime?

- Early Newtonian 1D simulations found little or no accretion close to the BHs, as binary torque carves a nearly empty cavity of 2a, and the circumbinary disk (CBD) is left behind, as the binary spirals inward fast (``decoupling'') – e.g. Pringle, 1991; Armitage+2002, Milosavljevic+2005.

- Modern 2D and 3D simulations find that binary torque "dam" does not hold, and accretion continues until approach to merger! – e.g. Noble+2012, D'Orazio+ 2013; Farris +2014; Ryan+2016, Tang+2018; Bowen+2017,2019.

- NR simulations hint at interesting dynamics, but are either too short or do not start from astrophysical initial conditions – e.g. Giacomazzo+2012; Gold+ 2013; Paschadilis+2021, Cattorini+2022.

  - ❖ Long-term, MRI resolving, GRMHD simulations are needed to "equilibrate" an accretion disk!
  - ❖ Realistic thermodynamics, plasma physics and radiation transport.



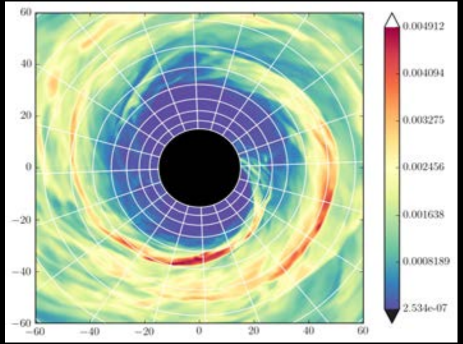
Paschadilis+2021

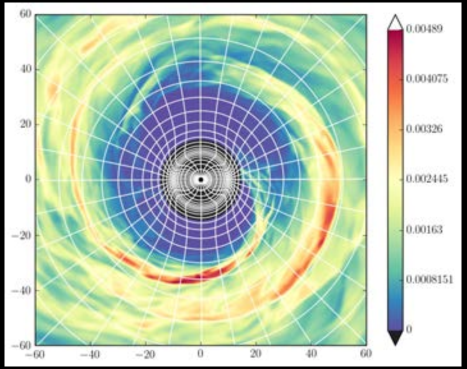
``Hand-off'' computational strategy:

Must resolve both **the MRI in the circumbinary disk and MHD dynamics** at the scale of the event horizons:

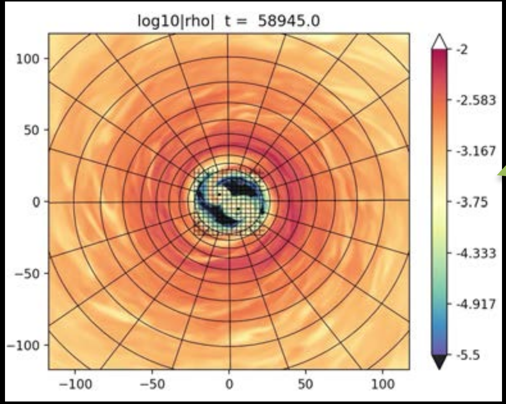
1. Perform a long-term, accurate, GRMHD simulation of a circumbinary disk in spherical coords, with a excised central cutout around the binary.
   - Harm3D adapted to evolve in dynamical GR –Noble+2006, 2012.
   - SphericalNR - Mewes++2018, 2019

1. After ``equilibration'', interpolate the computational domain into a new grid designed to resolve the physics near each BH





Warped curvilinear grids – Zilhão+2014



PatchworkMHD – New software infrastructure for problems of discrepant physical, temporal, scales and multiple geometries - Shiokawa+ 2018, Avara+ 2023

How do we efficiently simulate 10^7 cells for 10^7 steps?

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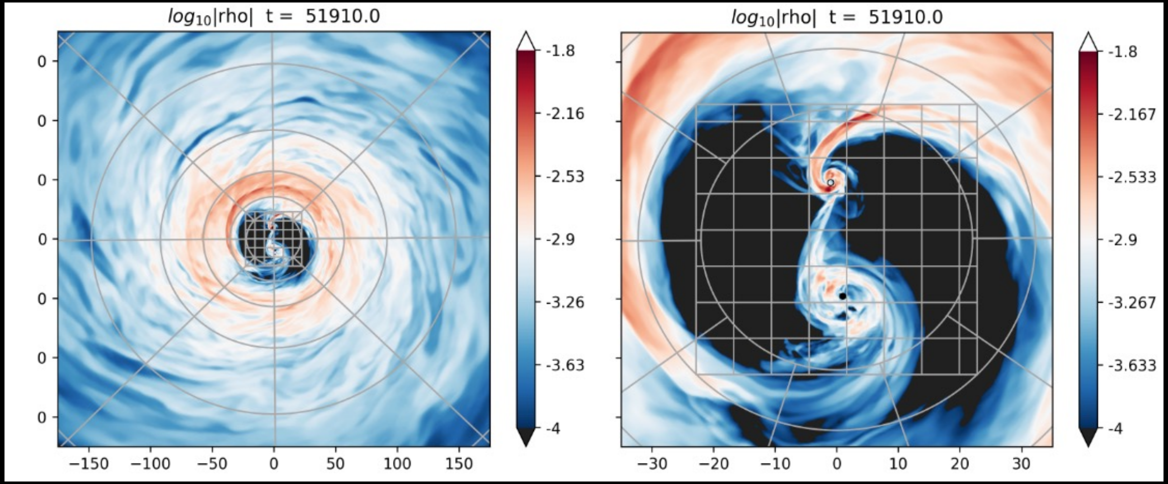
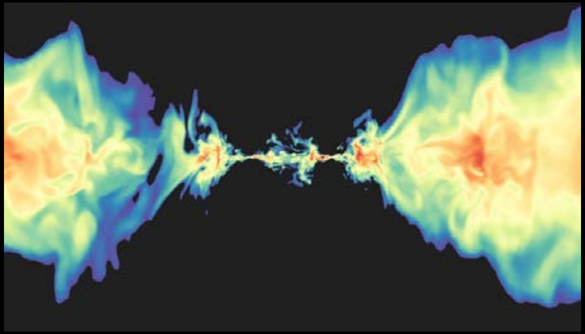
Accretion into a SMBBH before merger…

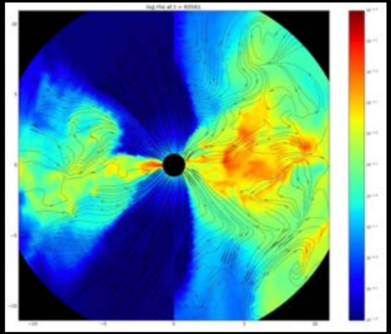
Noble++2012, Bowen+ 2017, 2018, 2019, Combi+2022, Avara+2023



Rich 3d structure of accretion disks



Mini-disks accretion nothing alike single BH accretion

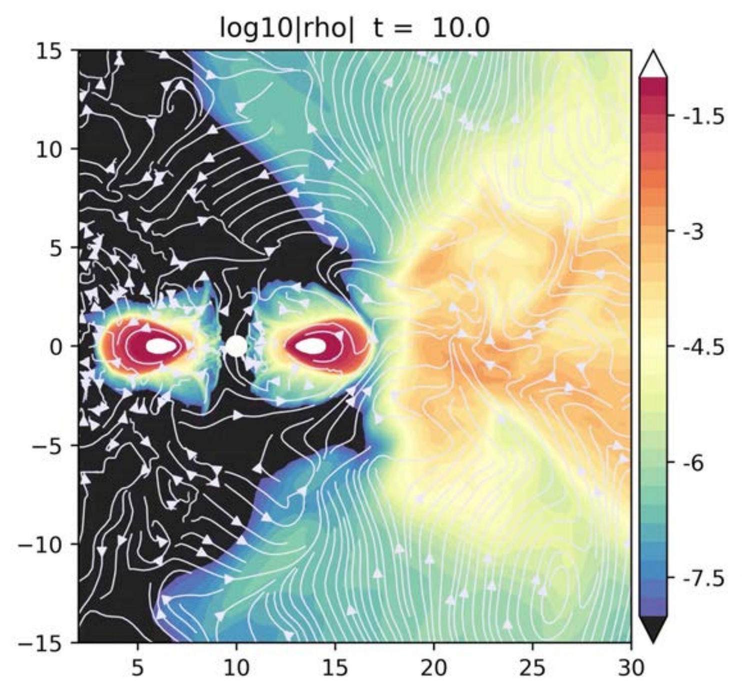


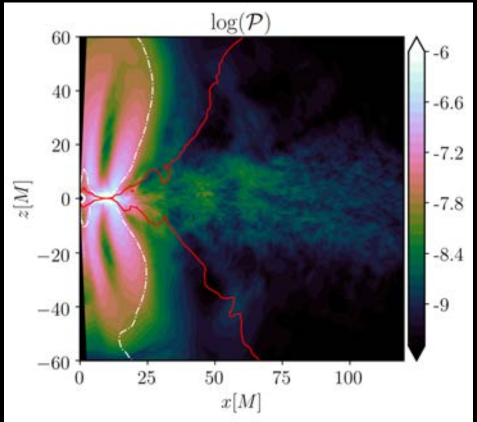
- A "lump" with characteristic periodicity generically form in the CBD.
- Accreting streams fall in the cavity and shock against the BH minidisks, which deplete and refill periodically at time scale close to one orbital period.
- The minisdisk exchange material through a periodic "sloshing".
- No real decoupling at these initial separations (~ 20 r_g)

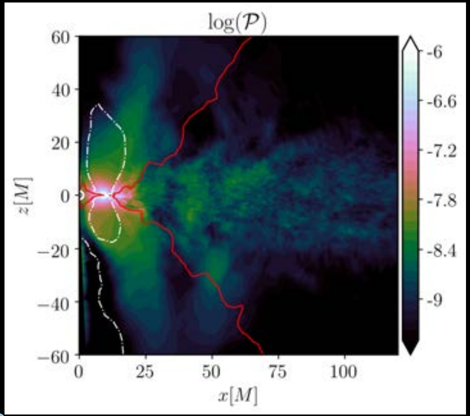
BH Spins and Jets!

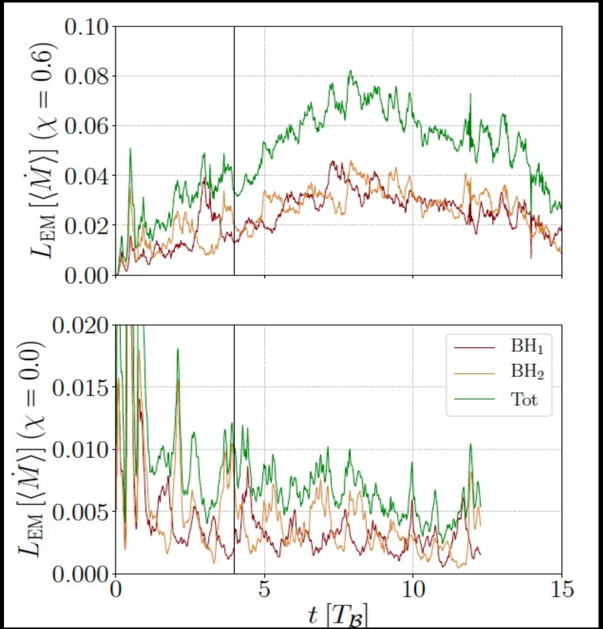
More magnetized mass + BH ergospheres means more jet-like structure!

Jet power modulated with the same periodic behavior that the filling/depletion cycle!







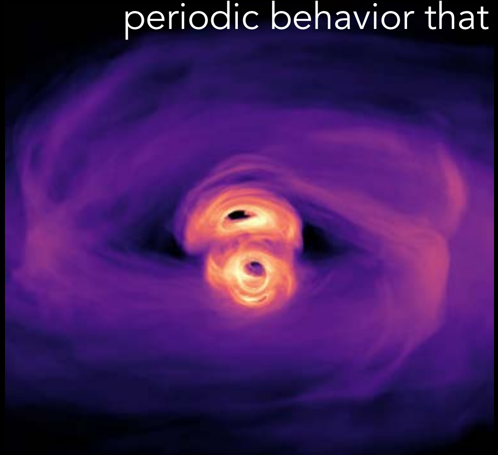


Outfows are nearly 10 times stronger than the non-spinning case!

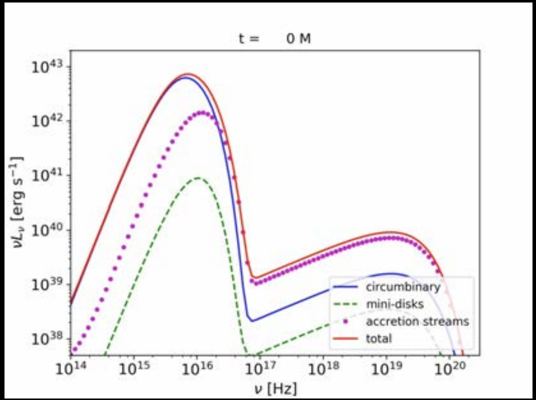
Combi+ 2022; Gutierrez+2023; Pelle+ in prep

"Radiation Transport"

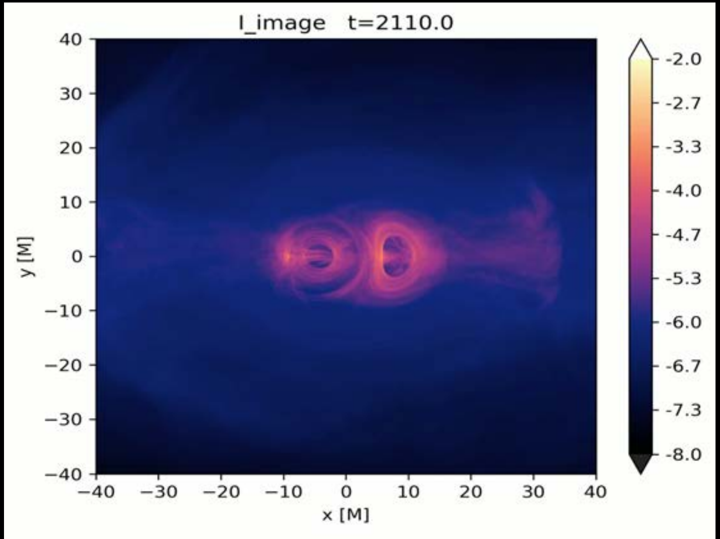
- Radiation transport (RT) via raytracing and cooling function – D'Ascoli+2018, Gutierrez+2022
  - ❖ Time varying spectrum shows that the minidisks around each of the BHs are the hottest features emitting bright X-rays relative to UV/EUV
  - ❖ Light curves and jet power modulated with the same periodic behavior that the filling/depletion cycle

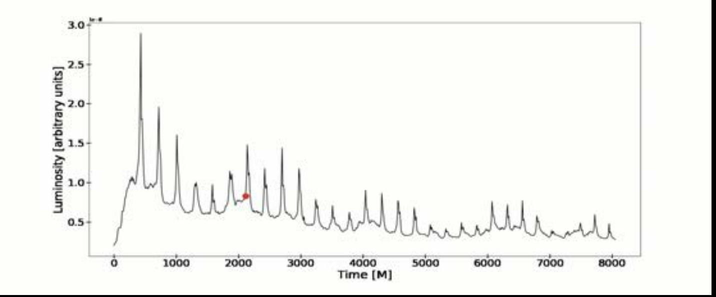


Intensity of X-rays (log scale) multiple-angle video in time, optically thin case

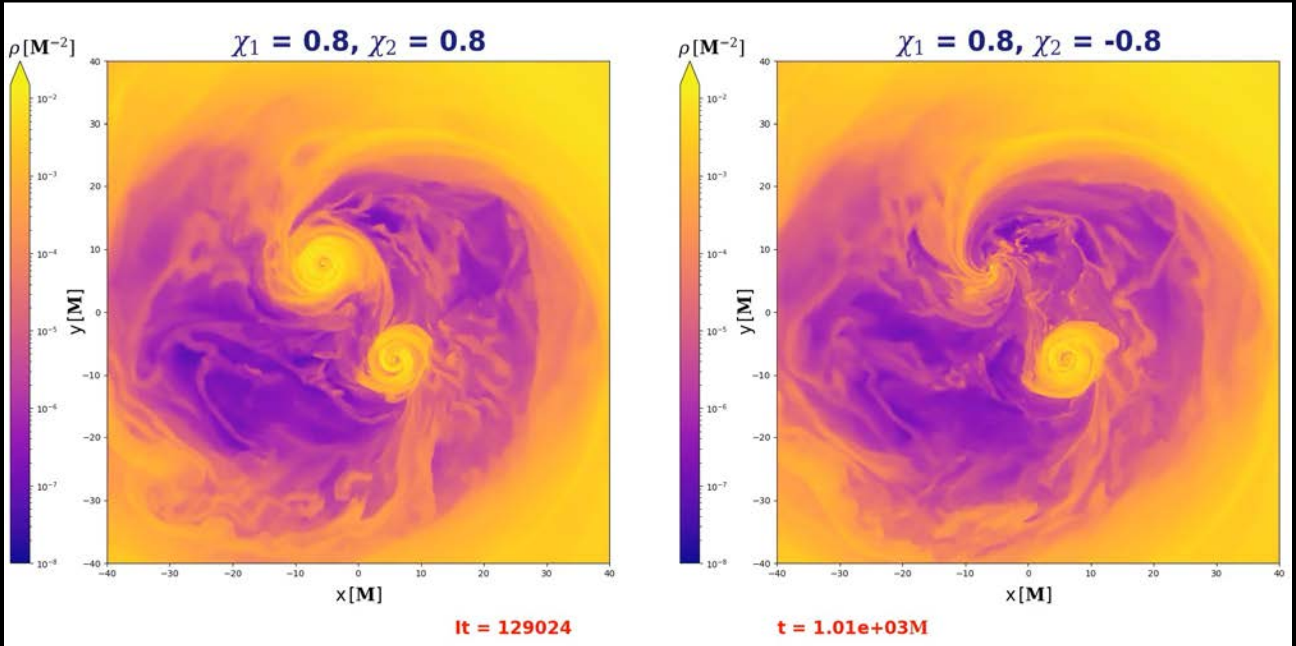


Spectra variability in time Face-on View,





NR simulations in full GRMHD from inspiral to merger

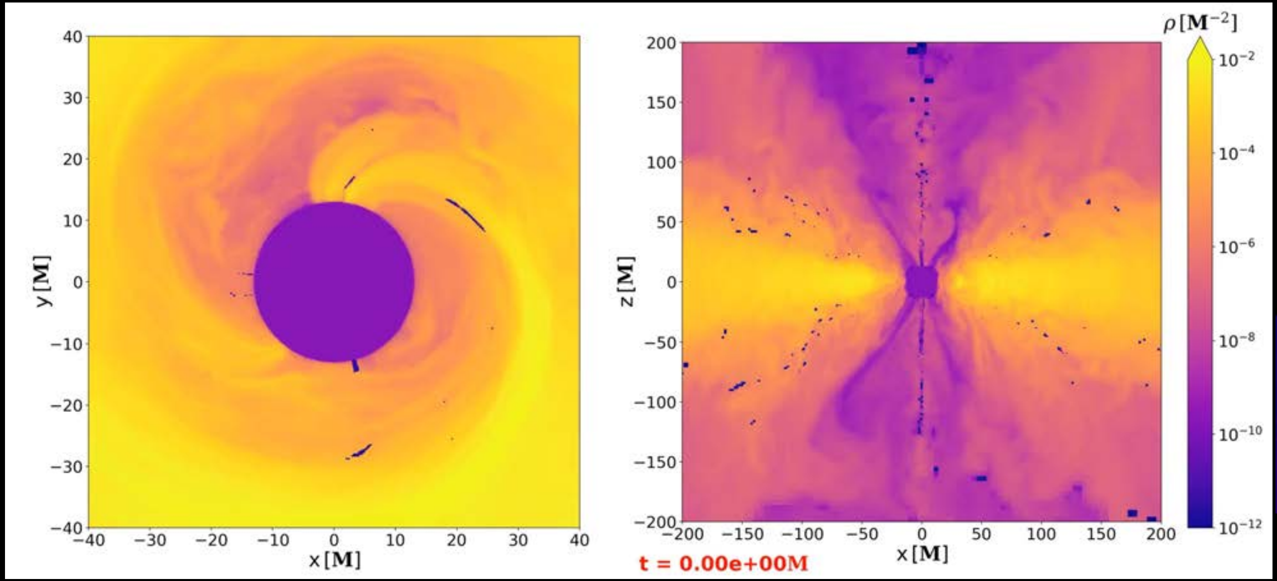


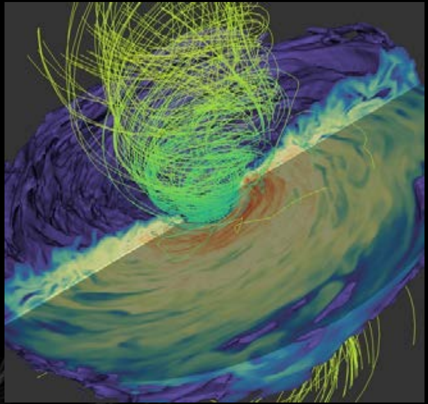
- First long-term simulations of various spins configurations and masses underway - Ennoggi++ in prep
- Hand-off of and equilibrated CBD to a full NR simulations in GRMHD with radiation transport (e.g. cooling/leakage)
- The magnitude and direction of the spins matters – e.g. Campanelli+2007

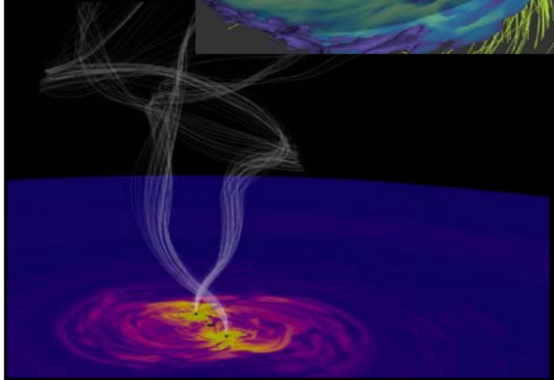
MRI resolving GRMHD needed for accretion in the CBD region, but in the physics of the ``cavity" is dominated by the BHs …

NR simulations in full GRMHD from inspiral to merger

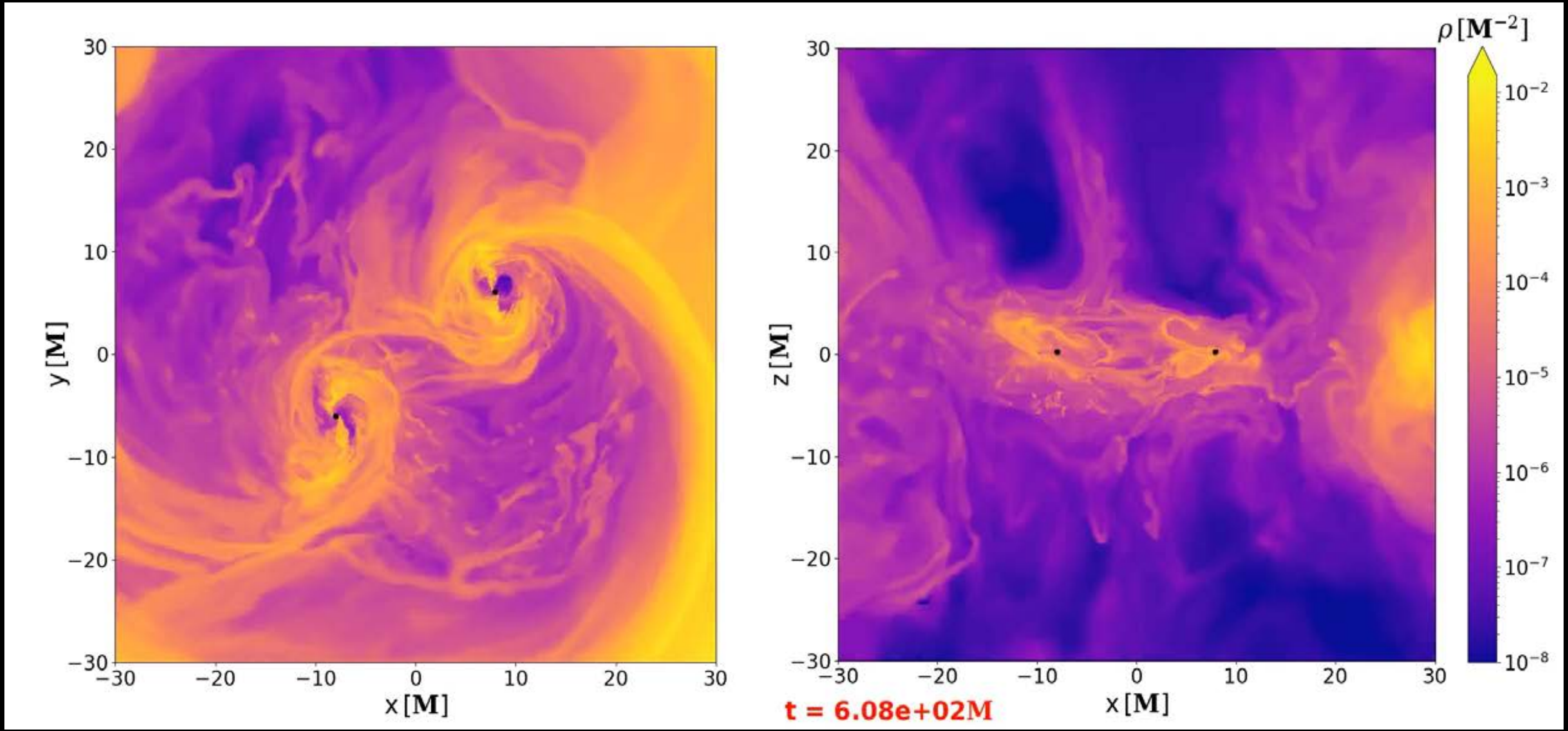
Powerful ``double” jets (e.g. Lorentz factor ≳100) that are modulated by accretion filling and refilling cycle …







NR simulations in full GRMHD from inspiral to merger



Interesting things could happens if the BH spins are oblique such as spin-flips and superkicks of the BH remnant – e.g. Campanelli+2007, Lousto+2015

Concluding Remarks

- NR simulations of merging compact binaries are key to the interpretation of multi-messenger observations, especially when powerful EM signals and high-energy particles in addition to GW.

- NR is in overall in good health, but more quantitative physics predictions require that we solve a number of important challenges in the next decade. Rapid cyberinfrastructure developments are underway and they will accelerate progress!

- Current facilities give us only a glimpse on new potential MMA discoveries.

- We must be ready to face the possibility that the universe can still surprise us a great deal!

Credits

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