A Decade of Discovery: Exploring the Uncharted Horizons of Gravitational Wave and Multimessenger Astronomy with Numerical Simulations

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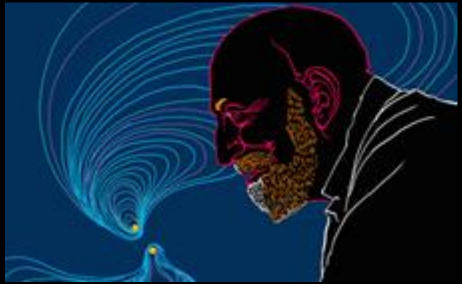
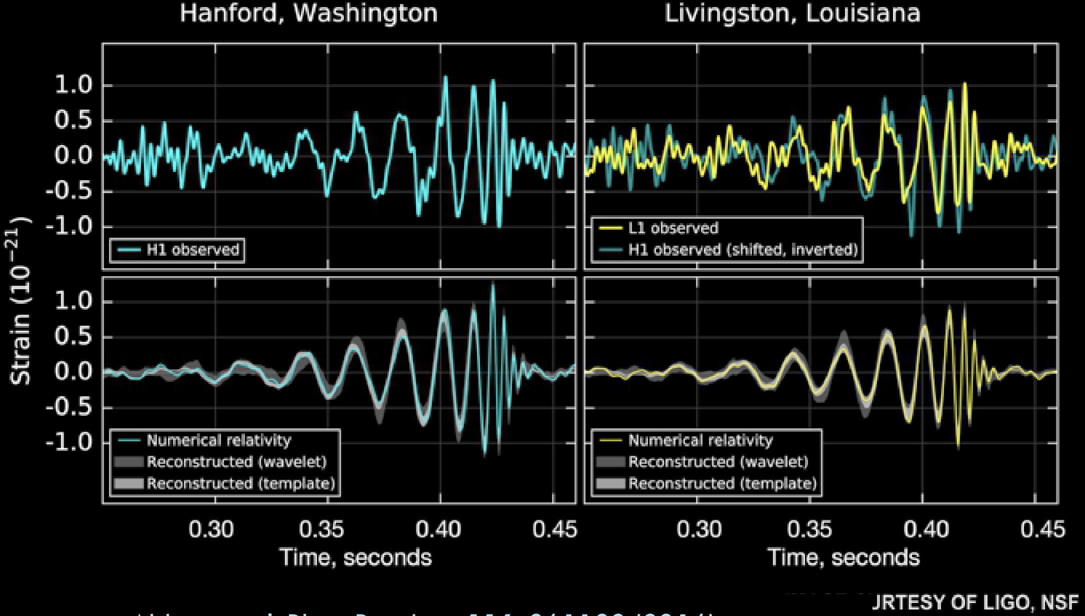
The role of simulations and modeling in GW observations…

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



The serendipitous case of GW150914

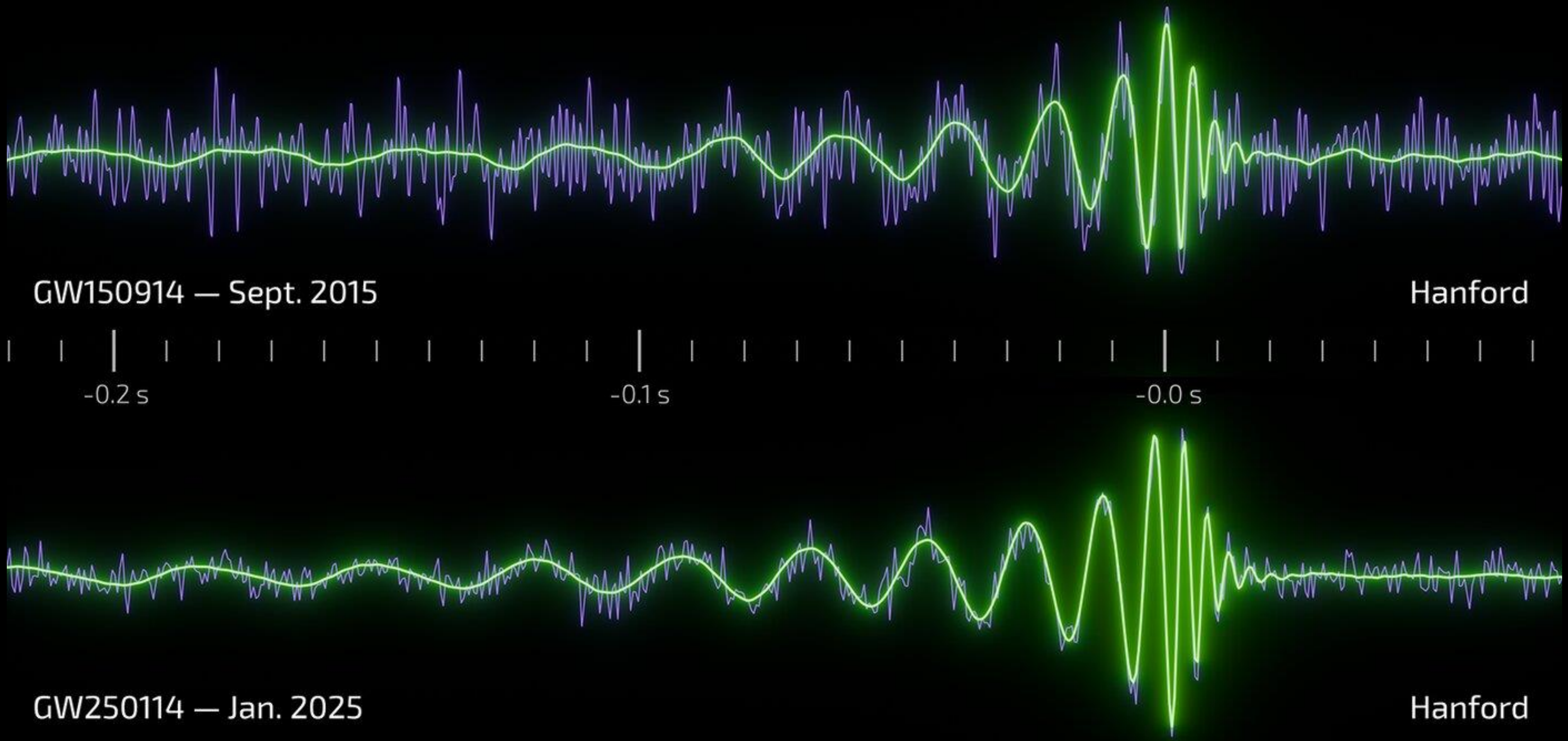


Abbott et al, Phys. Rev. Lett. **116**, 061102 (2016)

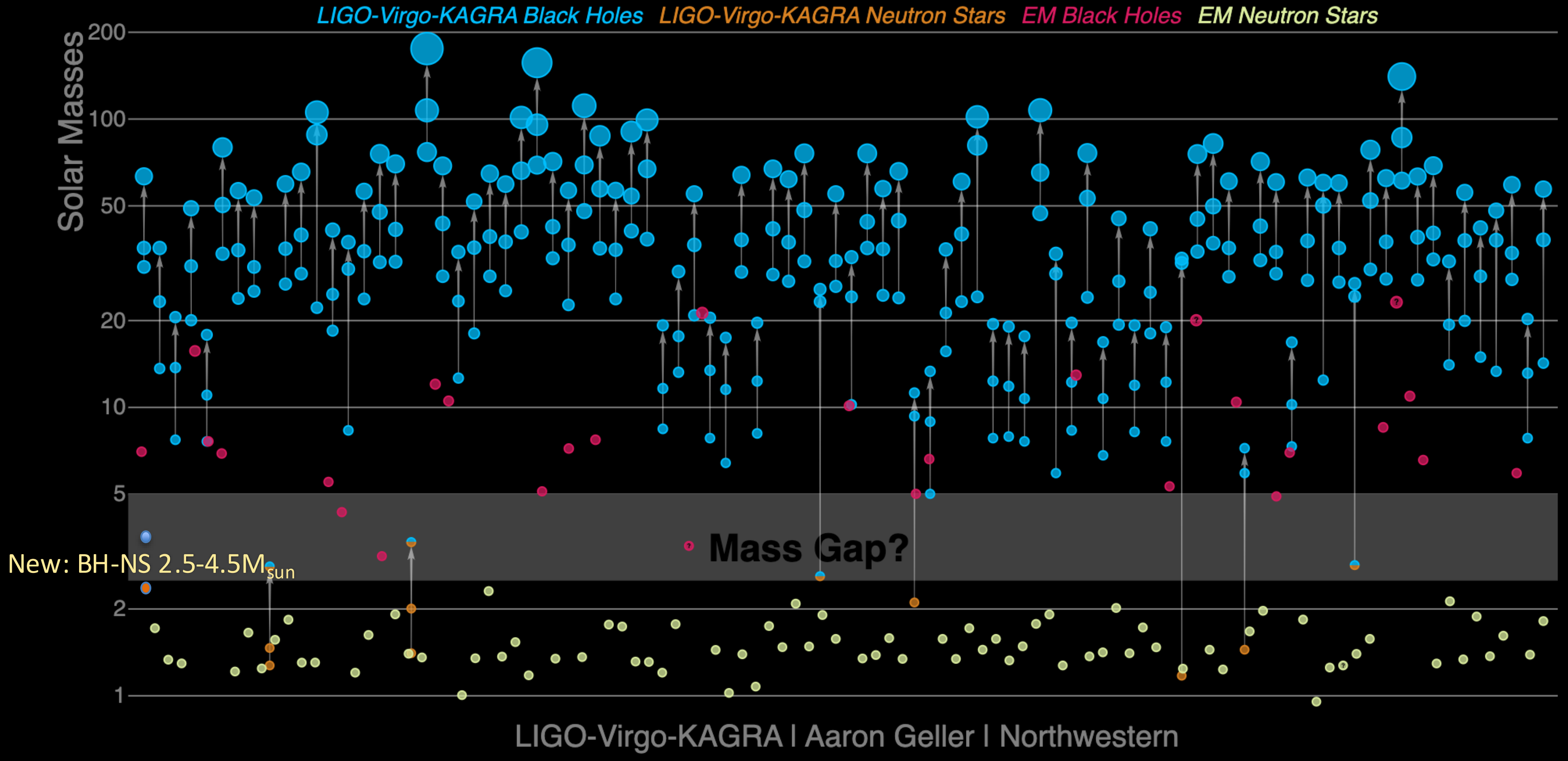
"I have bet these numerical relativists that gravitational waves will be detected from black-hole collisions before their computations are sophisticated enough to simulate them. I expect to win … but hope to lose, because the simulation results are crucial to interpreting the observed waves."

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

10 Years Later: LIGO Hears Loud and Clear



Masses in the Stellar Graveyard



200+ sources

NR simulations are routinely used to model GW waveforms from compact binary mergers!

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)

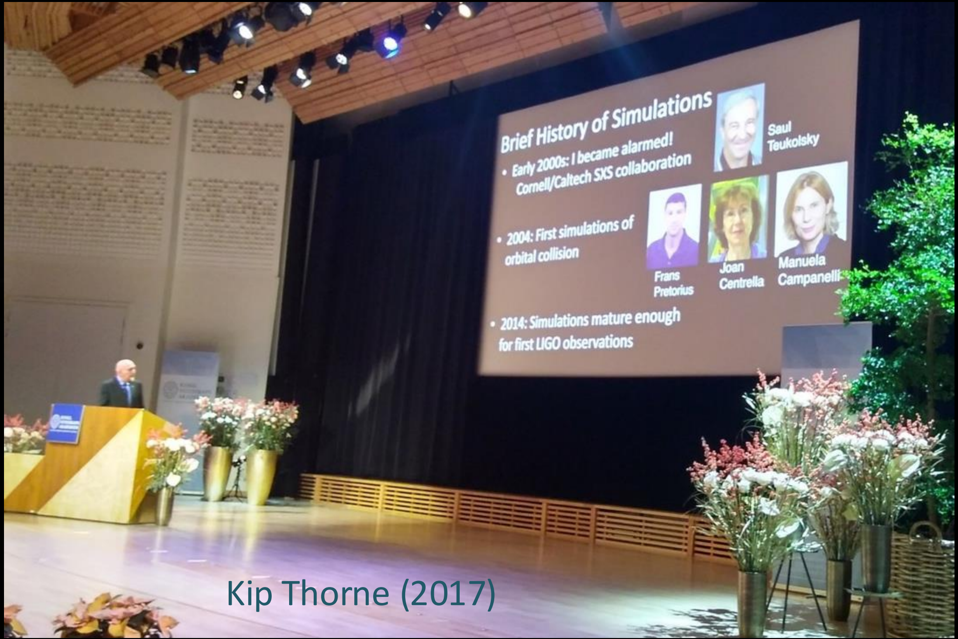
GR 1: Conference on the role of gravitation in physics
University of North Carolina, Chapel Hill [January 18-23, 1957]

``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 PRL 2005, Baker+PRL 2006, Campanelli+ PRL 2006
and codes didn't blow-up anymore …

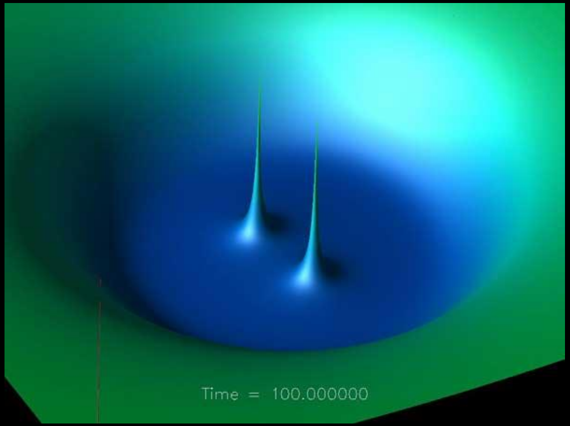


Kip Thorne (2017)

The Moving Punctures Approach

Campanelli, Lousto, Zlochower and Marronetti, PRL 2006

Allowed the punctures (no BH excision) to move across the grid …



Easy to implement and was quickly adopted by the greater NR community revolutionizing the field!

- This work highlighted by the Nobel Prize Committee and Kip Thorne in 2017!
- It is also one of the APS landmark papers of the century along with the one from Einstein himself!

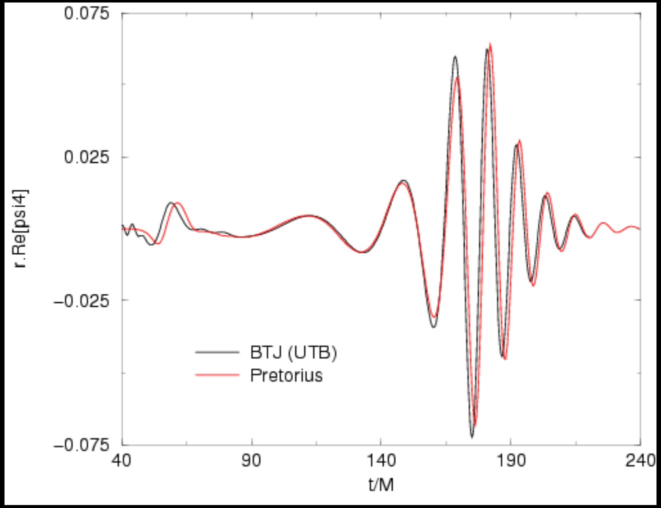
Replace ϕ $(O(\log r))$ with $\chi = e^{-4\phi}$ $(O(r^4))$

$$\partial_0 \alpha = -2\alpha K$$

$$\partial_t \beta^a = B^a,\ \partial_t B^a = 3/4 \partial_t \tilde{\Gamma}^a - \eta B^a$$

$$\alpha(t=0) = \psi_{BL}^{-2} \qquad \beta^i = B^i = 0.$$

- absorb singularities in the BSSN conformal factor to free the punctures
- use new shift condition to move the punctures



Baker, Campanelli, Pretorius and Zlochower 2007

NR Codes Today

Most of them still use the moving punctures approach!

einstein toolkit

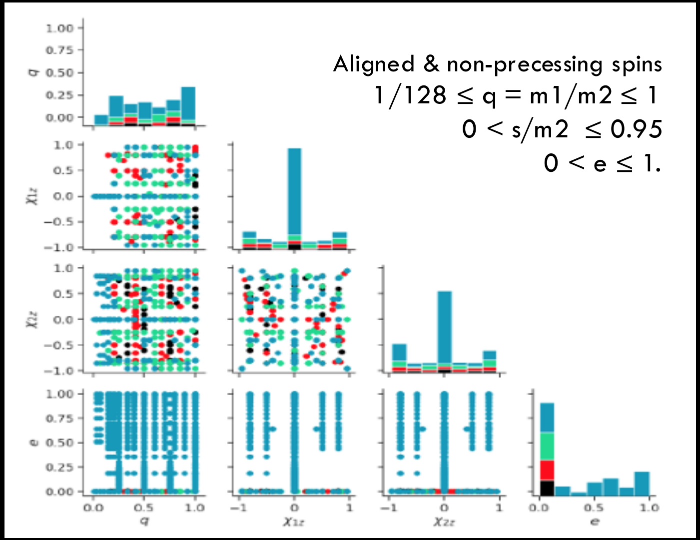
We are key software developers of the Einstein Toolkit - an open-source software platform of core computational tools to advance and support research in relativistic astrophysics and gravitational physics.

NSF funded us since 2007 for about 10 millions to support this software.

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

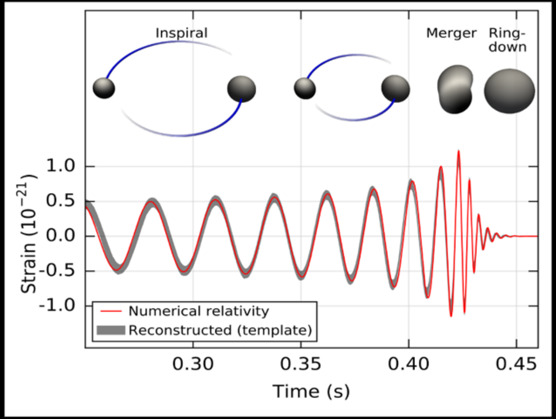
Catalogs of NR simulations

- GW waveform models are essential to infer source parameters.
- Today, there are thousands of such NR calculations and templates for a variety of BBH masses, spins, eccentricity, etc.



5000+ waveforms

- RIT waveform catalog, hundreds of eccentric BBHs - e.g. Healy+ 2022, Gayathri +2022
- Similarly, the SXS catalog, long waveforms via surrogate modeling – e.g. Boyle++ 2019



NR waveform modeling GW150914

The RIT Waveform Catalog is notable for its inclusion of waveforms characterized by high (precessing) spins, significant mass ratios, and eccentric configurations.

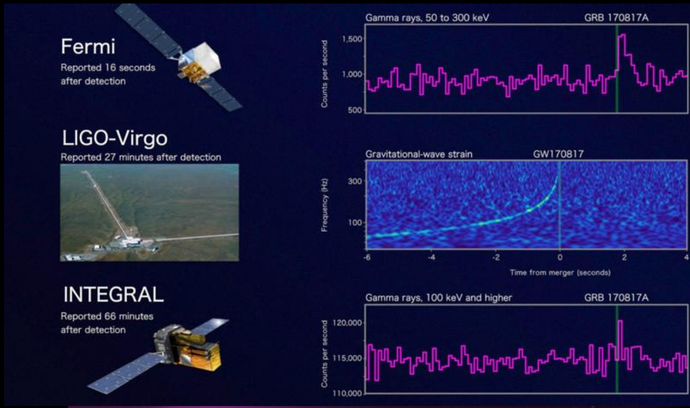
Hundreds publications in PRD and PRL on this topic, with funding from the NSF gravitational physics division

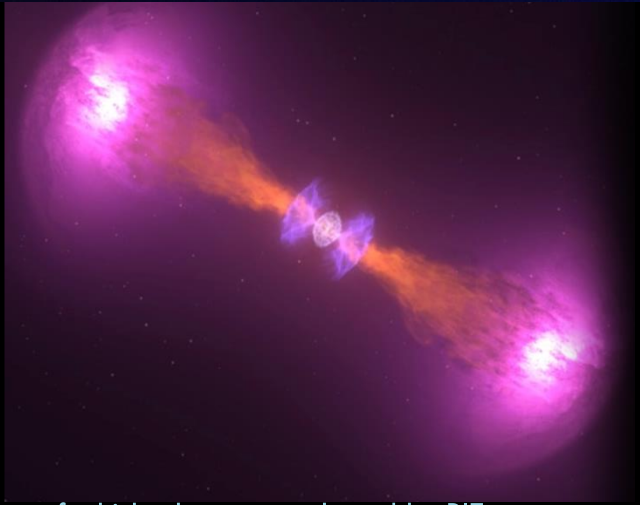
GW170817 & The Dawn of a Multimessenger Astronomy

- On August 17, 2017, the LIGO-Virgo detectors made the first observation of GWs from a binary neutron star (BNS) merger, kicking off the era of multimessenger astrophysics. This was the first event ever to be observed in both GWs and light.

- Timeline of Discoveries
  - 0s: GWs detected
  - +1.7s: Short Gamma-Ray Burst (sGRB)
  - +11 hours: Kilonova (optical/infrared counterpart)
  - +9 days: X-ray afterglow

- Key Scientific Breakthroughs
  - Confirmed that binary neutron star mergers are the cause of sGRBs.
  - Provided strong evidence that heavy elements like gold and platinum are created through the r-process in these mergers.
  - Offered a new, independent way to measure the expansion rate of the universe (the Hubble Constant).



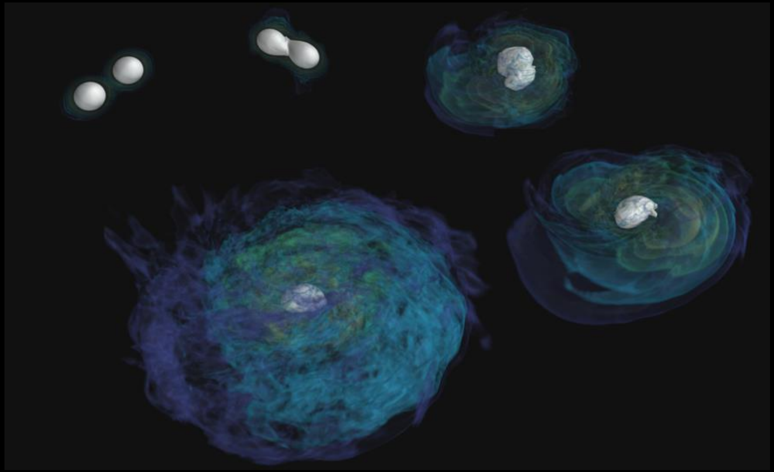


LIGO Scientific Collaboration & Virgo Collaboration + PRL 2027; Nature 2017
Kasen+ Nature 2017, Cowperthwaite + ApJ Letters 2017; and hundreds of more papers many of which where co-authored by RIT

The Post-GW170817 Era: Open Questions & The Simulation Challenge

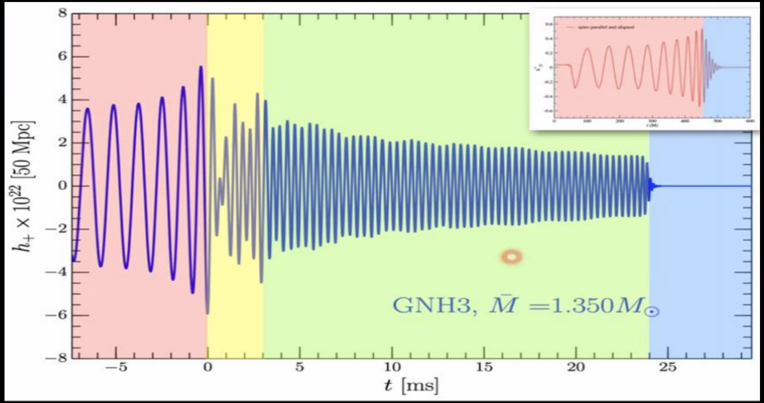
The discovery of GW170817 was revolutionary, but it left us with fundamental unanswered questions:

- What is the central engine of a sGRB ? 💥
- What is the origin of the distinct "blue" kilonova component ?
- How exactly are relativistic jets launched from the post-merger remnant?



Answering these requires decoding the GW signal. Unlike in binary black hole mergers, BNS waveforms depend sensitively on complex matter physics:

- The nuclear Equation of State (EoS)
- Magnetic Fields
- Neutrino Interactions



We need long-term (~seconds) GRMHD simulations with comprehensive physics to build self-consistent models of mass ejection and the resulting electromagnetic (EM) signatures.

See Radice+, *Annual Review of Nuclear and Particle Science*, Vol. 70:95-133 (2020)

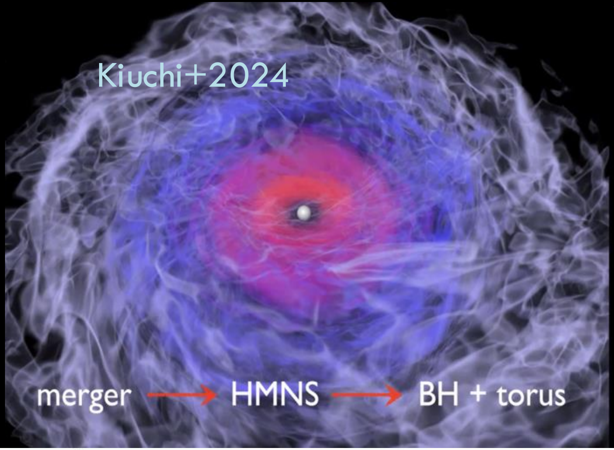
Computational Challenges in Neutron Star Mergers

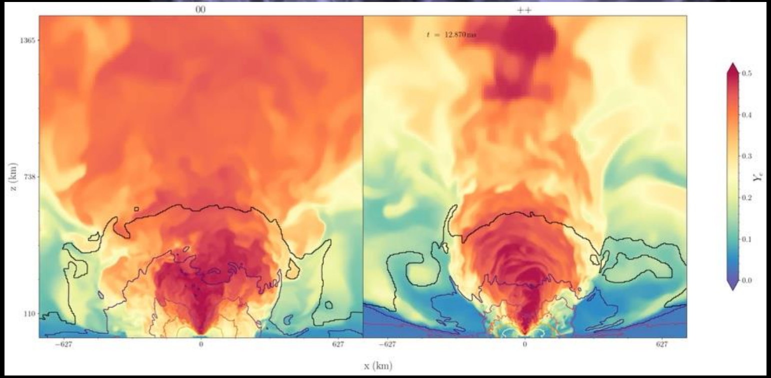
Turbulent Magnetohydrodynamics (GRMHD)

- Goal: Resolve MHD instabilities (like Kelvin-Helmholtz) to simulate the strong, organized magnetic fields that launch jets.
- Problem: This is computationally prohibitive, requiring the resolution of meter-scale physics.
- Current Limitation: Simulations are restricted to 50-100 meter scales and ~100 ms run times, necessitating artificially large initial magnetic fields.

Neutrino Transport & Nucleosynthesis

- Goal: Accurately model neutrinos, which set the ejected matter's composition (Y_e) and thus the kilonova's properties (color/brightness).
- Problem: A precise simulation requires solving the 6D Boltzmann equation, which is too computationally expensive.
- Current Limitation: Common approximation schemes (e.g., Leakage, M1) often omit key physics like neutrino oscillations and inelastic scattering, affecting the accuracy of nucleosynthesis predictions.

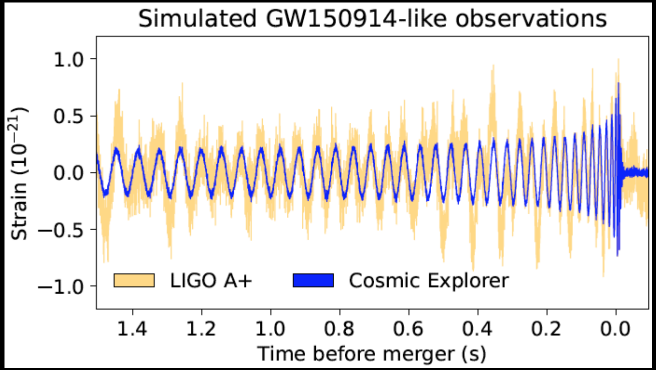




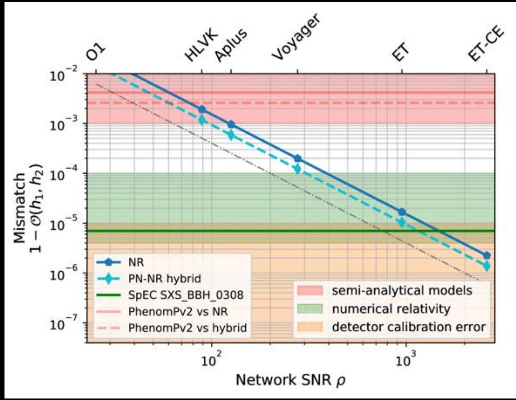
The effect of BNS spins on Y_e
Allen Wen, AST GRA and FINESST

Ready for Next-Generation GW Science?

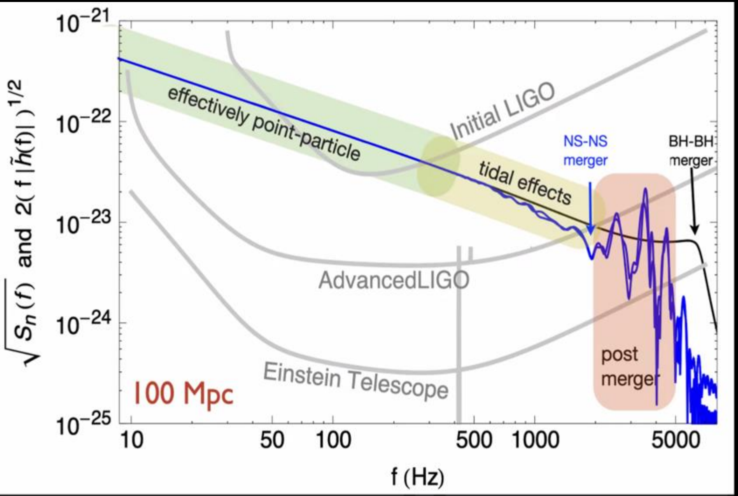
Waveform accuracy, length and parameter space coverage need to improve of at least an order of magnitude for future GW observations with SNR ~ O(1000) – e.g. Puerrer and Haster, 2020



Foucart++ snowmass 2022



Puerrer and Haster, 2020



Sources will be in band for longer periods of time which will require much longer waveforms and more accurate physics!

We can do multi-spectrum GW combining 3G + LISA – e.g. Vitale+2018, Sesana 2016, Breivik+2016, Rodriguez+2017

This will allow us to completely nail down the astrophysical origin and history of the sources, and their relation to the surrounding environment.

Supermassive black hole binaries

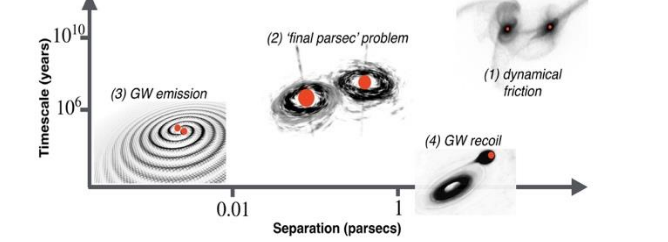
- SMBBH should form from post-galaxy-mergers; once into the AGN core they should accrete hot gas, emit powerful jets … - Begelman+1980;

- Dual-AGN should reach sub-pc scales and merge within Hubble time, via stellar dynamical friction, torques from gas, etc.

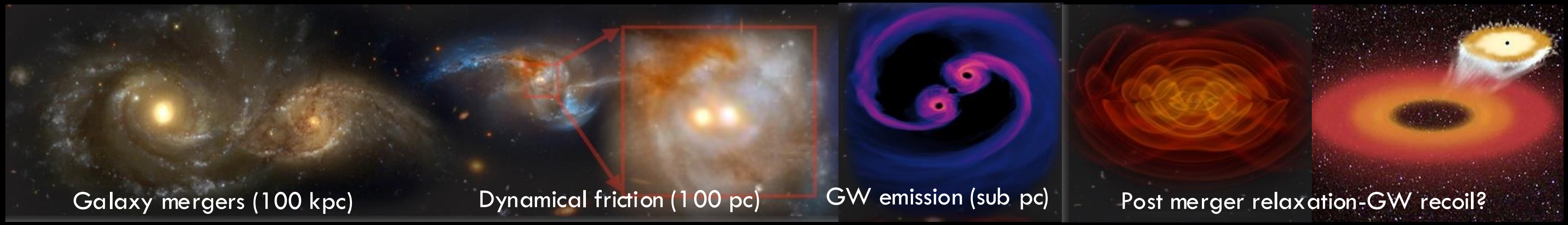
- Mergers due to GW emission, leading to recoils in some cases, are expected to occur in gas-rich environments leading to **EM emission:**

$L_{Edd} \sim 1.26 \times 10^{45} \frac{M}{M_\odot}$ erg/s

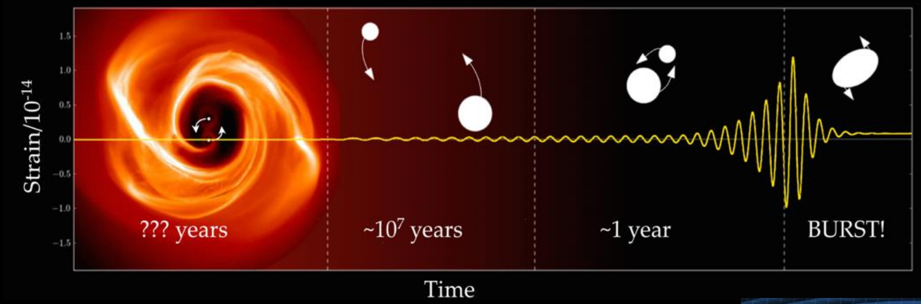
Taylor et al. 2019



- Once they are in the GW regime, SMBBH become optimal GW sources for both LISA ($M_{BH} \sim 10^6\ M_\odot$) and PTA ($M_{BH} \sim 10^9\ M_\odot$).



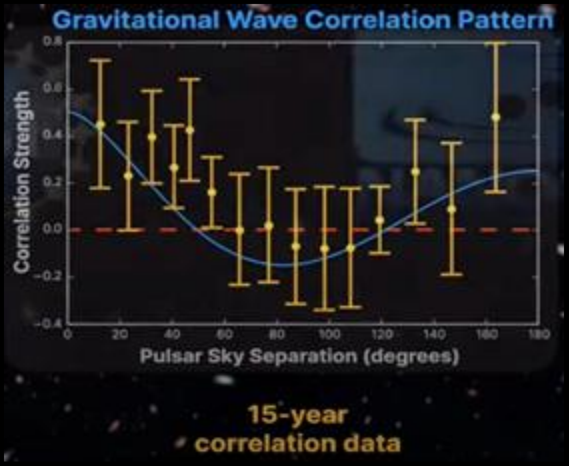
The hunt for low frequency GWs …

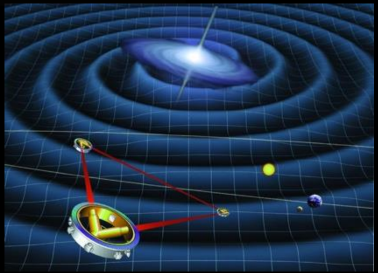


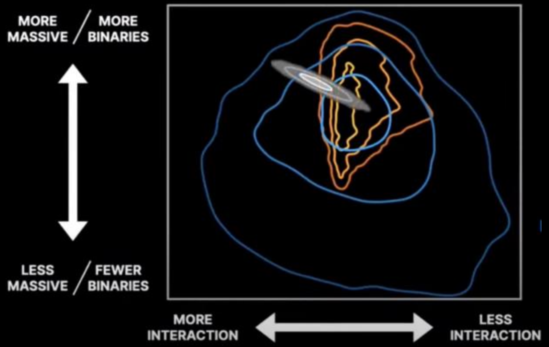
S. Burke-Spolaor +2018

PTA (NANOGrav) likely heard the hum from a universe filled with SMBBH inspirals

PTA+2023



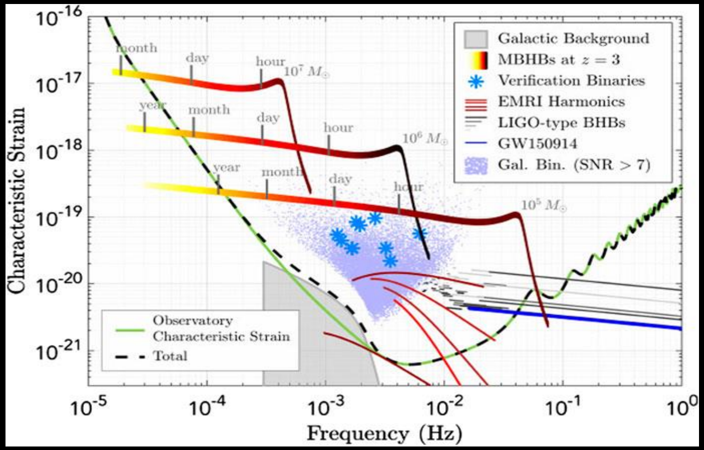




Model where BBH interact with their environments are favorite …

LISA's detection : SMBBH merger rate ~1/Year for ~$10^6 M_{sun}$ at z ~ 1

But watch for radiation feedback! - Li+2023



LISA sensitity curve - Sesana+2021

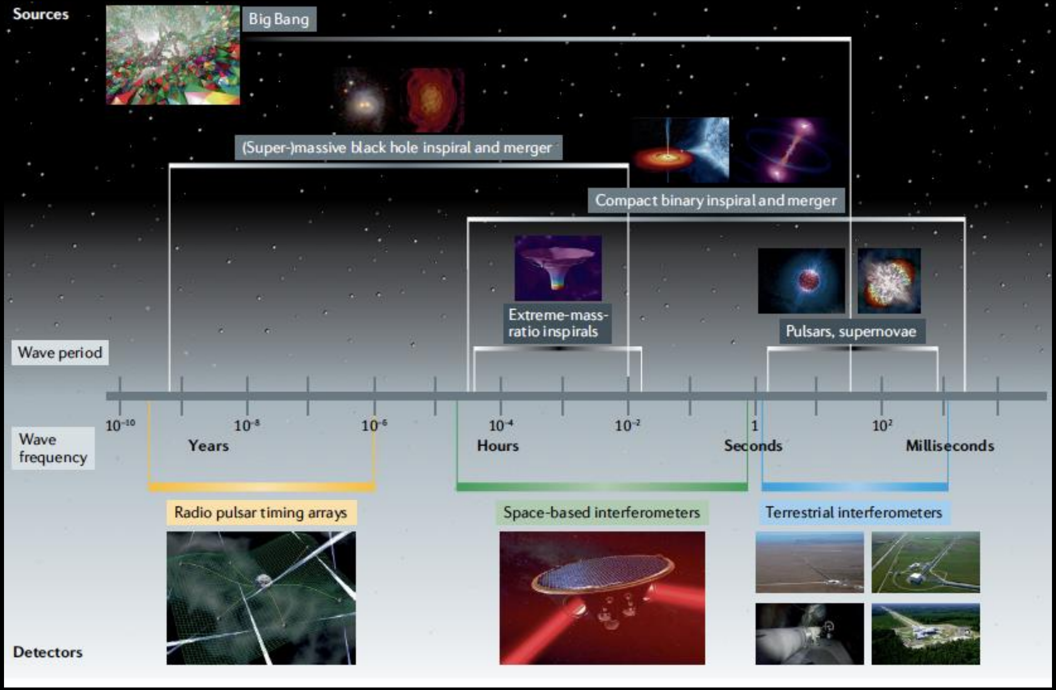
SMBBH as Multimessenger Astronomy sources

- Detection of gravitational radiation emitted by a MBHB constitutes the most direct evidence for the existence of such systems

- EM counterparts become necessary to constrain the location and properties of GW sources.

- **BBH mergers are fundamental to probe strong field gravity and to understand stellar evolution.**

- **They are also fundamental to the formation and accretion history of SMBHs across cosmic ages.**



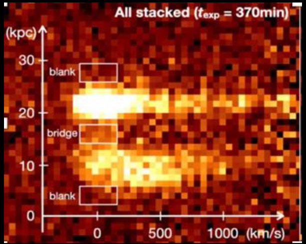
Can we distinguish EM signals SMBBH from single AGN?

There are ``numerous" observations of dual AGN systems with pairs of SMBHs; however, confirmed binaries are still rare …

How can we detect them?

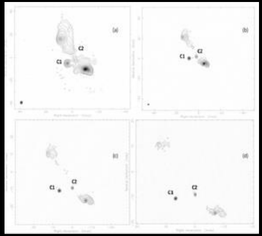
- Direct imaging of double nuclei with Very Long Baseline Interferometry (VLBI)
- Photometric measurements of **quasi-periodic** variability in the lightcurves of quasars (e.g **OJ287, PG1302-102**) or blazars (e.g **PKS2131**)
- Doppler-shifted emission lines in spectra of AGNs and quasars …
- Self-lensing, Reverberation mapping, etc

Many are binary quasars at z=6.05, separated by 12 kpc Matsuoka+2024;

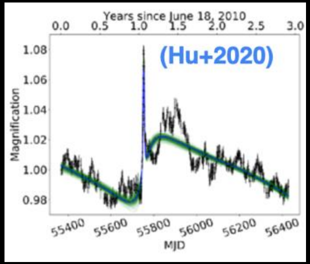


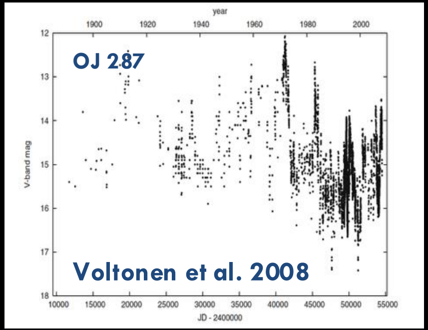
In the local universe: UGC 4211, z= 0.03,and at 230 pc separation- Koss+2024

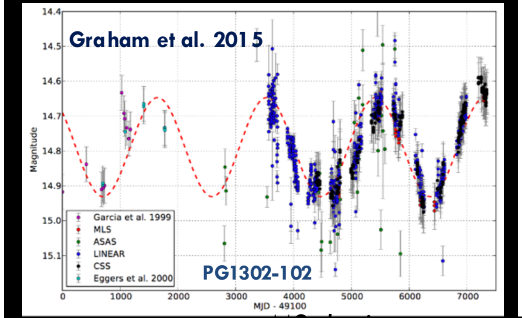
Double nuclei (radio) orbiting! 0402+379 - Bansal+2017, 12 years of multi-frequency VLBI observations

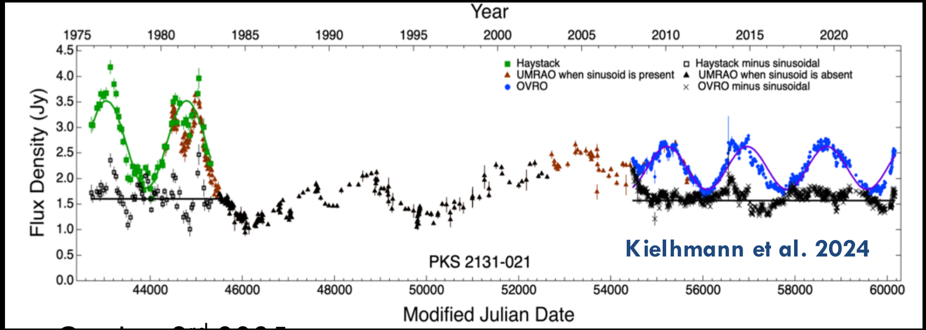


Self-lensing?





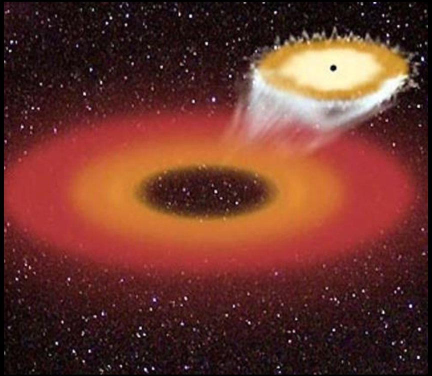




The case for recoiling BBH …

In 2007, our calculations predicted large recoiling merger remnants from BBH mergers if significant contribution of the total spin is in the orbital plane:

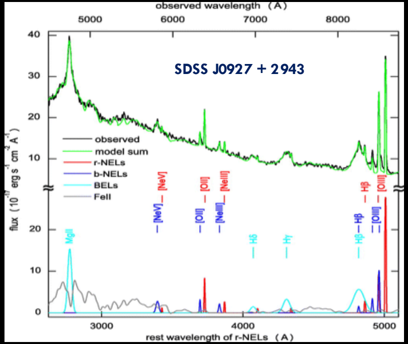
- Superkicks - Campanelli+2007,
- Hang-up kicks -Lousto+2011



- If large enough, the final BH remnant could be kicked out from galaxy
- This could impact many astrophysical scenarios including SMBH formation models

A recoiling SMBH in an AGN can retain the inner part of its accretion disk e.g Loeb 2007, Schields+2007

Astronomers searched for number of possible observational evidence for double-peaked emitters, off-set galactic nuclei, population of galaxies without SMBHs, x-rays afterglows, feedback trails, etc



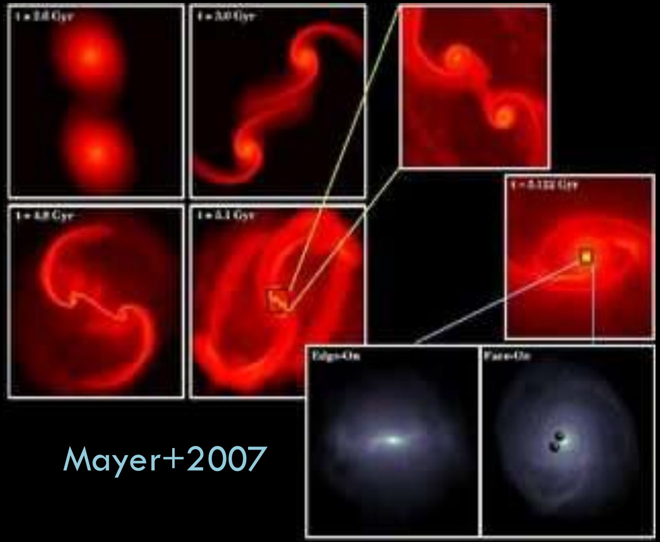
SDSS J0927 + 2943: blue NLR due to expanding gas from edge of bound disk of kicked BH. Red NLR is in host galaxy ionized by kicked AGN - Komossa+2008

But clear identification hasn't been easy because other interpretations are possible!

The identification of EM signals from SMBBH before, during and after merger requires realistic theoretical modeling.

Modeling SMBBH is challenging …

Relativistic SMBBH merger simulations must incorporate information obtained from simulations done at from kiloparsecs down to sub-parsec levels.



Mayer+2007

To explore the merger regime we need: general relativity; GRMHD (accurate at the scale of MRI/turbulence); realistic thermodynamics, plasma physics, and radiation transport.

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

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

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

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

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

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

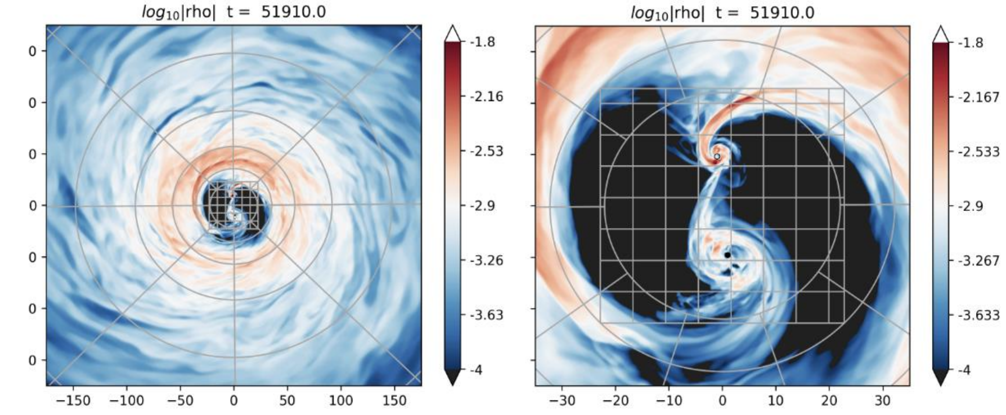
$$T_{\mu\nu} = T^{\text{fluid}}_{\mu\nu} + T^{\text{EM}}_{\mu\nu} + T^{\text{rad}}_{\mu\nu} + \ldots \quad \text{(energy} - \text{momentum tensor)}$$

TACC TEXAS ADVANCED COMPUTING CENTER FRONTERA

Accretion into a SMBBH before merger ...

Noble++2012, Bowen+2017, 2018, 2019, Noble+2021, Combi+2022, Avara+2023, Noble+2024

- Are there distinticve EM signals associated with the dynamics of the minidisks, streams, shoshing, lumps and dual jets as the binary approach merger?



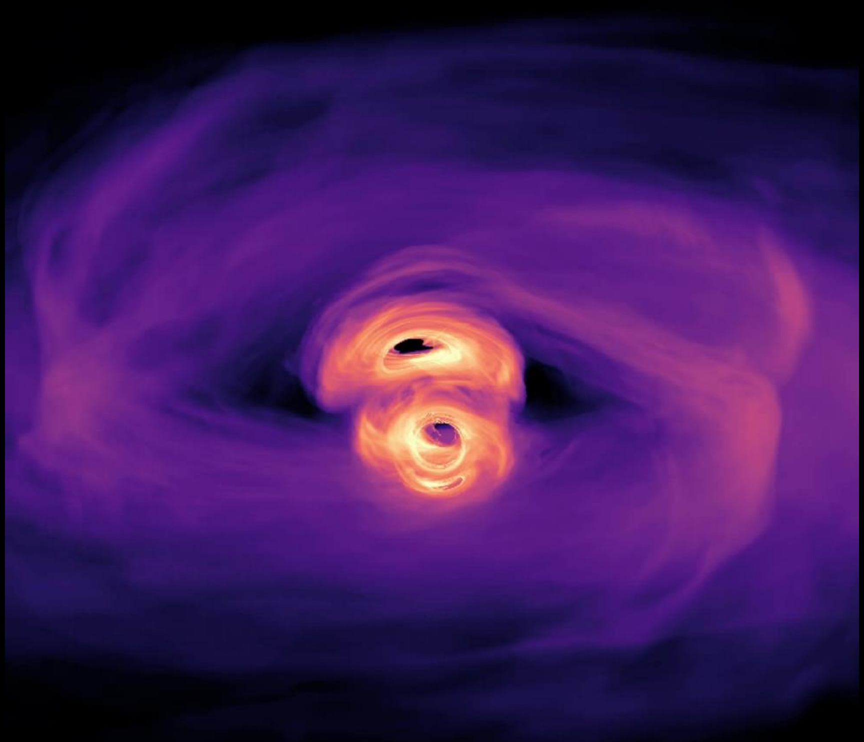
- Accreting streams primarily fall into the cavity due to gravity and shock against the BH minidisk, causing periodic depletion and refill on a timescale near one orbital period.

- The gas cycle in minidisks is mainly driven by the circumbinary disk "lump" within these streams.

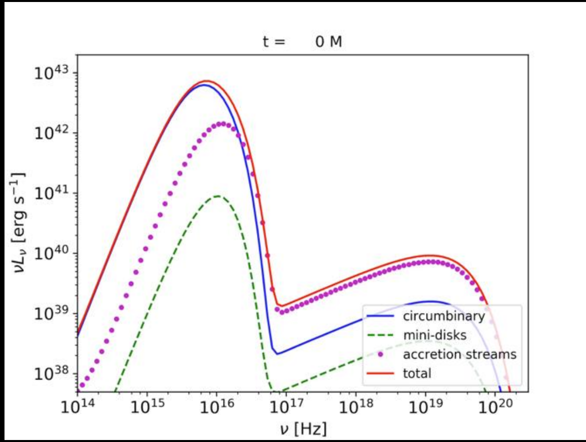
- Minidisks form quickly and exchange mass through periodic "sloshing," which contrasts with single black hole accretion.

Light from Accreting SMBBH

The first predicted time varying spectrum and light curves from accreting binary black holes approaching merger – D'Ascoli+2018, Gutierrez+ 2022

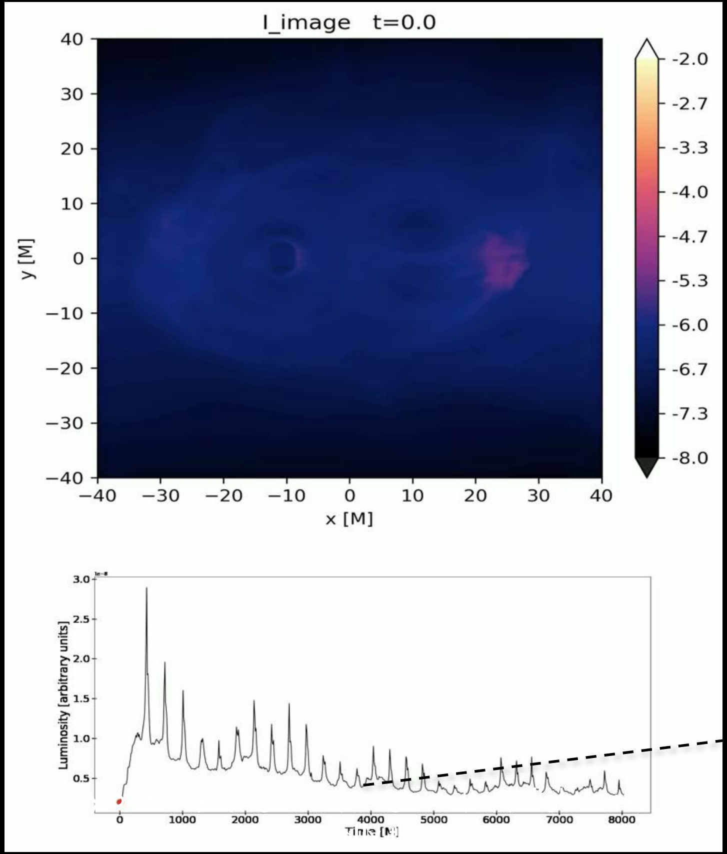


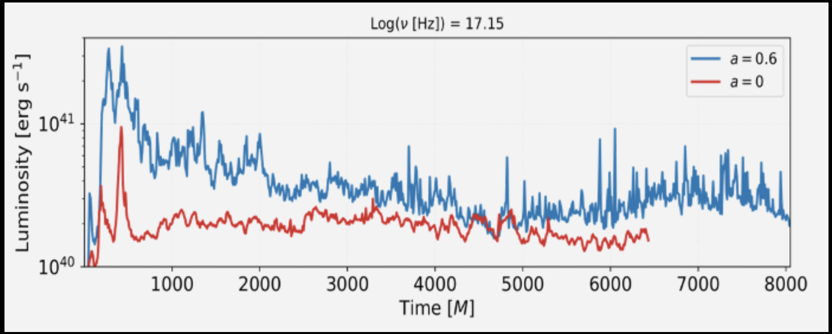
Intensity of X-rays (log scale) multiple-angle video in time, optically thin case



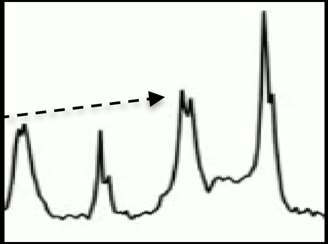
- We found that the minidisks around each of the BHs are the hottest features emitting hard X-rays relative to UV/EUV of CBD.
- Variability in the light curves and outflows follows that of accretion rate; brighter if the BHs are spinning!

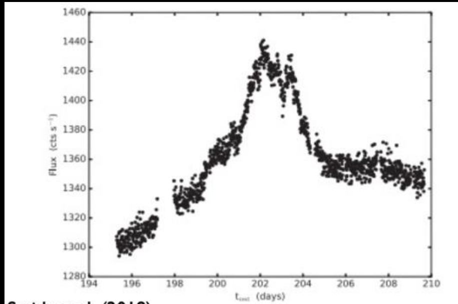
Light Curves display Self-lensing features





How self-lensing features depends on mass ratios, spins, accretion rates, etc – Porter+2024



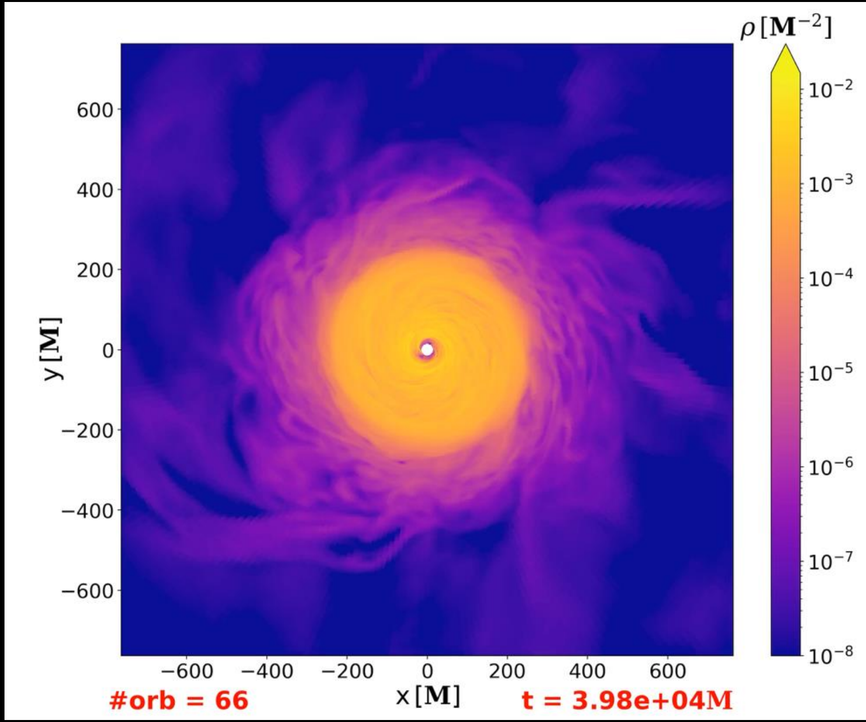


Smith et al. (2018)

Possible observation of SLF from AGN source known as Spikey, - Smith+2018

First long-term GRMHD simulations that reach merger …

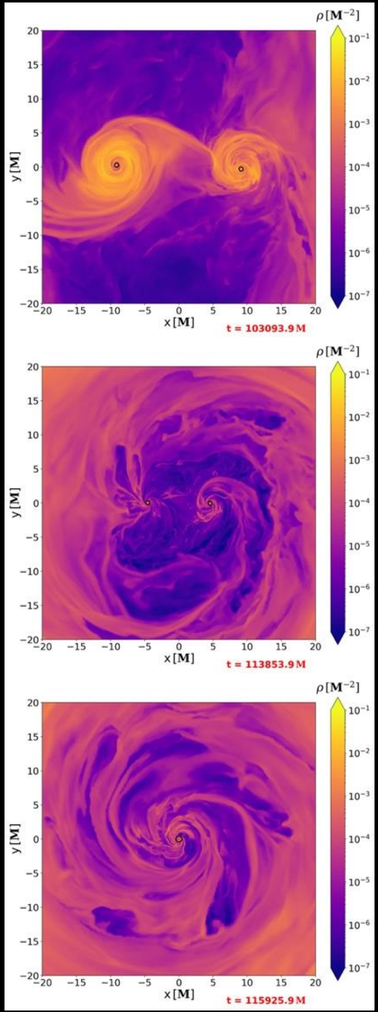
Over 250 binary orbits!



Minidisks around each black hole drain and dissolve as the binary shrinks, but the luminosity only drop by 50%!

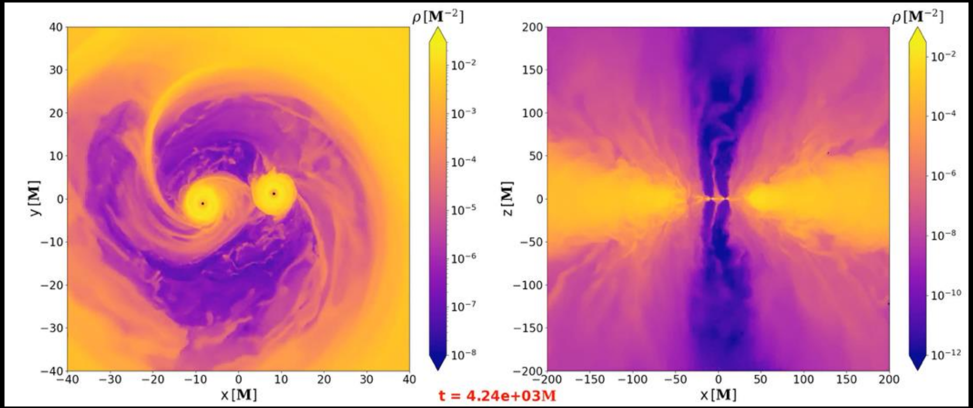
Unlike single black holes, thermal light during the final stages is powered by strong shocks, not disk turbulence.

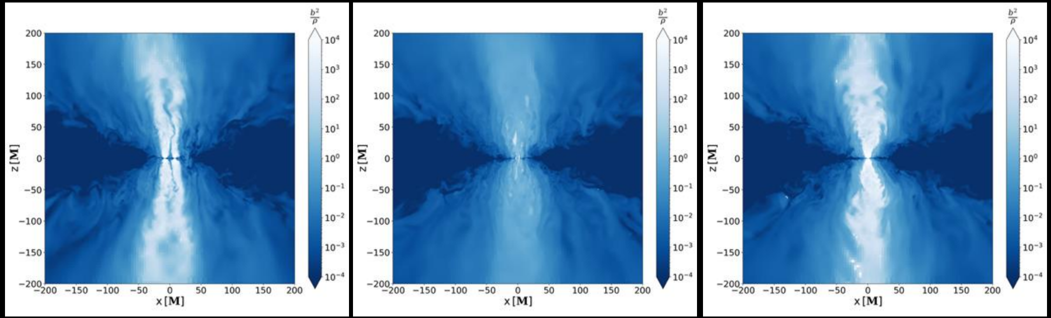
Ennoggi+, PRD 2025

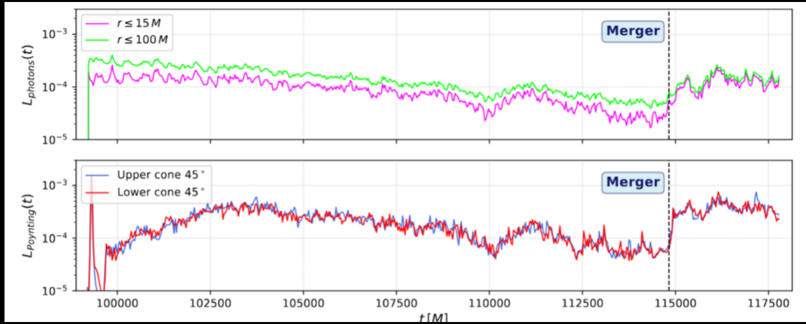


The merger of spinning, accreting SMBBH

- Luminosity briefly drops only by a factor a few, then spikes by 50% at merger and during the post-merger.
- Both photon and Poynting luminosities appears to be strongly correlated.



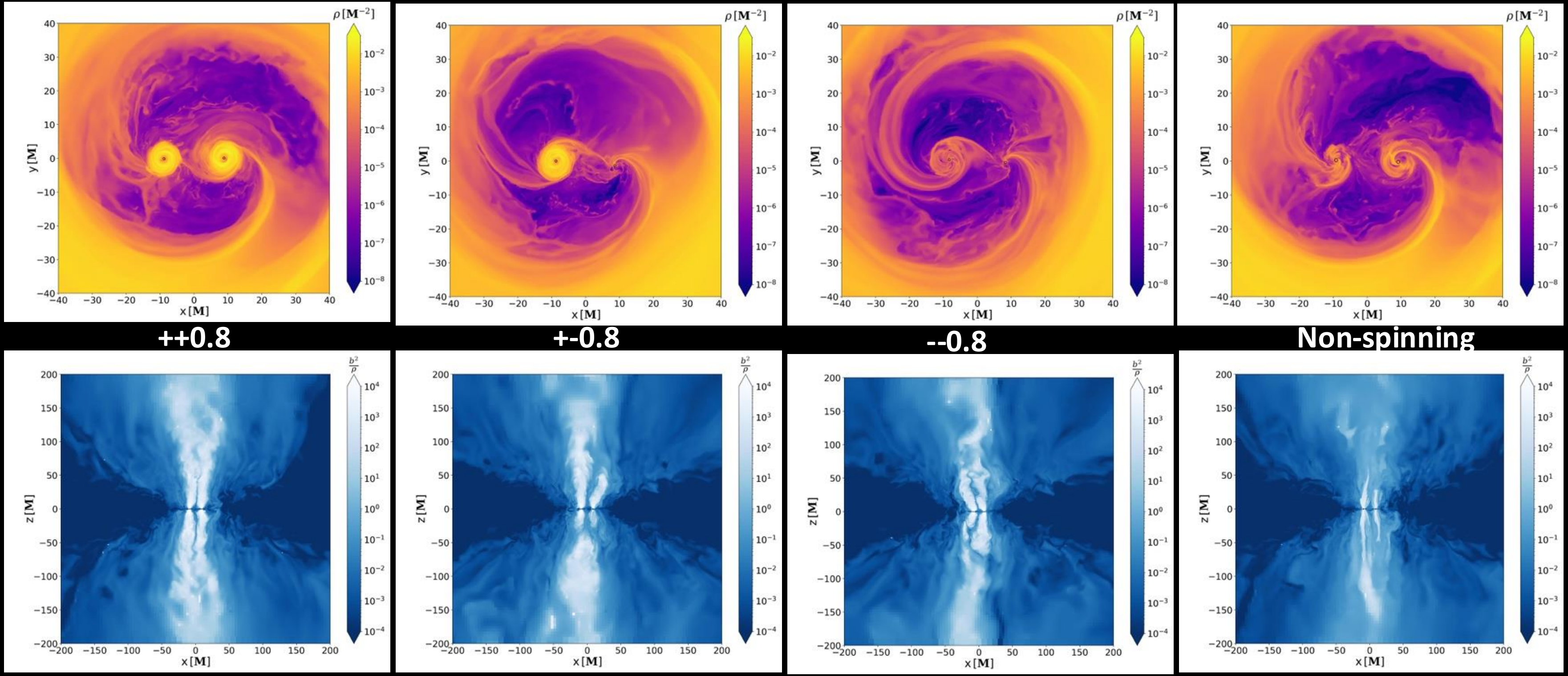




This unique "dip-then-jump" feature is a key observational fingerprint to help identify these mergers, even without a GW detection.

Ennoggi+, just submitted to PRL

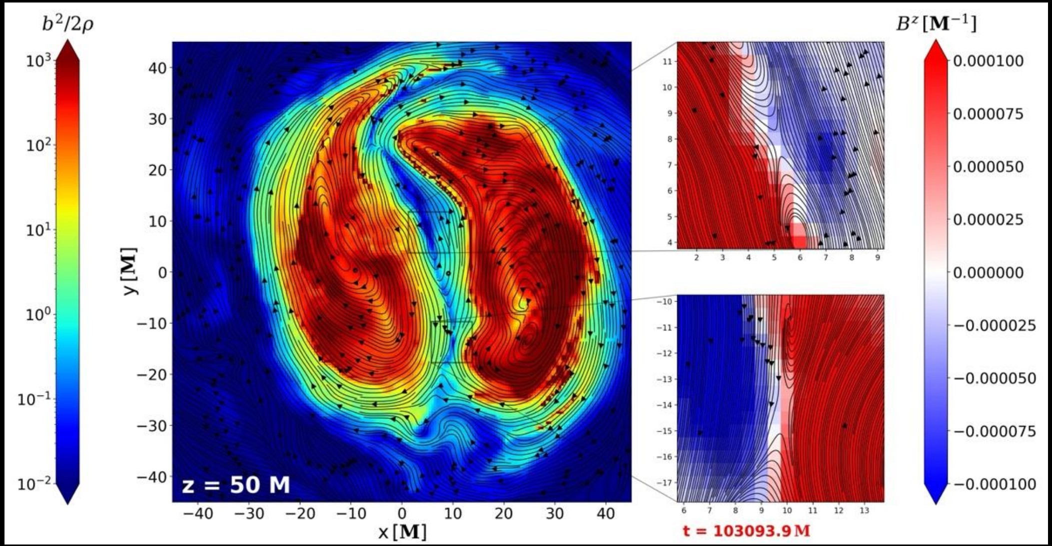
The effect of spins on minidisks and jets launching

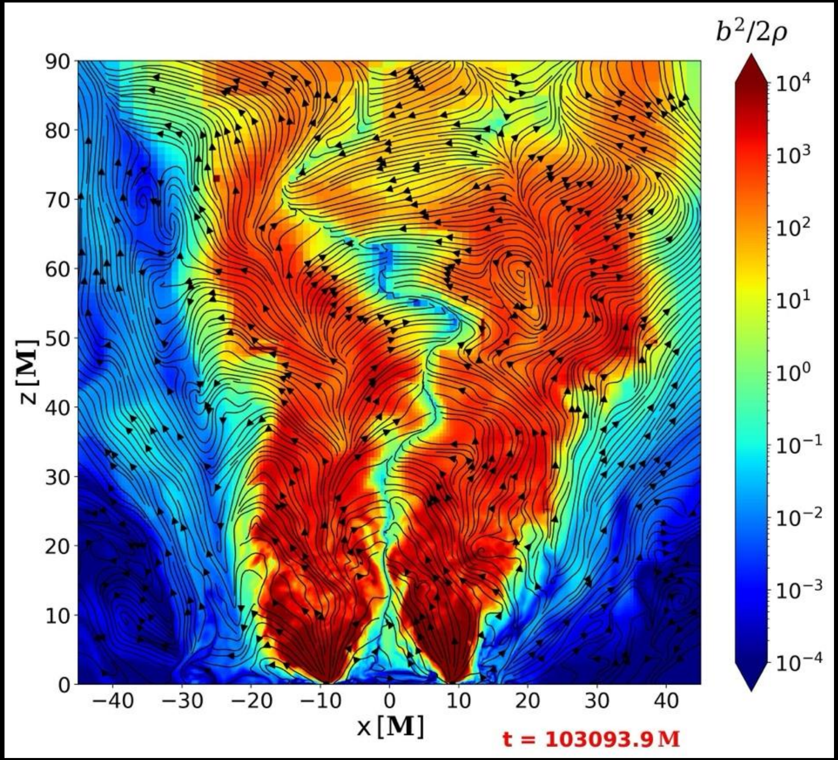


- The magnitude and direction of the spins affects orbital dynamics via spin-orbit interactions – e.g. Campanelli+2007
- Minidiscs physics affected by BH spins – Ennoggi+2025 in prep

Jet-jet interactions can amplify the EM signals!

Magnetic reconnection can occur in the jet interaction region:



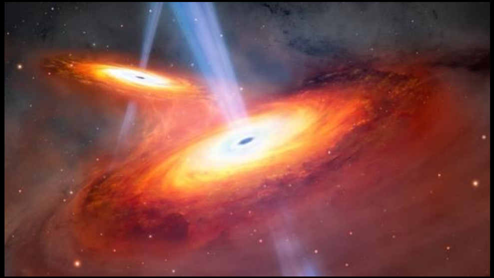


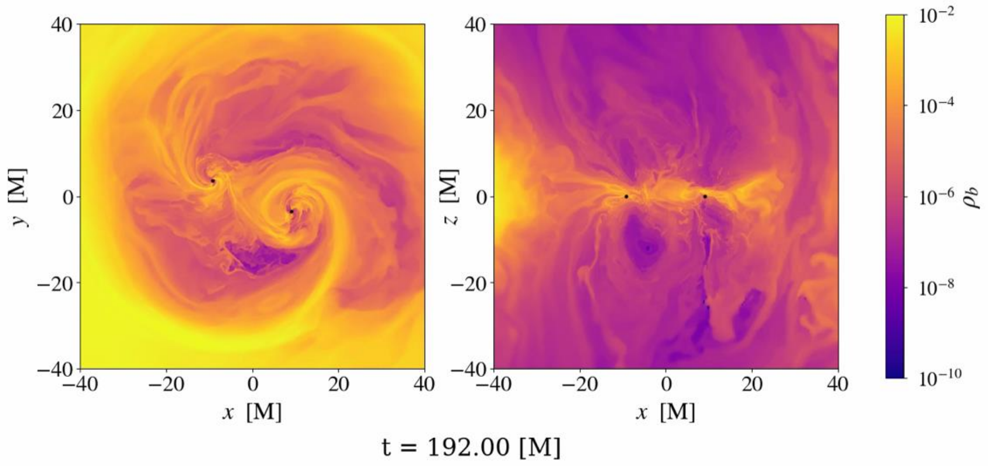
- In the jet interaction region, magnetic energy is converted into heat and kinetic energy..
- Electrons (and ions) are accelerated to extreme energies along the current sheet.
- These high-energy electrons then produce synchrotron and inverse Compton radiation.

De Simone, Ennoggi+ in prep

If the BH Spins are oblique …

BBH can display interesting merger dynamics due to precessing spins





Maria Chiara De Simone +, to be submitted to PRL

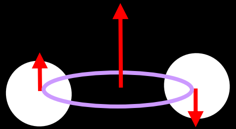
- BH spin – flip: Flip the spin of one of the BHs with respect to the orbital angular momentum **L** – Lousto & Healy, 2015
- L – Flip: 1:10 mass ratio BBH with spin of larger BH pointing down at oblique angle – Lousto & Healy, 2018
- Jet-jet interaction – Gutierrez+2024, Ressler+2024
- ``Superkicks" and ``Hang-up Kicks": the final BH remnant after merger can get a gravitational wave recoil of several thousands km/s is the BHs have oblique spins – Campanelli+2007, Lousto+2015

Kicks from Numerical Relativity Calculations

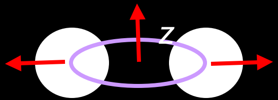
$$\vec{V}_{\rm recoil}(q,\vec{\alpha}) = V_m\,\hat{e}_1 + V_\perp(\cos\xi\,\hat{e}_1 + \sin\xi\,\hat{e}_2) + V_\|\,\hat{L},$$

NR calculations predicted large recoil velocities if significant contribution of the total spin is in the orbital plane:

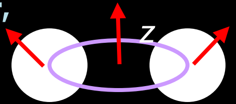
- ***Planar*** kicks up to ~ 400 km/s (**Herrmann+2007, Baker+2007, Gonzalez+2007)**

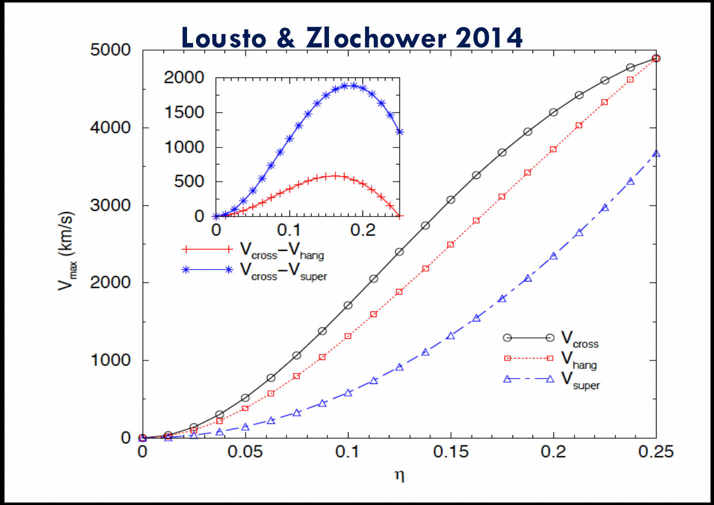


- ***Super-kicks*** up to ~ 4000 km/s (**Campanelli+2007, Tichy+2007)**

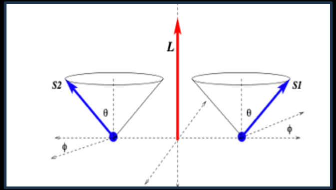


- ***Hang-up kicks*** up to ~5000 km/s (**Lousto & Zlochower, 2011)**



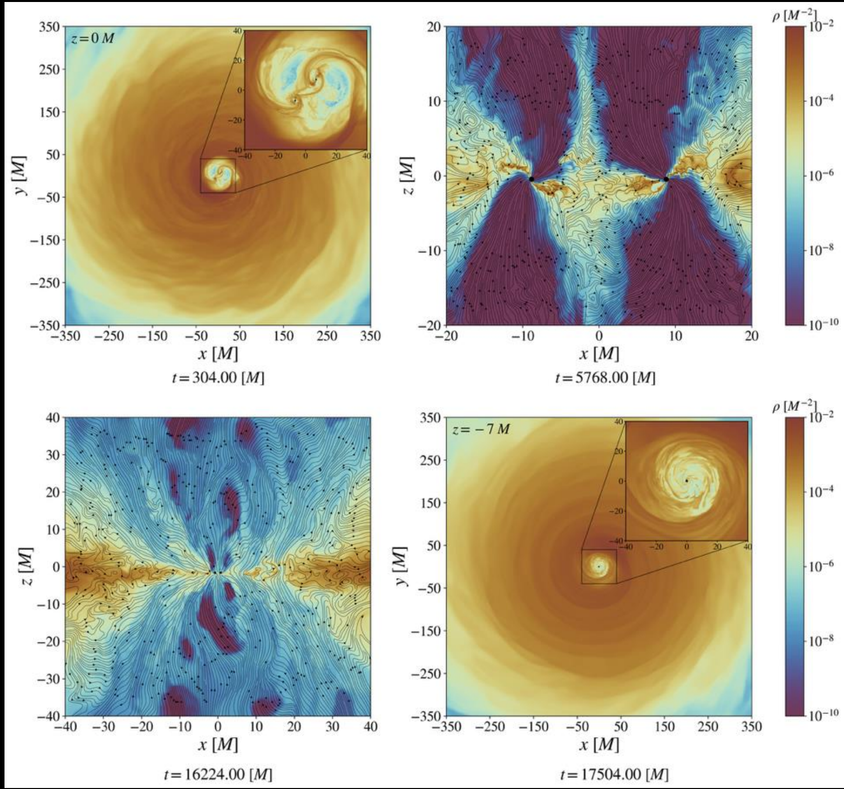


Hang-up effect: for spins aligned with L, spin-orbit coupling delays the merger, maximizing GW radiation (**Campanelli+ 2006)**



$$\eta = \frac{q}{(1+q)^2}$$

First Self-consistent GRMHD simulation of a Recoiling SMBBH …



De Simone +, just submitted to PRL

- Minidisks tilted by 45° in a direction normal to the spin axes; and theyare very warped!
- Jet aligned with spin axis ($z < 5\ M$) at close separations and aligned with orbital angular momentum at larger distances (**Cattorini2022, Kelly2021, Ressler2021**)
- Jet quenching before merger as minidisks disappear (**Ennoggi+2025**)
- Recoil along the negative z-axis due to symmetries of the system

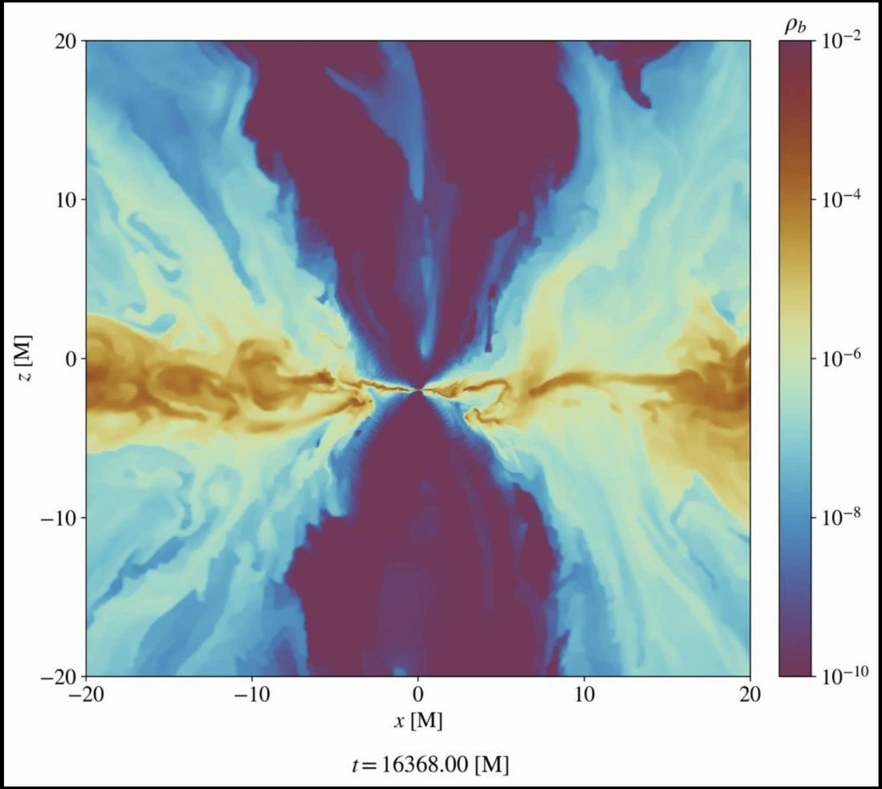
First Self-consistent GRMHD simulation of a Recoiling SMBBH …

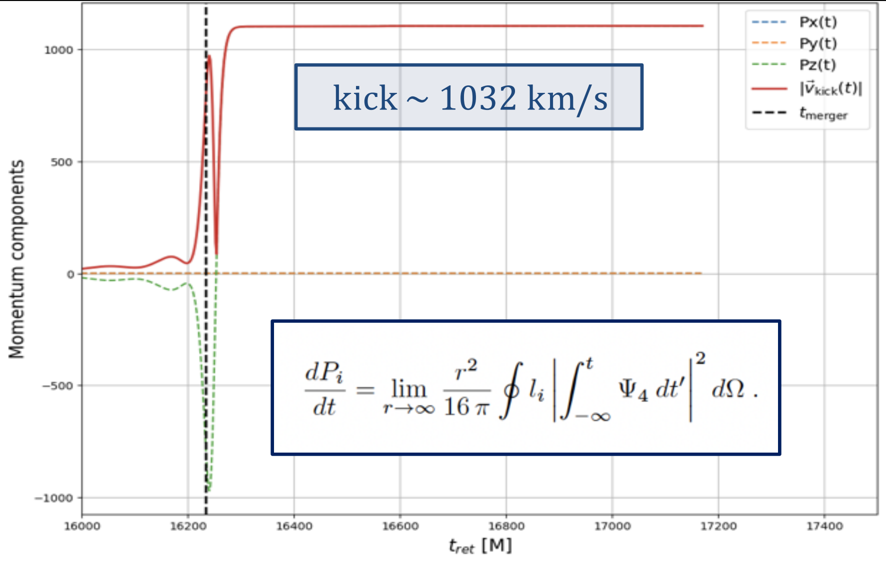
Does the recoiling SMBH retain the inner part of its disk?

$$R_{out} \sim \frac{GM}{v_{ej}^2} \sim 83000\ M$$

$$\chi_f = 0.82$$

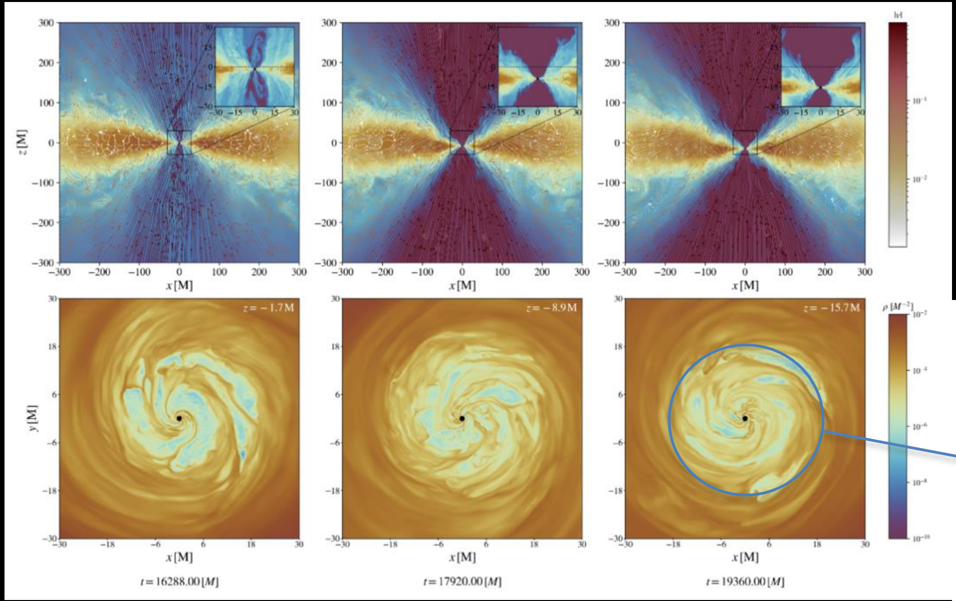
$$M_f = 0.93$$



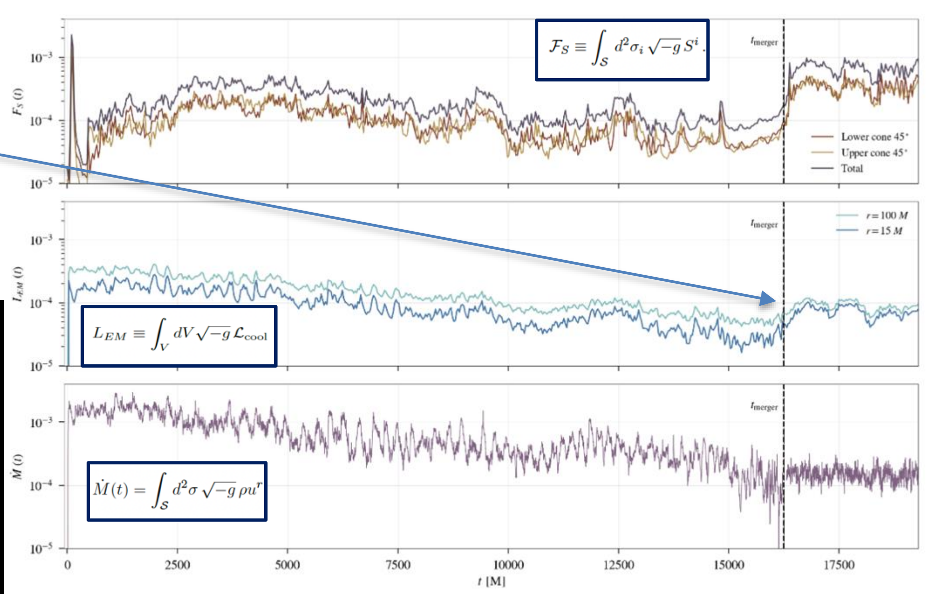


De Simone +, just submitted to PRL

Recoiling SMBBHs as potential multimessenger post-cursors …



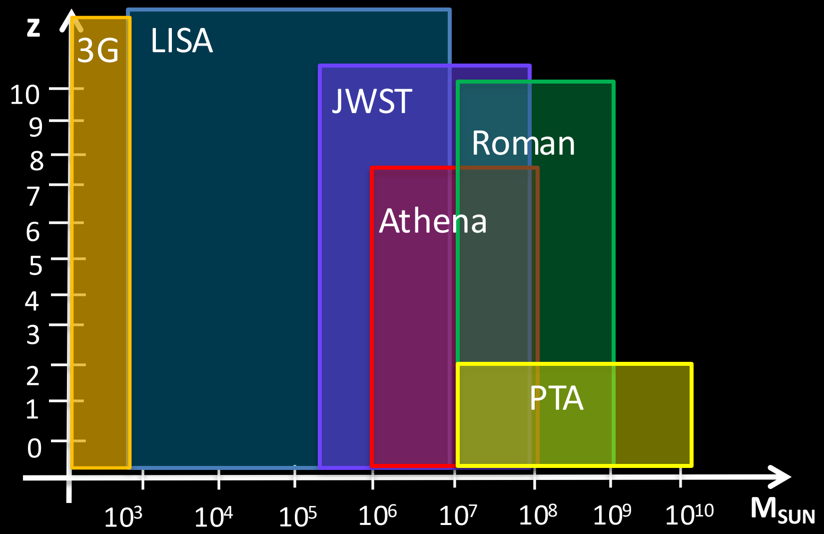
Most of the luminosity is coming from the region very close to the recoiling SMBH!



- Hints of periodic signatures in the light curve and pointing flux after merger.
- Postmerger EM signal as LISA MMA postcursor?

Concluding Remarks

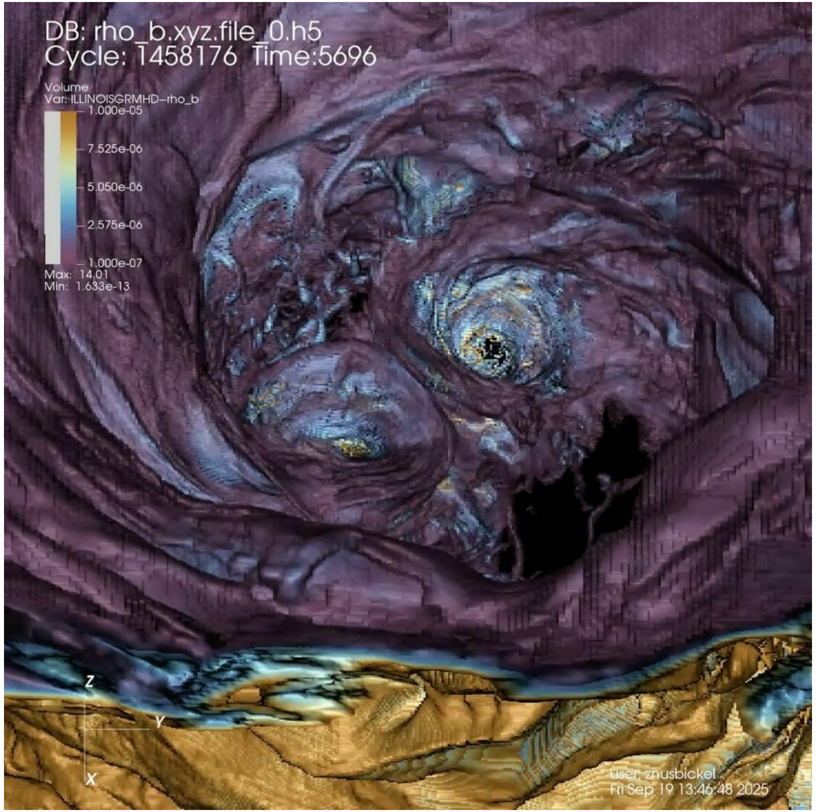
- In the next decade or two, there will be a revolution black hole astrophysics and GW science, unveiling populations of black holes, including binaries, across all cosmic epochs, and revealing their origins.



- JWST, Vera Rubin/LSST, Athena, Roman might uncover "many" binary-AGN in the haystack in the upcoming decade or two …

- We need to achieve better astrophysical realism and accuracy for magnetic field growth, radiation, microphysics treatments.

- The advent of CPU/GPU powered exascale+ supercomputers, augmented by AI and superchip technology, will only accelerate us in the path to discovery.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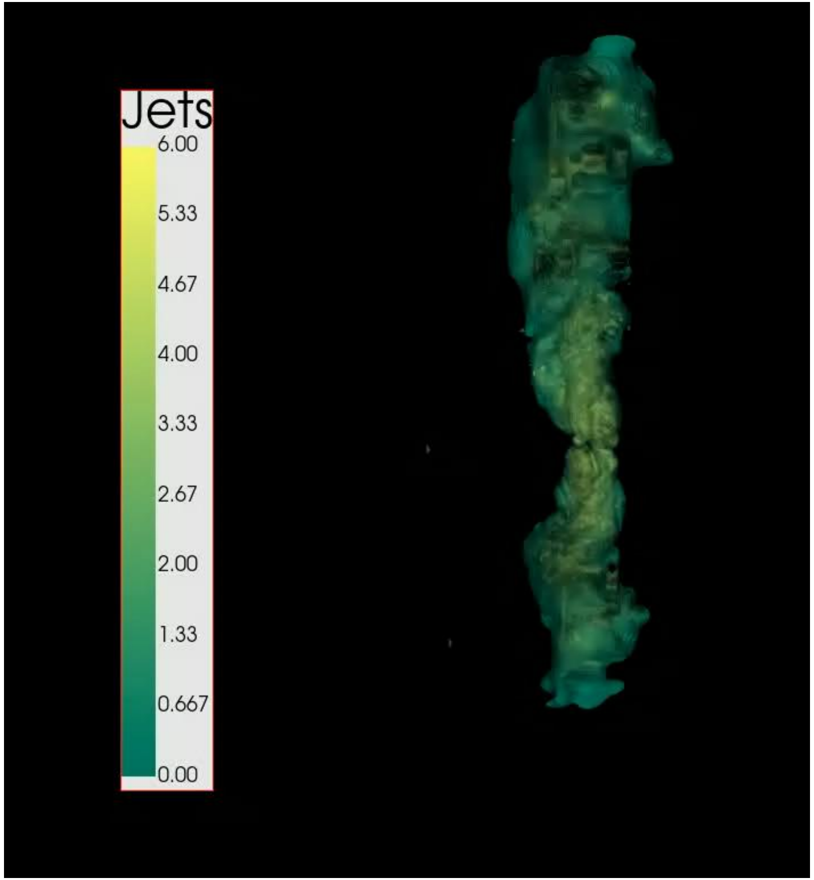
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