Binary black hole simulations with the Spectral Einstein Code

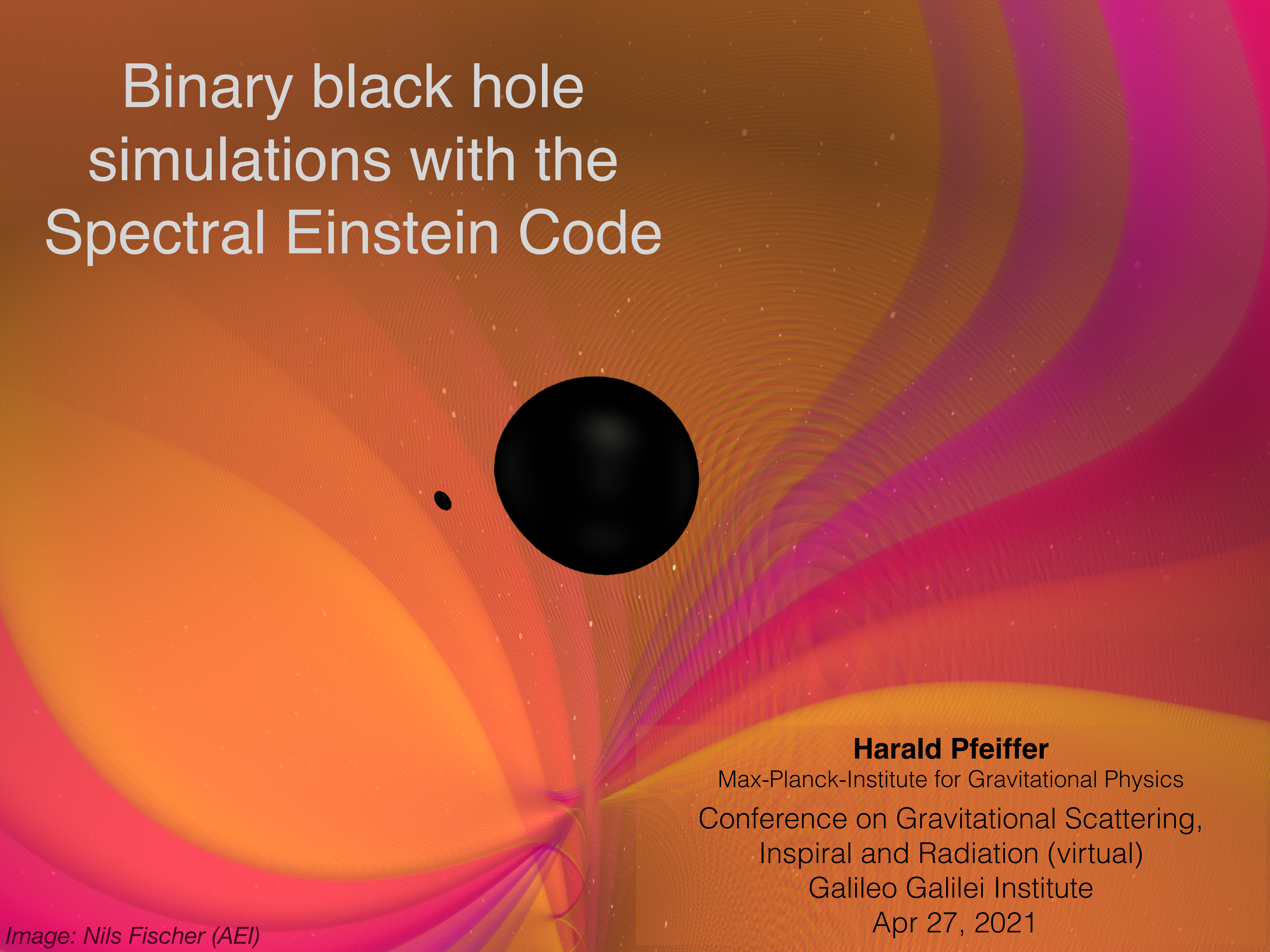


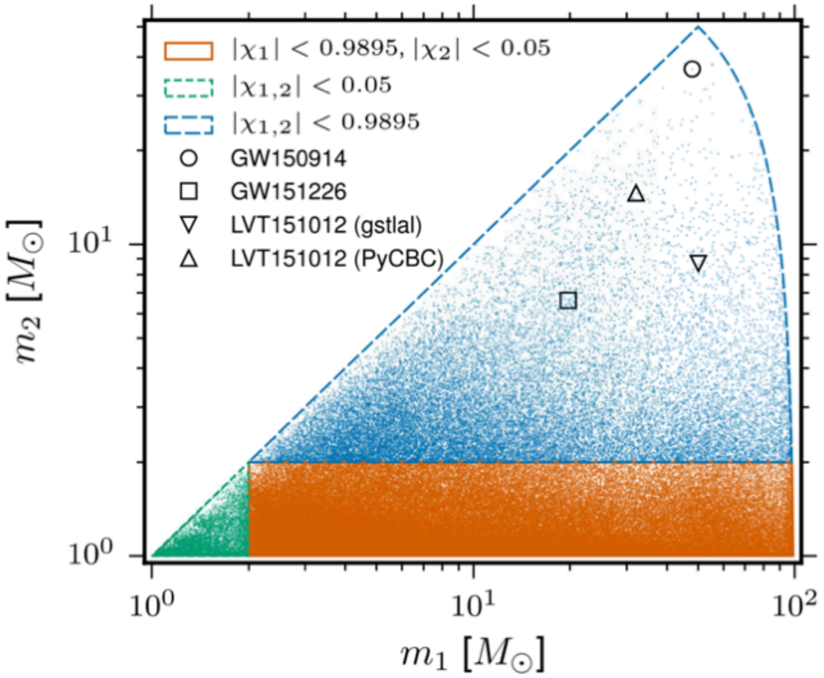
Image: Nils Fischer (AEI)

Harald Pfeiffer
Max-Planck-Institute for Gravitational Physics

Conference on Gravitational Scattering,
Inspiral and Radiation (virtual)
Galileo Galilei Institute
Apr 27, 2021

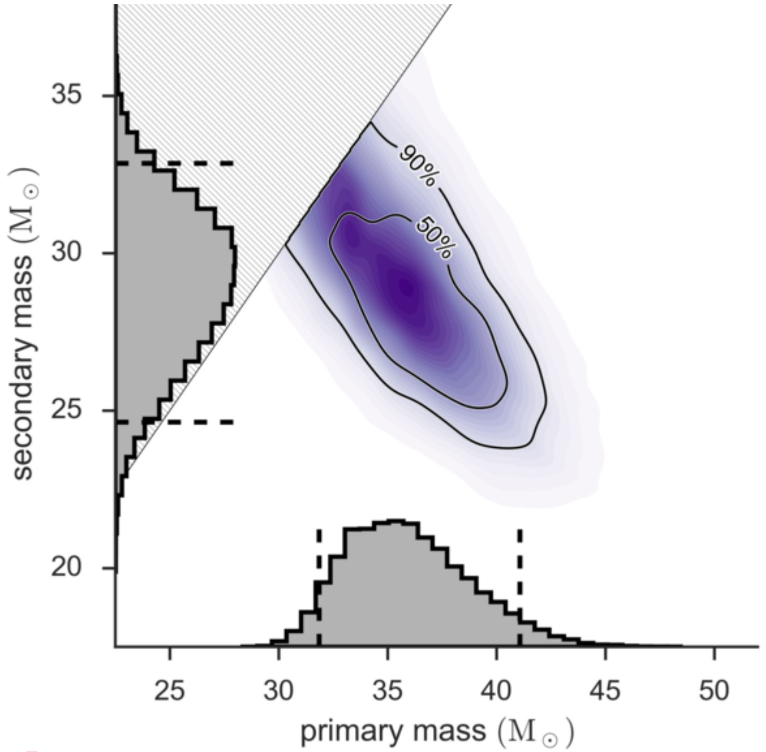
Waveform knowledge ***essential for GW astronomy***

Detection by matched filtering



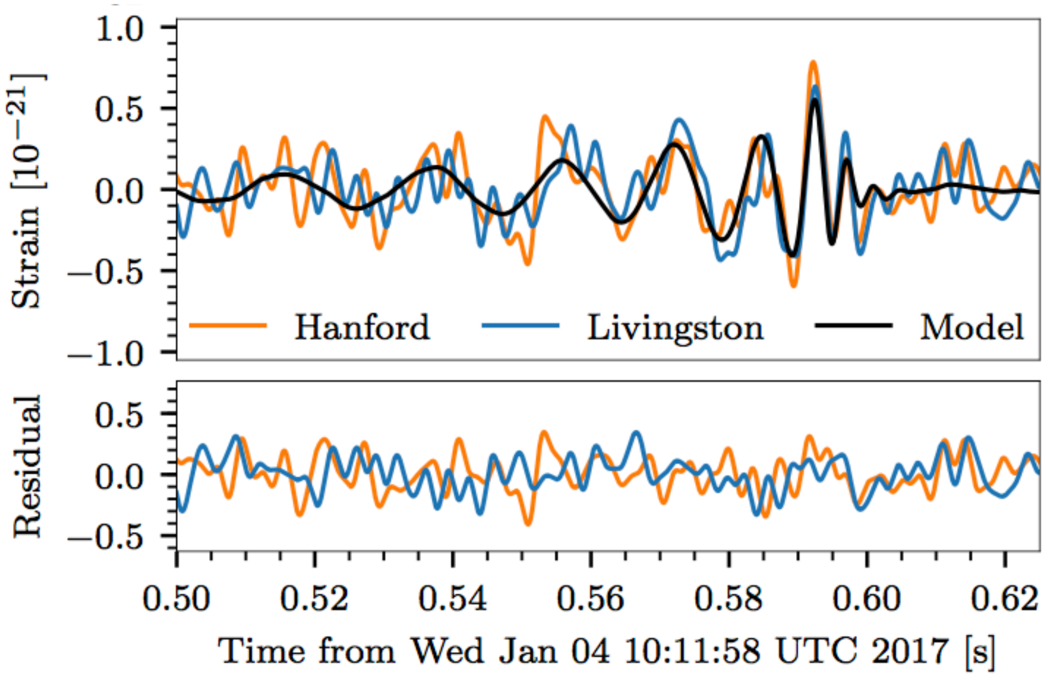
LIGO+Virgo, PRX 2016 (1606.04856)

Parameter estimation



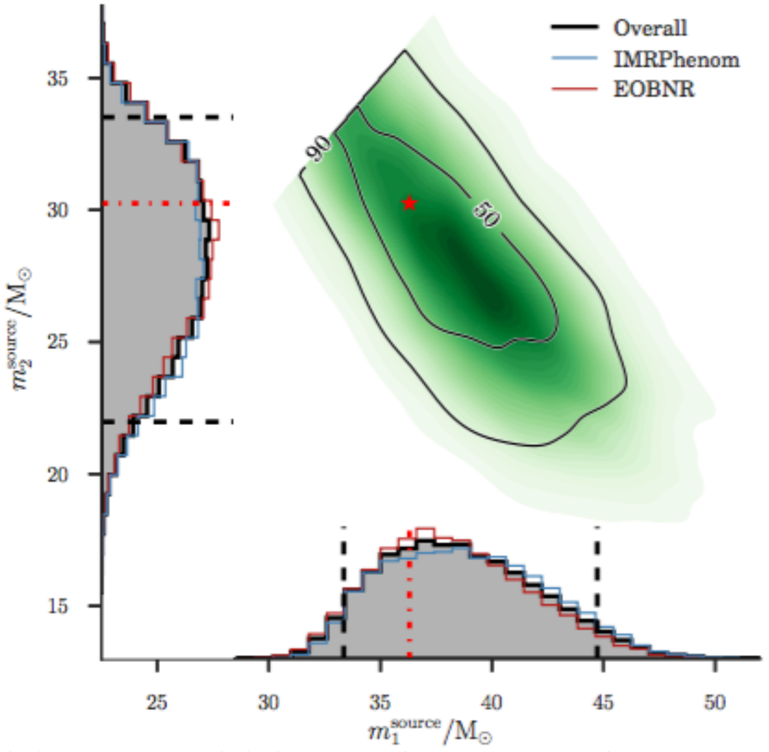
"GW150914" Abbott+ PRL 12016

Testing GR



LIGO+Virgo, PRL 2017 (1706.01812)

Validation



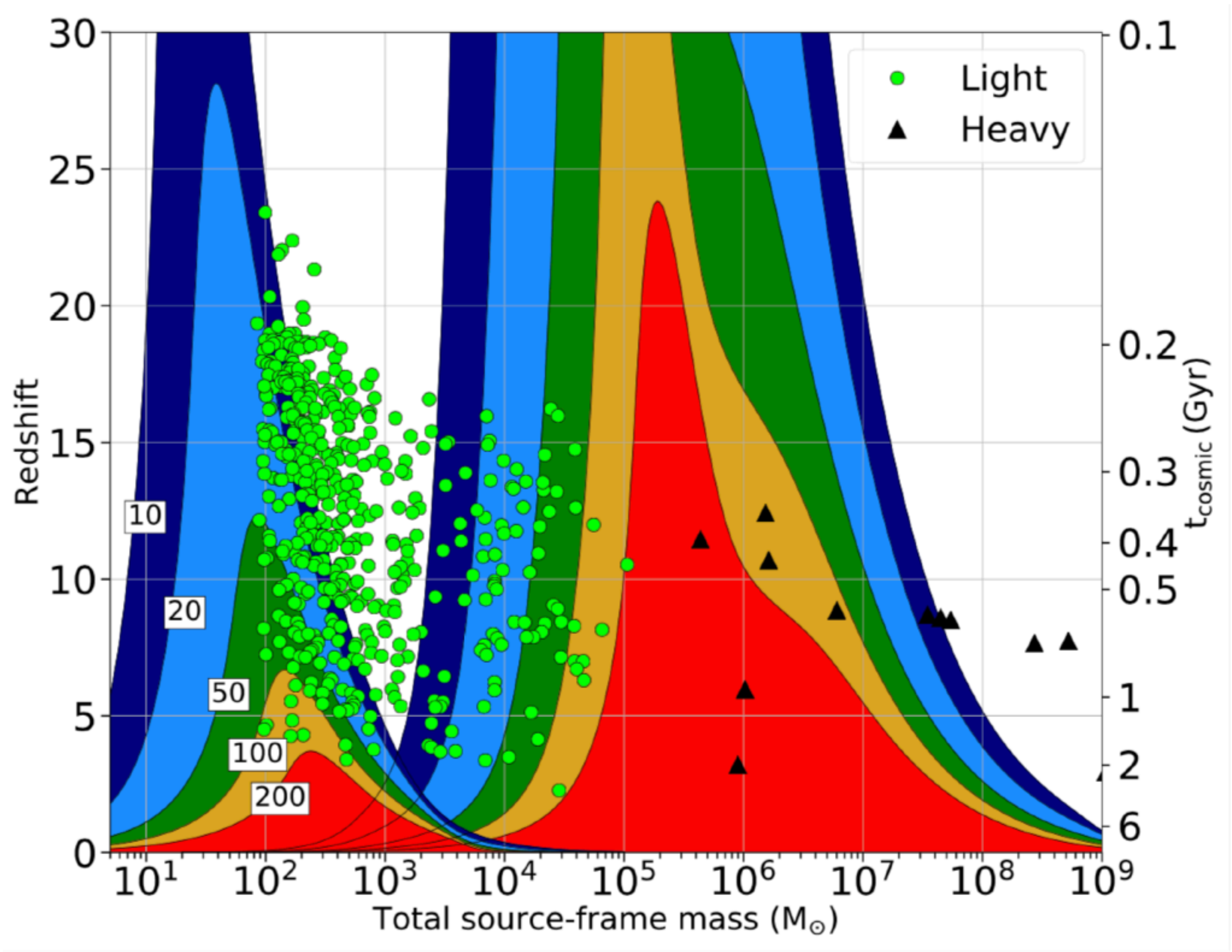
LIGO & Virgo: CQG 2017 (1611.07531)

This material is based upon work supported by NSF's LIGO Laboratory which is a major facility fully funded by the National Science Foundation.

In future, need ***higher accuracy*** for ***more diverse*** systems

3G & LISA: expected SNRs

needed accuracy ~ 1/SNR



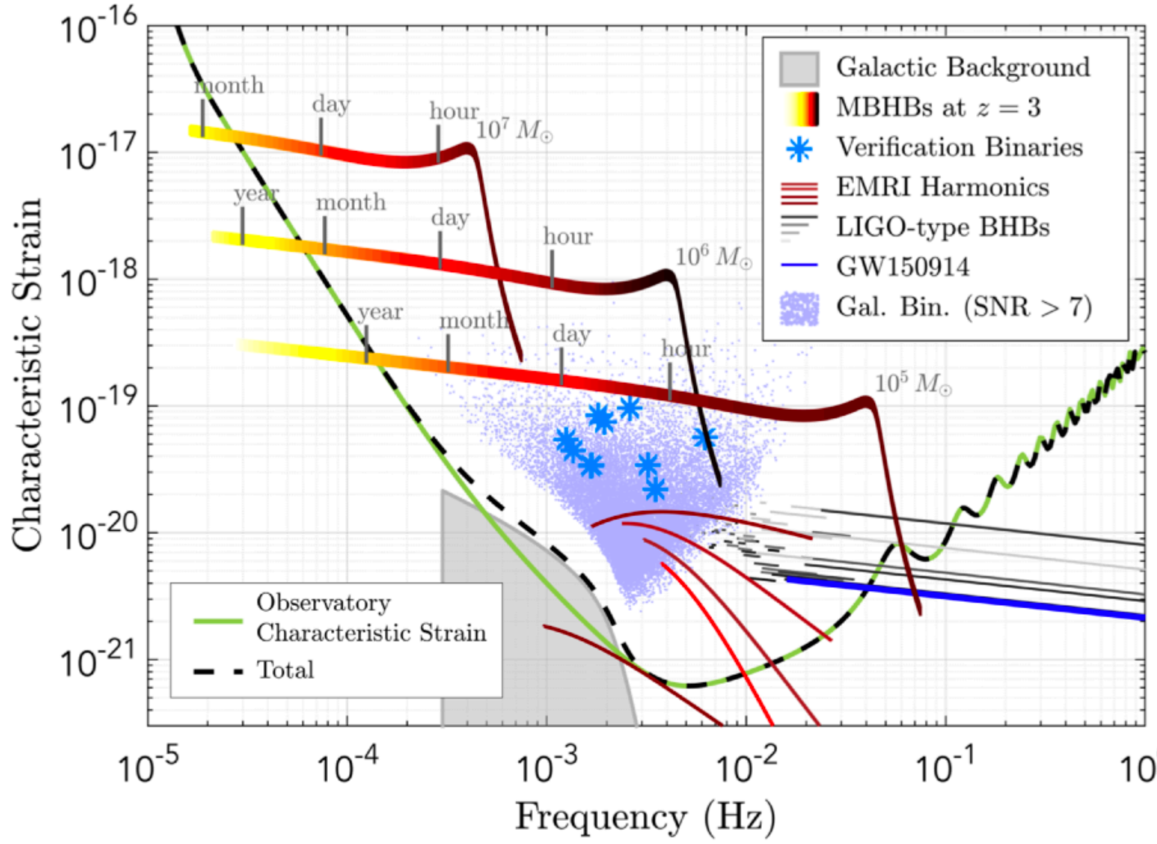
GWIC, https://gwic.ligo.org/3Gsubcomm/documents/science-case.pdf

LISA

among sources: BBH $q = 1\ldots10^{-6}$

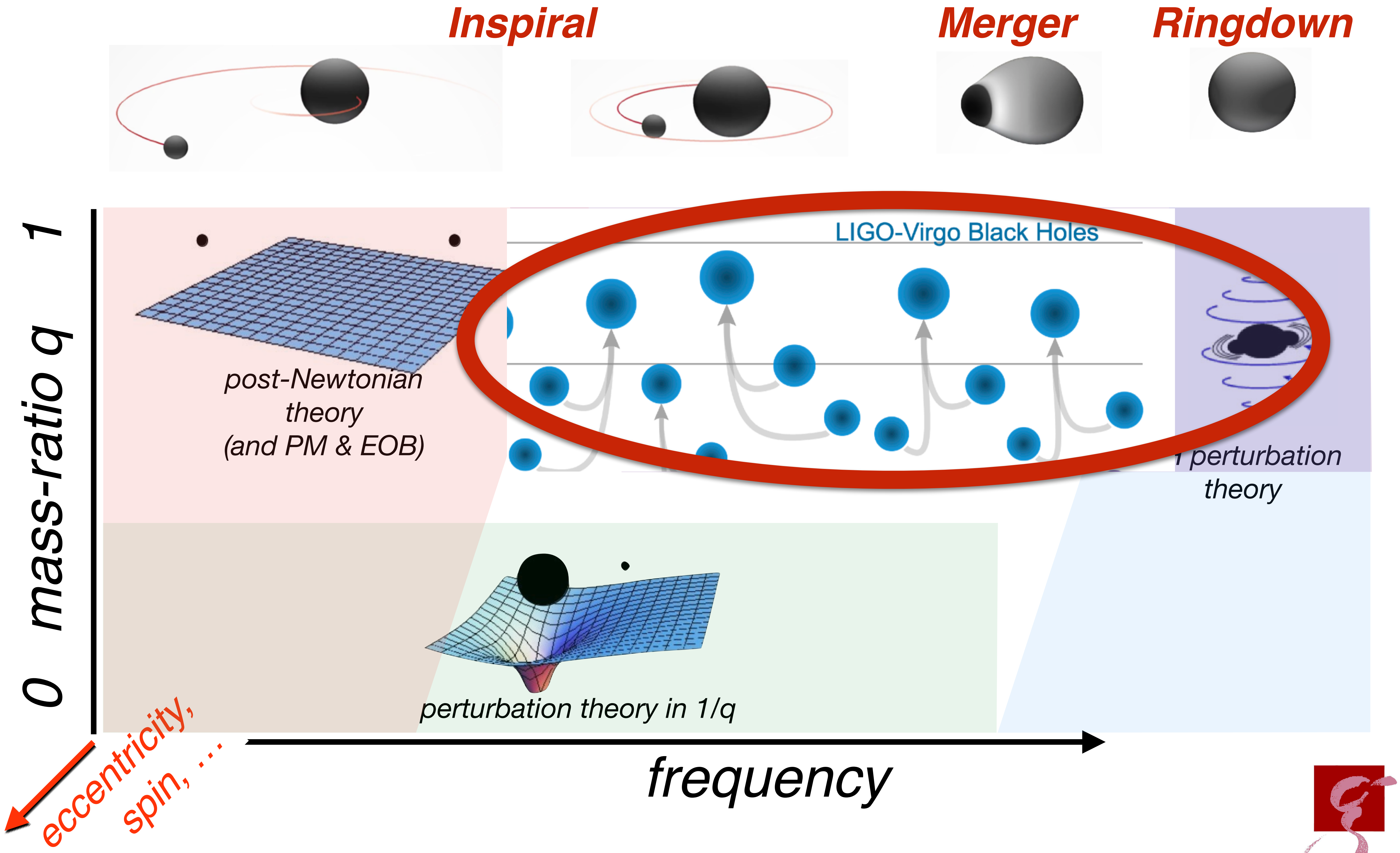
among science targets:

eccentricity measurement to $\delta e < 0.001$



LISA proposal 2017

Methods for modeling BBH



The first 50 Years of numerical relativity for BBH

1962 *ADM*
3+1 formulation

1964
Hahn-Lindquist
2 wormholes

1984
Unruh
excision

1992,3
Choptuik;
Abrahams+Evans
critical phenomena

1997
Brandt-Brügmann
puncture data

1994-98
BBH Grand Challenge

1999-00
AEI/PSU
grazing collisions

2000-04
AEI/UTB-NASA
revive crashing codes (Lazarus)

~2000 *Choptuik;*
Schnetter;Brügmann
mesh refinement

2005
Gundlach ea
constraint damping

2005 *Pretorius*
inspiral-merger-ringdown (IMR)
w/ harmonic

2005-06
Campanelli+; Baker+
IMR w/ BSSN &
moving punctures

2006-08
Scheel..HP+ *SXS*
IMR w/ spectral

2007-
Ajith, AEI, Jena
phenom GW models

2009-
UMD, SXS
EOB GW models

2011
Schmidt ea;
Boyle ea
Radiation aligned frame

2011
Lousto ea
q=100

2014-
precessing
GW models

2015
Szilagyi ea
175 orbits

1964 **~1999** **~2005** **2015**

1975-77
Smarr-Eppley
head-on collision

1979 *York*
kinematics and dynamics of GR

1989-95
Bona-Masso
modified ADM,
(hyperbolicity)

1994 *Cook*
Bowen-York
initial data

1994-95
NCSA-WashU
improved
head-on collision

1999
BSSN
evolution system

1999 *York*
conformal thin sandwich ID

1999-2005 *York,*
Cornell, Caltech, LSU
hyperbolic formulations

2000-02
Alcubierre
gauge conditions

2004
Brügmann ea
one orbit

2003-08
Cook, Pfeiffer ea
improved ID

2000 *Ashtekar*
isolated horizons

2006,07
Baker ea;
Gonzalez ea
non-spinning BBH kicks

2007 *SXS*
PN-NR comparison

2007-11
RIT; Jena; AEI;…
BBH superkicks

2008
all of NR
NINJA

2009-11
Bishop, …
Cauchy characteristic extraction

2010
Bernuzzi ea
C4z

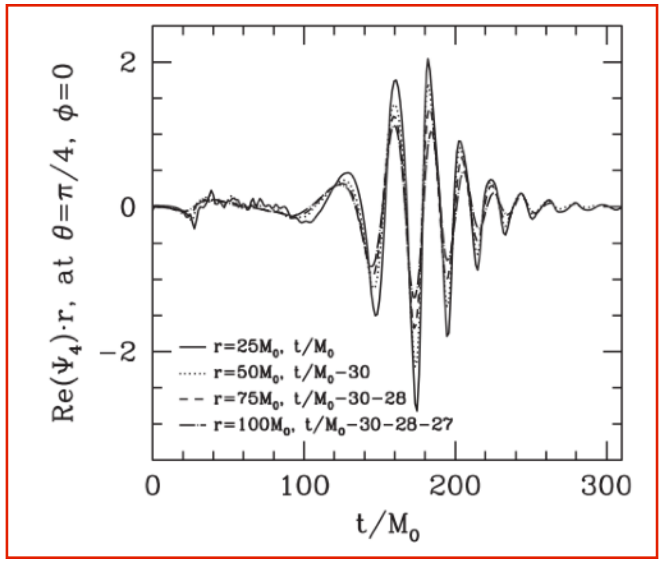
2011
Lovelace ea
S/M²=0.97

2011-
Le Tiec ea
self-force studies

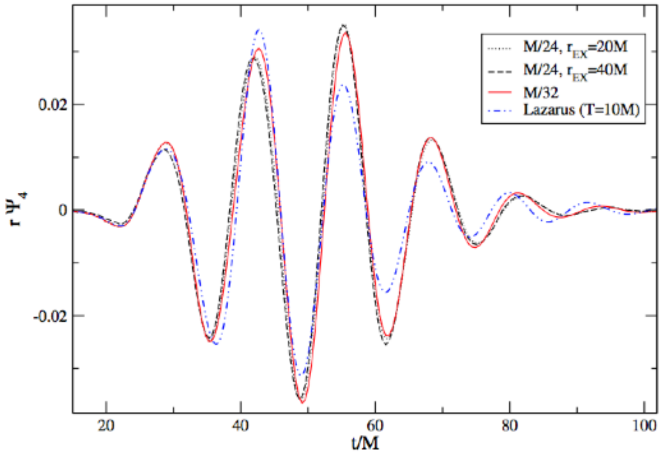
2013
GaTech; SXS
Precessing parameter studies

Courtesy Carlos Lousto,
updated by HP

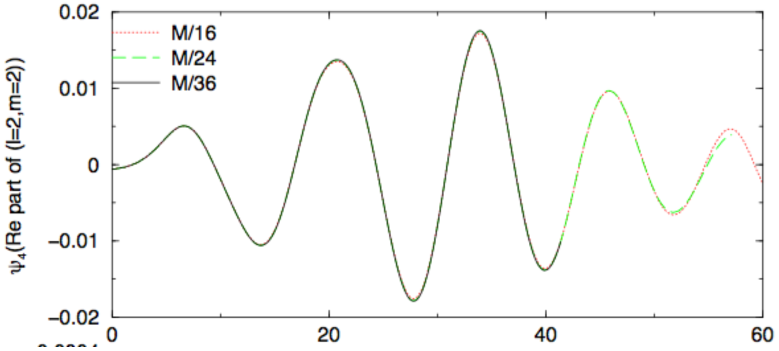
2005: First working BBH inspirals



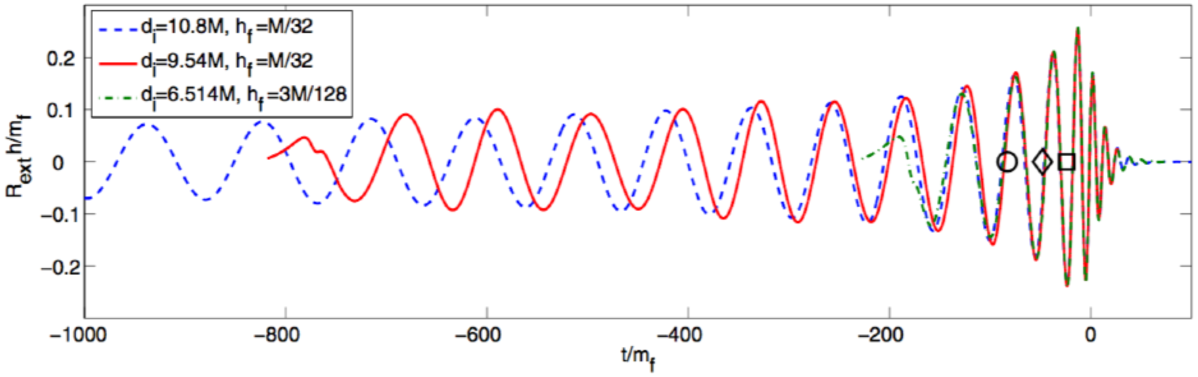
Pretorius 05



Baker+06



Campanelli+06



Baker+07

Important early result:

Simplicity of merger

Continuous transition inspiral → ringdown

Two approaches towards BBH simulations

"BSSN & Moving punctures"

LazEv, Maya, ETK, BAM,
Goddard, GRchombo

Puncture initial-data
$\chi \lesssim 0.9$ (but see Zlochower+ 17)

BSSN or CC4z

Moving puncture
mergers "easy"

Sommerfeld outer BC

4th to 8th order finite-difference

BHs advect through static grids

GW extrapolation
(Healy,Lousto '20 for LazEv COM correction)

"generalized harmonic & spectral"

SpEC (SXS collaboration)

Quasi-equilibrium excision data
$\chi \lesssim 0.999$

Generalized-Harmonic Evolution System

BH excision
mergers difficult

Constraint preserving,
minimally reflective outer BC

Spectral methods

Moving grid

long, phase-accurate inspirals

GW extrapolation & COM correction

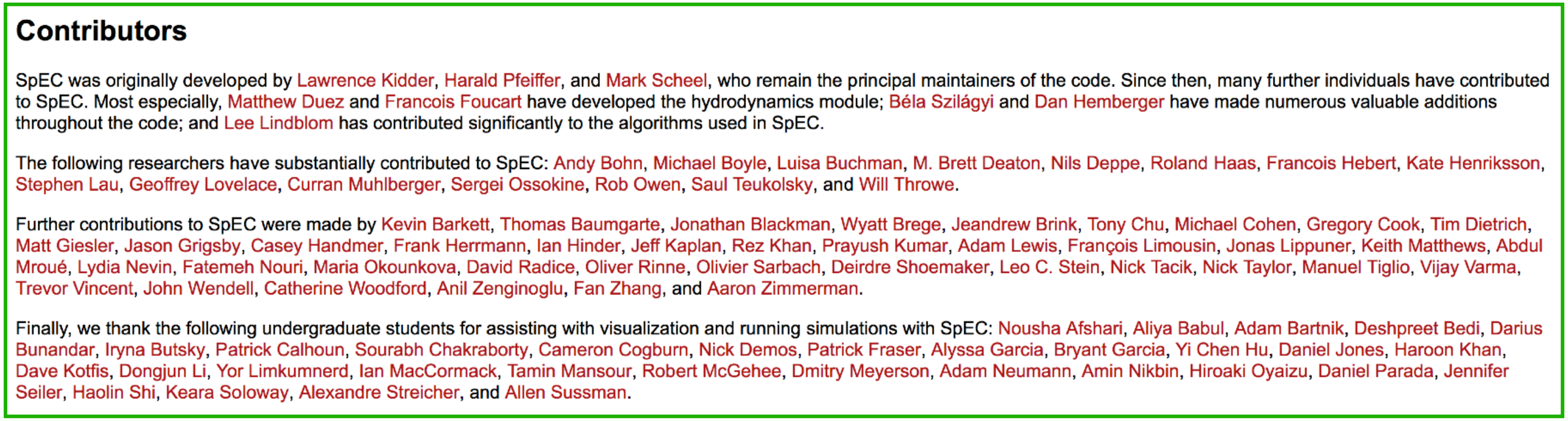
Cauchy-characteristic extraction
accurate m=0 modes, GW memory

Pretorius

Spectral Einstein Code (SpEC)

Simulating eXtreme Spacetimes collaboration

http://www.black-holes.org/SpEC.html



Contributors

SpEC was originally developed by Lawrence Kidder, Harald Pfeiffer, and Mark Scheel, who remain the principal maintainers of the code. Since then, many further individuals have contributed to SpEC. Most especially, Matthew Duez and Francois Foucart have developed the hydrodynamics module; Béla Szilágyi and Dan Hemberger have made numerous valuable additions throughout the code; and Lee Lindblom has contributed significantly to the algorithms used in SpEC.

The following researchers have substantially contributed to SpEC: Andy Bohn, Michael Boyle, Luisa Buchman, M. Brett Deaton, Nils Deppe, Roland Haas, Francois Hebert, Kate Henriksson, Stephen Lau, Geoffrey Lovelace, Curran Muhlberger, Sergei Ossokine, Rob Owen, Saul Teukolsky, and Will Throwe.

Further contributions to SpEC were made by Kevin Barkett, Thomas Baumgarte, Jonathan Blackman, Wyatt Brege, Jeandrew Brink, Tony Chu, Michael Cohen, Gregory Cook, Tim Dietrich, Matt Giesler, Jason Grigsby, Casey Handmer, Frank Herrmann, Ian Hinder, Jeff Kaplan, Rez Khan, Prayush Kumar, Adam Lewis, François Limousin, Jonas Lippuner, Keith Matthews, Abdul Mroué, Lydia Nevin, Fatemeh Nouri, Maria Okounkova, David Radice, Oliver Rinne, Olivier Sarbach, Deirdre Shoemaker, Leo C. Stein, Nick Tacik, Nick Taylor, Manuel Tiglio, Vijay Varma, Trevor Vincent, John Wendell, Catherine Woodford, Anil Zenginoglu, Fan Zhang, and Aaron Zimmerman.

Finally, we thank the following undergraduate students for assisting with visualization and running simulations with SpEC: Nousha Afshari, Aliya Babul, Adam Bartnik, Deshpreet Bedi, Darius Bunandar, Iryna Butsky, Patrick Calhoun, Sourabh Chakraborty, Cameron Cogburn, Nick Demos, Patrick Fraser, Alyssa Garcia, Bryant Garcia, Yi Chen Hu, Daniel Jones, Haroon Khan, Dave Kotfis, Dongjun Li, Yor Limkumnerd, Ian MacCormack, Tamin Mansour, Robert McGehee, Dmitry Meyerson, Adam Neumann, Amin Nikbin, Hiroaki Oyaizu, Daniel Parada, Jennifer Seiler, Haolin Shi, Keara Soloway, Alexandre Streicher, and Allen Sussman.

Spectral methods

- Expand in basis-functions, solve for coefficients

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

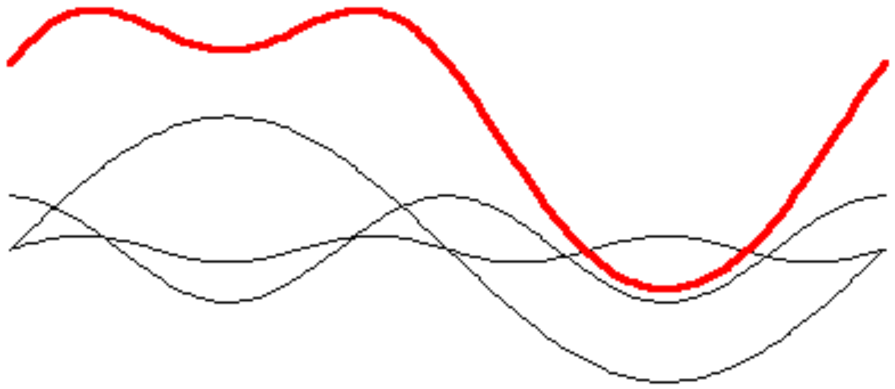
- Compute derivatives exactly

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

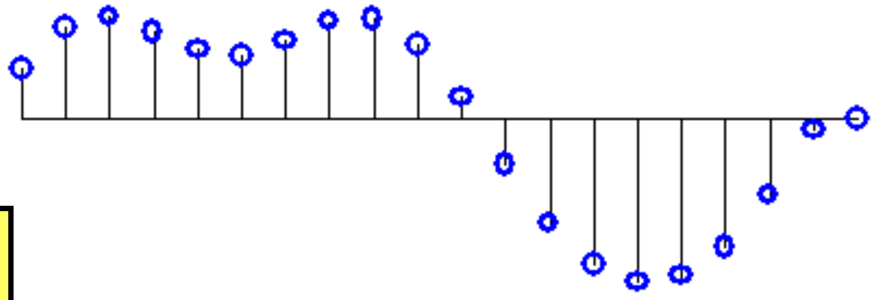
- Compute nonlinearities in physical space

- For smooth problems, ***exponential convergence***

Spectral

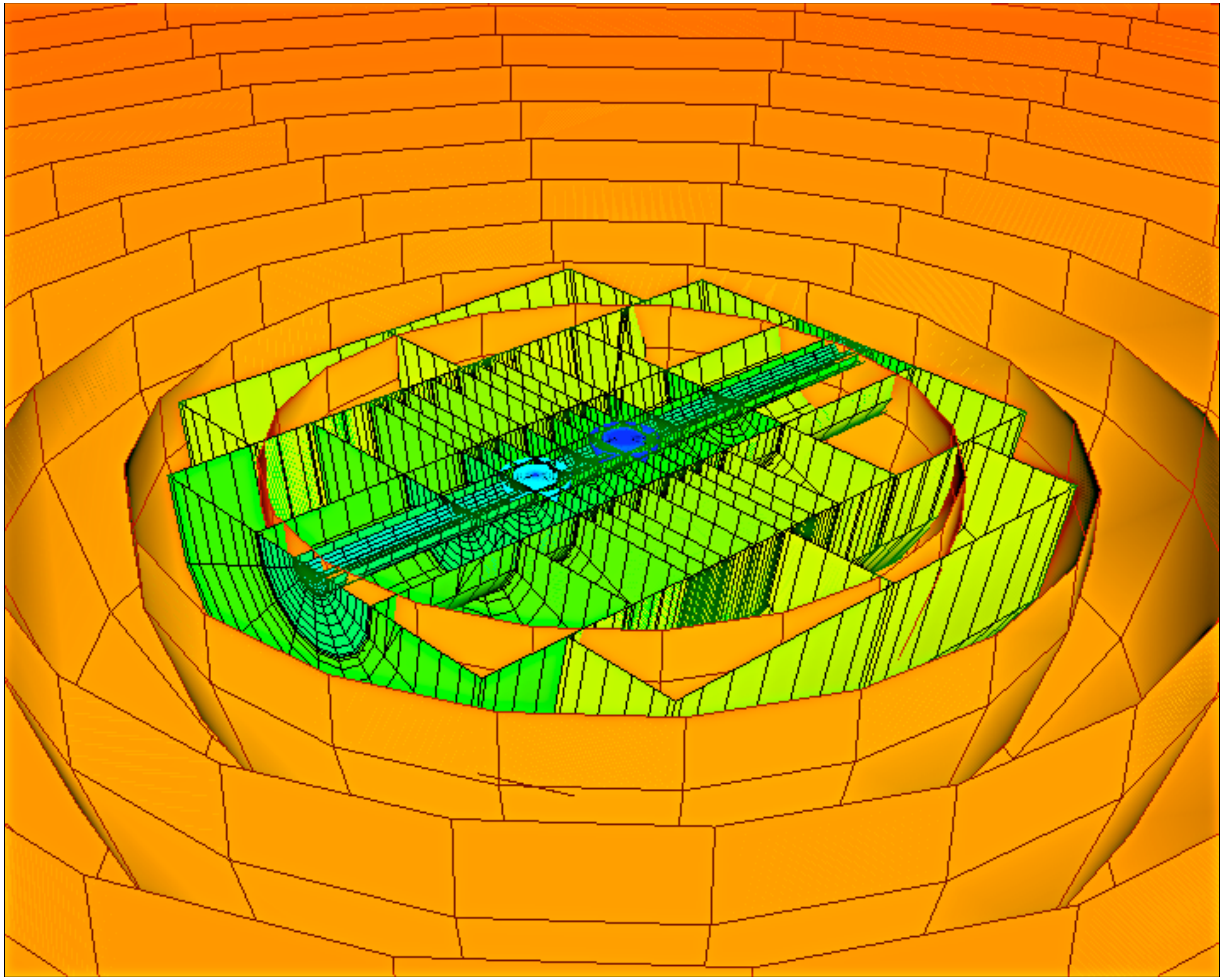


Finite differences



Domain-decomposition

- Many sub-domains, each with own basis-functions
  - Spheres
  - Blocks
  - Cylinders
- Advantages:
  - Excision of BH singularities
  - Adaptive Resolution
  - Parallelization



http://www.black-holes.org/SpEC.html

Einstein constraints: Formalism

$$\begin{tikzcd}
\boxed{\begin{array}{c} R + (\mathrm{tr}K)^2 - K^2 = 0 \\ \nabla\cdot(K - g\,\mathrm{tr}K) = 0 \end{array}} \arrow[r, bend left, "g = \psi^4\tilde{g}", "\text{Lichnerowicz 44}"'] & \begin{array}{l} \tilde{\nabla}^2\psi = \dots \\ \tilde{\nabla}\cdot(\frac{1}{\tilde{\sigma}}\tilde{\mathbb{L}}V) = \dots \end{array}
\end{tikzcd}$$

coupled nonlinear elliptic PDEs in 3D

$$K = \tfrac{1}{3}\mathrm{tr}K\, g + A$$

$$\begin{tikzcd}
A \arrow[r, "\text{conformal scaling}", "A = \psi^{-10}\tilde{A}"'] \arrow[d, "\text{TT decomp.}"'] & \tilde{A} \arrow[d, "\text{conformal TT decomp.}"] \\
A = A_{\mathrm{TT}} + \frac{1}{\sigma}(\mathbb{L}V) \arrow[r, "\text{conformal scaling}", "\begin{array}{c} A_{\mathrm{TT}} = \psi^{-10}\tilde{A}_{\mathrm{TT}} \\ \sigma = \psi^6\tilde{\sigma} \end{array}"'] & \tilde{A} = \tilde{A}_{\mathrm{TT}} + \frac{1}{\tilde{\sigma}}(\tilde{\mathbb{L}}V)
\end{tikzcd}$$

Hamiltonian picture ≡ Lagrangian picture

York(+) 72;74;99, HP,York 03

Applied to binary black holes

- Asymptotics/boundary conditions

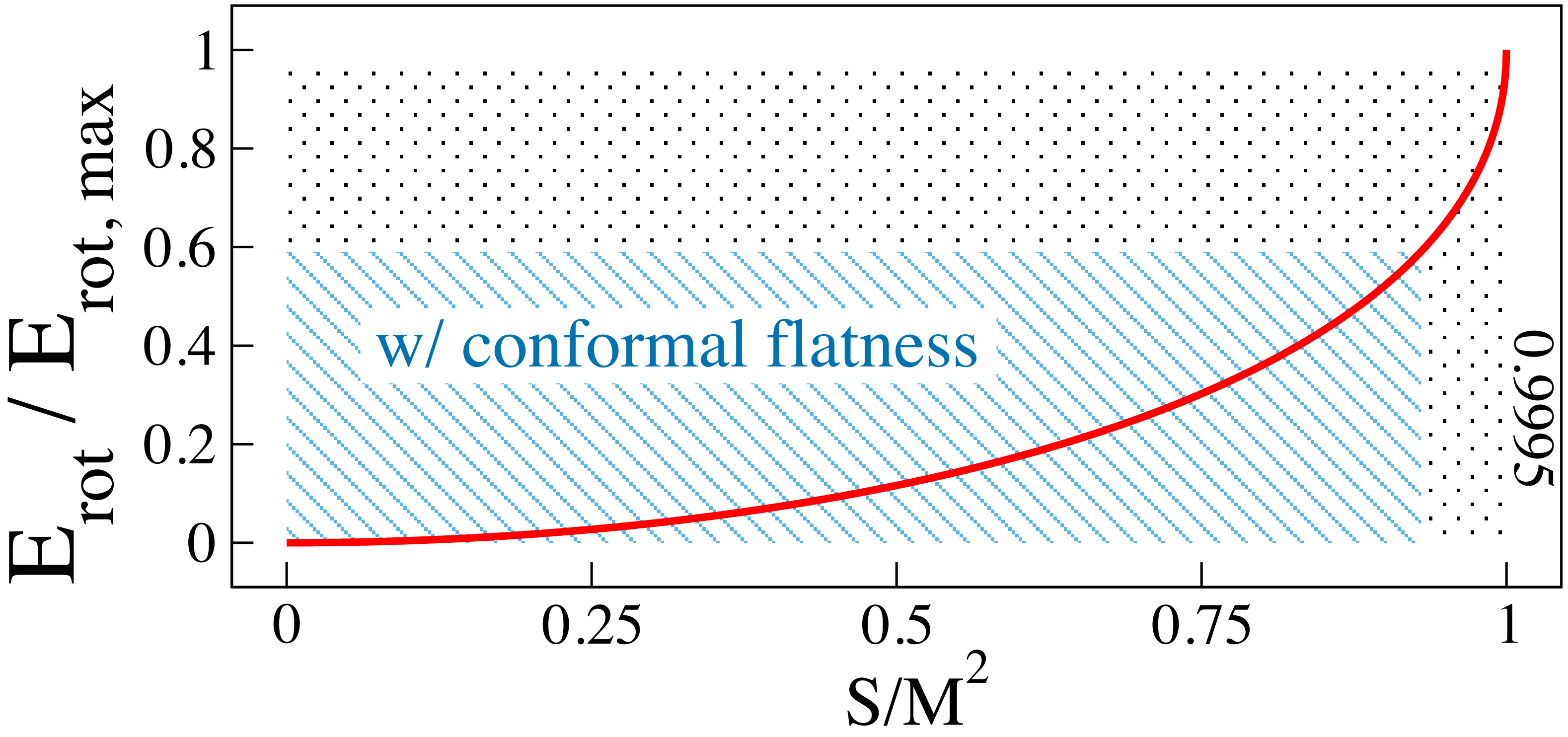
  Brandt, Brügmann 97; Cook,HP 04

- Elliptic solver

  HP+ 02, Ansorg 04

- Spins > 0.9

  Lovelace..HP+ 08

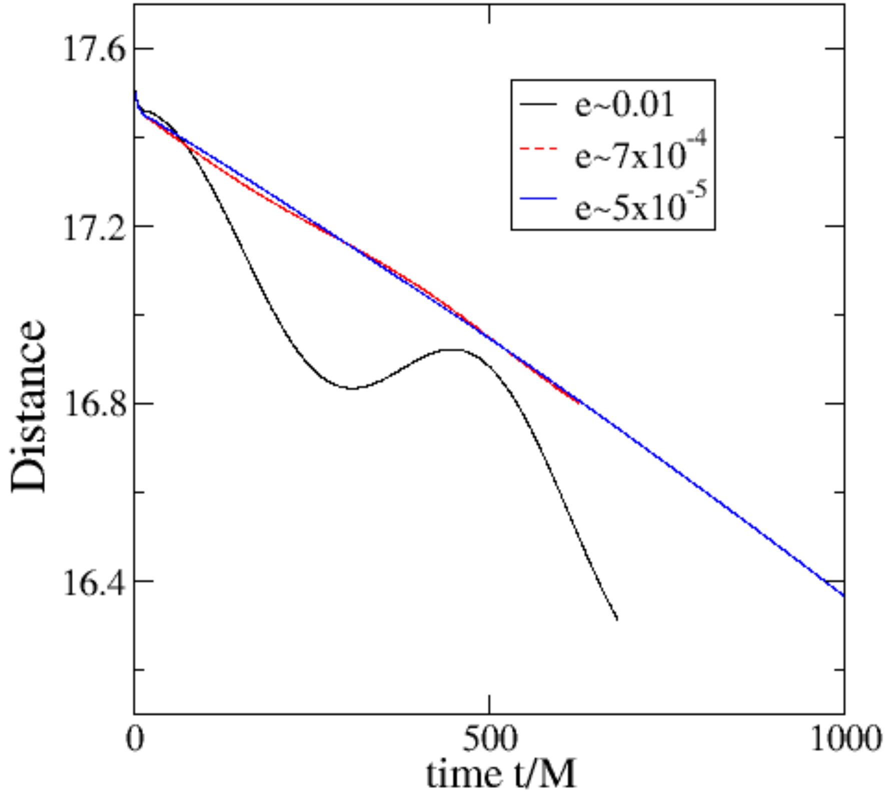


$$\tilde{\nabla}^2\psi = \dots$$

$$\tilde{\nabla}\cdot\left(\frac{1}{\tilde{N}}\tilde{\mathbb{L}}\beta\right) = \dots$$

$$\tilde{\nabla}^2\tilde{N} = \dots$$

- Control eccentricity



HP+ 05; Buonanno..HP+ 08
Chatziioannou, HP+ (in prep)

Einstein Evolution Equations

- Einstein's equations

$$0 = R_{ab}[g_{ab}] = -\frac{1}{2}\Box g_{ab} + \nabla_{(a}\Gamma_{b)} + \text{lower order terms}, \qquad \Gamma_a = -g_{ab}\Box x^b.$$

- Generalized harmonic coordinates $g_{ab}\Box x^b \equiv H_a(x^a, g_{ab})$
  (Friedrich 1985, Pretorius 2005; $H = 0$ used since 1920's)

$$\Box g_{ab} = \text{lower order terms.}$$

$\Rightarrow$ Constraint $C_a \equiv H_a - g_{ab}\Box x^b = 0$

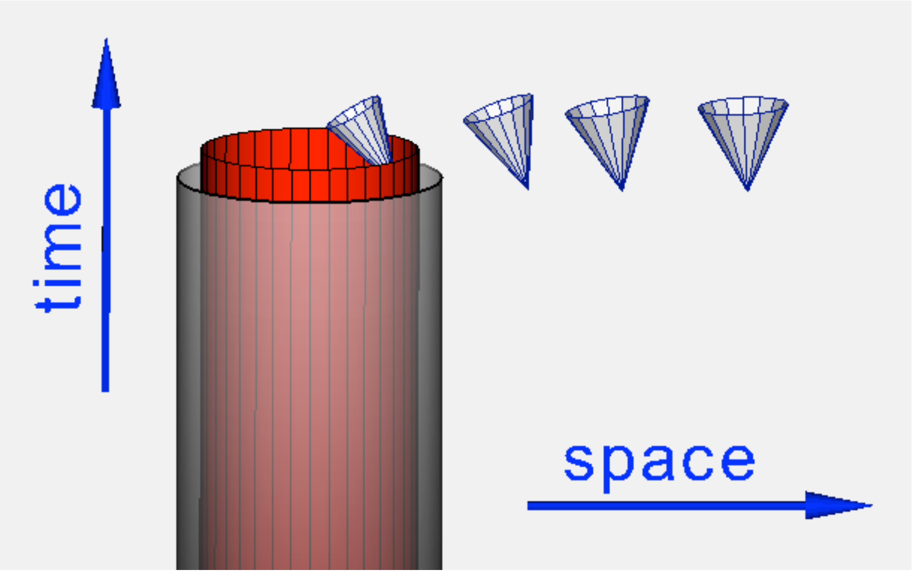
- Constraint damping (Gundlach, et *al.*, Pretorius, 2005)

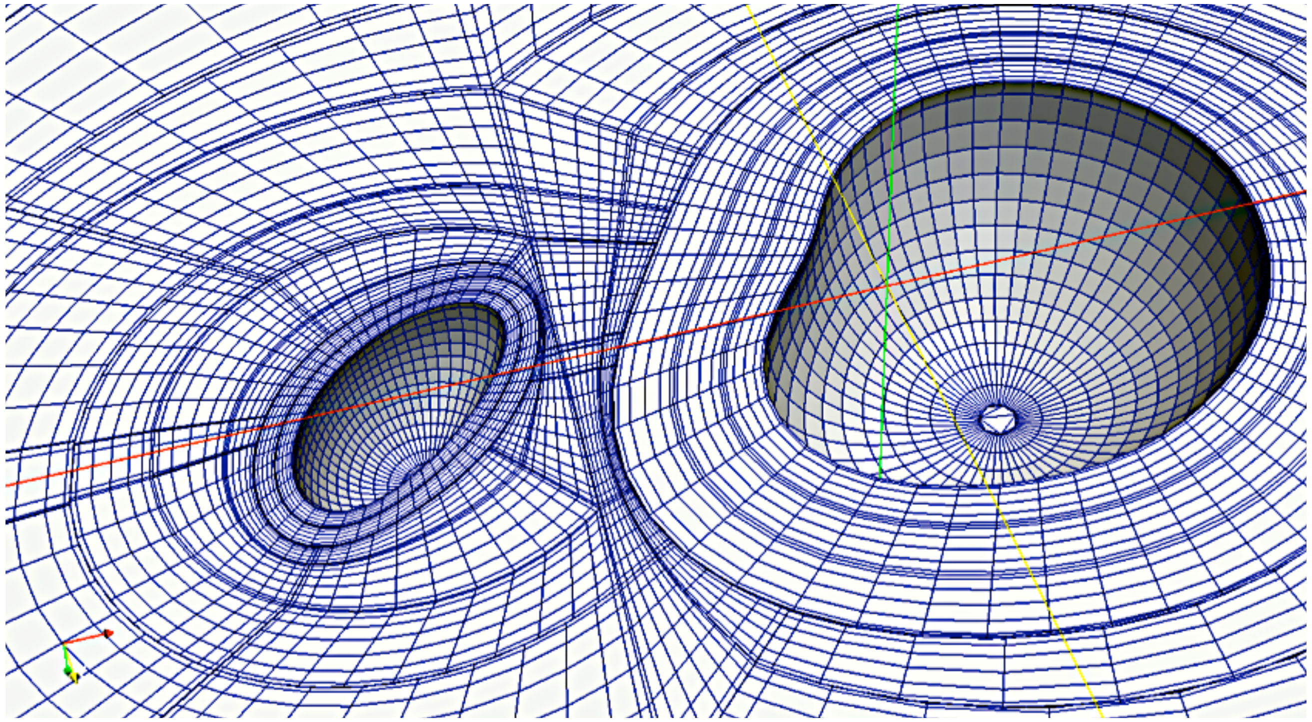
$$\Box g_{ab} = \gamma\left[t_{(a}C_{b)} - \frac{1}{2}g_{ab}t^c C_c\right] + \text{lower order terms}$$

$$\partial_t C_a \sim -\gamma C_a.$$

BH Excision

- Excise inside BH horizons
- Domain-decomposition **follows BHs continuously**, conforms to shape of AH



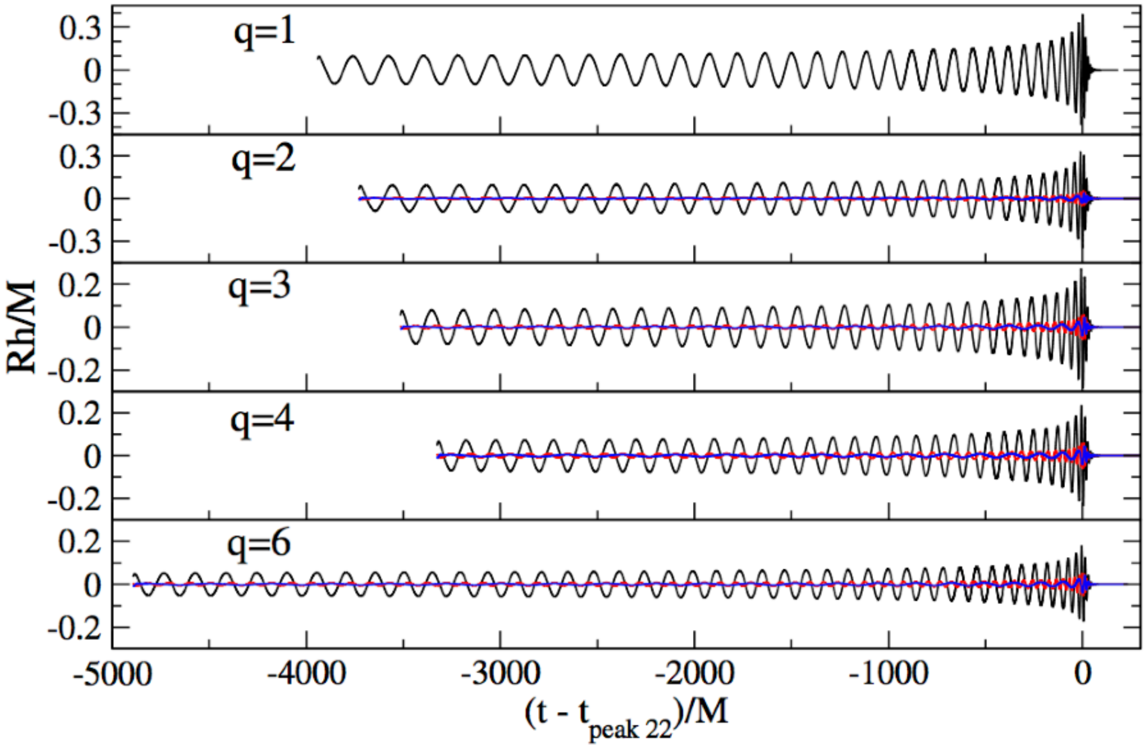


Scheel, HP+ 08, Szilagyi+ 08, Hemberger+ 13

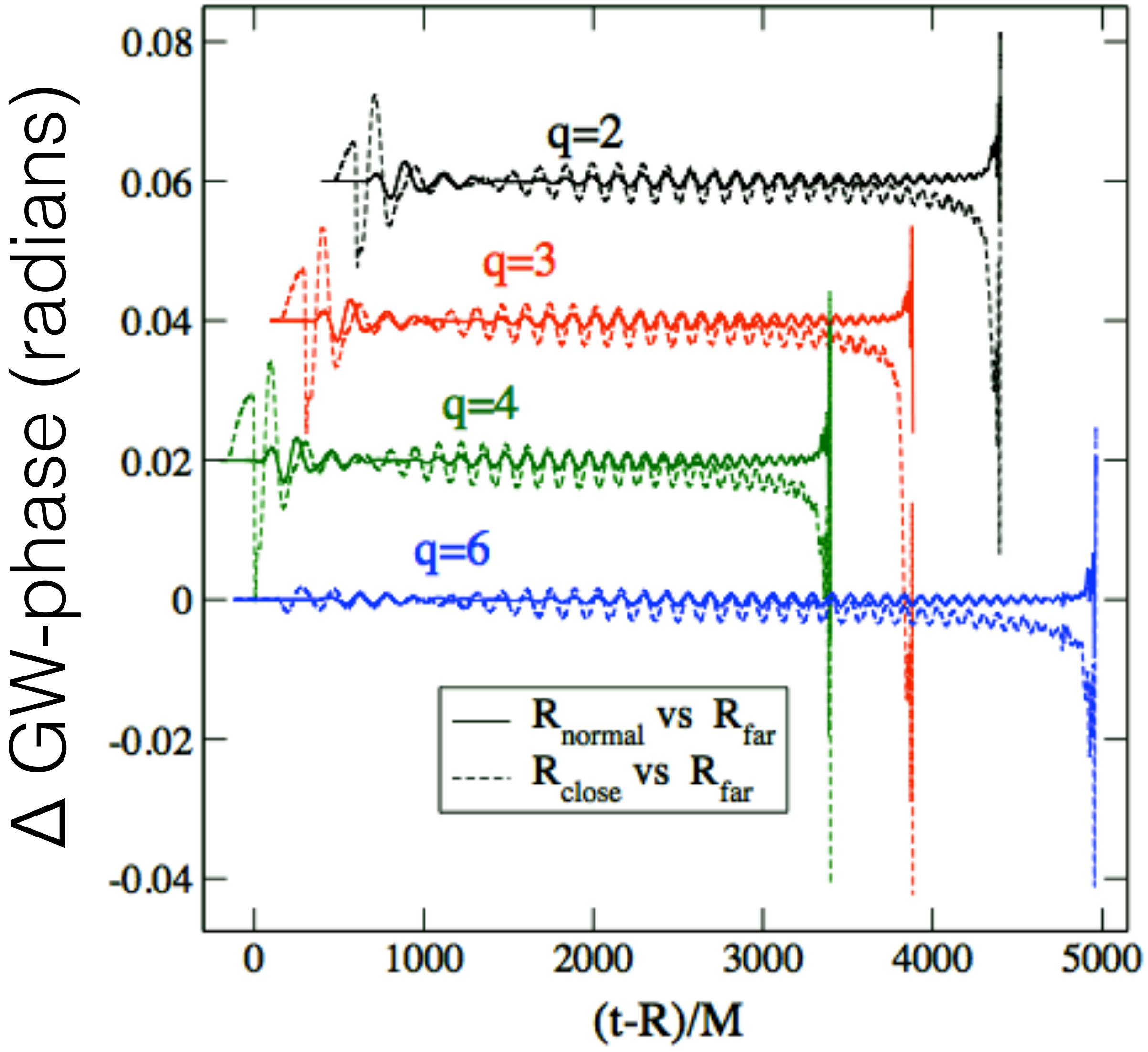
Outer boundary

- In SpEC:
  - **Constraint preserving**
  - **Minimally reflective**

Lindblom, Rinne+ 06

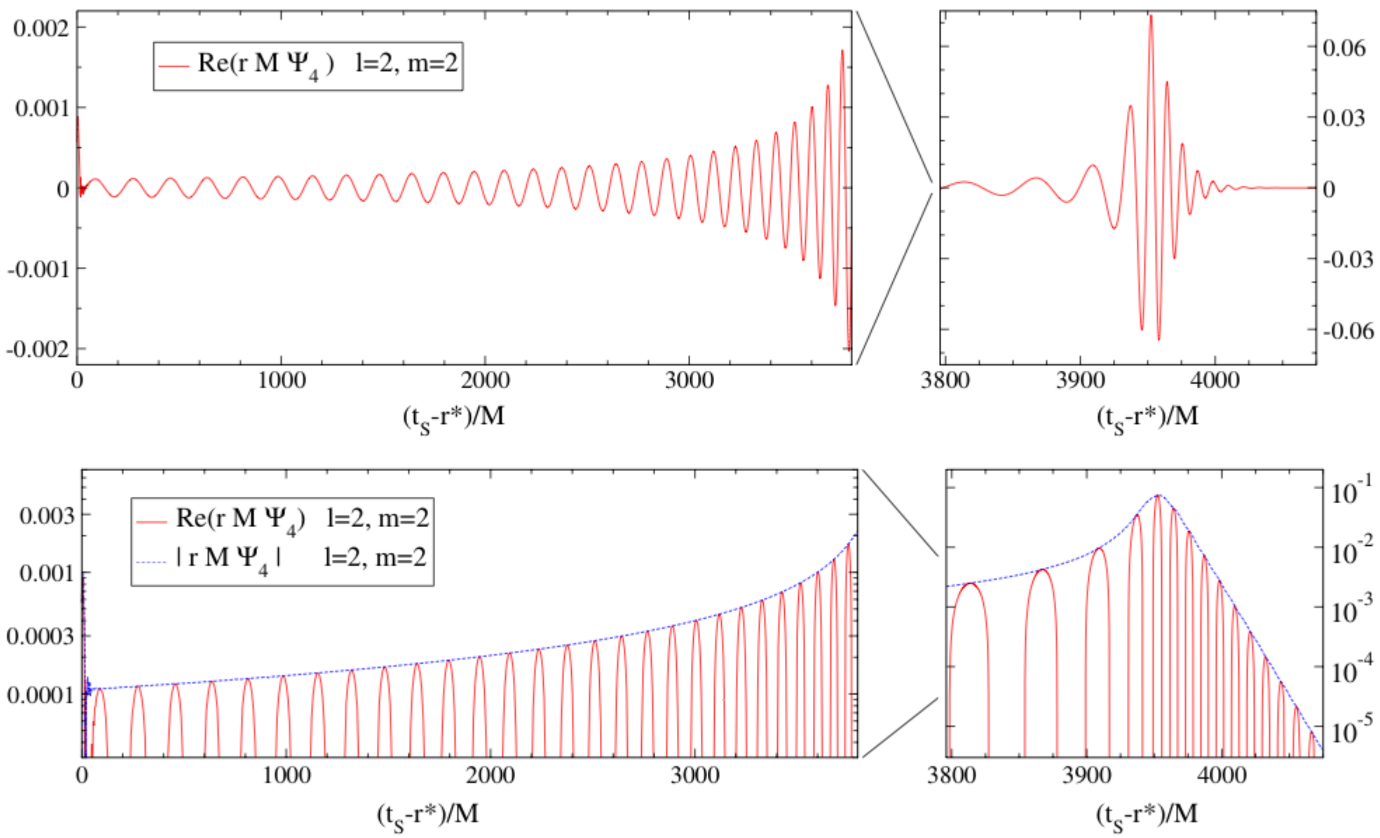


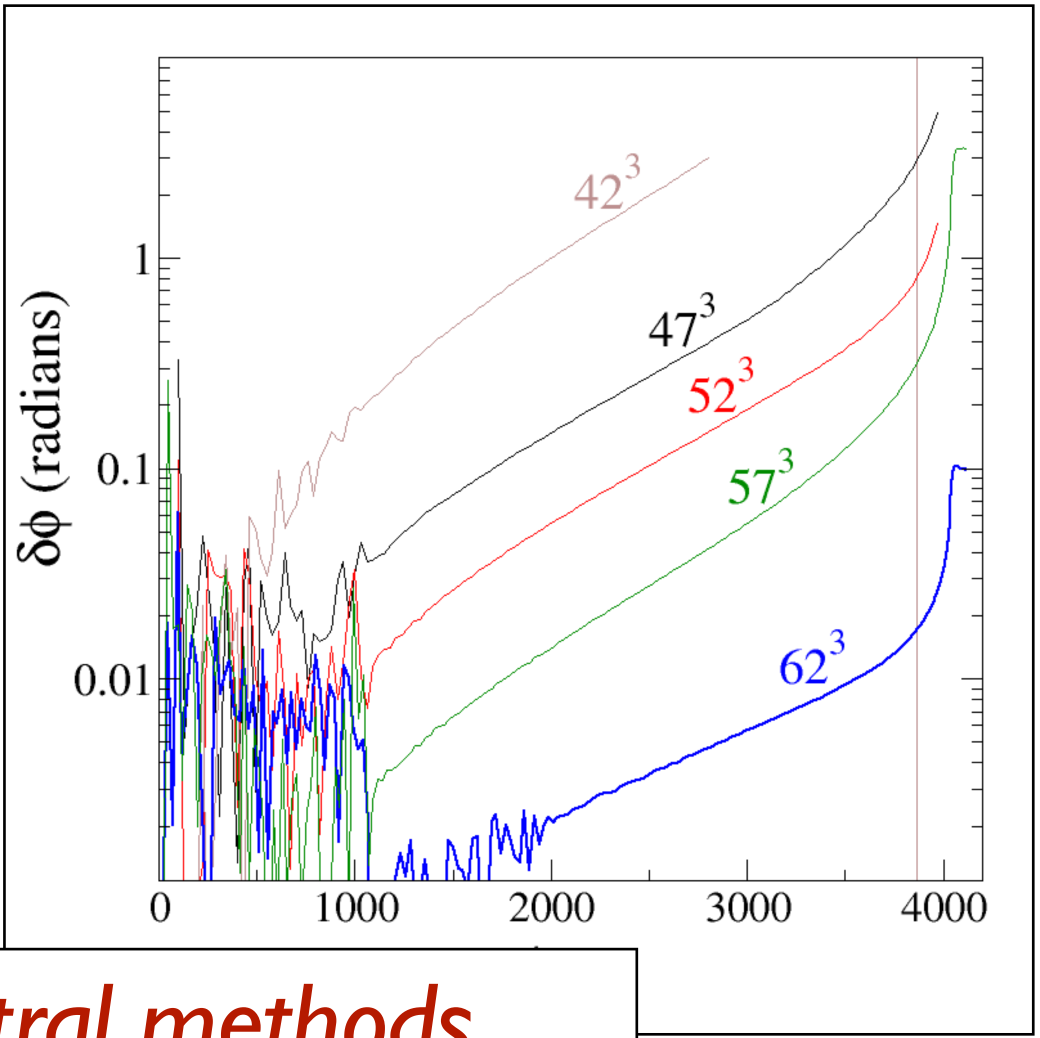
- Causally connected for long simulations



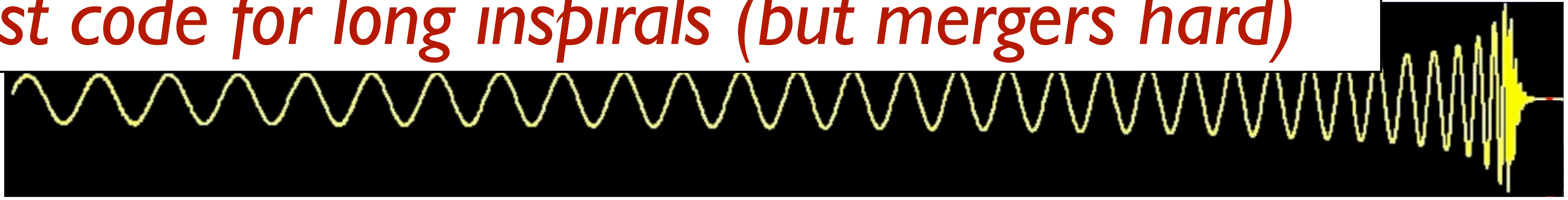
Buchman, HP, Scheel, Szilagyi, 2012

Accuracy of SpEC


GW precision data

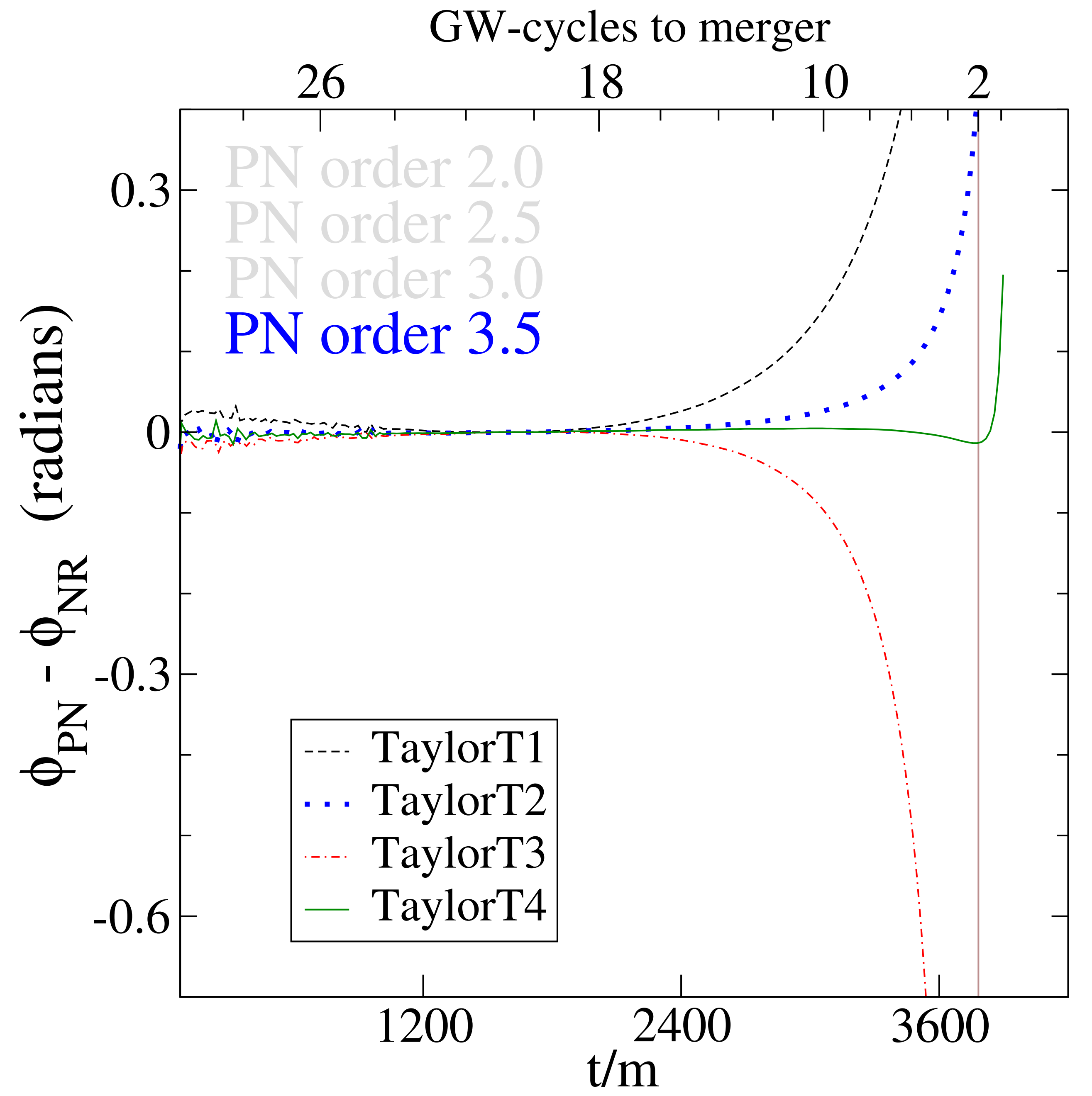


- *Rapid convergence due to spectral methods*
- *Small errors due to moving grid*
- *Best code for long inspirals (but mergers hard)*



Scheel,HP+ 09

post-Newtonian vs. NR



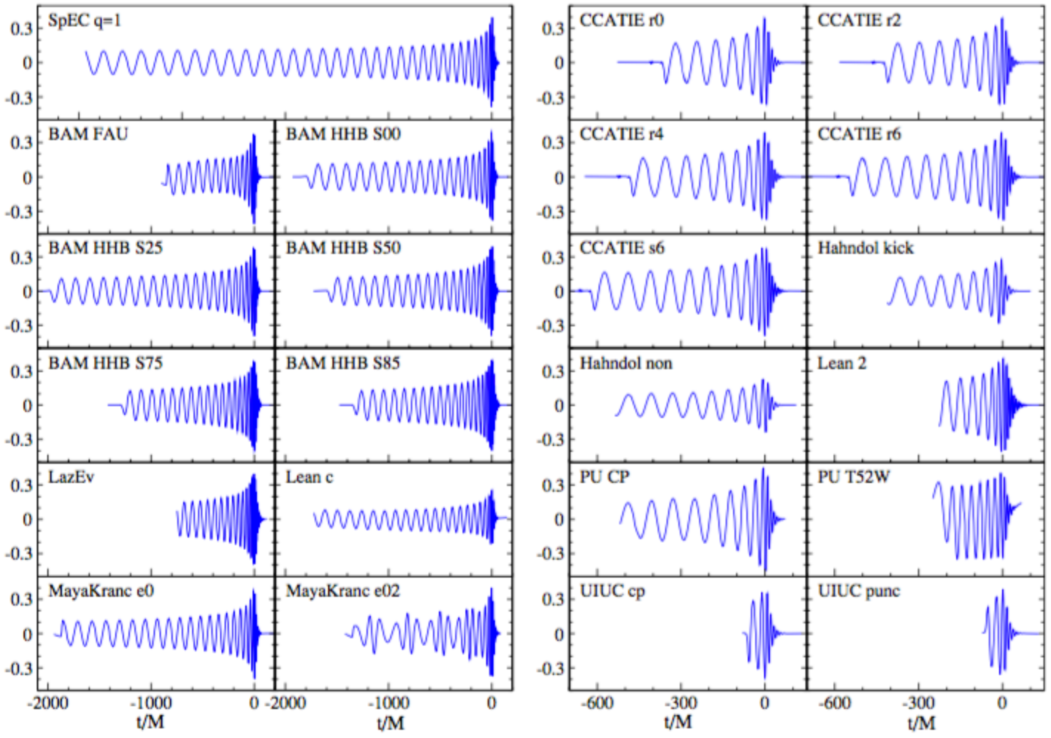
PN approximants
Equally justified approaches to derive inspiral rate from energy balance

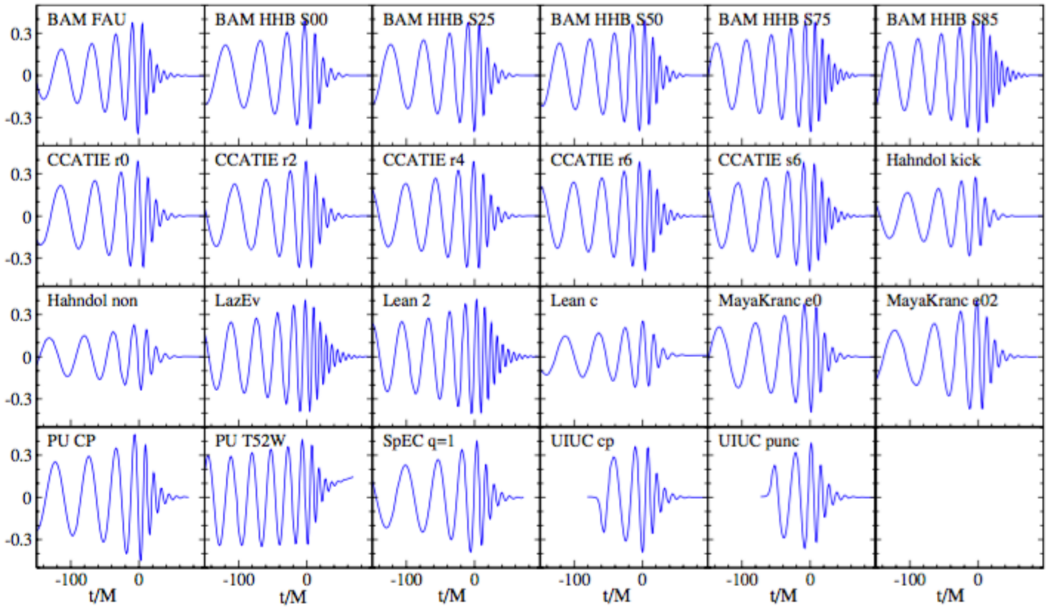
$$\frac{dE}{dt} = -F_{\mathrm{GW}}$$

Boyle..HP+ 07

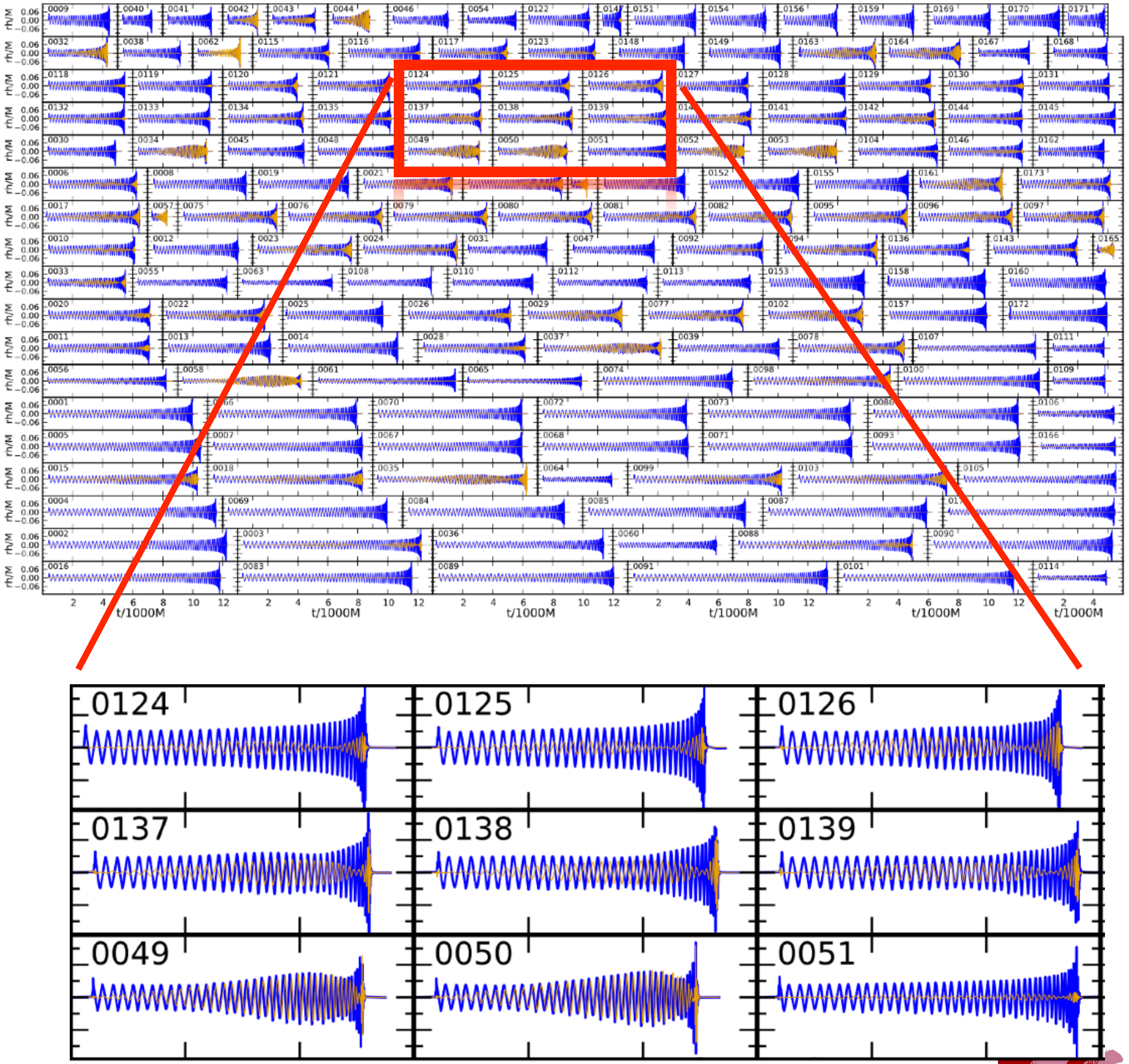
Parameter space exploration

NINJA *Aylott .. HP+ 09*





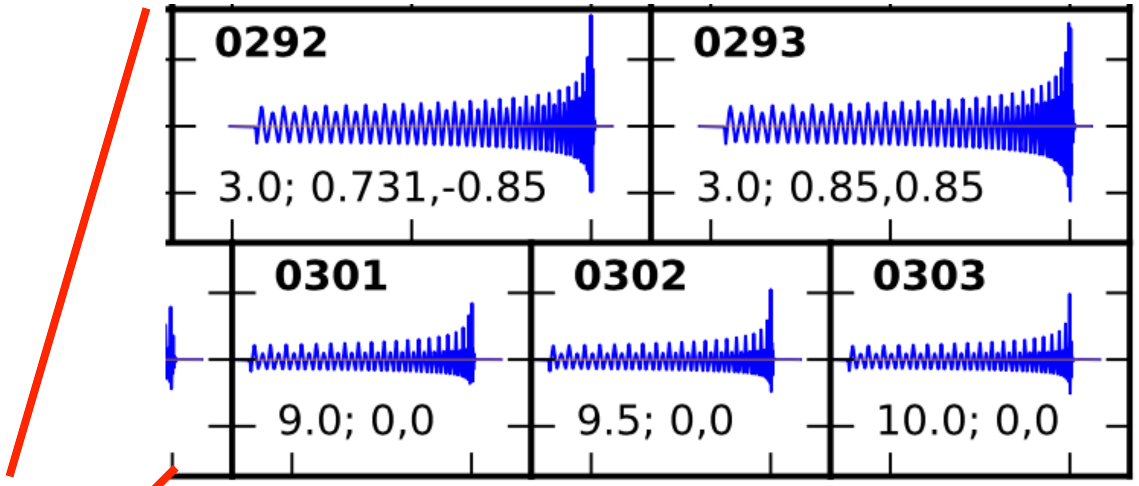
1st SXS Catalog *Mroue .. HP+ 13*



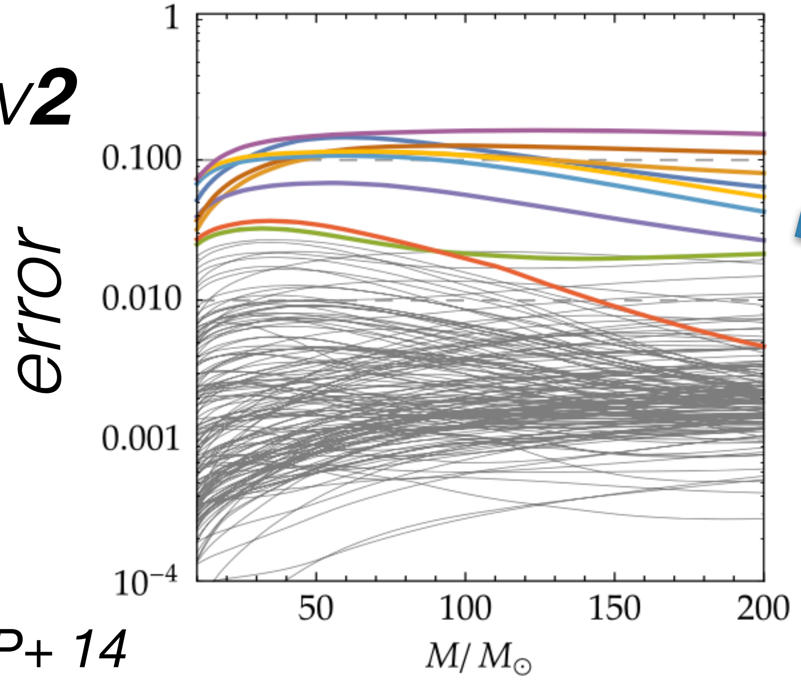
Improve analytical waveform models

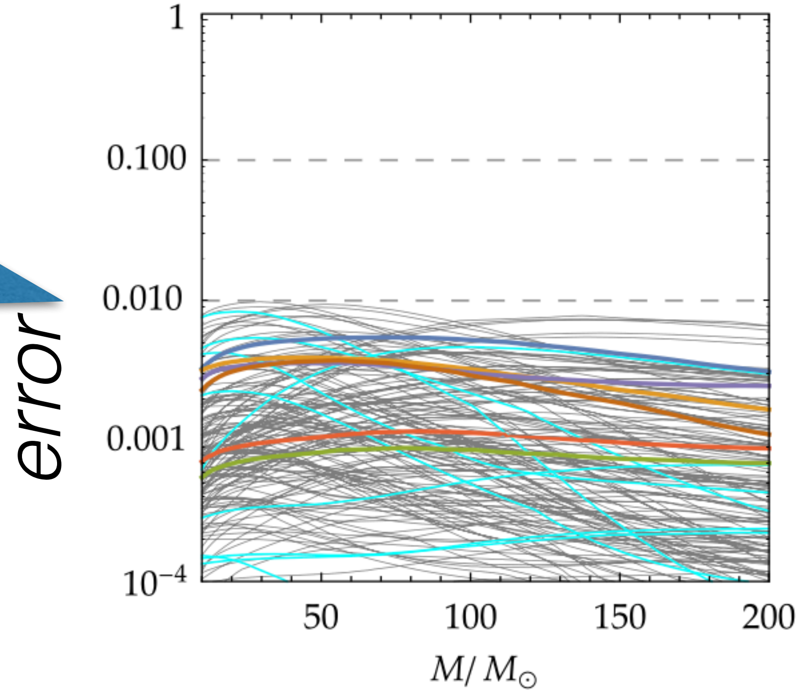
2nd SXS Catalog

Chu .. HP+ 15



*SEOBNRv**2***





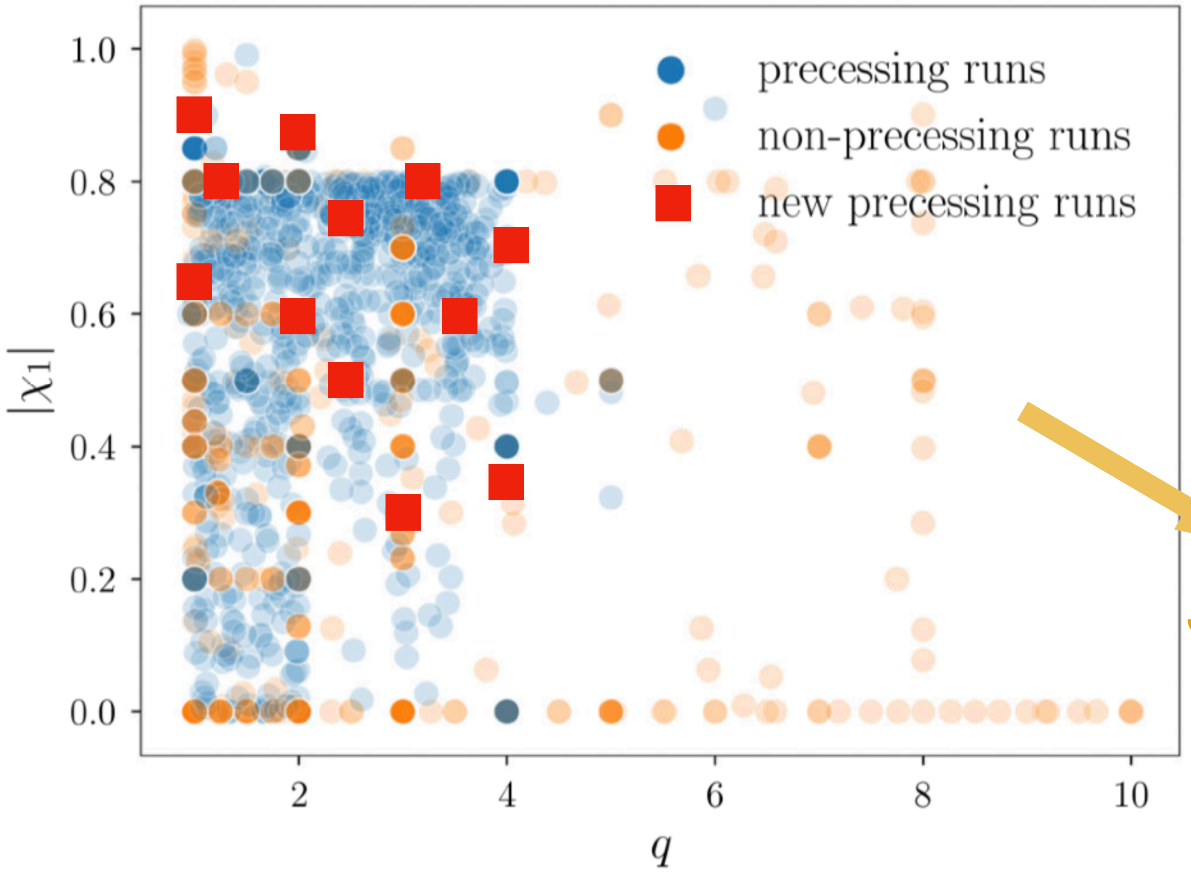
*SEOBNRv**4***

Bohe..HP+ 17

Taracchini..HP+ 14

Improve analytical waveform models

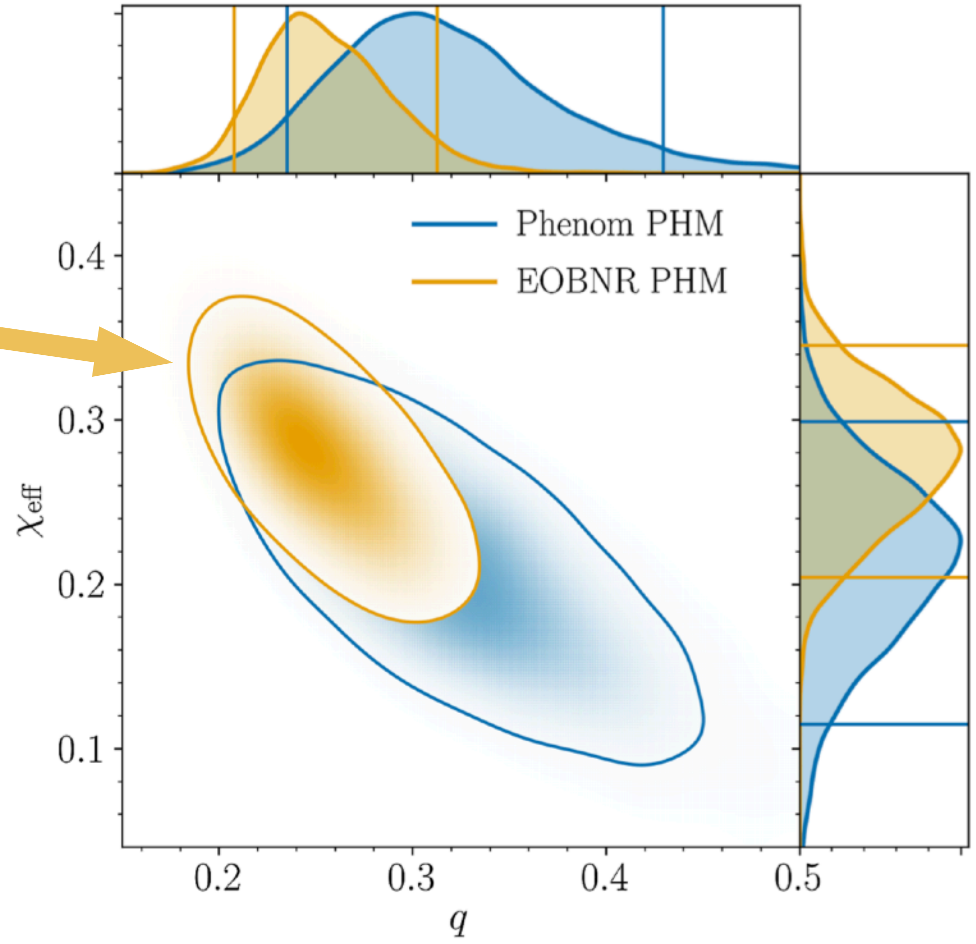
new highly precessing runs



Ossokine,..HP.. 20

LIGO/Virgo analysis (GW190412)

SEOBNRv4PHM



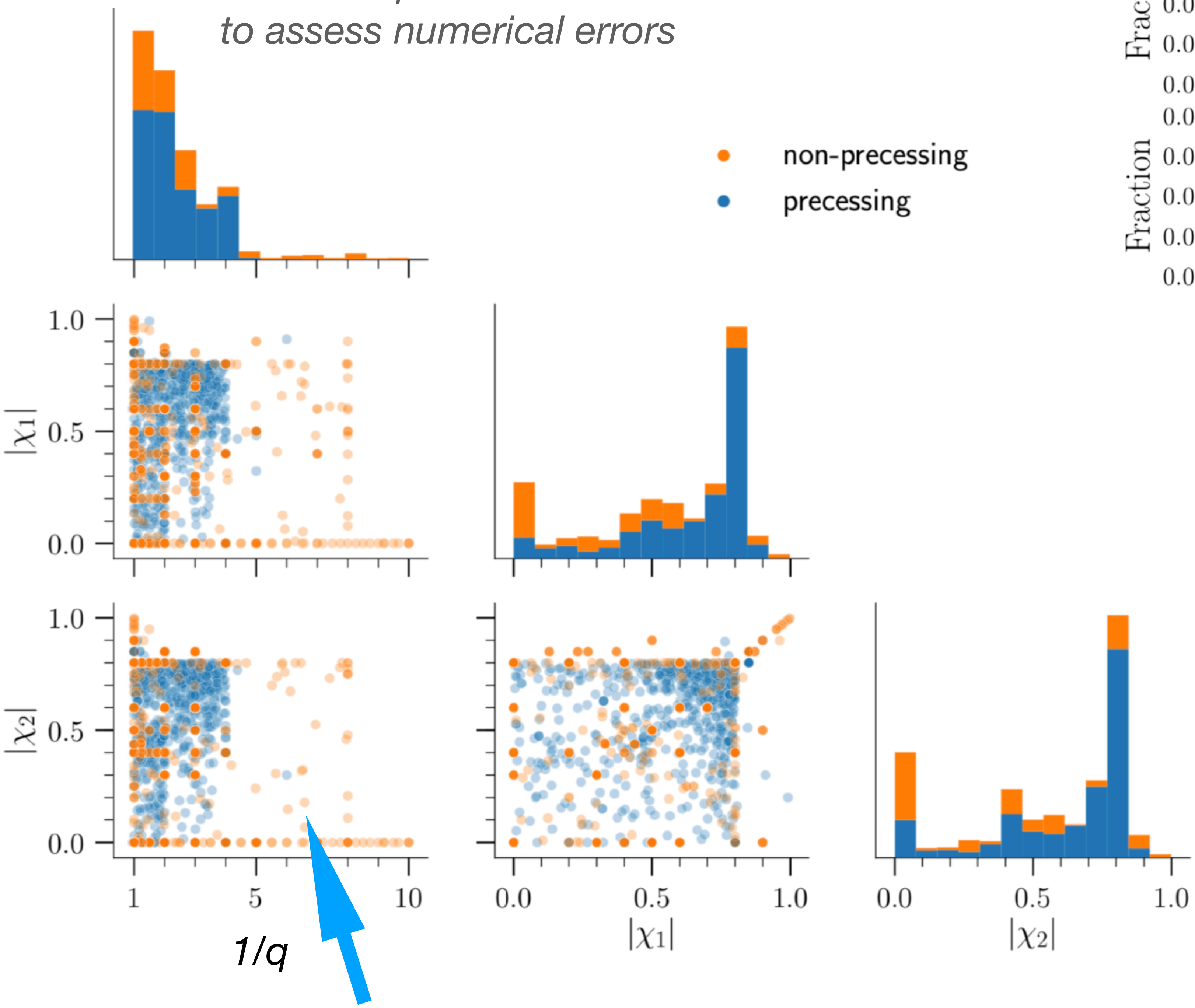
Abbott et al, PRD 102 043015 (2020)

This material is based upon work supported by NSF's LIGO Laboratory
which is a major facility fully funded by the National Science Foundation.

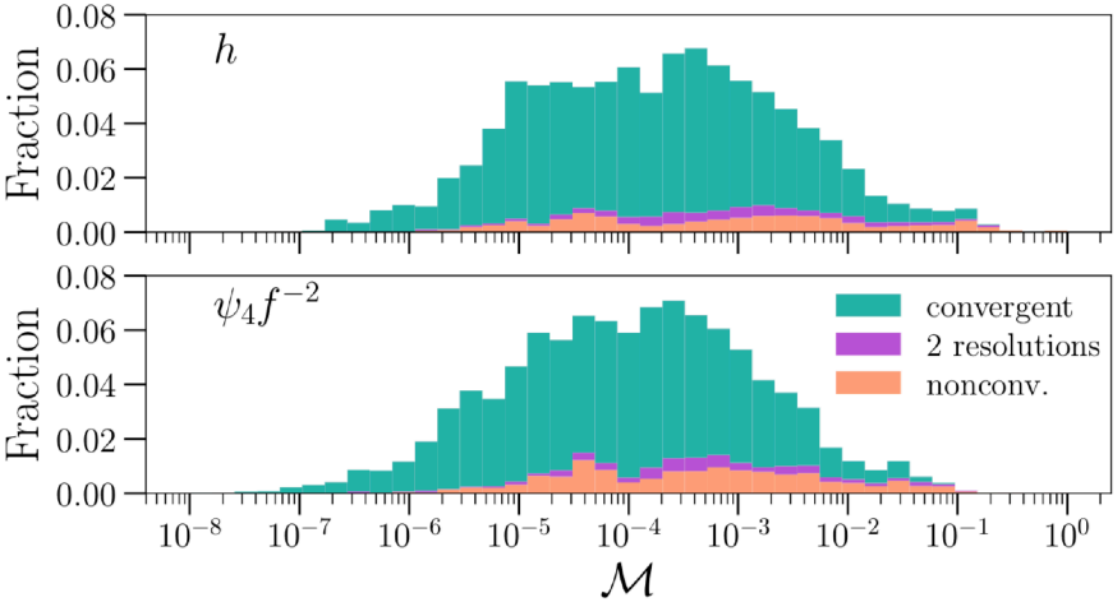
SXS waveform catalog 2019 edition

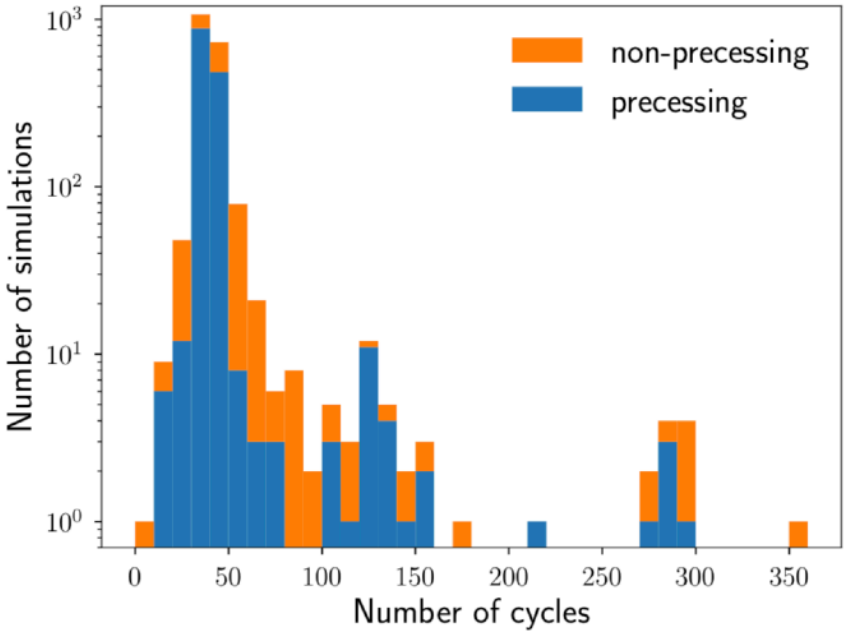
2018 Waveforms

all at multiple resolutions
to assess numerical errors



q<1/4 rare
q=1/10 highest public SpEC run

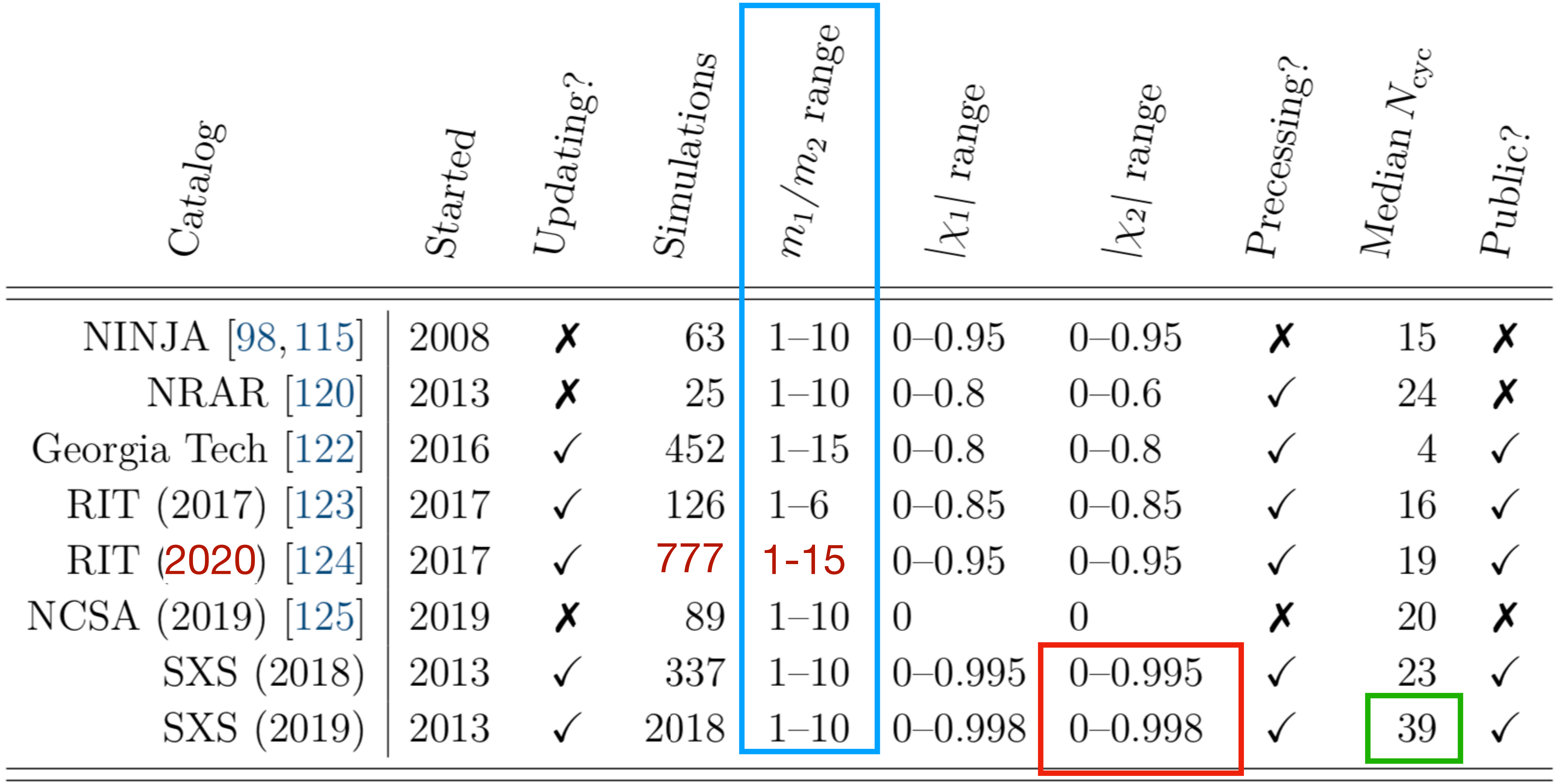




SXS Collaboration (Boyle, ..HP+)
CQG 2019 (1904.04831)

More parameter space exploration efforts

$q \geq 1/15$



Catalog	Started	Updating?	Simulations	m_1/m_2 range	$\|\chi_1\|$ range	$\|\chi_2\|$ range	Precessing?	Median N_{cyc}	Public?
NINJA [98, 115]	2008	✗	63	1–10	0–0.95	0–0.95	✗	15	✗
NRAR [120]	2013	✗	25	1–10	0–0.8	0–0.6	✓	24	✗
Georgia Tech [122]	2016	✓	452	1–15	0–0.8	0–0.8	✓	4	✓
RIT (2017) [123]	2017	✓	126	1–6	0–0.85	0–0.85	✓	16	✓
RIT (2020) [124]	2017	✓	777	1-15	0–0.95	0–0.95	✓	19	✓
NCSA (2019) [125]	2019	✗	89	1–10	0	0	✗	20	✗
SXS (2018)	2013	✓	337	1–10	0–0.995	0–0.995	✓	23	✓
SXS (2019)	2013	✓	2018	1–10	0–0.998	0–0.998	✓	39	✓

longest sims

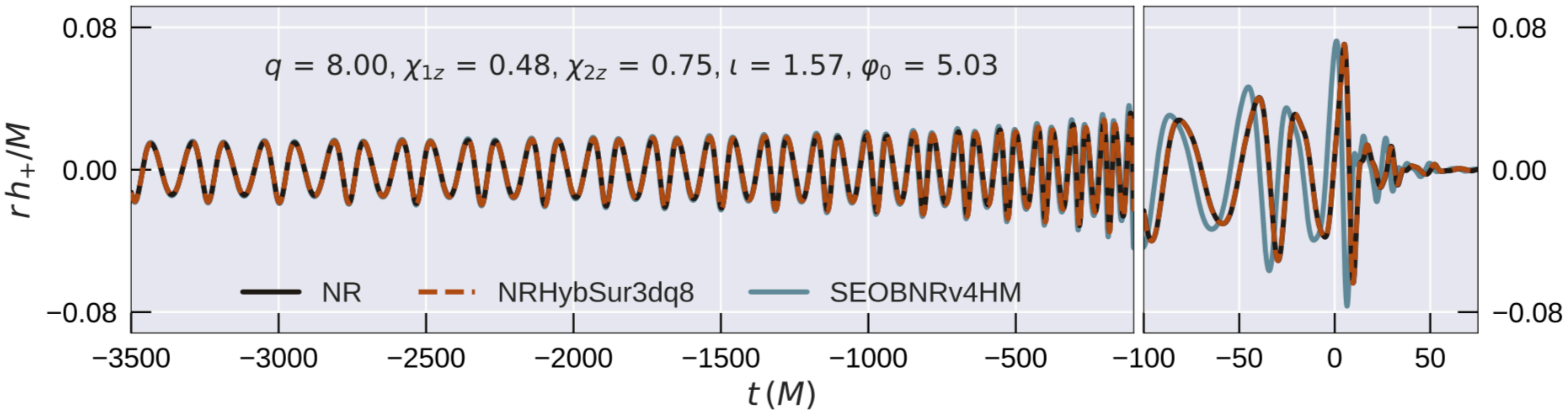
highest spins

SXS Collaboration (Boyle, ..HP+)
CQG 2019 (1904.04831)

And Palma group around Husa+ (data not public)

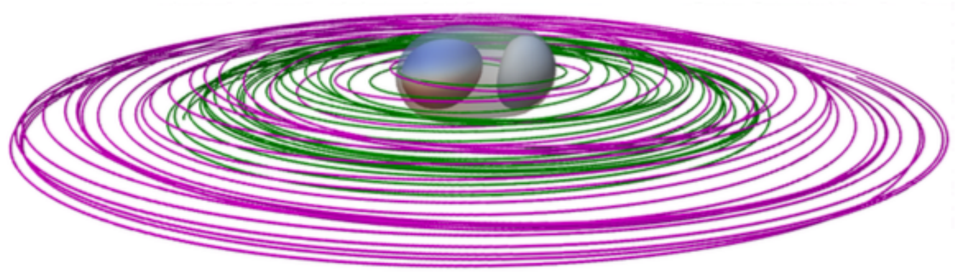
Main use for BBH simulations: waveform models

- state of the art: **Precession** and **higher modes**
- EOB models, Phenom models
- more recently: **NR surrogate models**
  - need O(1000) NR sims
  - nearly "automatic" model construction
  - model-accuracy $\sim$ NR-accuracy
  - but: only where NR is available & requires analytic early inspiral model



Blackman+ 15, Blackman+ 17a,b, Varma+ 18a,b, Varma+ 19a,b, Rifat+ 19, Taylor, Varma 20

Parameter space: NR records



$q=1$: **$S/M^2=0.998$**

$q<1$: $S/M^2=0.95$

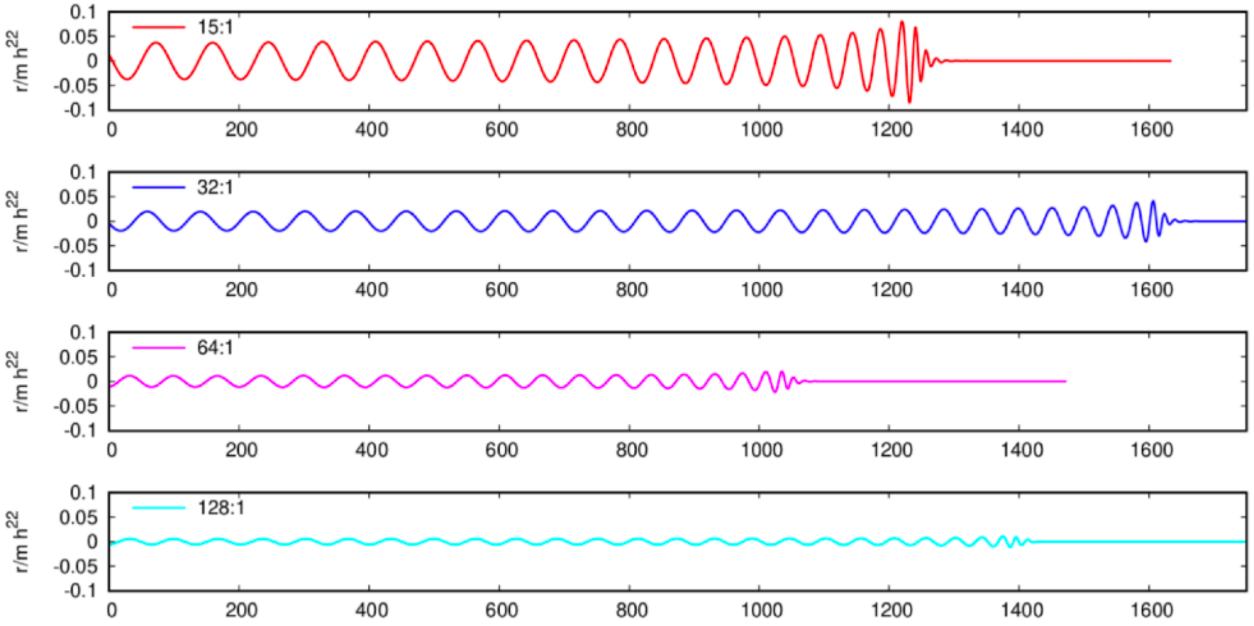
Scheel+ 14

Lovelace..HP+15

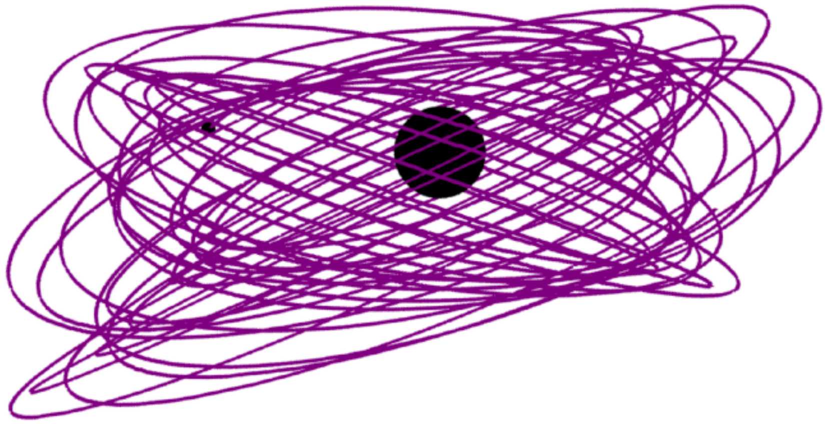
Boyle..HP+ 19

$q=1/128$

Lousto, Healy 20

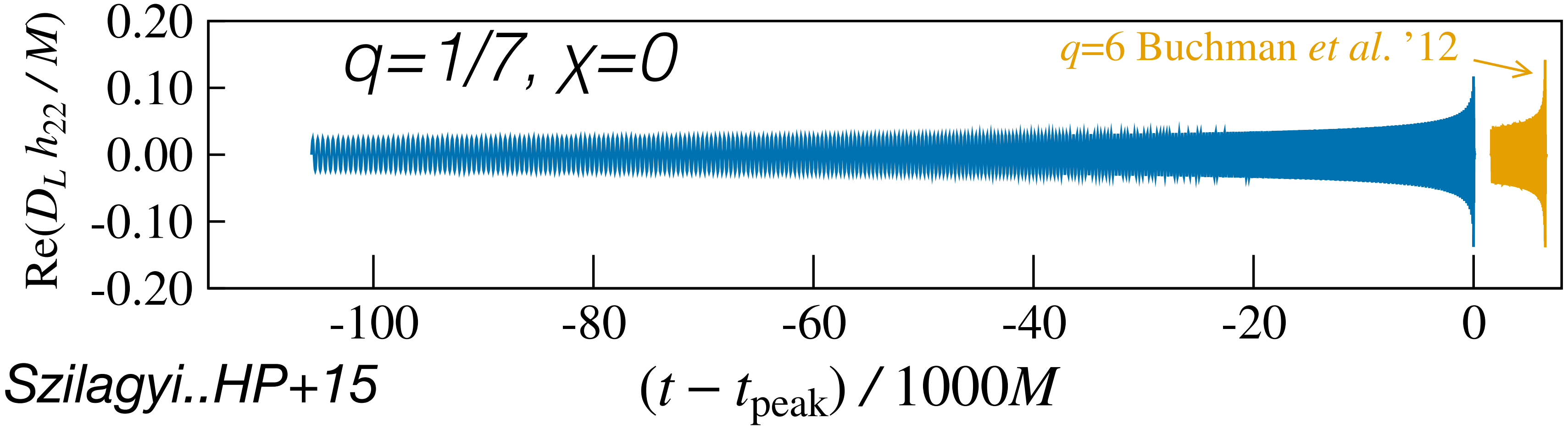


eccentric, precessing q=7



Lewis, Zimmerman, HP 17

350GW cycles



Szilagyi..HP+15

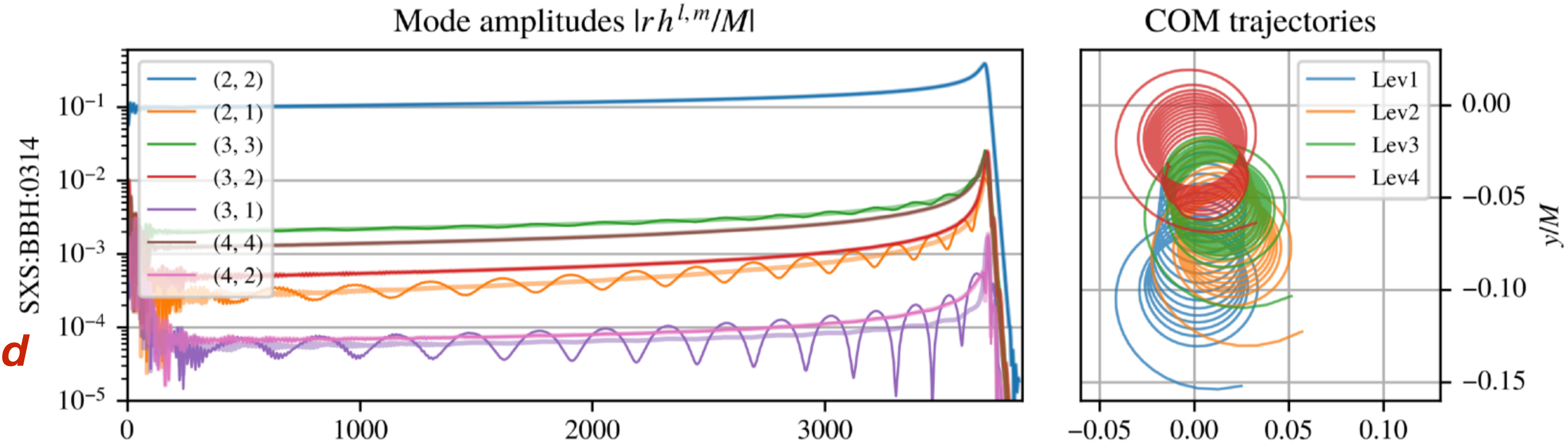
Recent (1)

Improved calculation of gravitational waves

Center of mass corrections

- in NR simulations, the center of mass typically drifts slowly away from the origin (on which GW extraction spheres are centered)
- SpEC corrects this since the 2019 catalog

*thin = **raw data***
thick = COM corrected



Woodford, Boyle, HP (PRD 2019)
Boyle..HP.. (SXS) (CQG 2019)

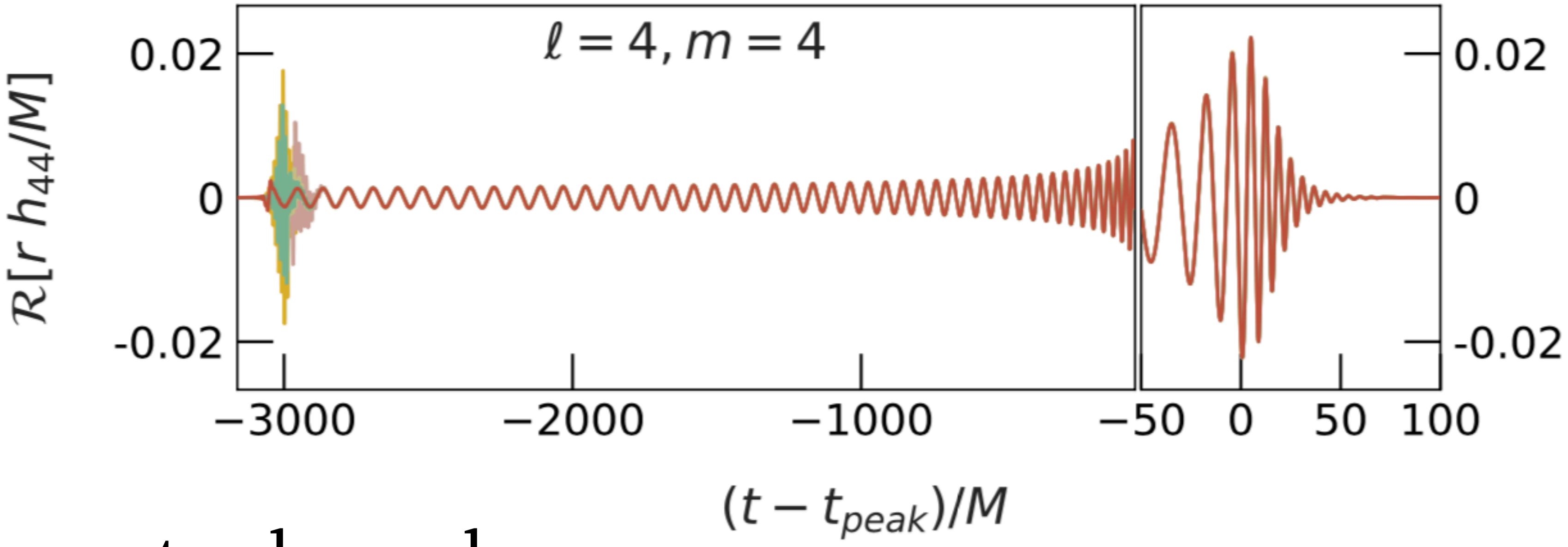
Weyl scalars, reduced junk radiation

- SpEC can now extract **all Weyl scalars** $\Psi_4, \ldots, \Psi_0$

Iozzo..HP.. (SXS) PRD 2021

- **Impact of initial burst of radiation** reduced:
  - different conformal data

Varma, Scheel, HP PRD 2018
Ma, Giesler, Scheel, Varma PRD 2021



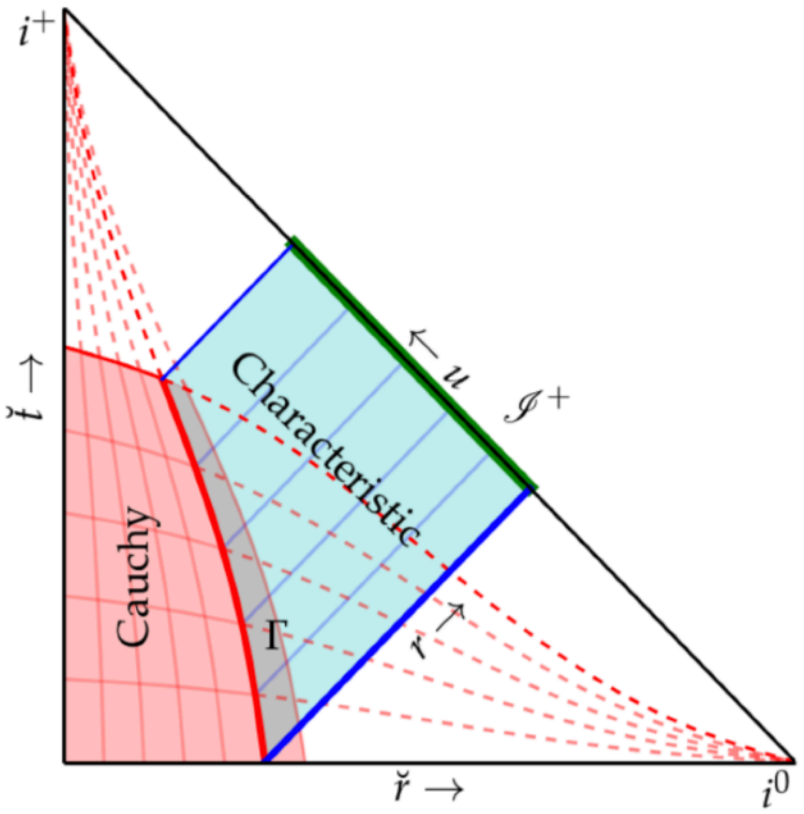
  - clip burst by resetting outer boundary
  - split numerical resolutions after burst

Cauchy Characteristic Extraction

- New spectral implementation

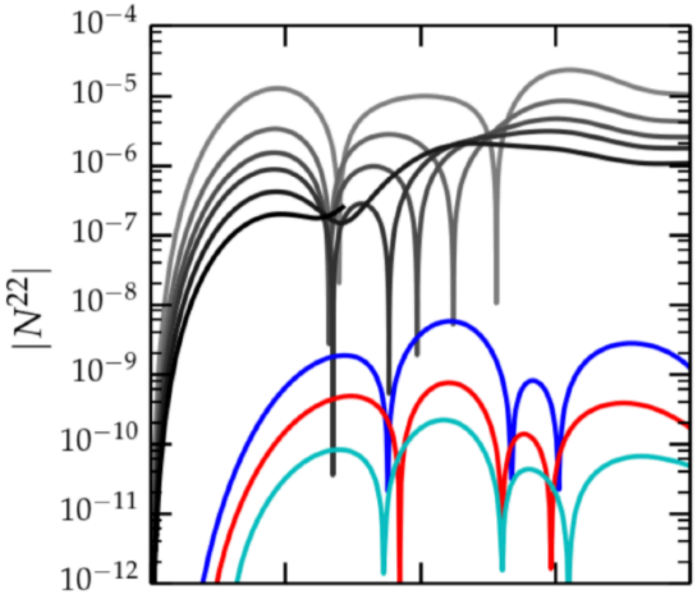
  Barkett+ PRD 2020 *Moxon, Scheel, Teukolsky PRD 2020*

  - faster, more accurate than PittNull code



test: GW for bouncing Schwarzschild BH

$$x \rightarrow x + a\ \sin^4(\Omega t)$$



BMS balance laws & GW memory

Ashtekar, De Lorenzo, Khera GRG 202

- Waveforms must satisfy balance laws

$$h = \frac{1}{2}\bar{\eth}^2\mathfrak{D}^{-1}\left[\frac{1}{4}\int_{-\infty}^{u}|\dot{h}|^2\,du - \left(\Psi_2 + \frac{1}{4}\dot{h}\bar{h}\right)\right]$$

- for finite length NR waveform, define

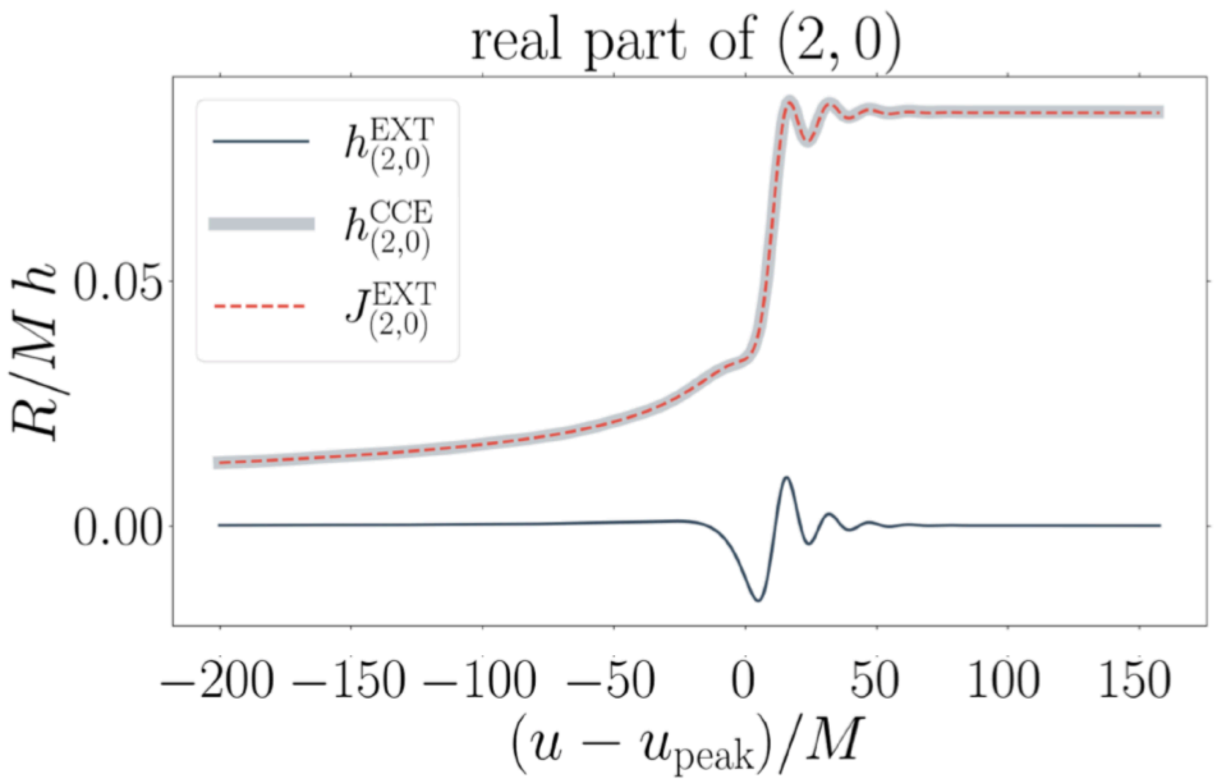
$$J \equiv \frac{1}{2}\bar{\eth}^2\mathfrak{D}^{-1}\left[\frac{1}{4}\int_{u_1}^{u}|\dot{h}|^2\,du - \left(\Psi_2 + \frac{1}{4}\dot{h}\bar{h}\right)\right] + \alpha$$

- two possibilities:
  - validity test: $h_{\mathrm{NR}} - J[h_{\mathrm{NR}}] \overset{?}{=} 0$
  - Improve: $h_{\mathrm{improved}} = J[h_{\mathrm{original}}]$

Mitman, Iozzo, Khera, .. HP.. PRD 2021
Iozzo, Khera .. HP.. 2104.07052

BMS balance laws & GW memory

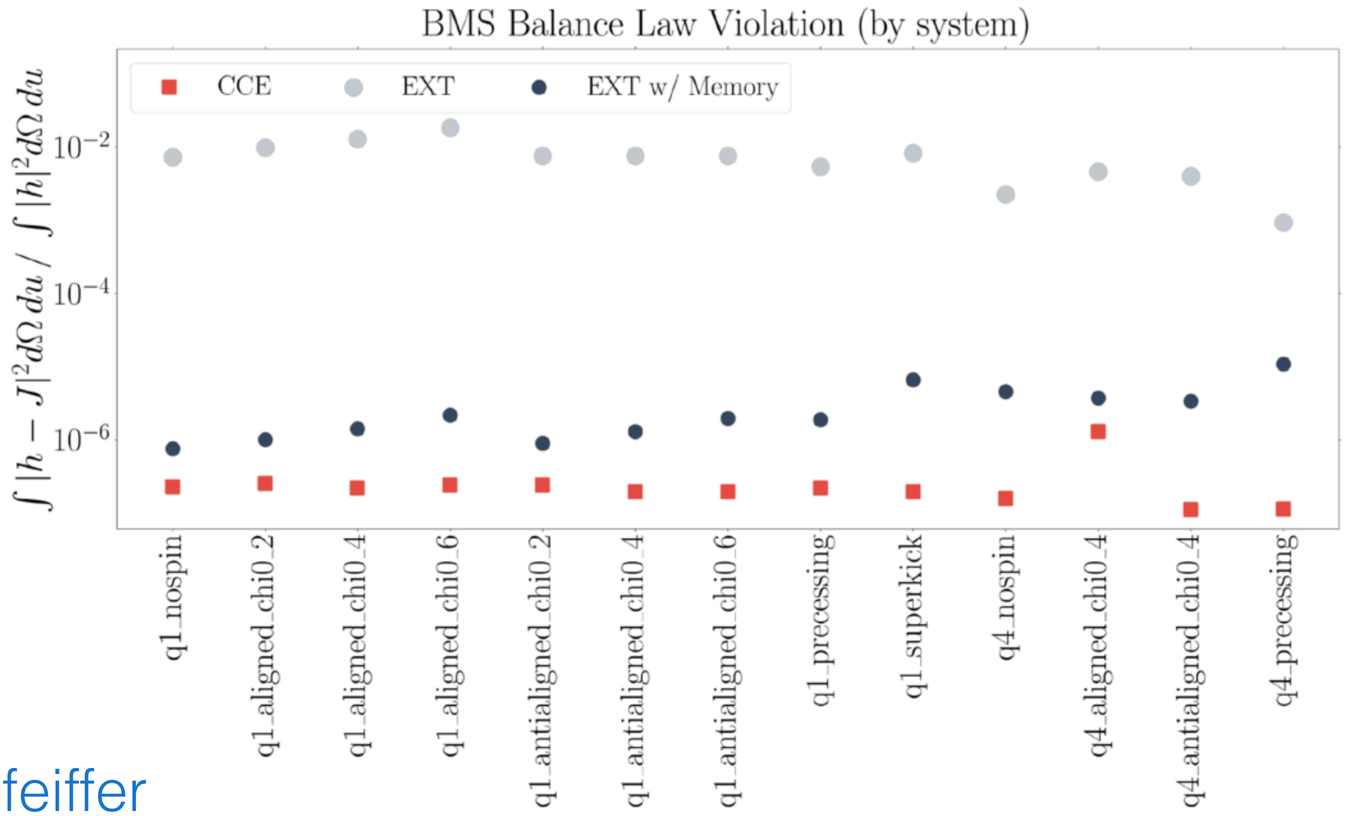
Mitman, Iozzo, Khera, .. HP.. PRD 2021
Iozzo, Khera .. HP.. 2104.07052



CCE

corrected standard SpEC $h_{2,0}$

standard (extrapolated) SpEC $h_{2,0}$



violation of BMS balance law for standard (extrapolated) SpEC GW

corrected standard SpEC GW

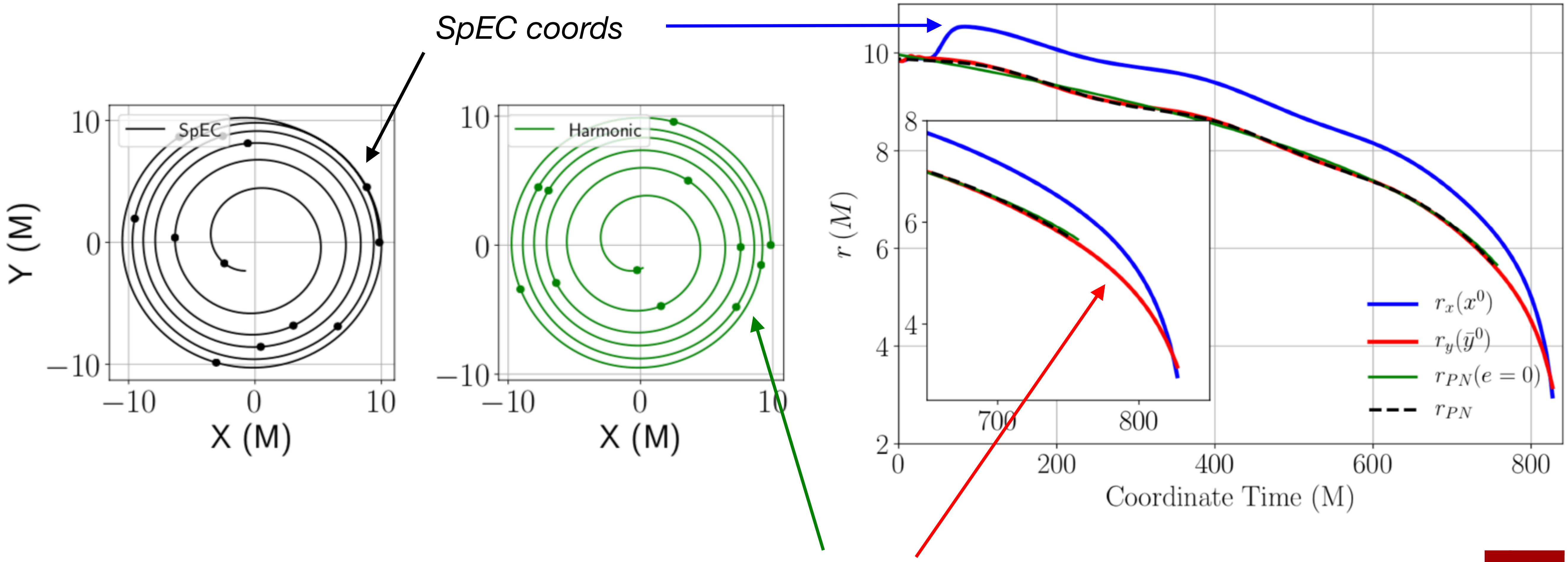
CCE

Recent (2)

Harmonic coordinates

Toward Harmonic Coordinates in NR

- **Prayush Kumar**, HP (in prep)
- **Evolve harmonic coordinates** as extra variables
  - easier contact with analytical calculations
  - at merger, harmonic coord singularities **outside** common AH



SpEC coords

Harmonic coords

Recent (3)

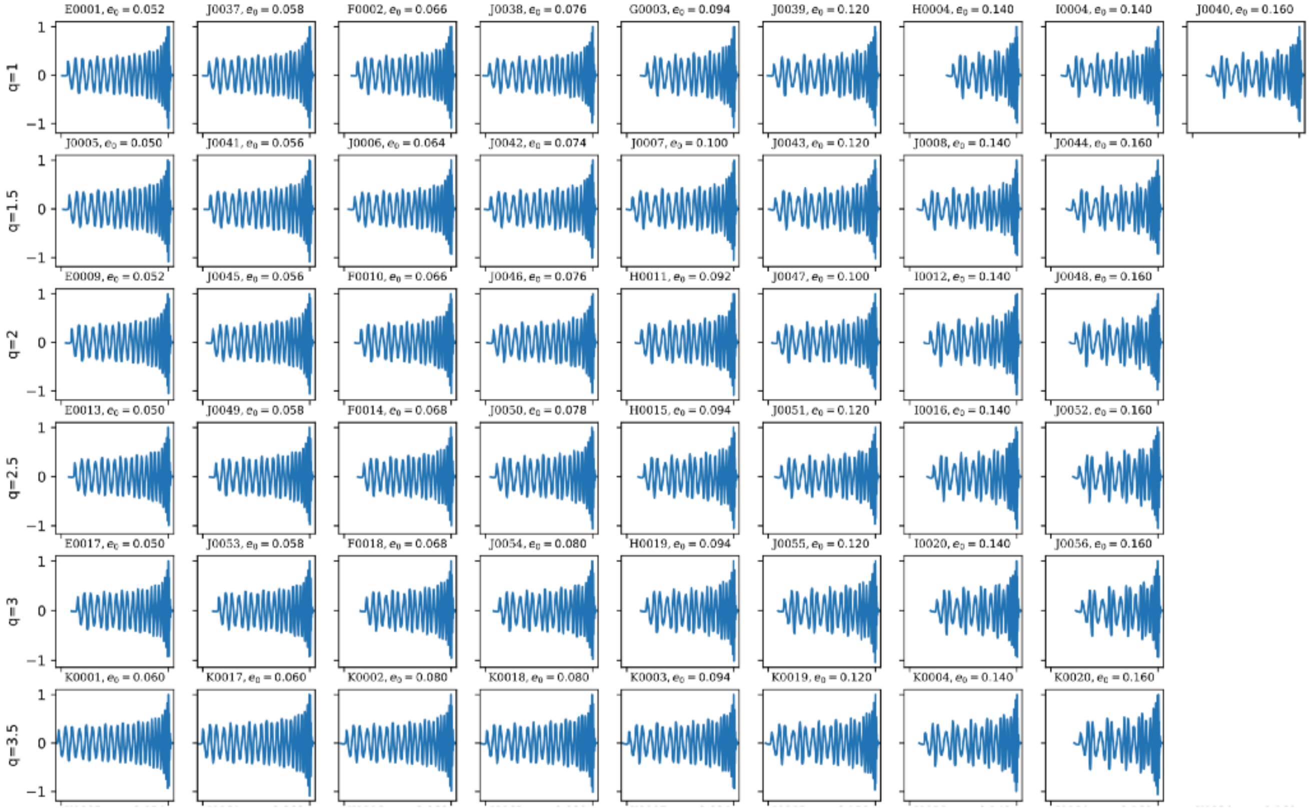
Eccentricity

Community is beginning to explore eccentricity

$q \geq 1/10,\, e_0 \leq 0.18$

energy emission
remnant properties

Huerta+ 1901.07038

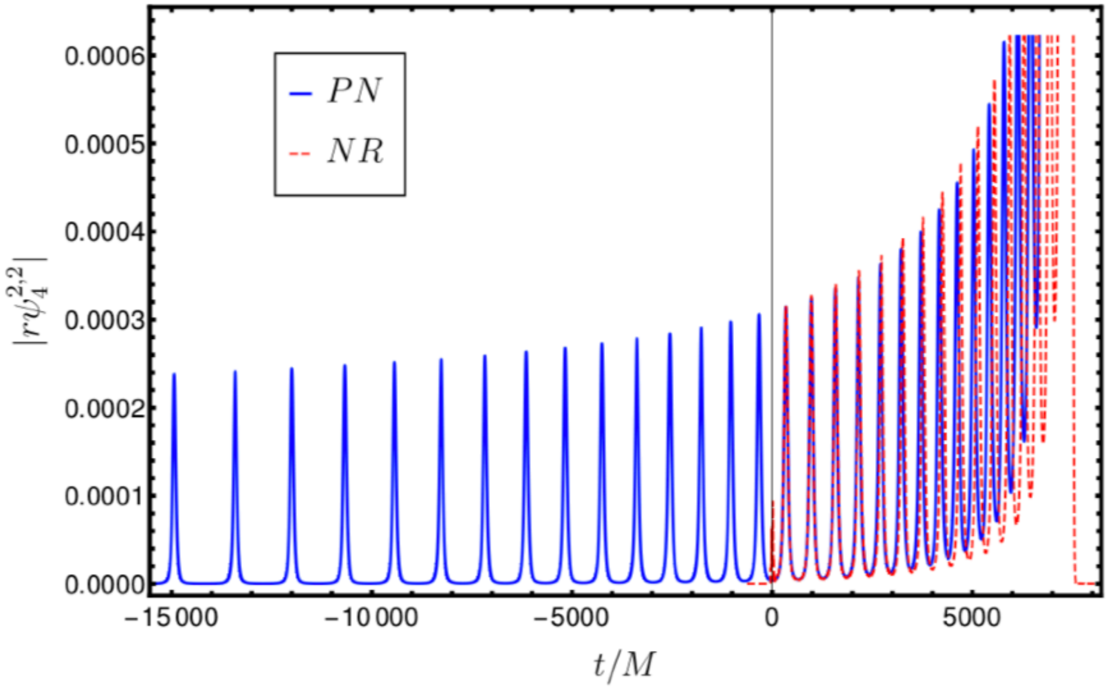


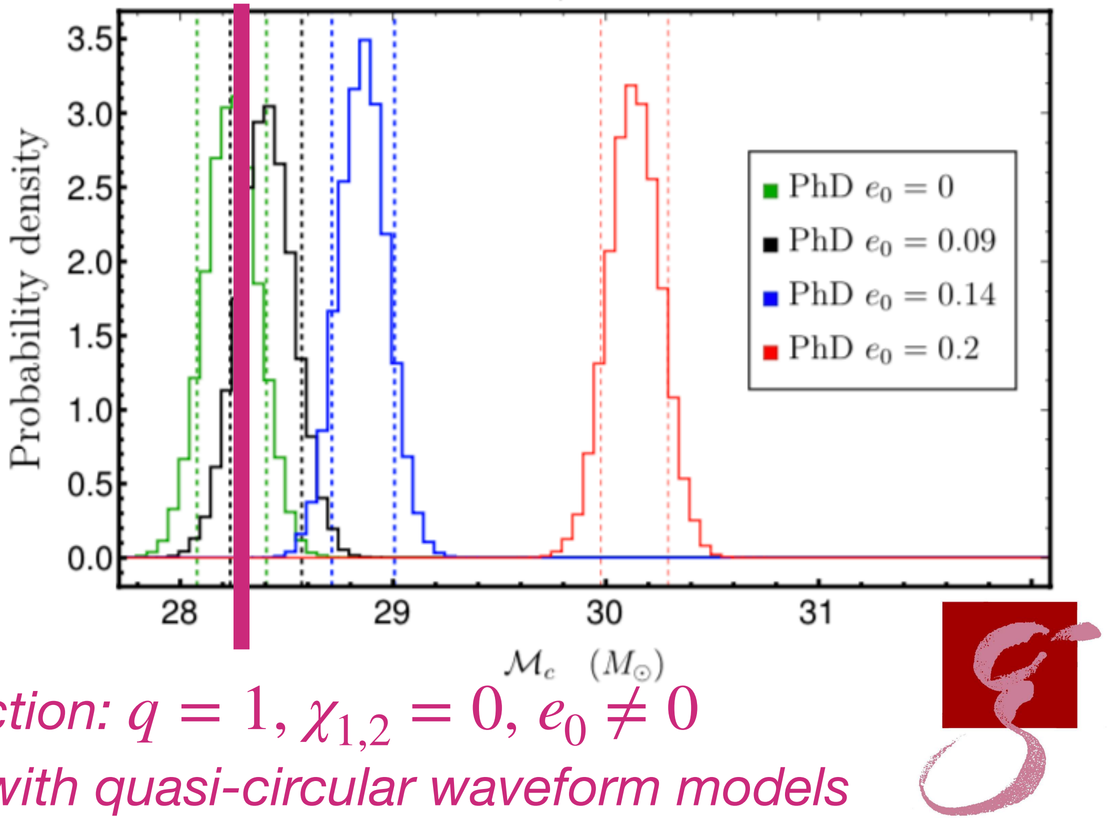
Eccentric waveform models w/ NR input:
Hinder+ 08, Huerta+ 16, Hinder+ 17,

$q \geq 1/4,\, \chi_{1,2} \leq 0.75$

hybridization & PE studies

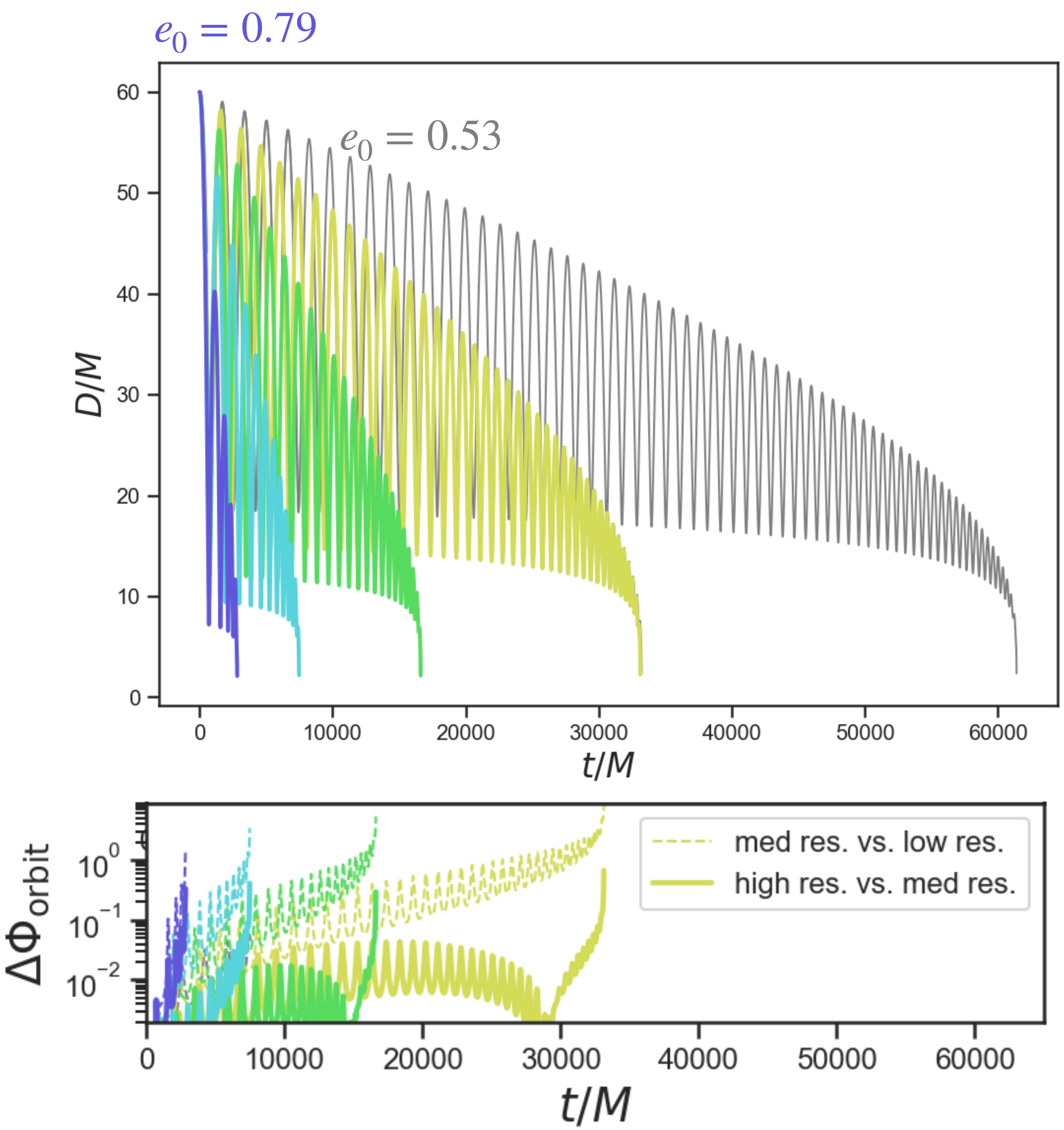
Ramos-Buades+ 1909.11011

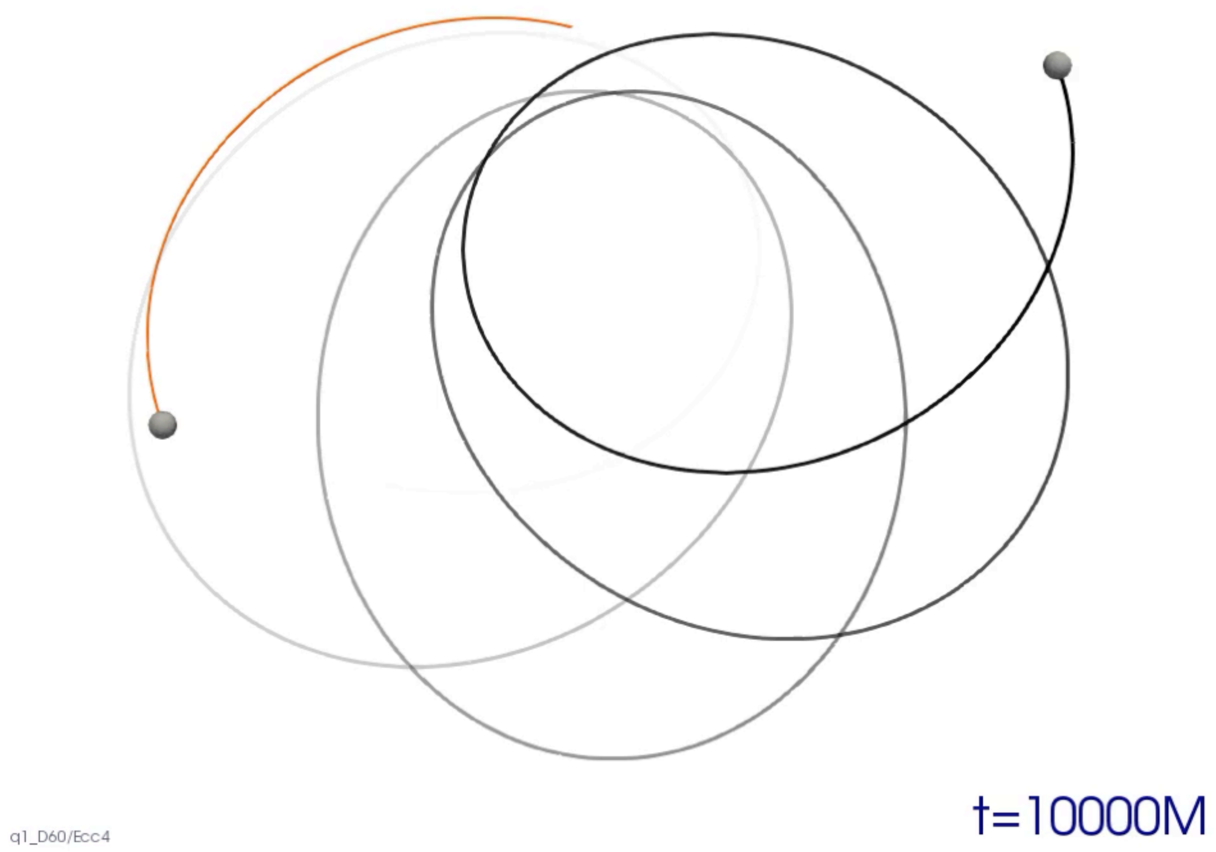




Injection: $q = 1, \chi_{1,2} = 0, e_0 \neq 0$
Recovery with quasi-circular waveform models

SpEC: highly eccentric inspirals (q=1)





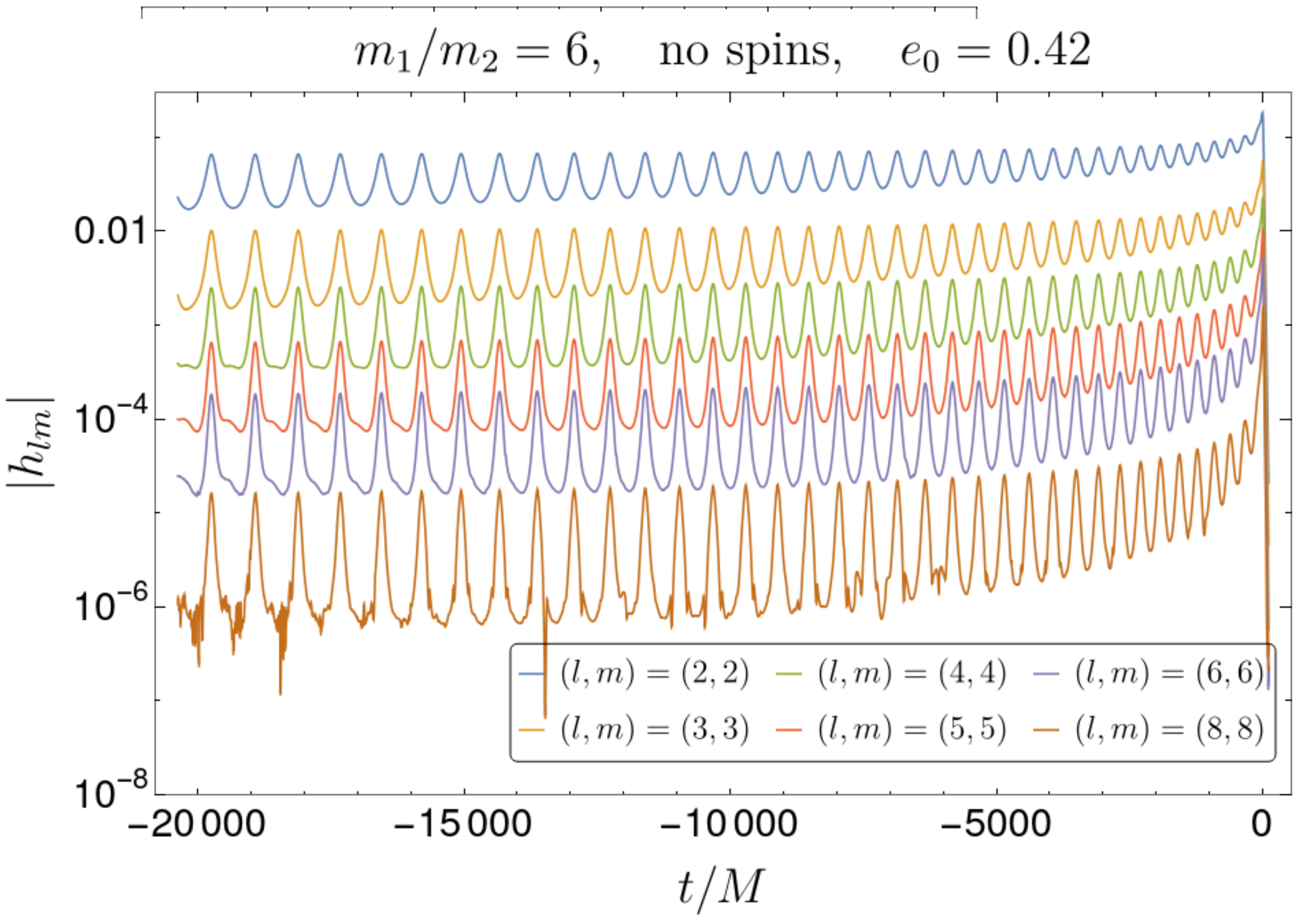
- NR phase-accurate to ~0.1rad
- eccentric PN expected to converge more slowly (Damour+ 04)

Ramos-Buades, Rüter, HP, SXS (in prep)

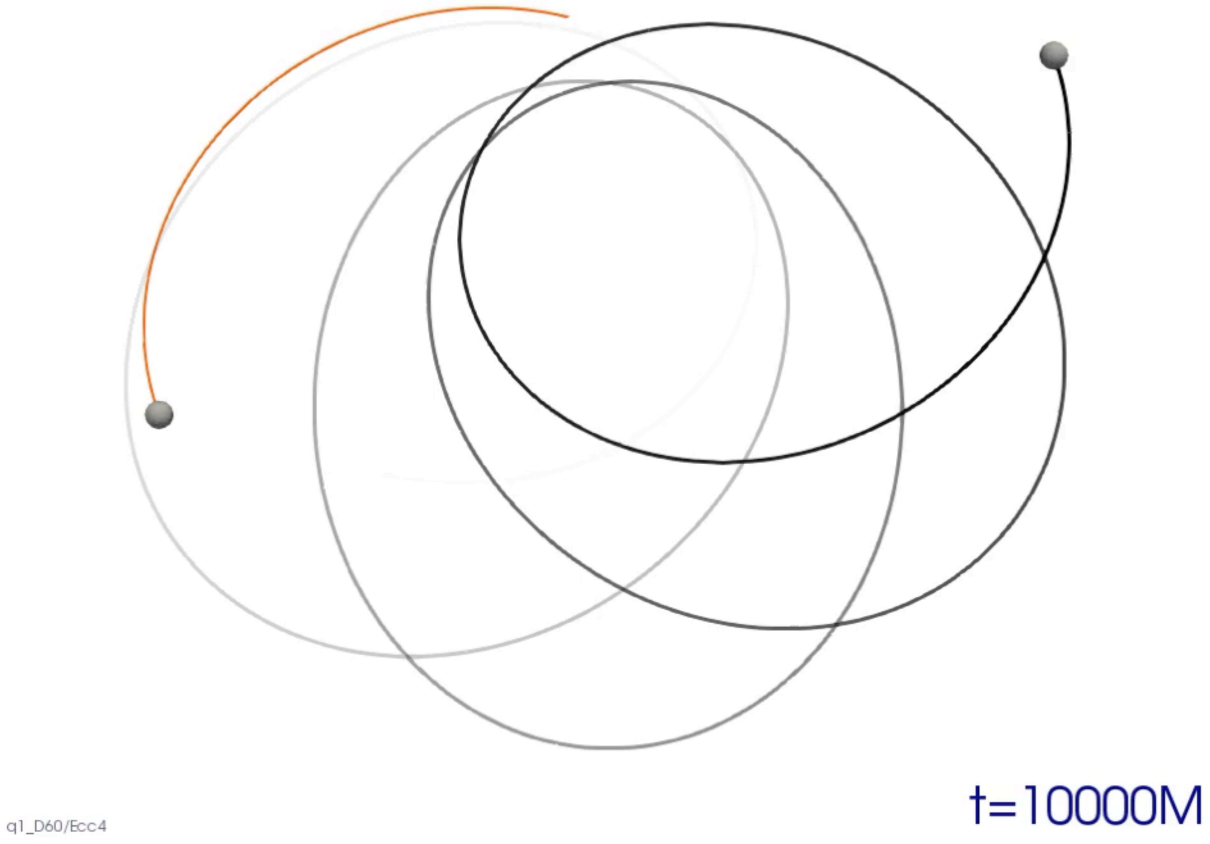
SpEC: highly eccentric inspirals (q=1)

(current) parameter space coverage

many clean higher modes



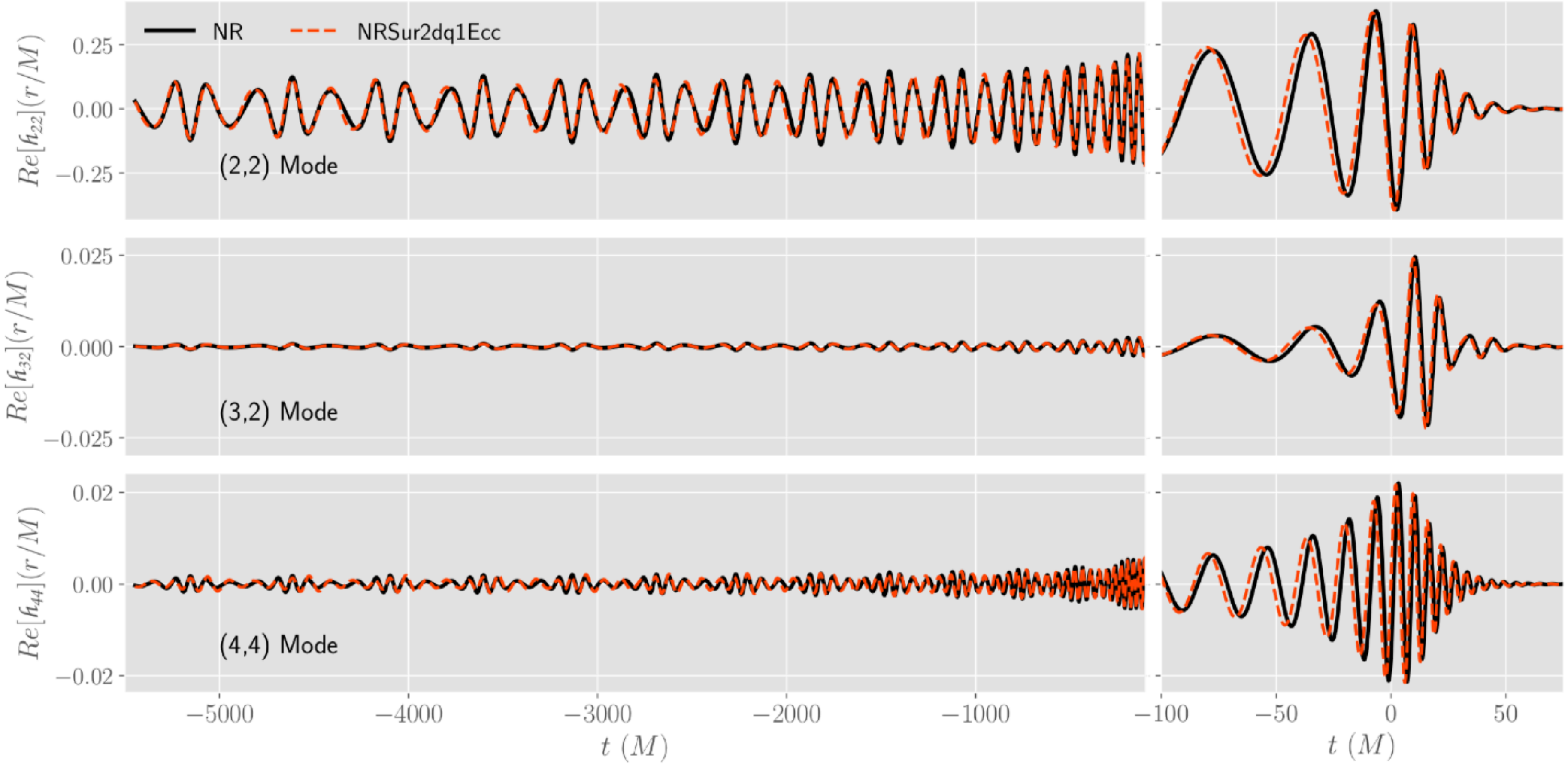
m_1/m_2



Ramos-Buades, Rüter, HP, SXS (in prep)

First eccentric surrogate model

- Built on SpEC runs
  - q=1, zero spin
  - e<0.2

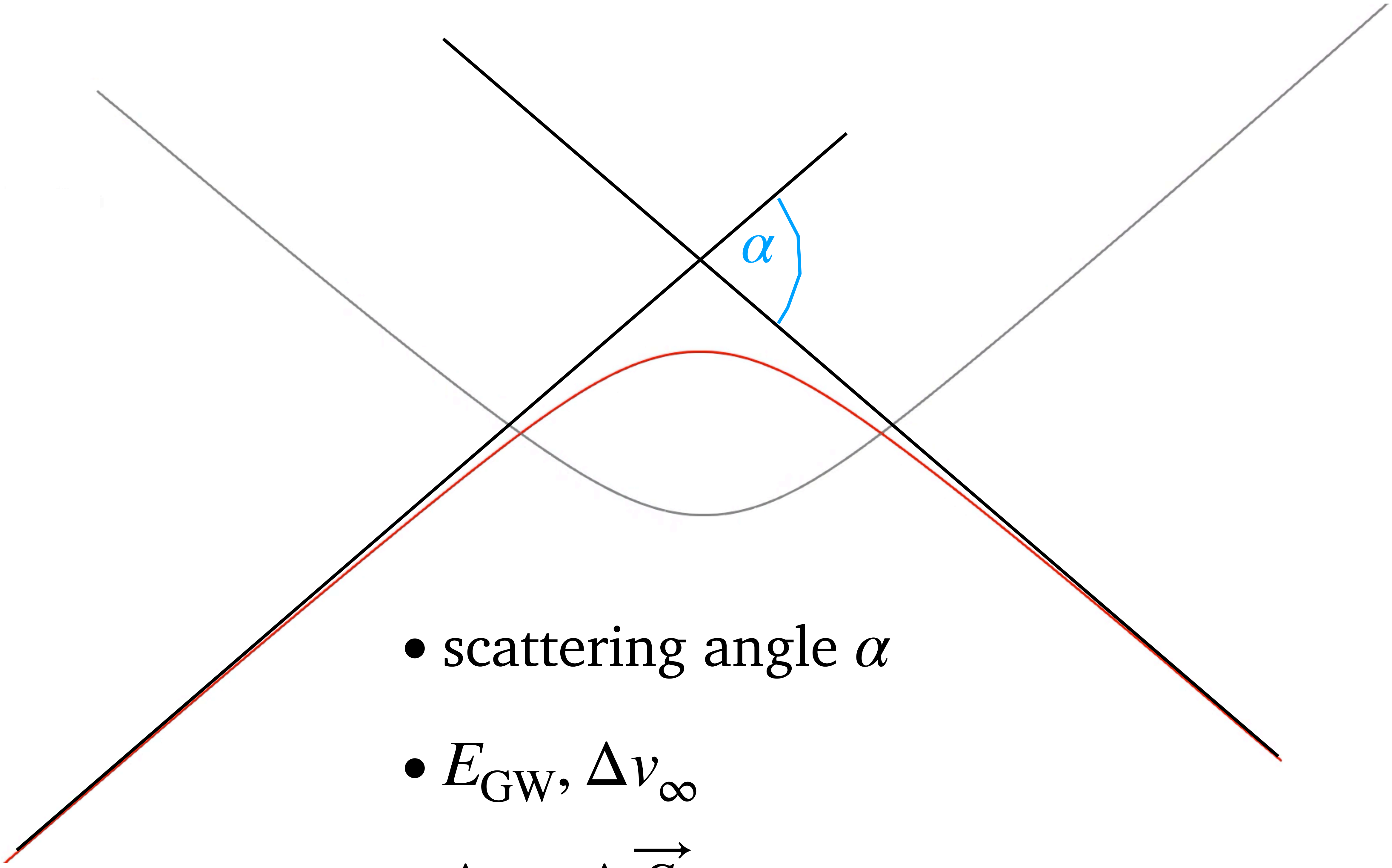


Islam, Varma, .. HP+ 21

Recent (4)

BBH scattering

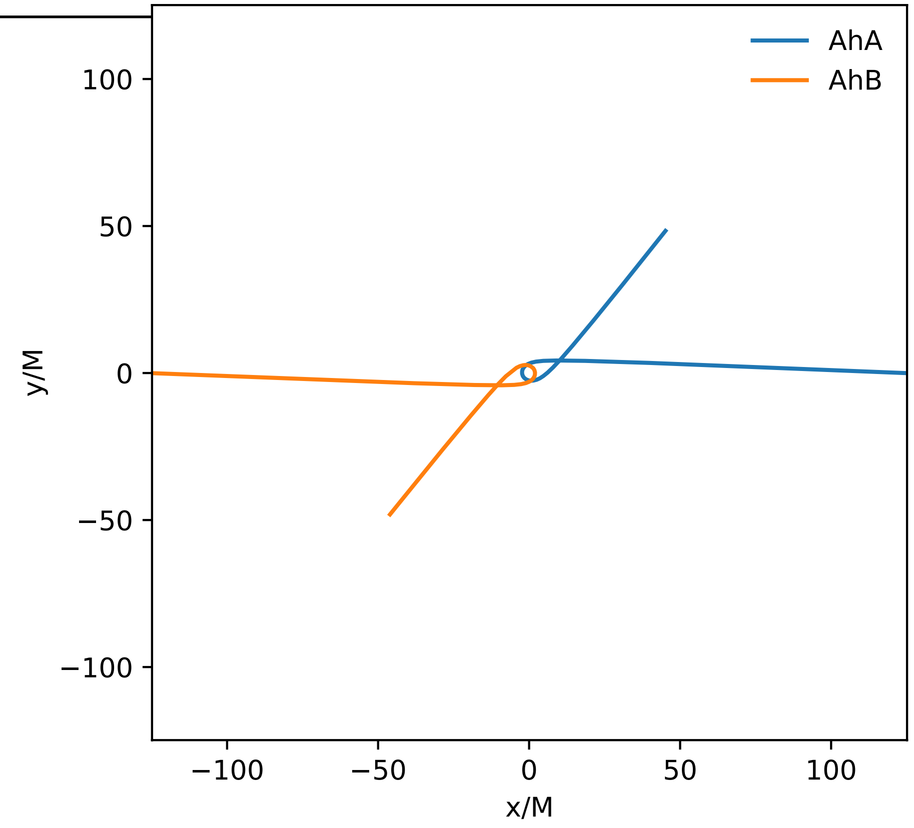
Recent (4): BH Scattering

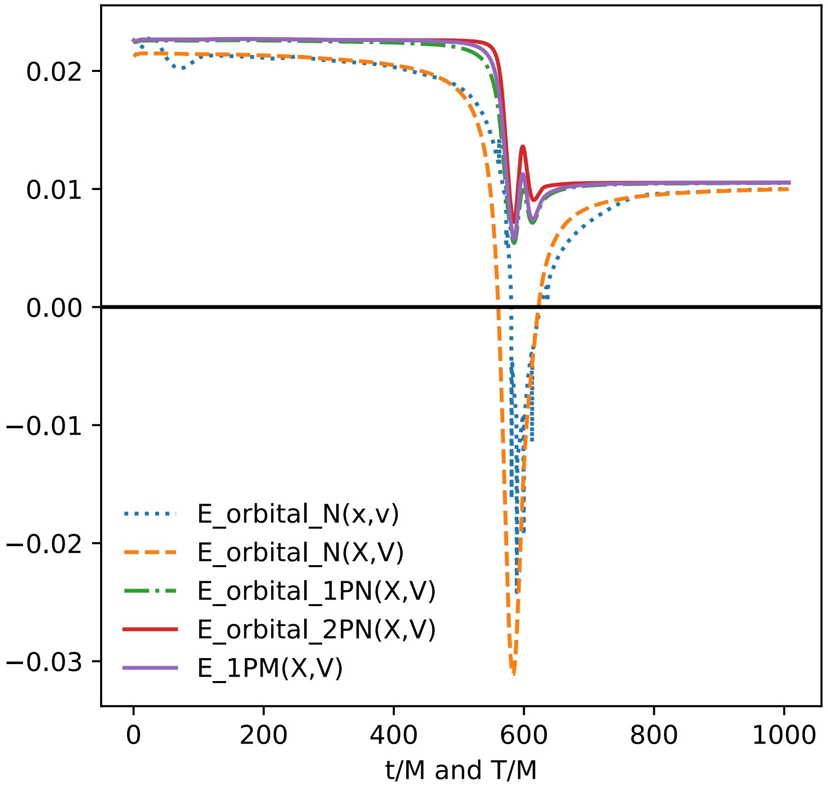


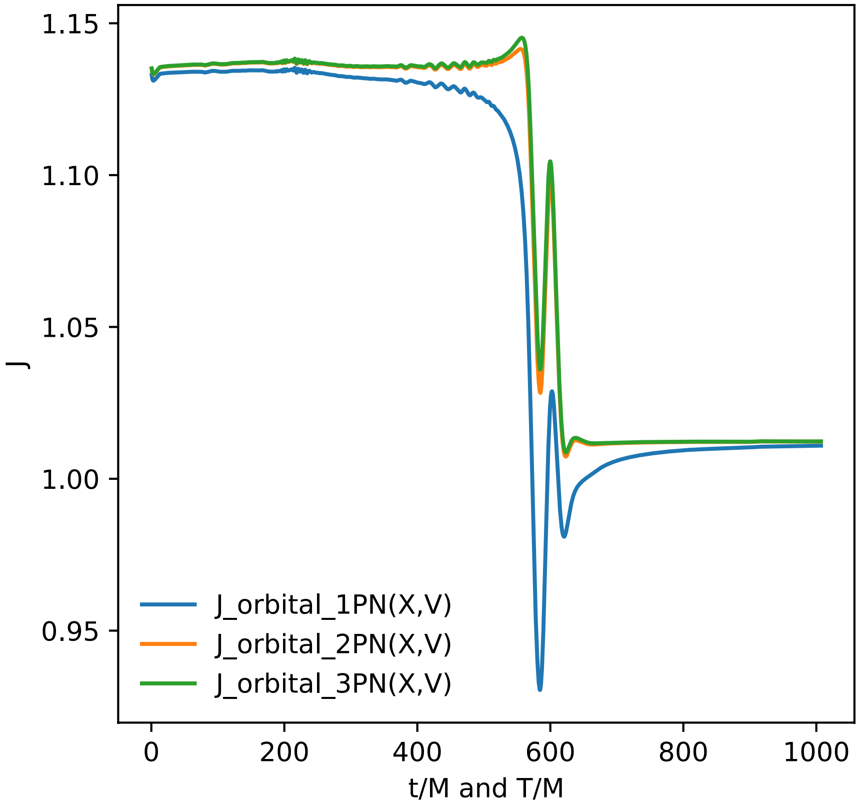
- scattering angle α
- E_{GW}, Δv_∞
- Δm_i, $\Delta \overrightarrow{S}_i$

Scattering in Harmonic Coordinates

- evolution in generalized harmonic coords
  - x,v
- Harmonic coords evolved along
  - **X, V**
- Post-Newtonian well converging
  - before / after encounter





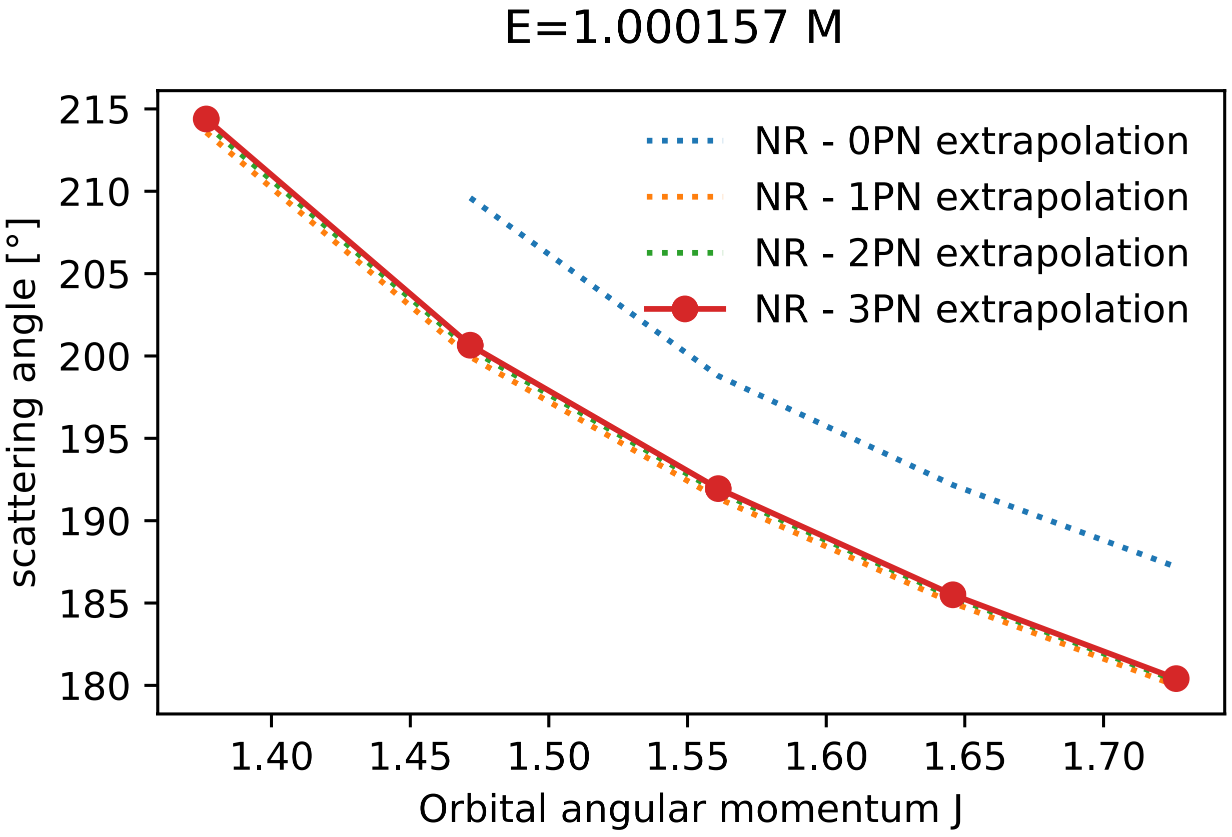


$q=1$, $J=1.025$, $E_{in}=0.0226$

Rüter, HP, SXS in prep

Error analysis of scattering angle

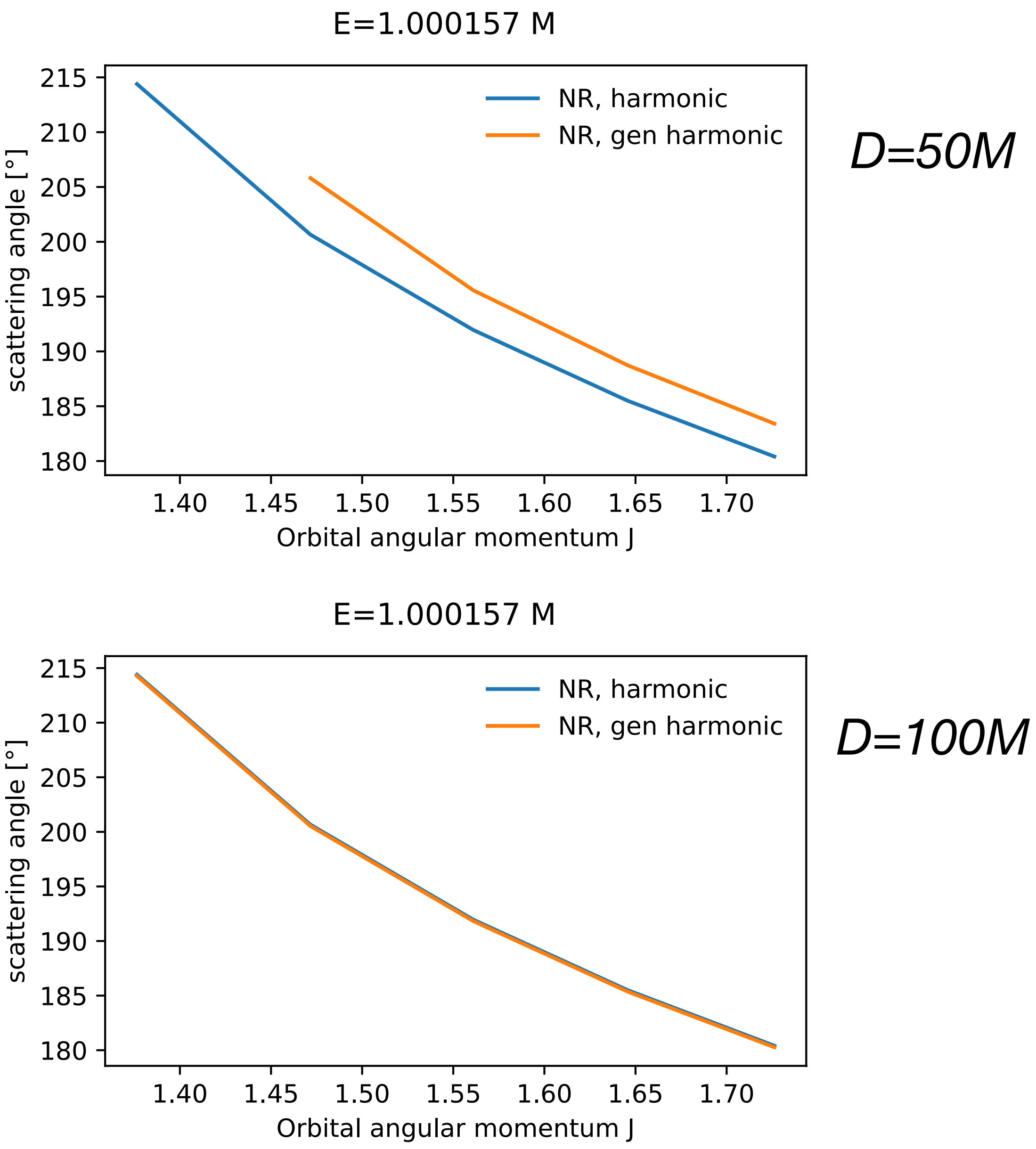
Extrapolate (finite) NR trajectories by PN of different order



Cumulative uncertainty due to
- numerical resolution
- initial conditions
- coordinates
- angle extraction

less than 1 degree

Harmonic coords reduce dependence on initial separation D

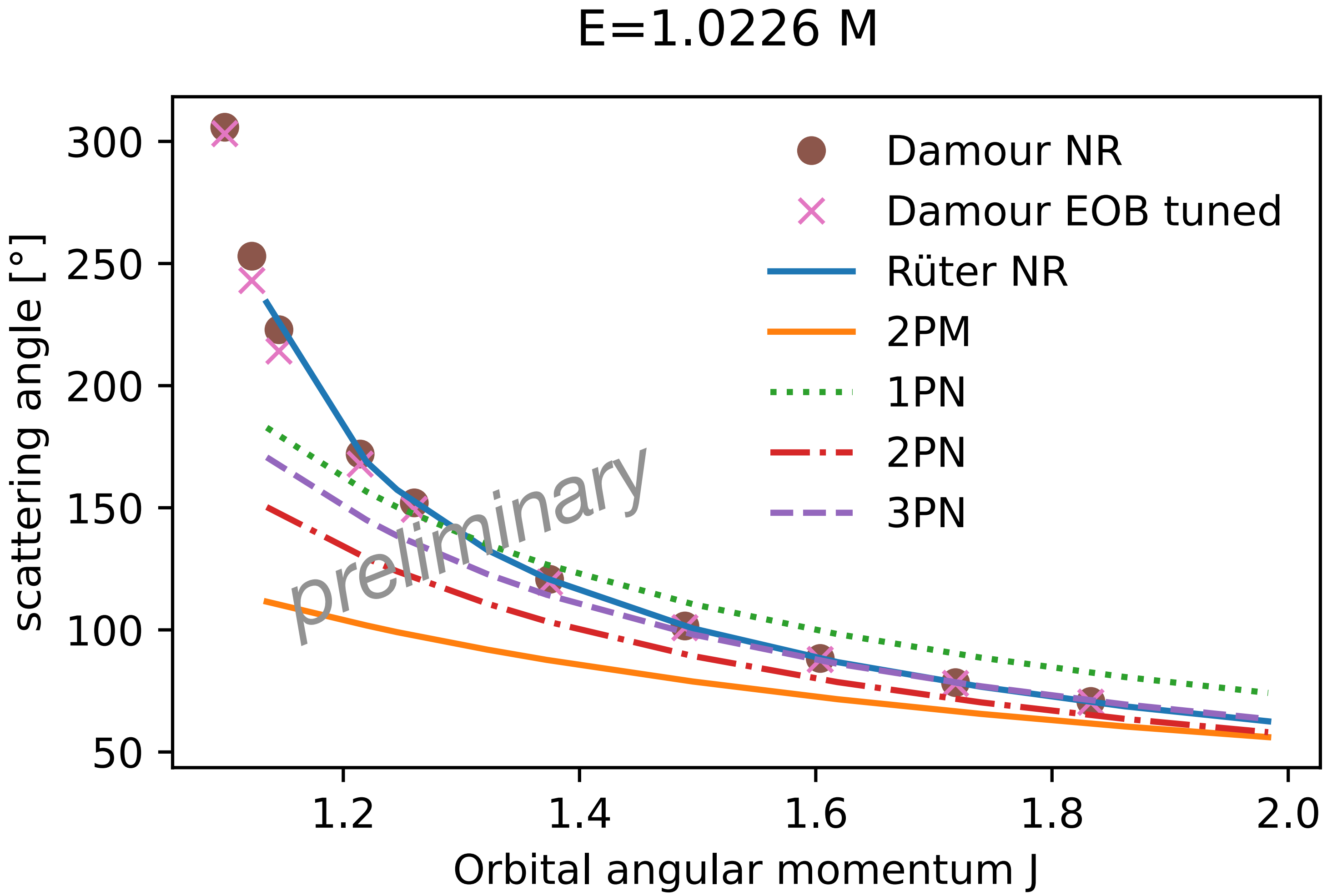


Rüter, HP, SXS in prep

PN: Memmesheimer, Gopakumar, Schäfer 04

scattering angles (q=1, spin zero)

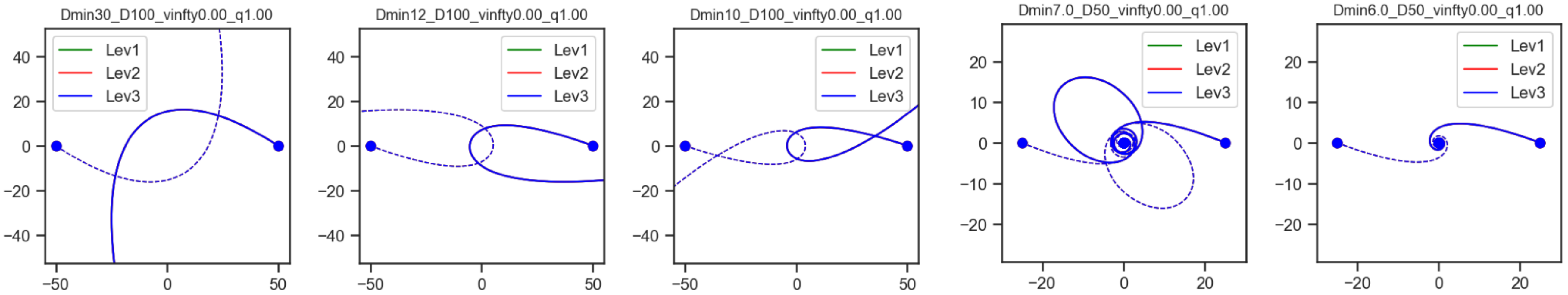
- Comparison w/ NR results of Damour+ 14
  - good agreement
  - validates both codes



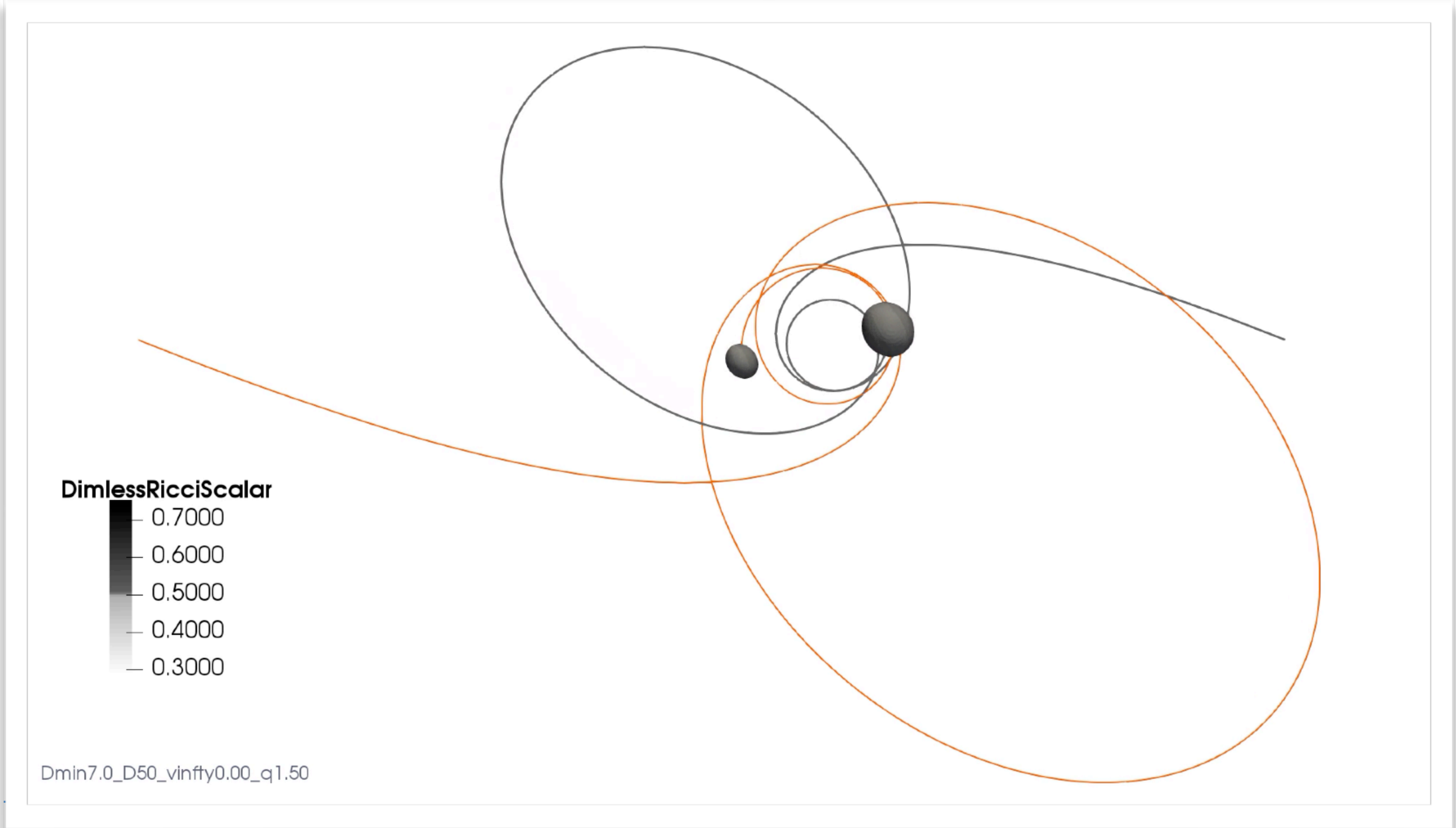
Rüter, HP, SXS in prep

PN: Memmesheimer, Gopakumar, Schäfer 04
2PM: taken from Vines, Steinhoff, Buonanno 19, originally Westpfahl 85

From scatter -> capture



q=2/3



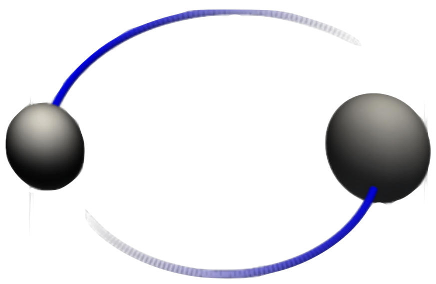
Recent (5)

Contact with gravitational self-force

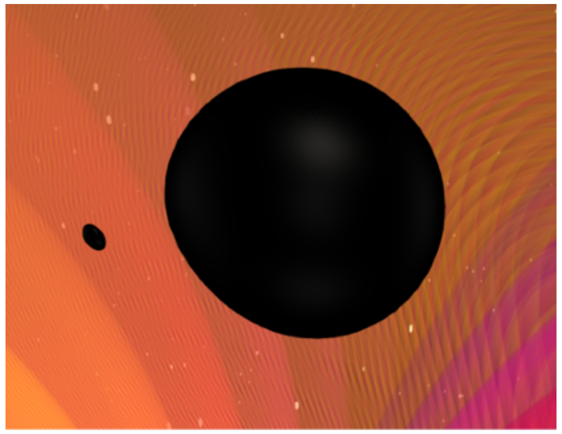
Bridging mass-ratio gap

q=1

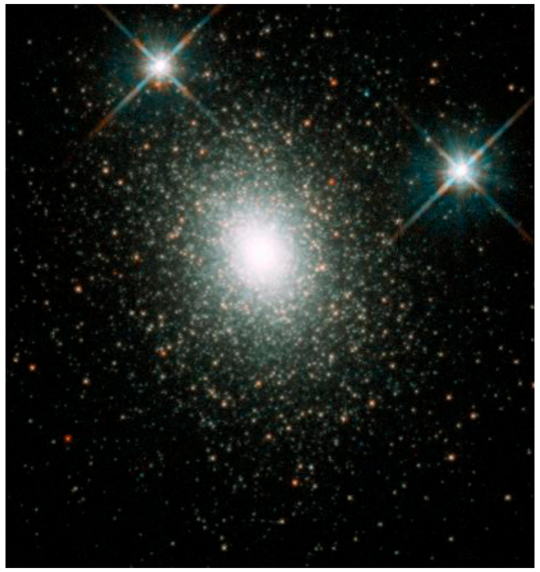
q=0


LVC

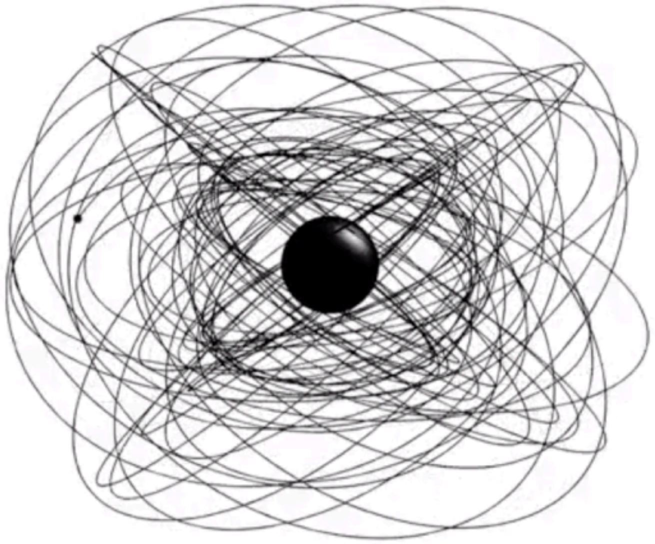
GW150914


Fischer, HP

GW190814


NASA

Intermediate mass BH
$(10+1000)M_\odot$
$(10^3+10^6)M_\odot$


S. Drasco

EMRI
$(10+10^6)M_\odot$

NR
$q \gtrsim 1/20$

Small-mass-ratio approximation (SMR)

expansion in q *or* $\nu = q/(1+q)^2$

Challenge for NR at small q

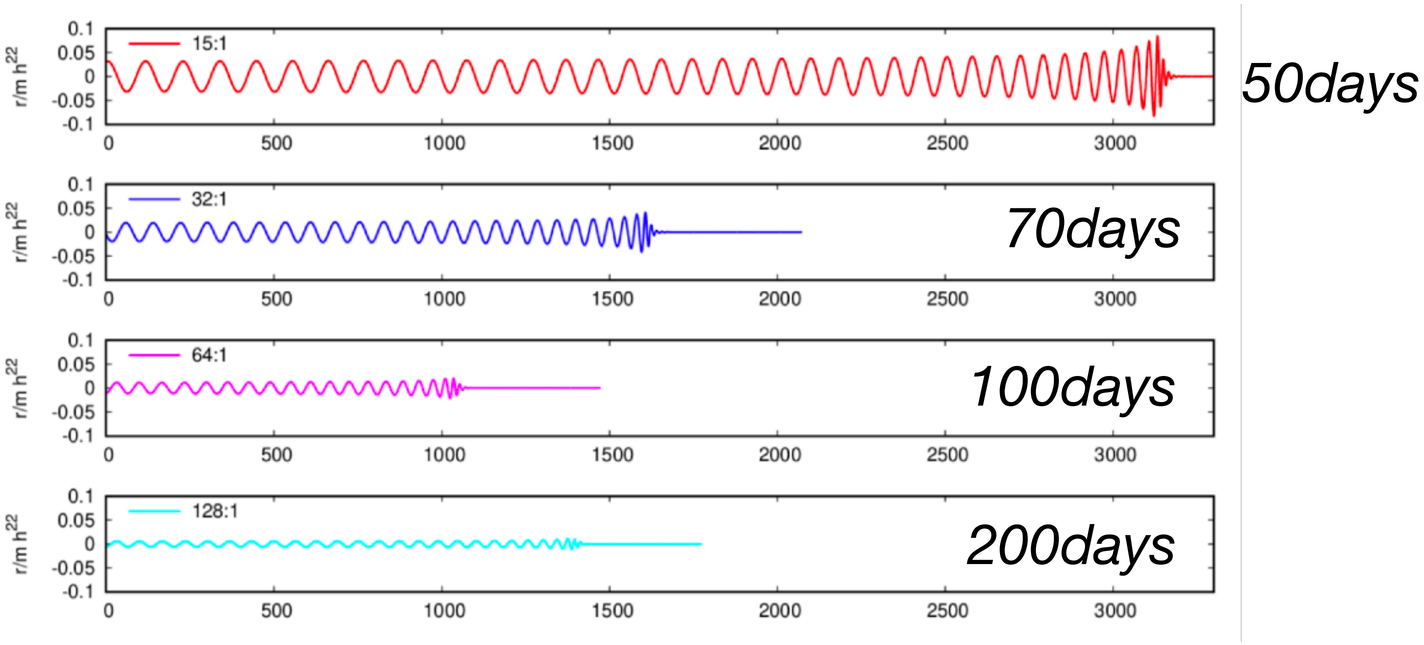
- Scaling of number of time-steps

$$\boxed{N_{\text{steps}} \propto \frac{1}{q^2}\frac{1}{(M\Omega_i)^{8/3}}}$$

q — more steps per orbit
(Courant limit — *numerics*)
q — more orbits per inspiral
(physics)
$(M\Omega)^{8/3}$ — start frequency

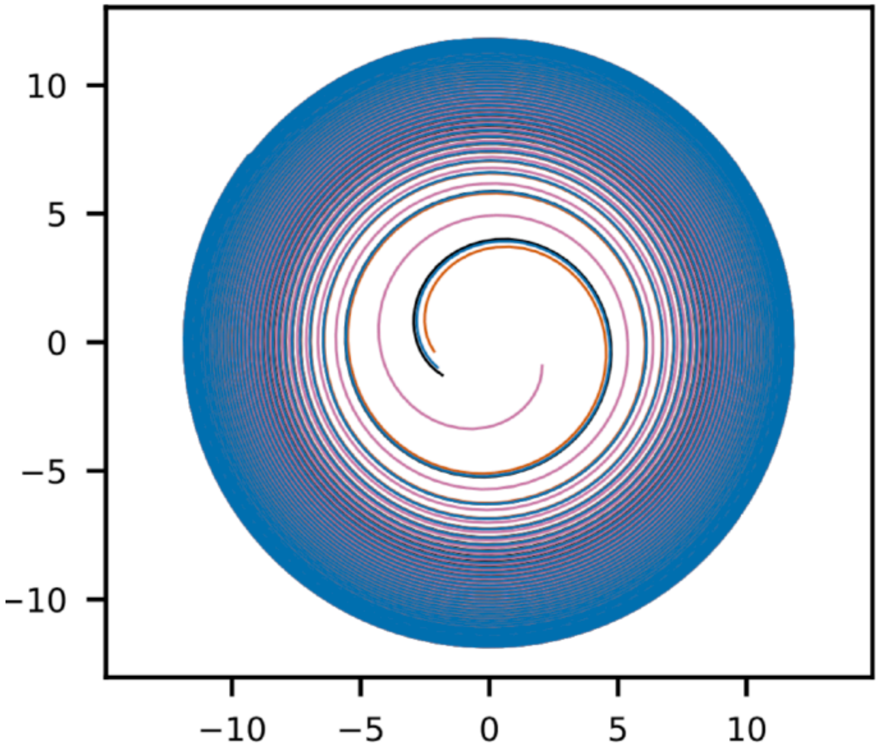
$\chi \gtrsim 0.6$: extra factor ~$1/(1-\chi_1)(1-\chi_2)$
χ_2 larger impact than χ_1

Lousto & Healy 2006.04818: q=1/15 .. 1/128 (!)



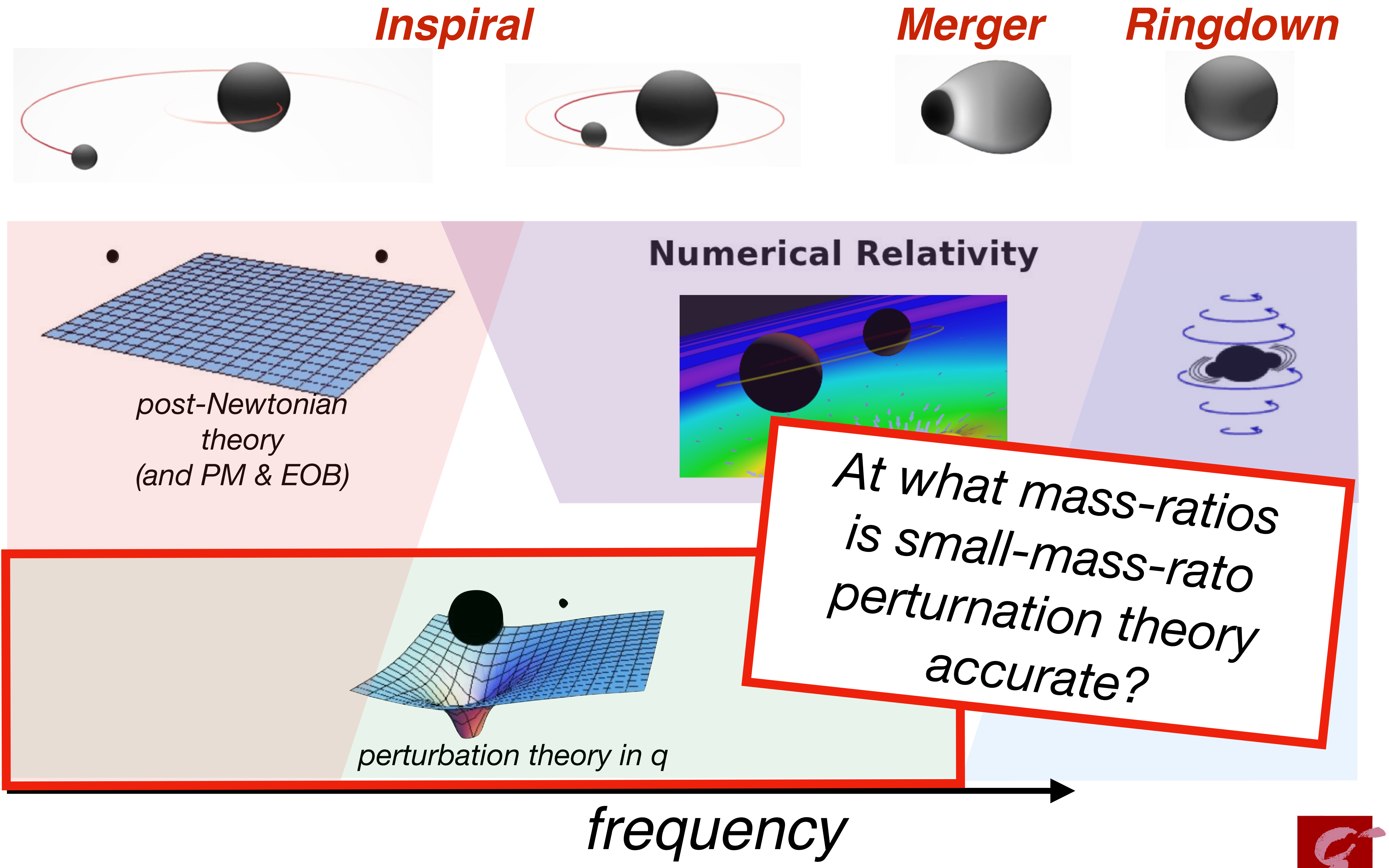
$q \leq 1/32$: *very limited convergence tests*

$q = 1/20, \chi_1 = 0, \chi_2 = 0$



SpEC, 4 resolutions
Ossokine, Fischer, Rüter, HP

Methods for modeling BBH



Inspiral **Merger** **Ringdown**

1 mass-ratio q 0

Numerical Relativity

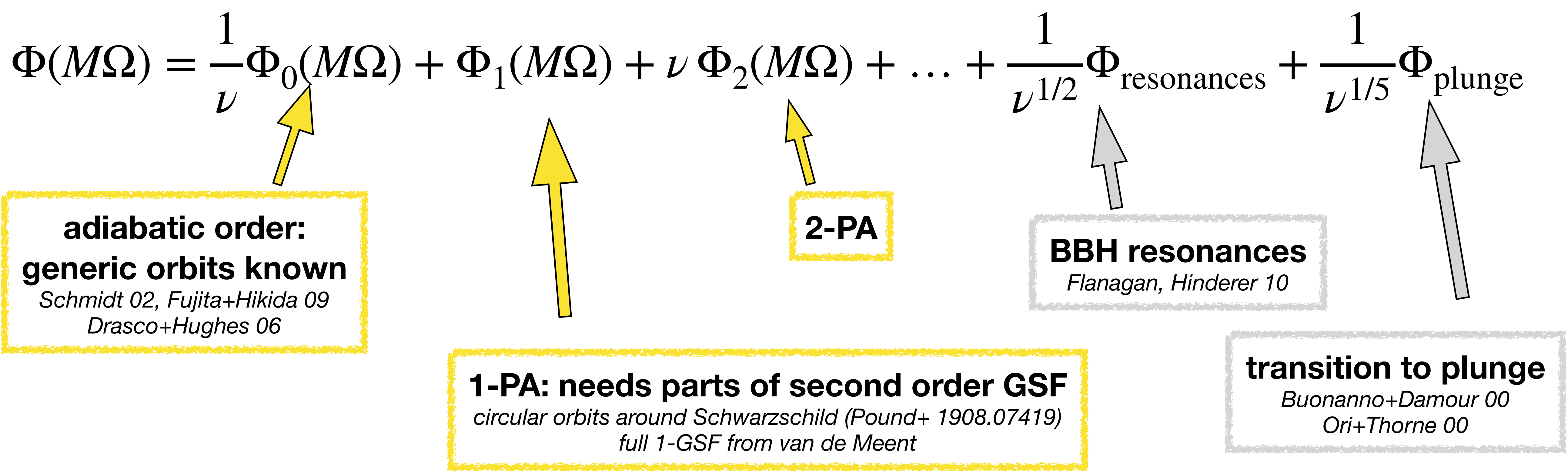
post-Newtonian theory (and PM & EOB)

perturbation theory in q

frequency

At what mass-ratios is small-mass-rato perturbation theory accurate?

SMR orbital phasing



$$\Phi(M\Omega) = \frac{1}{\nu}\Phi_0(M\Omega) + \Phi_1(M\Omega) + \nu\,\Phi_2(M\Omega) + \ldots + \frac{1}{\nu^{1/2}}\Phi_{\text{resonances}} + \frac{1}{\nu^{1/5}}\Phi_{\text{plunge}}$$

adiabatic order:
generic orbits known
Schmidt 02, Fujita+Hikida 09
Drasco+Hughes 06

1-PA: needs parts of second order GSF
circular orbits around Schwarzschild (Pound+ 1908.07419)
full 1-GSF from van de Meent

2-PA

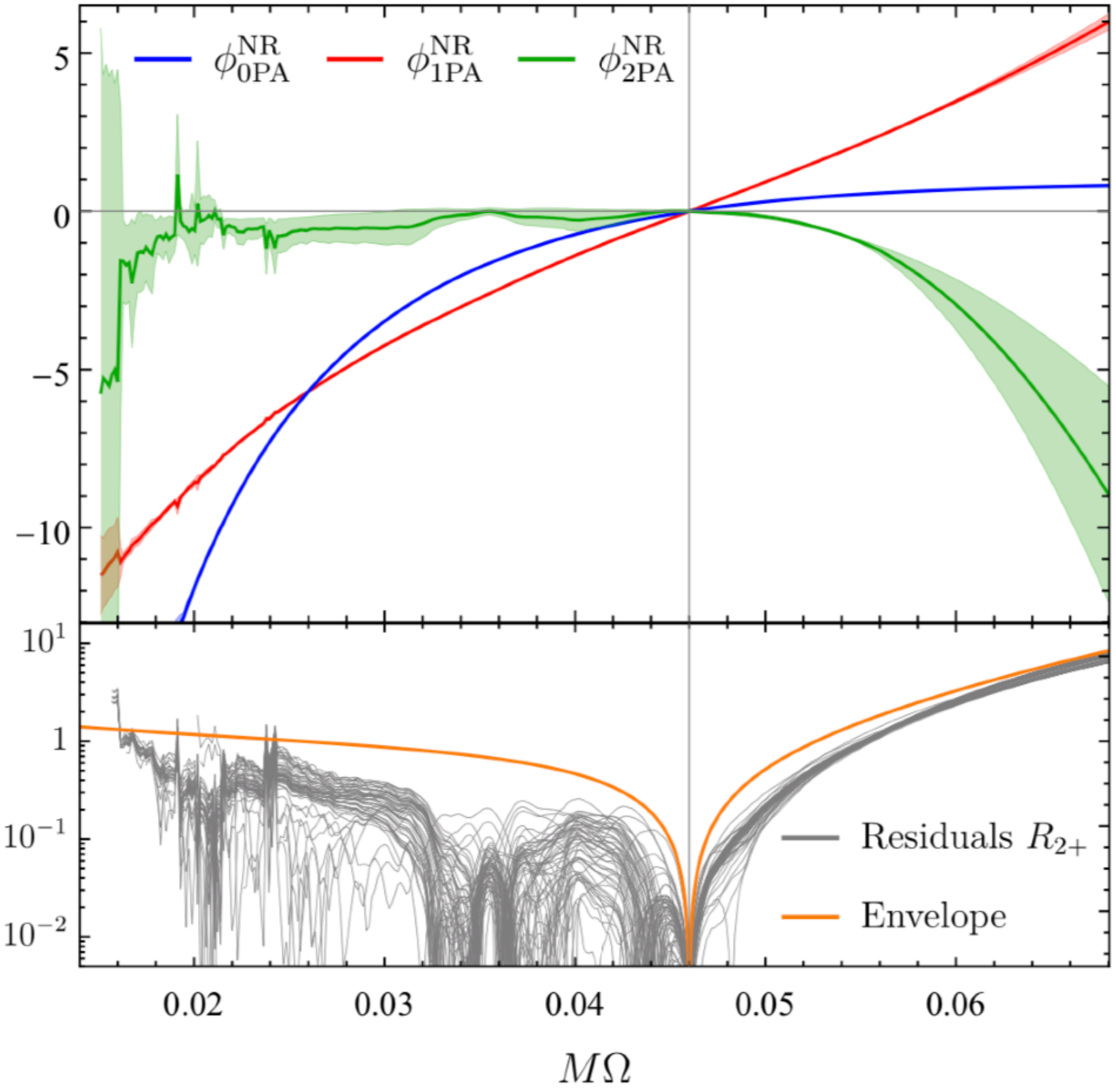
BBH resonances
Flanagan, Hinderer 10

transition to plunge
Buonanno+Damour 00
Ori+Thorne 00

SMR orbital phasing

$$\Phi(M\Omega) = \frac{1}{\nu}\Phi_0(M\Omega) + \Phi_1(M\Omega) + \nu\,\Phi_2(M\Omega) + \ldots + \frac{1}{\nu^{1/2}}\Phi_{\text{resonances}} + \frac{1}{\nu^{1/5}}\Phi_{\text{plunge}}$$

- $\Phi^{\rm NR}(M\Omega)$ from 55 SXS simulations with $q = 1\ldots 1/10$
- Fit to $\Sigma_k \nu^{k-1}\Phi_k(M\Omega)$
  - $\Phi_0(M\Omega)$ - agrees with 0PA
  - $\Phi_1(M\Omega)$ - hereby computed
  - $\Phi_2(M\Omega)$ - *remarkably small*



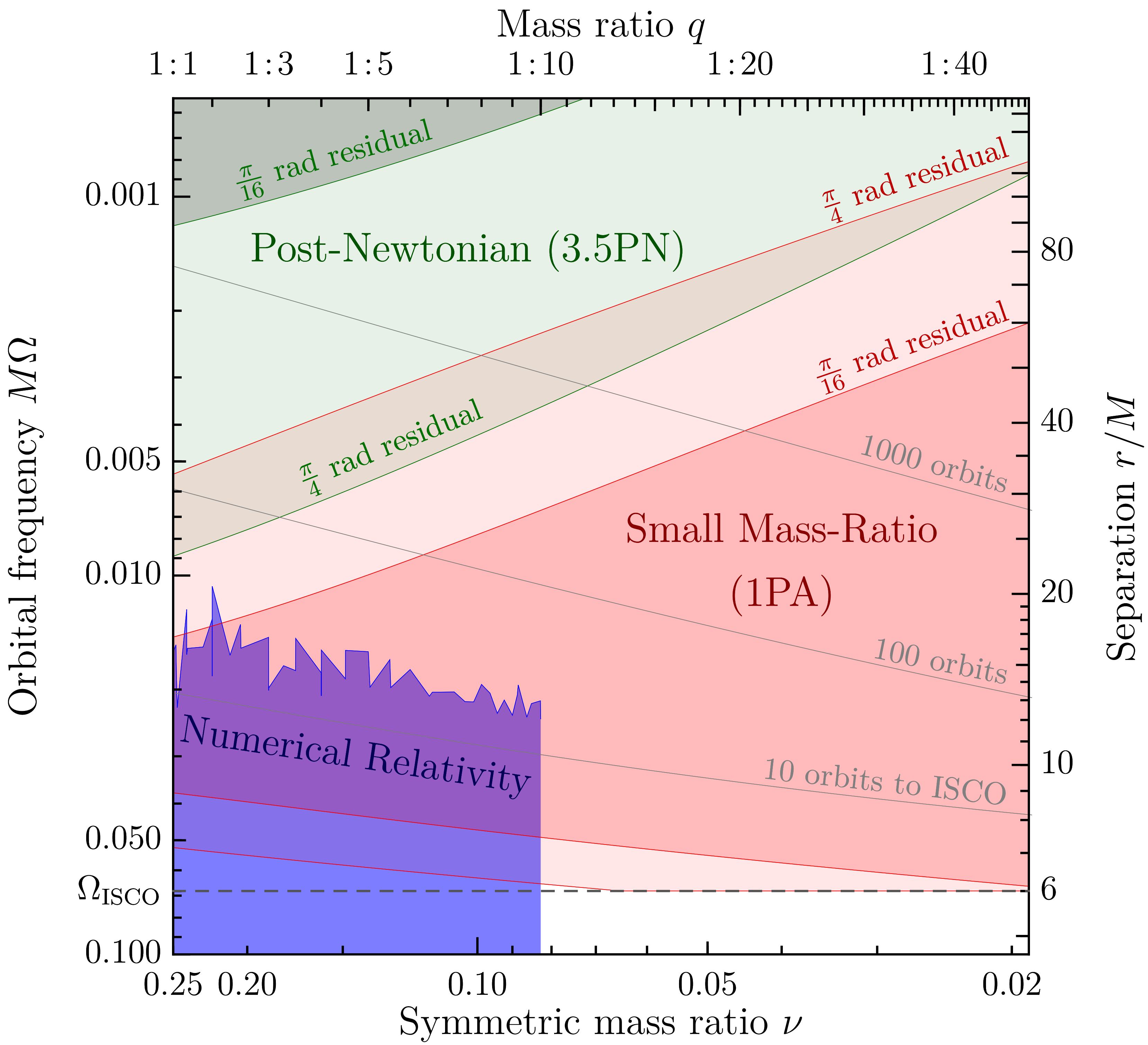
- Φ_1 contributes 10's of radians to orbital phase $\Rightarrow$ significant at *any* ν
- Φ_2 small only if expanded in ν (not in q) and written as function of $M\Omega$ (not $m_1\Omega$)

van de Meent, HP 2020

Applicability of approximation schemes

- For *non-spinning, quasi-circular*, at phase-errors *~1 radian*: **mass-ratio gap bridged!**

- Note: eccentric PN expected to converge more slowly (Damour+ 04)



van de Meent, HP 2006.12036

Summary

- NR simulations **accurate for today's GW detectors** and at parameters of GW events so far

- **Improvements under way** for future GW detectors:
    - accuracy
    - length
    - parameter space
    - high spins

- **Biggest challenges**
    - **high mass-ratio**
    - near extreme spins
    - high energy encounters

- Promising results for **eccentric inspirals** and **scattering encounters**