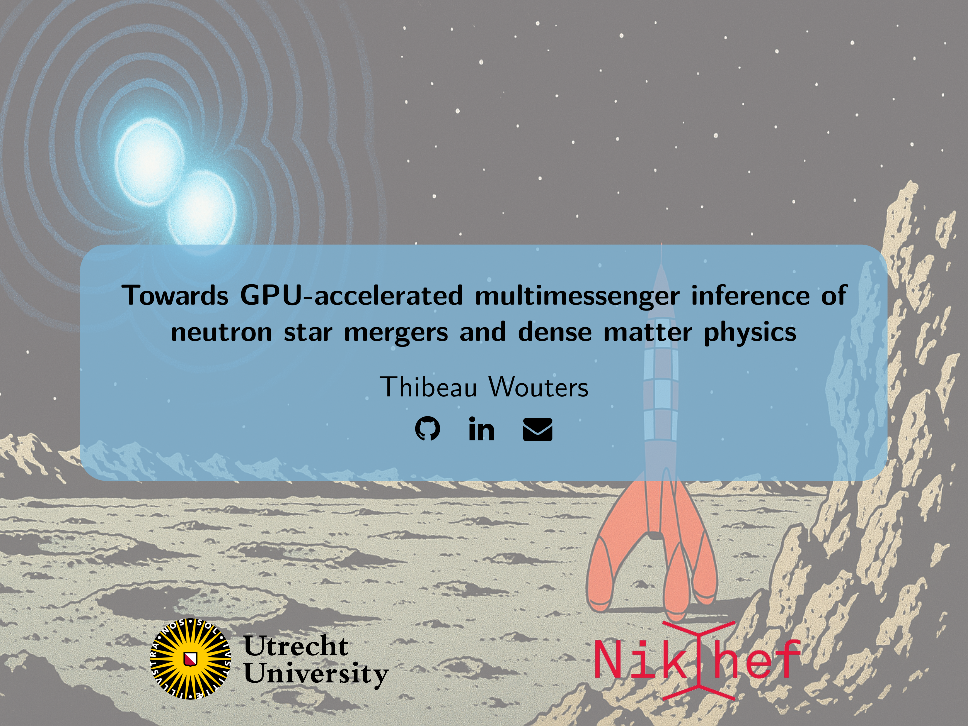

Towards GPU-accelerated multimessenger inference of neutron star mergers and dense matter physics

Thibeau Wouters

Utrecht University

Nikhef

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Neutron stars

- Neutron stars: supernova remnants, densest matter in the universe
- $m \sim 1.2 - 2.3 M_{\odot}$, $R \sim 10 - 13$ km

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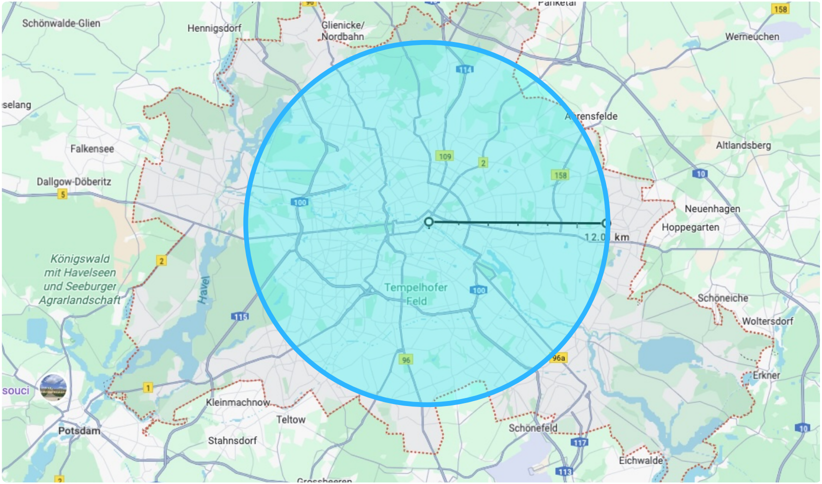
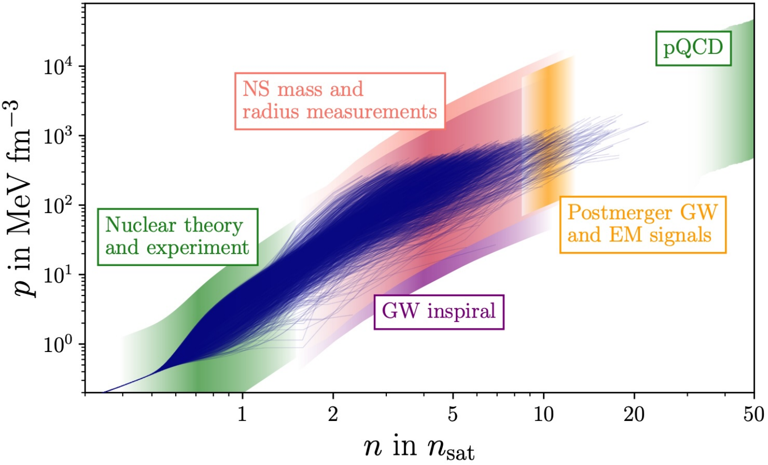


Equation of state

Neutron stars probe the high-density part of the equation of state (EOS) of dense nuclear matter [1]



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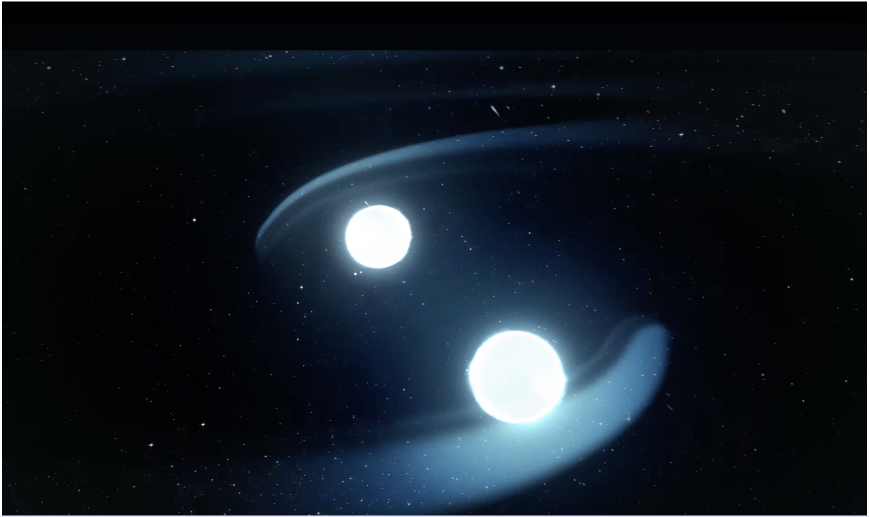

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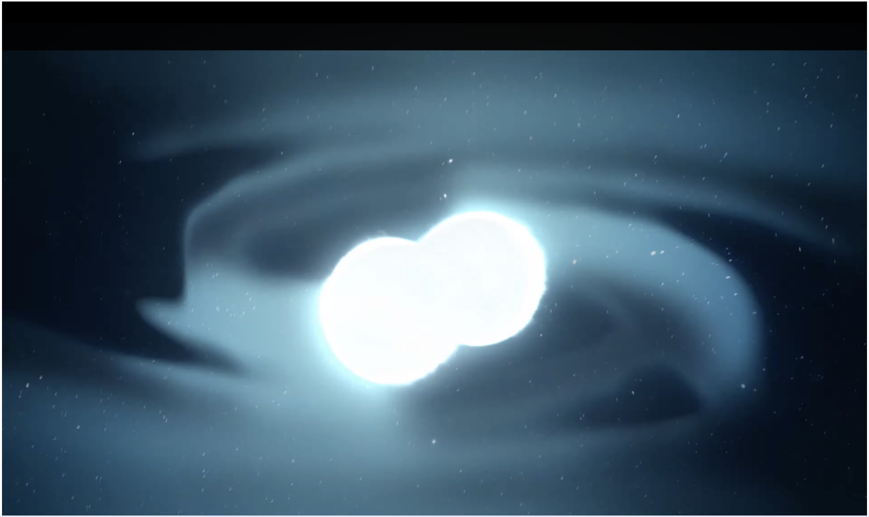

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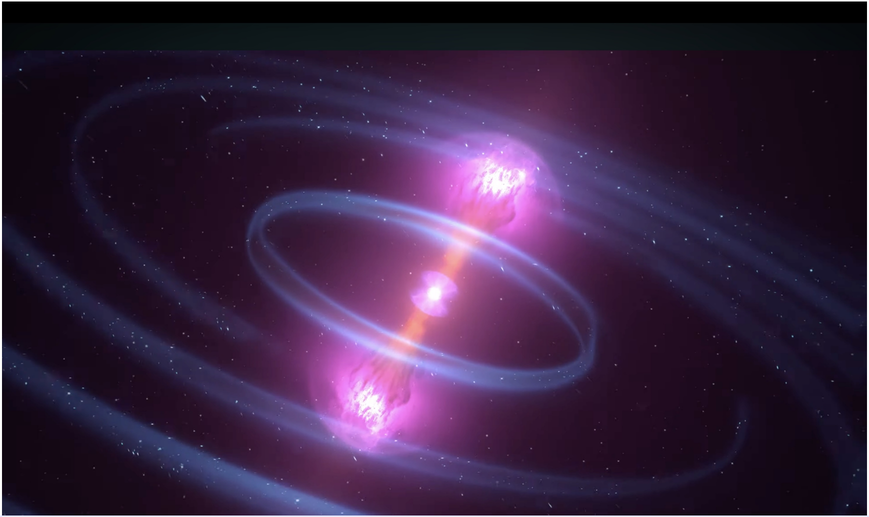

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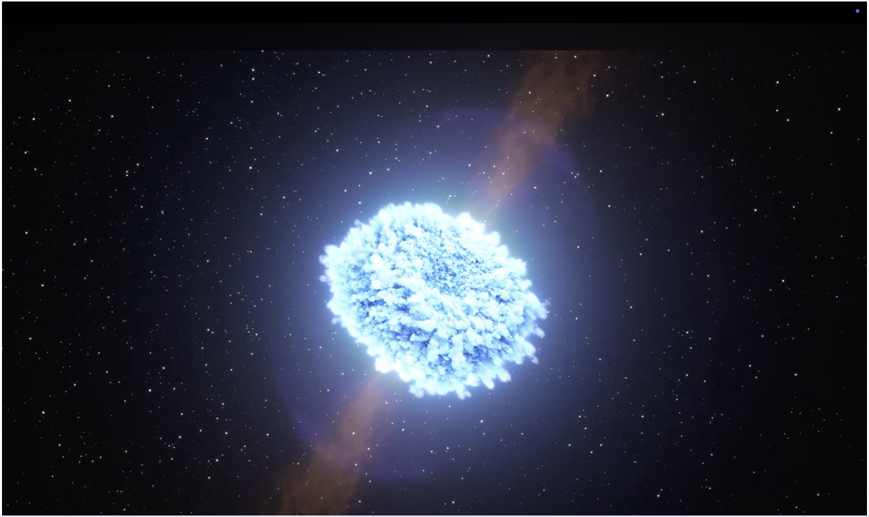

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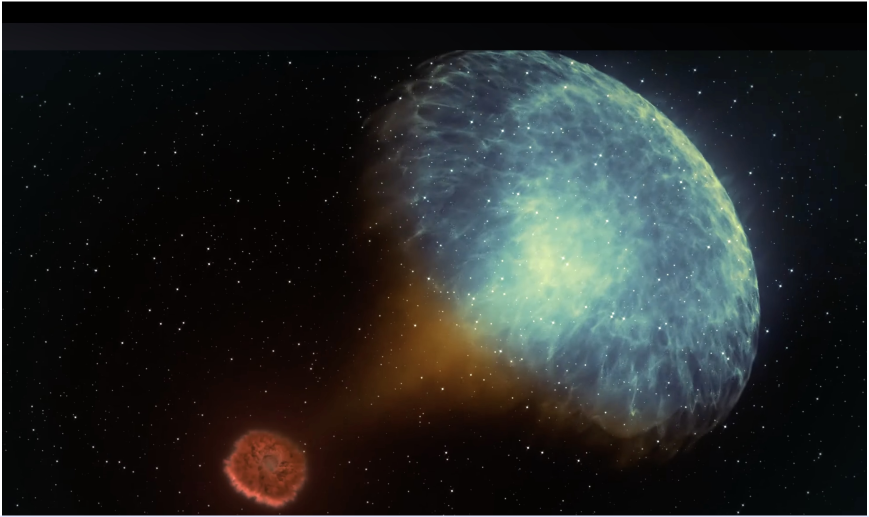

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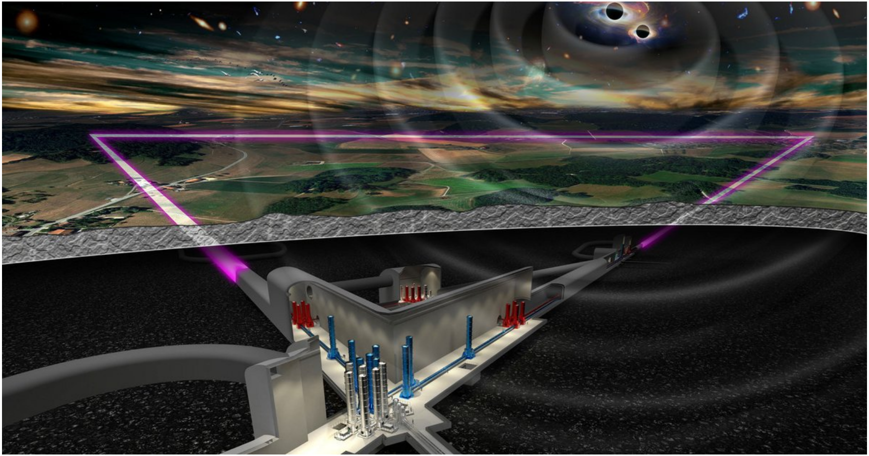
Future GW detectors: Einstein Telescope

Einstein Telescope: Third-generation ground-based GW detector [4, 5]



(or 2 L-shaped detectors...)

Future GW detectors: Einstein Telescope

Einstein Telescope: Third-generation ground-based GW detector [4, 5]

- Increased sensitivity
  - Louder signals
  - $10^5 - 10^6$ binary black hole mergers/year (now: $\sim 200/10$ years)
  - $10^4 - 10^5$ binary neutron star mergers/year (now: $2/10$ years)
  - $10^2 - 10^3$ multimessenger events/year (now: $1/10$ years)

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- Observe from 5 Hz (now: 20 Hz)
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    - Binary neutron star: 2 hours (vs 2 minutes now)
  - Signals will overlap: joint analysis needed

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  - Signals will overlap: joint analysis needed

Current software cannot handle the ET data analysis problem [6]

My research focus: why – how – what

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To make inference of multimessenger astrophysics scalable

- Prepare for future detectors
- Understand systematic effects through simulated data

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Without compromises to flexibility and accuracy

- Accelerate with GPU hardware, differentiable programming
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What?

GPU-accelerated Bayesian joint inference framework of neutron star mergers and dense matter physics

Contents

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Parameter estimation: Bayesian inference

How do we “measure” source parameters θ for data d?

Parameter estimation: Bayesian inference

How do we "measure" source parameters θ for data d?

Bayesian inference:

$$\text{posterior} = p(\theta|d,\mathcal{M}) = \frac{p(d|\theta,\mathcal{M})p(\theta|\mathcal{M})}{p(d|\mathcal{M})} = \frac{\text{likelihood} \times \text{prior}}{\text{evidence}}$$

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Ingredients:

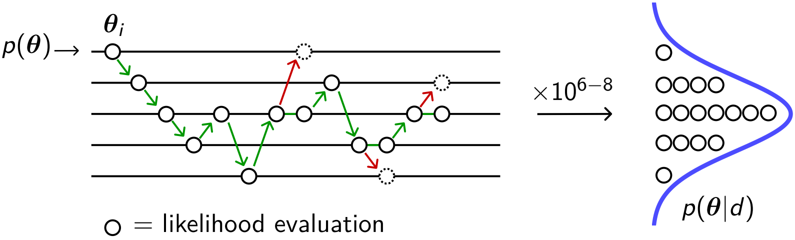
- Posterior: intractable, needs stochastic samplers
- Prior: specified by users, encode beliefs
- Likelihood: computational bottleneck
- Evidence: model selection

Parameter estimation: Markov chain Monte Carlo

How do we sample the posterior? Markov chain Monte Carlo

- N chains $\boldsymbol{\theta}_i$ explore posterior in parallel
- Evolve chains to new position: proposal
- Compute likelihood $\rightarrow$ accept/reject

Alternatives: nested sampling, sequential Monte Carlo



Computational aspects

$$\text{Total runtime} \approx N_{\text{likelihood}} \times \tau_{\text{likelihood}}$$

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In particular:

- Python: integrate into existing workflows
- Focus on arrays: widespread applications
- Numpy-like API: (`numpy` $\rightarrow$ `jax.numpy`)

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Gamechangers:

- GPU accelerators
- Composable function transformations: `jit`, `grad`, `vmap` & `pmap`

JAX – Function transformations

- `jit`: Just-in-time compilation

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- `jit`: Just-in-time compilation
- `grad`: Automatic differentiation:
  - Chain rule on computational graph
  - Exact gradients (up to machine precision), fast
- `vmap`, `pmap`: Vectorization, batch processing, parallelization
- These are composable, e.g.:
  - Higher-order derivatives: `grad(grad(f))`
  - Evolve N chains in parallel along gradient of the likelihood

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha * \texttt{vmap}(\texttt{jit}(\texttt{grad}(\texttt{logL}(\boldsymbol{\theta}))))$$

Computational aspects

$$\text{Total runtime} \approx N_{\text{likelihood}} \times \tau_{\text{likelihood}}$$

- $N_{\text{likelihood}}$: total number of likelihood evaluations
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Q: Given samples $\{x\} \sim p(x)$, how can we get $p(x)$?

- Evaluate density at any point
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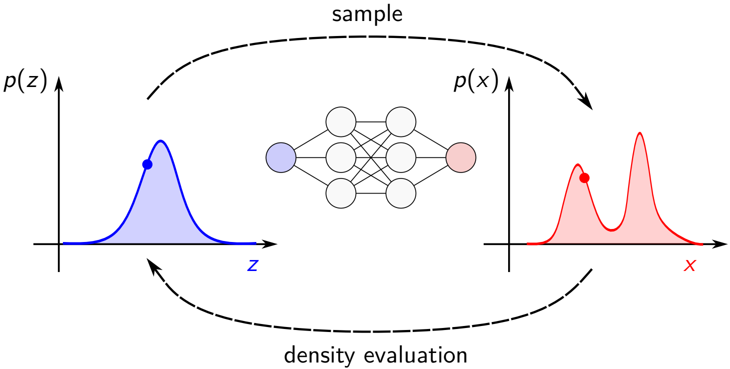
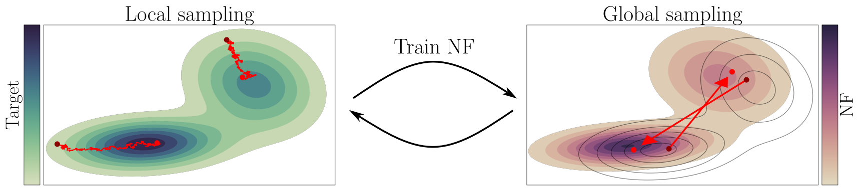
A: Normalizing flows: generative machine learning model, bijection between latent space (Gaussian) and data space



Contents

flowMC [8, 9]: normalizing flow-enhanced MCMC

1. Run gradient-based sampler (local sampler)
2. Train normalizing flow on MCMC chains
3. Propose samples from the normalizing flow (global sampler)
4. Repeat



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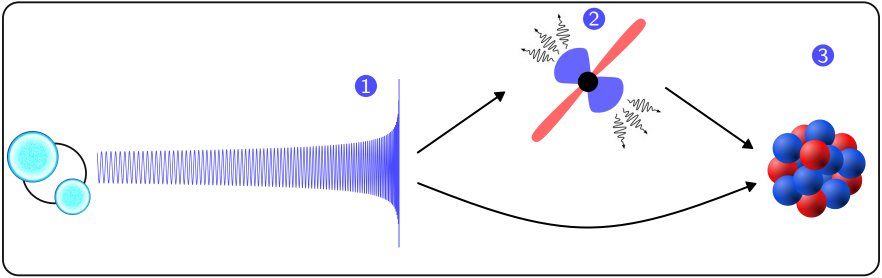
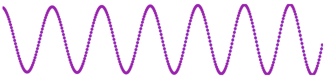
1. **Gravitational waves**
2. Electromagnetic counterparts
3. Nuclear equation of state



Gravitational waves: RIPPLE

- Waveforms on GPU: $\mathcal{O}(10^3)$ faster
- RIPPLE [10]: from LALSUITE to JAX



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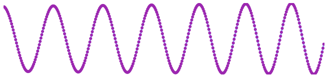

- Waveforms available in RIPPLE:
  - Binary black holes:
    - `IMRPhenomXAS`
    - `IMRPhenomD`
    - `IMRPhenomPv2`
  - Binary neutron stars:
    - `TaylorF2`
    - `IMRPhenomD_NRTidalv2`
    - `IMRPhenomPv_NRTidalv2` (by Nihar Gupte)
- Also see GWFAST [11] and SFTS [12]

Gravitational waves: Jim

Parameter estimation: Jim [13, 14]: ripple + flowMC

- Verified for binary neutron stars in current generation detectors [14]
- Matches bilby, passes *pp*-test

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Event	Waveform	Jim (1 GPU)	pBilby (480 cores)	RB-Bilby (24 cores)	ROQ-Bilby (24 cores)
GW170817	TF2	15.33 min	9.64 h	3.8 h	–
	NRTv2	25.59 min	10.99 h	4.11 h	1.65 h
GW190425	TF2	18.30 min	8.18 h	2.81 h	–
	NRTv2	21.20 min	4.91 h	2.42 h	0.97 h
Injection	TF2	24.76 min	–	–	–
	NRTv2	18.02 min	–	–	–

Gravitational waves: JIM

Parameter estimation: JIM [13, 14]: RIPPLE + FLOWMC

- Verified for binary neutron stars in current generation detectors [14]
- Matches BILBY, passes *pp*-test
- Runtime: from hours to minutes
- Up to $5 - 10\times$ more effective samples (normalizing flow)

	Effective sample size
JIM	4.1×10^4
pBILBY	6.5×10^3
RB-BILBY	5.8×10^3
ROQ-BILBY	7.4×10^3

Gravitational waves: JIM

Parameter estimation: JIM [13, 14]: RIPPLE + FLOWMC

- Verified for binary neutron stars in current generation detectors [14]
- Matches BILBY, passes *pp*-test
- Runtime: from hours to minutes
- Up to $5 - 10\times$ more effective samples (normalizing flow)
- More cost-effective/energy-efficient

		kWh	CO_2 [10^3 kg]	Trees
JIM		34	11	0.55
pBILBY		4127	1354	67.68
RB-BILBY		80	26	1.32
ROQ-BILBY	sampling	32	10	0.52
	precompute	27	9	0.44

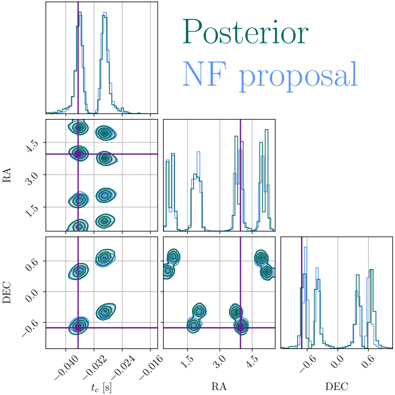
Einstein Telescope

Work in progress: showing proof-of-concepts!

Einstein Telescope

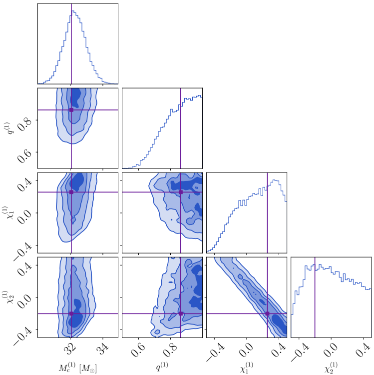
Work in progress: showing proof-of-concepts!

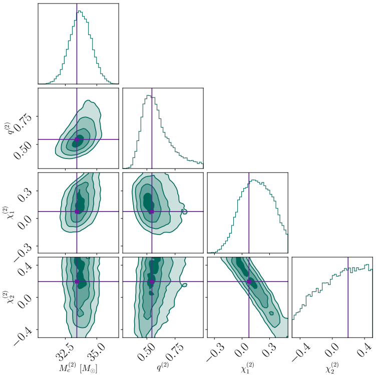
- ET posteriors are multimodal
- Normalizing flows help to jump between modes



Overlapping signals

- Assess scaling of Jim: BBH+BBH with LIGO-Virgo
  - 2 binary black hole mergers: 22 parameters
  - $M_c^{(1)} = 32 M_\odot$, $M_c^{(2)} = 33 M_\odot$, $\Delta t = 70$ ms
  - $\mathrm{SNR}^{(1)} = 25.76$, $\mathrm{SNR}^{(2)} = 25.24$
  - 1h28m on H100 GPU (vs several days on 16 CPUs [15])





Open call

- Recently: nested samplers in JAX for GW [16]
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- Bridge between LALSUITE and RIPPLE?

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Get in touch if you are interested! We need you!

JIM developers $\cap$ waveform developers $=$ **you**?

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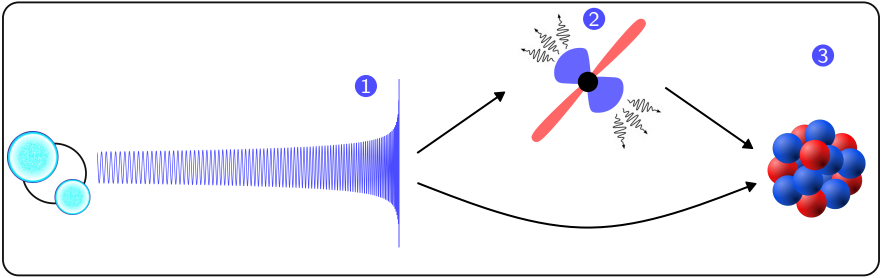
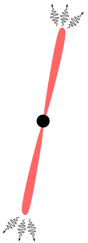
1. Gravitational waves
2. **Electromagnetic counterparts**
3. Nuclear equation of state

+ flowMC



Electromagnetic counterparts (Hauke Koehn)

- Predicting a GRB afterglow is slow
- Code libraries too large to 'jaxify': neural network emulators for inference: FIESTA [17]

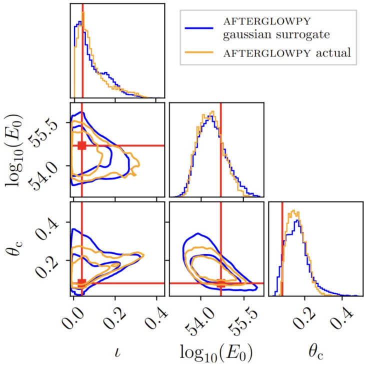


FIESTA

- 1m36s
- 1 H100 GPU

AFTERGLOWPY

- 4 hours
- 30 CPUs



Electromagnetic counterparts (Hauke Koehn)

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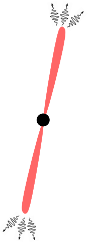
- Scales well for systematics 'nuisance parameters'



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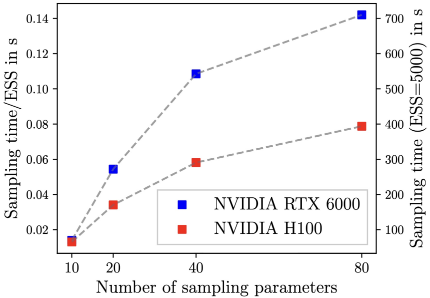

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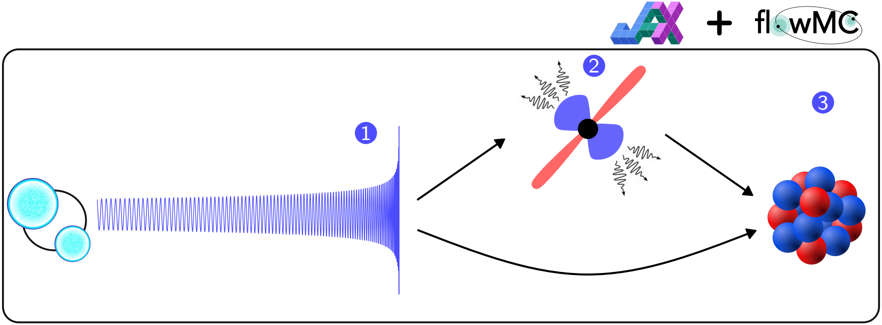
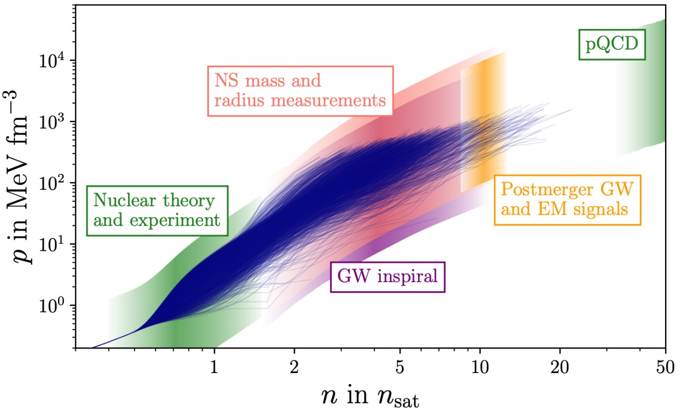


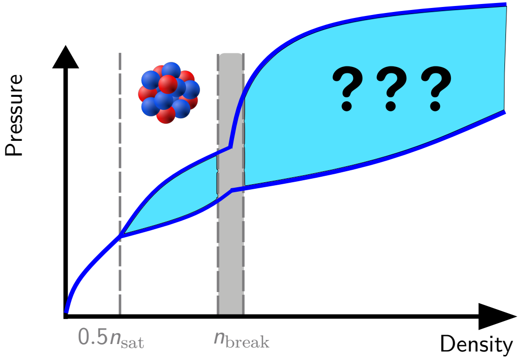
Equation of state inference – warmup

- How do we constrain the EOS from neutron star observations?
- Define parametrization and likelihood



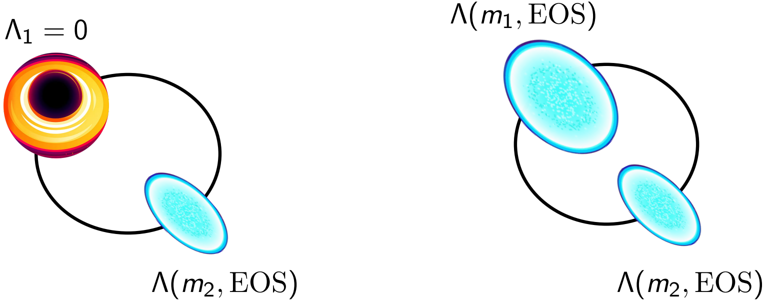
Equation of state inference – parametrization

- $n \leq \frac{1}{2} n_{\rm sat}$: fixed crust
- $\frac{1}{2} n_{\rm sat} \leq n \leq n_{\rm break}$: metamodel EOS, nuclear physics inspired
- $n \leq n_{\rm break}$: agnostic extension
- > 26 (!) parameters $\boldsymbol{\theta}_{\rm EOS}$



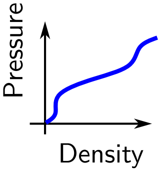
Tidal deformability

- Neutron stars are tidally deformed in a binary, quantified by tidal deformability Λ: affect phase of GWs
- Neutron stars: $\Lambda = \Lambda(m, \mathrm{EOS})$, black holes: $\Lambda = 0$
- GWs give us $p(m_1, m_2, \Lambda_1, \Lambda_2 | d)$ for EOS inference



Equation of state

- To predict neutron star properties, we solve the TOV equations: ordinary differential equations (ODEs)



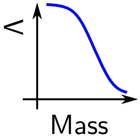
$\longrightarrow$

Solve TOV equations

$$\frac{\mathrm{d}p}{\mathrm{d}r} = -\frac{\varepsilon(r) m(r)}{r^2} \frac{\left[1 + \frac{p(r)}{\varepsilon(r)}\right]\left[1 + \frac{4\pi r^3 p(r)}{m(r)}\right]}{\left[1 - \frac{2m(r)}{r}\right]}$$

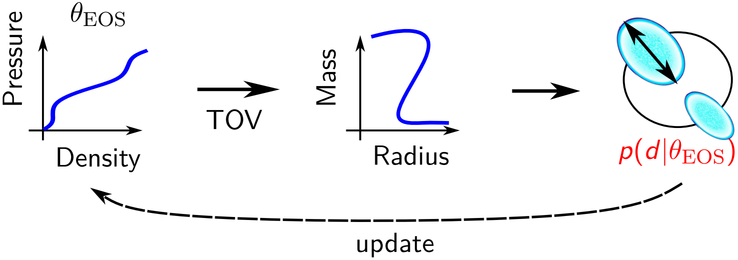
$$\frac{\mathrm{d}m}{\mathrm{d}r} = 4\pi r^2 \varepsilon(r)\,,$$

$\longrightarrow$



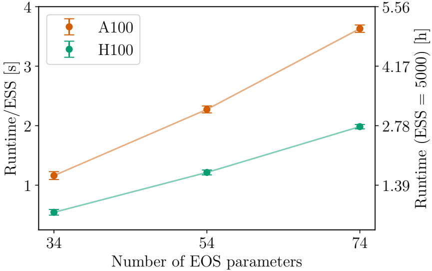
Equation of state

- To predict neutron star properties, we solve the TOV equations: ordinary differential equations (ODEs)
- Done for each sample $\theta_{\rm EOS}$: costly likelihood
- How to make this scalable without compromises?



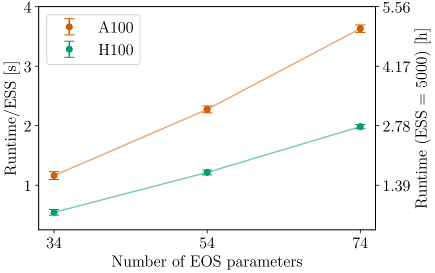
Jester

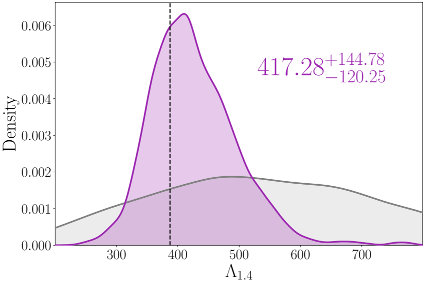
- Jester [18]: JAX-based TOV solver
  - 1000× faster, without compromises
  - Full inference in ∼hours



Jester

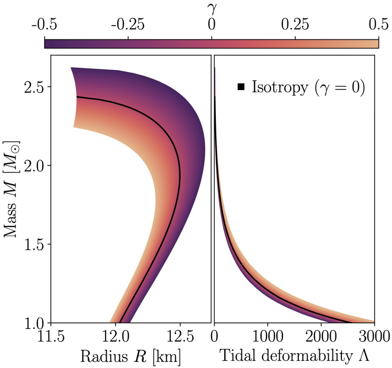
- Jester [18]: jax-based TOV solver
  - 1000× faster, without compromises
  - Full inference in ~hours
- Jim+Jester: from GWs to EOS in a few hours
  - Example: 20 binary neutron stars in O5
- Enable systematics studies in EOS inference





Anistropy in neutron stars (Peter T. H. Pang)

- Anistropic pressure: $\gamma \propto p - p_t$



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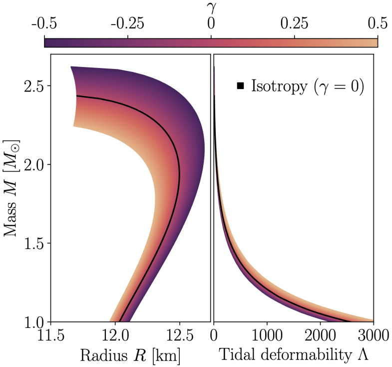
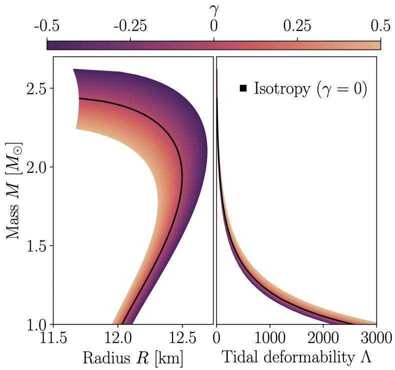
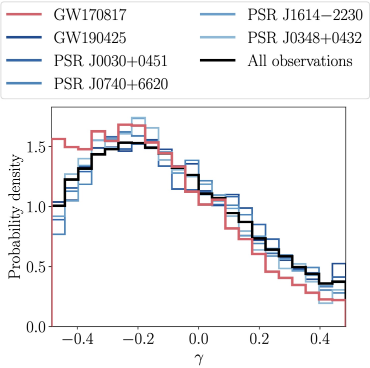
- Magnetic fields, dark matter clusters, superfluids...



Anistropy in neutron stars (Peter T. H. Pang)

- Anistropic pressure: $\gamma \propto p - p_t$
- Magnetic fields, dark matter clusters, superfluids...
- Preference for negative anisotropy, but weak evidence [19]





Auto-differentiable ODE solvers

- ODE solvers written in JAX are auto-differentiable
- Frame inference as optimization problem:
  - Gradient descent on loss function $\mathcal{L}(\boldsymbol{\theta}_{\rm EOS})$

Auto-differentiable ODE solvers

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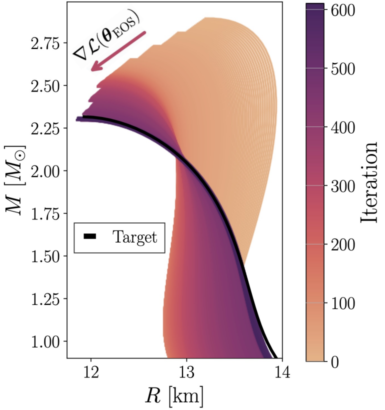
  - Gradient descent on loss function $\mathcal{L}(\boldsymbol{\theta}_{\text{EOS}})$

$$\mathcal{L}(\boldsymbol{\theta}_{\text{EOS}}) = \frac{1}{N} \sum_{i=1}^{N} \left| \frac{R_i(\boldsymbol{\theta}_{\text{EOS}}) - \hat{R}_i}{\hat{R}_i} \right|$$



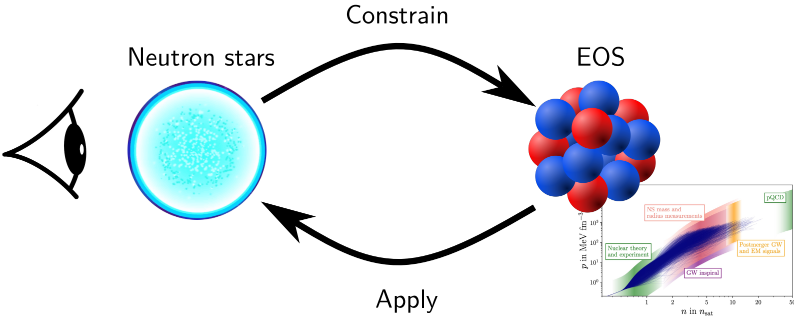
Contents

Neutron star data analysis loop

Data analysis of neutron stars forms a **loop**:

1. Constraining the EOS with neutron star observations
2. Applying EOS knowledge in neutron star data analysis (e.g., GW)

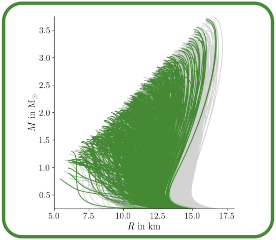
How can we efficiently perform Step 2?



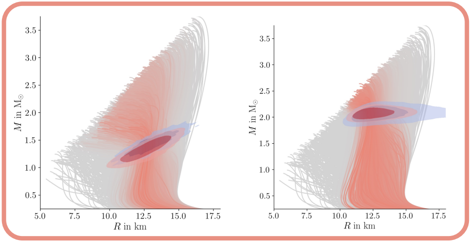
Case study

- Take constraints on EOS from:
  - **Radio timing**: EOS must support $2\,M_\odot$ neutron stars
  - **Chiral EFT** ($\chi_{\rm EFT}$): nuclear theory predictions (valid $< 2n_{\rm sat}$)
  - **NICER**: Mass-radius observations of neutron stars

Chiral EFT



NICER



- How can we use this information in GW analyses?

Equation of state-informed priors

- This should enter the prior on Λ_i

$$\mathcal{P}(\theta_{\mathrm{GW}}|d) \propto \mathcal{L}(d|\theta_{\mathrm{GW}})\pi(\theta_{\mathrm{GW}})$$

- By default, we choose **agnostic priors**: e.g. $\Lambda_{1,2} \sim \mathcal{U}(0, 5000)$

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- **But**, we have prior knowledge from the EOS:
  - Masses m_i determined by $M_{\rm max}$ (or population)
  - $\Lambda_i = \Lambda_i(m_i, \mathrm{EOS})$

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- **But**, we have prior knowledge from the EOS:
  - Masses m_i determined by $M_{\rm max}$ (or population)
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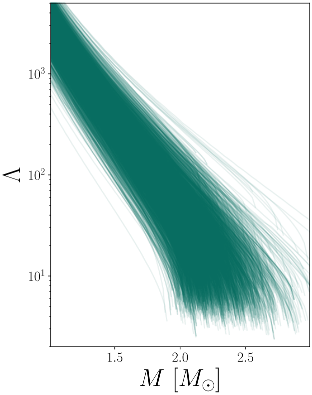
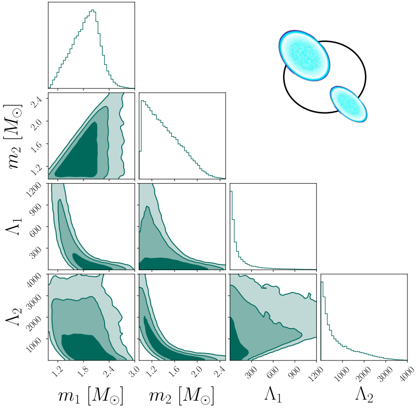
- **Equation of state-informed prior**: take EOS uncertainty into account

$$\pi(m_1, m_2, \Lambda_1, \Lambda_2) = \int {\rm d}\theta_{\rm EOS}\ \pi(m_1, m_2|\theta_{\rm EOS})\pi(\Lambda_1, \Lambda_2|m_1, m_2, \theta_{\rm EOS}) \times \pi(\theta_{\rm EOS})$$

Equation of state-informed priors

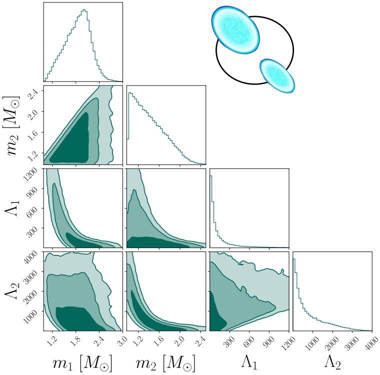
- Example: EOSs with $M_{\max} > 2.0 M_\odot$
- Sample to produce $\pi(m_1, m_2, \Lambda_1, \Lambda_2)$

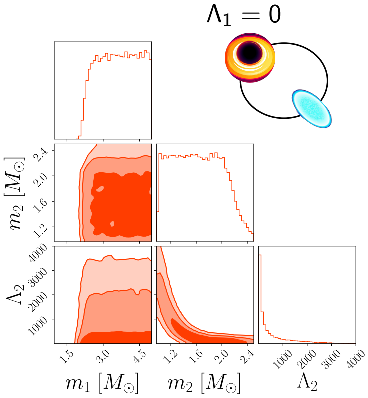




Source classification

- Similar to the **binary neutron star (BNS)** prior, we can also construct a **neutron star-black hole (NSBH)** prior
  - BH mass in $[M_{\max}(\mathrm{EOS}), 5\,\mathrm{M}_\odot]$
- Classify events with Bayesian model selection





Neural priors

- Masses can also be informed by populations
  - Uniform (agnostic)
  - Gaussian
  - Double Gaussian
- (BNS/NSBH) $\times$ (3 populations) $\times$ (3 EOS constraints) $=$ 18 priors
- Emulate with normalizing flow: **neural priors**

Neural priors

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  - Uniform (agnostic)
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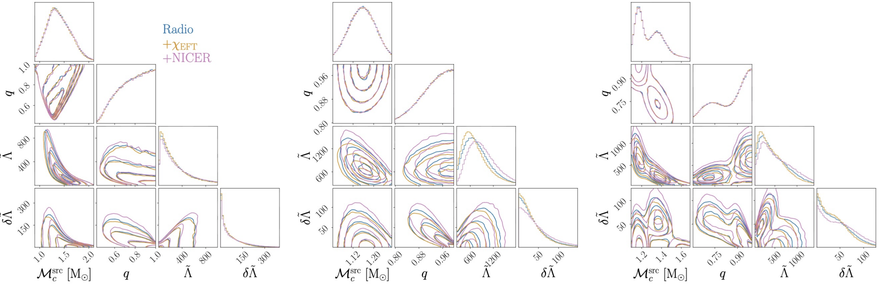
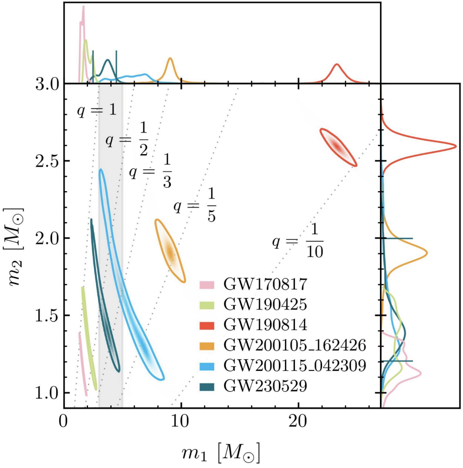


Application

- Implemented in BILBY
- Consider three "low-mass" GWs

- GW170817
- GW190425
- GW230529



GW170817 – classification

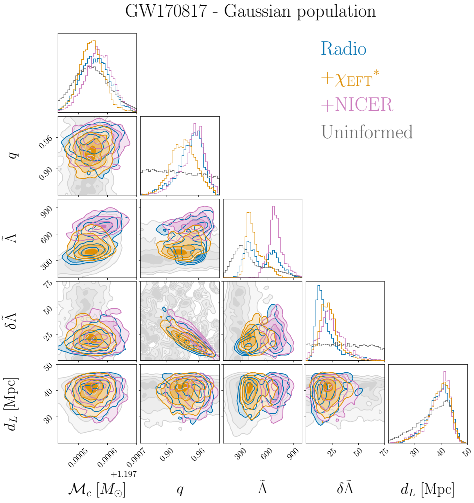
Showing $\log_{10}$ Bayes factors: negative = less preferred

- Strongly prefer BNS over NSBH
- Gaussian population, EOS inconclusive

Source	Population	EOS Constraints	GW170817
BNS	Uniform	Radio	-0.76
		$+\chi_{\mathrm{EFT}}$	-0.52
		+NICER	-0.86
	Gaussian	Radio	-0.14
		$+\chi_{\mathrm{EFT}}$	**ref.**
		+NICER	-0.05
	Double Gaussian	Radio	-0.43
		$+\chi_{\mathrm{EFT}}$	-0.26
		+NICER	-0.73
NSBH	Uniform	Radio	-224.11
		$+\chi_{\mathrm{EFT}}$	-224.11
		+NICER	-224.12
	Gaussian	Radio	-224.13
		$+\chi_{\mathrm{EFT}}$	-224.13
		+NICER	-224.13
	Double Gaussian	Radio	-224.12
		$+\chi_{\mathrm{EFT}}$	-224.13
		+NICER	-224.12

GW170817 – parameter constraints

- More equal mass ratio $q \geq 0.9$
- $\tilde{\Lambda}$ bimodal, resolved by extra EOS information



GW190425 – classification

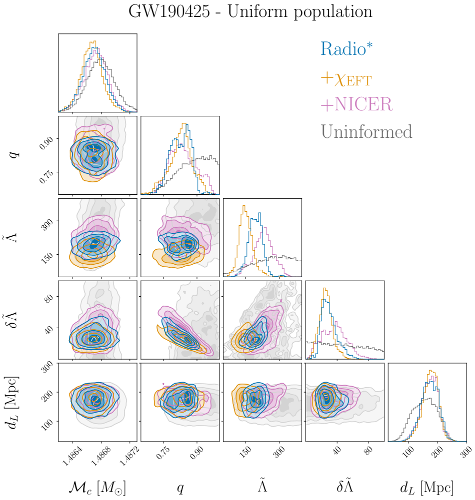
Showing $\log_{10}$ Bayes factors: negative = less preferred

- Prefer BNS over NSBH, but less conclusive
- Most consistent with uniform population

Source	Population	EOS Constraints	GW190425
BNS	Uniform	Radio	**ref.**
		$+\chi_{\mathrm{EFT}}$	-0.09
		+NICER	-0.11
	Gaussian	Radio	-8.51
		$+\chi_{\mathrm{EFT}}$	-6.57
		+NICER	-4.42
	Double Gaussian	Radio	-0.76
		$+\chi_{\mathrm{EFT}}$	-0.56
		+NICER	-0.89
NSBH	Uniform	Radio	-1.10
		$+\chi_{\mathrm{EFT}}$	-1.10
		+NICER	-1.19
	Gaussian	Radio	-0.82
		$+\chi_{\mathrm{EFT}}$	-1.01
		+NICER	-0.98
	Double Gaussian	Radio	-1.65
		$+\chi_{\mathrm{EFT}}$	-3.40
		+NICER	-2.12

GW190425 – parameter constraints

- Less equal masses ($q \leq 0.9$)
- Higher distances



GW230529 – classification

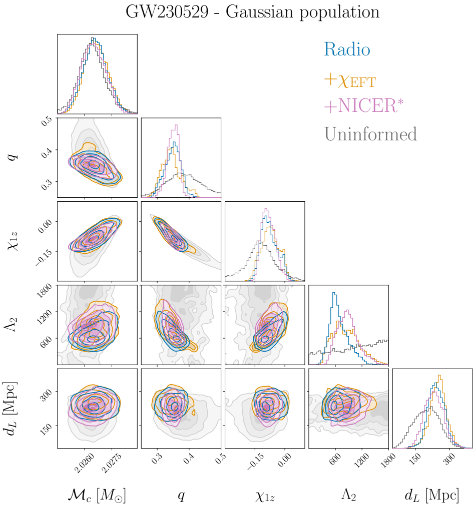
Showing $\log_{10}$ Bayes factors: negative = less preferred

- Decisive evidence for NSBH over BNS
- Weak evidence for population or EOS (low SNR)

Source	**Population**	**EOS Constraints**	**GW230529**
BNS	Uniform	Radio	-13.23
		$+\chi_{\mathrm{EFT}}$	-13.31
		+NICER	-13.23
	Gaussian	Radio	-18.90
		$+\chi_{\mathrm{EFT}}$	-18.86
		+NICER	-18.88
	Double Gaussian	Radio	-13.84
		$+\chi_{\mathrm{EFT}}$	-13.79
		+NICER	-13.98
NSBH	Uniform	Radio	-0.16
		$+\chi_{\mathrm{EFT}}$	-0.28
		+NICER	-0.42
	Gaussian	Radio	-0.28
		$+\chi_{\mathrm{EFT}}$	-0.28
		+NICER	**ref.**
	Double Gaussian	Radio	-0.18
		$+\chi_{\mathrm{EFT}}$	-0.08
		+NICER	-0.06

GW230529 – parameter constraints

- Mass ratio more constrained $\rightarrow \chi_{1z}$ more constrained
- Higher distances



Contents

Conclusion

- Progress on scalable Bayesian inference, with minimal compromises
- Accelerate likelihood-based inference with
  - JAX: GPU for faster likelihoods, automatic differentiation
  - Normalizing flows to aid in inference (sampling, priors)
- GWs: verified for LVK, work in progress for ET
  - Waveform experts more than welcome!
- Kilonova/GRB: emulators for fast inference
- EOS: scalable inference, open up systematics studies

Let's talk!

Thanks for listening!

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Evidence calculation: HARMONIC I

Evidence Z can be computed from posterior samples with HARMONIC [22] with the harmonic mean estimator

$$\begin{aligned}\rho \equiv \mathbb{E}_{P(\theta|d)}\left[\frac{1}{L(\theta)}\right] &= \int \mathrm{d}\theta \frac{1}{\mathcal{L}(\theta)} P(\theta|d) \\ &= \int \mathrm{d}\theta \frac{1}{\mathcal{L}(\theta)} \frac{\mathcal{L}(\theta)\pi(\theta)}{Z} = \frac{1}{Z}\end{aligned}$$

Therefore, estimate ρ with posterior samples:

$$\hat{\rho} = \frac{1}{N}\sum_{i=1}^{N} \frac{1}{\mathcal{L}(\theta)}, \quad \theta_i \sim P(\theta|d)$$

Evidence calculation: HARMONIC II

Can be interpreted as importance sampling

$$\rho = \int \mathrm{d}\theta \frac{1}{Z} \frac{\pi(\theta)}{P(\theta|d)} P(\theta|d)\,,$$

but with target = prior and sampling density = posterior. Therefore, importance sampling is inefficient – how to solve?
New proposal:

$$\begin{aligned}
\rho &= \mathbb{E}_{P(\theta|d)} \left[\frac{\varphi(\theta)}{\mathcal{L}(\theta)\pi(\theta)} \right] \\
&= \int \mathrm{d}\theta \, \frac{\varphi(\theta)}{\mathcal{L}(\theta)\pi(\theta)} \, P(\theta|d) \\
&= \int \mathrm{d}\theta \, \frac{\varphi(\theta)}{\mathcal{L}(\theta)\pi(\theta)} \, \frac{\mathcal{L}(\theta)\pi(\theta)}{Z} = \frac{1}{Z}
\end{aligned}$$

Evidence calculation: HARMONIC III

Use the following estimator:

$$\hat{\rho} = \frac{1}{N} \sum_{i=1}^{N} \frac{\varphi(\theta_i)}{\mathcal{L}(\theta_i)\pi(\theta_i)}, \quad \theta_i \sim P(\theta|d)$$

Replace the target distribution π with φ: only requirement is that it is normalized

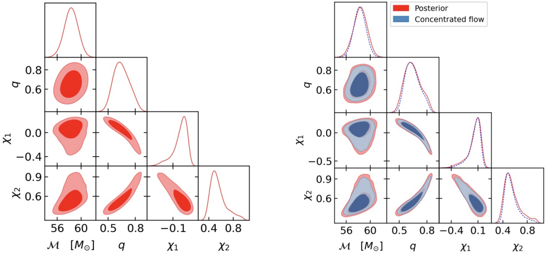
In practice, this can be achieved with a normalizing flow [23].

This has been verified to give accurate evidences (similar values as nested sampling) when GW posteriors are used [24].

HARMONIC with JIM [24]

Table 1: Total wall times to compute the evidence estimates for the examples discussed in the main text. We run BILBY on 16 CPU cores and JIM + `harmonic` on 1 GPU.

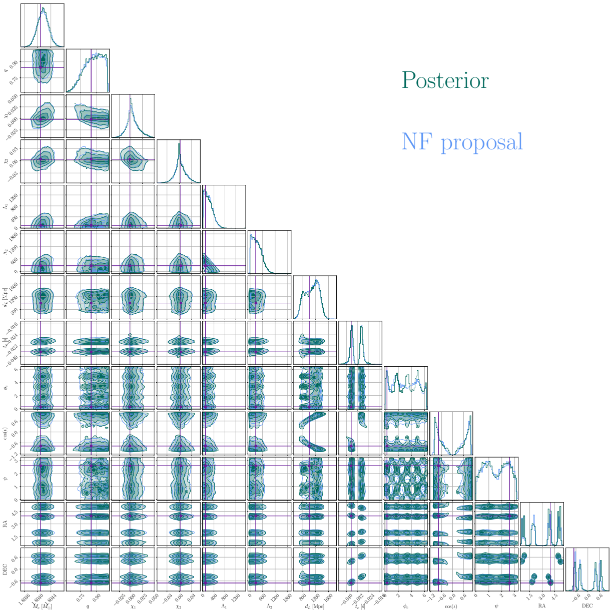
Example	Method	$\log(z)$	Sampling time	Evidence estimation time
4D	BILBY	390.33 ± 0.11	31.3 min	–
	JIM + `harmonic`	$390.360^{+0.006}_{-0.006}$	3.4 min	1.9 min
11D	BILBY	378.29 ± 0.15	3.5 h	–
	JIM + `harmonic`	$378.420^{+0.09}_{-0.08}$	11.8 min	2.4 min



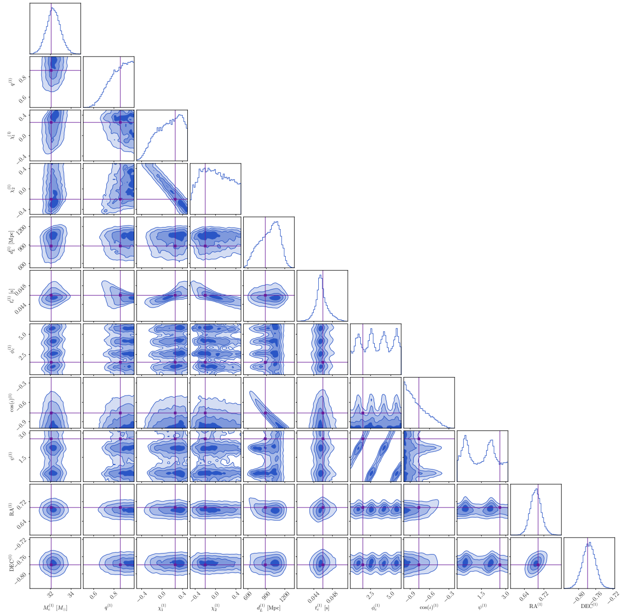
(a) BILBY (b) JIM + `harmonic`

Figure 1: Corner plots for the 4-dimensional posterior samples from (a) BILBY and (b) JIM used for inference (solid red) alongside the concentrated flow at $T = 0.8$ used in the learned harmonic mean (dashed blue).

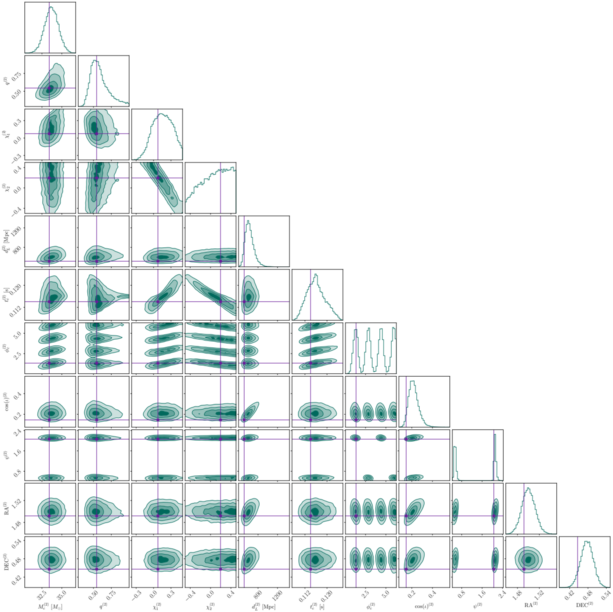
BNS in ET-Δ example: all parameters



Overlapping signals: all parameters signal A

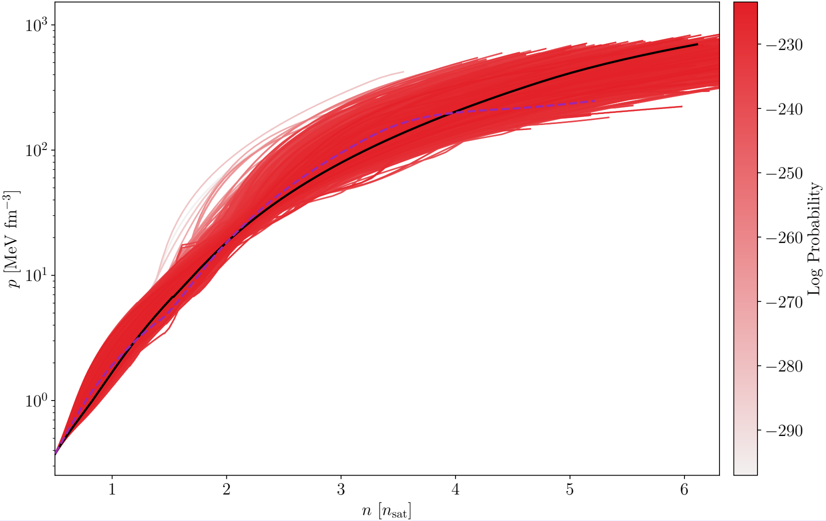


Overlapping signals: all parameters signal B



Equation of state O5 projection with 20 BNS: EOS

- **Purple**: target
- **Red**: posterior EOS samples (**black**: maximum log posterior)



Equation of state O5 projection with 20 BNS: NS