

# Scalable Bayesian inference for 3G: Leveraging hardware acceleration and normalizing flows

Thibeau Wouters



Utrecht  
University

Nikhef



# Contents

① Introduction

② Methods

③ Applications

④ Conclusion

# Parameter estimation in 3G

Parameter estimation is done with **Bayesian inference**:

$$p(\theta|d) \propto p(d|\theta)p(\theta)$$

posterior  $\propto$  likelihood  $\times$  prior

- Sample the posterior: MCMC or nested sampling
- $\mathcal{O}(10^6)$  likelihood evaluations: computational bottleneck

# Parameter estimation in 3G

Parameter estimation is done with **Bayesian inference**:

$$p(\theta|d) \propto p(d|\theta)p(\theta)$$

posterior  $\propto$  likelihood  $\times$  prior

- Sample the posterior: MCMC or nested sampling
- $\mathcal{O}(10^6)$  likelihood evaluations: computational bottleneck

What about **3G** detectors?

- ET will observe  $\mathcal{O}(10^5)$  events per year
- Signals will be longer and have higher SNRs

# Parameter estimation in 3G

Parameter estimation is done with **Bayesian inference**:

$$p(\theta|d) \propto p(d|\theta)p(\theta)$$

posterior  $\propto$  likelihood  $\times$  prior

- Sample the posterior: MCMC or nested sampling
- $\mathcal{O}(10^6)$  likelihood evaluations: computational bottleneck

What about **3G** detectors?

- ET will observe  $\mathcal{O}(10^5)$  events per year
- Signals will be longer and have higher SNRs

**Premise:** Current software will not scale to 3G [1]

# Contents

① Introduction

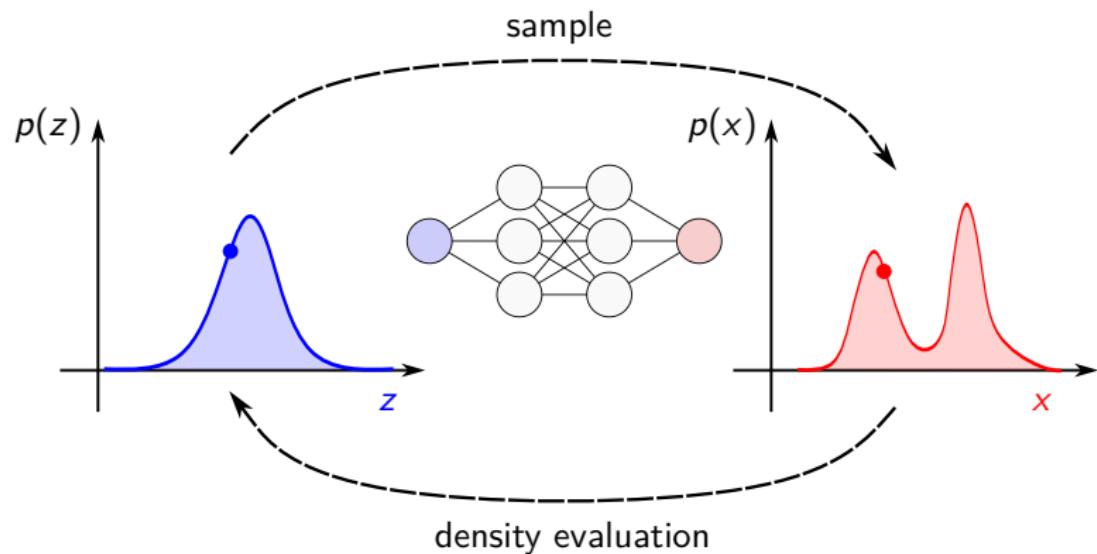
② Methods

③ Applications

④ Conclusion

# Normalizing flows (NFs)

- Trainable bijection between **latent** and **data** spaces
- Sample and evaluate complicated densities



# JAX & FLOWMC

Accelerate Python with JAX :

- Use GPU accelerators
- Automatic differentiation → gradient-based samplers



# JAX & FLOWMC

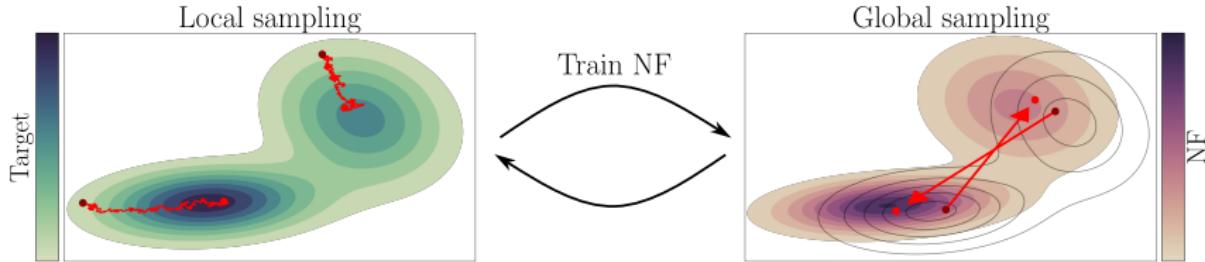
Accelerate Python with JAX :

- Use GPU accelerators
- Automatic differentiation → gradient-based samplers



FLOWMC [2, 3]:

- MCMC + normalizing flows in JAX
- Training data: MCMC chains → **no pre-training**



# Contents

① Introduction

② Methods

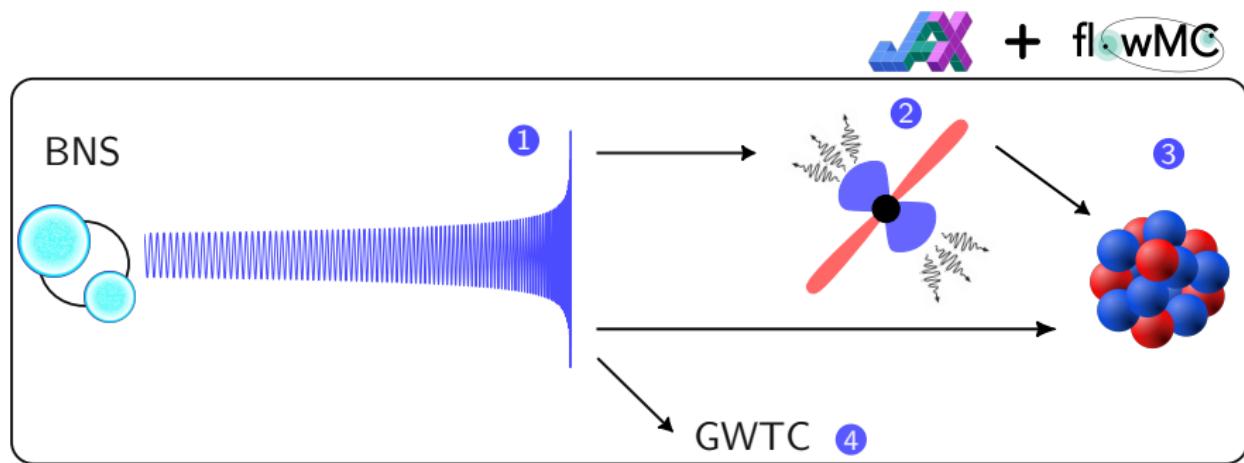
③ Applications

④ Conclusion

# Overview

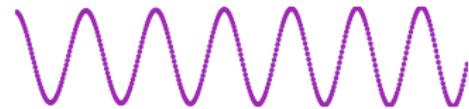
Analyzing a multi-messenger **binary neutron star** (BNS) signal:

- ① Gravitational waves
- ② Electromagnetic counterparts
- ③ Nuclear equation of state
- ④ Gravitational wave transient catalogue



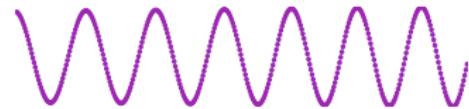
# Gravitational waves

- Waveforms on GPU:  $\mathcal{O}(10^3)$  faster
- From LALSUITE to JAX: RIPPLE  [4]



# Gravitational waves

- Waveforms on GPU:  $\mathcal{O}(10^3)$  faster
  - From LALSUITE to JAX: RIPPLE  [4]
- 



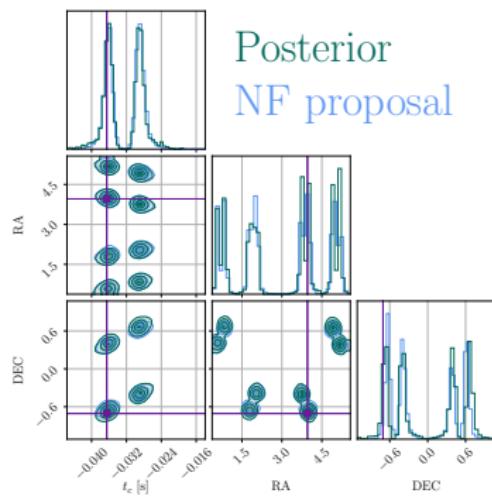
- Parameter estimation: JIM  [5, 6]
- ✓ BNS in LVK analyzed in  $\sim 15$  min

# Gravitational waves

- Waveforms on GPU:  $\mathcal{O}(10^3)$  faster
- From LALSUITE to JAX: RIPPLE  [4]



- Parameter estimation: JIM  [5, 6]
- ✓ BNS in LVK analyzed in  $\sim 15$  min
- Ongoing work for ET – example:
  - BNS,  $f_{\min} = 20$  Hz, SNR = 21
  - ET- $\Delta$
  - IMRPhenomD\_NRTidalv2
  - 30 mins on H100 GPU



# Overlapping signals

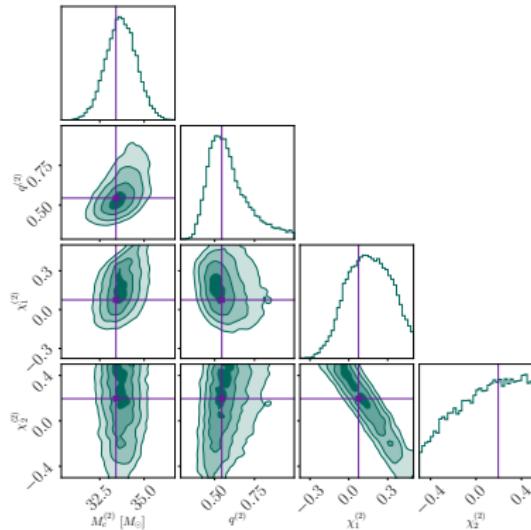
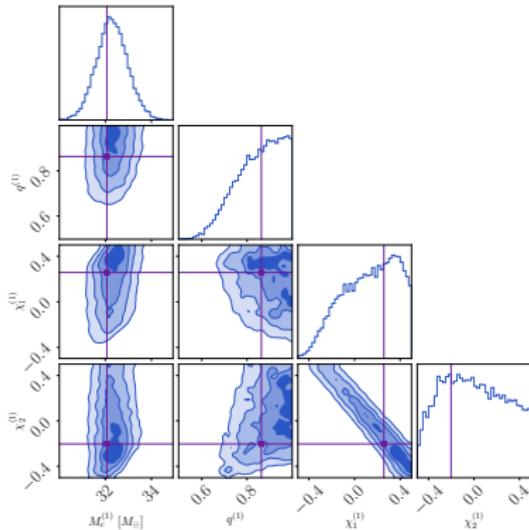
(Luca Negri, Justin Janquart, James Alvey, Uddipta Bhardwaj)

- Assess scaling of JIM: BBH+BBH in O5 with LVK
  - IMRPhenomD → 22 parameters (joint parameter estimation)
  - $M_c^{(1)} = 32M_\odot$ ,  $M_c^{(2)} = 33M_\odot$ ,  $\Delta t = 70$  ms
  - $\text{SNR}^{(1)} = 25.76$ ,  $\text{SNR}^{(2)} = 25.24$

# Overlapping signals

(Luca Negri, Justin Januart, James Alvey, Uddipta Bhardwaj)

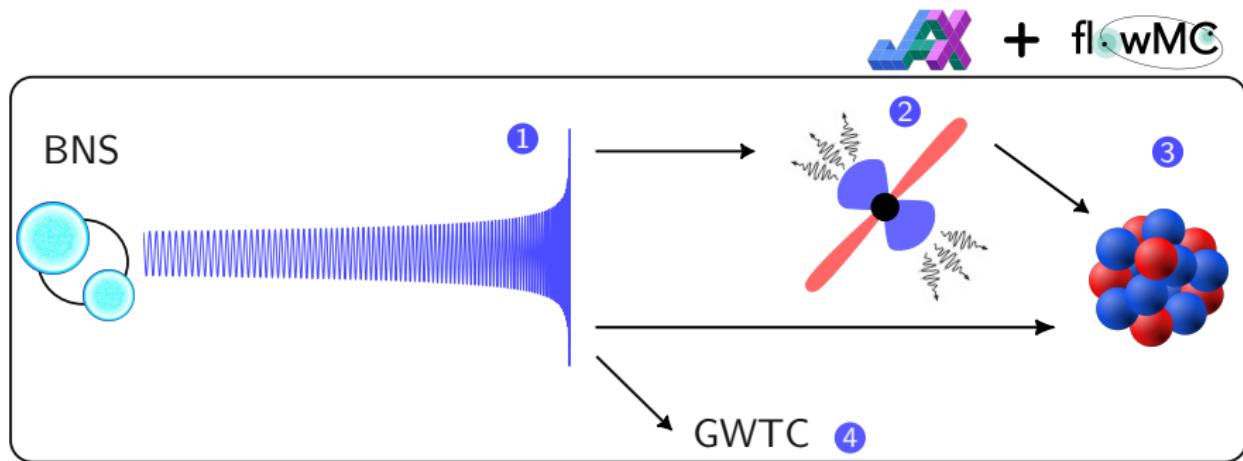
- Assess scaling of JIM: BBH+BBH in O5 with LVK
  - IMRPhenomD → 22 parameters (joint parameter estimation)
  - $M_c^{(1)} = 32M_\odot$ ,  $M_c^{(2)} = 33M_\odot$ ,  $\Delta t = 70$  ms
  - $\text{SNR}^{(1)} = 25.76$ ,  $\text{SNR}^{(2)} = 25.24$
  - **1h28m** on H100 (vs 23 days on 16 CPUs [7])



# Overview

Analyzing a multi-messenger **binary neutron star** (BNS) signal:

- ① Gravitational waves
- ② Electromagnetic counterparts
- ③ Nuclear equation of state
- ④ Gravitational wave transient catalogue

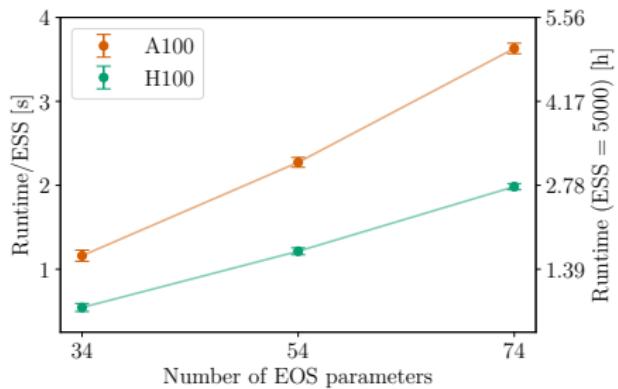


## Equation of state inference (Peter T.H. Pang)

- Likelihood involves solving TOV equations (EOS → NS): slow!

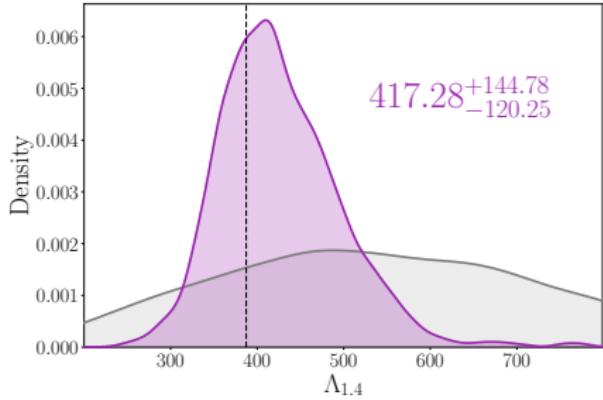
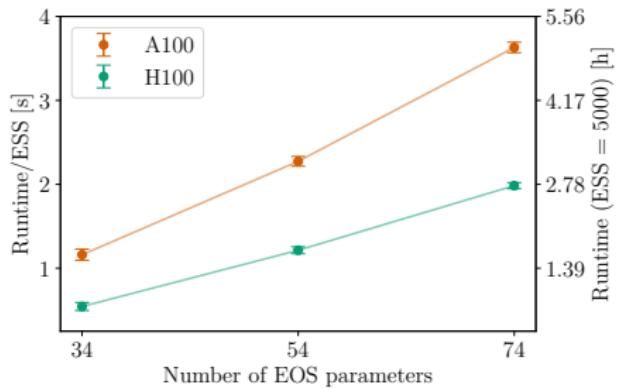
# Equation of state inference (Peter T.H. Pang)

- Likelihood involves solving TOV equations (EOS → NS): slow!
- JESTER  [8]: JAX-based TOV solver
  - Full inference in  $\sim$ hours
  - No need for machine learning surrogates



# Equation of state inference (Peter T.H. Pang)

- Likelihood involves solving TOV equations (EOS → NS): slow!
- JESTER  [8]: JAX-based TOV solver
  - Full inference in  $\sim$ hours
  - No need for machine learning surrogates
- End-to-end analysis: constrain EOS from 20 BNS in O5



# Contents

① Introduction

② Methods

③ Applications

④ Conclusion

# Conclusion

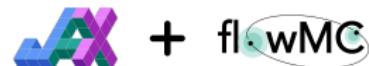
- Progress on scalable Bayesian inference software for 3G, with minimal amount of pre-training
- Hybrid acceleration: GPUs + normalizing flow proposals
  - JAX/GPU: faster likelihoods
  - FLOWMC: sampling converges faster
- Goal: joint multimessenger analyses in  $\sim$ hours
- Weakness: need waveform models in JAX!

Let's talk!

# Thank you for your attention!

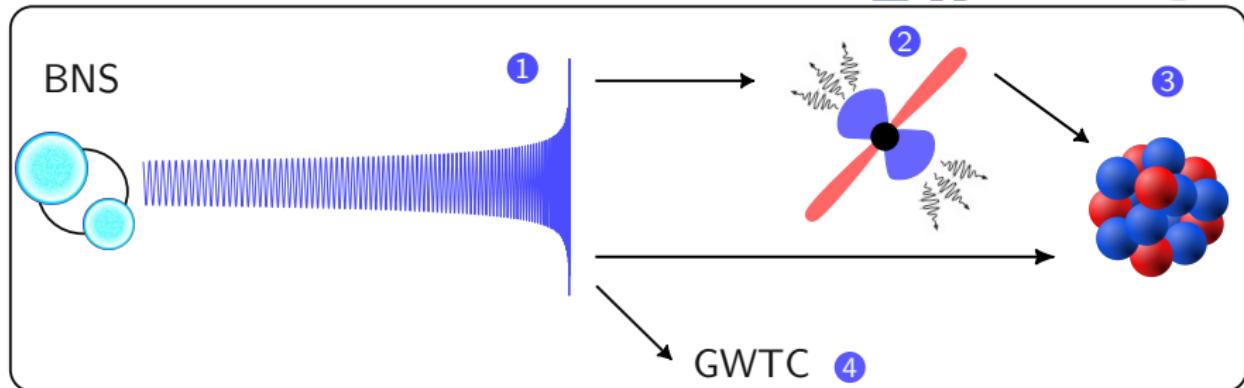
Software written in JAX:

- FLOWMC [2, 3]
- JIM [5, 6] ① ② ④
- FIESTA ②
- JESTER [8] ③
- HARMONIC [9–11]



+

flowMC



# References I

- [1] Qian Hu and John Veitch. "Costs of Bayesian Parameter Estimation in Third-Generation Gravitational Wave Detectors: a Review of Acceleration Methods". In: (Dec. 2024). arXiv: [2412.02651 \[gr-qc\]](https://arxiv.org/abs/2412.02651).
- [2] Marylou Gabrié, Grant M. Rotskoff, and Eric Vanden-Eijnden. "Adaptive Monte Carlo augmented with normalizing flows". In: *Proc. Nat. Acad. Sci.* 119.10 (2022), e2109420119. DOI: [10.1073/pnas.2109420119](https://doi.org/10.1073/pnas.2109420119). arXiv: [2105.12603 \[physics.data-an\]](https://arxiv.org/abs/2105.12603).
- [3] Kaze W. k. Wong, Marylou Gabrié, and Daniel Foreman-Mackey. "flowMC: Normalizing flow enhanced sampling package for probabilistic inference in JAX". In: *J. Open Source Softw.* 8.83 (2023), p. 5021. DOI: [10.21105/joss.05021](https://doi.org/10.21105/joss.05021). arXiv: [2211.06397 \[astro-ph.IM\]](https://arxiv.org/abs/2211.06397).
- [4] Thomas D. P. Edwards et al. "Differentiable and hardware-accelerated waveforms for gravitational wave data analysis". In: *Phys. Rev. D* 110.6 (2024), p. 064028. DOI: [10.1103/PhysRevD.110.064028](https://doi.org/10.1103/PhysRevD.110.064028). arXiv: [2302.05329 \[astro-ph.IM\]](https://arxiv.org/abs/2302.05329).
- [5] Kaze W. K. Wong, Maximiliano Isi, and Thomas D. P. Edwards. "Fast Gravitational-wave Parameter Estimation without Compromises". In: *Astrophys. J.* 958.2 (2023), p. 129. DOI: [10.3847/1538-4357/acf5cd](https://doi.org/10.3847/1538-4357/acf5cd). arXiv: [2302.05333 \[astro-ph.IM\]](https://arxiv.org/abs/2302.05333).
- [6] Thibreau Wouters et al. "Robust parameter estimation within minutes on gravitational wave signals from binary neutron star inspirals". In: *Phys. Rev. D* 110.8 (2024), p. 083033. DOI: [10.1103/PhysRevD.110.083033](https://doi.org/10.1103/PhysRevD.110.083033). arXiv: [2404.11397 \[astro-ph.IM\]](https://arxiv.org/abs/2404.11397).

## References II

- [7] Justin Janquart et al. "Analyses of overlapping gravitational wave signals using hierarchical subtraction and joint parameter estimation". In: *Mon. Not. Roy. Astron. Soc.* 523.2 (2023), pp. 1699–1710. DOI: [10.1093/mnras/stad1542](https://doi.org/10.1093/mnras/stad1542). arXiv: [2211.01304](https://arxiv.org/abs/2211.01304) [gr-qc].
- [8] Thibeau Wouters et al. "Leveraging differentiable programming in the inverse problem of neutron stars". In: (Apr. 2025). arXiv: [2504.15893](https://arxiv.org/abs/2504.15893) [astro-ph.HE].
- [9] Jason D. McEwen et al. *Machine learning assisted Bayesian model comparison: learnt harmonic mean estimator*. 2023. arXiv: [2111.12720](https://arxiv.org/abs/2111.12720) [stat.ME]. URL: <https://arxiv.org/abs/2111.12720>.
- [10] Alicja Polanska et al. *Learned harmonic mean estimation of the marginal likelihood with normalizing flows*. 2024. arXiv: [2307.00048](https://arxiv.org/abs/2307.00048) [stat.ME]. URL: <https://arxiv.org/abs/2307.00048>.
- [11] Alicja Polanska et al. "Accelerated Bayesian parameter estimation and model selection for gravitational waves with normalizing flows". In: *38th conference on Neural Information Processing Systems*. Oct. 2024. arXiv: [2410.21076](https://arxiv.org/abs/2410.21076) [astro-ph.IM].
- [12] Kurzgesagt. *Figures taken from "Neutron Stars - The Most Extreme Things that are not Black Holes"*. Accessed on May 14, 2025. 2019. URL: <https://www.youtube.com/watch?v=udFxKZRyQt4>.

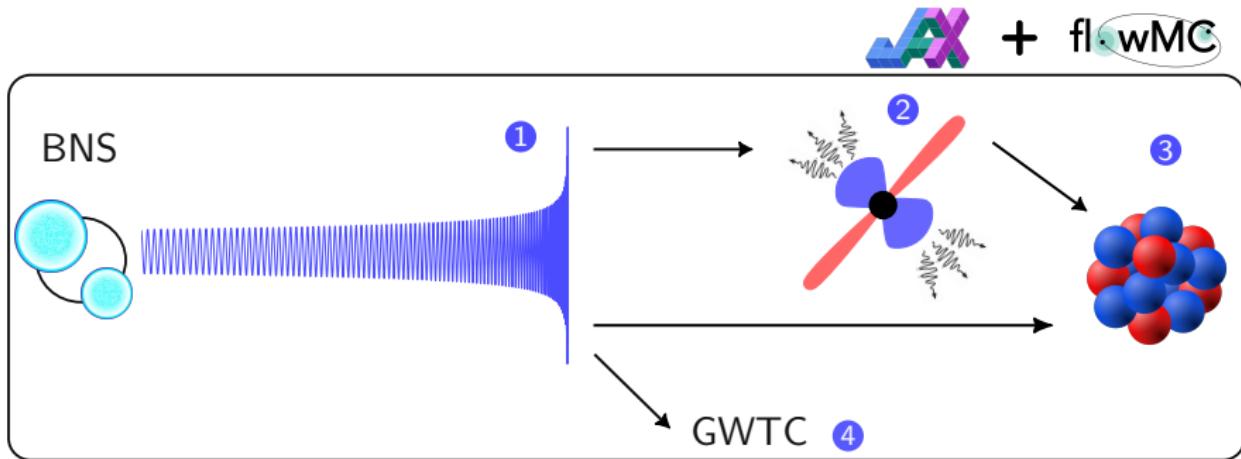
## References III

- [13] Hergé. *Cover figure created with ChatGPT using this input figure from the comic Destination Moon.* Accessed on May 14, 2025. 2019. URL: <https://www.youtube.com/watch?v=udFxKZRyQt4>.
- [14] Geoffrey Ryan et al. "Gamma-Ray Burst Afterglows in the Multimessenger Era: Numerical Models and Closure Relations". In: *Astrophys. J.* 896.2 (2020), p. 166. DOI: 10.3847/1538-4357/ab93cf. arXiv: 1909.11691 [astro-ph.HE].

# Overview

Analyzing a multi-messenger **binary neutron star** (BNS) signal:

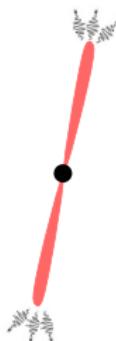
- ① Gravitational waves
- ② Electromagnetic counterparts
- ③ Nuclear equation of state
- ④ Gravitational wave transient catalogue



- BNS mergers lead to kilonovae, **gamma-ray bursts (afterglows)**
- Numerical models are expensive (e.g. AFTERGLOWPY [[14](#)])

# Electromagnetic counterparts (Hauke Koehn, Tim Dietrich)

- BNS mergers lead to kilonovae, **gamma-ray bursts (afterglows)**
- Numerical models are expensive (e.g. AFTERGLOWPY [14])
- Neural network surrogates for inference: FIESTA 

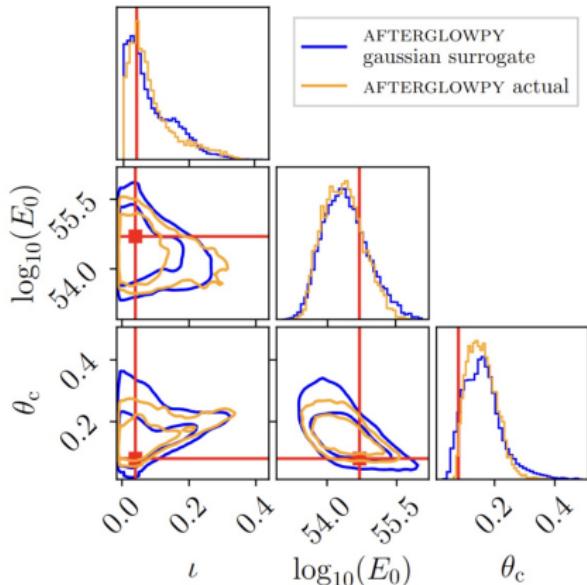


## FIESTA

- 1m36s
- 1 H100 GPU

## AFTERGLOWPY

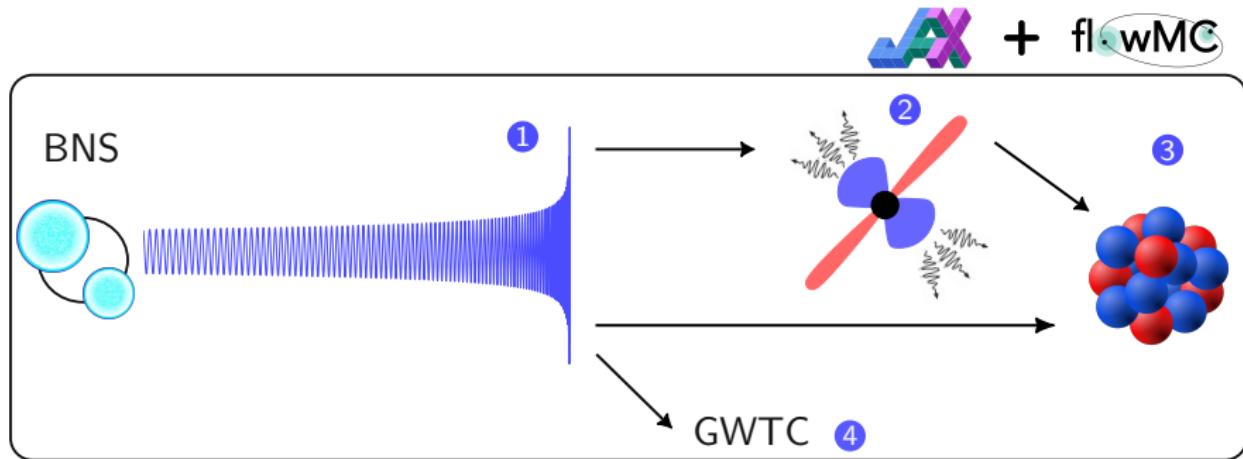
- 4 hours
- 30 CPUs



# Overview

Analyzing a multi-messenger **binary neutron star** (BNS) signal:

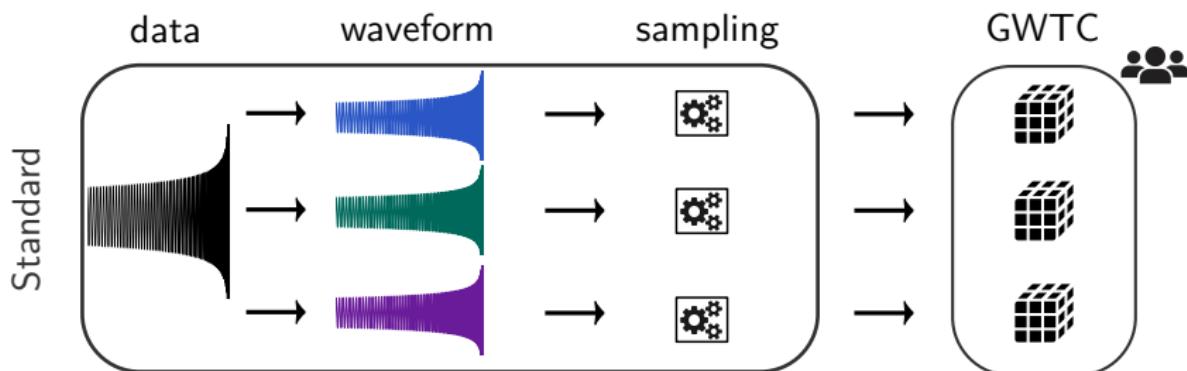
- ① Gravitational waves
- ② Electromagnetic counterparts
- ③ Nuclear equation of state
- ④ **Gravitational wave transient catalogue**



# Constructing GWTCs (Thomas Ng, Kaze Wong)

GWTCs do not scale well in **memory**:

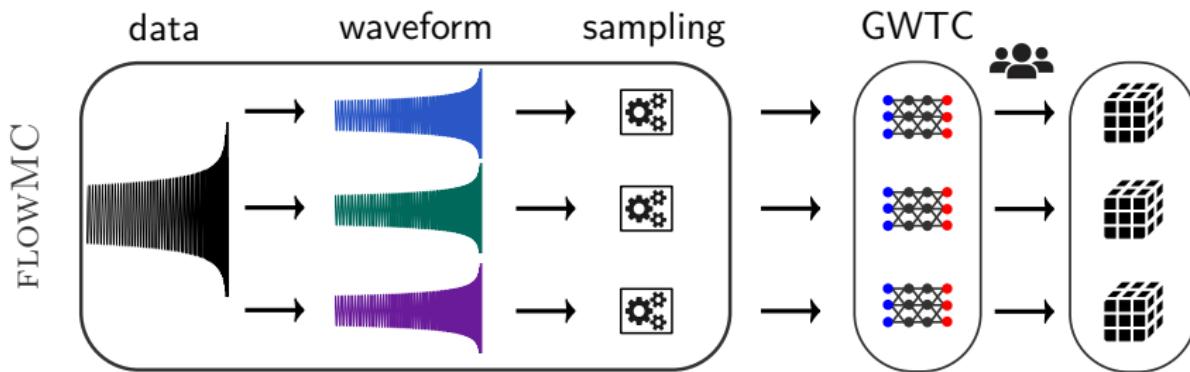
- GWTC stores several samples (different waveforms)
- Standard: fixed sample size,  $\sim 100$  MB



# Constructing GWTCs (Thomas Ng, Kaze Wong)

GWTCs do not scale well in **memory**:

- GWTC stores several samples (different waveforms)
- Standard: fixed sample size,  $\sim 100$  MB
- FLOWMC: generate samples from normalizing flows,  $\sim 10$  MB



## Evidence calculation: HARMONIC I

Evidence  $Z$  can be computed from posterior samples with HARMONIC [9] with the **harmonic mean estimator**

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

Therefore, estimate  $\rho$  with posterior samples:

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

## Evidence calculation: HARMONIC II

Can be interpreted as importance sampling

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

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

New proposal:

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

## 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  $\pi$  with  $\varphi$ : only requirement is that it is normalized

In practice, this can be achieved with a normalizing flow [10].

This has been verified to give accurate evidences (similar values as nested sampling) when GW posteriors are used [11].

# HARMONIC with JIM

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	$390.33 \pm 0.11$	31.3 min	—
	JIM + harmonic	$390.360^{+0.006}_{-0.006}$	3.4 min	1.9 min
11D	BILBY	$378.29 \pm 0.15$	3.5 h	—
	JIM + harmonic	$378.420^{+0.09}_{-0.08}$	11.8 min	2.4 min

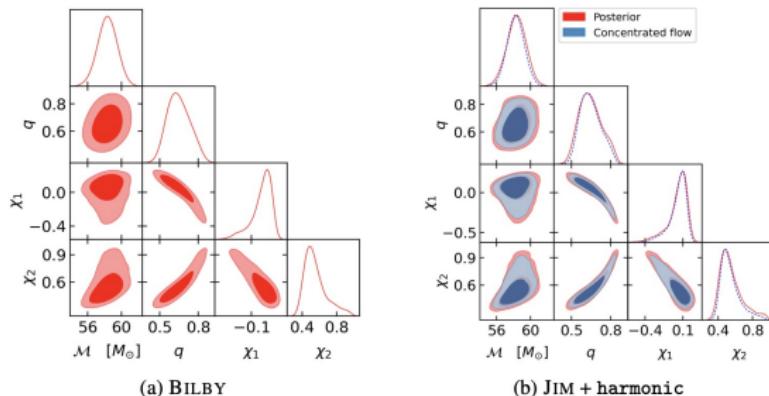
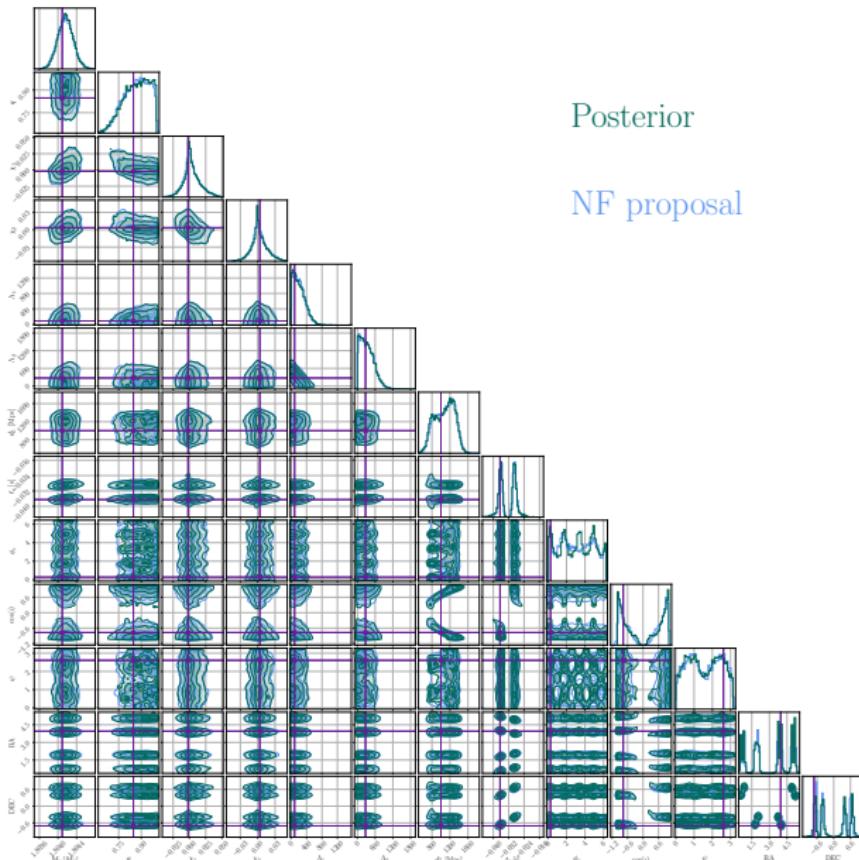
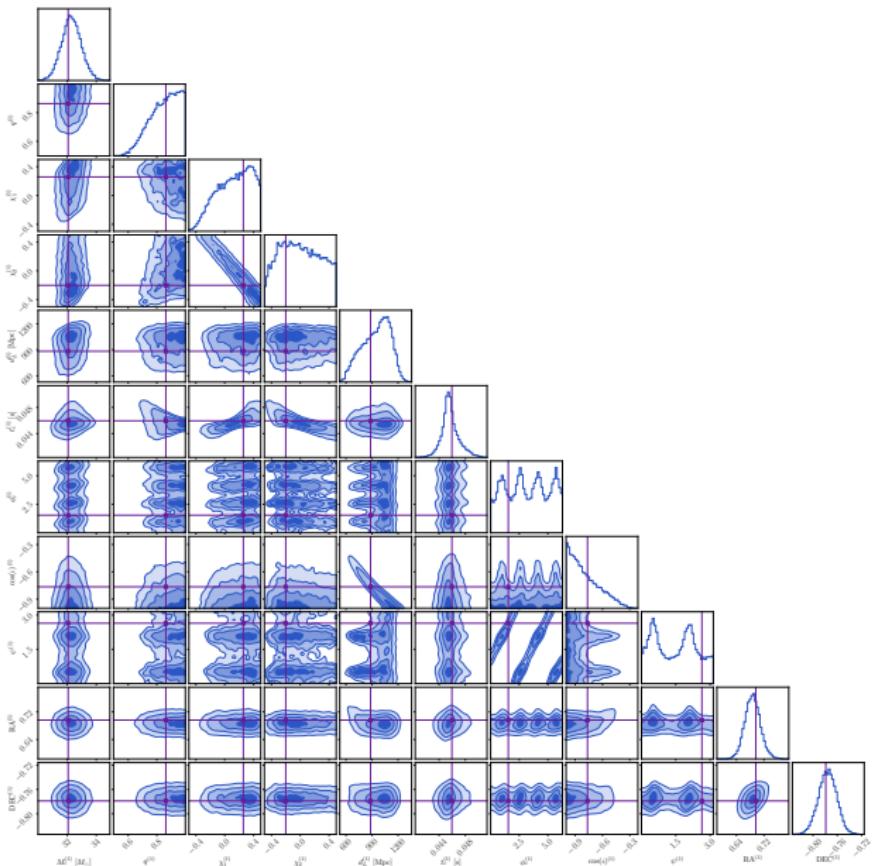


Figure 1: Corner plots for the 4-dimensional posterior samples from (a) BILBY and (b) JIM used for inference (solid red) alongside the concentrated flow at  $T = 0.8$  used in the learned harmonic mean (dashed blue).

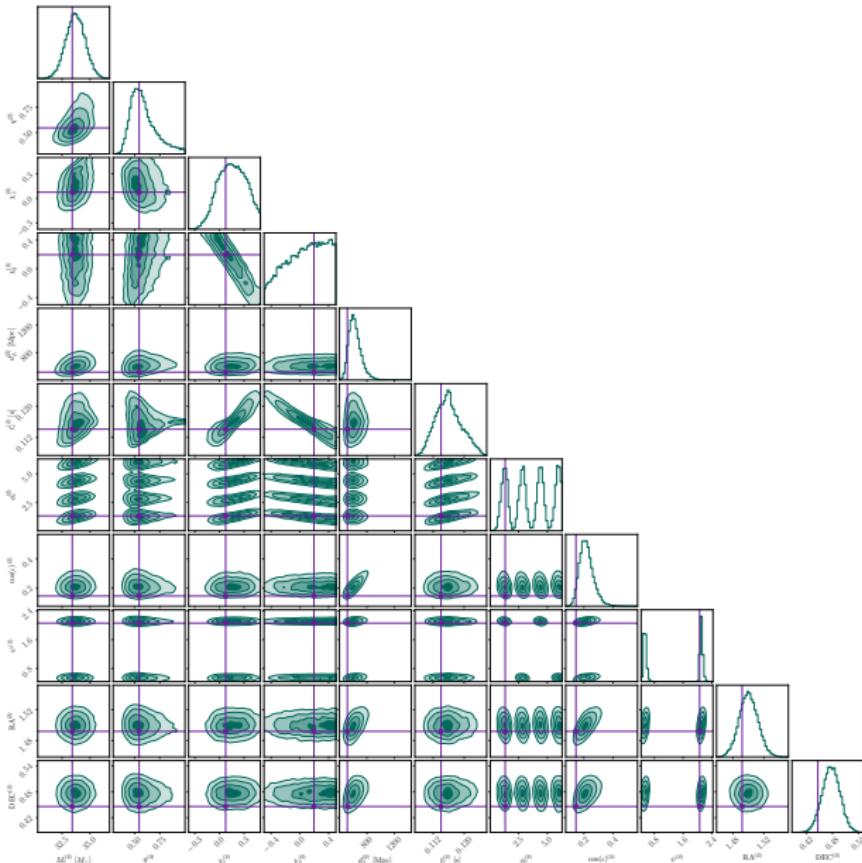
# BNS in ET- $\Delta$ example: all parameters



# Overlapping signals: all parameters signal A

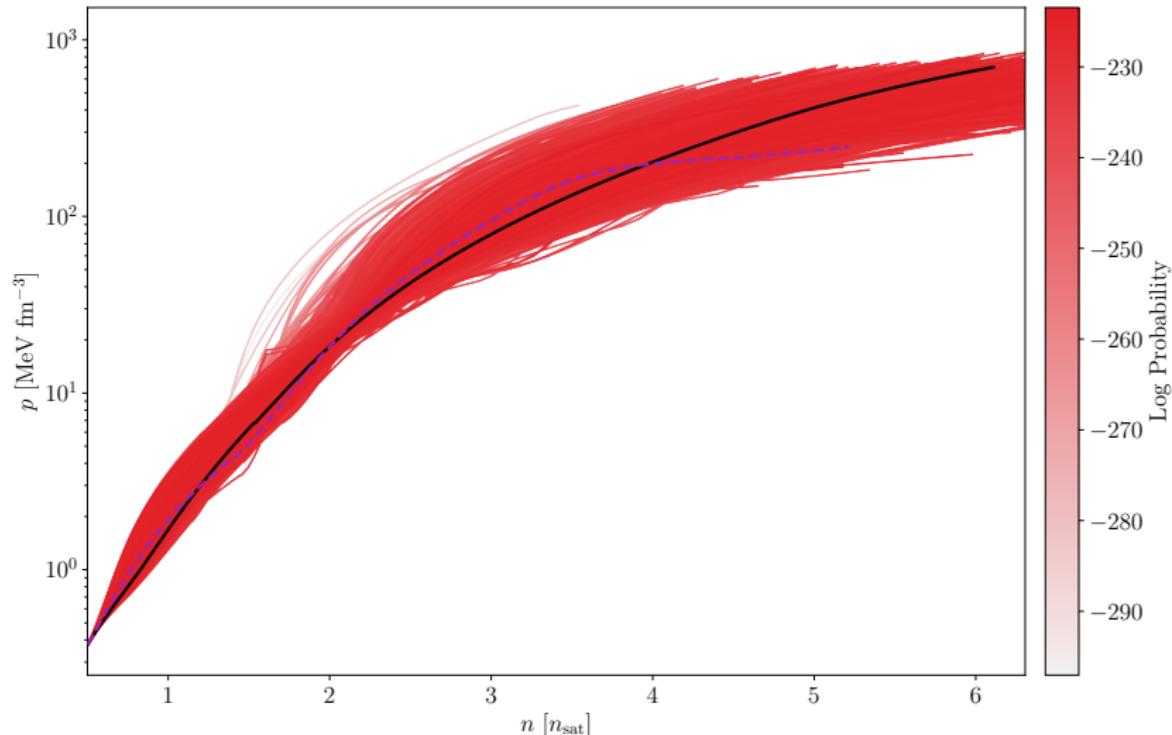


# Overlapping signals: all parameters signal B



# 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

