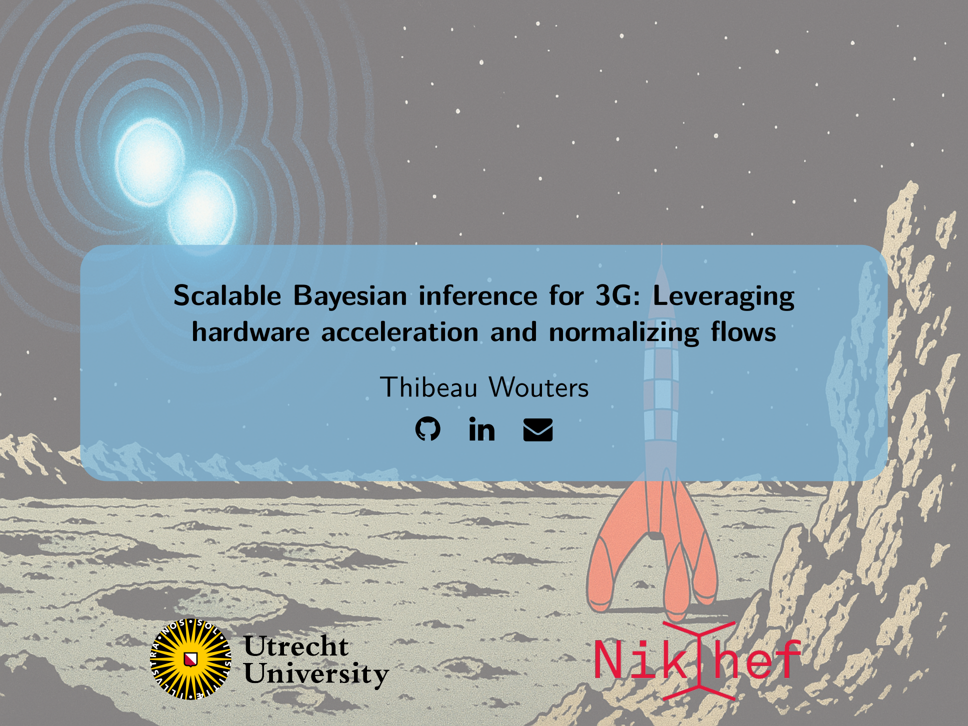

Scalable Bayesian inference for 3G: Leveraging hardware acceleration and normalizing flows

Thibeau Wouters

Utrecht University

Nikhef

Contents

Parameter estimation in 3G

Parameter estimation is done with Bayesian inference:

$$\text{posterior} \propto \frac{\text{likelihood} \times \text{prior}}{\text{evidence}}$$

- Sample the posterior: MCMC or nested sampling
- $\mathcal{O}(10^6) - \mathcal{O}(10^8)$ likelihood evaluations per inference

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

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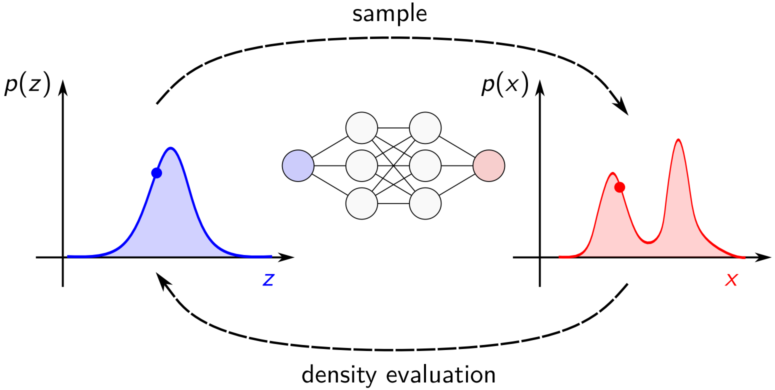
Premise: Current software will not scale to 3G [1]

Contents

Normalizing flows (NFs)

- Trainable bijection between latent and data spaces
- Sample and evaluate complicated densities
- Used as proposal distribution, trained from MCMC chains



JAX & FLOWMC

Accelerate Python with JAX:

- Use GPU accelerators
- Automatic differentiation → gradient-based samplers
- Just-in-time (JIT) compilation

JAX & flowMC

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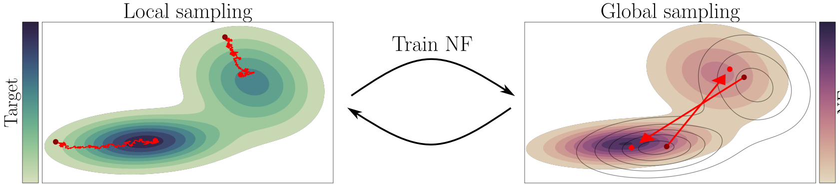
flowMC [2, 3]: MCMC + normalizing flows in JAX

- MCMC chains as training data → no pre-training
- Also see NESSAI [4, 5]



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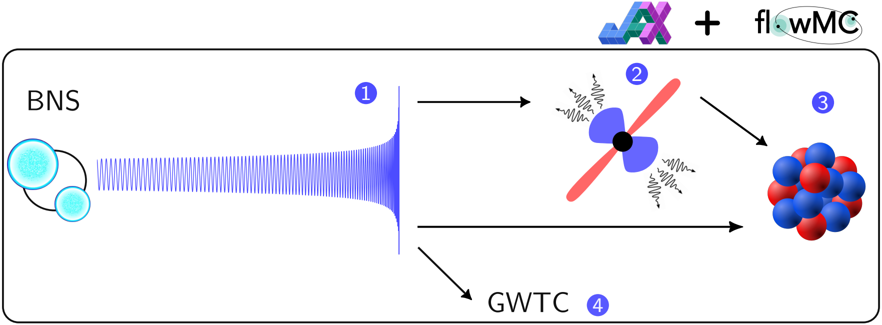
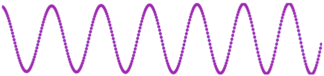


Gravitational waves

- Waveforms on GPU: $\mathcal{O}(10^3)$ faster
- From LALSUITE to JAX: RIPPLE [6]



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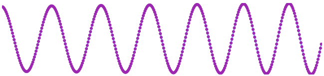

- Parameter estimation: JIM [7, 8]
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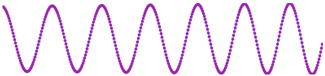
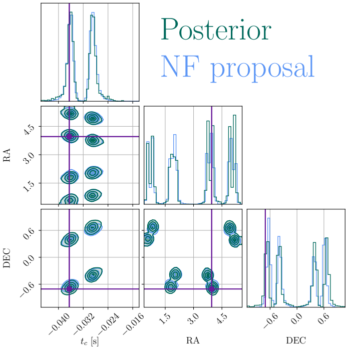


- Parameter estimation: JIM [7, 8]
- BNS in LVK analyzed in ~ 15 min
- Ongoing work for ET – example:
  - BNS, $f_{\min} = 20$ Hz, SNR $= 21$
  - ET-Δ, `IMRPhenomD_NRTidalv2`
  - 30 mins on H100 GPU
- Evidence? HARMONIC [9]



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

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

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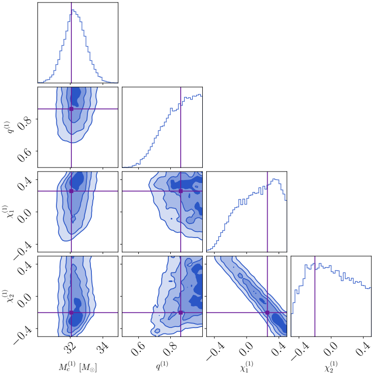
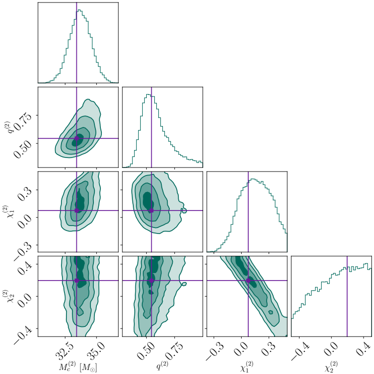
  - $\mathrm{SNR}^{(1)} = 25.76$, $\mathrm{SNR}^{(2)} = 25.24$
  - 1h28m on H100 (vs 23 days on 16 CPUs [10])





Overview

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

1. Gravitational waves
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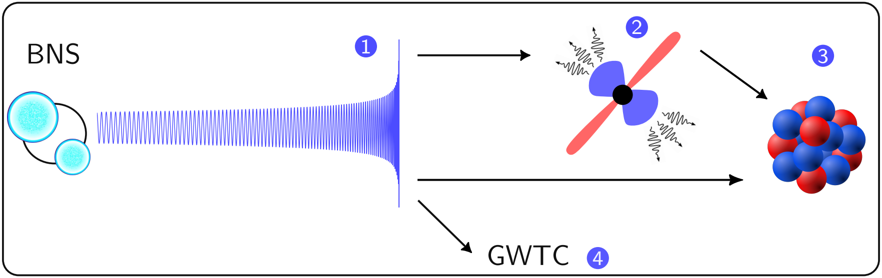
3. Nuclear equation of state
4. Gravitational wave transient catalogue



Electromagnetic counterparts (Hauke Koehn, Tim Dietrich)

- BNS mergers lead to kilonovae, gamma-ray bursts (afterglows)
- Numerical models are too expensive (e.g. AFTERGLOWPY [11])

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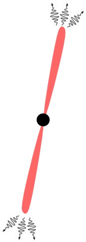
- BNS mergers lead to kilonovae, gamma-ray bursts (afterglows)
- Numerical models are too expensive (e.g. AFTERGLOWPY [11])
- Neural network surrogates for inference: FIESTA

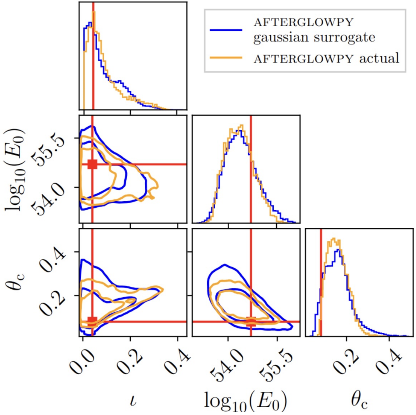


FIESTA

- 1m36s
- 1 H100 GPU

AFTERGLOWPY

- 4 hours
- 30 CPUs



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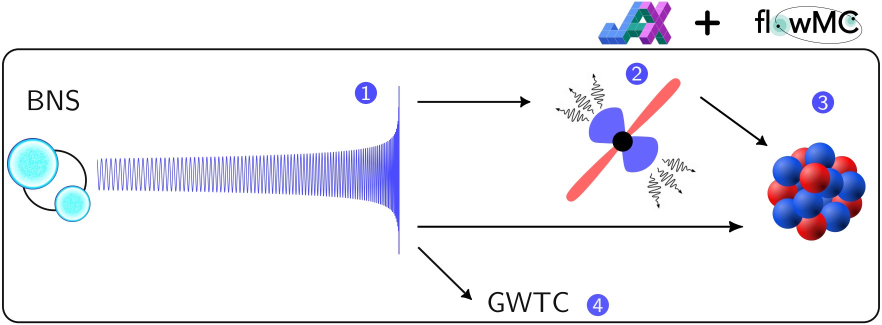

Equation of state inference (Peter T.H. Pang)

- Goal: infer nuclear equation of state (EOS) of neutron stars [12]
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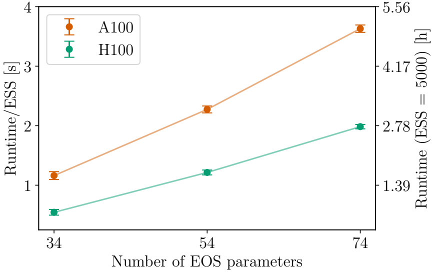

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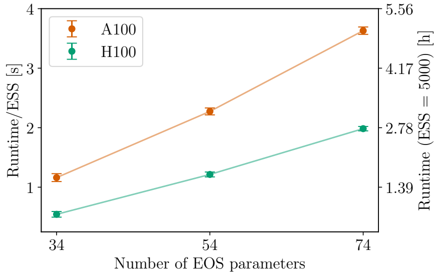
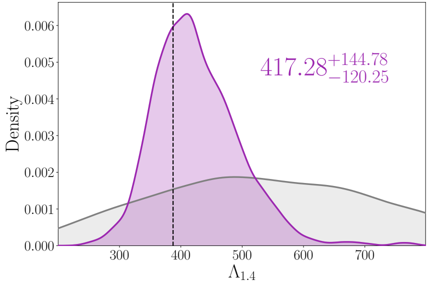
- End-to-end analysis: constrain EOS from 20 BNS in O5





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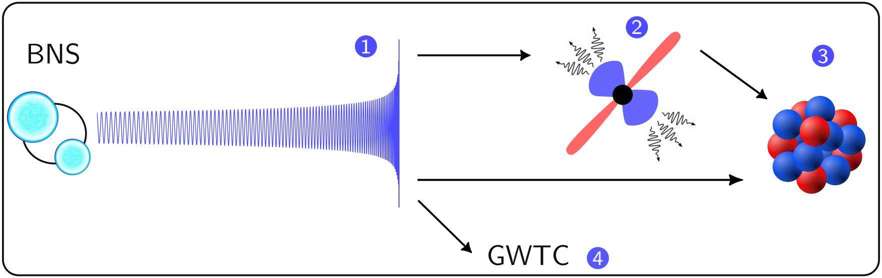
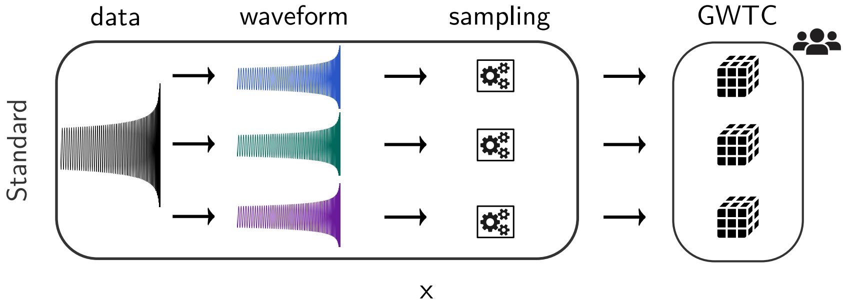


Constructing GWTCs (Thomas Ng, Kaze Wong)

GWTCs do not scale well in memory:

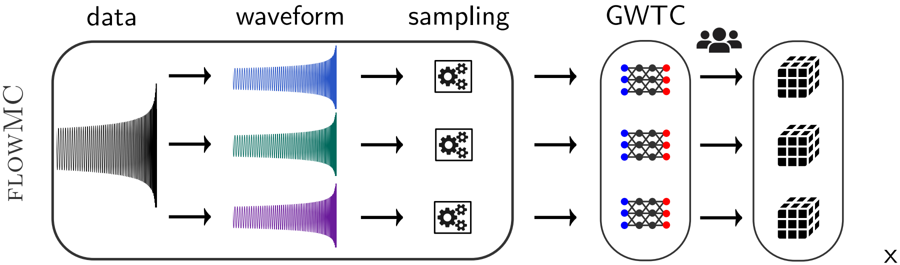
- GWTC stores several samples (different waveforms)
- Standard: fixed sample size, ~ 100 MB



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



Conclusion

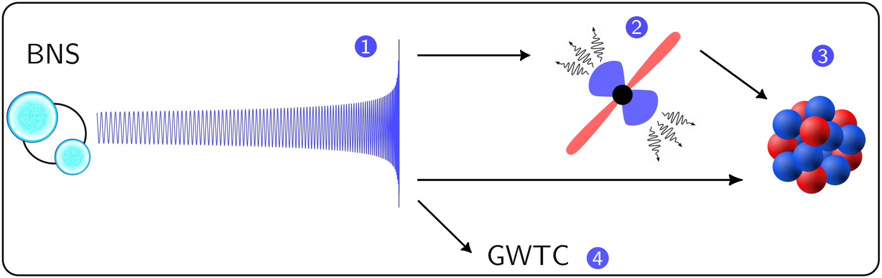
- Progress on scalable Bayesian inference software for 3G, with minimal amount of pre-training
- Hybrid acceleration: GPUs + normalizing flow proposals
  - JAX/GPU: likelihoods faster
  - FLOWMC: sampling converges faster
- Goal: joint multimessenger analyses in ~hours (NMMA [14] in JAX)
- To do
  - GW injection studies for ET
  - More waveform models in JAX
  - Equation of state study with ET data

Let's talk!

Thank you for your attention!

Software written in JAX:

- FLOWMC [2, 3]
- JIM [7, 8] 1 2 4
- FIESTA 2
- JESTER [13] 3
- HARMONIC [9, 15, 16]



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Evidence calculation: HARMONIC I

Evidence Z can be computed from posterior samples with HARMONIC [15] with the harmonic mean estimator

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

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

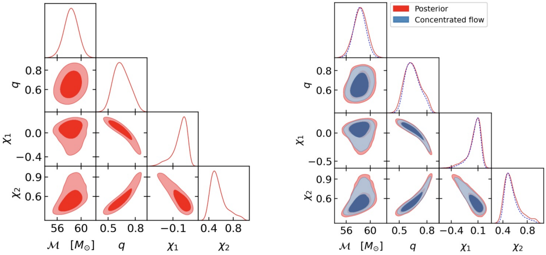
In practice, this can be achieved with a normalizing flow [16].

This has been verified to give accurate evidences (similar values as nested sampling) when GW posteriors are used [9].

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.

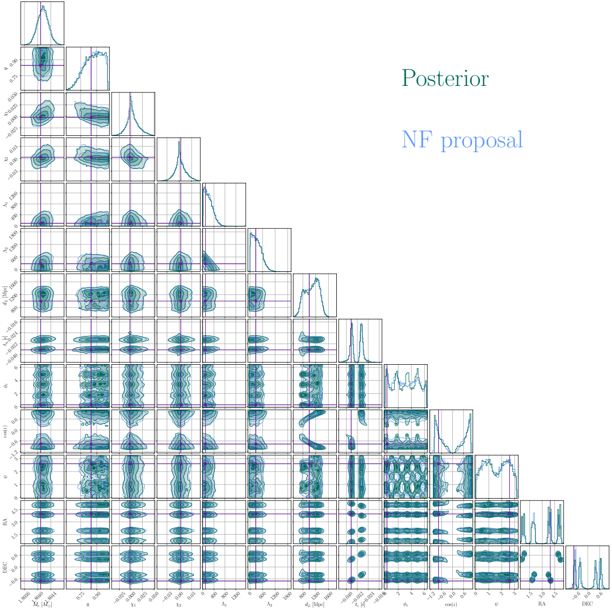
Example	Method	$\log(z)$	Sampling time	Evidence estimation time
4D	BILBY	390.33 ± 0.11	31.3 min	–
	JIM + `harmonic`	$390.360^{+0.006}_{-0.006}$	3.4 min	1.9 min
11D	BILBY	378.29 ± 0.15	3.5 h	–
	JIM + `harmonic`	$378.420^{+0.09}_{-0.08}$	11.8 min	2.4 min



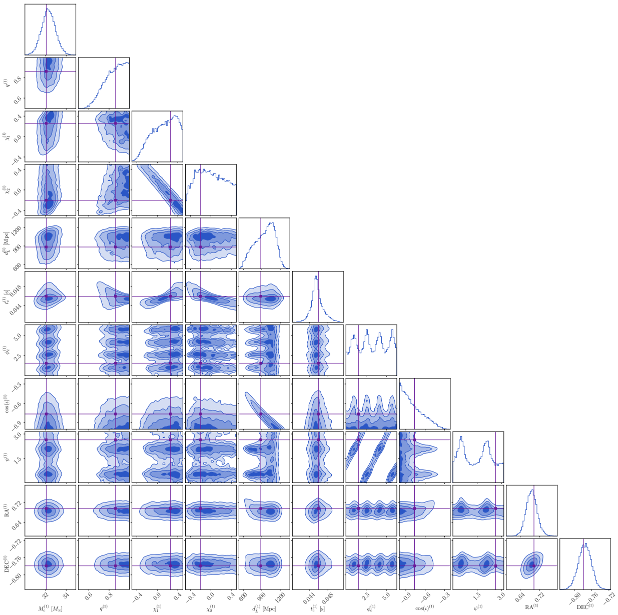
(a) BILBY (b) JIM + `harmonic`

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).

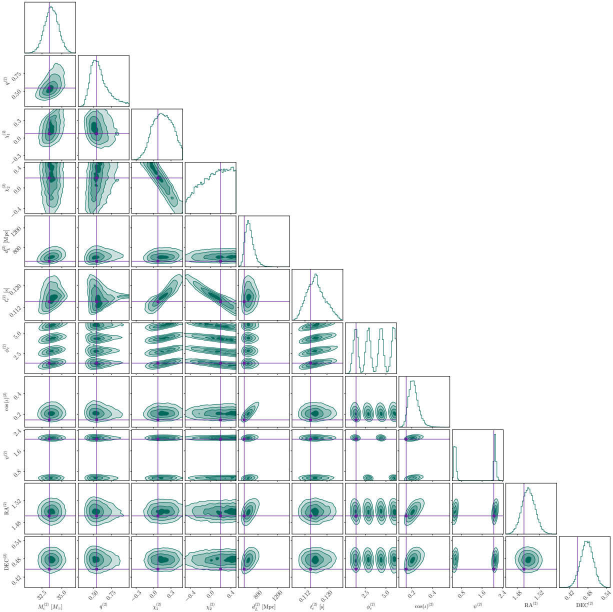
BNS in ET-Δ example: all parameters



Overlapping signals: all parameters signal A

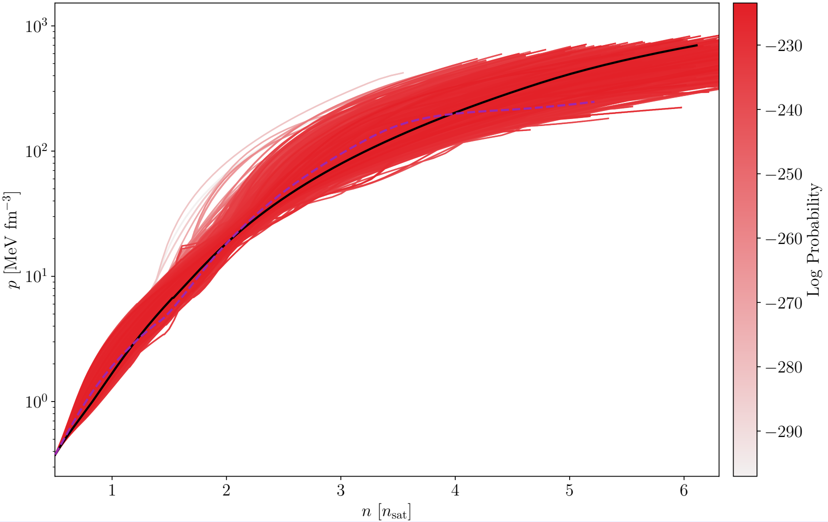


Overlapping signals: all parameters signal B



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