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

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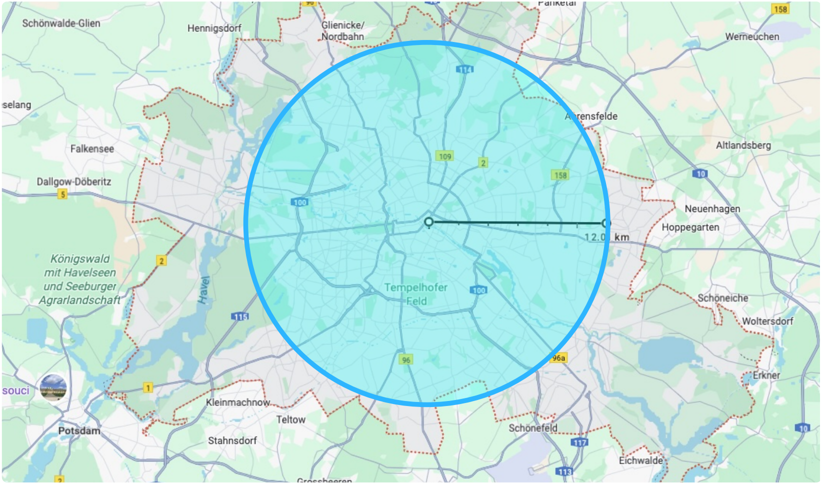
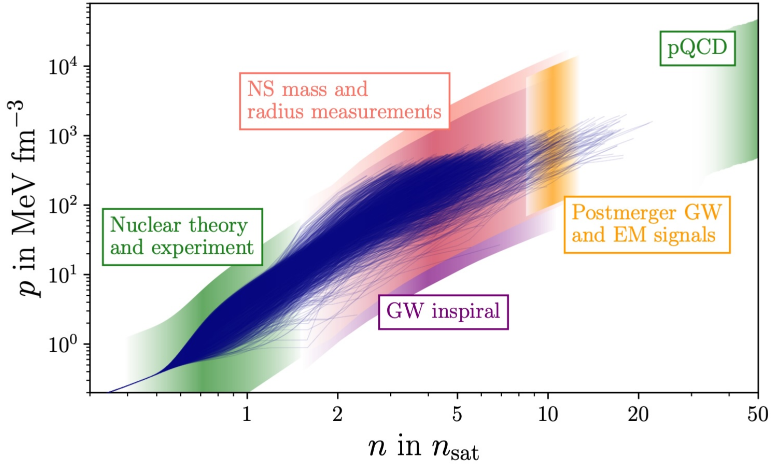
Neutron stars

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



Equation of state

Neutron stars uniquely probe the equation of state (EOS) of dense nuclear matter [1]



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Multimessenger astrophysics

Observe neutron star mergers through gravitational waves and electromagnetic radiation: GW170817 [2, 3]

TODO: Snapshots

Contents

Future GW detectors: Einstein Telescope

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

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

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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  - $10^4 - 10^5$ binary neutron star mergers/year (now: 2/10 years)
  - $10^2 - 10^3$ multimessenger events/year (now: 1/10 years)
- Observe from 5 Hz (now: 20 Hz)
  - Longer signals: binary neutron star: 2 hours vs 2 minutes
  - Signals will overlap

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

My research focus: why – how – what

Why?

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

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Parameter estimation: Bayesian inference

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

Bayesian inference:

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

Ingredients:

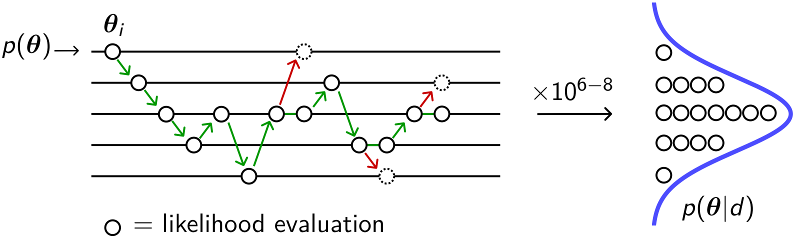
- Prior: specified by users
- Likelihood: often costly
- Posterior: intractable, needs stochastic samplers
- Evidence: model selection

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

Alteratives: nested sampling, sequential Monte Carlo



Computational aspects

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How can we optimize this?

Contents

jax "is a Python library for accelerator-oriented array computation and program transformation, designed for high-performance numerical computing and large-scale machine learning." [7]

In particular:

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

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In particular:

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- Numpy-like API: (`numpy` → `jax.numpy`)

Gamechangers:

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

JAX – Function transformations

- `jit`: Just-in-time compilation to XLA (CPU/GPU/TPU)

TODO: Some figure for autodiff

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JAX – Function transformations

- `jit`: Just-in-time compilation to XLA (CPU/GPU/TPU)
- `grad`: Automatic differentiation: compute gradients with chain rule
- `vmap`, `pmap`: Vectorization, batch processing, parallelization
- Composable, e.g.:
  - Higher-order derivatives: `jaxgrad(jaxgrad(f))`
  - Evolve N chains in parallel along gradient of the likelihood

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

TODO: Some figure for autodiff

Computational aspects

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Normalizing flows

Q: Given samples $\{x\} \sim p(x)$, how can we get $p(x)$?

- Evaluate density at any point
- Generate new samples

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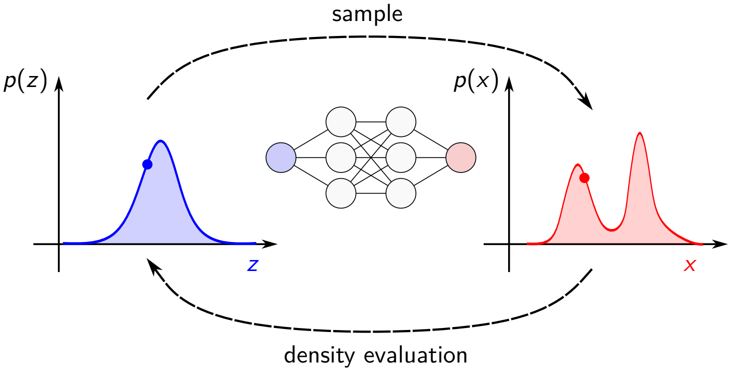
A: Normalizing flows: generative machine learning model, bijection between latent space (Gaussian) and data space



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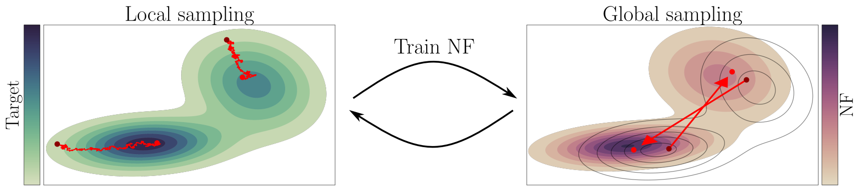
flowMC

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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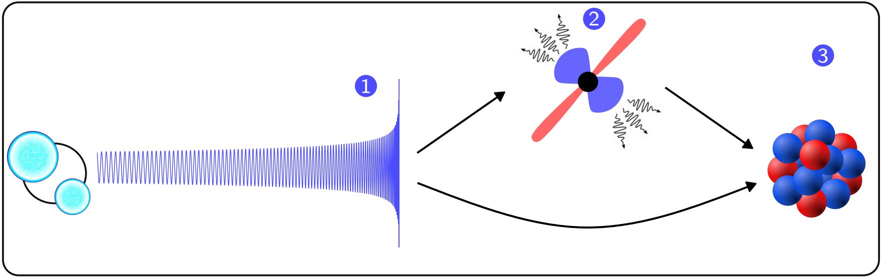
Overview

Analyzing a multi-messenger **binary neutron star** signal:

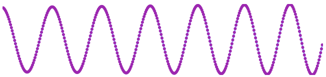
1. **Gravitational waves**
2. Electromagnetic counterparts
3. Nuclear equation of state

JAX + flowMC



Gravitational waves: RIPPLE

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



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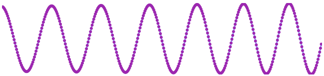

- Waveforms on GPU: $\mathcal{O}(10^3)$ faster
- RIPPLE [10]: from LALSUITE to JAX
- Waveforms available in RIPPLE:
  - Binary black holes:
    - `IMRPhenomXAS`
    - `IMRPhenomD`
    - `IMRPhenomPv2`
  - Binary neutron stars:
    - `TaylorF2`
    - `IMRPhenomD_NRTidalv2`
    - `IMRPhenomPv_NRTidalv2` (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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- Verified for binary neutron stars in current generation detectors [14]
- Matches bilby, passes *pp*-test
- Runtime: from hours to minutes

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

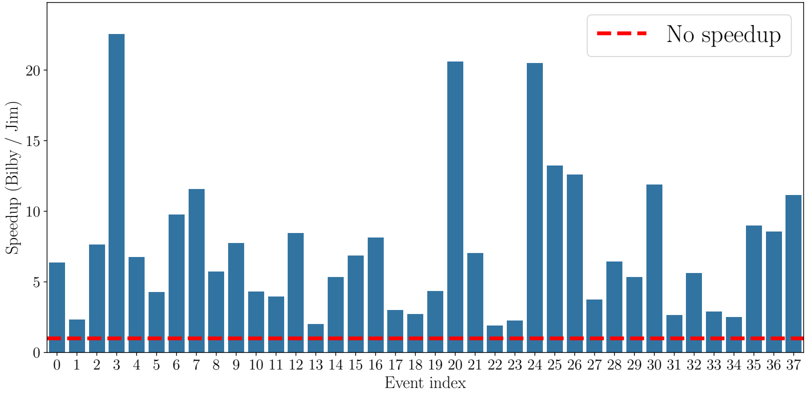
Gravitational waves: JIM

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

- Re-analyze GWTC-3 with `IMRPhenomPv2`
- JIM on A800 GPU: on average $\sim$ 7 times faster than BILBY on 16 CPUs, **without compromises**
- Work in progress!



Einstein Telescope

Work in progress: showing proof-of-concepts!

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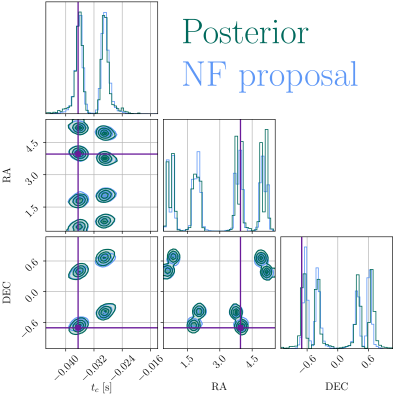
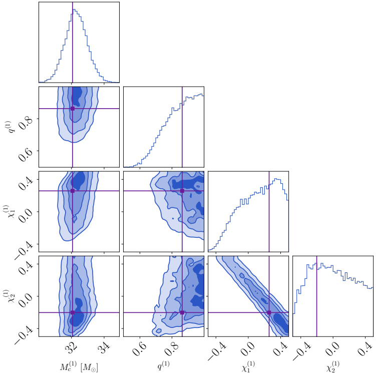
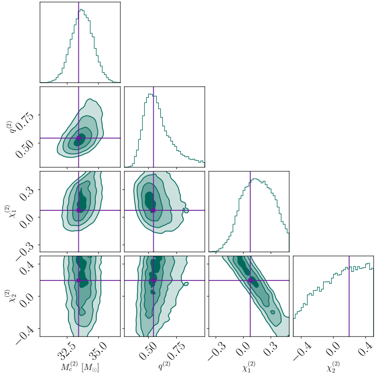
- ET posteriors are multimodal
- Normalizing flows help to jump between modes



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])





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2. **Electromagnetic counterparts**
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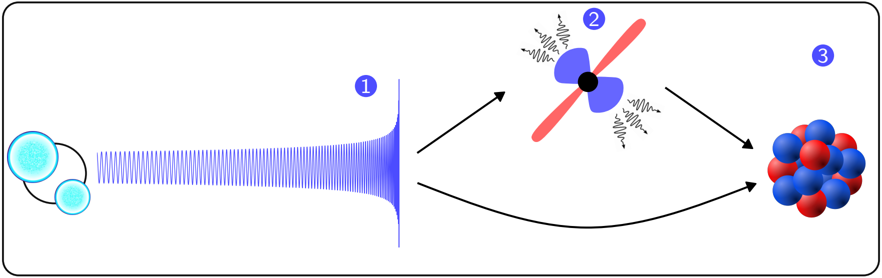

Electromagnetic counterparts (Hauke Koehn, Tim Dietrich)

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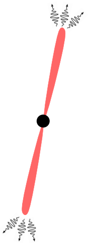
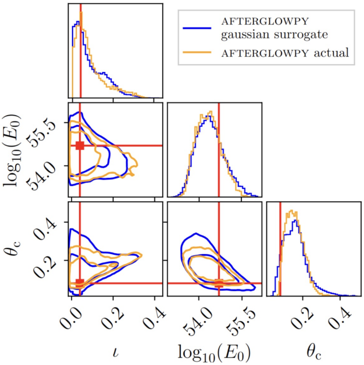


FIESTA

- 1m36s
- 1 H100 GPU

AFTERGLOWPY

- 4 hours
- 30 CPUs



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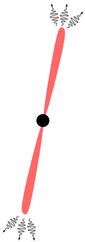
- Kilonovae and GRB afterglows
- Code libraries too large to 'jaxify' (e.g. AFTERGLOWPY [16])
- Neural network emulators for inference: FIESTA [17]
- Scales well for systematics 'nuisance parameters'



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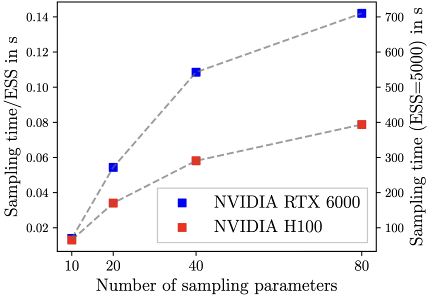

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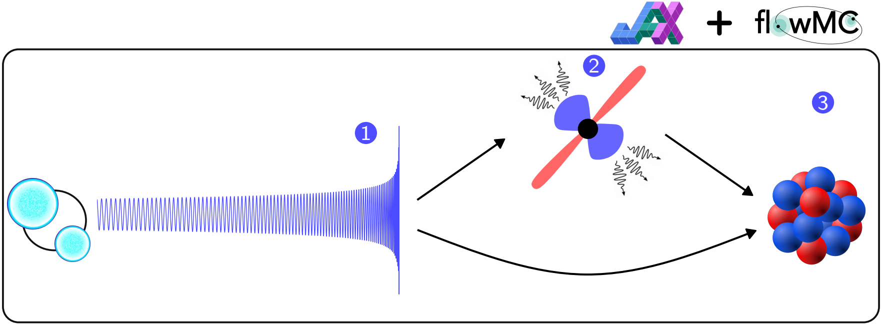
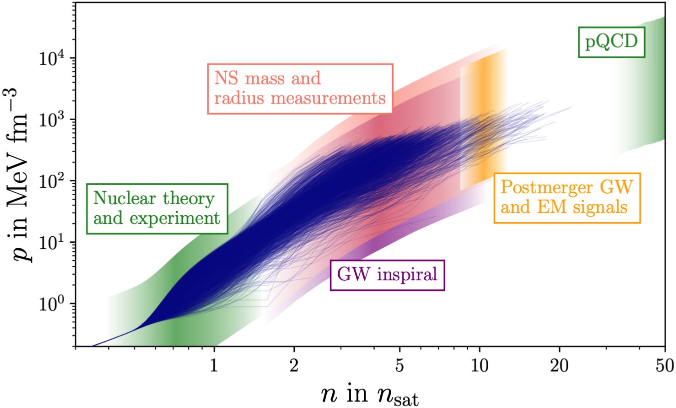


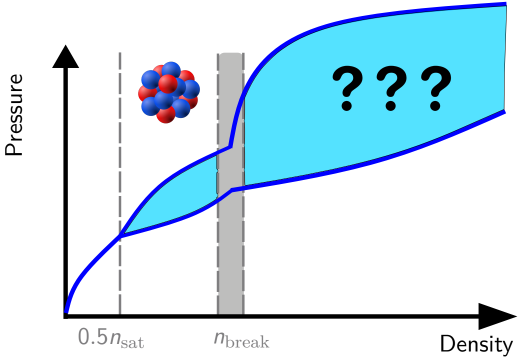
Equation of state inference – warmup

- How do we constrain the EOS from neutron star observations?
- Define parametrization and likelihood
- GWs from binary neutron stars inspiral as example



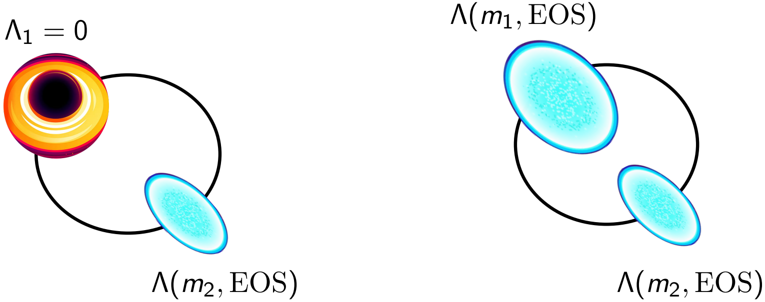
Equation of state inference – parametrization

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



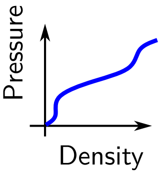
Tidal deformability

- 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

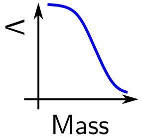
- To predict neutron star properties, we solve the TOV equations: ordinary differential equations (ODEs)



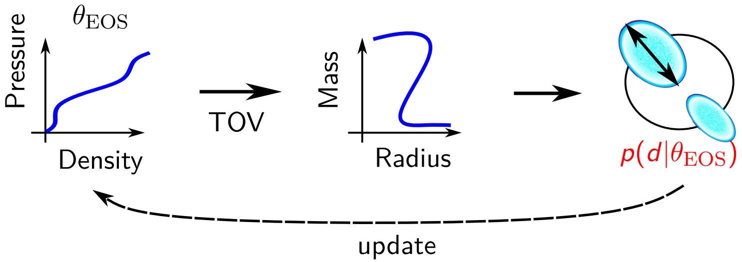
Solve TOV equations

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

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

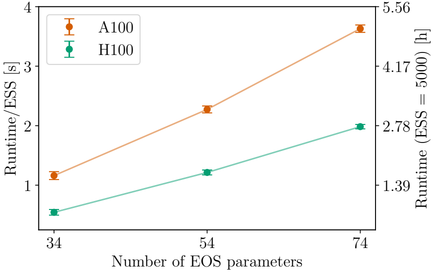


- To predict neutron star properties, we solve the TOV equations: ordinary differential equations (ODEs)
- Done for each sample θ_{EOS}: costly likelihood
- How to make this scalable without compromises?

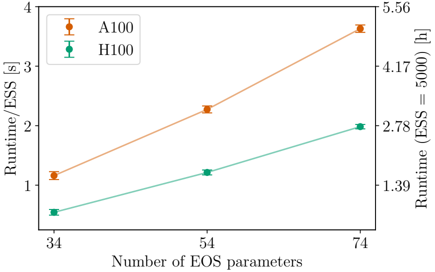


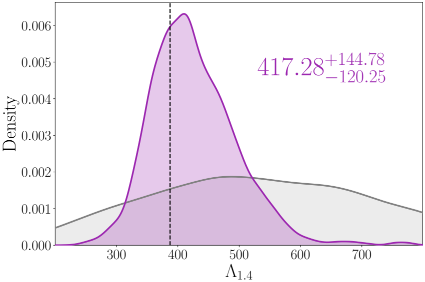
Jester

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



- JESTER [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
- Open up possibilities to study systematics in EOS inference





Auto-differentiable ODE solvers

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

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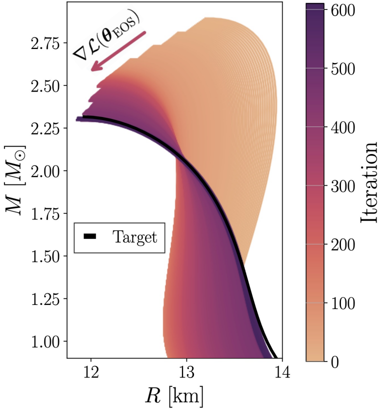
- Frame inference as optimization problem:
  - Gradient descent on loss function $\mathcal{L}(\boldsymbol{\theta}_{\rm EOS})$

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



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and now, for something completely different...

Contents

Conclusion

- Progress on scalable Bayesian inference, with minimal pre-training
- Hybrid acceleration: GPUs + normalizing flow proposals
  - JAX/GPU: faster likelihoods
  - FLOWMC: sampling converges faster
- Simulators in JAX can remove the need for emulators (GW, TOV)
- Auto-differentiable ODE solvers: inference as optimization problem

Let's talk!

Thanks for listening!

References I

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Evidence calculation: HARMONIC I

Evidence Z can be computed from posterior samples with HARMONIC [21] 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:

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

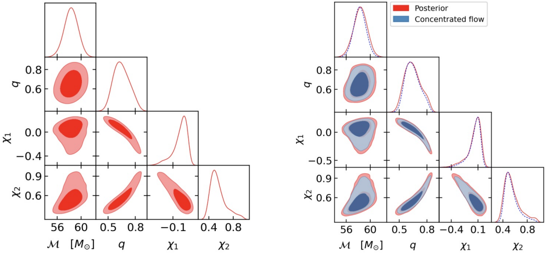
Replace the target distribution π with φ: only requirement is that it is normalized

In practice, this can be achieved with a normalizing flow [22].

This has been verified to give accurate evidences (similar values as nested sampling) when GW posteriors are used [23].

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.

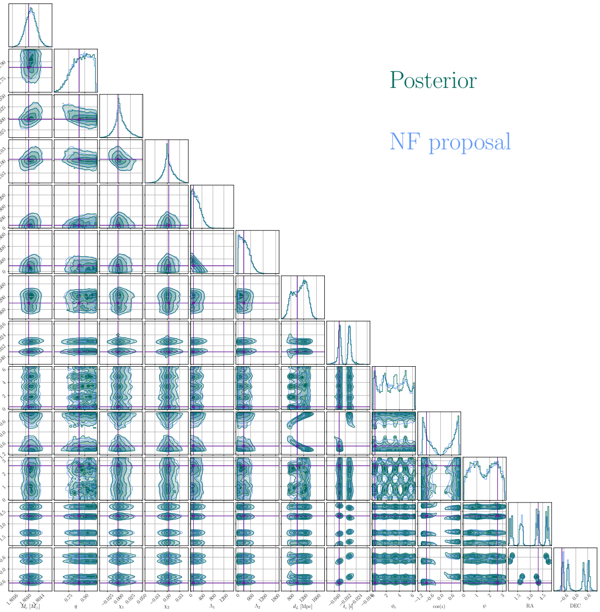
Example	Method	$\log(z)$	Sampling time	Evidence estimation time
4D	BILBY	390.33 ± 0.11	31.3 min	–
	JIM + `harmonic`	$390.360^{+0.006}_{-0.006}$	3.4 min	1.9 min
11D	BILBY	378.29 ± 0.15	3.5 h	–
	JIM + `harmonic`	$378.420^{+0.09}_{-0.08}$	11.8 min	2.4 min



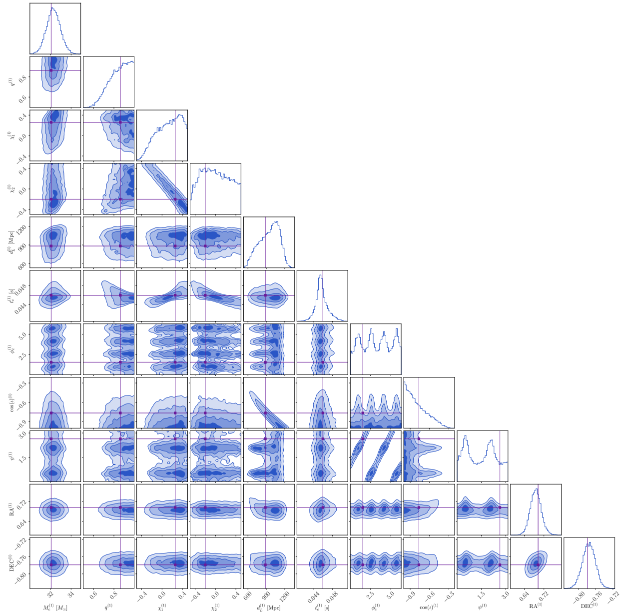
(a) BILBY (b) JIM + `harmonic`

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).

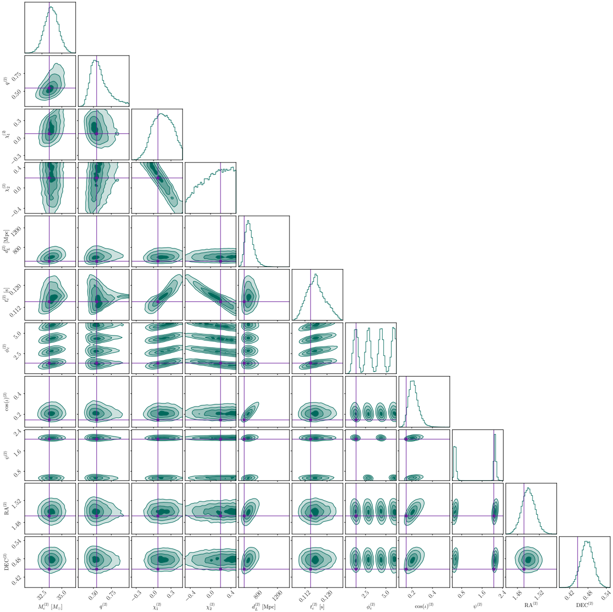
BNS in ET-Δ example: all parameters



Overlapping signals: all parameters signal A

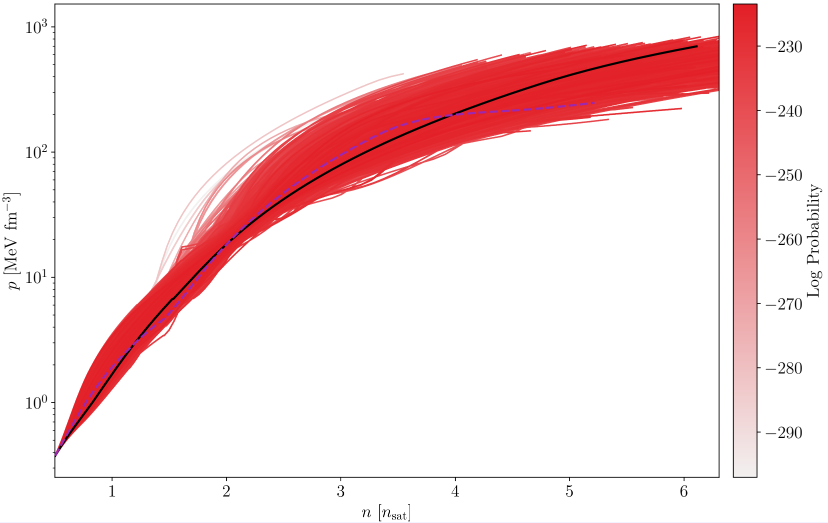


Overlapping signals: all parameters signal B



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