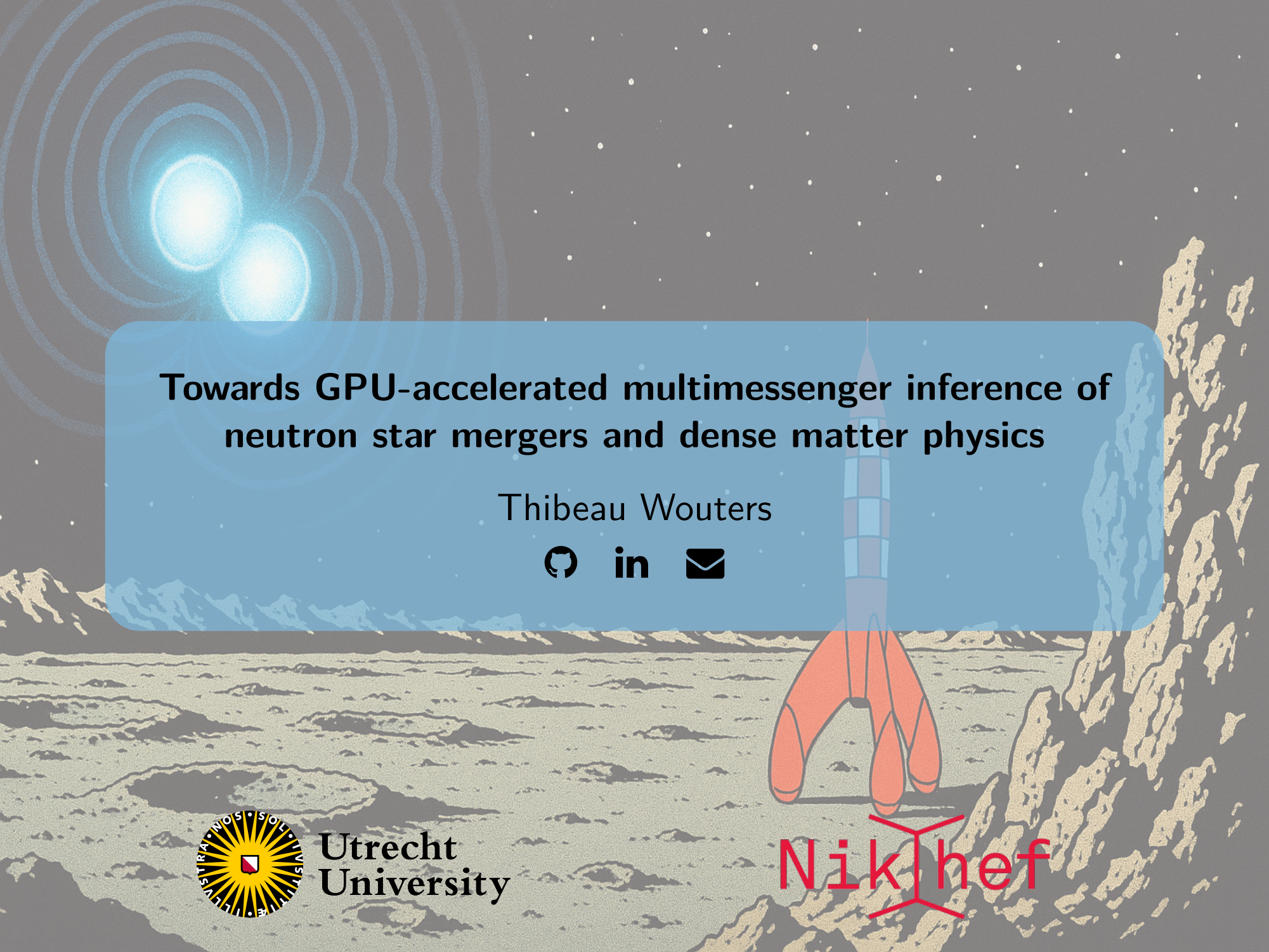

Towards GPU-accelerated multimessenger inference of neutron star mergers and dense matter physics

Thibeau Wouters

Utrecht University

Nikhef

Table of Contents

1. Introduction
2. Methods
3. Applications
4. Outlook and conclusion

Contents

1. Introduction
   - Neutron stars and equation of state
   - Multimessenger astrophysics
   - Future detectors and challenges
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1. Introduction
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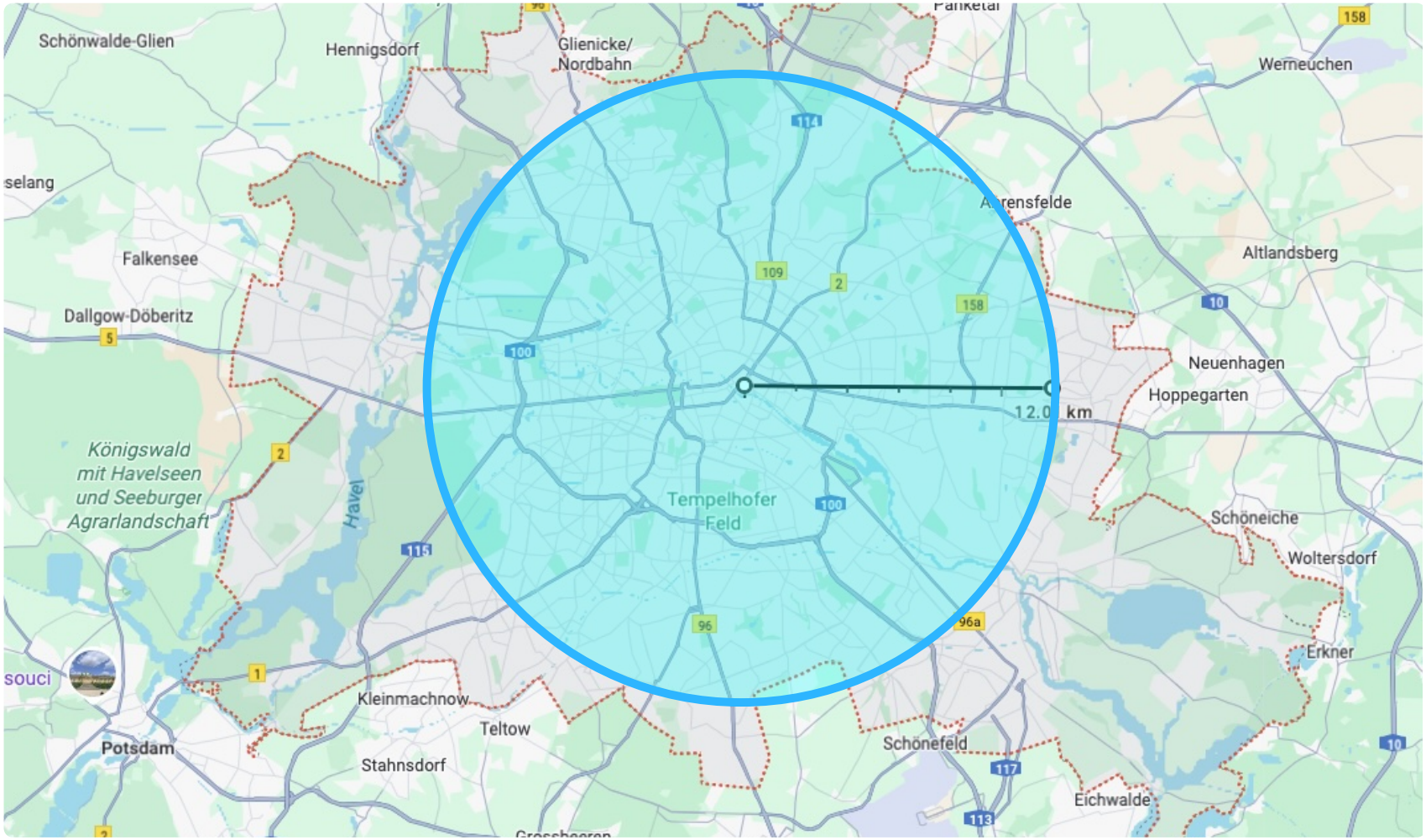
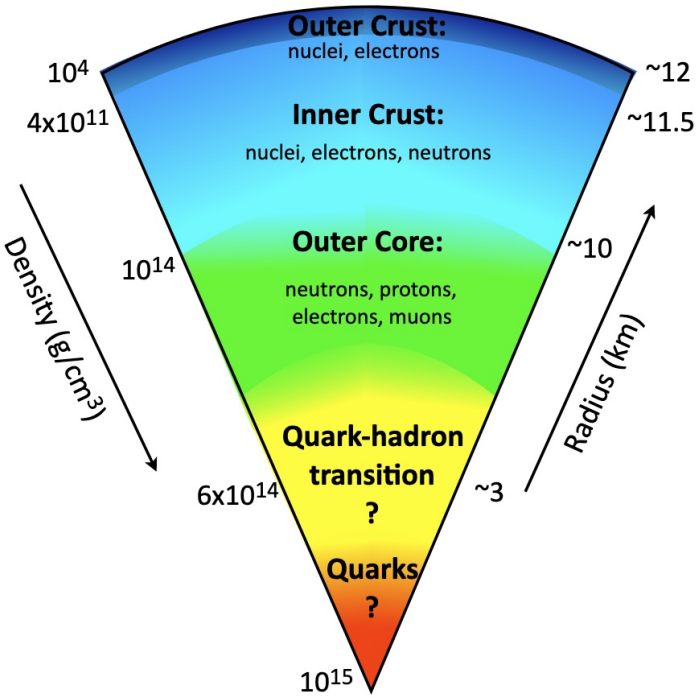
Neutron stars

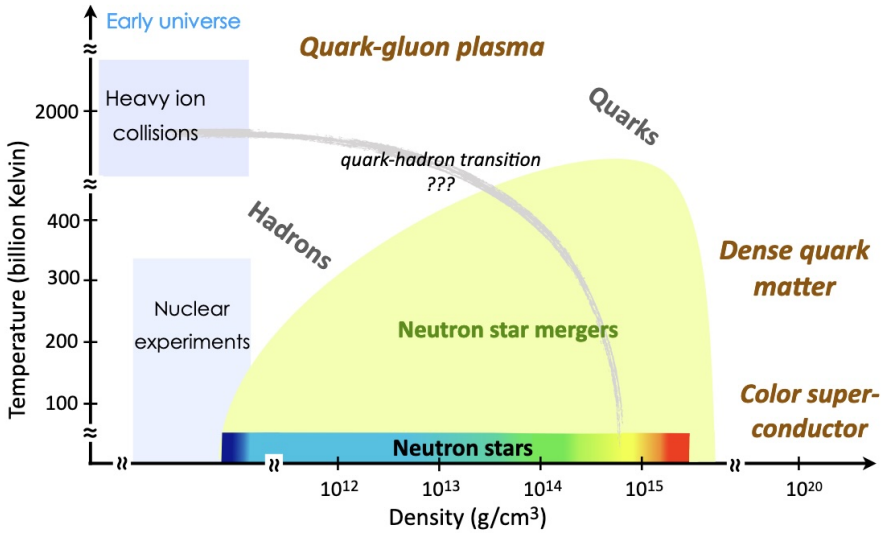
- Neutron stars: supernova remnants, densest matter in the universe
- $m \sim 1.2 - 2.3 M_\odot$, $R \sim 10 - 13$ km



Neutron stars

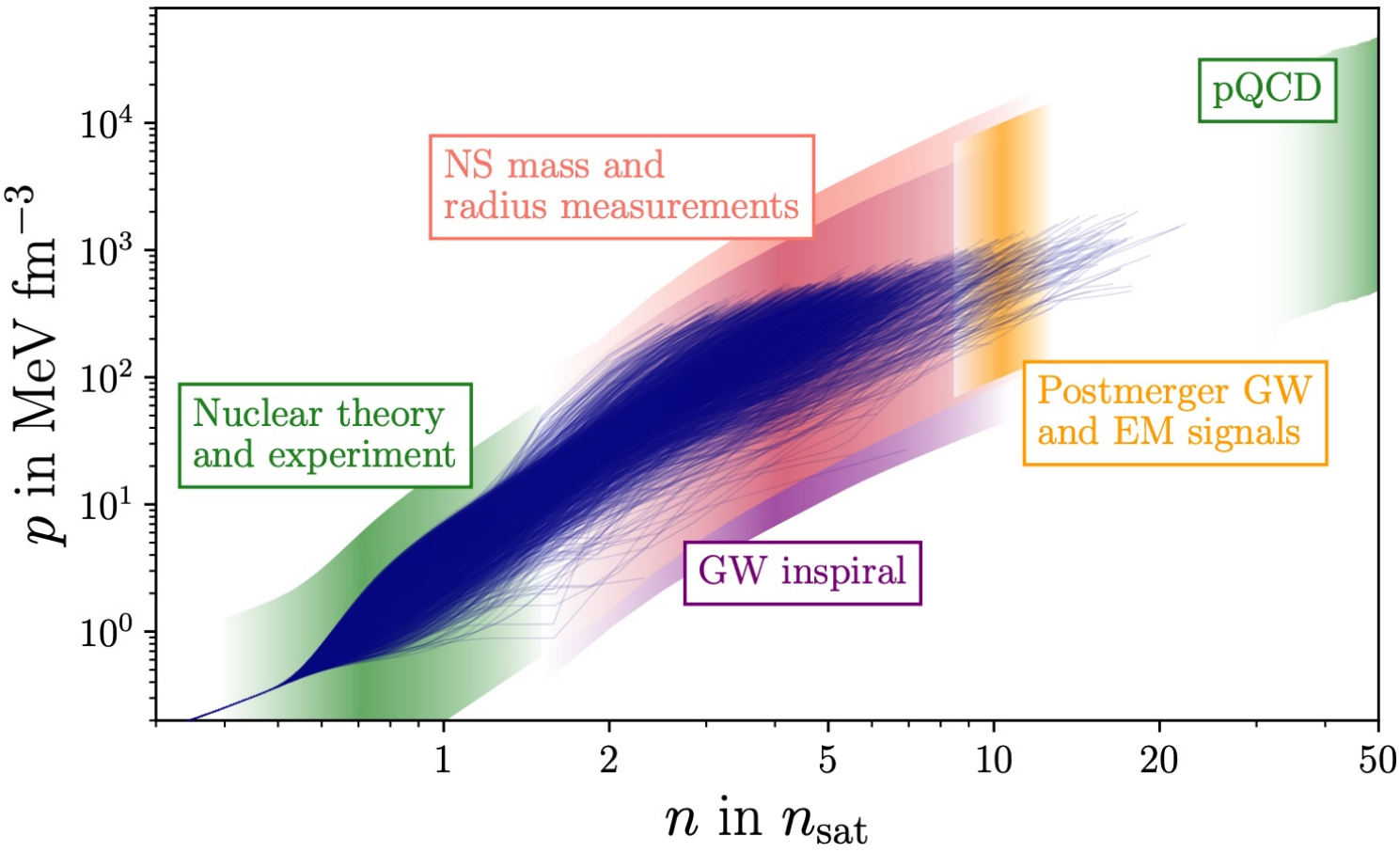
- Neutron stars: supernova remnants, densest matter in the universe
- $m \sim 1.2 - 2.3 M_\odot$, $R \sim 10 - 13$ km
- Cosmic laboratories for fundamental physics





Equation of state

- Neutron stars uniquely probe the cold equation of state (EOS) of dense nuclear matter [1]
- How to determine the EOS from neutron stars?



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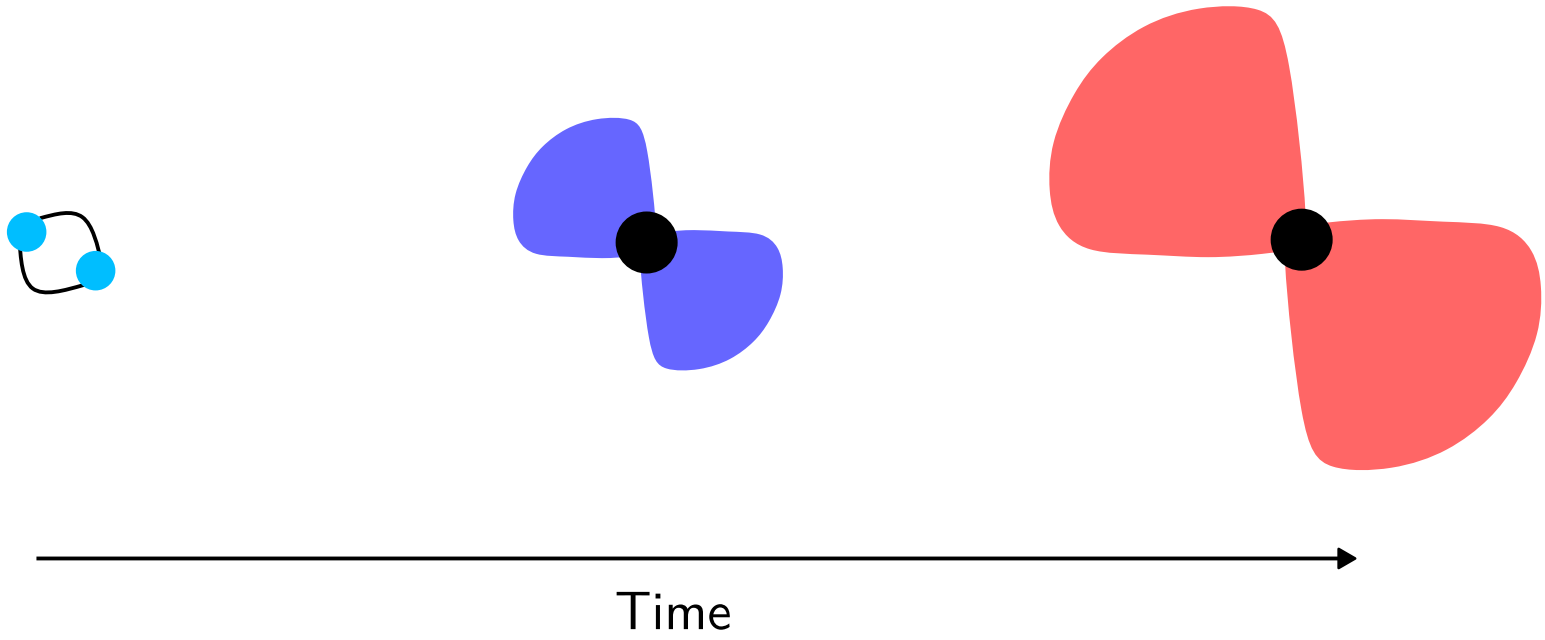
Multimessenger astrophysics

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

TODO: Snapshots

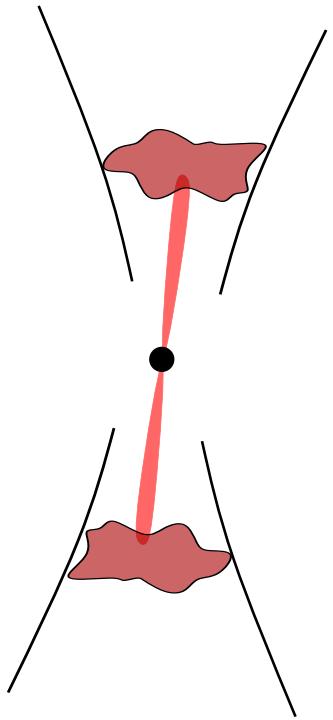
Kilonovae

- Electromagnetic counterpart of a binary neutron star merger [4]
- Lasts days-weeks, isotropic
- Powered by radioactive decay of heavy elements: r-process
- Ejecta depend on EOS TODO: how and put in the slide



Gamma-ray bursts afterglow

- Short gamma-ray burst: relativistic jet launched after merger (~ 1 s)
- Afterglow: broadband emission from radio to X-rays
- Lasts weeks-years



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Future GW detectors: Einstein Telescope

Einstein Telescope: Third-generation ground-based GW detector [5, 6]

Current software cannot handle the ET data analysis problem [7]

Future GW detectors: Einstein Telescope

Einstein Telescope: Third-generation ground-based GW detector [5, 6]

- 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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  - $10^2 - 10^3$ 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 [7]

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
- Use machine learning to assist inference, not replace it

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

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   - JAX
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   - FLOWMC
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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:

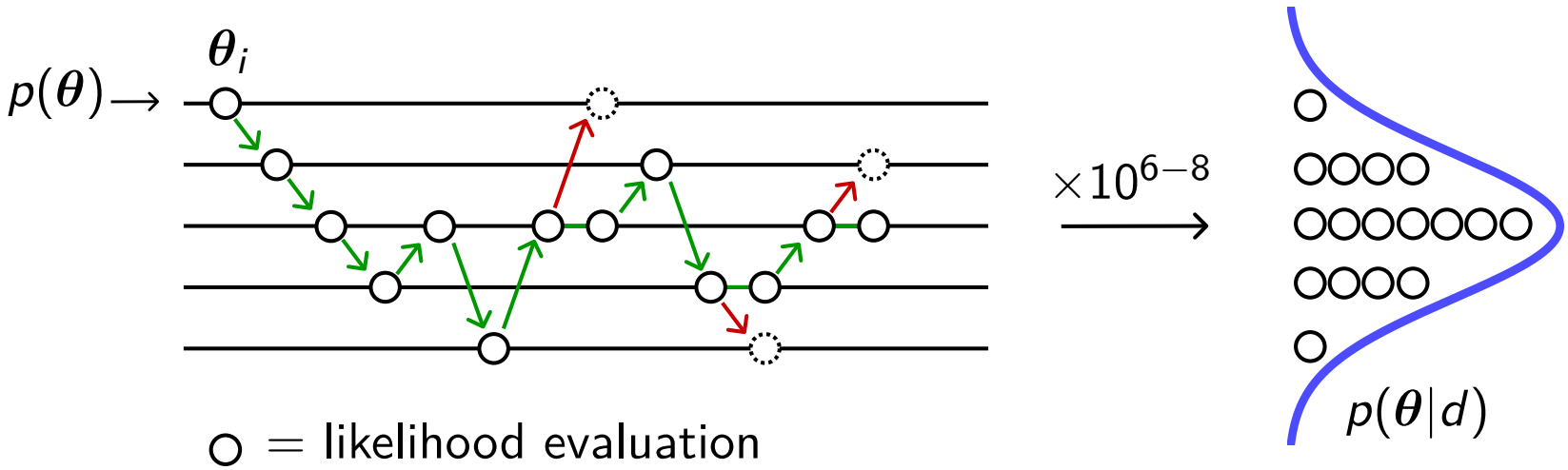
- Prior: specified by users
- Likelihood: often costly
- Posterior: intractable, needs stochastic samplers
- Evidence: model selection

Parameter estimation: Markov chain Monte Carlo

How do we sample the posterior? Markov chain Monte Carlo

- N chains θ_i explore posterior in parallel
- Evolve chains to new position: proposal
- Compute likelihood $\rightarrow$ accept/reject

Alteratives: nested sampling, sequential Monte Carlo



Computational aspects

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

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JAX

jax "is a Python library for accelerator-oriented array computation and program transformation, designed for high-performance numerical computing and large-scale machine learning." [8]

In particular:

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

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

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

TODO: Some figure for autodiff

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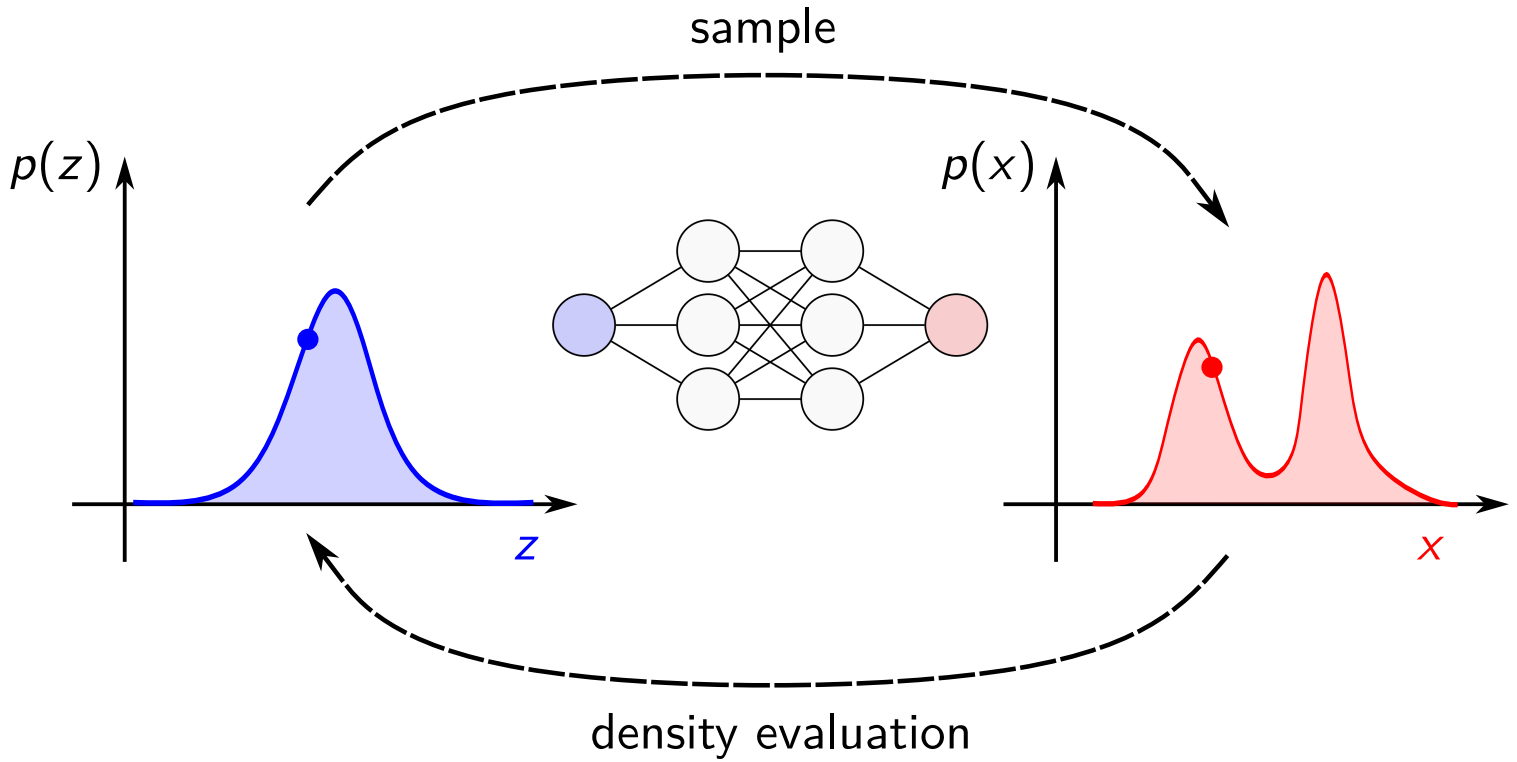
A: Normalizing flows: generative machine learning model, bijection between latent space (Gaussian) and data space



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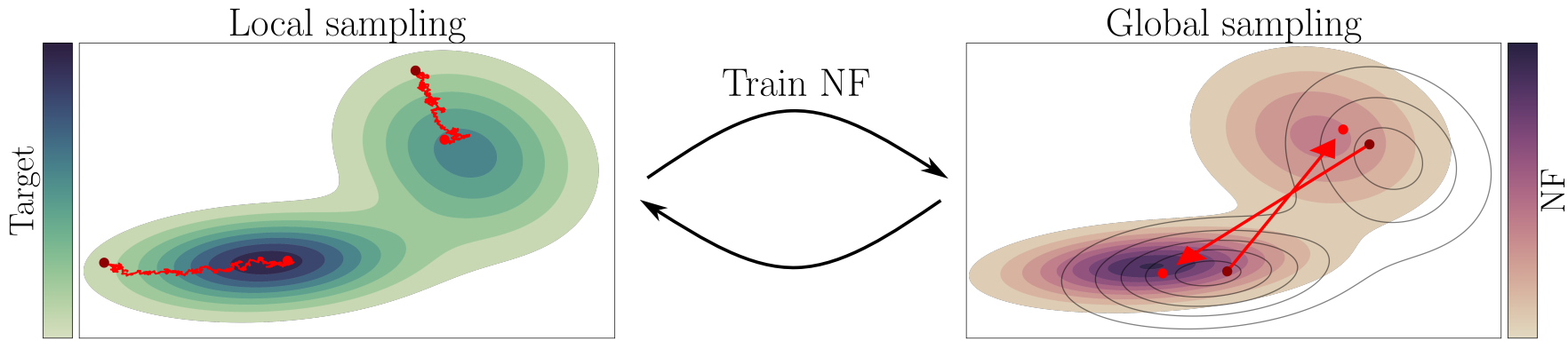
FLOWMC [9, 10]: normalizing flow-enhanced MCMC

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



Contents

1 Introduction

2 Methods

3 Applications

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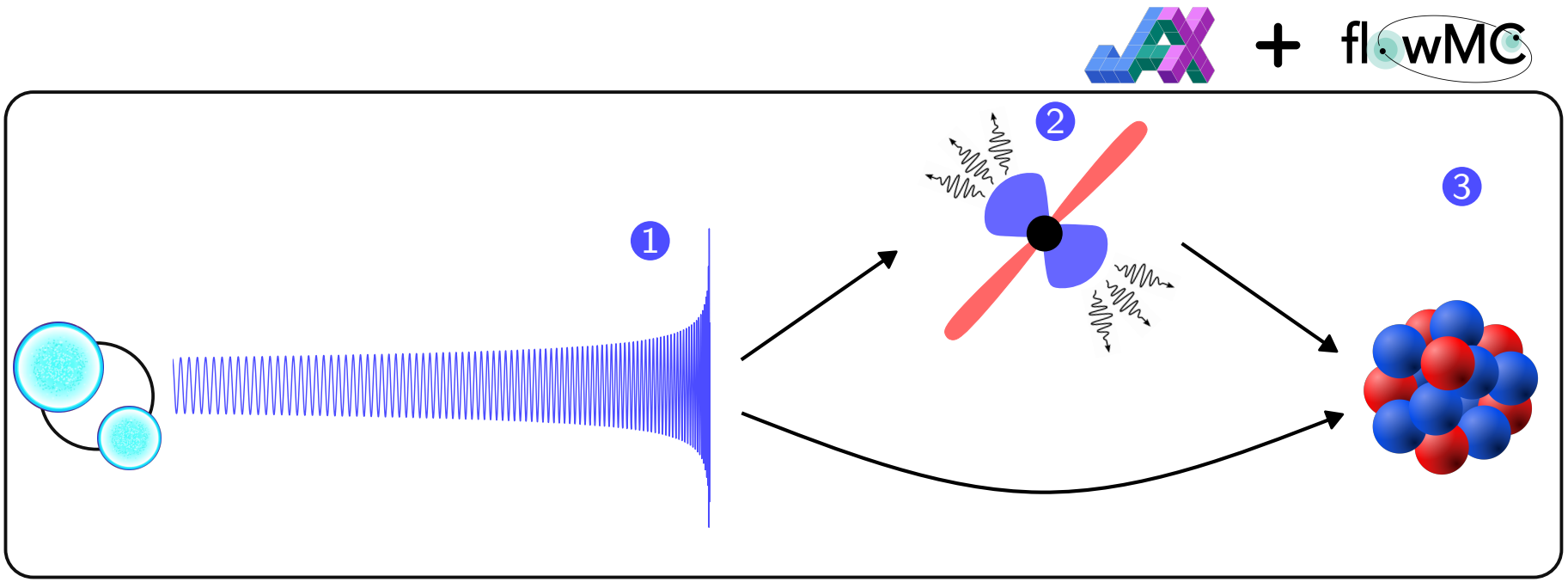
Overview

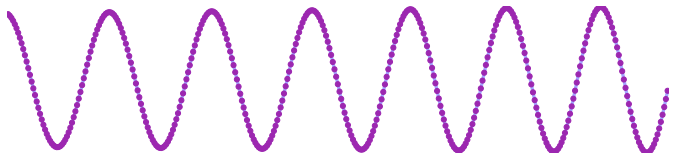
Analyzing a multi-messenger **binary neutron star** signal:

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



Gravitational waves: RIPPLE

- Waveforms on GPU: $\mathcal{O}(10^3)$ faster
- RIPPLE [11]: from LALSUITE to JAX



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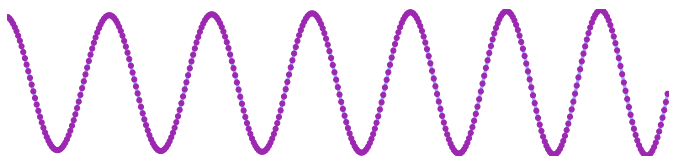

- Waveforms available in RIPPLE:
  - Binary black holes:
    - `IMRPhenomXAS`
    - `IMRPhenomD`
    - `IMRPhenomPv2`
  - Binary neutron stars:
    - `TaylorF2`
    - `IMRPhenomD_NRTidalv2`
    - `IMRPhenomPv_NRTidalv2` (by Nihar Gupte)
- Also see GWFAST [12] and SFTS [13]

Gravitational waves: JIM

Parameter estimation: JIM [14, 15]: RIPPLE + FLOWMC

- Verified for binary neutron stars in current generation detectors [15]
- Matches BILBY, passes *pp*-test

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- 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

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- 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

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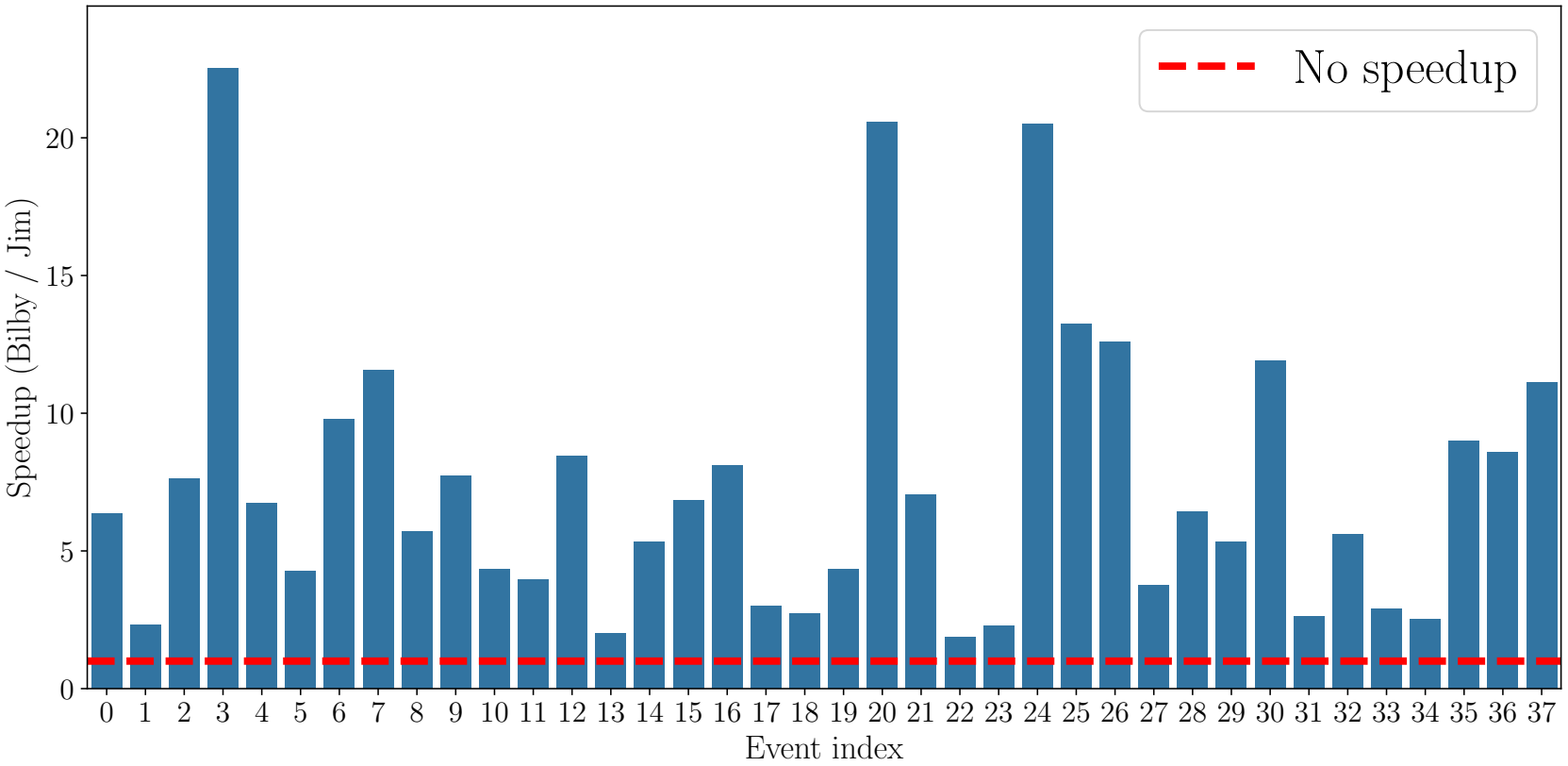
- Matches BILBY, passes *pp*-test
- Runtime: from hours to minutes
- Up to $5 - 10\times$ more effective samples (normalizing flow)
- More cost-effective/energy-efficient

		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

Gravitational waves: JIM reanalysis – Thomas Ng

- Re-analyze GWTC-3 with `IMRPhenomPv2`
- JIM on A800 GPU: on average ~ 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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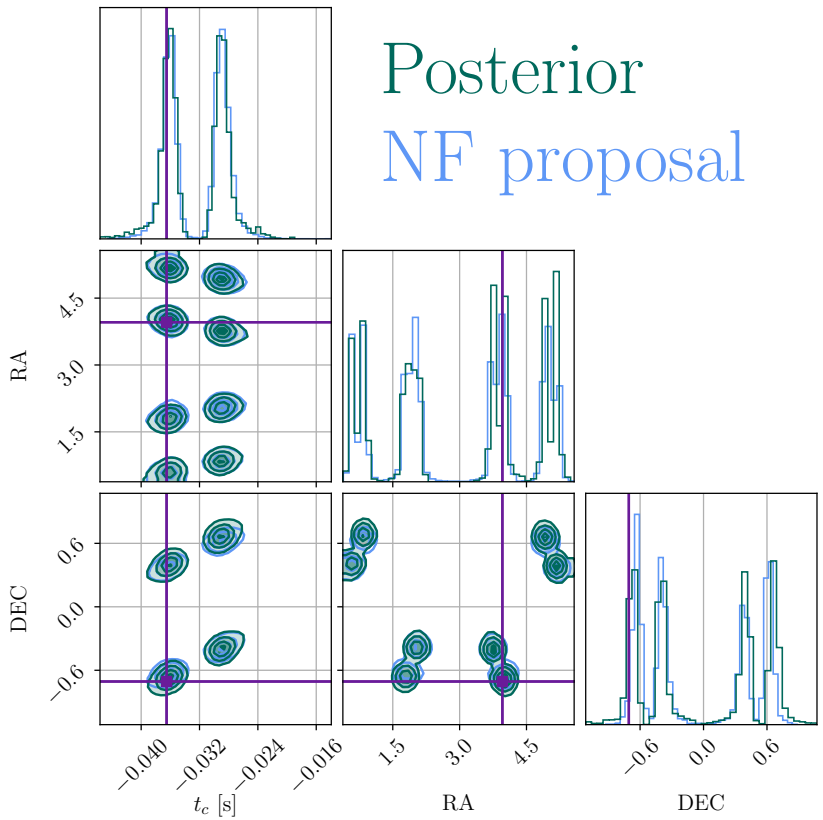
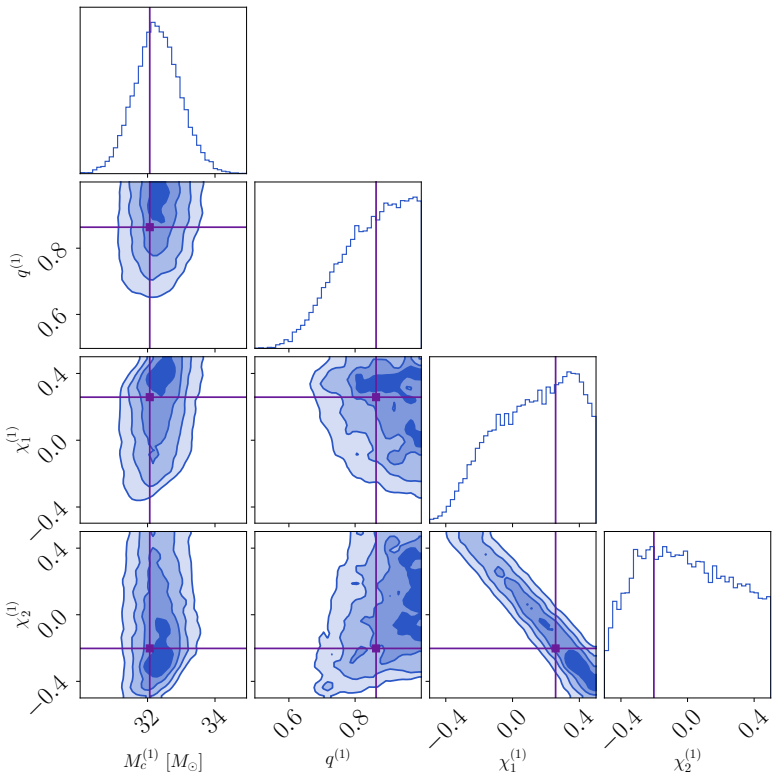
Work in progress: showing proof-of-concepts!

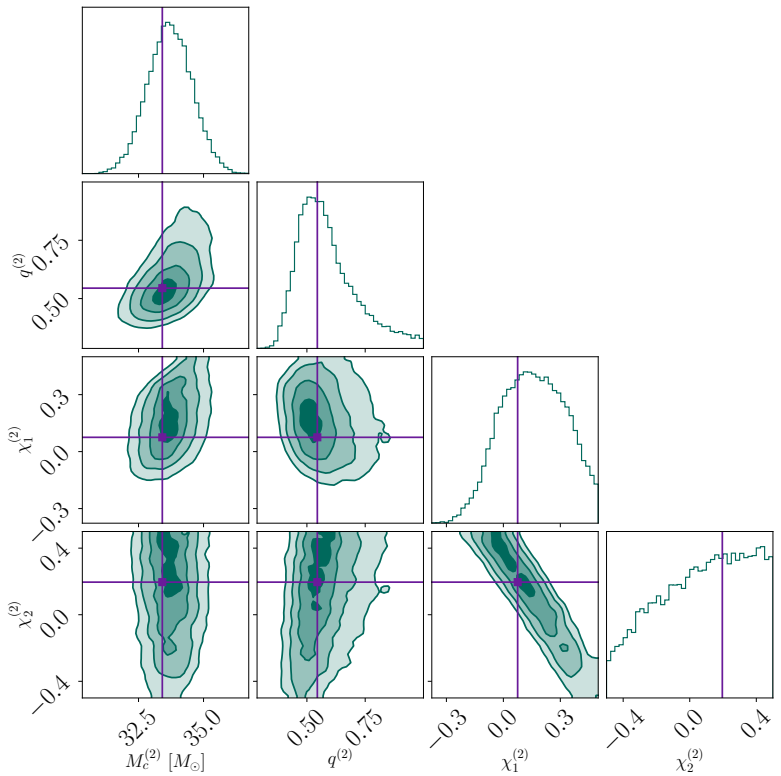
- ET posteriors are multimodal
- Normalizing flows help to jump between modes



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 [16])





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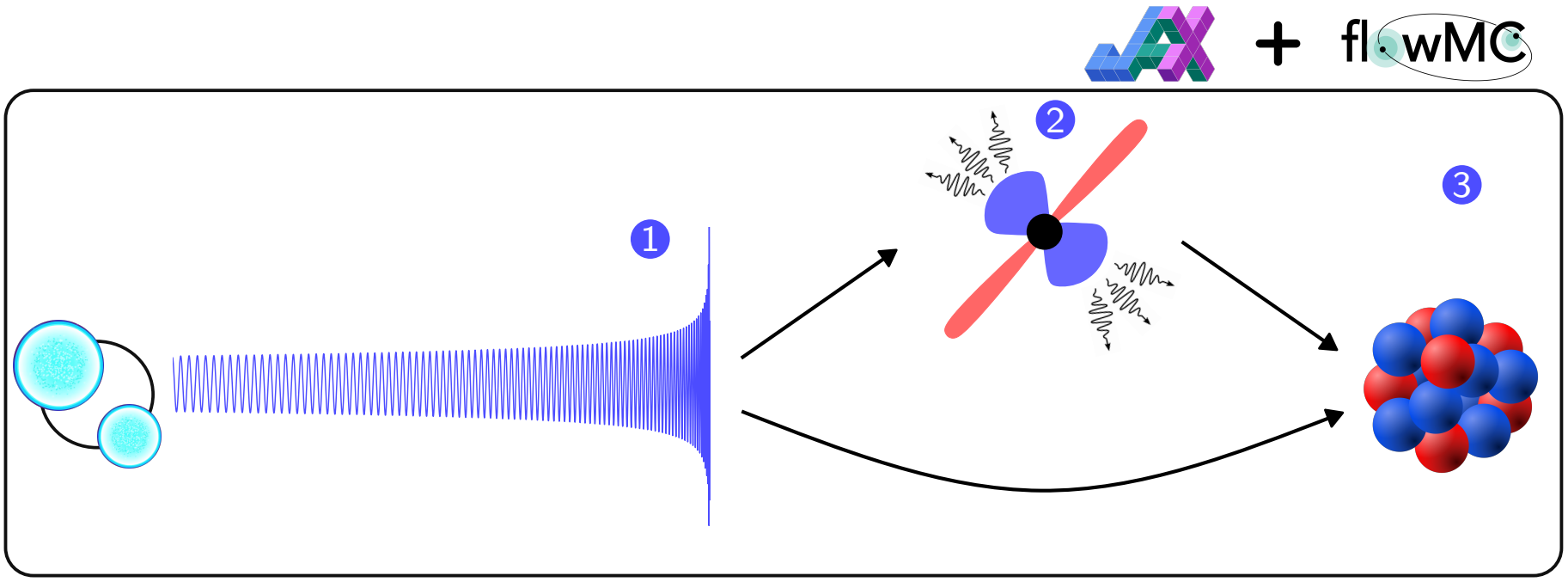
1. Gravitational waves
2. **Electromagnetic counterparts**
3. Nuclear equation of state



Electromagnetic counterparts (Hauke Koehn, Tim Dietrich)

- Kilonovae and GRB afterglows
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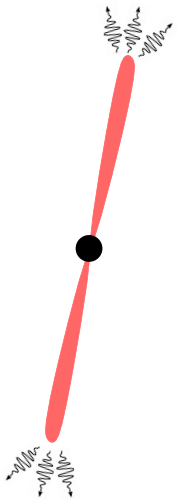
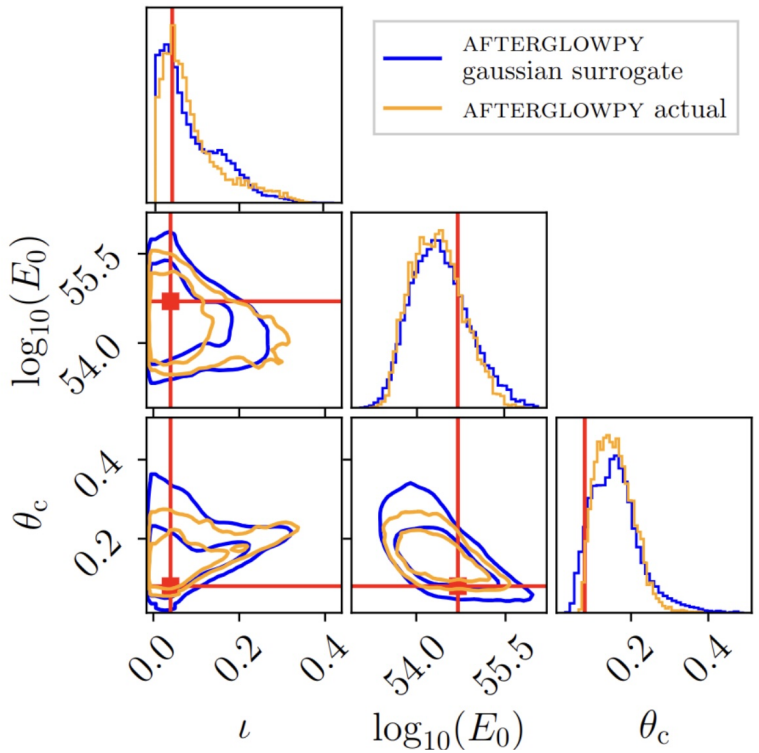


FIESTA

- 1m36s
- 1 H100 GPU

AFTERGLOWPY

- 4 hours
- 30 CPUs



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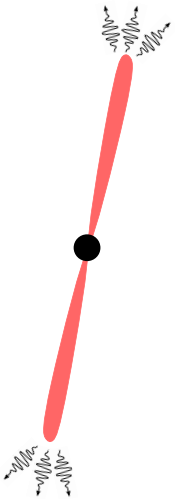
- Kilonovae and GRB afterglows
- Current libraries too large to 'jaxify' (e.g. AFTERGLOWPY [17])
- Neural network emulators for inference: FIESTA [18]
- Scales well for systematics 'nuisance parameters'



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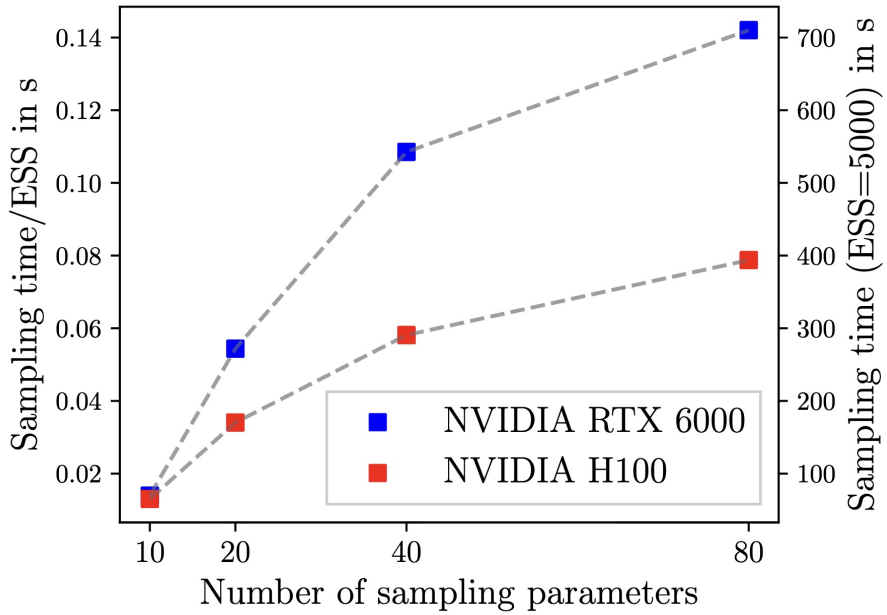

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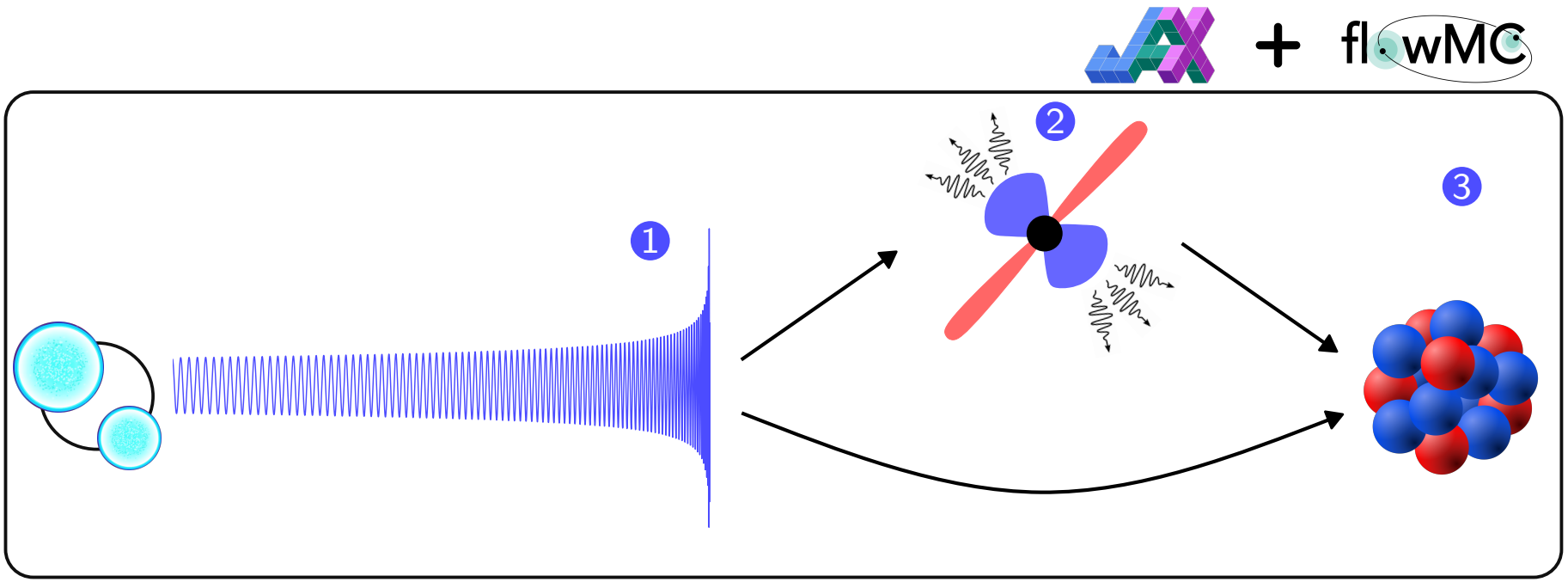
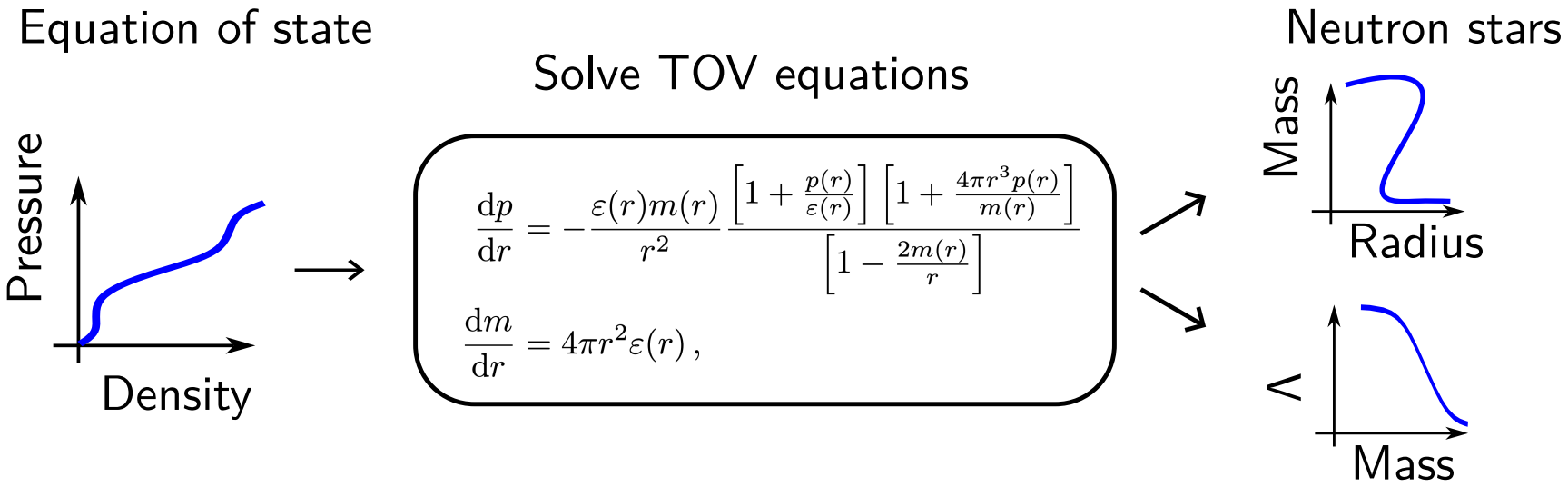
3. **Nuclear equation of state**



Equation of state inference

- Masses, radii, and tidal deformation of neutron stars
- Uniquely determined by the equation of state, have to solve the TOV equations

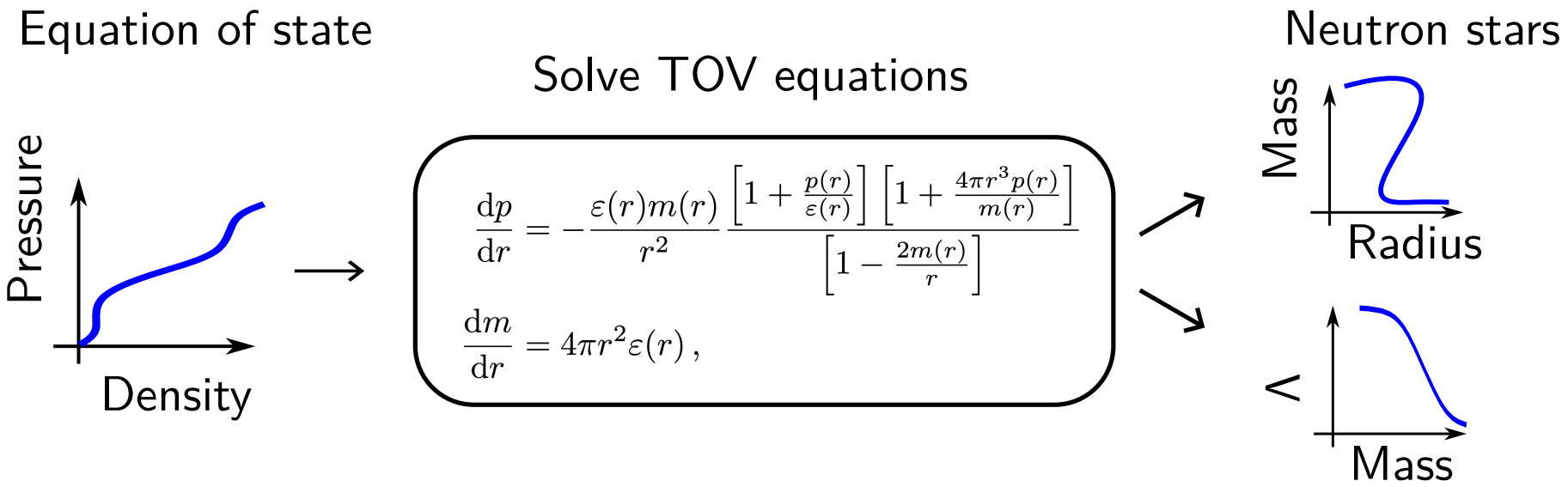


Equation of state

- Parametrization θ_{EOS}: constrain with Bayesian inference

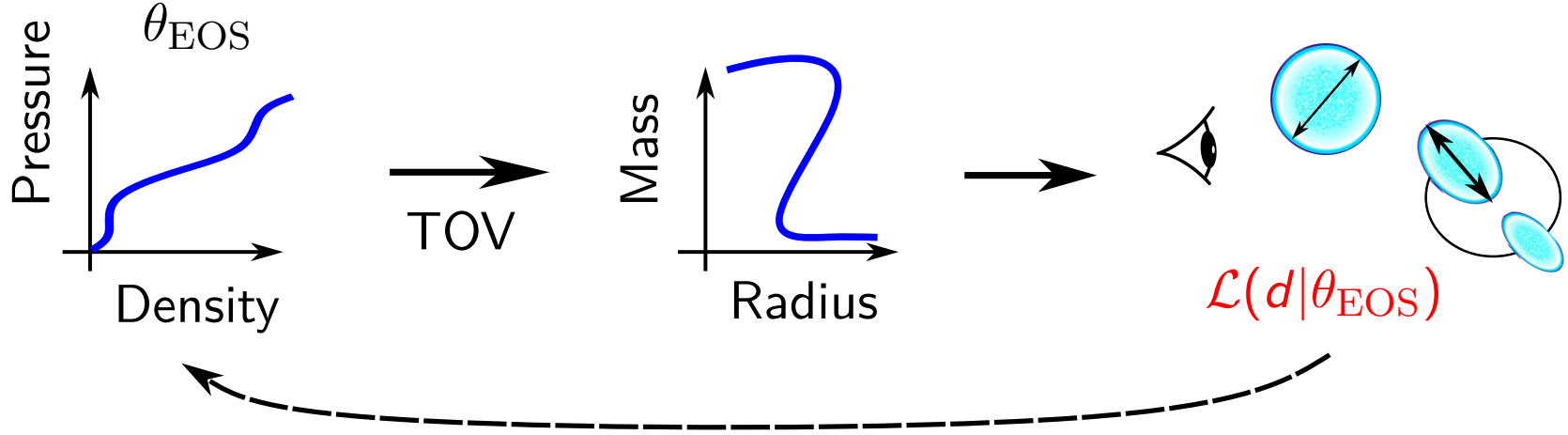
Equation of state

- Parametrization θ_{EOS}: constrain with Bayesian inference
- To predict neutron star properties, we solve the TOV equations: ordinary differential equations (ODEs)



Equation of state

- Parametrization θ_{EOS}: constrain with Bayesian inference
- To predict neutron star properties, we solve the TOV equations: ordinary differential equations (ODEs)
- Done for each sample θ_{EOS}: costly likelihood



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- Solving TOV equations (EOS $\rightarrow$ NS) is slow

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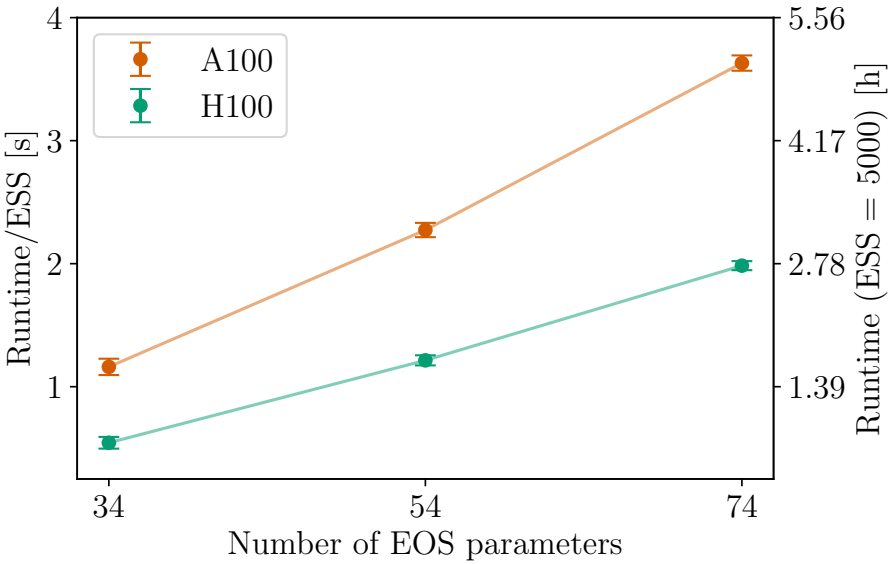
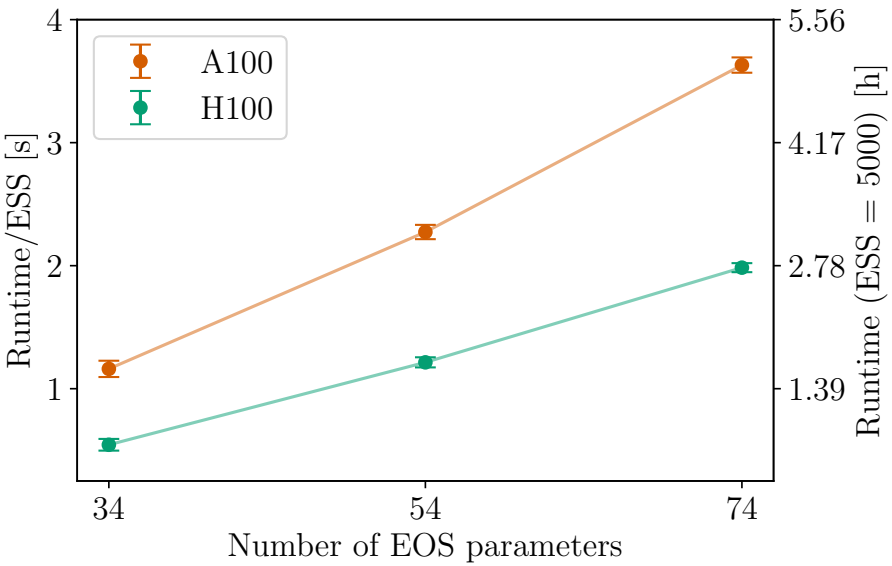
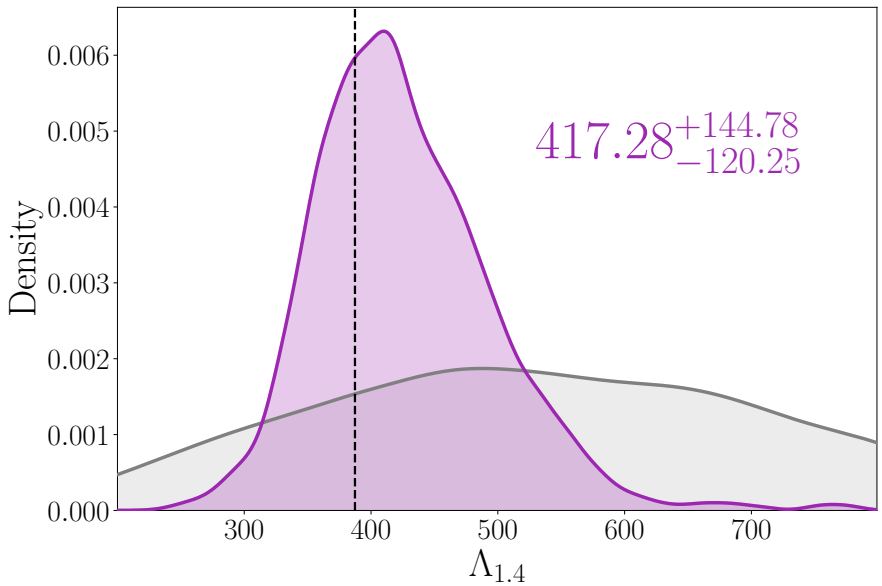


JESTER (Peter T.H. Pang)

- Solving TOV equations (EOS $\rightarrow$ NS) is slow
- JESTER [19]: JAX-based TOV solver
  - Full inference in ∼hours
  - No need for ML emulators
- End-to-end analysis: from gravitational waves of neutron star mergers to the equation of state
  - Example: 20 BNS in O5





Auto-differentiable ODE solvers

- ODE solvers in JAX are auto-differentiable (DIFFRAX )
- Frame inference as optimization problem:
  - Gradient descent on loss function $\mathcal{L}(\theta_{\mathrm{EOS}})$

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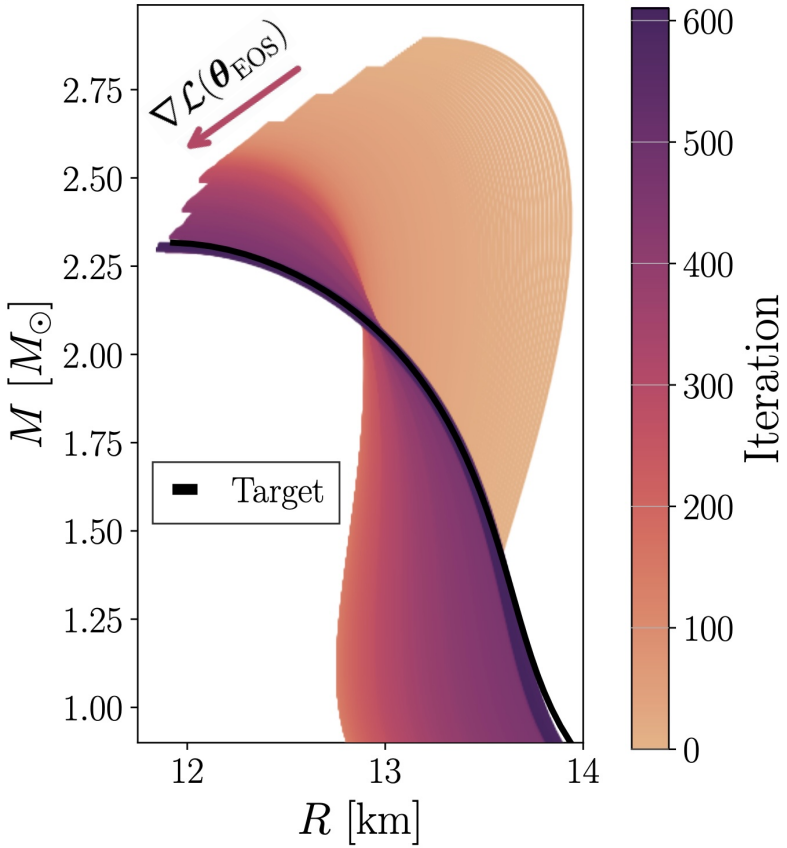
$$\mathcal{L}(\boldsymbol{\theta}_{\rm EOS}) = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{R_i(\boldsymbol{\theta}_{\rm EOS}) - \hat{R}_i}{\hat{R}_i}\right|$$



Contents

1 Introduction

2 Methods

3 Applications

4 Outlook and conclusion

Conclusion

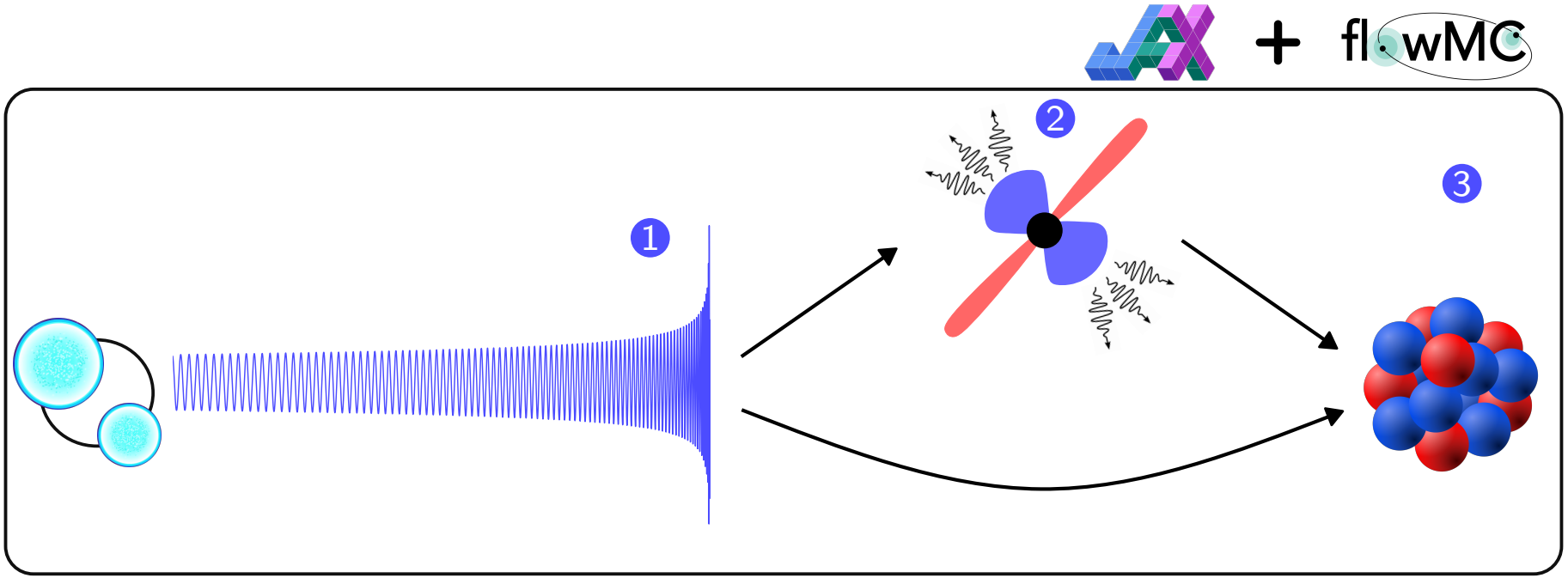
- Progress on scalable Bayesian inference, with minimal pre-training
- Hybrid acceleration: GPUs + normalizing flow proposals
  - JAX/GPU: faster likelihoods
  - FLOWMC: sampling converges faster
- Simulators in JAX can remove the need for emulators (GW, TOV)
- Auto-differentiable ODE solvers: inference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

Let's talk!

Thank you for your attention!

Software written in JAX:

- FLOWMC [9, 10]
- JIM [14, 15] ❶ ❷ ❹
- FIESTA ❷
- JESTER [19] (built with DIFFRAX) ❸
- HARMONIC [20–22]



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Evidence calculation: HARMONIC I

Evidence Z can be computed from posterior samples with HARMONIC [20] 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

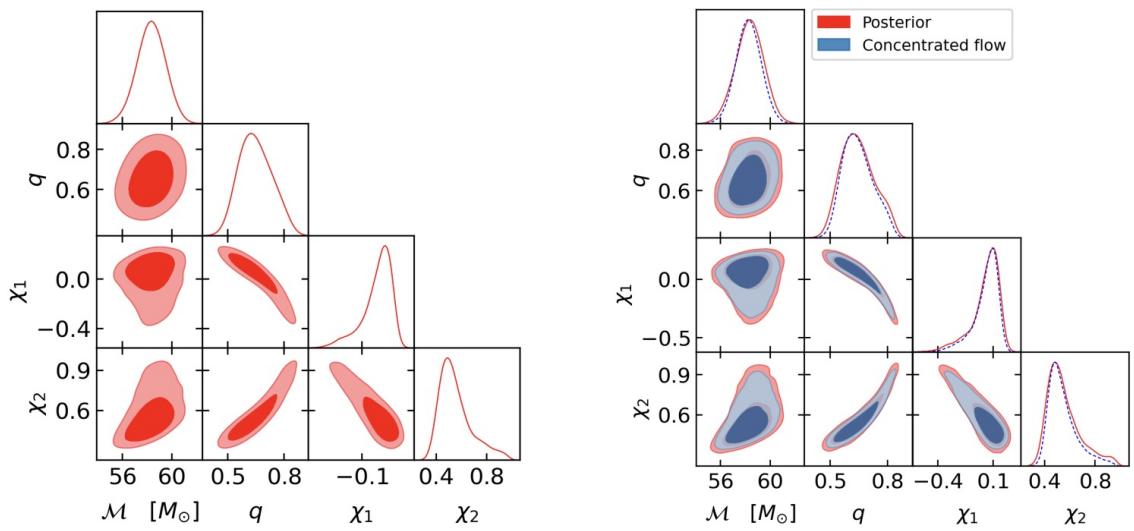
In practice, this can be achieved with a normalizing flow [21].

This has been verified to give accurate evidences (similar values as nested sampling) when GW posteriors are used [22].

HARMONIC with JIM [22]

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.

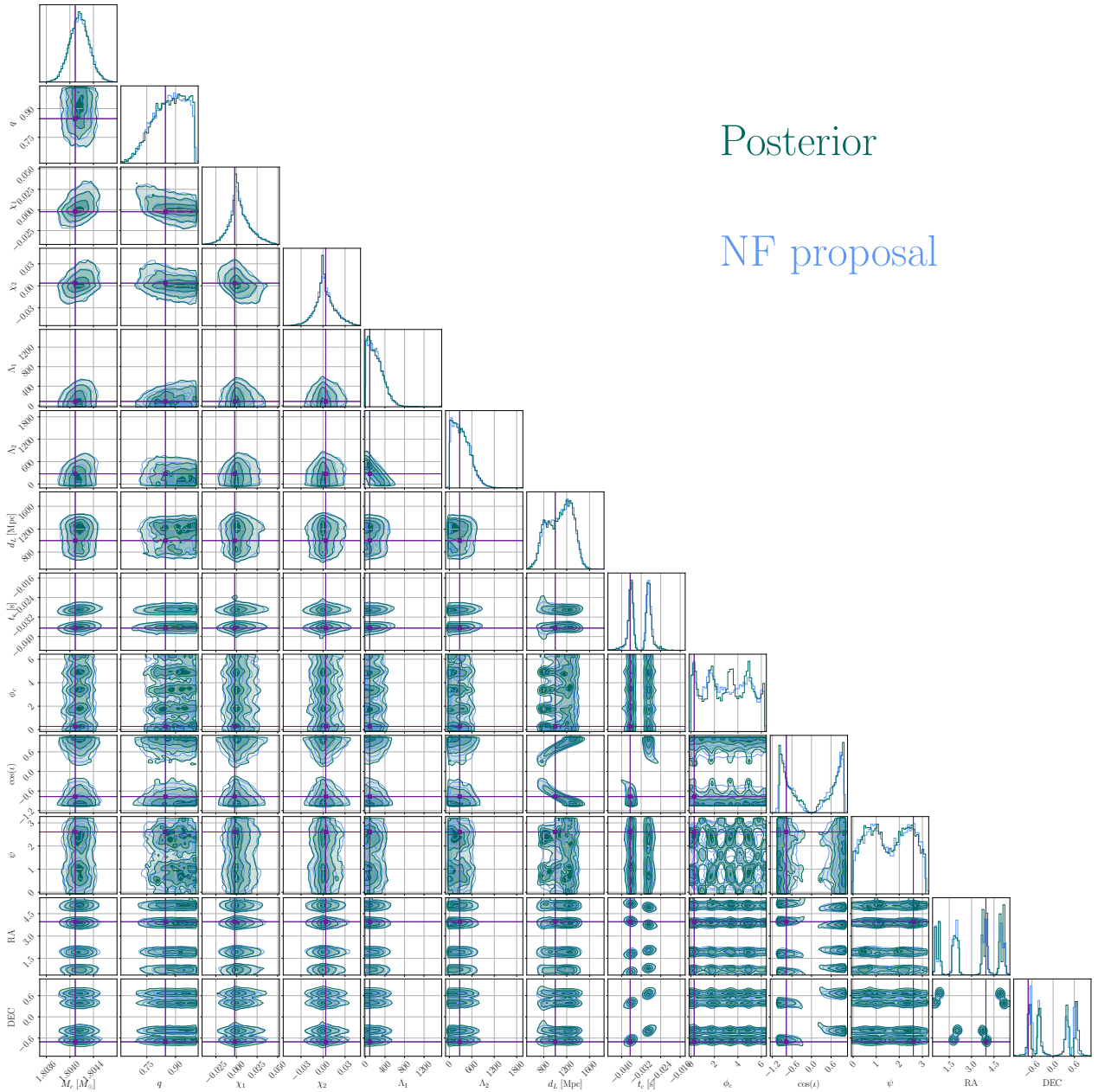
Example	Method	$\log(z)$	Sampling time	Evidence estimation time
4D	BILBY	390.33 ± 0.11	31.3 min	–
	JIM + `harmonic`	$390.360^{+0.006}_{-0.006}$	3.4 min	1.9 min
11D	BILBY	378.29 ± 0.15	3.5 h	–
	JIM + `harmonic`	$378.420^{+0.09}_{-0.08}$	11.8 min	2.4 min



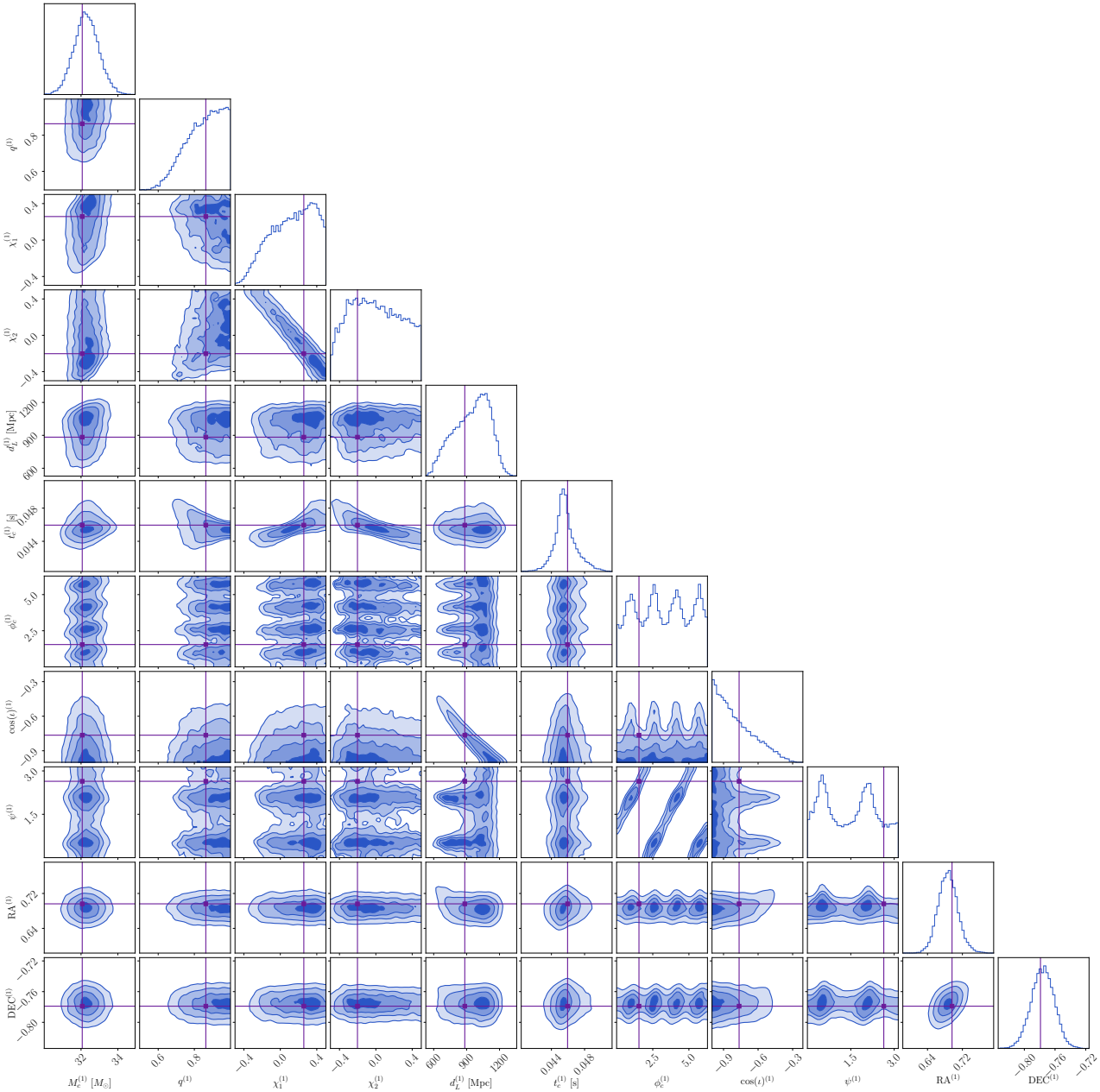
(a) BILBY (b) JIM + `harmonic`

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).

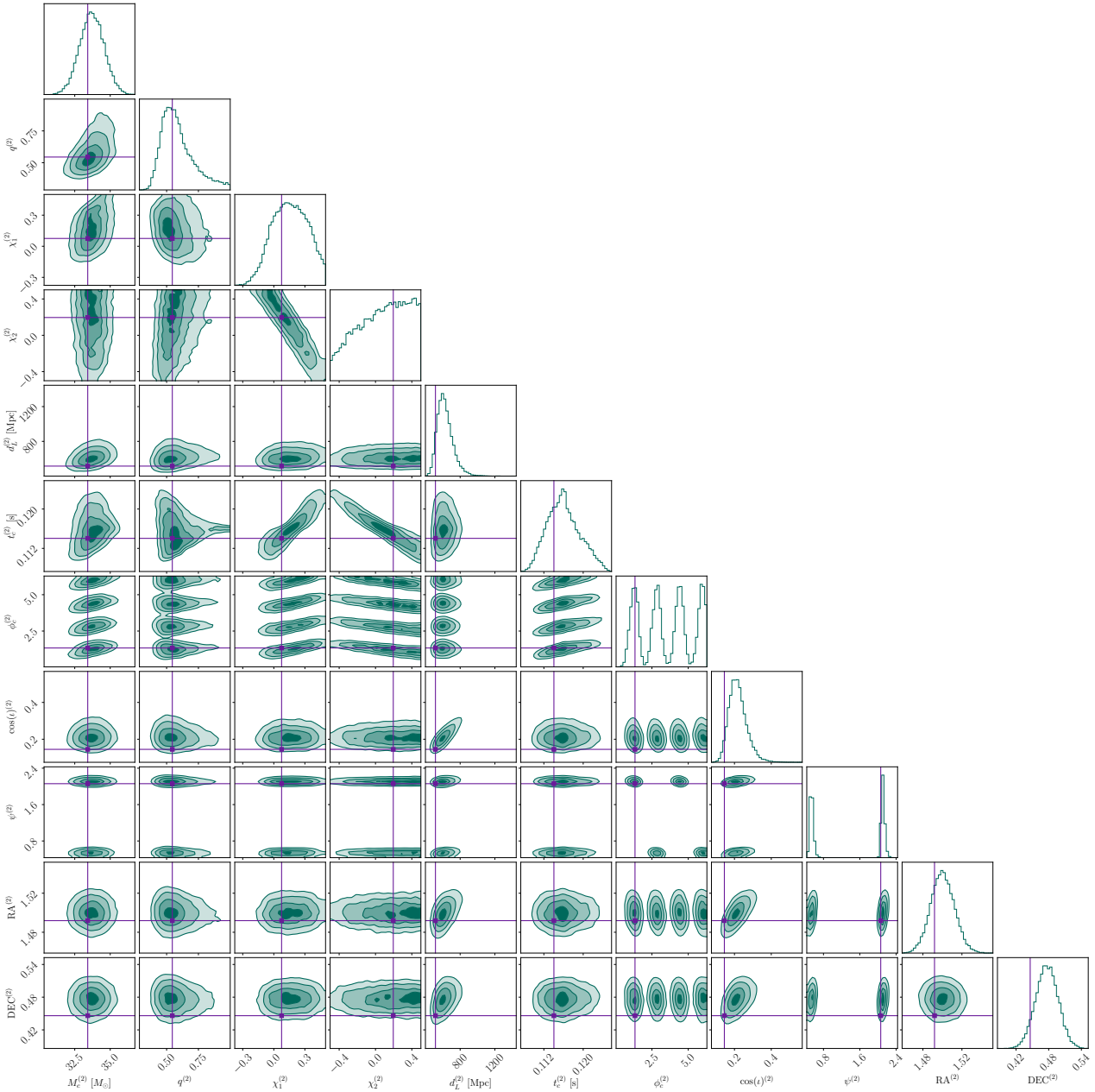
BNS in ET-Δ example: all parameters



Overlapping signals: all parameters signal A

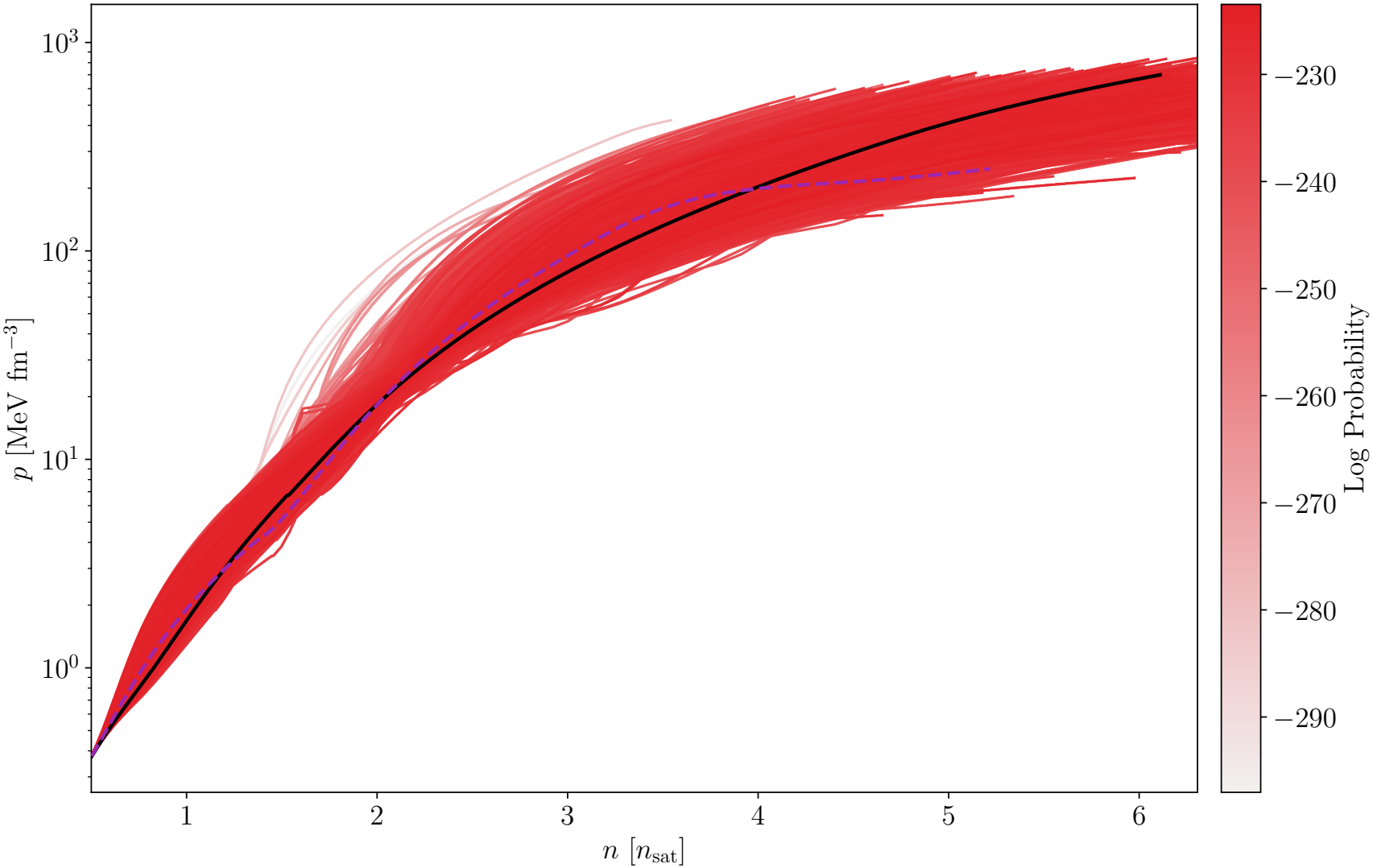


Overlapping signals: all parameters signal B



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