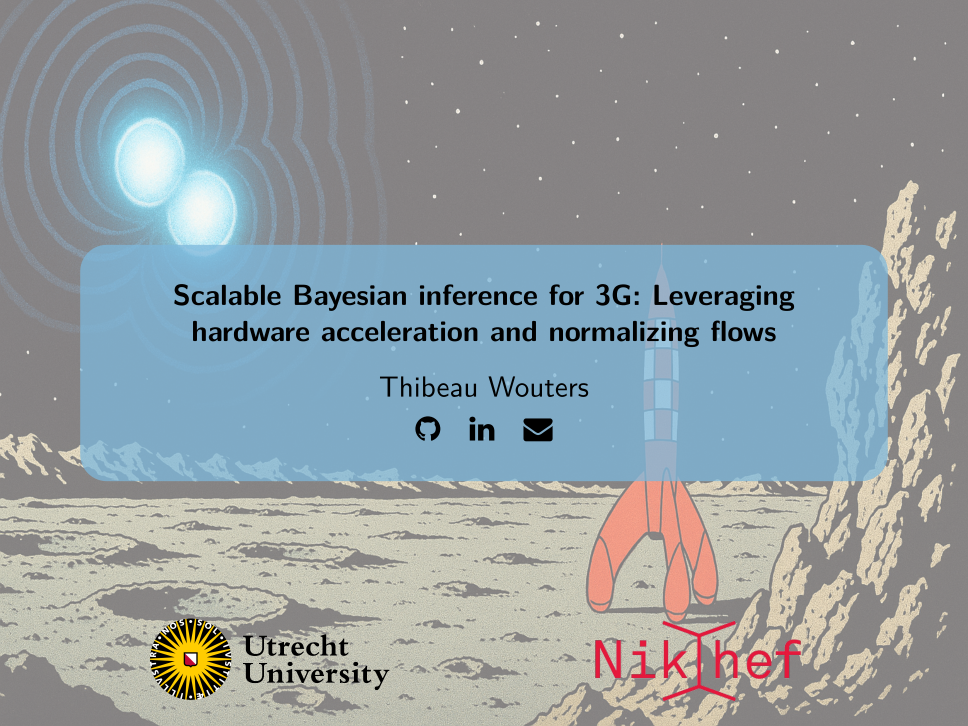

Scalable Bayesian inference for 3G: Leveraging hardware acceleration and normalizing flows

Thibeau Wouters

Utrecht University

Nikhef

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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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What about 3G detectors?

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

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

Towards scalable inference

Ingredients to make inference scalable:

- Hardware acceleration: GPUs for parallel computations
- Normalizing flows (NFs): neural density estimators

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- Hybrid approach: faster likelihoods + NF proposals
  - + No pre-training: more flexibility
  - − Re-implement software
  - Also see Luca Negri's poster: neural likelihood estimators

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- **Hybrid approach: faster likelihoods + NF proposals → this talk**
  - \+ No pre-training: more flexibility
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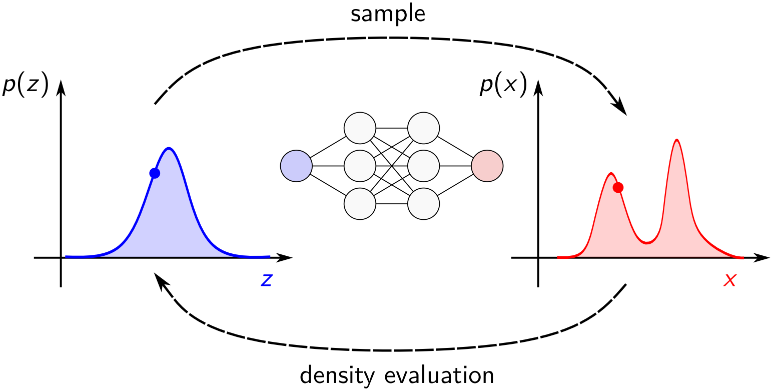
Normalizing flows (NFs)

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



Acceleration with JAX features:

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

JAX & FLOWMC

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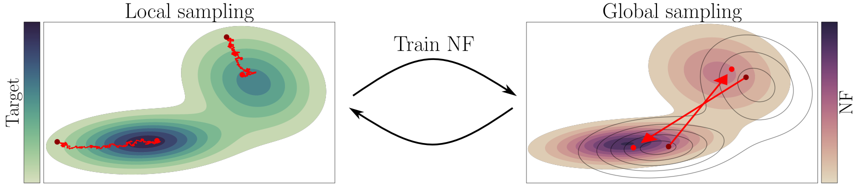
FLOWMC [7, 8]: MCMC + normalizing flows + JAX

- MCMC chains as training data: no pre-training
- Also see NESSAI [9, 10]



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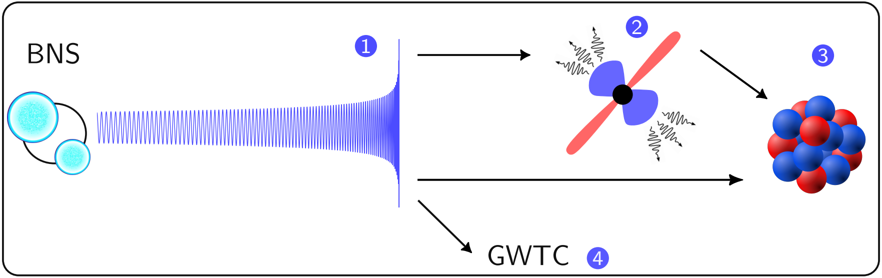
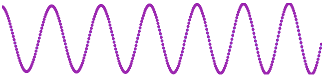
Analyzing a multi-messenger **binary neutron star** (BNS) signal:

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



Gravitational waves

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



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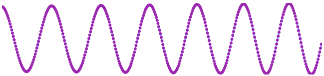

- Parameter estimation: JIM [12, 13]
- BNS in LVK analyzed in $\sim$ 15 min

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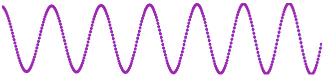
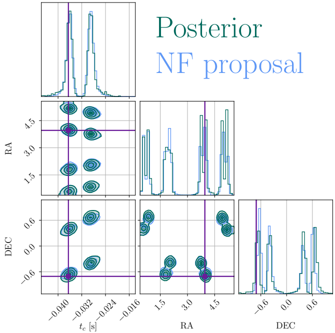


- Parameter estimation: JIM [12, 13]
- BNS in LVK analyzed in ~ 15 min
- Ongoing work for ET – example:
  - BNS, $f_{\min} = 20$ Hz, SNR $= 21$
  - ET-Δ, `IMRPhenomD_NRTidalv2`
  - 30 mins on H100 GPU
- Evidence: HARMONIC [14]



Overlapping signals

- In 3G, we expect to see overlapping signals
- Assess scaling: BBH+BBH in LVK

Either 61 or 102 or one of the later ones, need to check in detail

Overview

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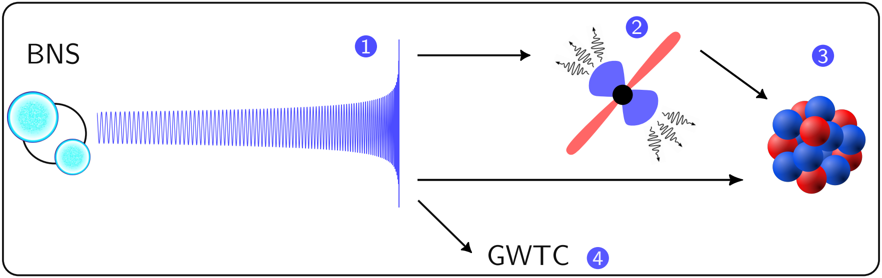
+ flowMC



Electromagnetic counterparts (Hauke Koehn, Tim Dietrich)

- BNS mergers lead to kilonovae, gamma-ray bursts
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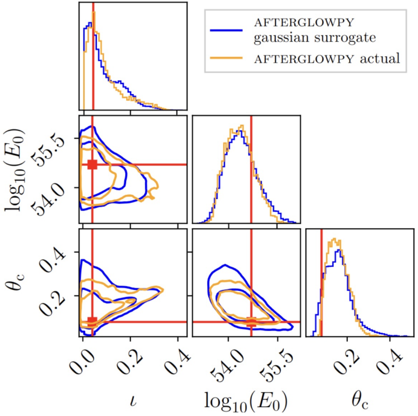
- BNS mergers lead to kilonovae, gamma-ray bursts
- Numerical models are too expensive (e.g. AFTERGLOWPY [15])
- Neural network surrogates for inference: FIESTA

FIESTA surrogates

- 1m36s
- 1 H100 GPU

AFTERGLOWPY

- 4 hours
- 30 CPUs



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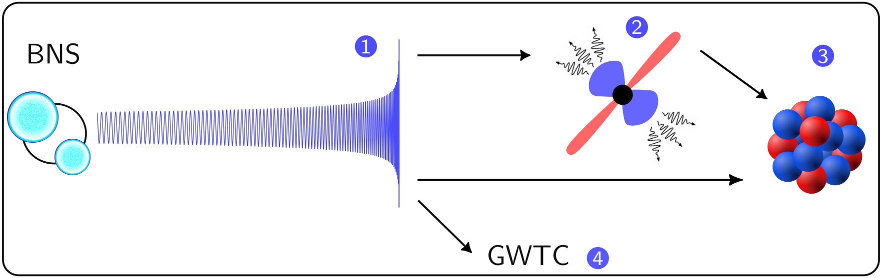

Equation of state inference

- Goal: infer nuclear equation of state (EOS) of neutron stars [16]
- Computational bottleneck: solve TOV equations

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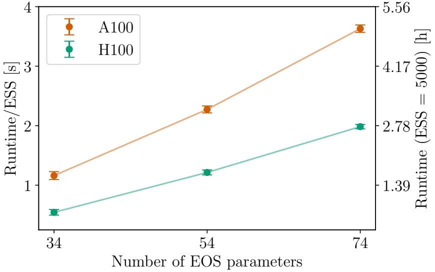
  - Full inference in ∼hours
  - No need for machine learning surrogates



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- JESTER [17]: JAX-based TOV solver
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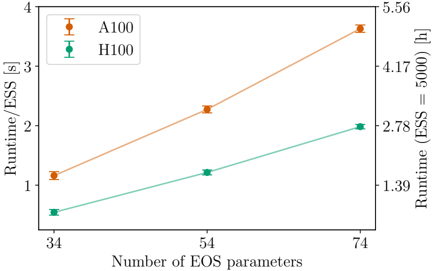
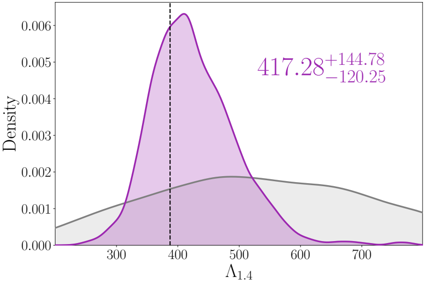
- End-to-end analysis: constrain EOS from 20 BNS in O5





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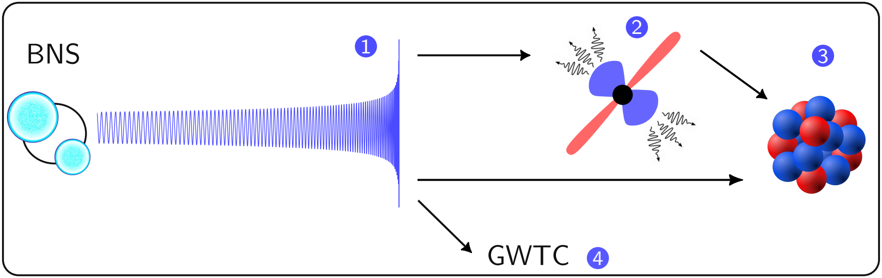
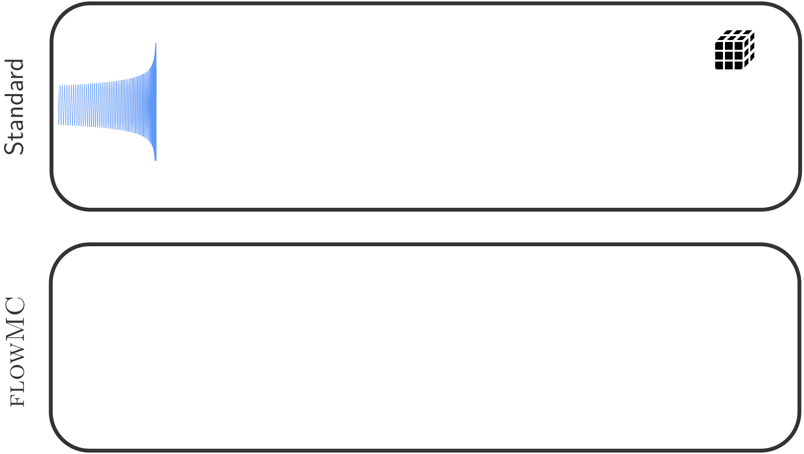


Gravitational wave transient catalogue

How can we use the trained normalizing flow proposal from FlowMC?



Conclusion

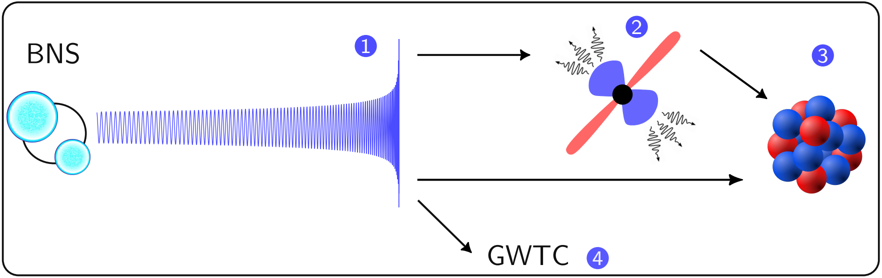
- Progress on scalable Bayesian inference software for 3G, with minimal amount of pre-training
- Hybrid acceleration: GPU + normalizing flow
  - JAX/GPU: likelihoods faster
  - FLOWMC: sampling converges faster
- Goal: joint multimessenger analyses in ~hours (NMMA [18] in JAX)
- To do
  - GW injection studies for ET
  - More waveform models in JAX
  - Equation of state study with ET data

Let's talk!

Thank you for your attention!

Software:

- FLOWMC [7, 8]
- JIM [12, 13] 1 2 4
- FIESTA 2
- JESTER [17] 3
- HARMONIC [14, 19, 20]



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Evidence calculation: HARMONIC I

Evidence Z can be computed from posterior samples with HARMONIC [19] 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 [20].

This has been verified to give accurate evidences (similar values as nested sampling) when GW posteriors are used [14].

BNS in ET-Δ example: all parameters