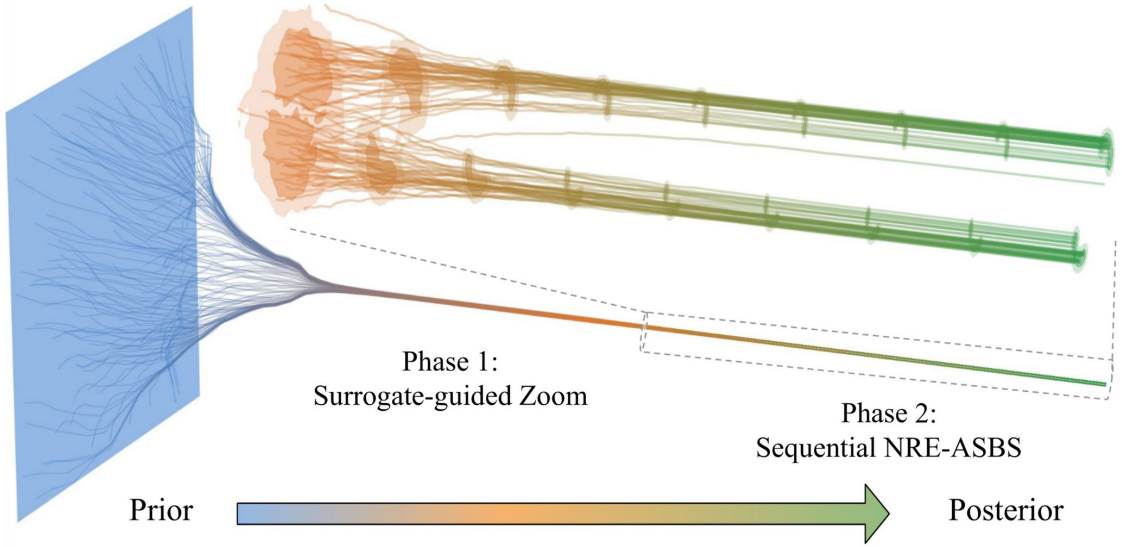
Rapid Simulation Based Inference

Uros Zivanovic, Rahul Srinivasan, Roberto Trotta and Andre Scaffidi

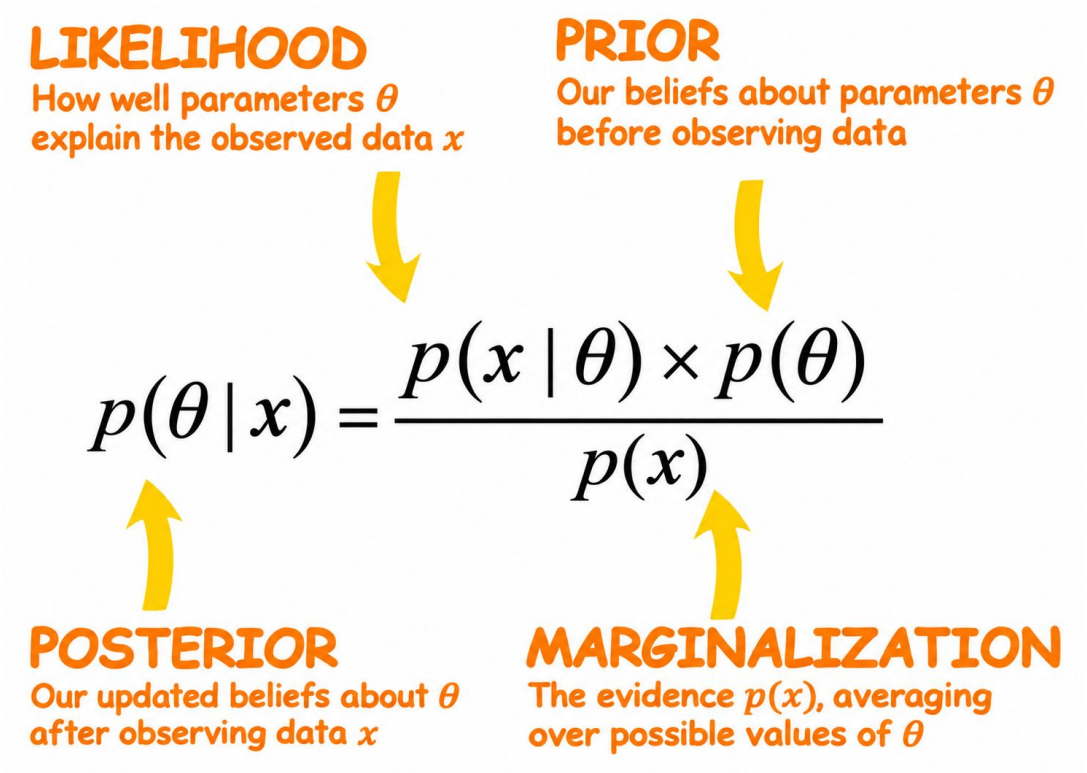


imprs-is
EMPIRICAL INFERENCE
MAX PLANCK INSTITUTE FOR INTELLIGENT SYSTEMS

NEURAL INFORMATION PROCESSING SYSTEMS

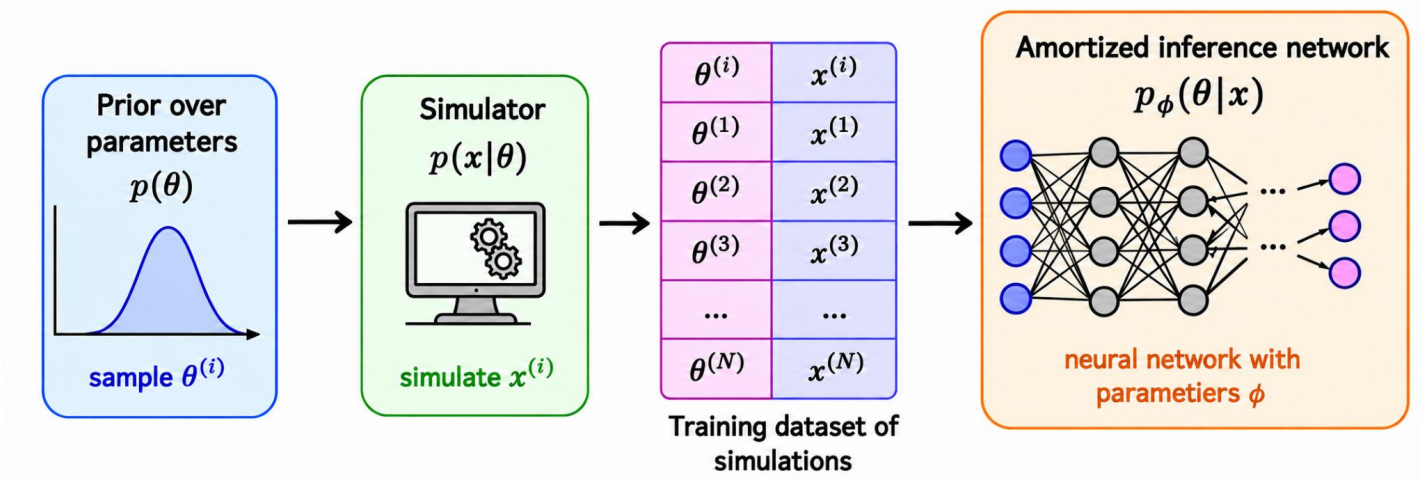
SISSA DATASCIENCE
Machine Learning for the Natural Sciences

Bayesian inference



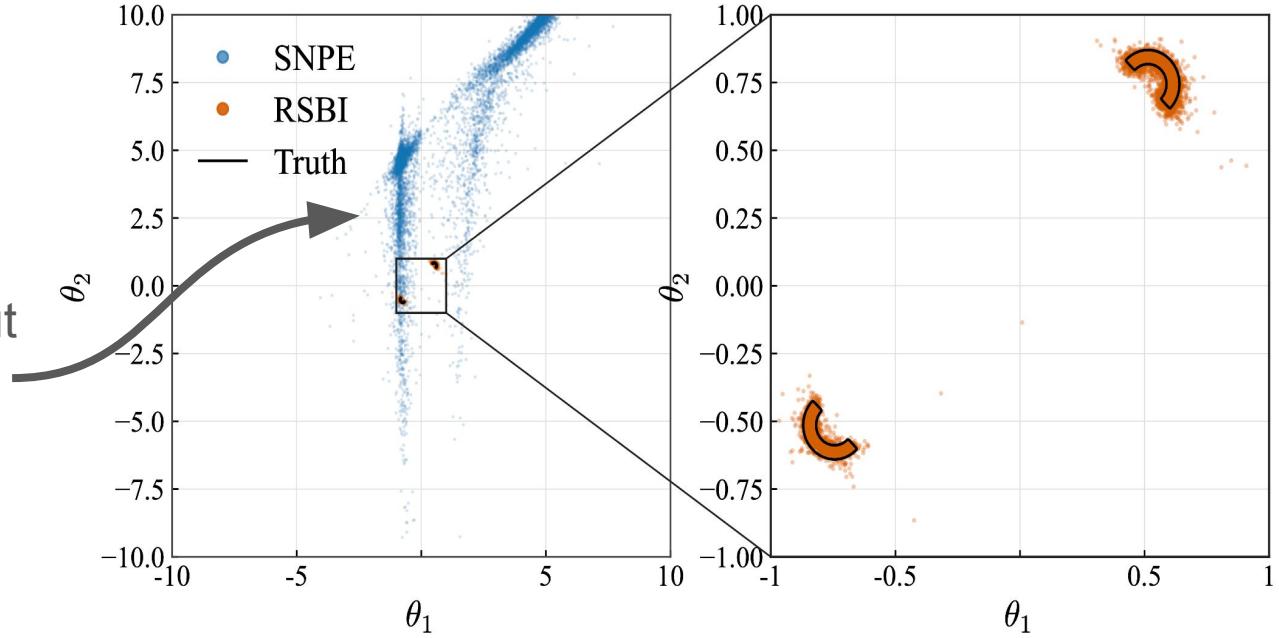
Simulation Based Inference (SBI)

- Goal is to learn posterior distribution from simulator, parameter pairs.
- Usually done via learning a density family (e.g normalising flow).



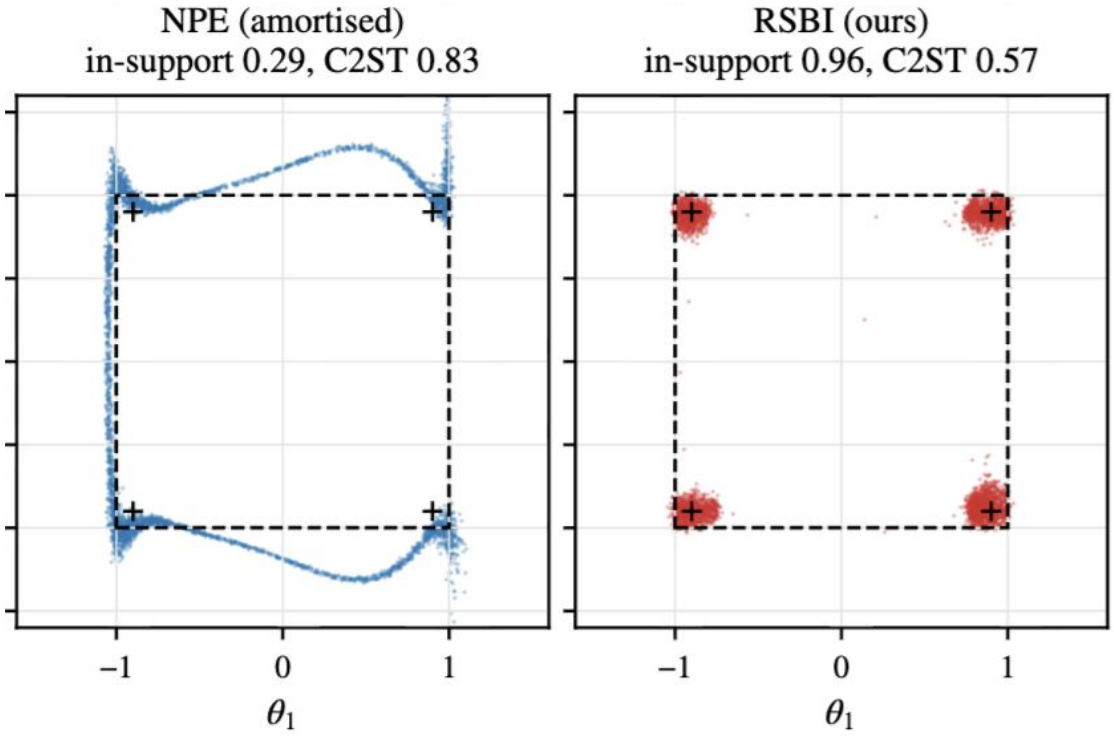
Where do standard SBI methods fall flat?

They spend time simulating (θ,x) pairs out here!

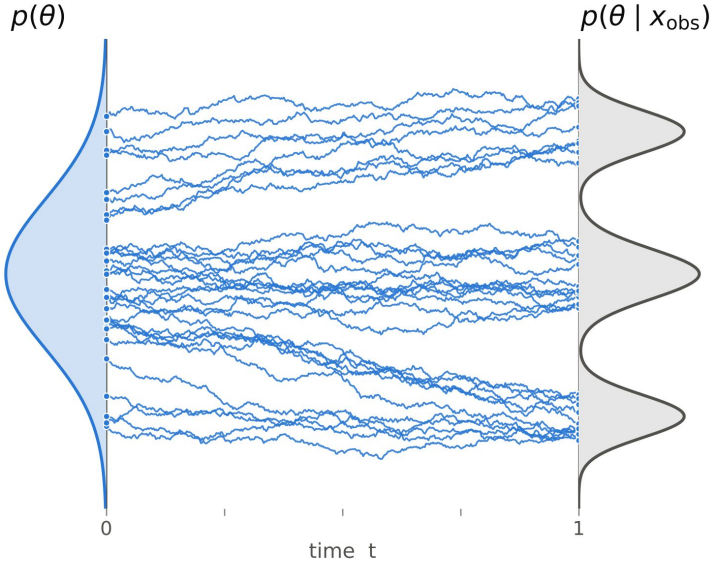


Where do standard SBI methods fall flat?

SBI methods that learn density estimators cana suffer from leakage



Diffusion for SBI:
Adjoint Schrödinger Bridge (SB) Sampling



Sampling from a Boltzmann distribution:

$$v(x) = \frac{e^{-E(x)/T}}{Z}, \qquad Z = \int_{\mathcal{X}} e^{-E(x)/T} dx < \infty$$

Schrödinger Bridge formulation:

$$u^* = \arg\min_u D_{\mathrm{KL}}(p^u || p^{\mathrm{base}}) = \arg\min_u \mathbb{E}_{\mathbb{X}\sim p^u}\left[\int_0^1 \frac{1}{2}||u_t(X_t)||^2 dt\right],$$

$$\text{s.t. } dX_t = \sigma_t u_t(X_t)dt + \sigma_t dW_t, \quad X_0 \sim \mu(X_0), \quad X_1 \sim v(X_1).$$

What is RSBI?

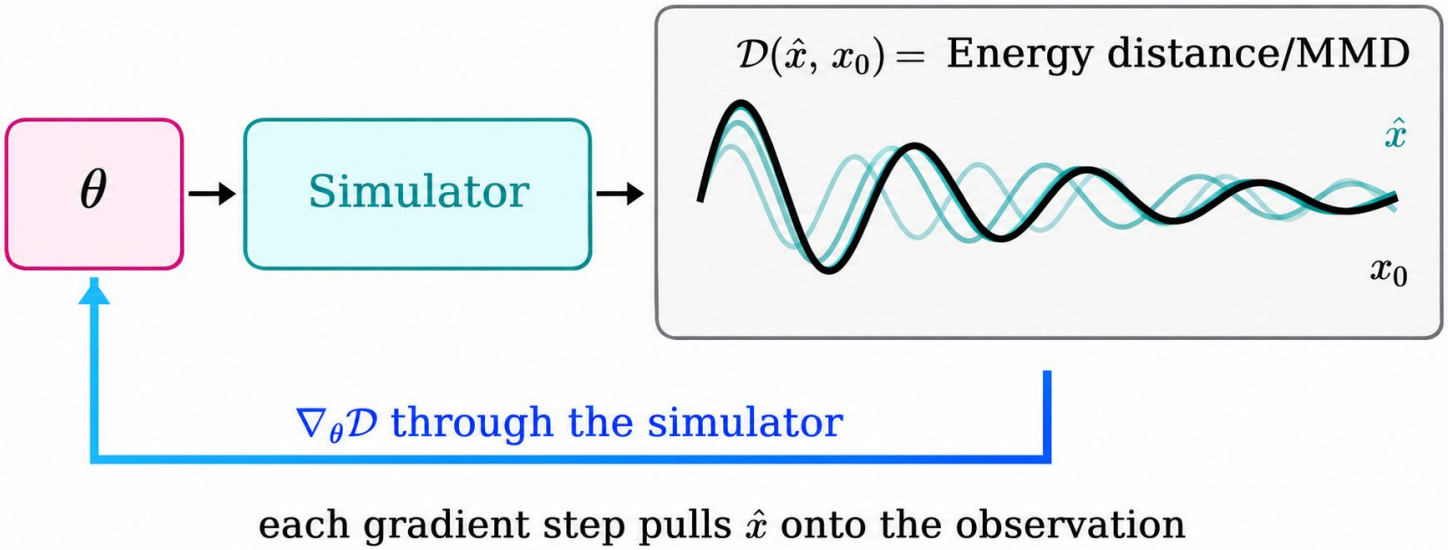
RSBI is a **two-phase diffusion-based SBI** method.

1) Leverage simulator gradients to ‘zoom in’ on posterior mass.
2) Refine the posterior modes

What is RSBI?

RSBI is a **two-phase diffusion-based SBI** method.

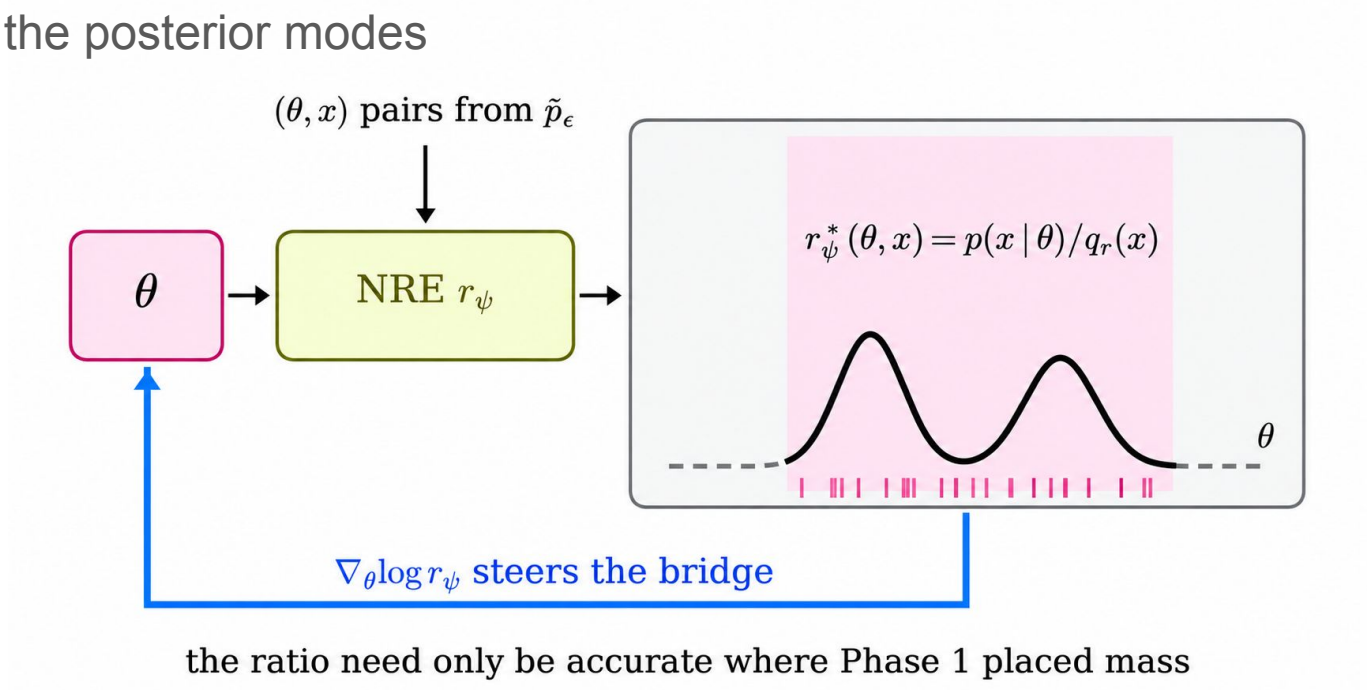
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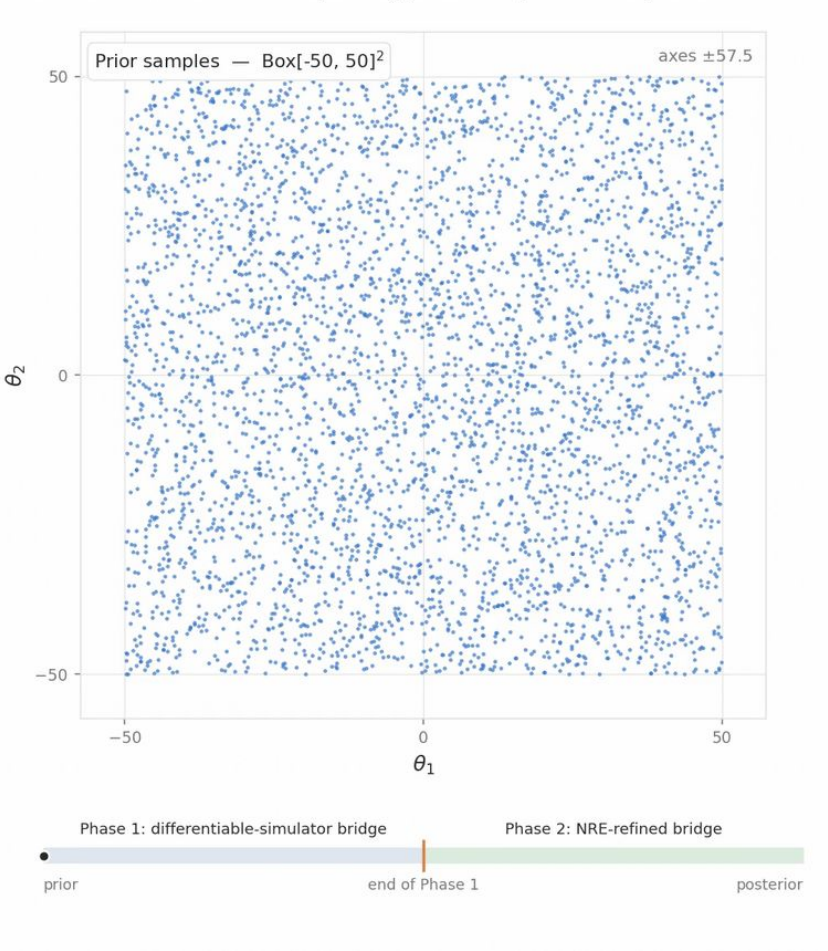


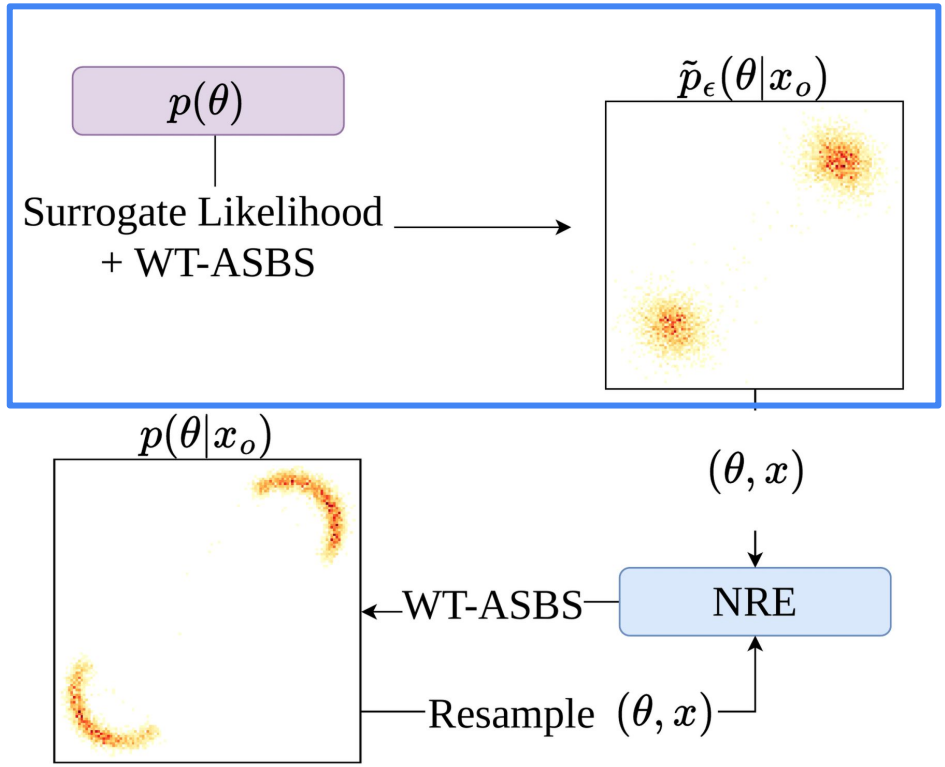
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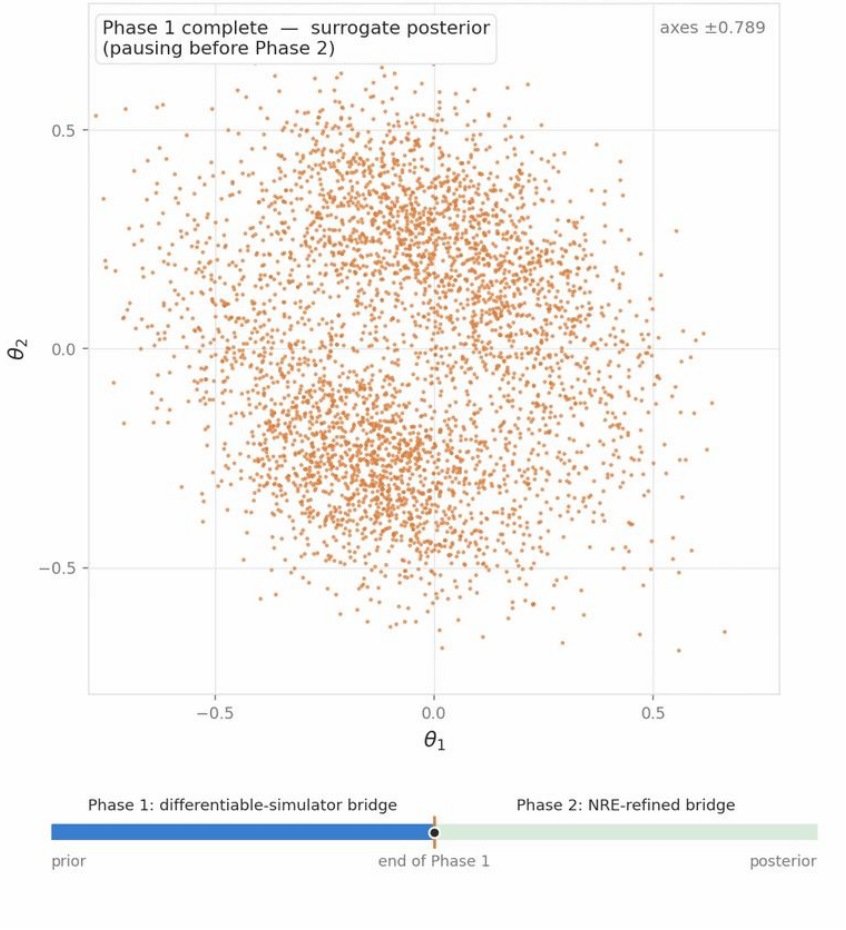
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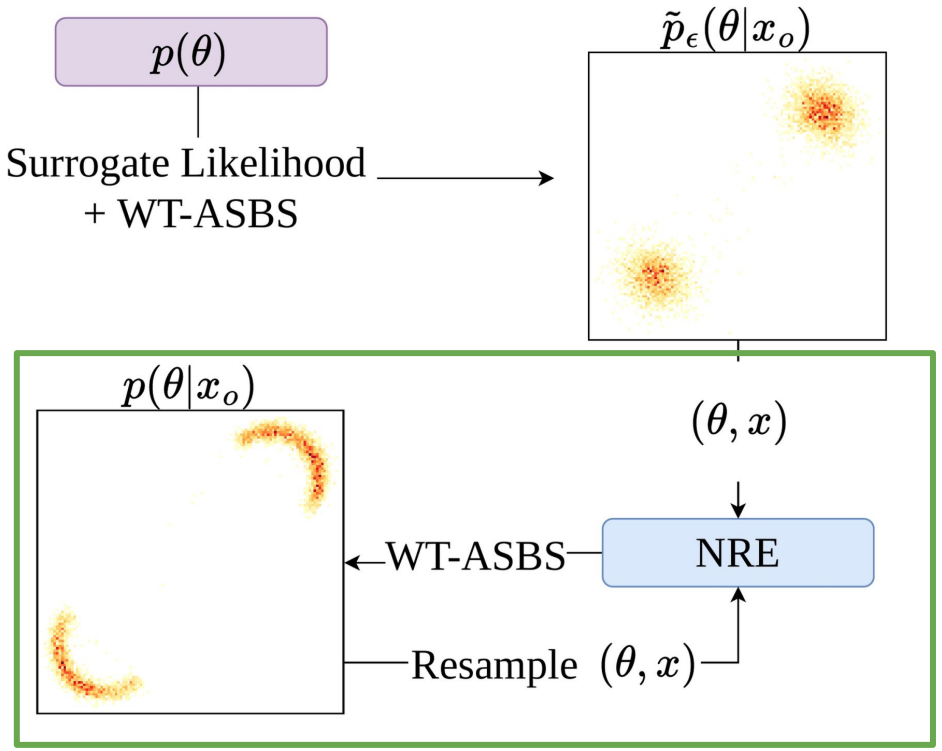
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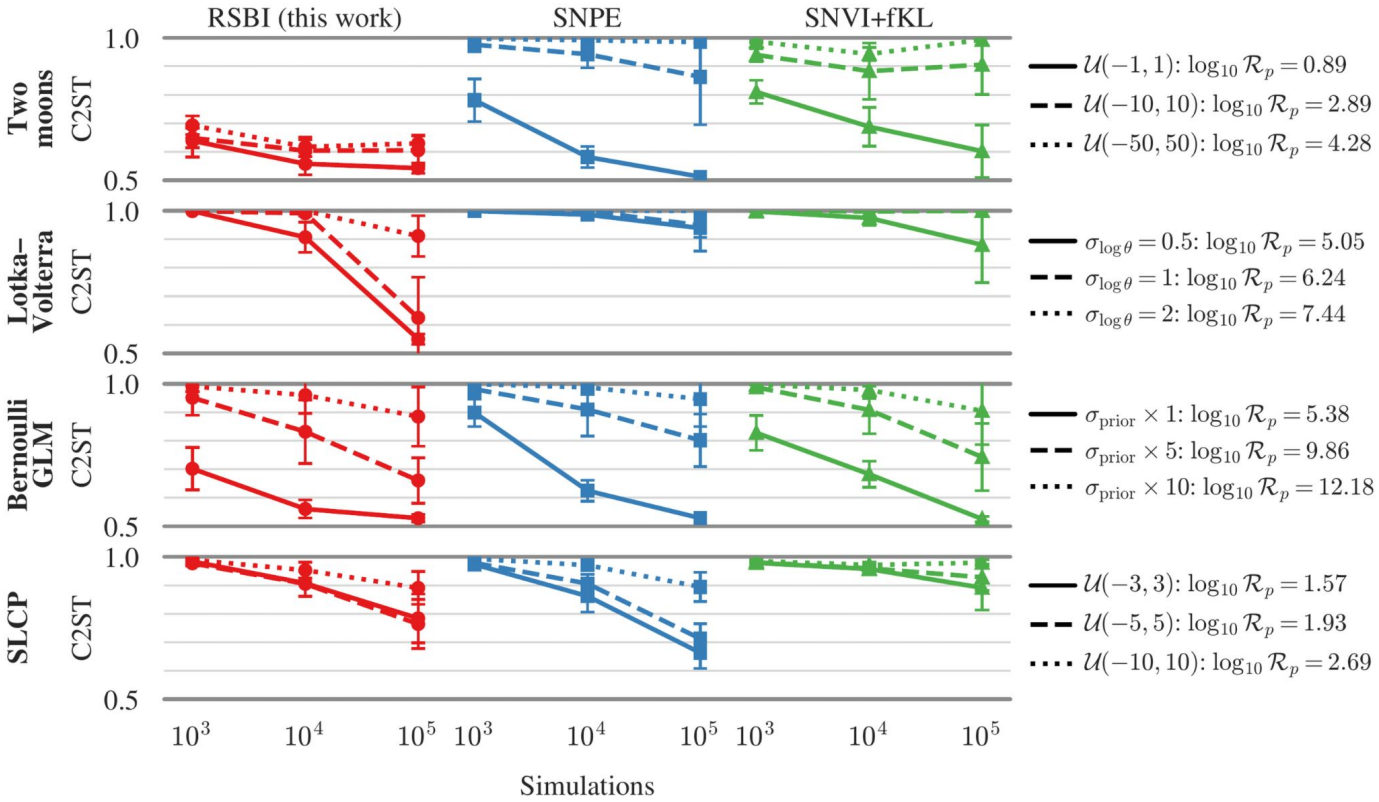

Prior samples — Box[-50, 50]²
axes ±57.5
50
0
−50
θ_2
−50
0
50
θ_1
Phase 1: differentiable-simulator bridge
Phase 2: NRE-refined bridge
prior
end of Phase 1
posterior


$p(\theta)$
Surrogate Likelihood
+ WT-ASBS
$\tilde{p}_\epsilon(\theta|x_o)$
$p(\theta|x_o)$
(θ, x)
WT-ASBS
NRE
Resample (θ, x)

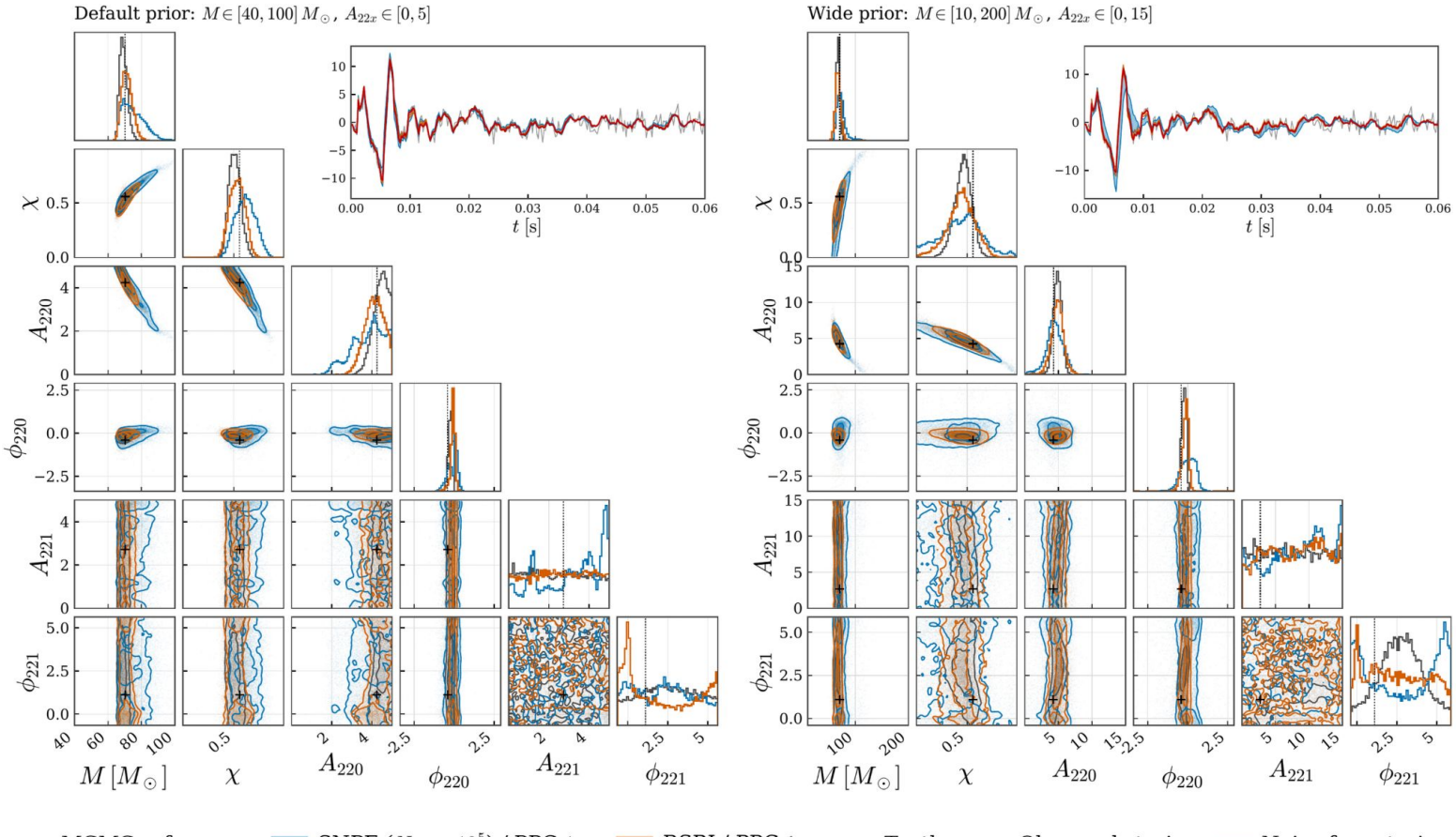

Phase 1 complete — surrogate posterior
(pausing before Phase 2)
axes ±0.789
0.5
0.0
−0.5
θ_2
−0.5
0.0
0.5
θ_1
Phase 1: differentiable-simulator bridge
Phase 2: NRE-refined bridge
prior
end of Phase 1
posterior


$p(\theta)$
Surrogate Likelihood
+ WT-ASBS
$\tilde{p}_\epsilon(\theta|x_o)$
$p(\theta|x_o)$
(θ, x)
WT-ASBS
NRE
Resample (θ, x)

Benchmarks


RSBI (this work)
SNPE
SNVI+fKL
Two moons
Lotka–Volterra
Bernoulli GLM
SLCP
C2ST
1.0
0.5
10^3
10^4
10^5
Simulations
$\mathcal{U}(-1, 1)$: $\log_{10} \mathcal{R}_p = 0.89$
$\mathcal{U}(-10, 10)$: $\log_{10} \mathcal{R}_p = 2.89$
$\mathcal{U}(-50, 50)$: $\log_{10} \mathcal{R}_p = 4.28$
$\sigma_{\log\theta} = 0.5$: $\log_{10} \mathcal{R}_p = 5.05$
$\sigma_{\log\theta} = 1$: $\log_{10} \mathcal{R}_p = 6.24$
$\sigma_{\log\theta} = 2$: $\log_{10} \mathcal{R}_p = 7.44$
$\sigma_{\text{prior}} \times 1$: $\log_{10} \mathcal{R}_p = 5.38$
$\sigma_{\text{prior}} \times 5$: $\log_{10} \mathcal{R}_p = 9.86$
$\sigma_{\text{prior}} \times 10$: $\log_{10} \mathcal{R}_p = 12.18$
$\mathcal{U}(-3, 3)$: $\log_{10} \mathcal{R}_p = 1.57$
$\mathcal{U}(-5, 5)$: $\log_{10} \mathcal{R}_p = 1.93$
$\mathcal{U}(-10, 10)$: $\log_{10} \mathcal{R}_p = 2.69$

Science use case: gravitational wave ringdown



Thanks! Check us out!

