SimulationBasedInference.jl: A flexible toolkit for Bayesian inference with process-based models

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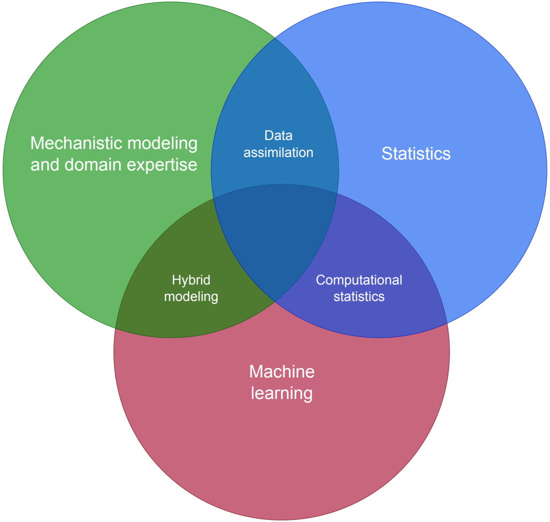
What is simulation-based inference?



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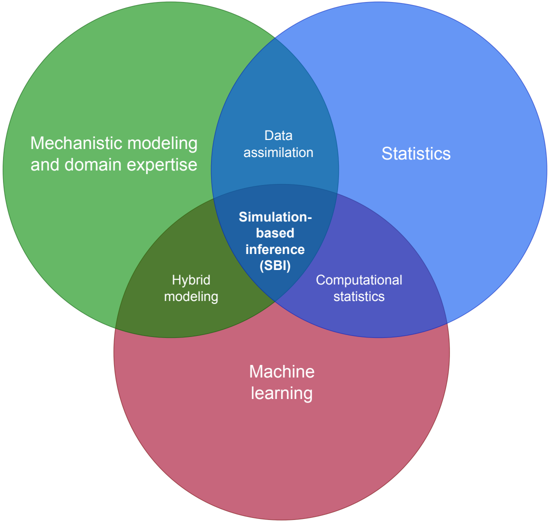

Bayesian inverse modeling

Let $\mathbf{s} = \mathcal{M}(\mathbf{x}, \mathbf{s}_0)$ represent a forward model (simulator) $\mathcal{M}$ with latent states $\mathbf{s}$, unknown or partially known inputs $\mathbf{x}$, and observation operator $\mathbf{y} = \mathcal{G}(\mathbf{s})$.

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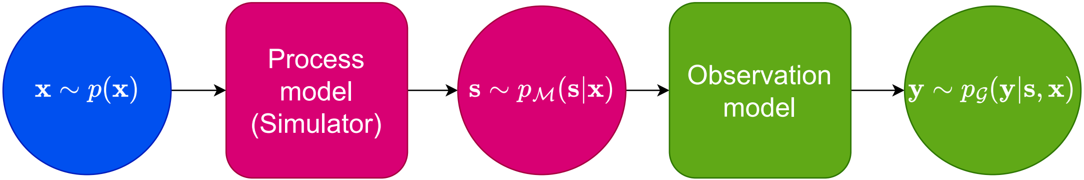

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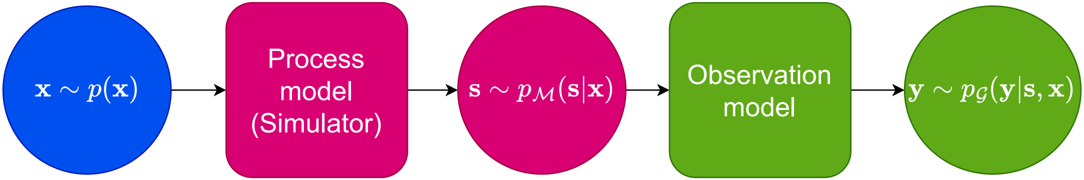

The Bayesian inverse problem given observations $\mathbf{y}$ is then:

$$p(\mathbf{s}, \mathbf{x}|\mathbf{y}) \propto p_{\mathcal{G}}(\mathbf{y}|\mathbf{s}, \mathbf{x}) p_{\mathcal{M}}(\mathbf{s}|\mathbf{x}) p(\mathbf{x}) \tag{1}$$

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- **Emulation** of the simulator using (possibly physics-informed) ML
- **Data-driven estimation** of the observation noise/error model
- **Amortized inference** via neural density estimators (NDEs)

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- Integrate with state-of-the-art software for **probabilistic** and **differentiable** programming

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- 100% free and open source

What if I don't know Julia?

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- That's OK! Minimal Julia familiarity is required to use the package at a basic level.
- It is possible to define a simulator that wraps code in other languages like python, C, or Fortran.
- You can also consider similar recently developed **python** frameworks like **sbi**[1] and **bayesflow**[2].

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Example: Linear ODE

```julia
using SimulationBasedInference, OrdinaryDiffEq

# define dynamics
f(u,p,t) = -p[1]*u;
# define "true" parameters
p = [0.2];
# define simulation time span
tspan = (0.0,10.0);
# initial state
u0 = [1.0]
# define ODE problem
ode_prob = ODEProblem(f, u0, tspan, p)
```

Example: Linear ODE

```
# define the observable
t_save = 0.1:0.1:10.0
observable = ODEObservable(
    :y, ode_prob, t_save, samplerate=0.01
)

# define the "forward problem"
forward_prob = SimulatorForwardProblem(
    ode_prob,
    observable,
    # can add more observables here...
)
```

Example: Linear ODE

```
# define prior and likelihood (omitted for brevity)
simulator_prior = ...
likelihood = ...

# define inference problem
inference_prob = SimulatorInferenceProblem(
    forward_prob,
    forward_solver,
    simulator_prior,
    likelihood,
);
```

Example: Linear ODE

```
# solve with ensemble importance sampling
enis_sol = solve(inference_prob, EnIS());

# solve with ensemble smoother
esmda_sol = solve(inference_prob, ESMDA());

# solve with ensemble Kalman sampling
eks_sol = solve(inference_prob, EKS());

# solve with Hamiltonian Monte Carlo (HMC)
hmc_sol = solve(inference_prob, MCMC(NUTS()));
```

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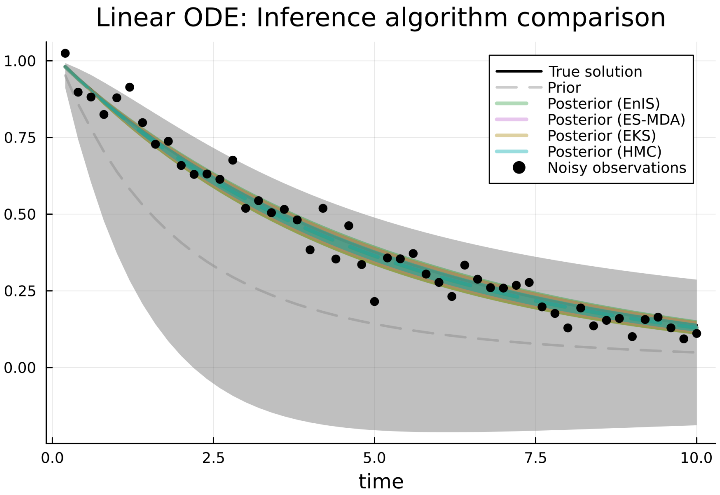
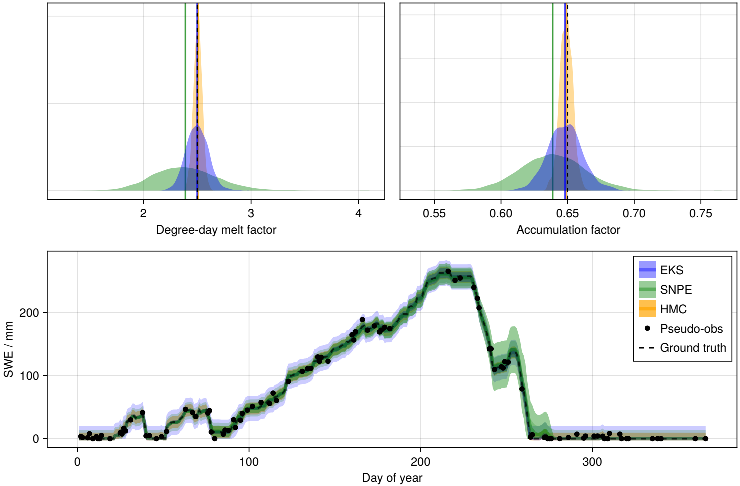
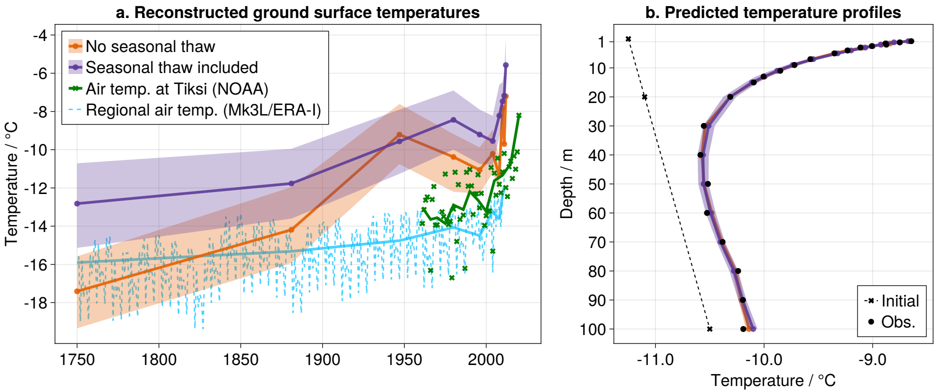


Example: Degree-day snow modeling



Calibration of degree-day snow melt model from synthetic pseudo-observations

Example: Surface temperature inversion with EKS



Groenke et al. 2024. *Robust reconstruction of historical climate change from permafrost boreholes*. JGR: Earth Surface. In review.

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- There are numerous avenues for the application of ML in improving the tractability of SBI in scientific workflows.
- SimulationBasedInference.jl provides a flexible and user-friendly framework for applying SBI to scientific models both big and small.

Thank you!

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