MIT Uncertainty Quantification (MUQ) Library

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SIAM UQ 2016

MUQ: philosophy

"A small change in algorithm or application should only require a small change in code"

Goals:

- Provide a sandbox for playing with different models and algorithms
  - Facilitate constructive modeling
  - Extensible and easily hybridized algorithms
- Reduce distance and time between algorithms and applications

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Target audiences:

- Algorithm developers
- Application scientists and engineers

MUQ: outline

1. **Modeling framework**
   - Constructing combined (physical + statistical) models with high-level structure
   - Graphical modeling technique to easily combine sub models

2. **Algorithm framework**
   - *Example:* Markov chain Monte Carlo stack — using mathematical structure in software design

3. **MUQ development update**
   - Use of MUQ in our research

MUQ: modeling

Unique modeling approach:

1. **Graphically** building physical and statistical models
   - Connect models and algorithms to *expose underlying structure*

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   - Apply MCMC (and other algorithms) to a *wide variety of applications*
3. "Grey-box" approach: MUQ **wraps around existing models**, but uses any new or available problem structure
4. Built-in tools to **implement physical models**

Graphical models in MUQ

- Physical & statistical models are implemented separately (`ModPieces`)

```
# create submodels
theta = VectorPassthroughModel()
prior = GaussianDensity(mu, sig)
f = ForwardModel()
like = GaussianDensity()
post = DensityProduct()
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Graphical models in MUQ

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Parameters: θ

Forward model:
$f(\theta)$

Likelihood:
$\pi(d|f(\theta))$

Prior:
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Posterior:
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Graphical models in MUQ

- Submodels are connected — becoming **graphs** (`ModGraphs`)

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Add submodels to the graph:

```
# Add graph nodes
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G.AddNode(theta, 'Parameter')
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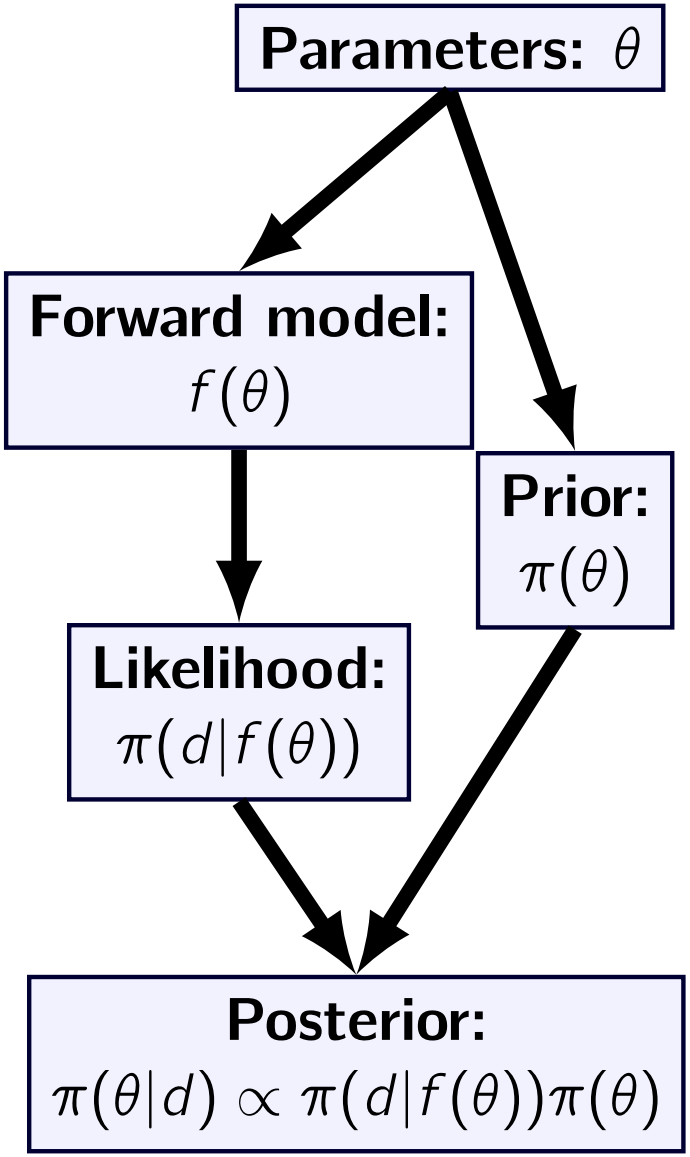
Connect nodes with edges:

```
# Add graph edges
G.AddEdge('Parameters', 'Forward Model', 0)
G.AddEdge('Forward Model', 'Likelihood', 0)
G.AddEdge('Likelihood', 'Posterior', 0)

G.AddEdge('Parameters', 'Prior', 0)
G.AddEdge('Prior', 'Posterior', 1)
```



Advantages of graph-based modeling

1. Relates *implementation structure* to *intuitive interpretation*

```
# use a different forward model
g = AnotherForwardModel()
G.SwapNode('Forward Model', g)
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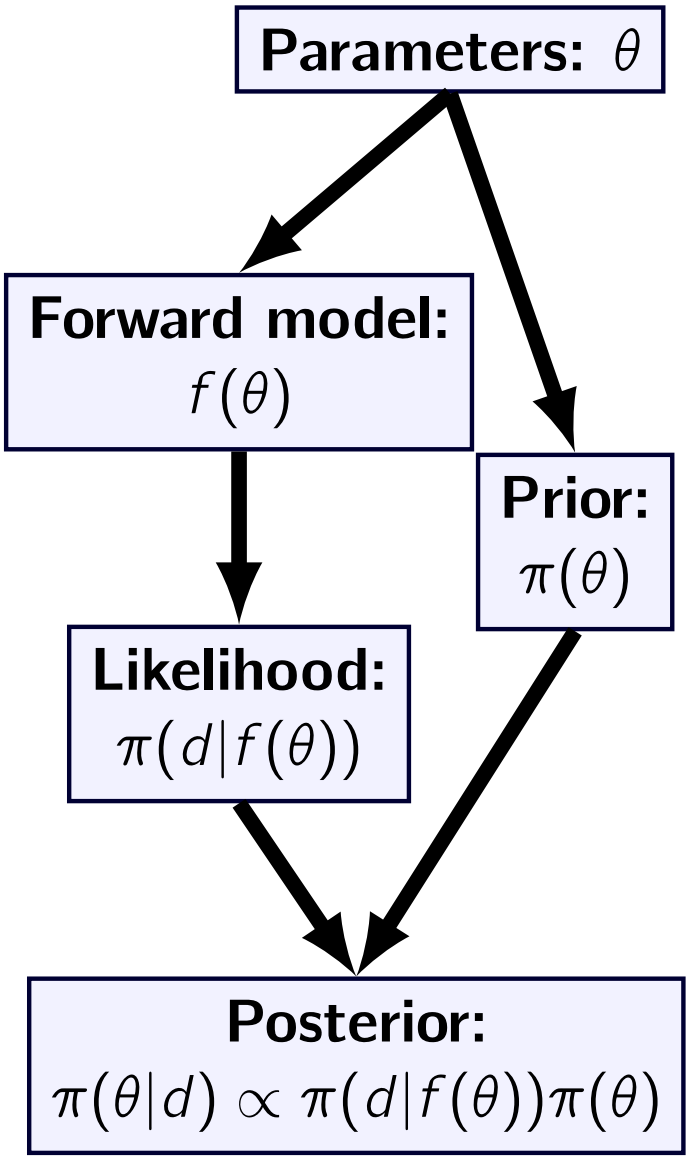

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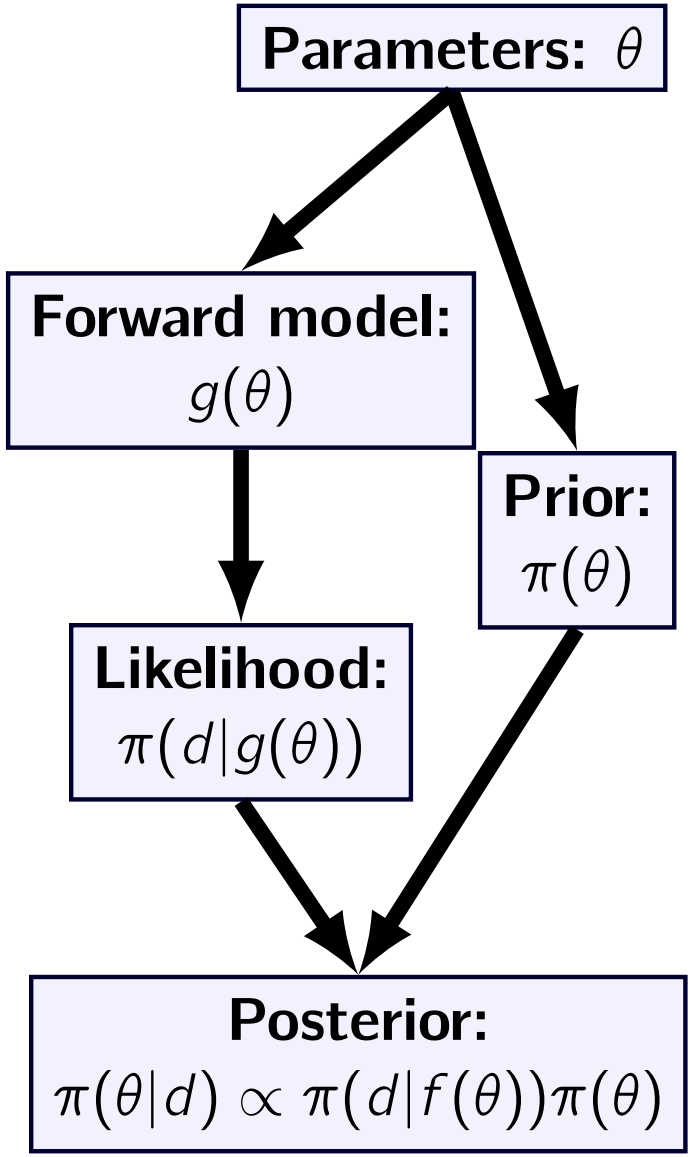

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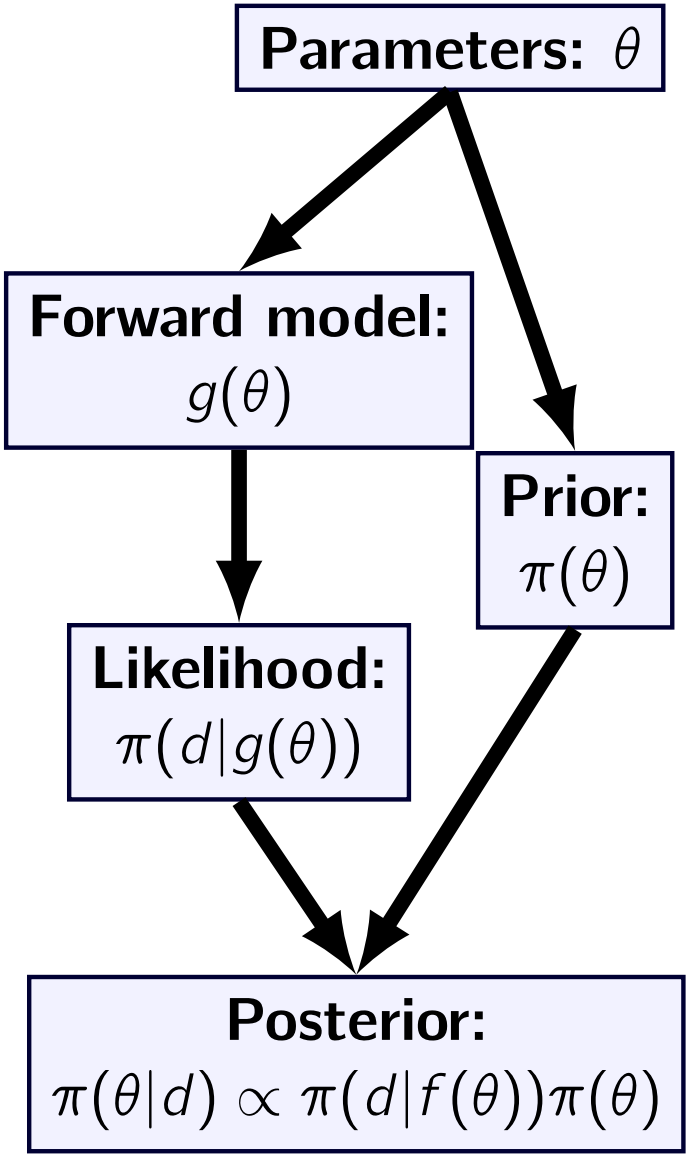
3. "Grey-box" wrapper around existing models



Grey-box wrapper: Using existing models (C++)

- Existing implementation becomes a submodel
- The user only needs to write a **MUQ/existing solver interface:**

```
class ModelWrapper : public muq::Modeling::ModPiece {
  public:
    // A way to create the submodel
    ModelWrapper(inputSizes, outputSize) :
       ModPiece(inputSizes, outputSize)

  private:
    // Grey-box implementation
    Eigen::VectorXd EvaluateImpl(std::vector<Eigen::VectorXd>
        const& inputs) {
      Eigen::VectorXd output(outputSize);
      /* ***** CALL EXISTING CODE HERE ***** */
      return output;
    }
};
```

Grey-box wrapper: Using existing models (Python)

- Existing implementation becomes a submodel
- The user only needs to write a **MUQ/existing solver interface:**

```
class ModelWrapper(libmuqModelling.ModPiece):
    # a way to create the submodel
    def __init__(self, inputSizes, outputSize):
        libmuqModelling.ModPiece.__init__(inputSizes, outputSize)

    # Grey-box implementation
    def EvaluateImpl(self, inputs):
        # #### CALL EXISTING CODE HERE #### #
        # existing code returns output (list type)
        return output
```

Derivative implementation (C++)

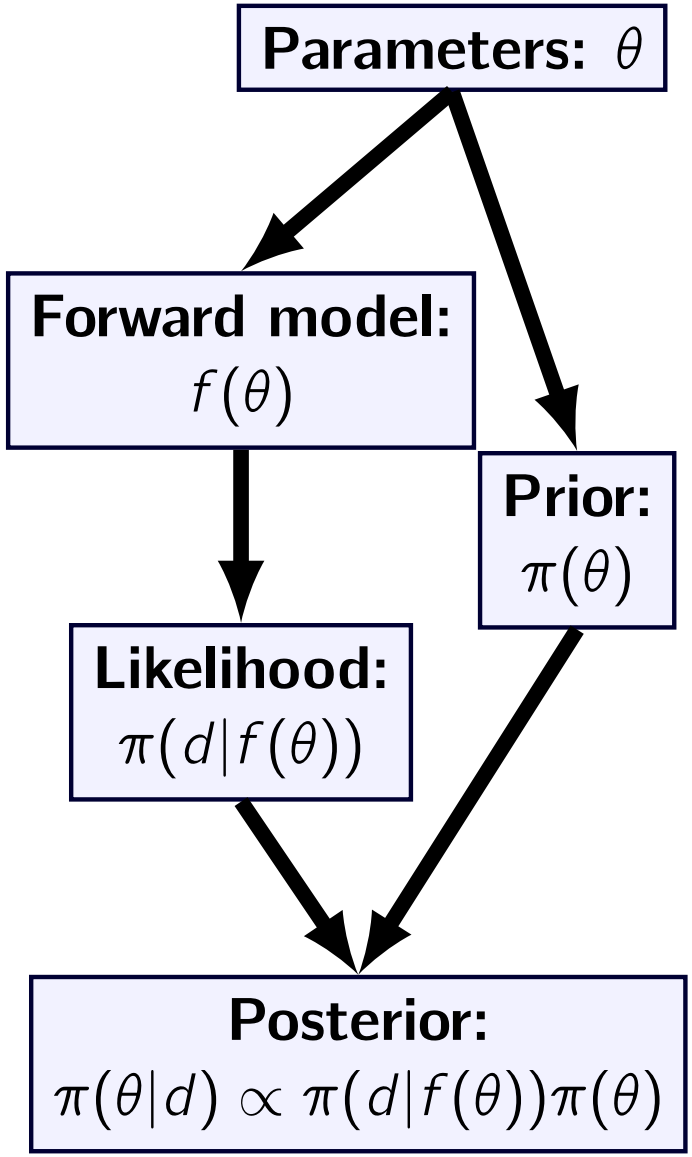
- User may optionally implement derivative information
  Gradient, Jacobian, Jacobian's action, and/or Hessian
- The user only needs to write a **MUQ/existing solver interface:**

```
class ModelWrapper : public muq::Modeling::ModPiece {
    // Model implementation
    Eigen::VectorXd EvaluateImpl(std::vector<Eigen::VectorXd>
        const& inputs) { return output; }
    // Derivative implementation

    virtual Eigen::VectorXd
        GradientImpl(std::vector<Eigen::VectorXd> const& inputs,
        Eigen::VectorXd const& sensitivity,
        int const inputDimWrt) override {
            return gradient;
        }
};
```

Model derivatives

1. Option to include user implemented derivatives



Model derivatives

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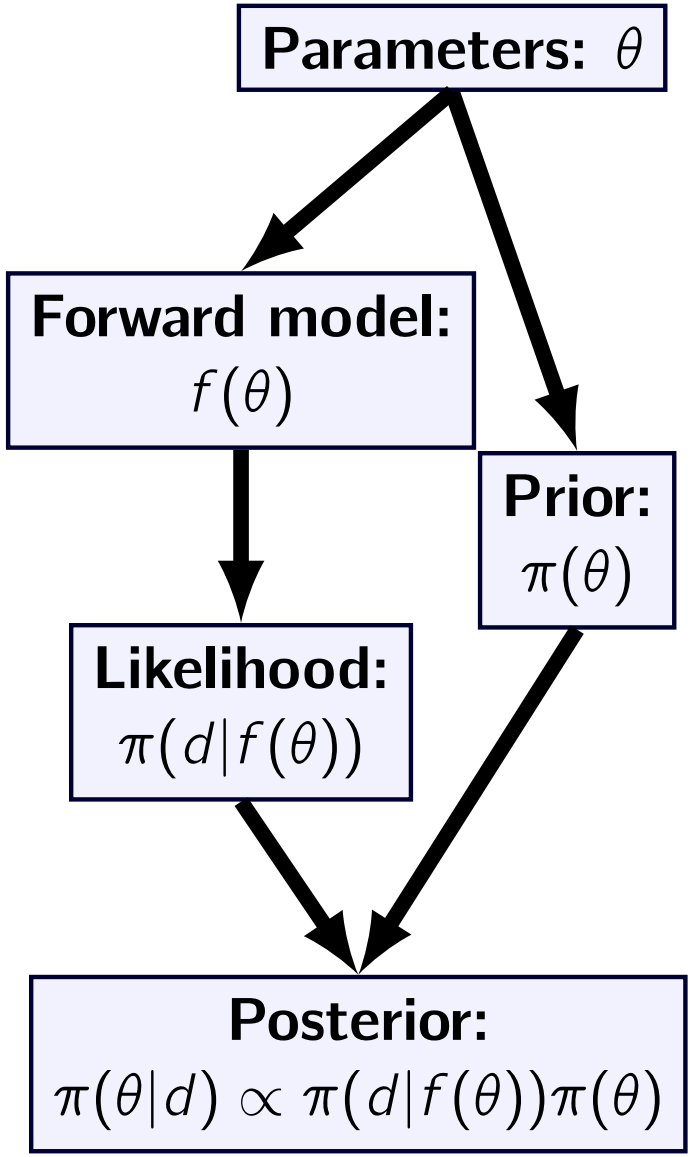
2. Defaults to finite difference if analytic derivatives are not implemented



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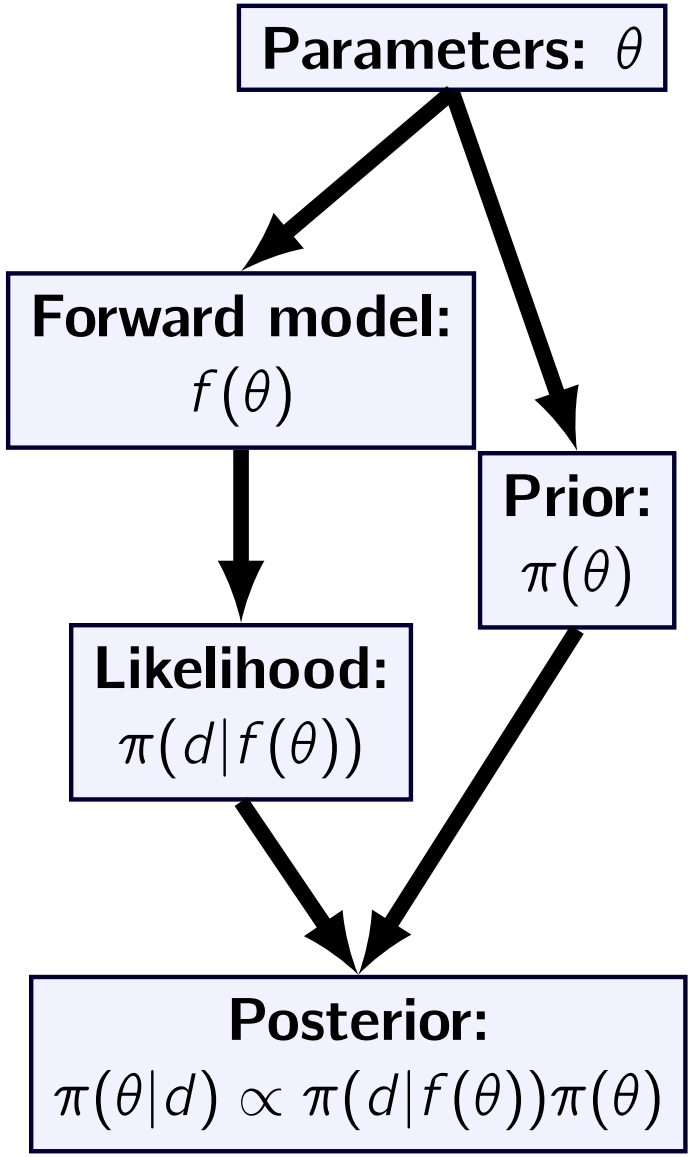
3. Computes derivative of the graph's output via the chain rule



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   - Component-wise functions (`exp`, `sin`, ...)
   - Component-wise sum
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   - *and many more* ...

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   - Numerical integration of ODEs, state-discretized PDEs
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   - *and many more* ...
3. `Sundials` interface
   - Numerical integration of ODEs, state-discretized PDEs
   - Root-finding algorithms
4. Transient and steady PDE solver
   - User must implement the *weak form*
   - Derivative information computed via automatic differentiation (`Sacado`)
   - *Finite element method* spatial discretization (`LibMesh`)

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MUQ: MCMC

Question

What are the fundamental components of an MCMC algorithm?

Metropolis-Hastings MCMC:

1. Save current state
$$\theta^{(k)} = \theta$$
2. Propose new state
$$\theta' \sim q(\theta'|\theta)$$
3. Accept or reject
$$\alpha = \min\left\{1, \frac{\pi(\theta')}{\pi(\theta)}\frac{q(\theta|\theta')}{q(\theta'|\theta)}\right\}$$

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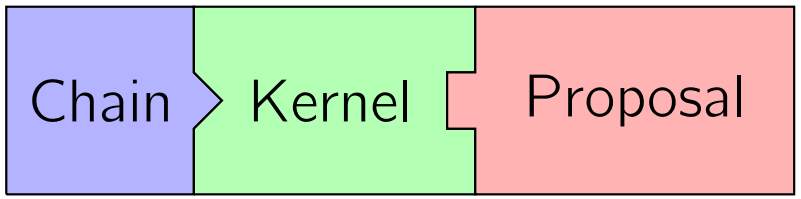

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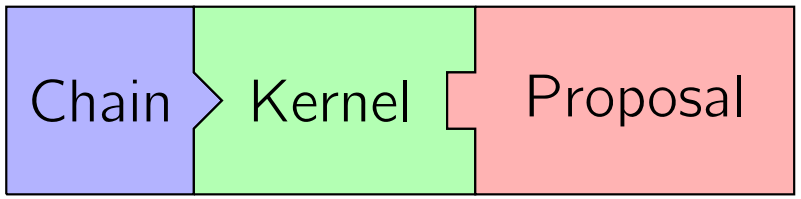
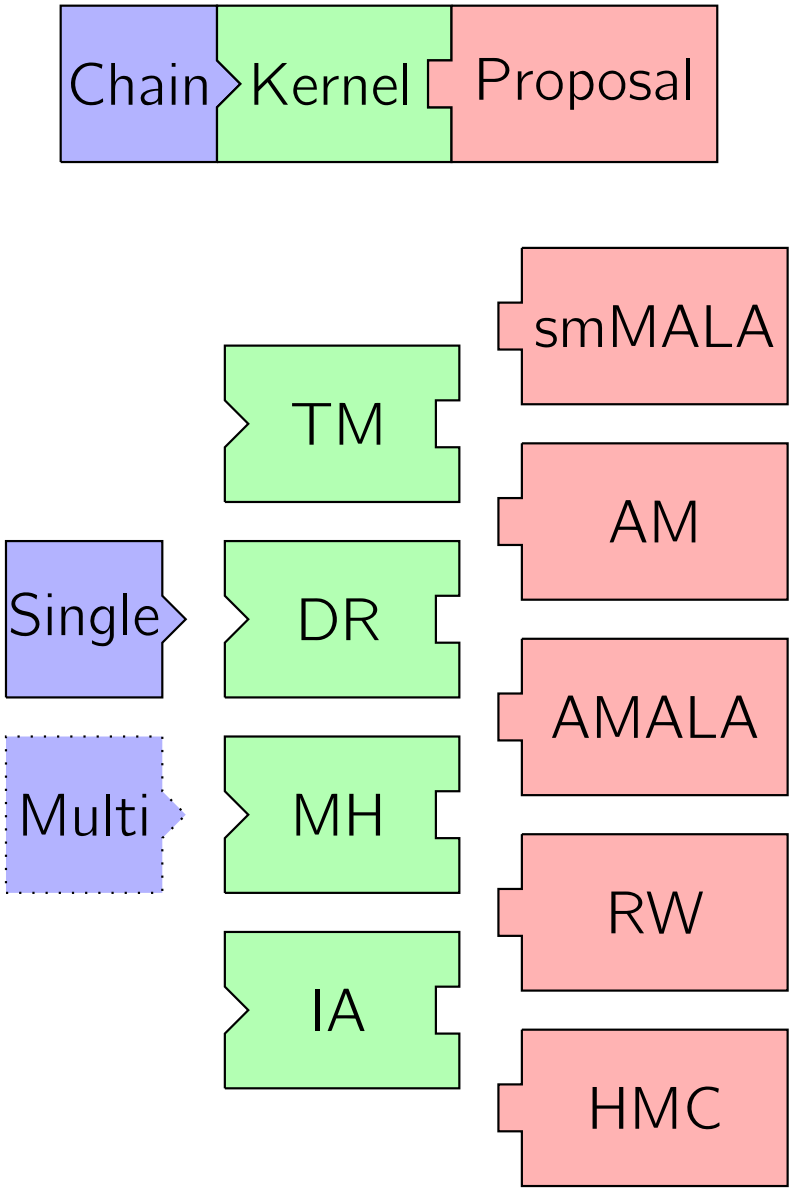


- We copy this structure with C++ classes
- Easily extendable
- Many possible configurations (> 30)

MUQ: full MCMC framework



Advantages:

- New proposals used with any kernel
- Focus efforts on *new* features
- Changing components is trivial
- Extensive performance comparisons are straightforward

```
// MH + AMALA:
ps.put("MCMC.Kernel","MH");
ps.put("MCMC.Proposal","AMALA");

// TM + RW:
ps.put("MCMC.Kernel","TransportMap");
ps.put("MCMC.Proposal","MHProposal");
```

MCMC and models

Observation:

Many MCMC algorithms rely on specific problem structure.

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Problem iterates through graph and extracts important structure:

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- etc. . .

No extra effort: **Structure automatically defined in "grey-box" model.**

Beyond MCMC

Lessons learned:

- Design code to mimic the mathematics
  - Allows us easily add new components without duplicate code
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  - Enables algorithms to exploit high-level structure
  - Still allows arbitrary model implementations (e.g., legacy code)

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Notes:

- Similar structure exists in our optimization algorithms
- More complicated chains being tested (DILI, DILI+maps, etc.)

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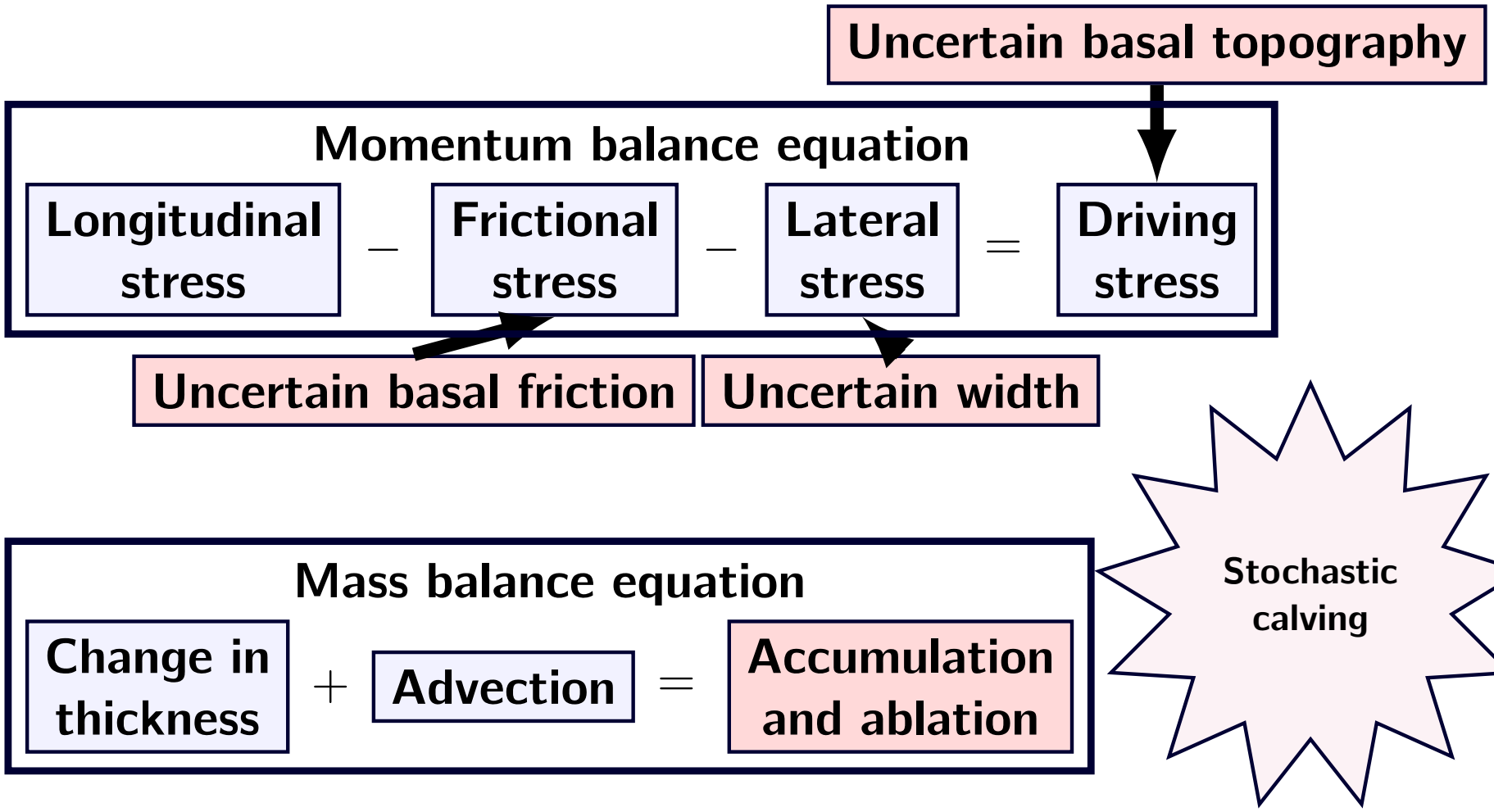
MUQ usage: ice sheet modeling

Solve conservation equations with *uncertain input parameters* . . .



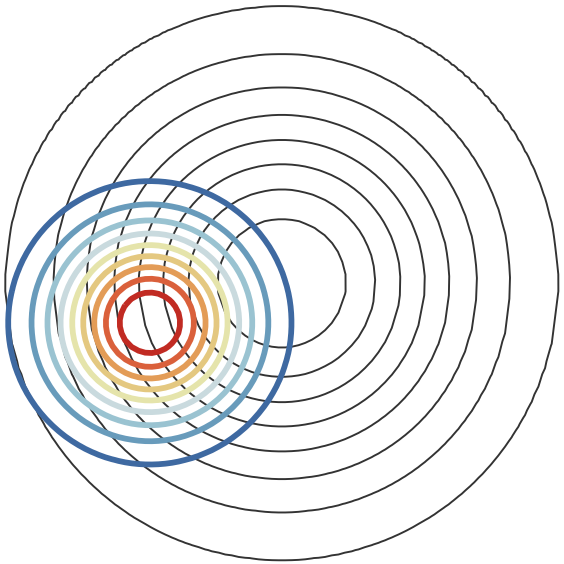
. . . computed field are used within UQ algorithms (e.g., Monte Carlo, optimization, MCMC, importance sampling ect. . . .)

MUQ usage: map-accelerated MCMC

Use nonlinear variable transformation to "precondition" target density.

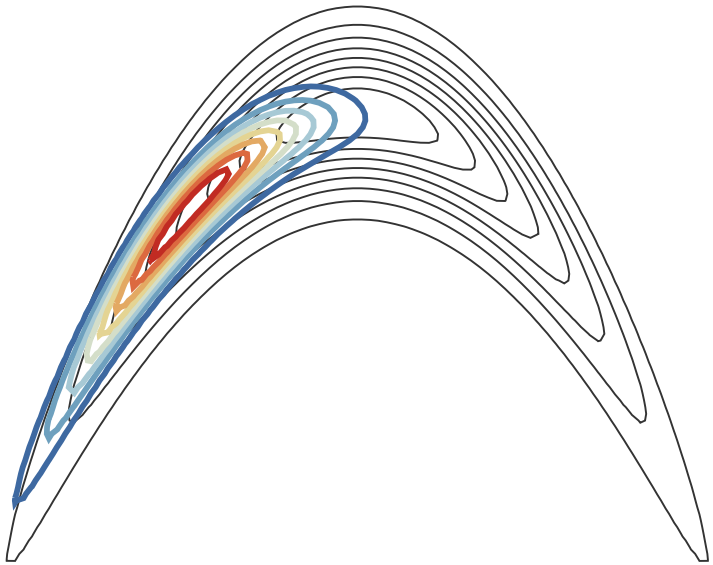
reference proposal

$q_r(r'|r) = N(r, \sigma^2 I)$



mapped proposal

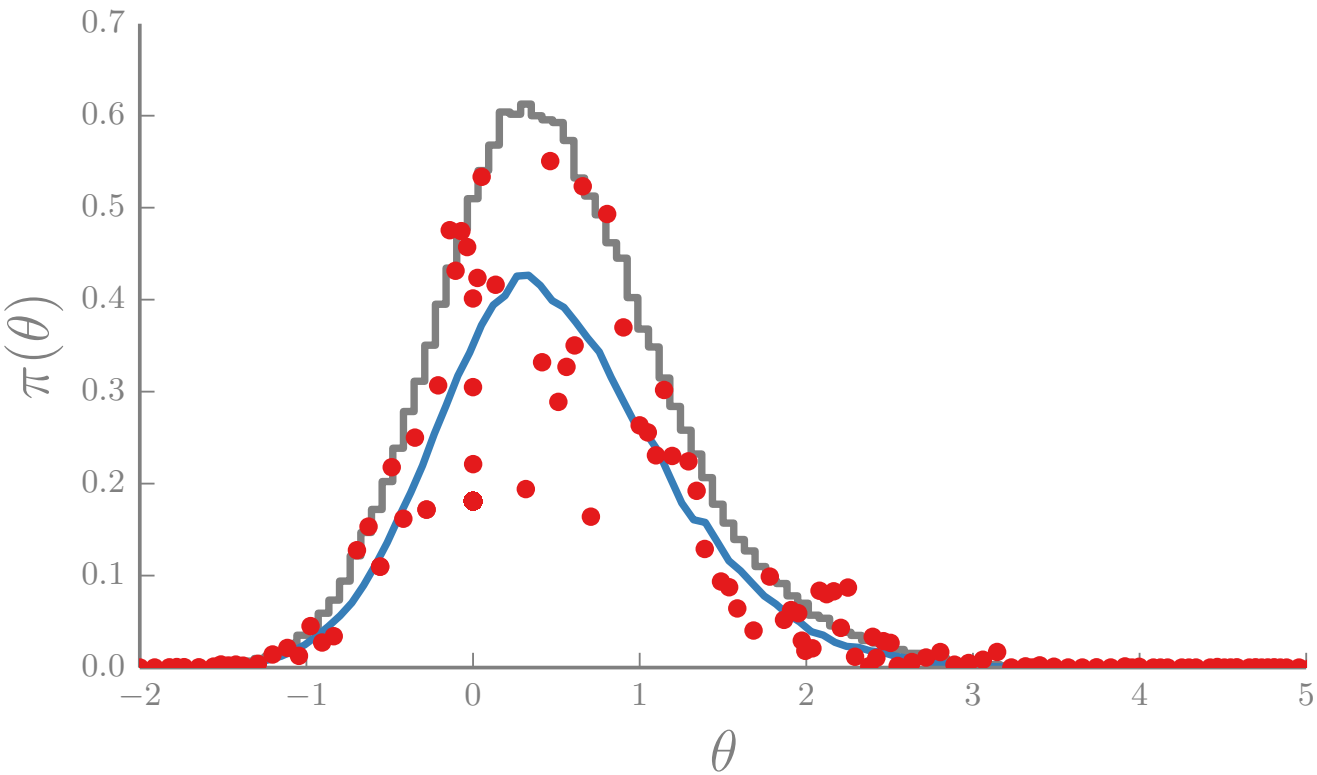
$q_\theta(\theta'|\theta) = q_r\left(\tilde{T}(\theta')|\tilde{T}(\theta)\right)\left|\det D\tilde{T}(\theta')\right|$



The exchangeability of MCMC components makes testing many reference proposals easy

MUQ usage: characterizing marginal distributions

- Build a surrogate model of the marginal using stochastic evaluations



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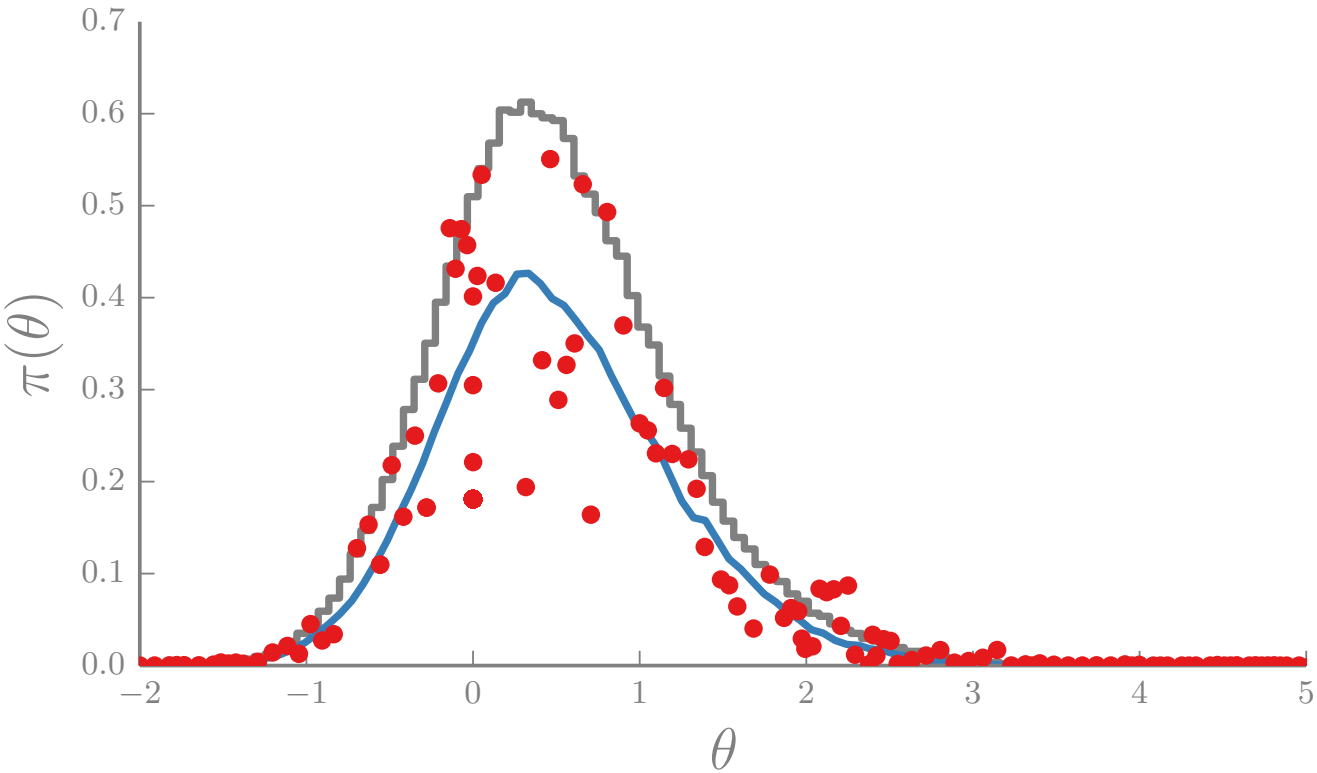
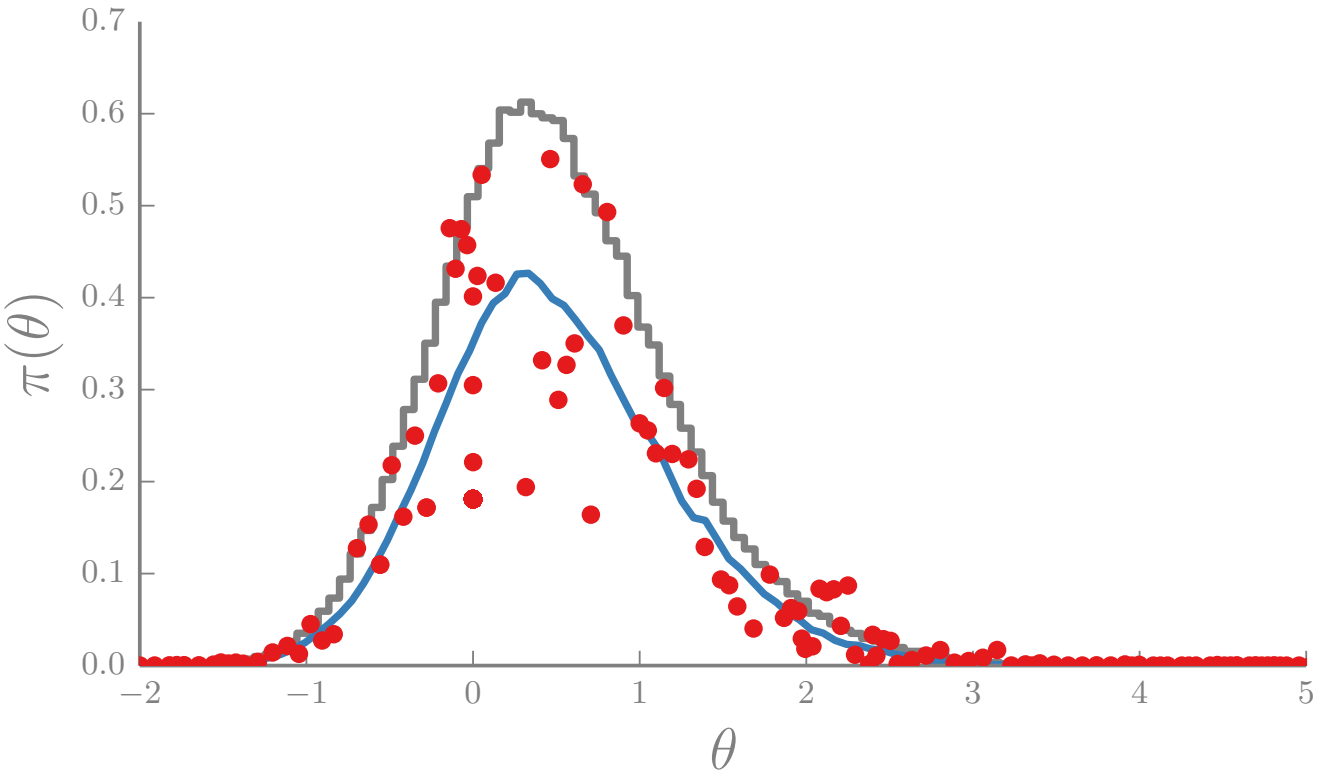


MUQ usage: characterizing marginal distributions

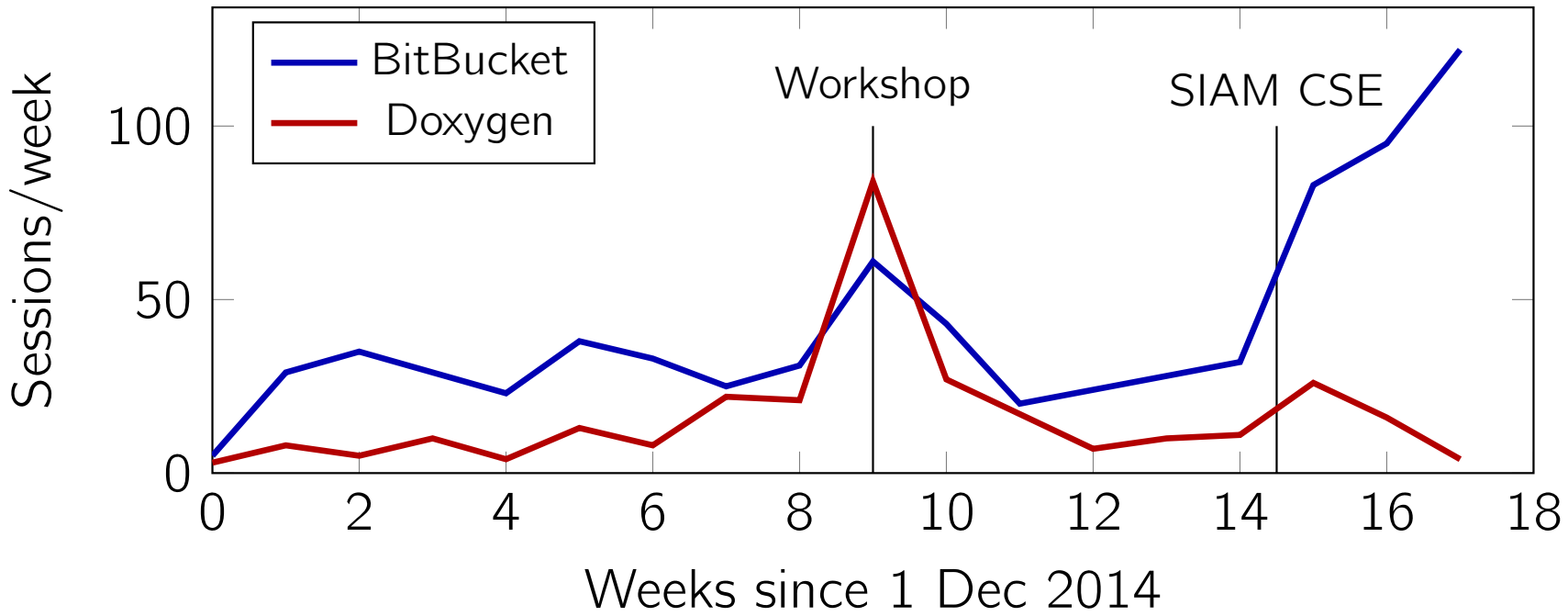
- Build a surrogate model of the marginal using stochastic evaluations
- Using the surrogate to evaluate the acceptance ratio does **not** affect the proposal
- We can easily combine many proposal methods (e.g., MH, AM, DRAM, . . .) with surrogate modeling



MUQ: development notes

Development improvements:

Google analytics:



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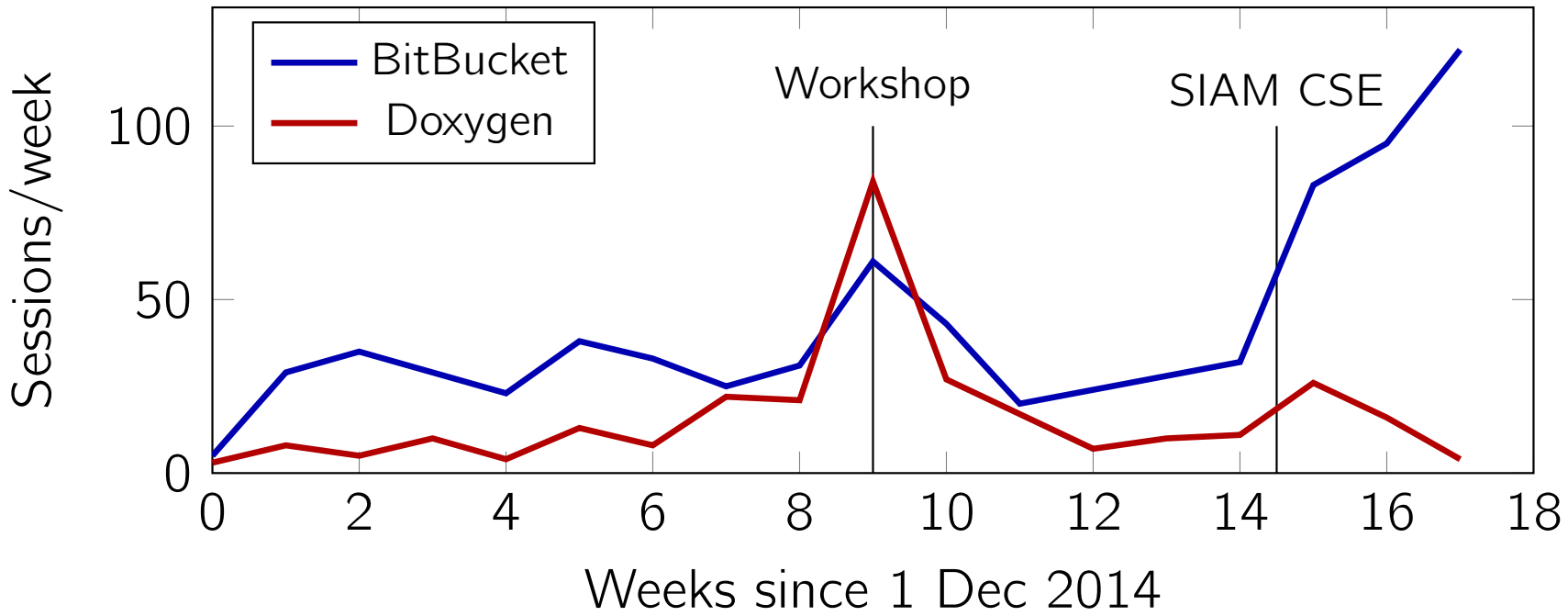

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- Extensive testing for corrent and/or consistent perfermance
  - Automated code testing for verification with Jenkins

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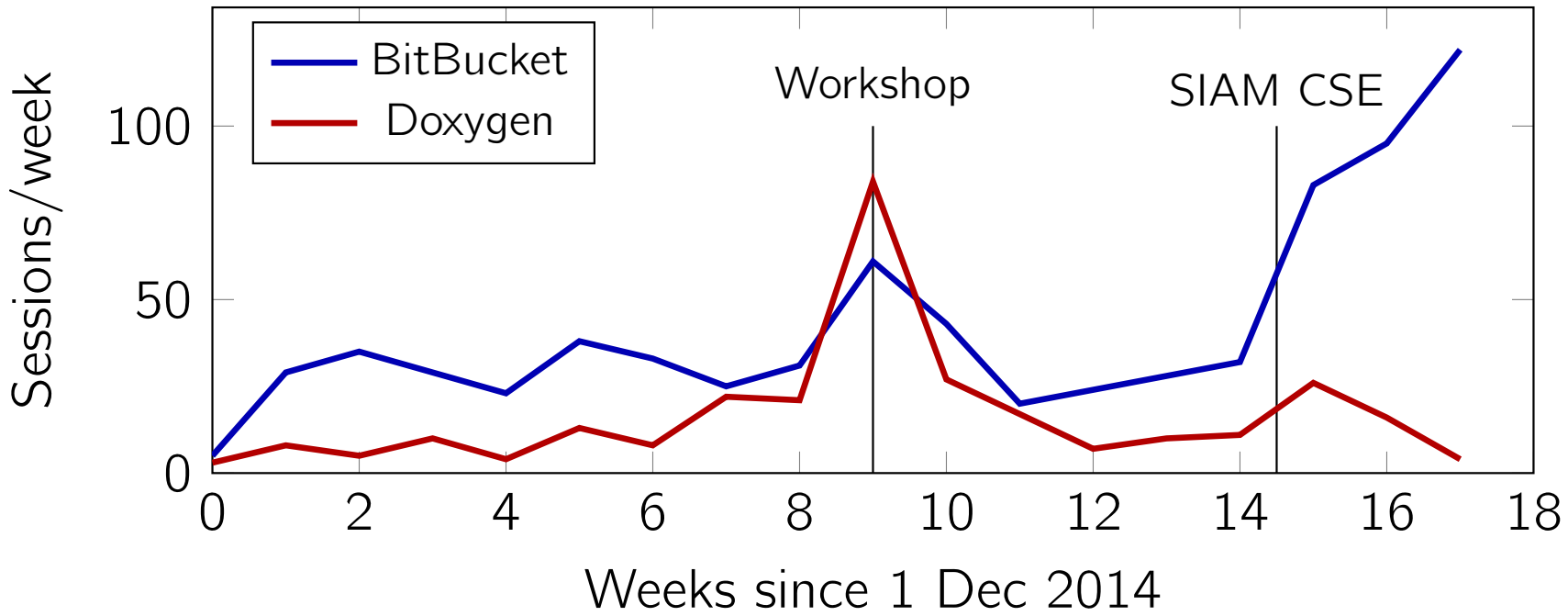

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