Quantum Uncertainty Quantification for Physical Models using ToQ.jl

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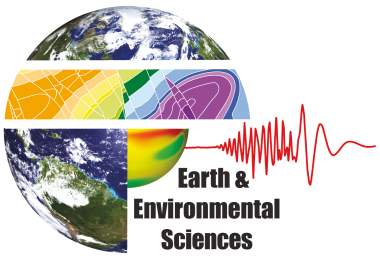

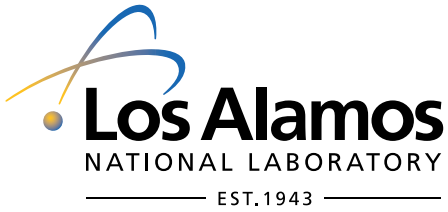

Programming D-Wave machines

0^{th} order approximation

$$\hat{\mathbf{q}} = \min_{\mathbf{q}\in\{0,1\}^n} \sum_{i=1}^{n} a_i q_i + \sum_{i=1}^{n}\sum_{j=1}^{i-1} b_{ij} q_i q_j$$

1^{st} order approximation

$$\mathbf{q} \sim e^{-\beta\left(\sum_{i=1}^{n} a_i q_i + \sum_{i=1}^{n}\sum_{j=1}^{i-1} b_{ij} q_i q_j\right)}$$

- The core task of programming a D-Wave machine is to assemble

$$\sum_{i=1}^{n} a_i q_i + \sum_{i=1}^{n}\sum_{j=1}^{i-1} b_{ij} q_i q_j$$

in such a way that one of the above approximations will be useful

How can ToQ.jl help?

- ToQ.jl makes it relatively easy to assemble a “logical QUBO”
  - Don’t have to worry about the sparsity of b_{ij}
  - Don’t have to worry about the bounds on a_i and b_{ij}
  - Do have all the features of Julia
- ToQ.jl makes it very easy to use different backends
  - dw
  - Python SAPI
  - qbsolv
- ToQ.jl makes it very easy to write hybrid classical/quantum programs
  - Use Julia to write the classical part
  - Use Julia+ToQ.jl to interact with the D-Wave
- Sidenote: ToQ.jl is a misnomer and has nothing to do with D-Wave’s ToQ – name change coming soon

Assembling a logical QUBO
Coloring the map of Canada

- Color the 13 Canadian provinces with 3 colors
- Assign exactly one of three colors to each province
- No two neighboring provinces can have the same color

Assembling a logical QUBO
Coloring the map of Canada

- Color the 13 **Canadian provinces** with 3 colors
- Assign exactly one of three colors to each province
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```
provinces = ["BC", "YK", "NW", "AB",...
neighbors = Dict()
neighbors["BC"] = ["YK", "NW", "AB"]
neighbors["YK"] = ["BC", "NW"]
neighbors["NW"] = ["YK", "BC", "AB", "SK",
"NV"]
neighbors["AB"] = ["BC", "NW", "SK"]
neighbors["SK"] = ["AB", "NW", "MT"]
neighbors["NV"] = ["NW", "MT"]
neighbors["MT"] = ["NV", "SK", "ON"]
neighbors["ON"] = ["MT", "QB"]
neighbors["QB"] = ["ON", "NB", "NL"]
neighbors["NB"] = ["QB", "NS"]
neighbors["NS"] = ["NB"]
neighbors["PE"] = []
neighbors["NL"] = ["QB"]
```

Assembling a logical QUBO
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- **Color the 13 Canadian provinces with 3 colors**
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```
m = ToQ.Model("canada_model", "laptop",
"c4-sw_sample", "workingdir", "c4")

@defvar m red[1:length(provinces)]
@defvar m green[1:length(provinces)]
@defvar m blue[1:length(provinces)]
```

Assembling a logical QUBO
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$$-(q_1 + q_2 + q_3) + 2(q_1q_2 + q_1q_3 + q_2q_3)$$

```
for i = 1:length(provinces)
  @addterm m -1 * red[i]
  @addterm m -1 * green[i]
  @addterm m -1 * blue[i]
  @addterm m 2 * red[i] * green[i]
  @addterm m 2 * red[i] * blue[i]
  @addterm m 2 * green[i] * blue[i]
end
```

Assembling a logical QUBO
Coloring the map of Canada

- Color the 13 Canadian provinces with 3 colors
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$$r_1 r_2 + g_1 g_2 + b_1 b_2$$

```
for j = 1:length(provinces)
 for k = 1:j - 1
  if provinces[k] in neighbors[provinces[j]]
   @addterm m red[j] * red[k]
   @addterm m green[j] * green[k]
   @addterm m blue[j] * blue[k]
  end
 end
end
```

I’ve got the QUBO, now what?
Coloring the map of Canada

```
#sample with dw
ToQ.solve!(m; numreads=100, param_chain=2)
#load the first dw sample
@loadsolution m energy occurrences isvalid 1
#print the first dw sample
println(hcat(red.value, blue.value, green.value))

#sample with Python SAPI
ToQ.solvesapi!(m; num_reads=100, param_chain=2)
#load the first SAPI sample
@loadsolution m energy occurrences isvalid 1
#print the first SAPI sample
println(hcat(red.value, blue.value, green.value))

#solve with qbsolv
ToQ.qbsolv!(m; minval=-13 * w1)
#print the qbsolv solution
println(hcat(red.value, blue.value, green.value))
```

Coloring arbitrary maps with 25 lines

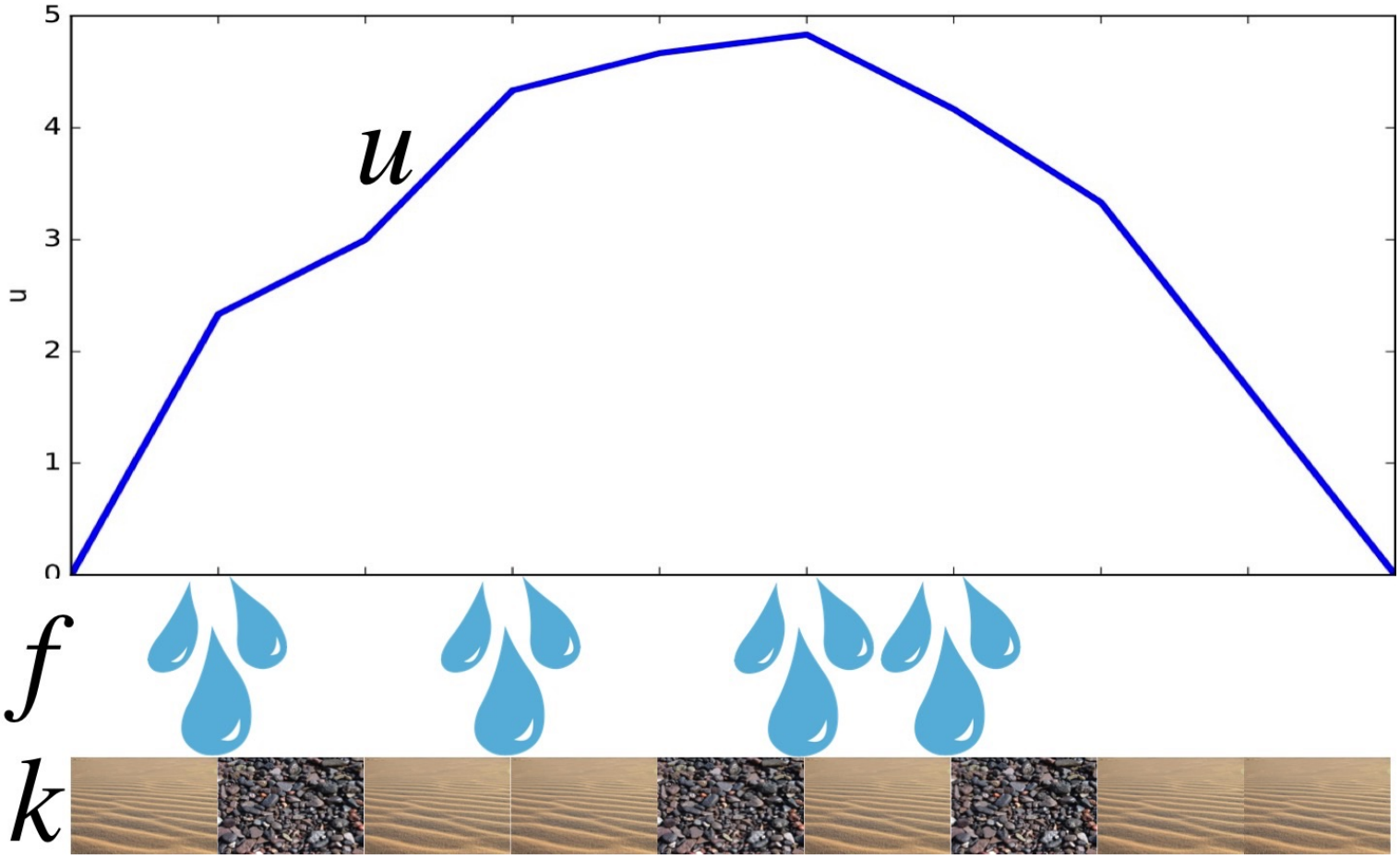
```
function colormap(regions, neighbors, numcolors; w1=1, w2=1)
 colornames = ["red", "orange", "yellow", "green", "blue", "indigo", "violet"]
 m = ToQ.Model("mapcolor", "laptop", "c4-sw_sample", "workingdir", "c4")
 @defvar m colors[1:length(regions), 1:numcolors]
 for i = 1:length(regions)
  for j = 1:numcolors
   @addterm m -w1 * colors[i, j]
   for k = 1:j - 1
    @addterm m 2 * w1 * colors[i, j] * colors[i, k]
   end
  end
 end
 for j = 1:length(regions)
  for k = 1:j - 1
   if regions[k] in neighbors[regions[j]]
    for i = 1:numcolors
     @addterm m w2 * colors[j, i] * colors[k, i]
    end
   end
  end
 end
 ToQ.qbsolv!(m; minval=-length(regions) * w1)
 result = Dict(zip(regions, map(i->colornames[indmax(vec(colors.value[i, :]))], 1:length(regions))))
 return result
end

counties, county_neighbors = parseusa("county_adjacency.txt")
usa_answer = colormap(counties, county_neighbors, 4)
```

Uncertainty Quantification: a long story short

- The developed UQ methods are not “ready for prime time”
- **However**, there are clear paths for improvement that could be pursued with more time & effort

The physics problem

$$\nabla \cdot (k \nabla u) = f$$



The physics problem

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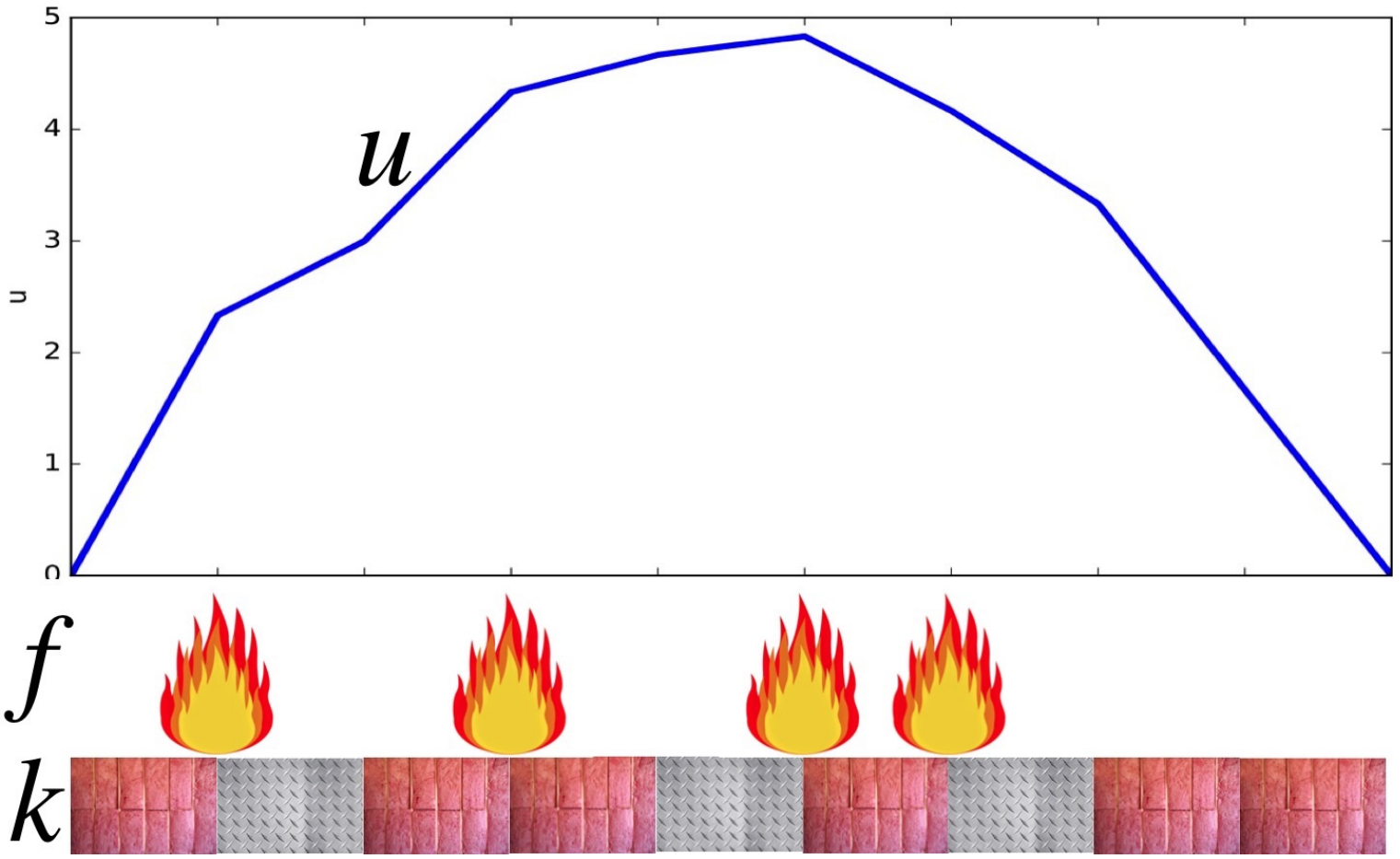
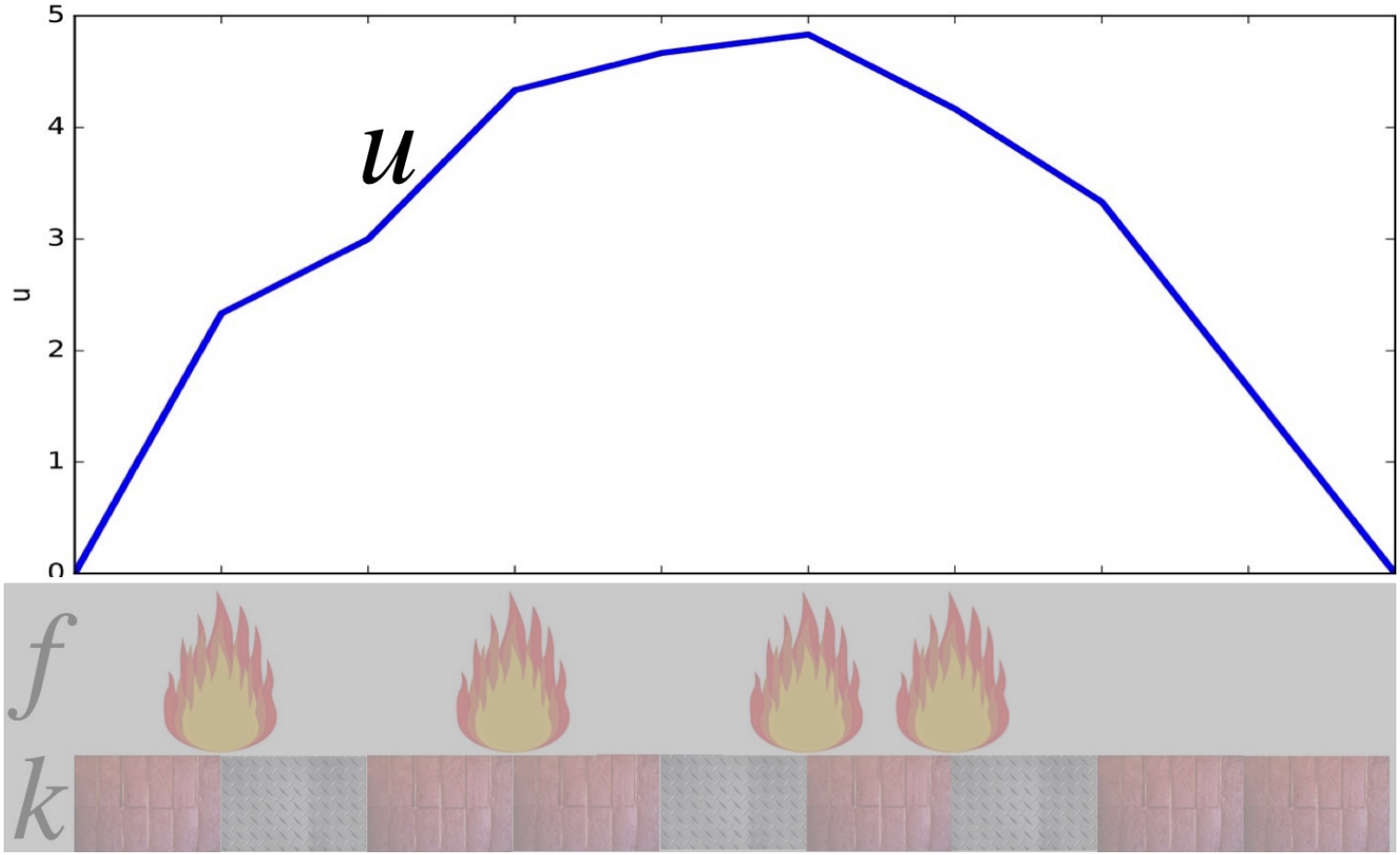


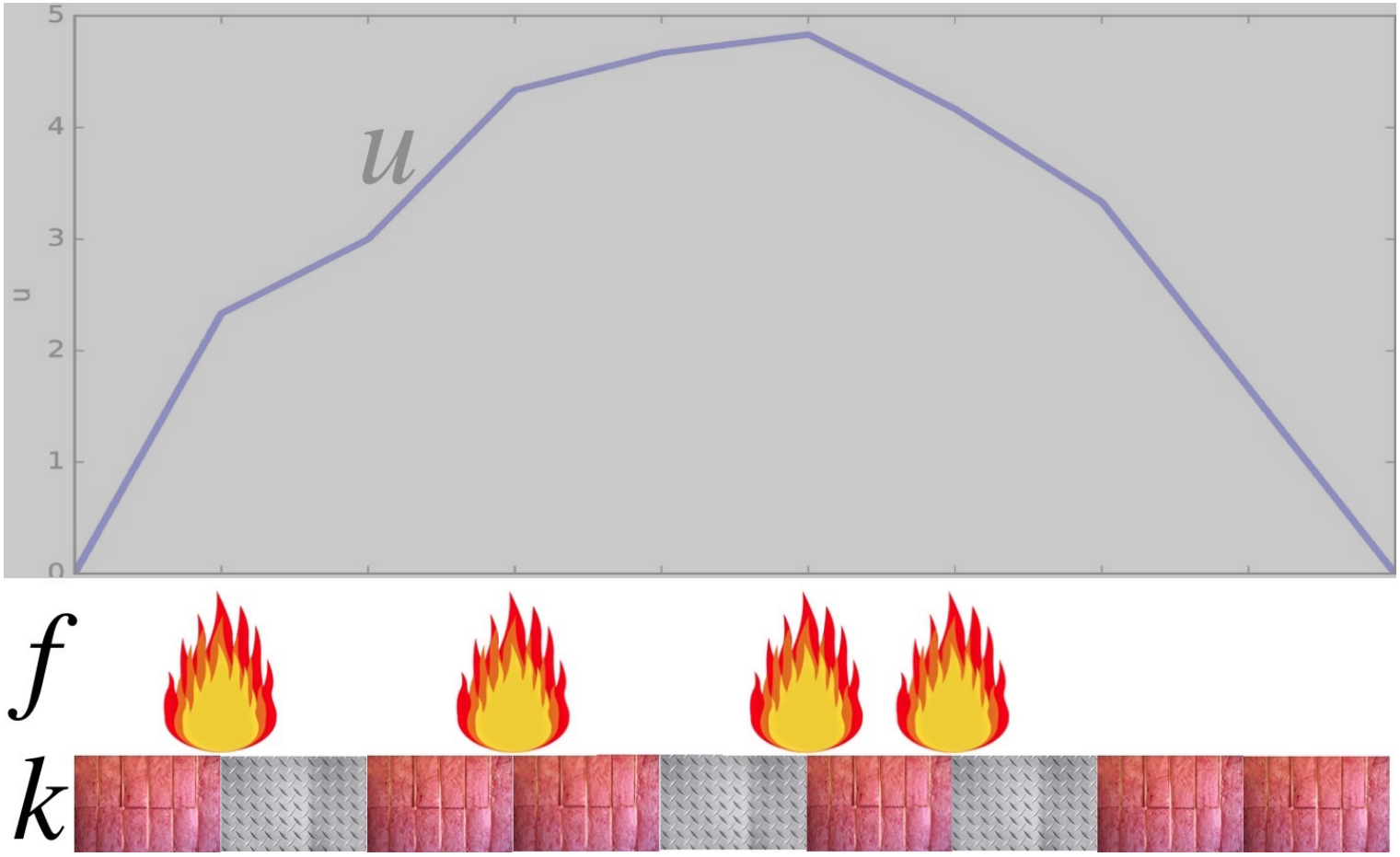
What we know

$$\nabla \cdot (k \nabla u) = f$$



What we don't know

$$\nabla \cdot (k \nabla u) = f$$



The uncertainty quantification

Two sets of bits that will be represented on the D-Wave hardware: the q_i bits are used to represent k and the r_i bits are used to represent f.

$$\begin{aligned} u_i - \hat{u}_i &\sim N(0,1) \\ k_i &= k_{low} + q_i(k_{high} - k_{low}) \\ f_i &= -r_i \\ 0 &= k_{i-1}u_{i-1} - (k_{i-1} + k_i)u_i + k_i u_{i+1} - f_i \end{aligned}$$

$$H(\mathbf{q}, \mathbf{r}) = \sum_{i=2}^{N-1} \left[k_{i-1}u_{i-1} - (k_{i-1} + k_i)u_i + k_i u_{i+1} - f_i\right]^2 \quad (1)$$

Get samples from the D-Wave with likelihood

$$\exp(-\beta H^*(\mathbf{q}, \mathbf{r}))$$

use importance sampling to estimate statistics of k and f.

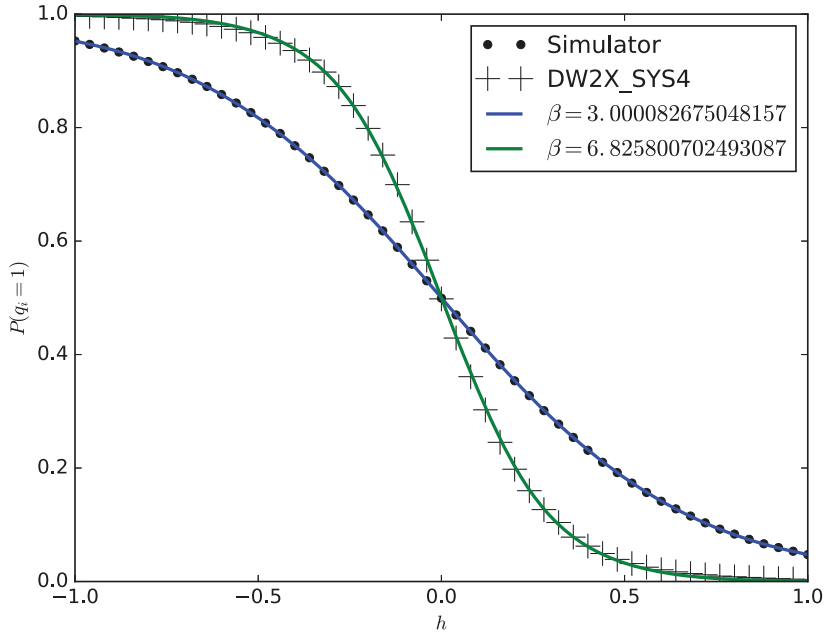
Boltzmann approximation? Effective temperature?

1^{st} order approximation

$$\mathbf{q} \sim e^{-\beta\left(\sum_{i=1}^{n} a_i q_i + \sum_{i=1}^{n}\sum_{j=1}^{i-1} b_{ij} q_i q_j\right)}$$

Let $a_i = h \; \forall i$ and $b_{ij} = 0 \; \forall i, j$

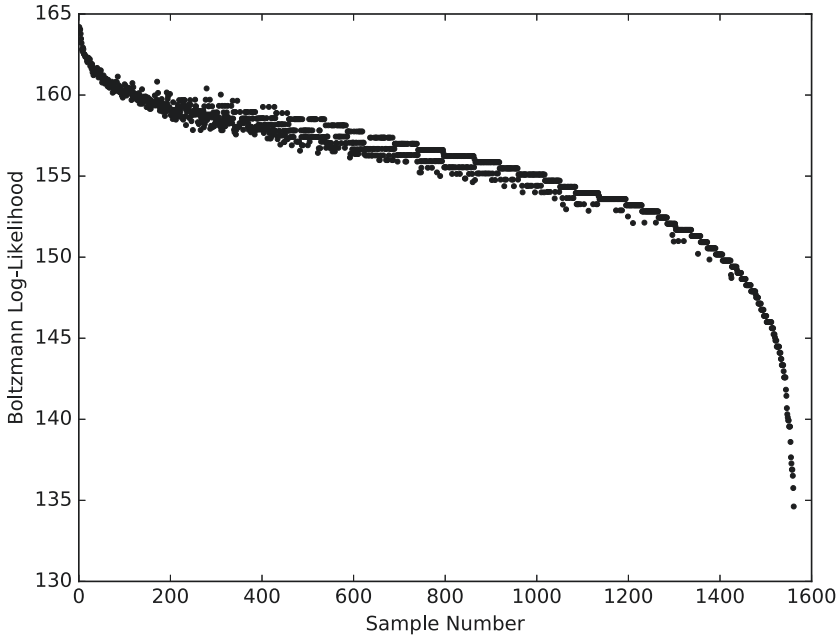
$$P(q = 1; h, \beta) = \frac{\exp(-\beta h)}{\exp(-\beta h) + 1}$$



$$\hat{\beta} = \arg\min_{\beta} \sum_{i=1}^{N} (P(q = 1; h_i, \beta) - \sum_{j=1}^{M} q_j^i / M)^2$$

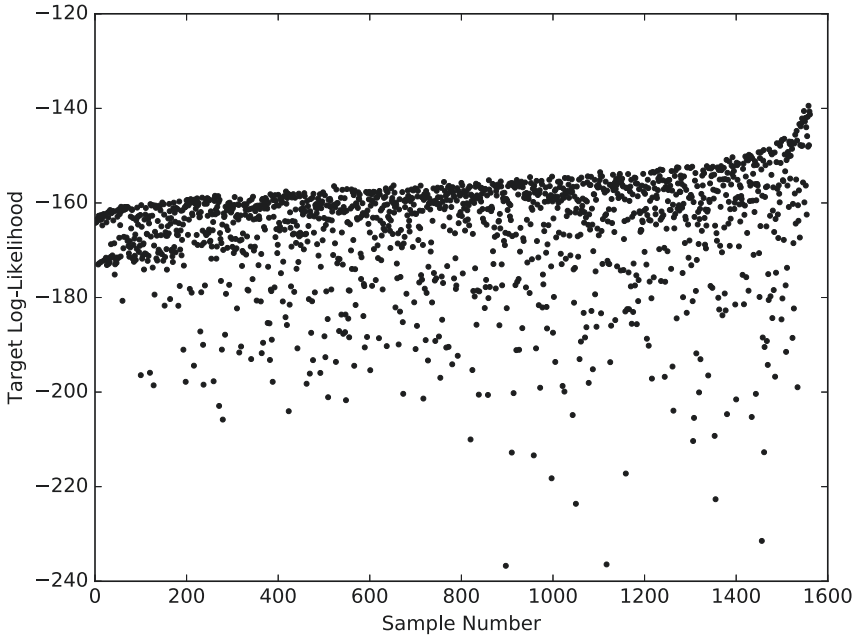
Importance sampling: Boltzmann→Target

Boltzmann



$$e^{-\beta\left(\sum_{i=1}^{n} a_i q_i + \sum_{i=1}^{n} \sum_{j=1}^{i-1} b_{ij} q_i q_j\right)}$$

Target



$$\frac{f(\mathbf{q})}{e^{-\beta\left(\sum_{i=1}^{n} a_i q_i + \sum_{i=1}^{n} \sum_{j=1}^{i-1} b_{ij} q_i q_j\right)}}$$

Possible next steps

- Use a better approximation for the D-Wave sampling likelihood
  - Results that are being presented today?
  - $\exp\left\{-\beta\left[\sum_i (1+\epsilon_i) a_i q_i + \sum_{i<j} (1+\epsilon_{ij}) b_{ij} q_i q_j\right]\right\}$
  - Better Boltzmann sampling from D-Wave
  - Finish off each sample with a short MCMC chain
- Reduce the impact of embedding
  - D-Wave's "product X"

Conclusion

- Importance sampling did not work well here, but we can and (someone) will do better in the future
- ToQ.jl is available on GitHub
  - https://github.com/losalamos/ToQ.jl
- Many thanks to the D-Wave team for their help along the way