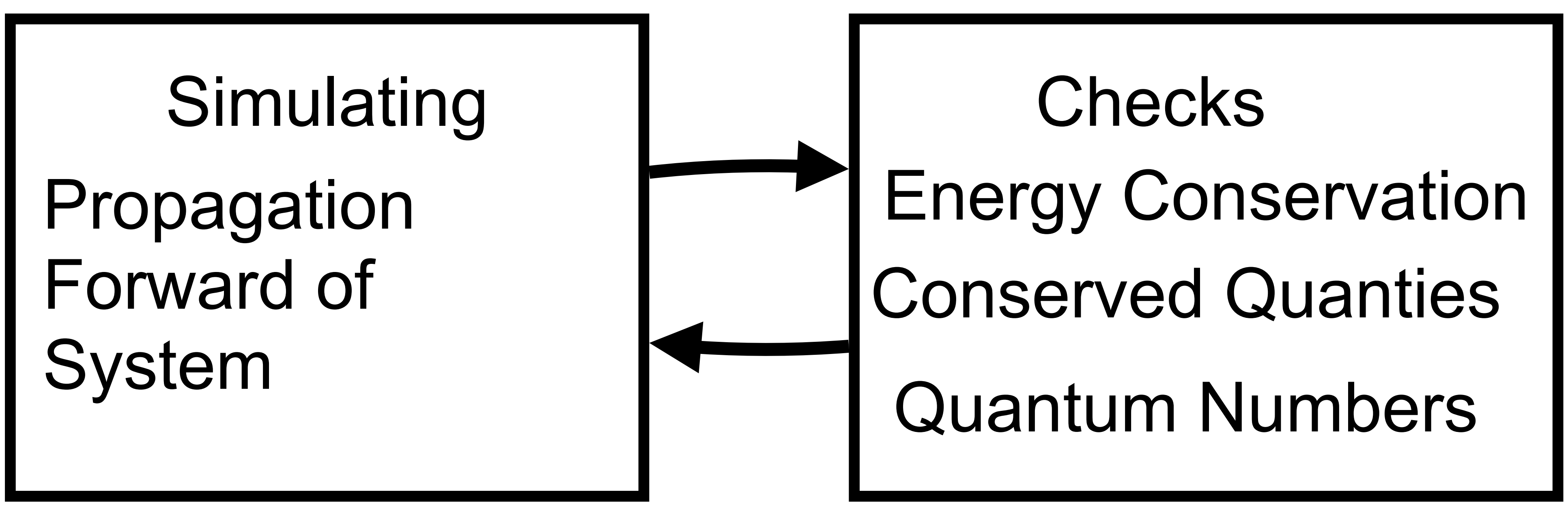
Making MC Better

- In this simulation part of this class
  - We have learned that simulations are not accurate
  - There are a few things we can do to make it better
    - Key is to have a notion of when we are going wrong



Correcting

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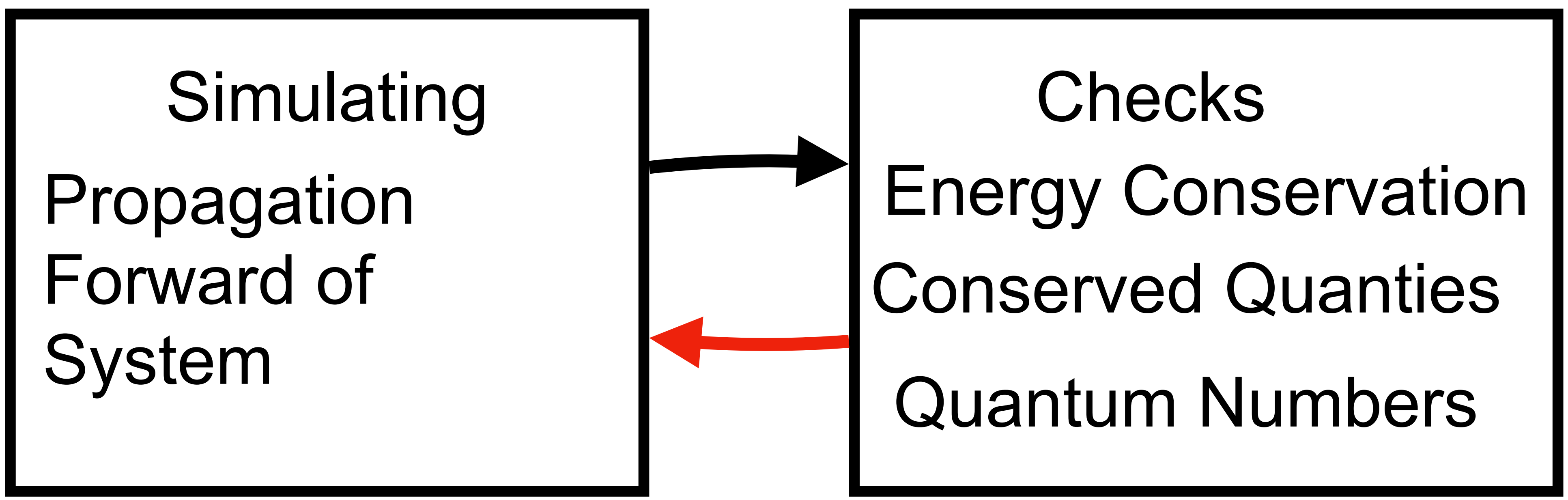
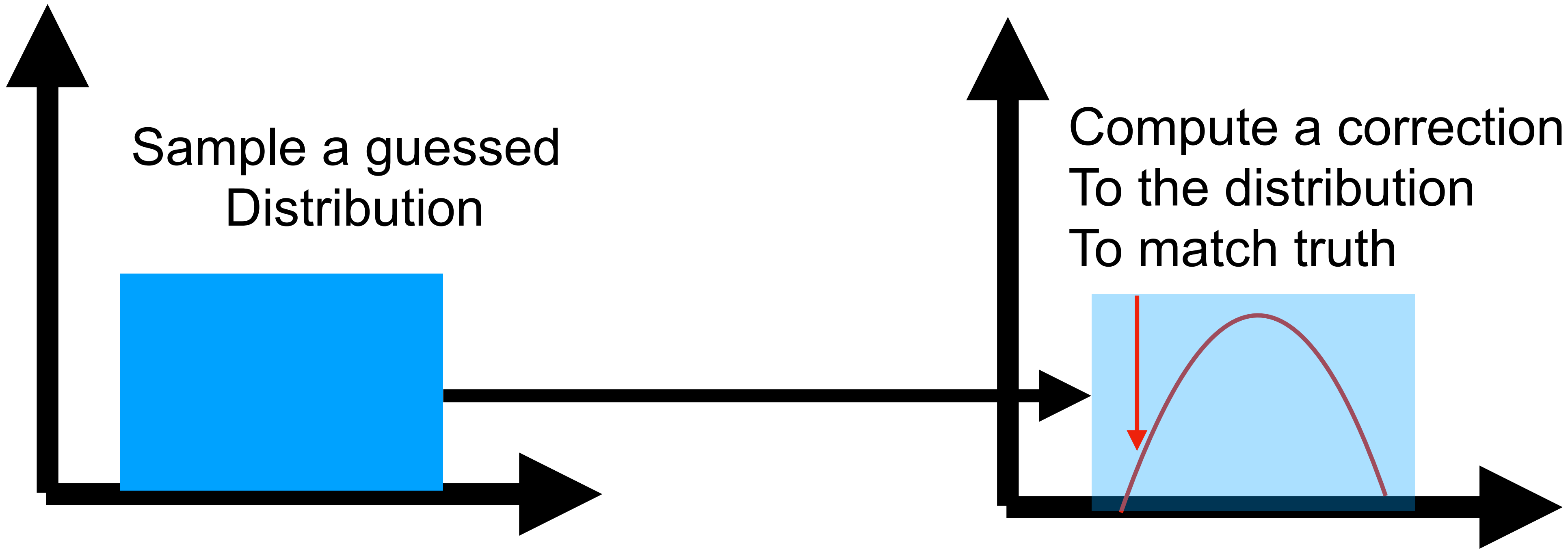
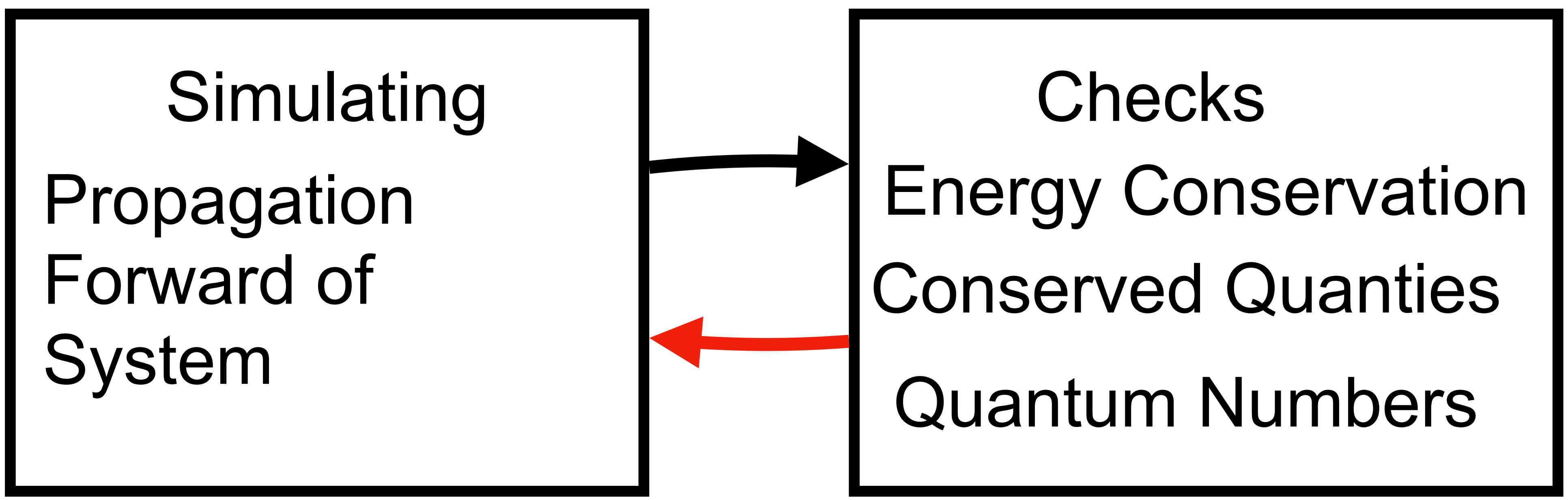


Correct Our Simulation Through a Probabilistic Rescaling

Markov Chain MC





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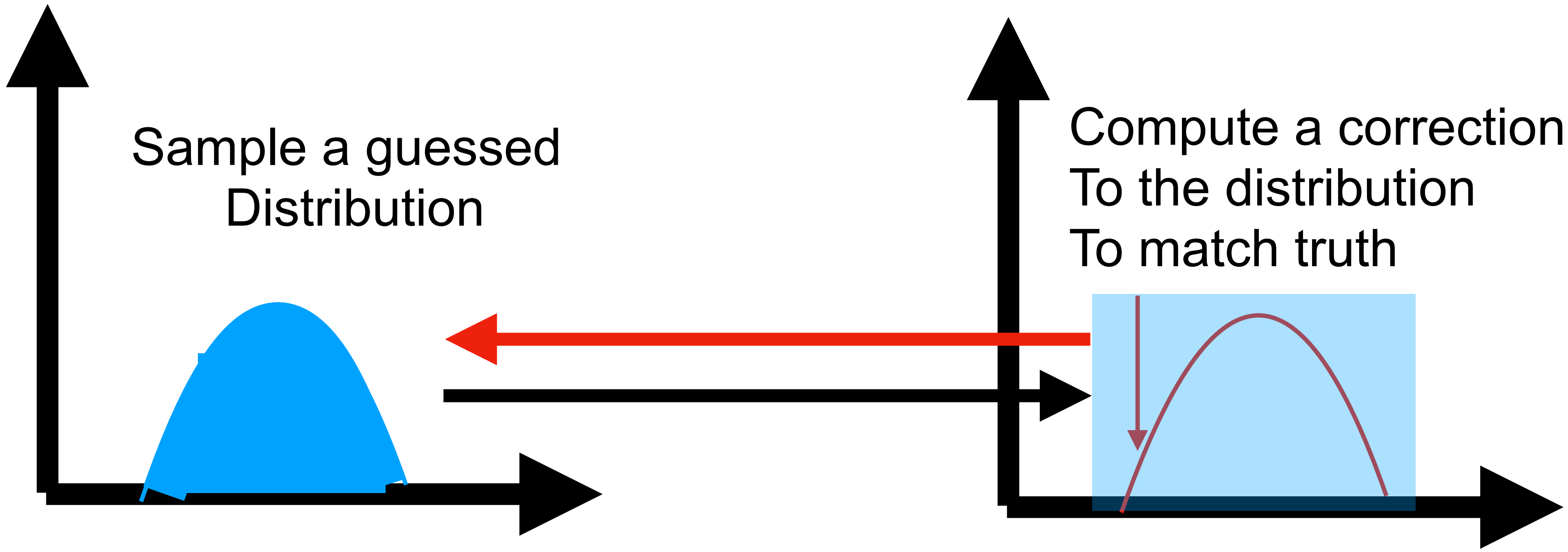


Simulating

Propagation
Forward of
System

Checks

Energy Conservation

Conserved Quanties

Quantum Numbers

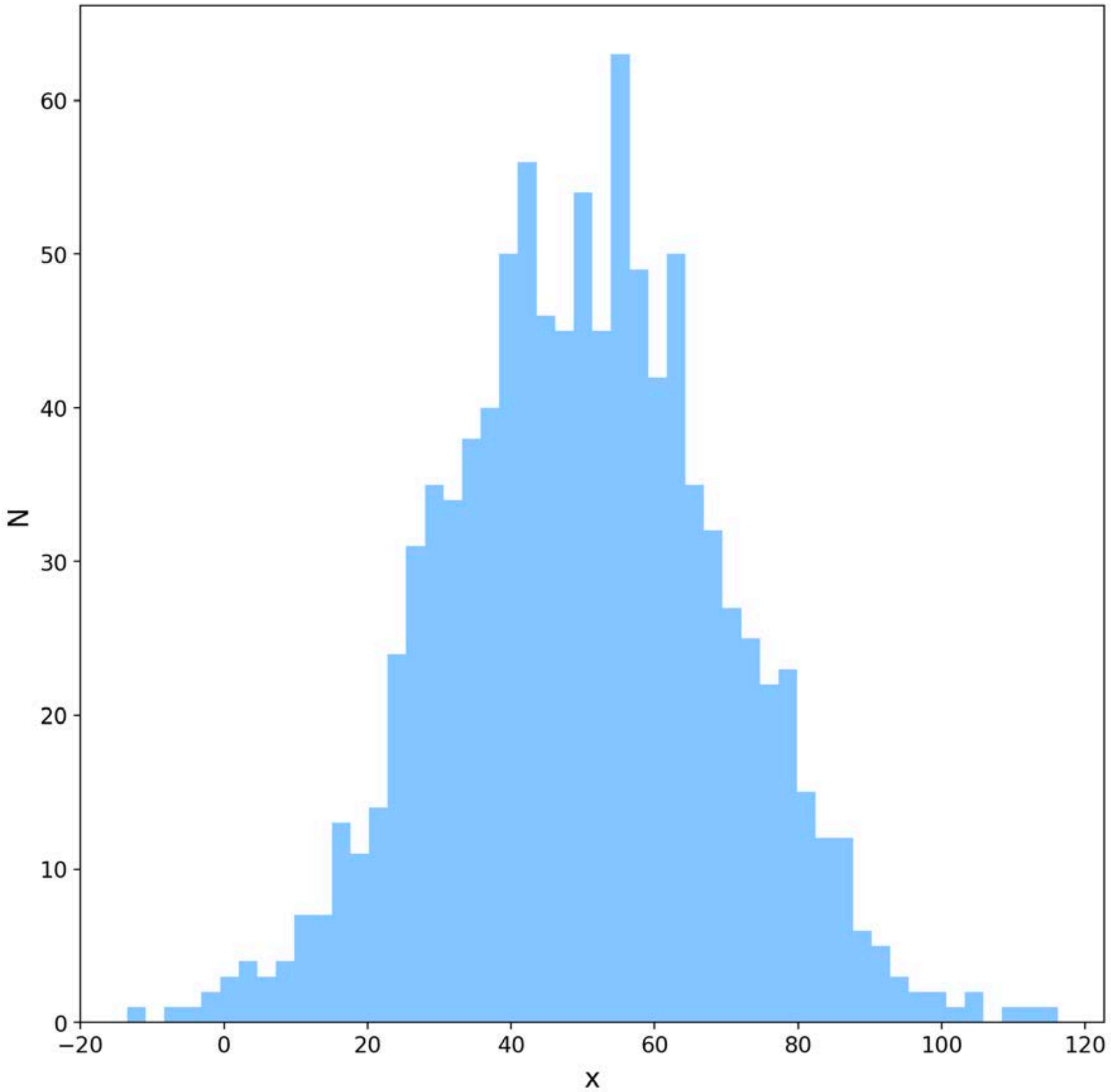
Correct Our Simulation Through a Probabilistic Rescaling

Metropolis-Hastings

- Step 0: Randomly sample a parameter $\boldsymbol{x_1}$
- Step 1: Sample a new parameter $\mathbf{x_2}$
    - Use a chosen “Proposal Function”
    - Compute the probability of stepping $\mathbf{x_2}$ to stepping $\mathbf{x_1}$
- Step 2: Sample a flat distribution from 0 to 1 ($\mathbf{s_2}$)
    - Accept $\mathbf{x_2}$ if $s_2 < \dfrac{p(x_2)}{p(x_1)}$
- Step 3 : Go back to step 1

Fitting a Guassian

- Strategy to randomly sample mean(μ) and sigma σ
  - Accept the values for μ, σ if probability is higher
  - Keep accepting/rejecting until we hit equilibrium



Log(Probability)

$$\log(\mathcal{L}) = \sum_i \log\left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(\mu-x_i)^2}{\sigma^2}}\right)$$
$$= \sum_i \left(\frac{x_i-\mu}{\sigma}\right)^2 - \frac{1}{2}\log\left(2\pi\sigma^2\right)$$

Accepted μ, σ yield the best fits

Visualizing in Bayes

Posterior probability of the model in light of the data

Likelihood function of the data given the model

Prior probability of the model

$$\boxed{P(\text{model}|\text{data})} = \frac{\boxed{P(\text{data}|\text{model})}\,\boxed{P(\text{model})}}{P(\text{data})}$$

Equilibrated Best Fit

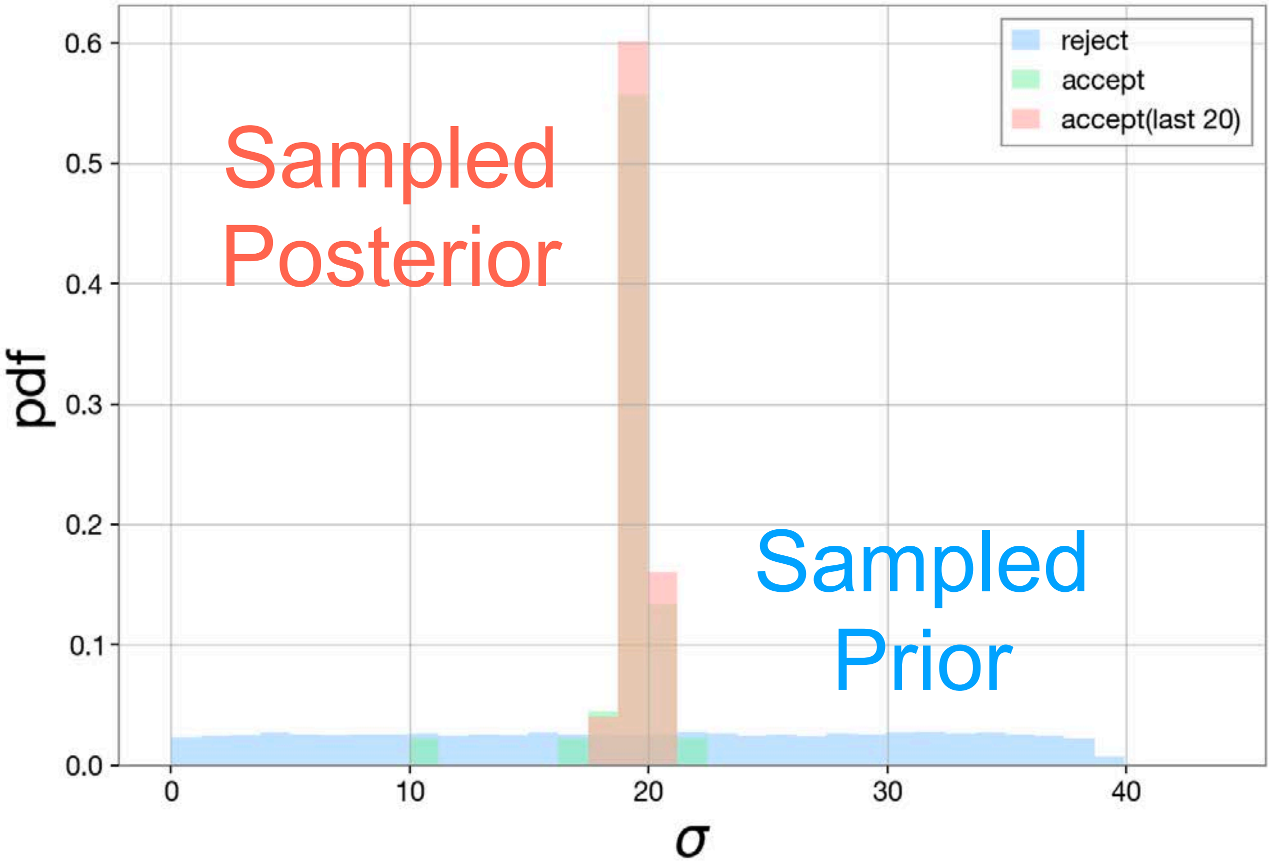
Sampled Distribution
Aka Proposal

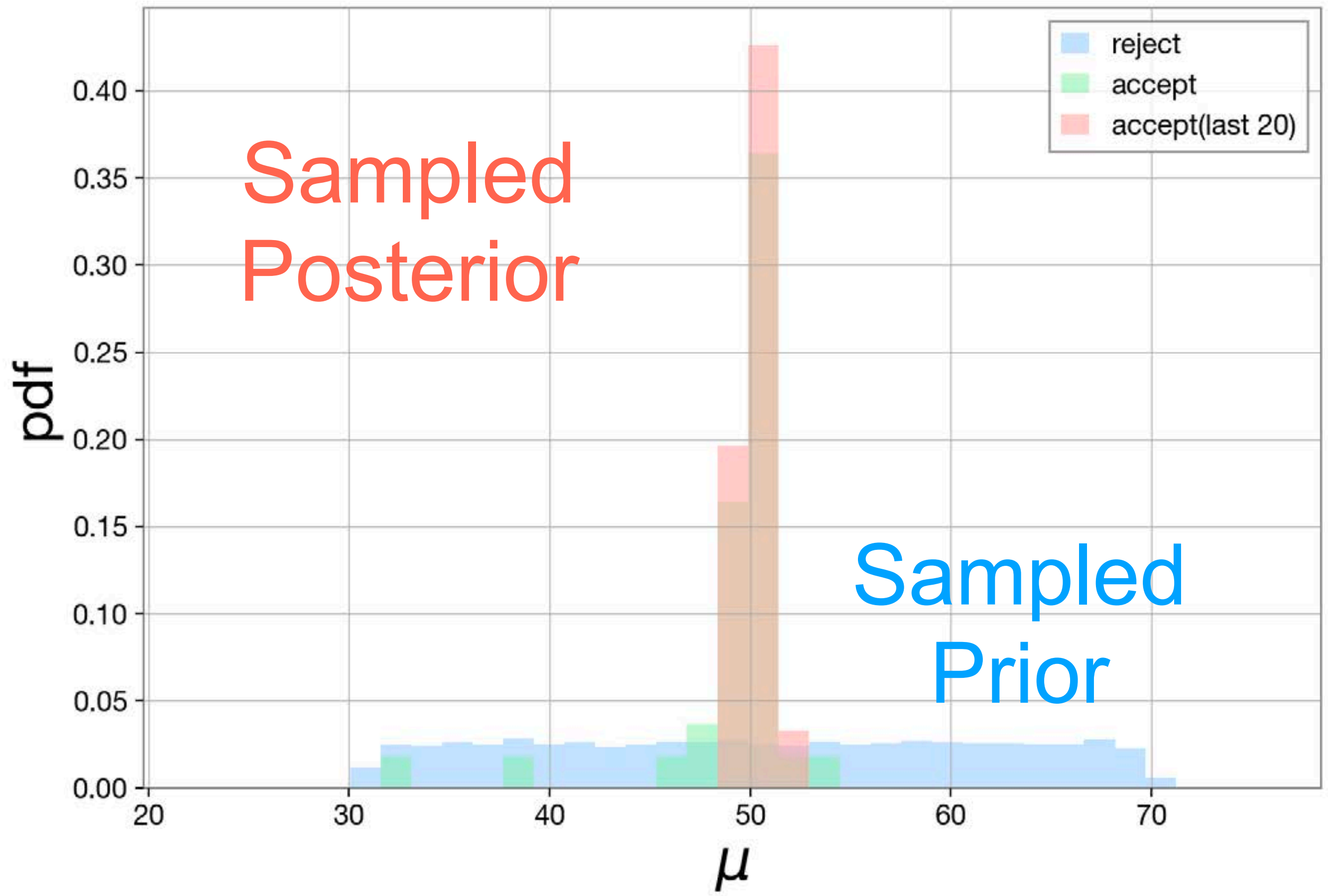
Probability Driving
Decision

Evidence [can typically be absorbed into the normalization of the posterior]

The Likelihood reweights the Prior to the Posterior

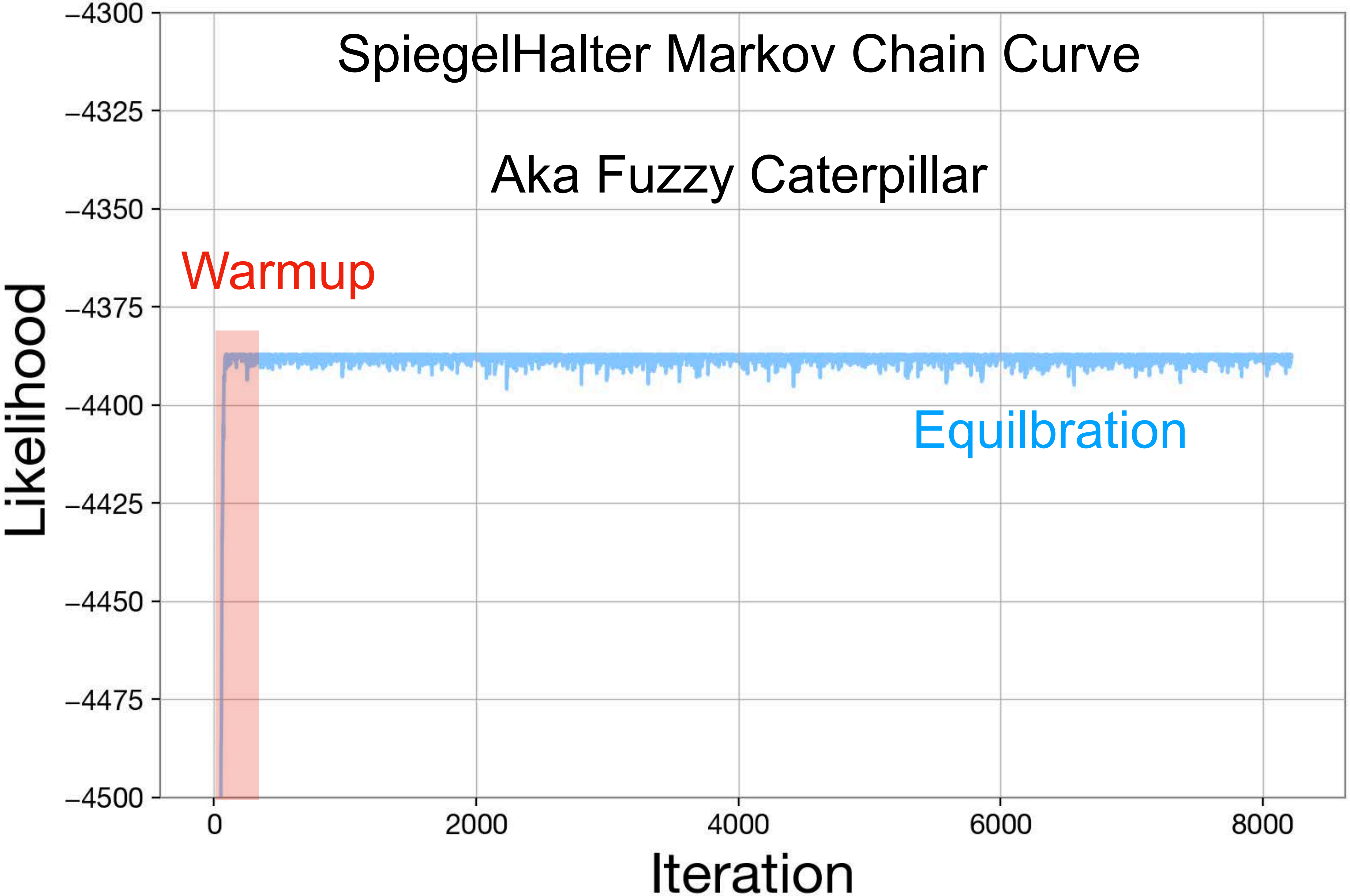
Best Fit Paramters



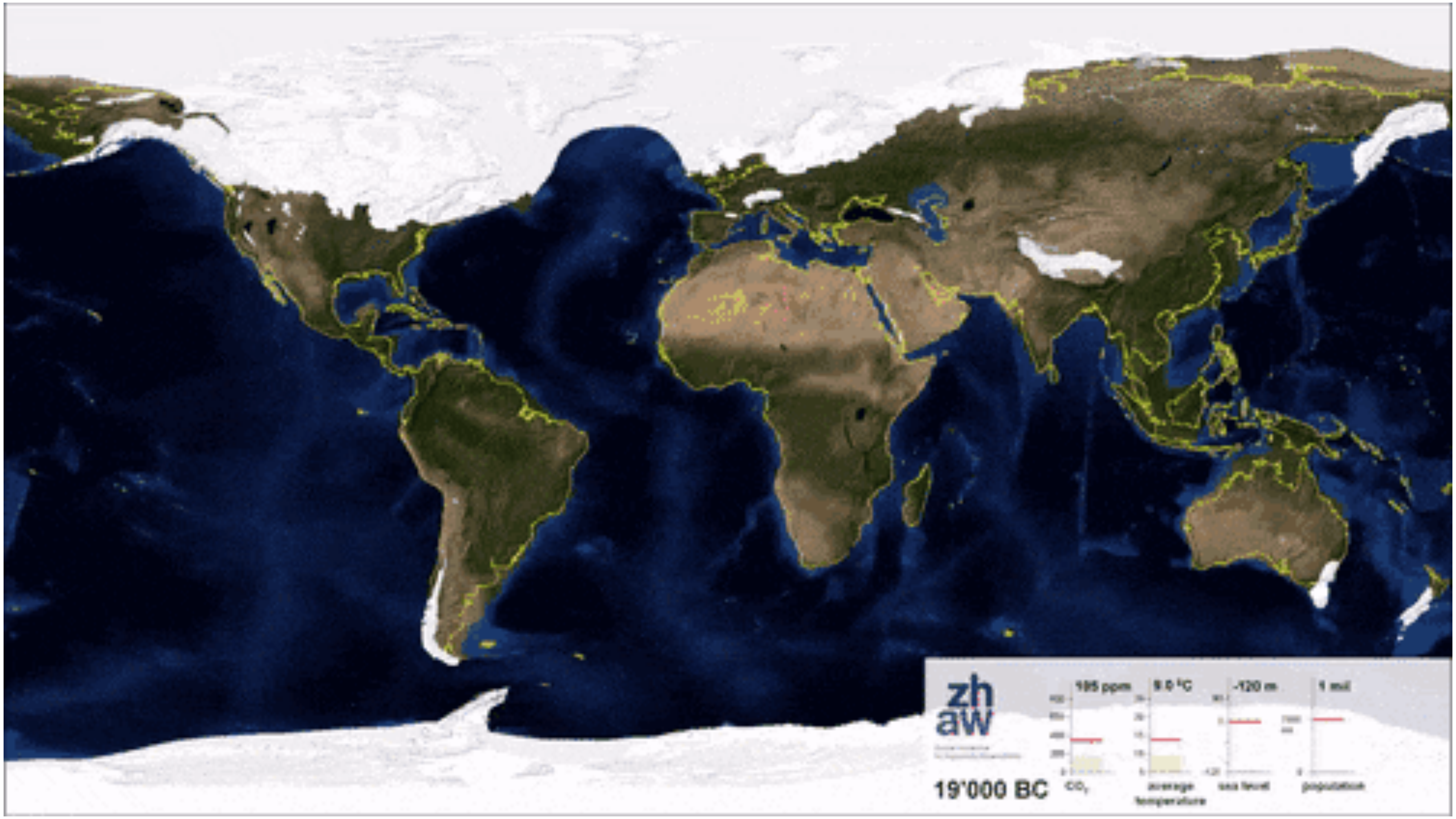


- This is where I start to hint that there are limitations here
- What we are doing is running a check
  - We are not taking a derivative (No gradients or Hessians)

Best Fit Paramters

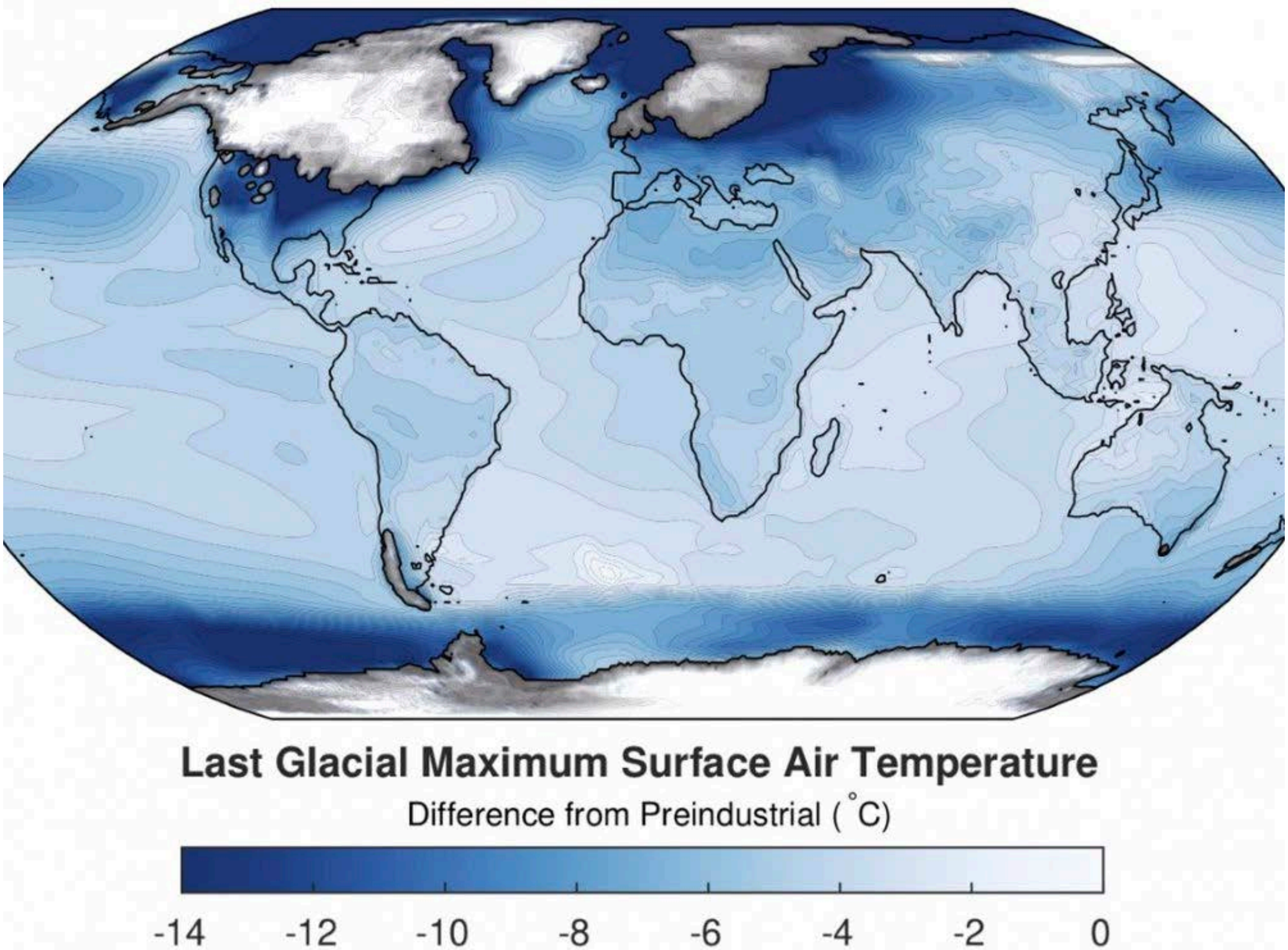


The Ice Age



- Ice age had a profound impact on the earth
- Crazy to think humans were alive at this time

The Ice Age


Last Glacial Maximum Surface Air Temperature
Difference from Preindustrial (°C)
-14
-12
-10
-8
-6
-4
-2
0

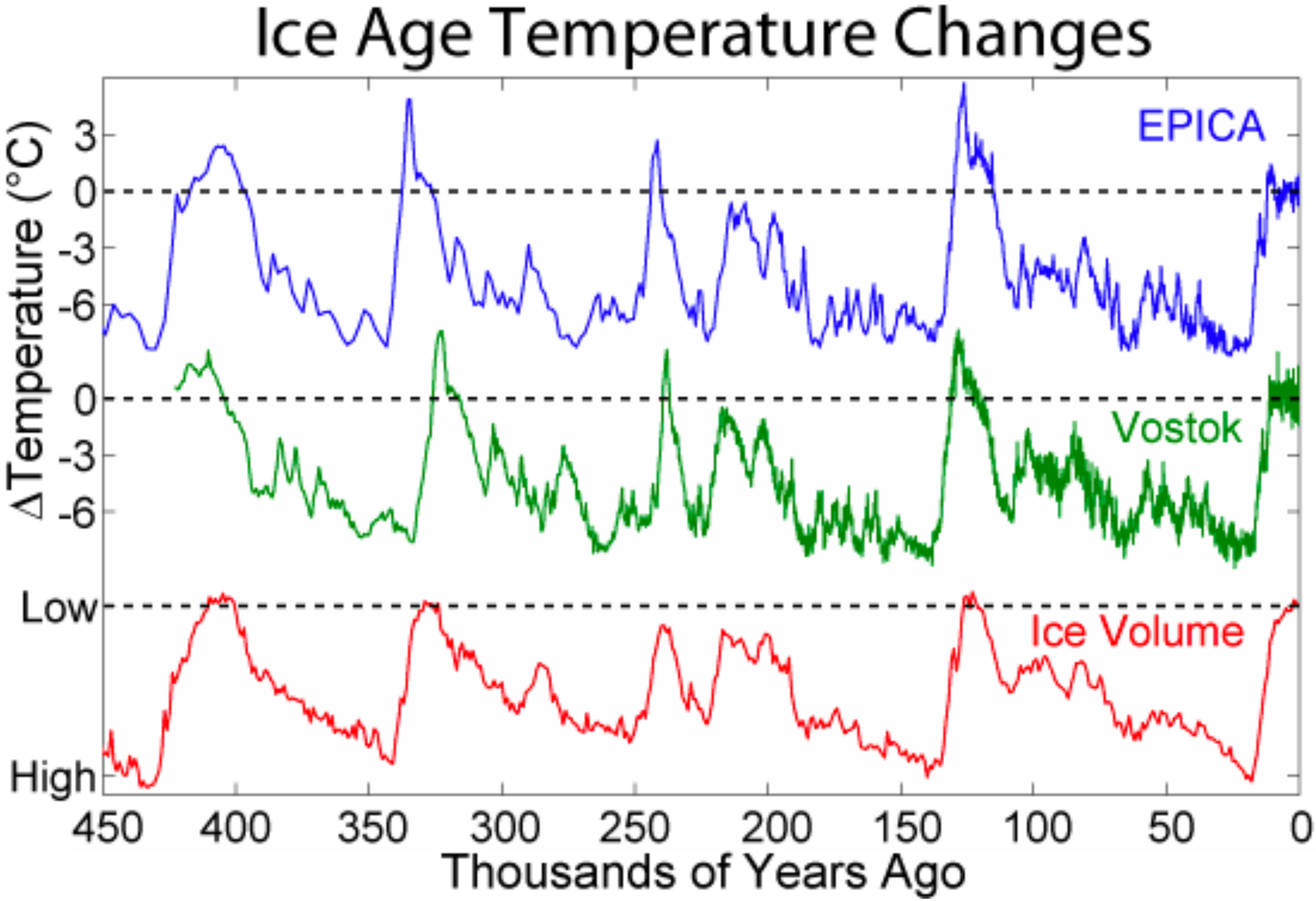
Ice Core Temps

The dark band in this ice core from the West Antarctic Ice Sheet Divide (WAIS Divide) is a layer of volcanic ash that settled on the ice sheet approximately 21,000 years ago. — Credit: Heidi Roop, NSF

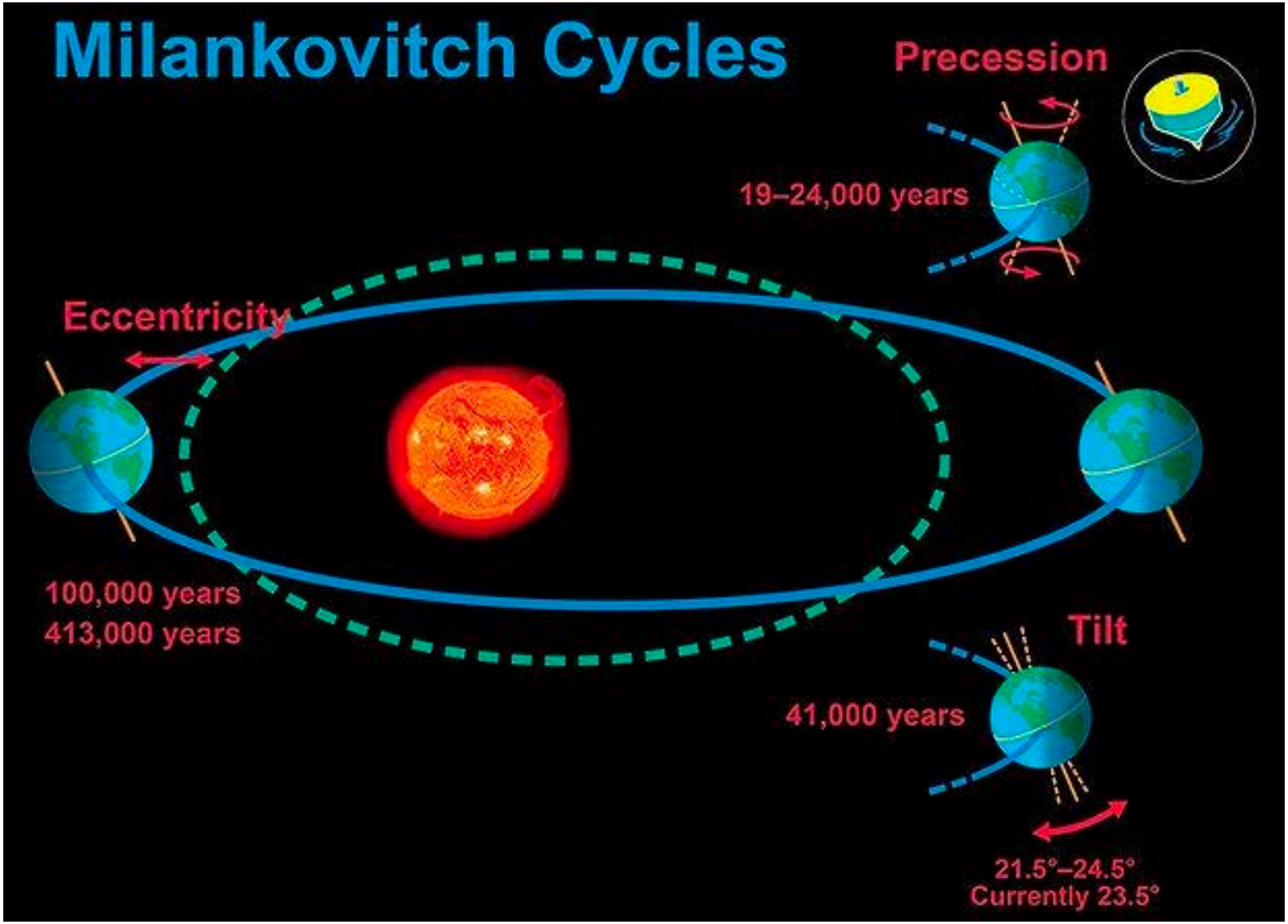
Ice Core

Ice Core recovery has been
A critical element In many
locations on earth

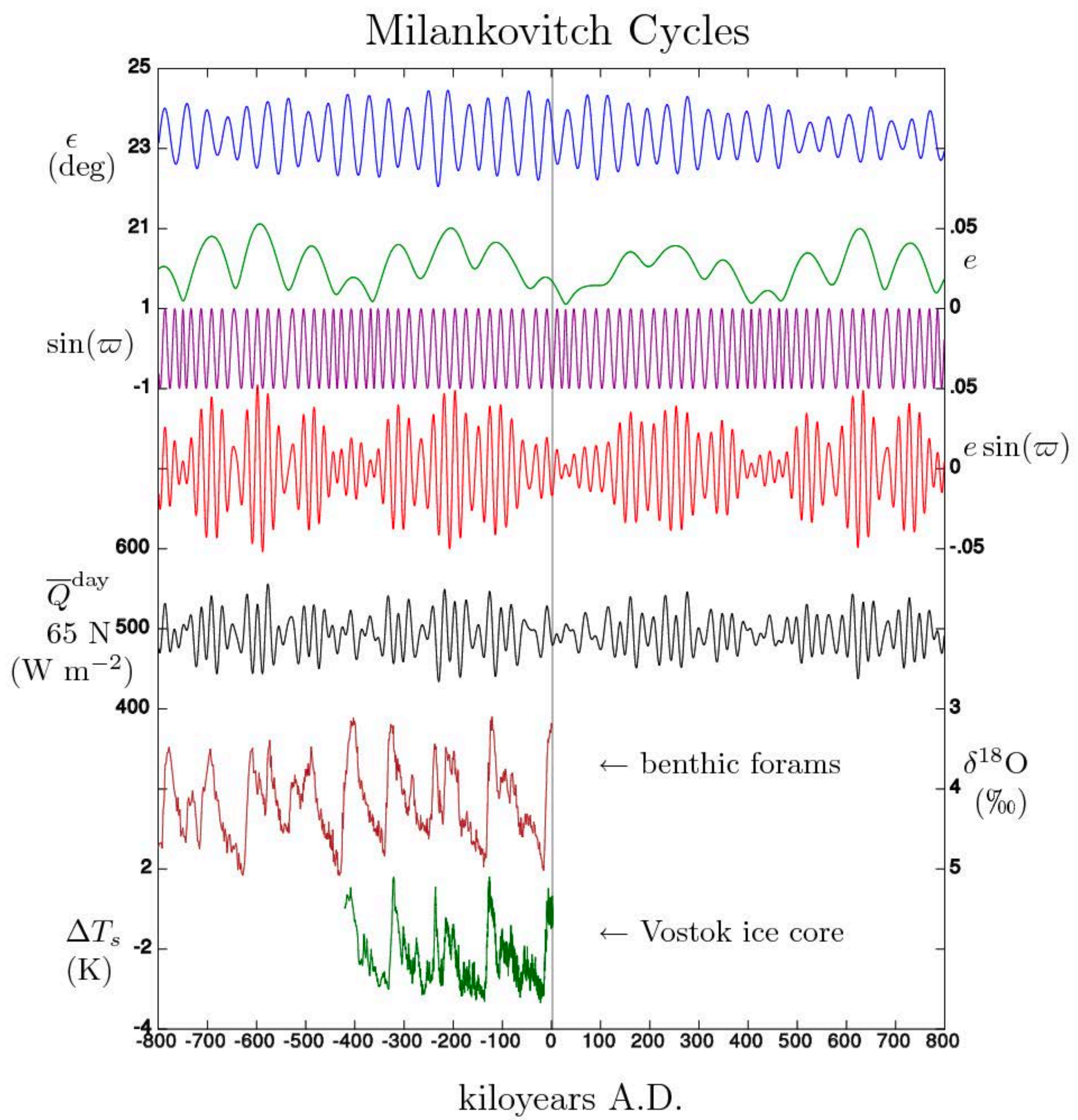
Ice Age over time



Milhanovitch Cycles

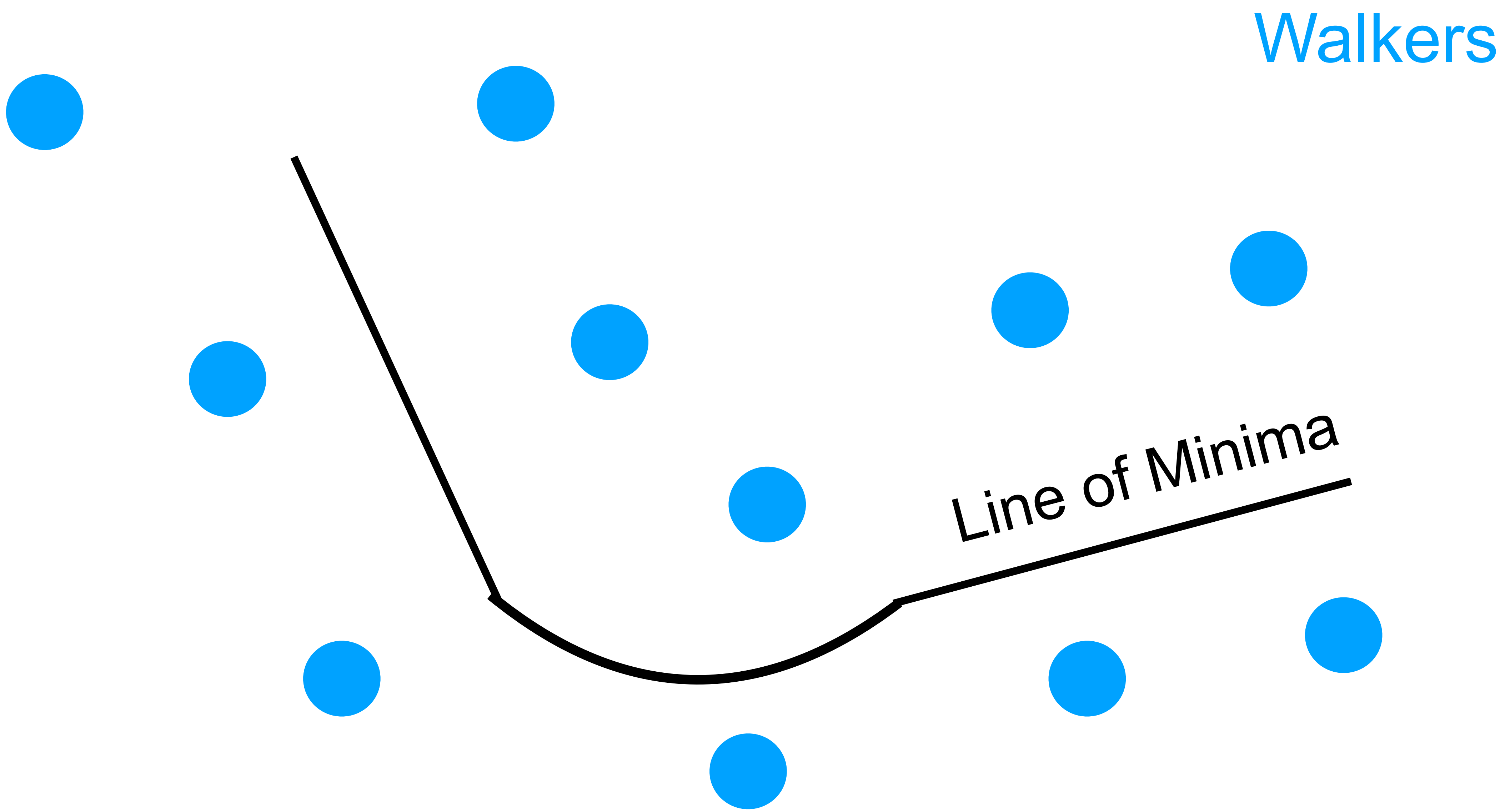


Scale of Eccentricity



Speeding up MCMC

- We can consider having many walkers probe our space
  - Many walkers at the same time speed up convergence



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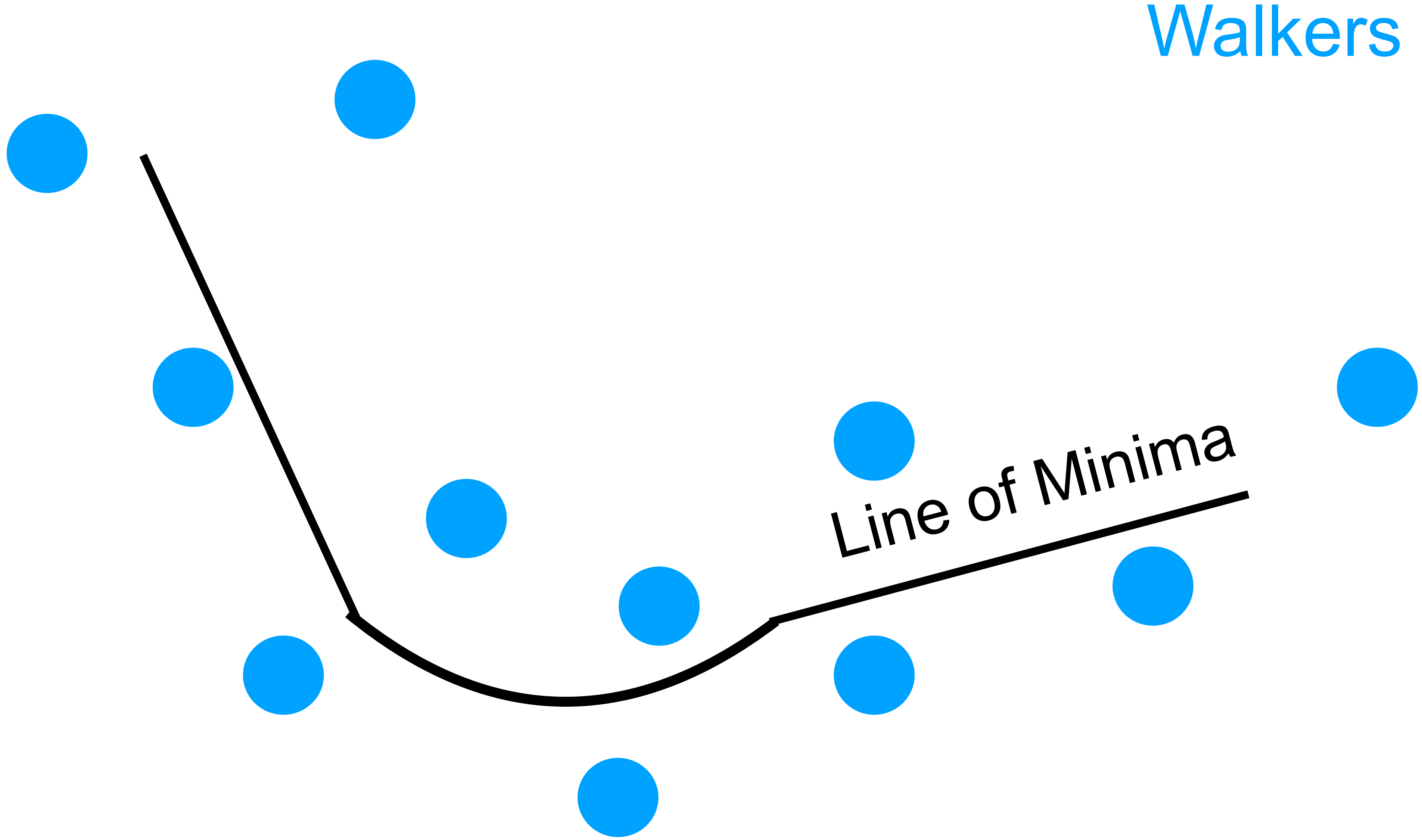

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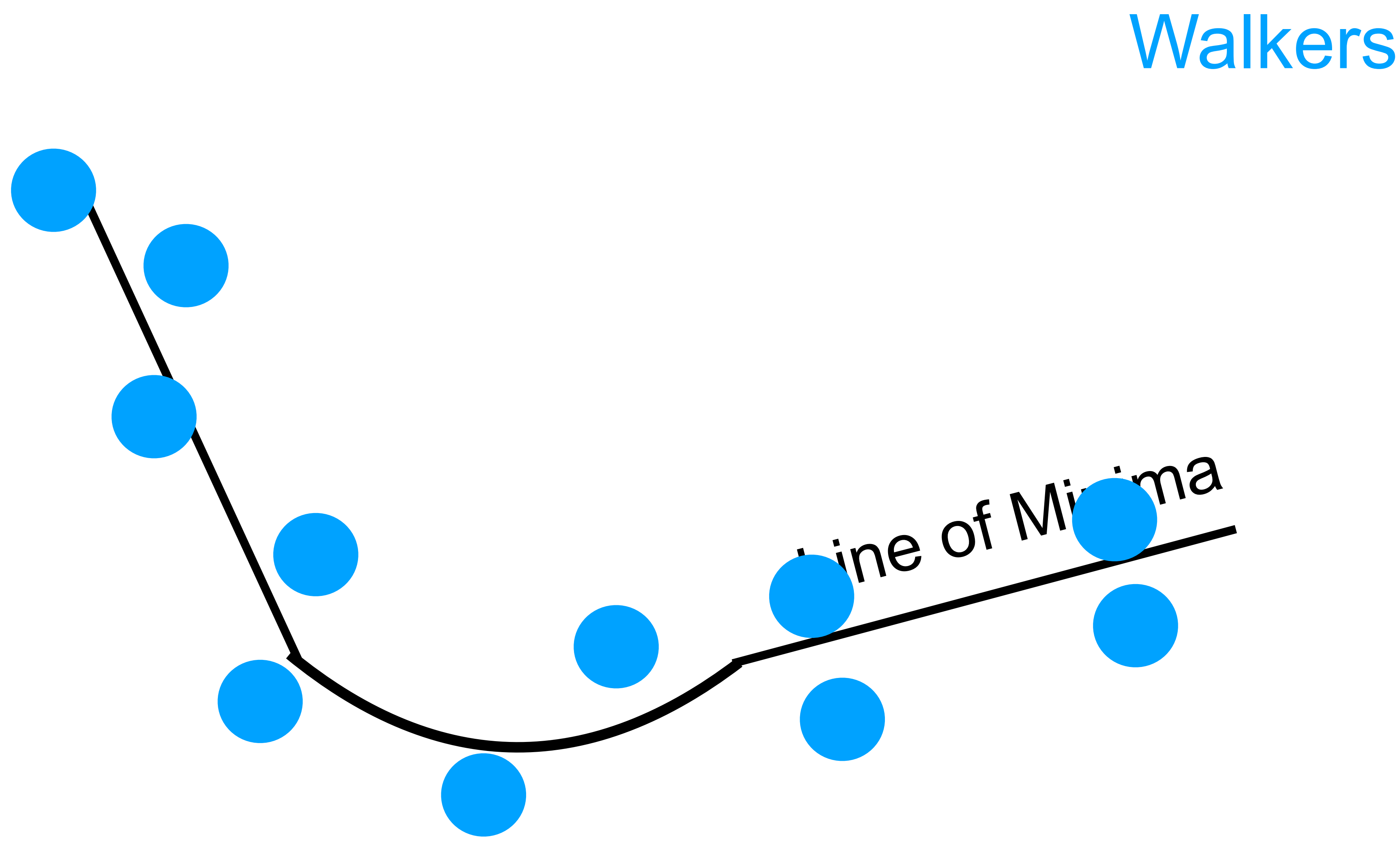
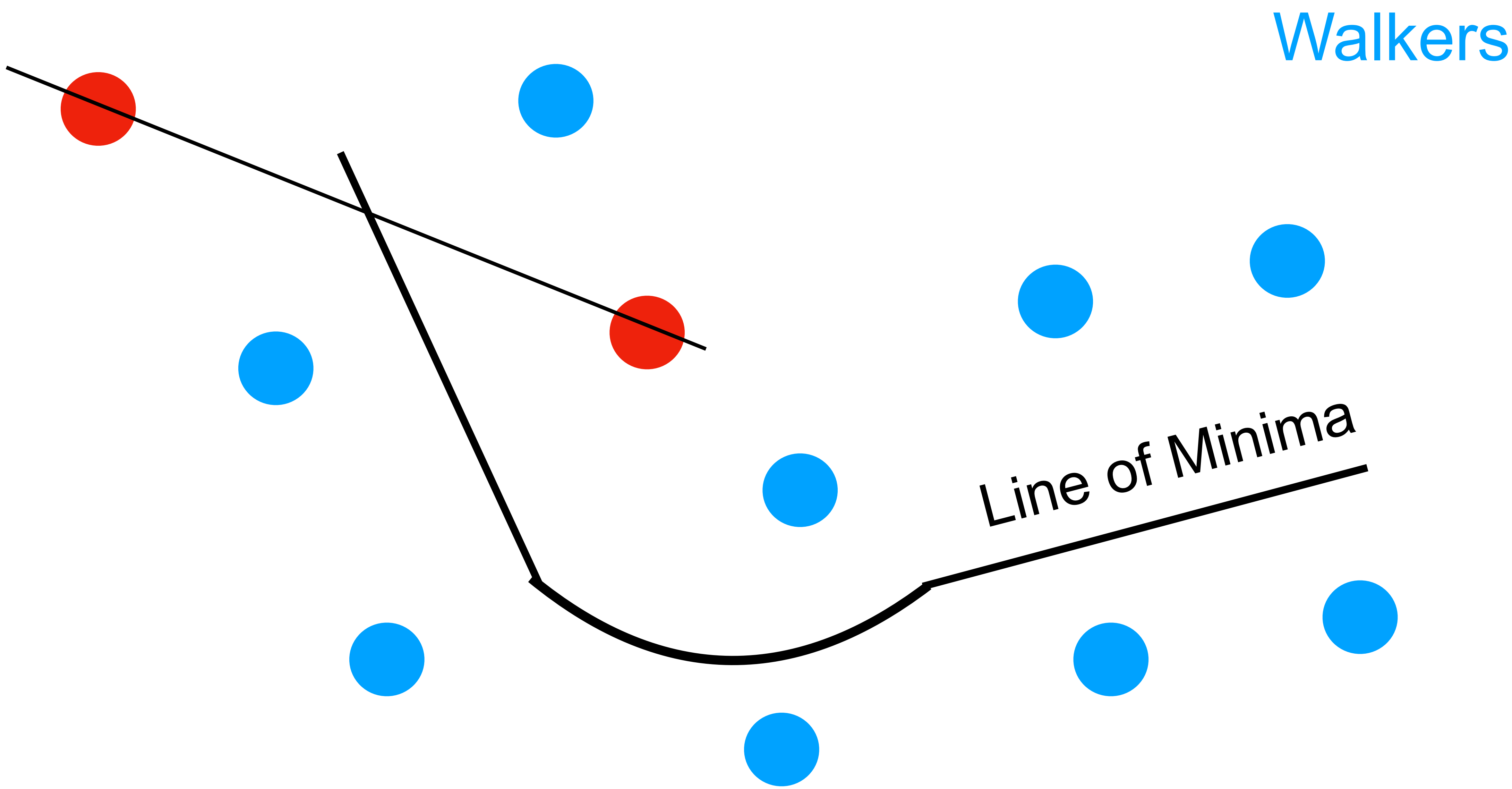


Updating w/Random Points

- We randomly choose a pair of points
  - Move one of the points along the line between them



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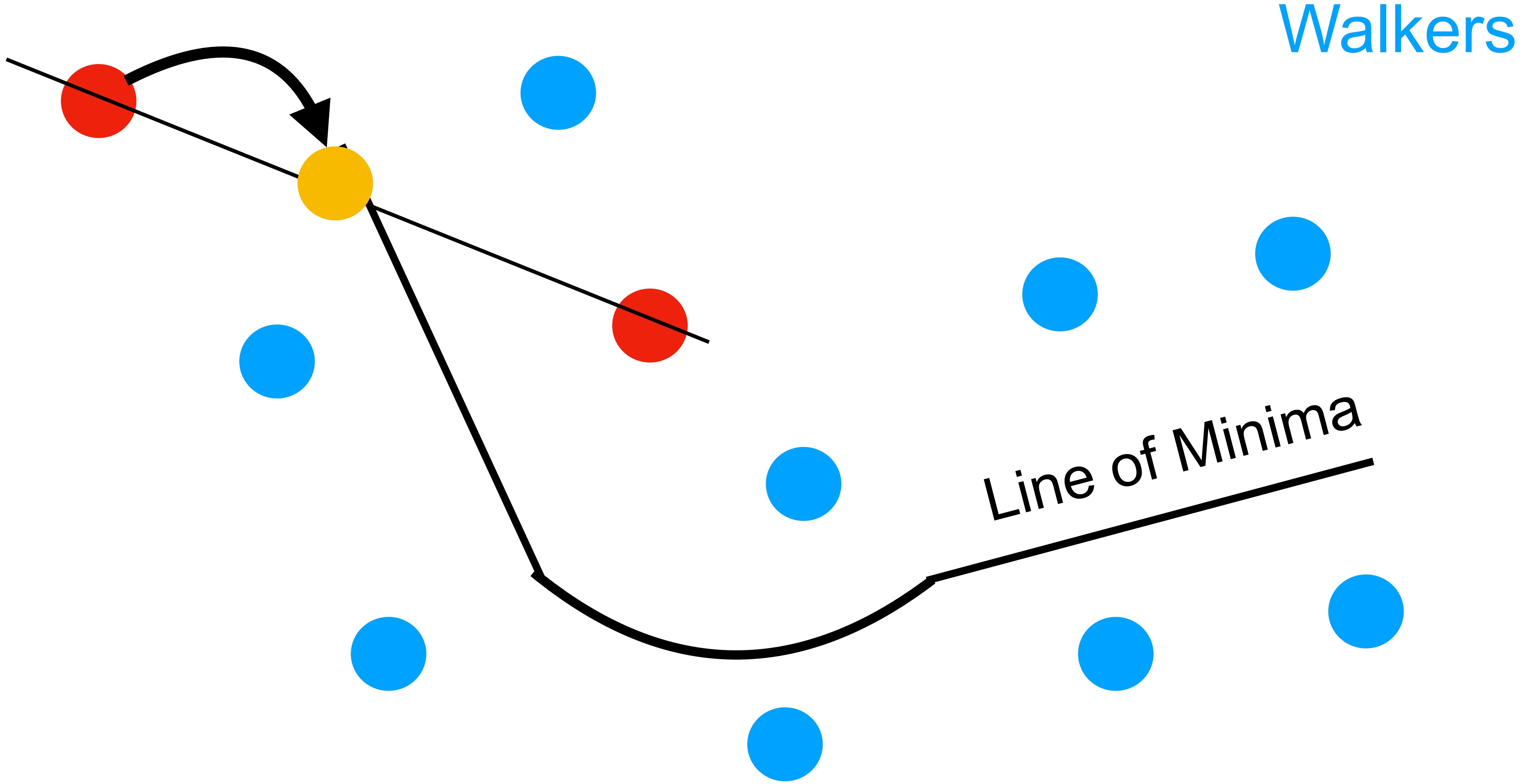

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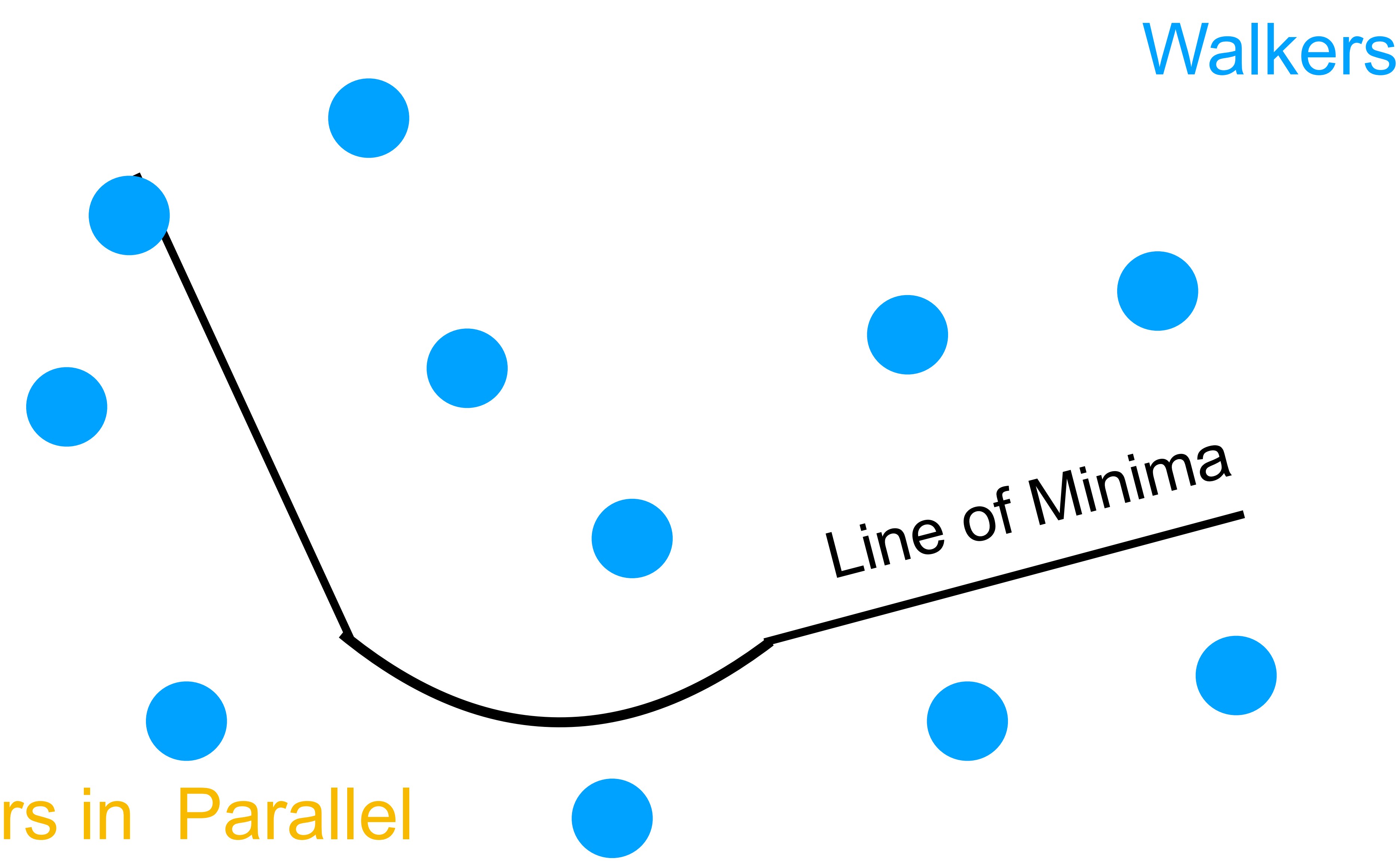


We can Update
All of the Walkers in Parallel

Quantum Monte Carlo

- Can use the same MCMC to populate a wave function
  - We can then scan paramaters to solve Shroedinger's Eq

$$\boxed{\psi(\vec{r}\,|\,\vec{\theta}) = Ae^{-r/\theta_0}}$$

Guess a Form for the wavefunction

$$\boxed{p(\vec{r}\,|\,\vec{\theta}) = \frac{\psi^*(\vec{r}\,|\,\vec{\theta})\psi(\vec{r}\,|\,\vec{\theta})}{\langle\psi\,|\,\psi\rangle}}$$

We can define probability from wavefunction

$$\boxed{w_{i+1} = \frac{p(\overrightarrow{r_{i+1}}\,|\,\vec{\theta})}{p(\overrightarrow{r_i}\,|\,\vec{\theta})}}$$

Our proposal Doesn't need integral Aka $\langle\psi\,|\,\psi\rangle$

Multiple Walkers Populate

- The key is to MCMC evolve the wave function many times
  - We can use the aggregate Particles solve QM stuff

$$\sum_j \psi_j(\vec{r}\,|\,\vec{\theta}) = Ae^{-r/\theta_0}$$

Guess a Form for the wavefunction

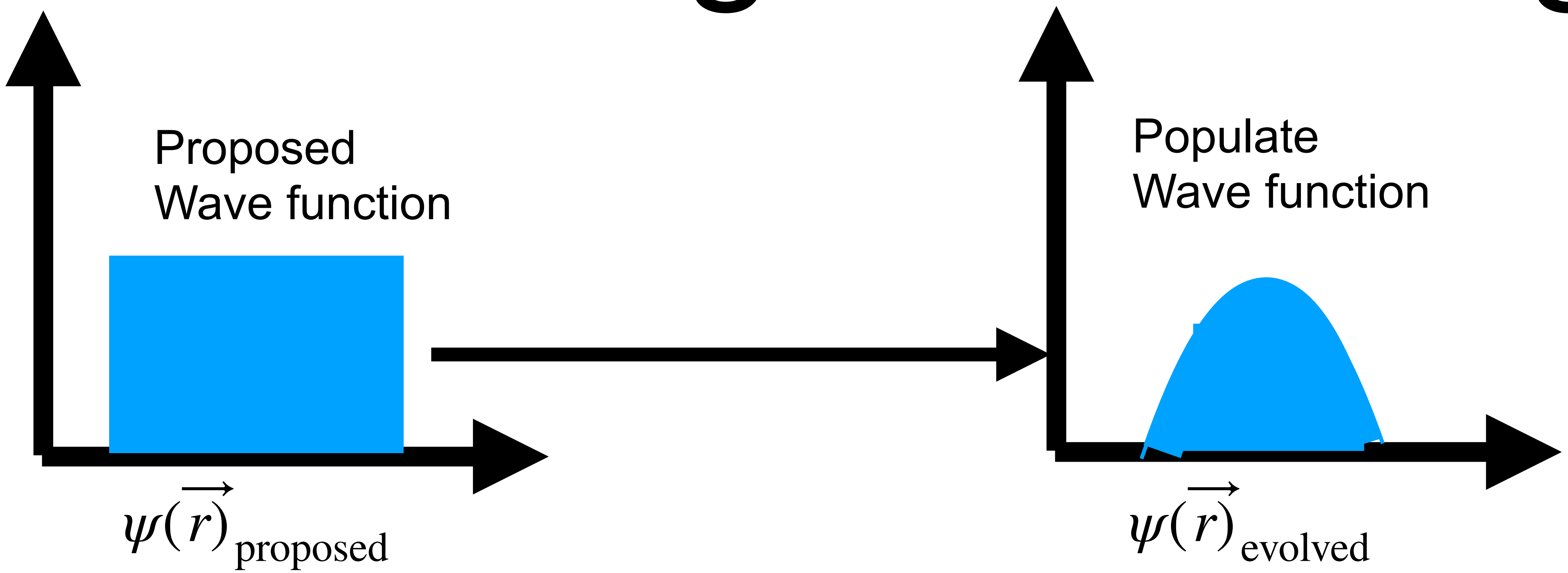
$$\sum_j p_j(\vec{r}\,|\,\vec{\theta}) = \frac{\psi_j^*(\vec{r}\,|\,\vec{\theta})\psi_j(\vec{r}\,|\,\vec{\theta})}{\langle\psi|\psi\rangle}$$

We can define probability from wavefunction

$$\sum_j w_{i+1}^j = \frac{p_j(\overrightarrow{r_{i+1}}\,|\,\vec{\theta})}{p_j(\overrightarrow{r_i}\,|\,\vec{\theta})}$$

Our proposal Doesn't need $\langle\psi|\psi\rangle$

Solving Schroedinger



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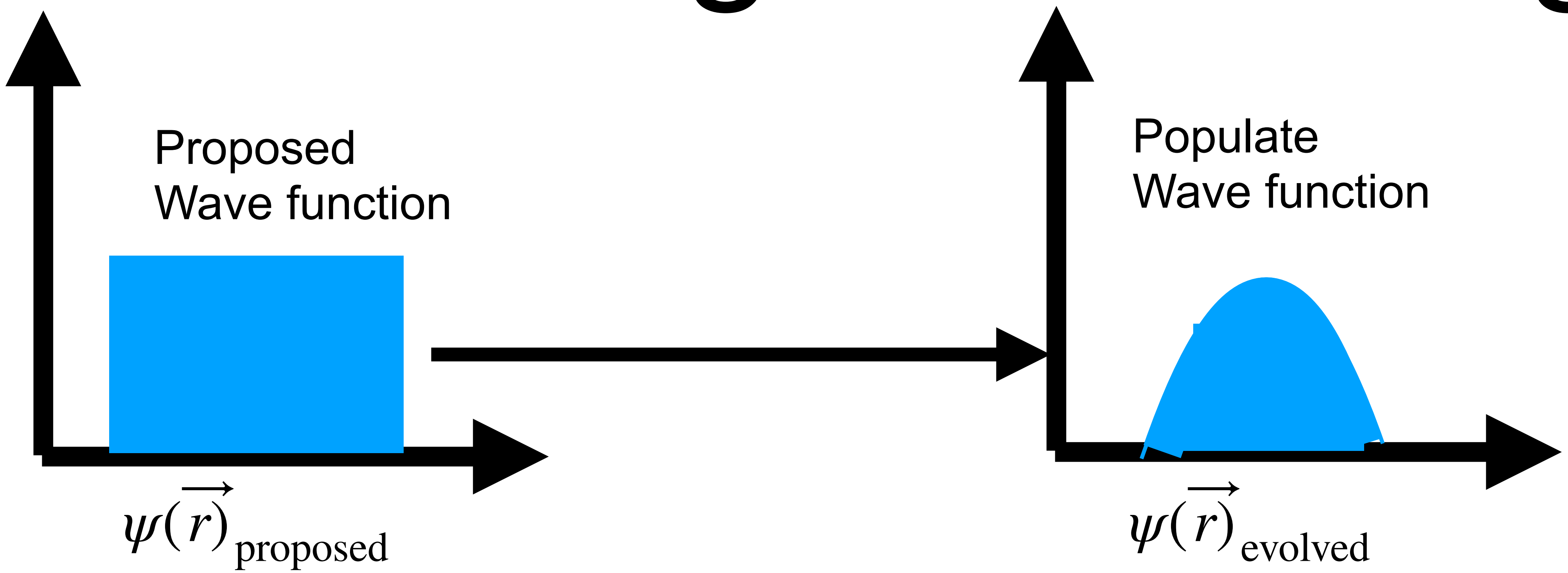
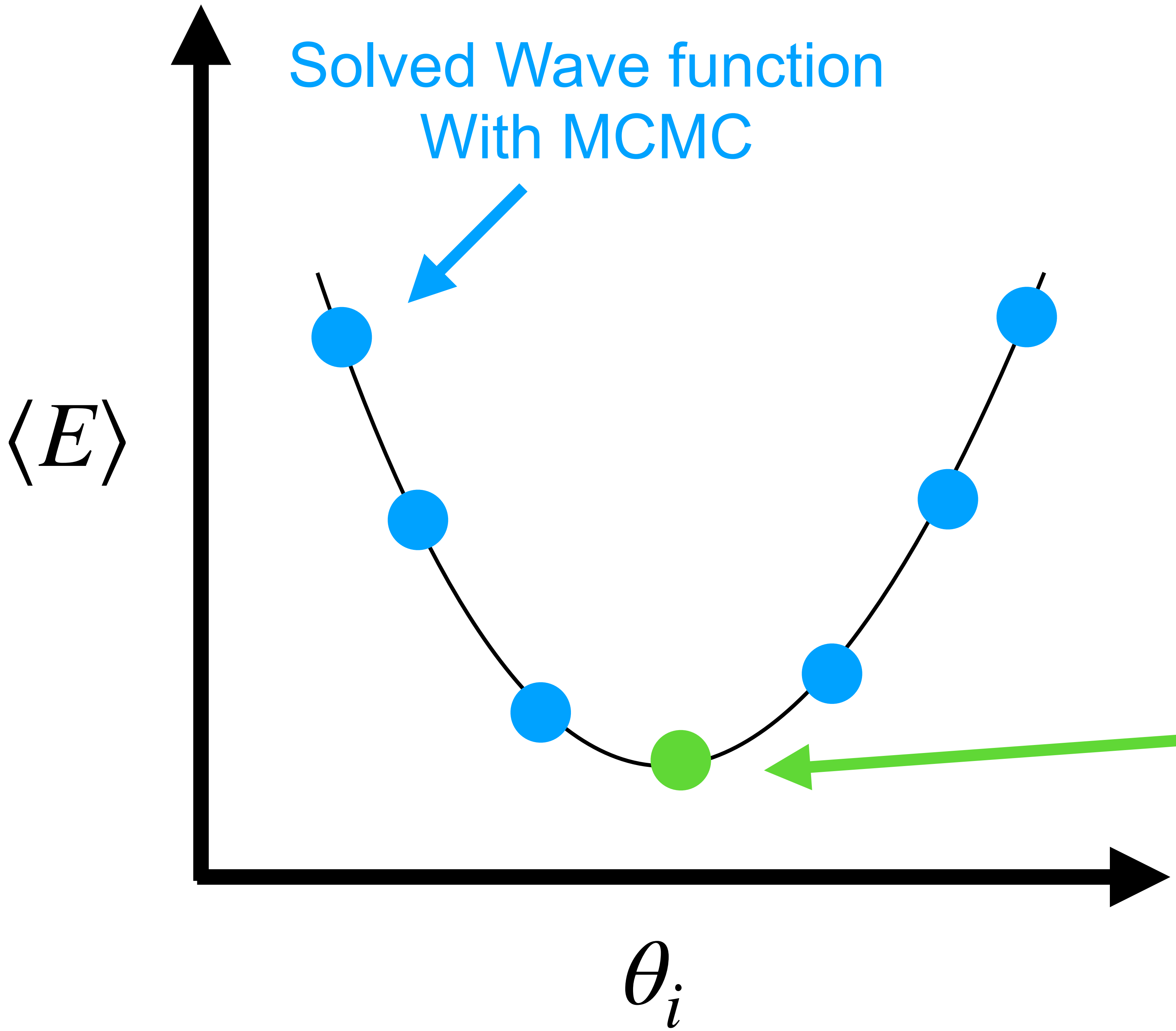


- Once we have the evolved wave funciton
  - We can compute expectations
  - No need to integrate (Realy this is MC integration)

$$\boxed{\langle E\rangle = \sum_j p_j(\vec{r}\,|\,\vec{\theta})E_j(\vec{r}\,|\,\vec{\theta}) = \sum_j \psi_j^*(\vec{r}\,|\,\vec{\theta})\psi_j(\vec{r}\,|\,\vec{\theta})E_j(\vec{r}\,|\,\vec{\theta})}$$

Solving Schroedinger



Our goal is to minimize the Energy given a wave functional form

Image Sources

ice age evolution gif

link: https://x.com/galka_max/status/839170821574832134

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ice age surface air temperature

link: https://www.smithsonianmag.com/smart-news/ice-age-temperature-science-how-cold-180975674/

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ice core

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