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Optimizing Replica Exchange

October 12, 2008 | Jan H. Meinke, Jülich Supercomputing Centre

Sampling Complex Energy Landscapes

Systems with frustration

→ rough energy landscape

→ difficult sampling

Parallel Tempering/Replica Exchange

Multiple independent replicas in parallel at different values of the control parameter (often temperature)

Exchange of replicas according to exchange criterion

$$P_{ex}(i,j)=\min\left(1,\mathrm{e}^{(\beta_i-\beta_j)(E_i-E_j)}\right)$$

Leads to random walk of replica in control parameter space

→ Faster relaxation especially at low temperatures

Choosing a Temperature Scale

Picking the range

Picking the number of replica

Choosing a discretization

- Linear in beta = 1/k_bT
- Geometric series beta_(i+1) / beta_i = const.
- Linear in T
- Any other discretization

Quality Measures

Goals

- Accelerate equilibration at low temperatures
- Minimize correlation time

Measure

- Correlation time at T_0
- Round trip time of replica

Optimizing the Temperature Scale

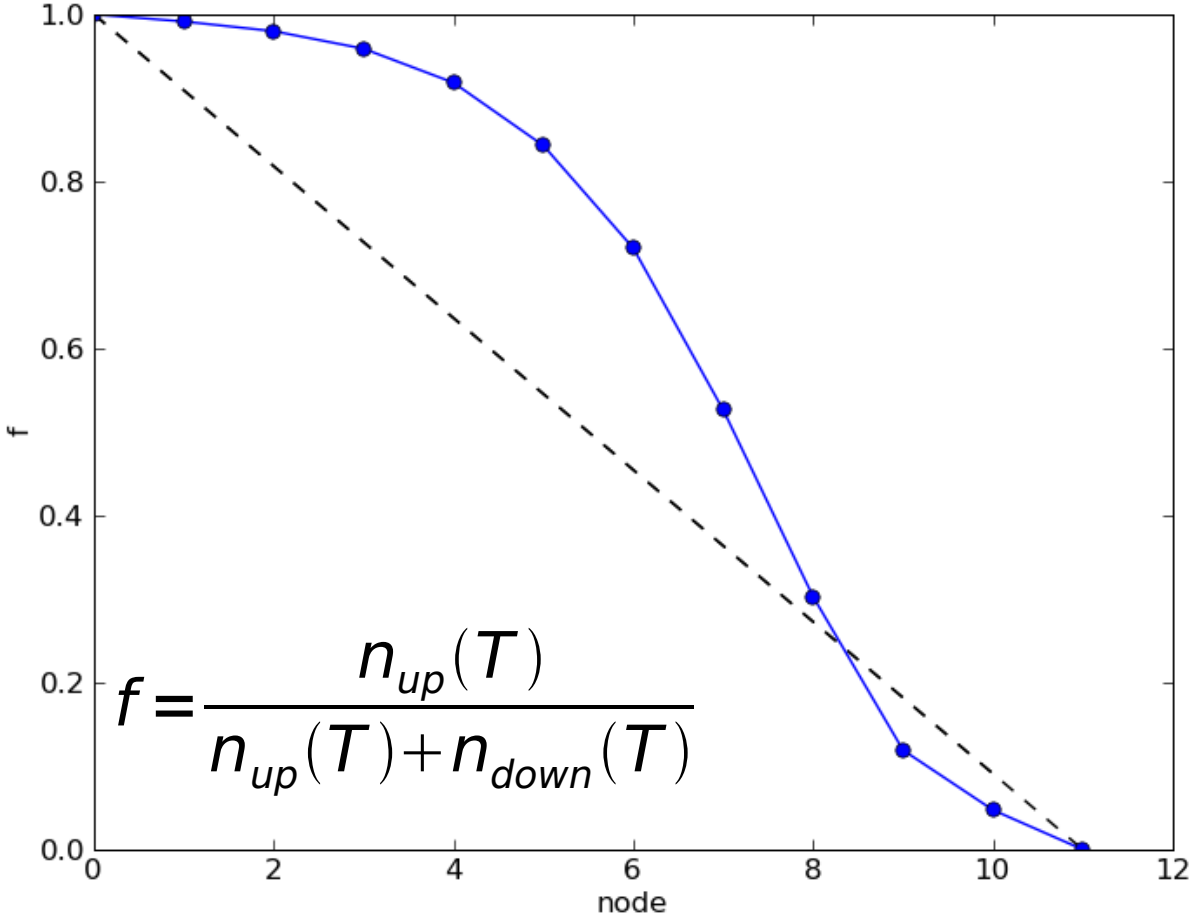
Goal

- Minimize average round trip time

Approach

- Equal probabilities ...
- Specific heat (fluctuation of energy)
- Flow

Optimizing the Temperature Scale



$$f = \frac{n_{up}(T)}{n_{up}(T) + n_{down}(T)}$$

Optimizing the Temperature Scale

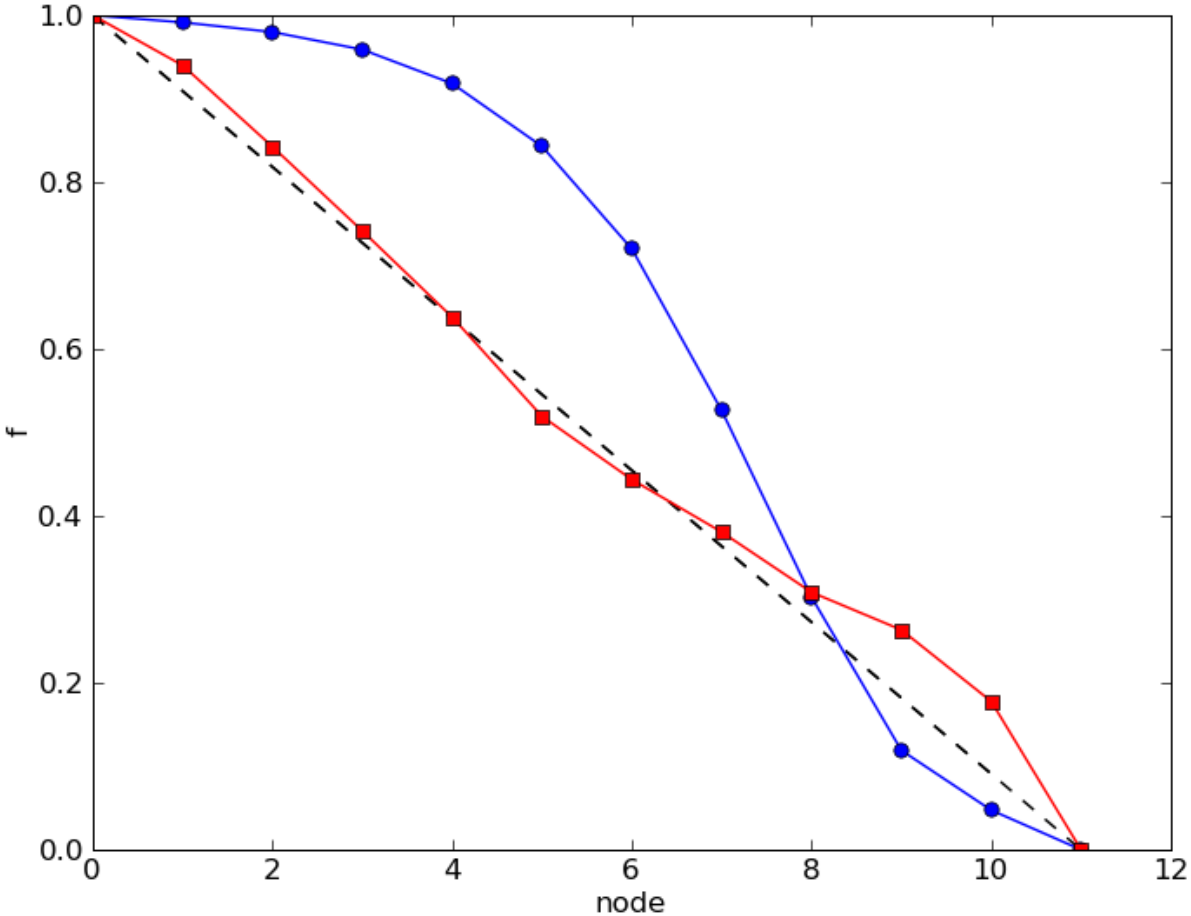
f defines a steady state current j

$$j = D(T)\eta(T)\frac{df}{dT}$$

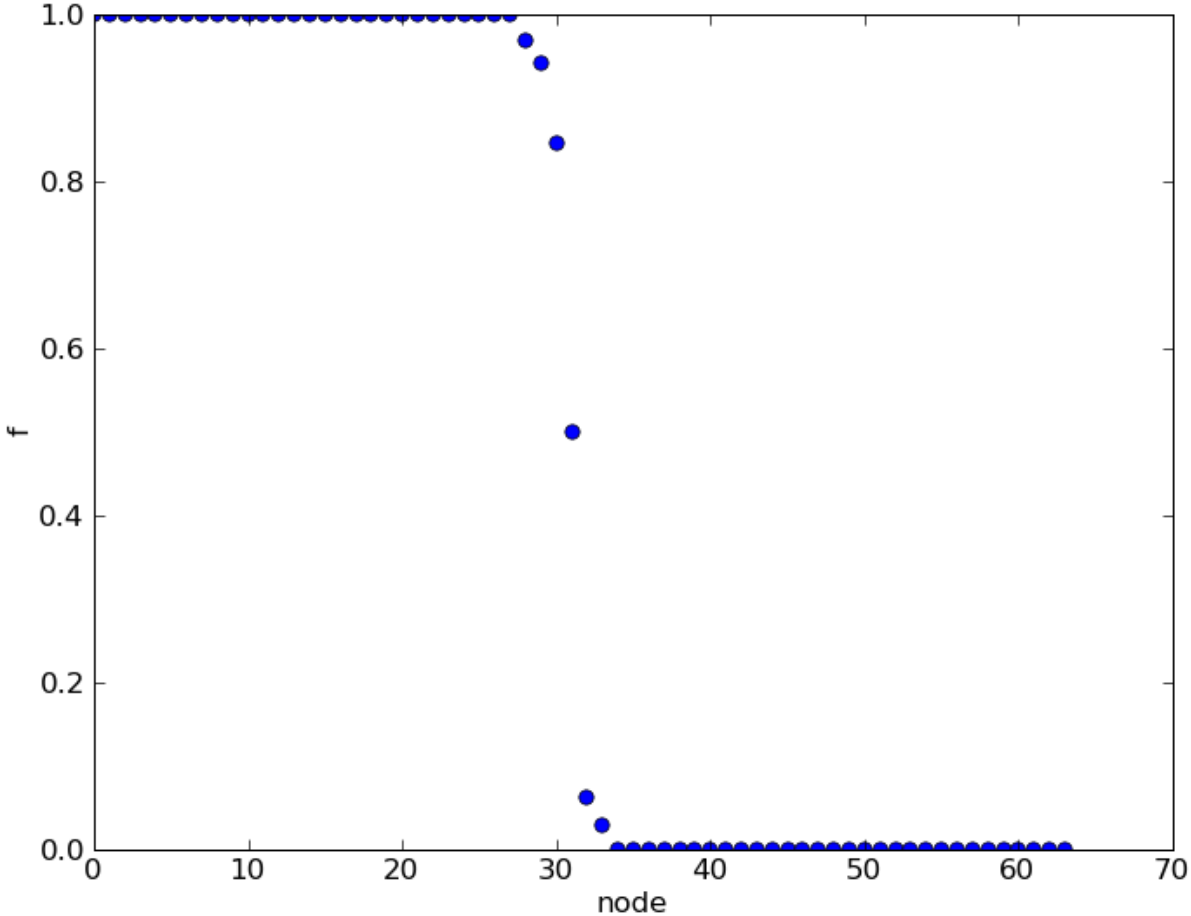
Maximize j via iterative scheme.

Trebst, S., Troyer, M. & Hansmann, U.H.E. *J Chem Phys* 124, 174903(2006).

Optimizing the Temperature Scale

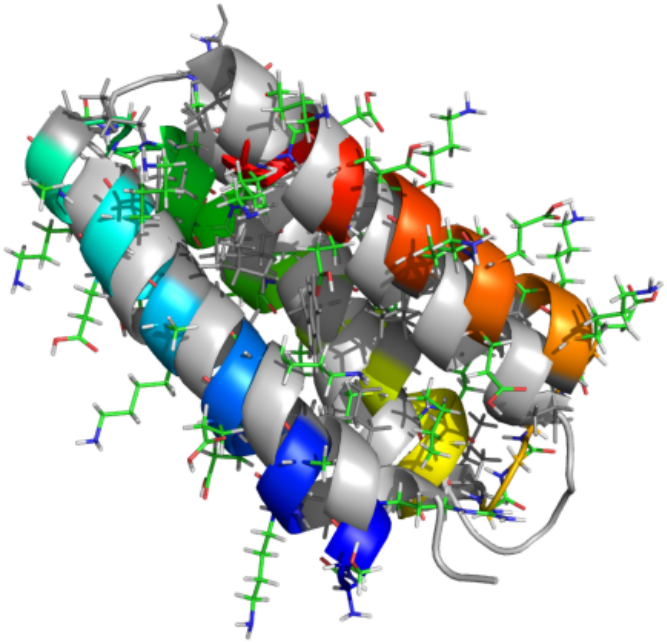


What to do with Bad Statistics



1LQ7

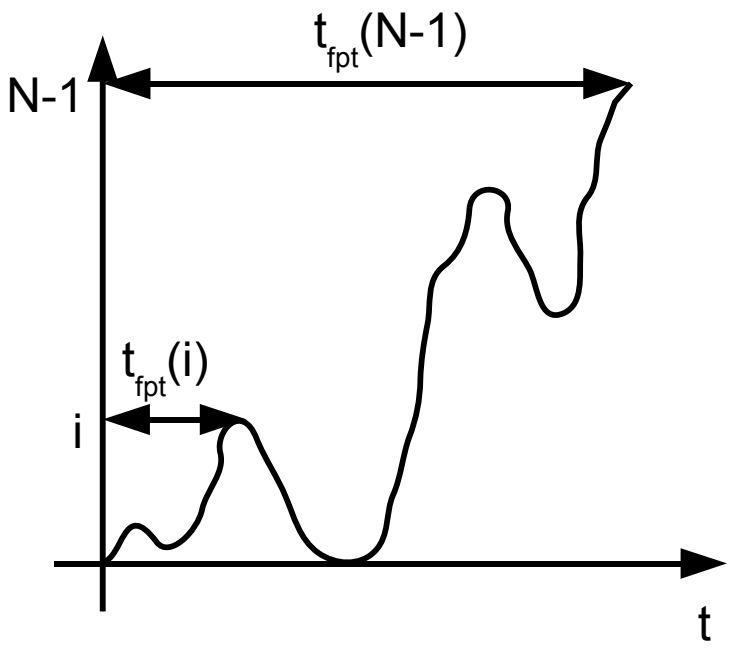
Designed 3-helix bundle



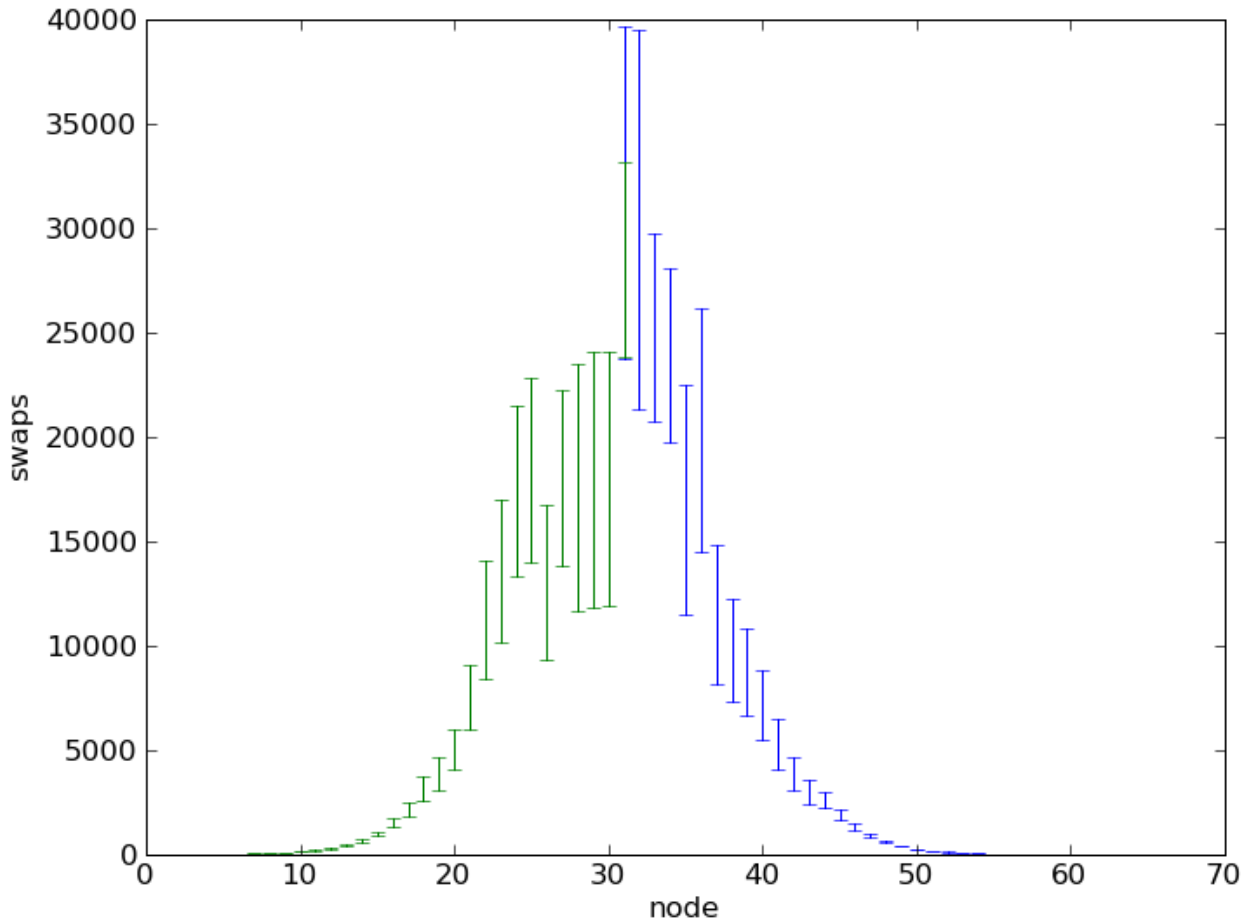
First Passage Times (FPT)

First passage time to node i:

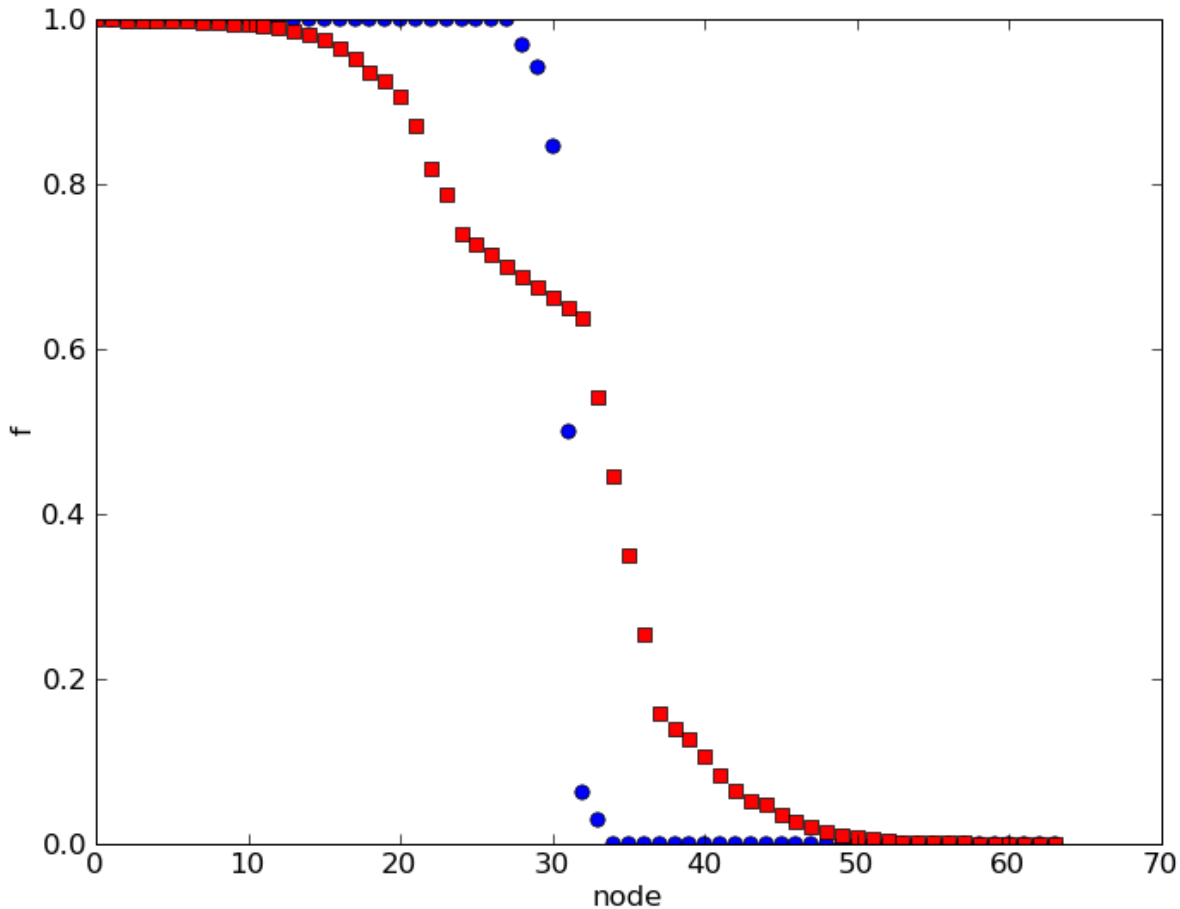
- time to get from boundary to node i.



First Passage Times



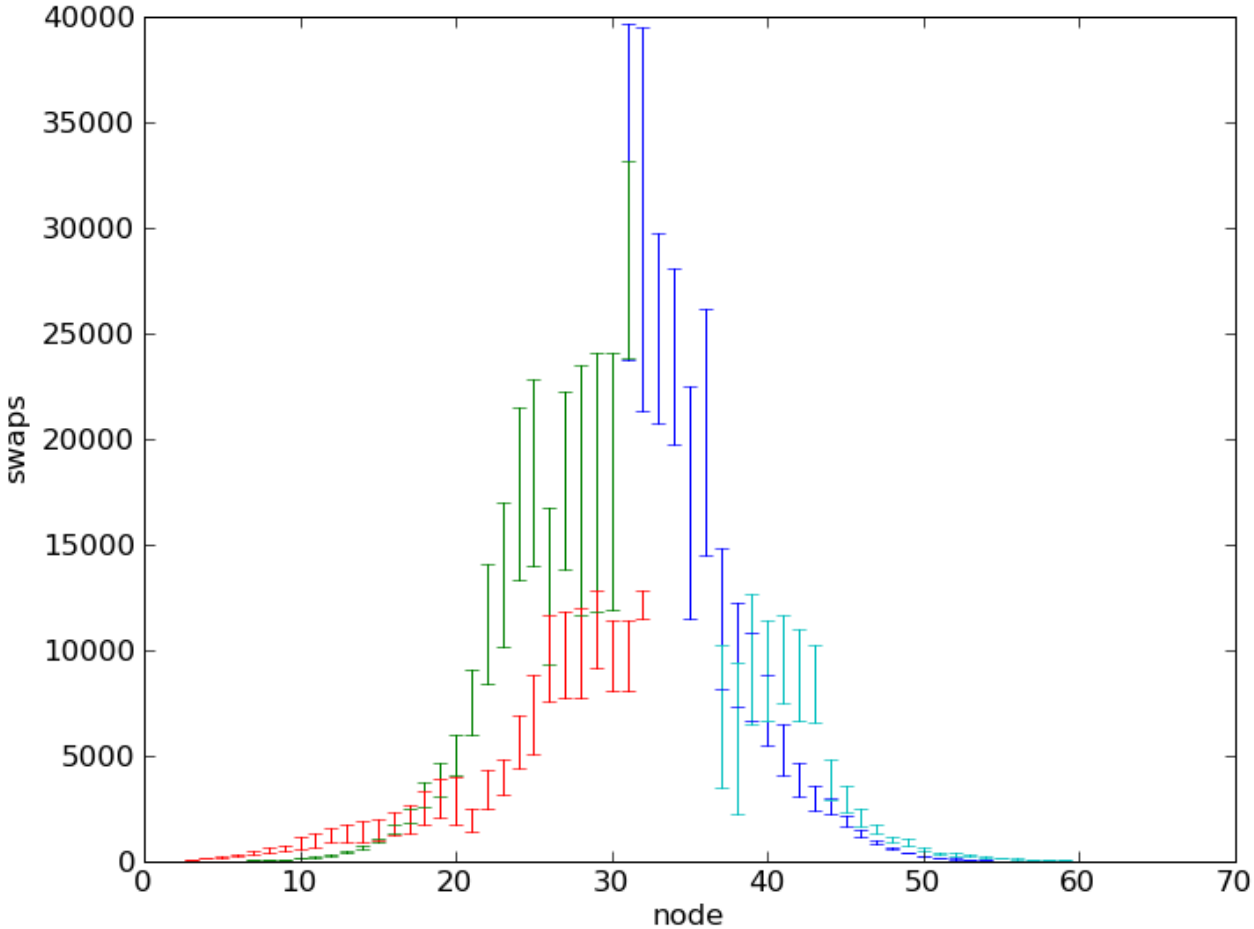
Flow distribution from FPT



Temperature Optimization Based on Flow from FPT

1. Start with any (sensible) temperature discretization
2. Measure first passage times
3. Extrapolate first passage times if necessary
4. Estimate flow distribution based on first passage times
5. Determine new temperature discretization
6. Continue at 2

First Iteration



Summary

Optimize the temperature discretization

Iterative scheme based of flow analysis

First passage times allow estimate of flow even with limited statistics