



Sampling vs. Analysis Transitions

Focus on rates  
leaving A

Flux and crossing probability are identical.

Difference: conditional transition probability

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A	—	$k_{A \rightarrow B}$	$k_{A \rightarrow C}$

$$k_{A \rightarrow B} = \Phi_{A_0} P(\lambda_{A_n} | \lambda_{A_0}) P(B | \lambda_{A_n})$$

$$k_{A \rightarrow C} = \Phi_{A_0} P(\lambda_{A_m} | \lambda_{A_0}) P(C | \lambda_{A_m})$$

In MSTIS, we sample the transition  $A \rightarrow$  anything

These are the “sampling transitions.”



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- “sampling transitions”: actually used in the sampling, to minimize the amount of work we need to do.
- “analysis transitions,” or just “transitions”: contain all the individual reactions of interest, up to  $N(N-1)$  for  $N$  states.
- `TransitionNetwork` builds both