

ToyFold

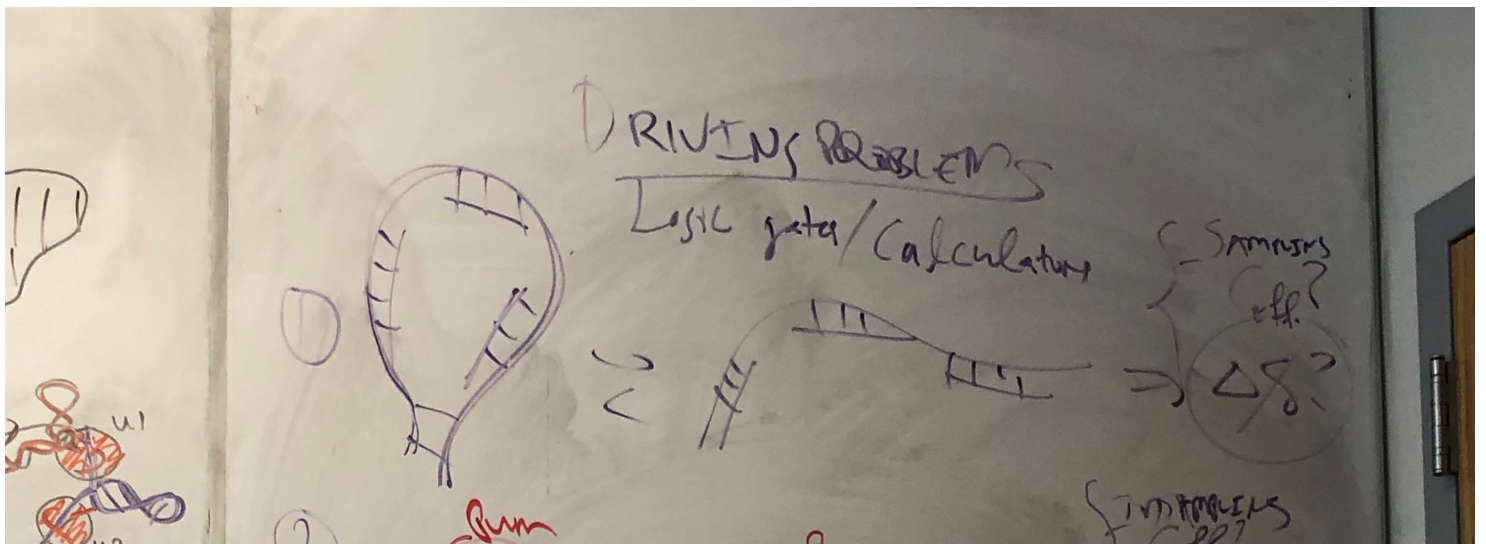
Calculations and simulations of RNA tertiary structure in a 2D toy model

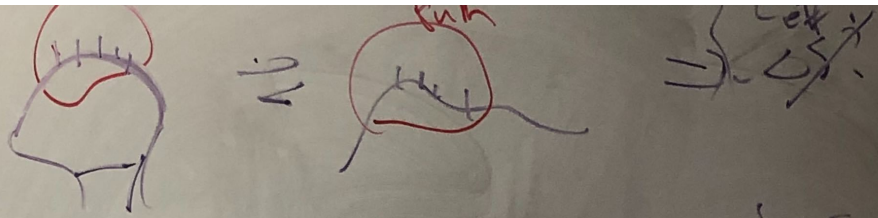
Goals

- Bead model of RNA-like folding in 2D.
- Allow rapid simulations to test partition function calcs -- including tertiary structure -- in MATLAB.
- Test factorization of free energy in terms of local motif energy (including K_d); motif modularity costs; tertiary closure.
- Test simple analytic representations of translation/rotation $SE(2)$ distributions in tertiary closure costs, including Gaussian models and harmonic transforms.
- Easy-to-understand visualization in 2D.

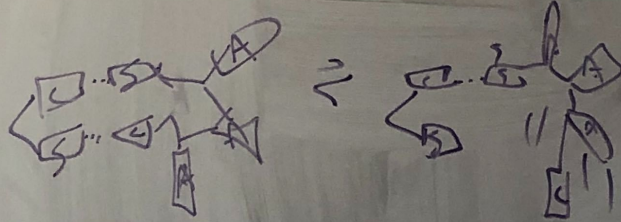
Notes

- Go to 'large-N' limit where beads have large alphabet to define unambiguous pairings for secondary and tertiary structure.
- use springs to connect nearest neighbor beads at R .
- define a flat-bottom well potential to connect paired beads at $2 \times R$. Will allow pseudoknots.
- create a simple A-minor type tertiary interaction for one bead color and cognate *pair* of beads.
- Goal (for a paper) -- compare analytical predictions of ΔG with numerical simulations for a bunch of designed structures, including: hairpin, pseudoknots, kissing loops, cdiAMP-riboswitch-like squares, and P4-P6 like A-minor conformations.



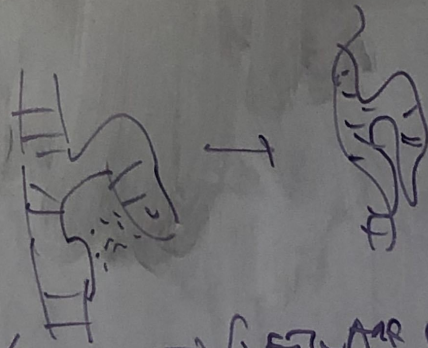


③



50 samples
off?

④ FARFAR sum



50 samples
off?

1. (Lassen function) \Rightarrow SOFTWARE EFFICIENCY?
 \Rightarrow NEU TOOLKIT.
2. Numerical efficiency/accuracy?