

# BarMap & SundialsWrapper

advanced RNA folding kinetics

Stefan Badelt

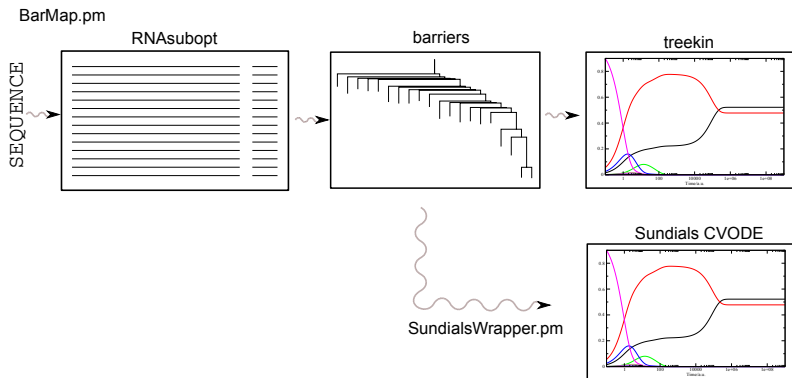
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# Outline – BarMap.pm & SundialsWrapper.pm

Two libraries ...

- BarMap.pm
  - interface to RNA folding kinetics on static landscapes
  - kinetics on time-varying energy landscapes
- SundialsWrapper.pm
  - solving arbitrary CRNs using the Sundials CVODE C-library



# Outline – BarMap.pm & SundialsWrapper.pm

Two libraries ...

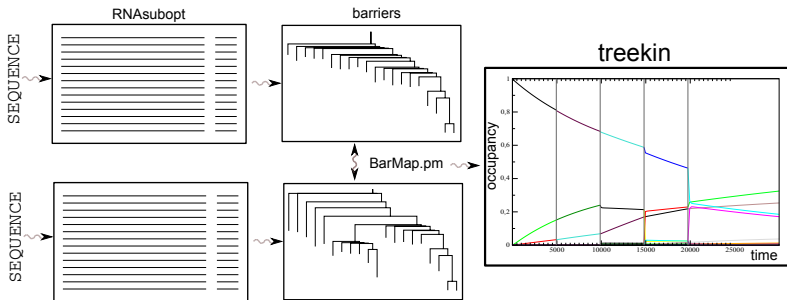
- BarMap.pm
  - interface to RNA folding kinetics on static landscapes
  - kinetics on time-varying energy landscapes
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...and many tools:

- BarMapSimulator.pl
  - simulations on time-varying energy landscapes
- interkin.pl
  - kinetics of (multiple) pairwise interacting RNAs
- transkin.pl
  - co-transcriptional folding of long RNA molecules
- ...

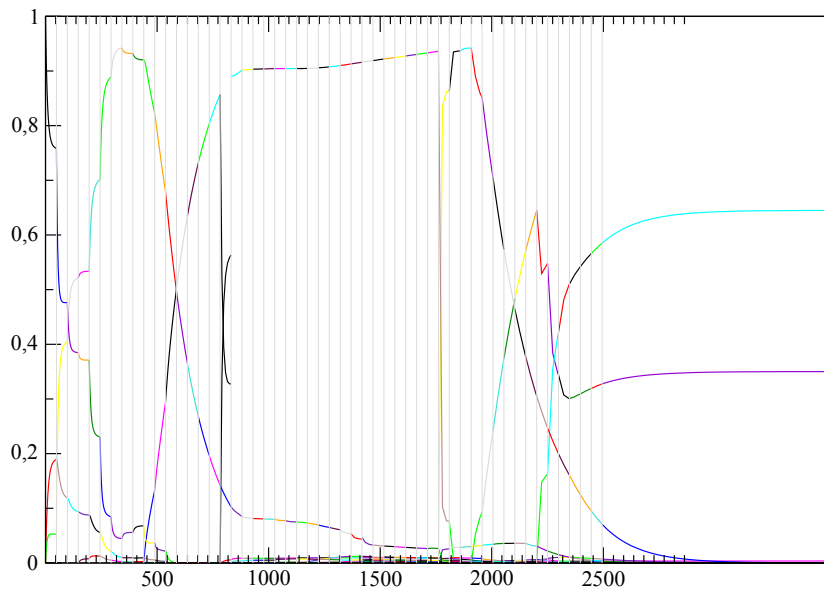
# BarMap library

- BarMapSimulator.pl
  - kinetics on time-varying energy landscapes



Ivo L. Hofacker, Christoph Flamm, Christian Heine, Michael T. Wolfinger, Gerik Scheuermann, and Peter F. Stadler, **BarMap: RNA folding on dynamic energy landscapes**, RNA, (2010)

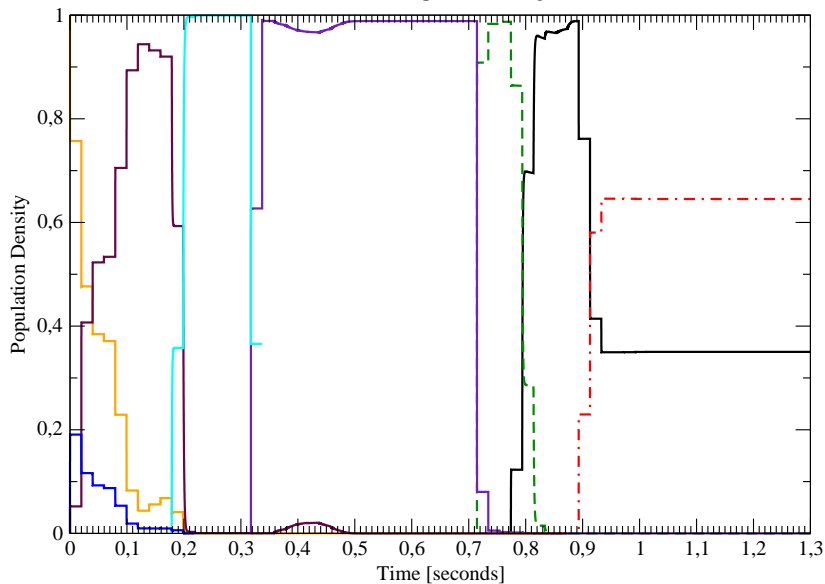
## BarMap and co-transcriptional folding



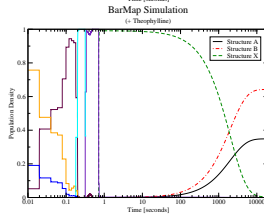
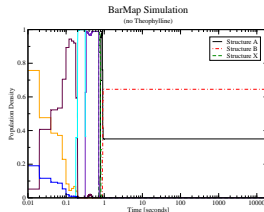
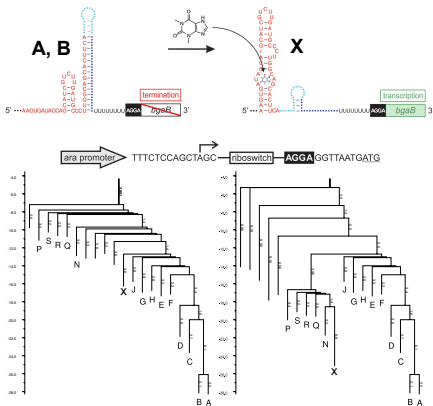
# BarMap and co-transcriptional folding

## BarMap Simulation

co-transcriptional folding



# BarMap including ligand interactions

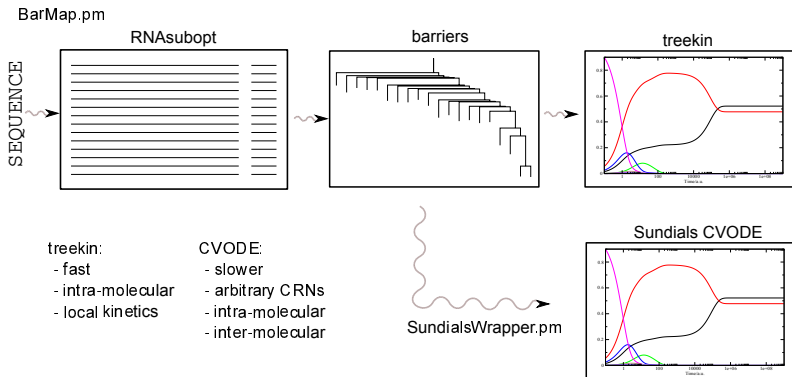


Stefan Badelt, Stefan Hammer, Christoph Flamm, and Ivo L. Hofacker,  
**Thermodynamic and kinetic folding of riboswitches,**  
 Methods in Enzymology, Elsevier, in press.

Manja Wachsmuth, Sven Findeiß, Nadine Weissheimer, Peter F. Stadler and Mario Mörl,  
**De novo design of a synthetic riboswitch that regulates termination transcription, NAR, (2012)**

# SundialsWrapper library

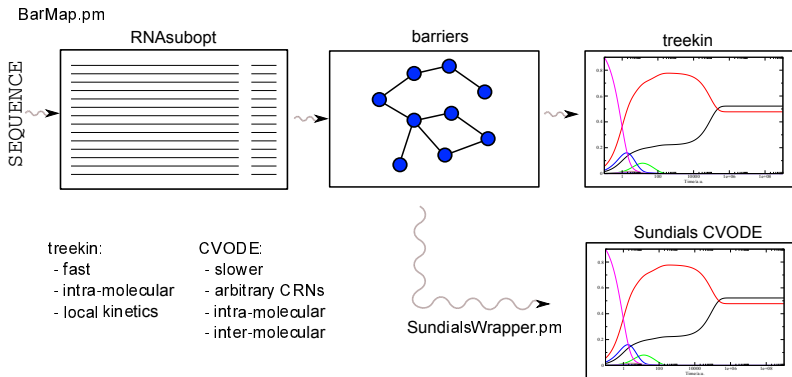
- SundialsWrapper.pm
  - solving arbitrary CRNs using the Sundials CVODE C-library





# SundialsWrapper library

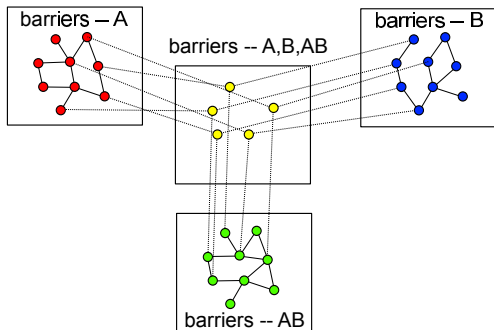
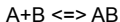
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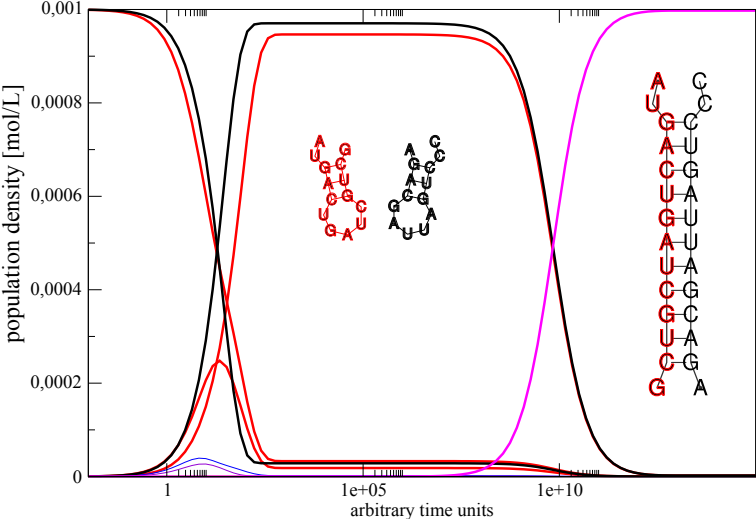
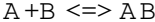
# interkin.pl kinetics of interacting molecules

- compute intra-molecular rates for each monomer
- compute intra-molecular rates for all interacting dimers
- compute transition rates between monomers and dimers

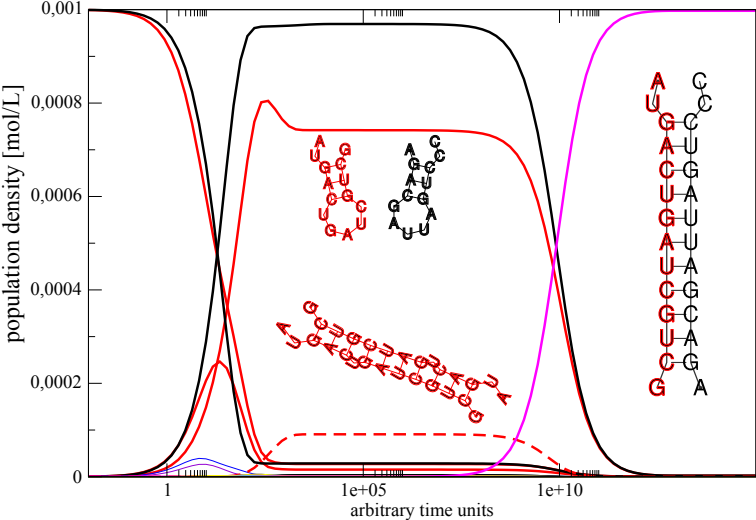
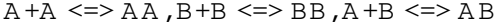
simulation of the reaction:



# RNA folding of interacting molecules



# RNA folding of interacting molecules



## transkin.pl co-transcriptional folding of large RNAs

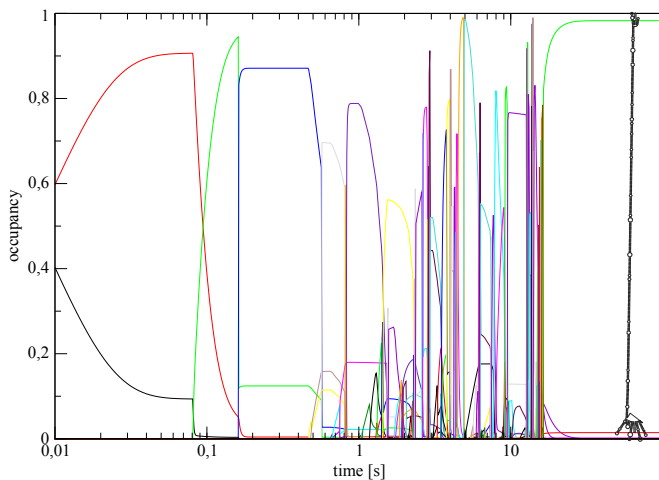
$\mathcal{S} = ()$

for each RNAsequence of the growing chain

- 1  $s =$  MFE-structure of current sequence,  
unless  $s \in \mathcal{S}$  {  
     $\mathcal{S} = \mathcal{S} + s$   
    compute refolding rates to all currently populated structures  
}
- 2 simulate CRN using SundialsWrapper

# transkin.pl co-transcriptional folding of large RNAs

cotranscriptional folding (843nt)



# thanks to

## This work

Ivo L. Hofacker

Christoph Flamm



... and the whole TBI group

## Design Projects:

–*XOR riboswitches*

Peter F. Stadler

Mario Mörl

Regula Arreger

Gesine Domin

–*RNAprions*

Sabine Müller

Sonja Petkovic

–*co-transc. folding of 3' UTRs*

Andrea Tanzer

Michael T. Wolfinger

Michael Jantsch

Konstantin Licht

Mansoureh Tajaddod

tbi



universität  
wien



FWF

Der Wissenschaftsfonds.

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