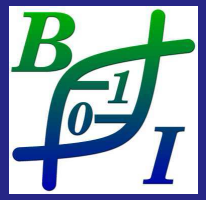


The Energy Landscape Library

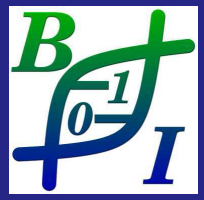
- A Platform for Generic Algorithms

Andreas Richter, Sebastian Will and *Martin Mann*

Albert-Ludwigs-University Freiburg
Bioinformatics at the Department of Computer Science

Winterseminar Bled 2007

EU - project Embio



Overview

The Energy Landscape Library
- a Platform for Generic Algorithms

What we need to know:

- What for ?
- What we have !
- What we want . . .

The Energy Landscape Library
- a Platform for Generic Algorithms

What we need to know:

- What for ? ✘
- What we have !
- What we want . . .

The ELL

Martin Mann

Energy Landscapes

- A set of states of a given energy model
- An energy for each state
- A neighborhood definition between states

An example - RNA structure space

- State = RNA structure for a fixed sequence
- Energy = minimum free energy
- Neighbors = differ in one bond in the structure

Based on that . . .

- Local Minimum : all neighbored states have higher energy
- Saddle Points : minimum barrier height between two minima
- . . .

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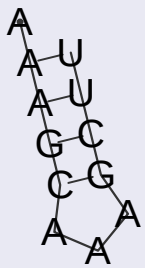

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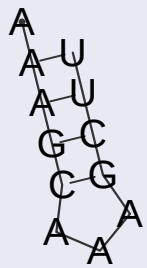

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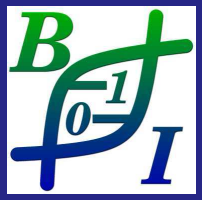


What for?

Study of Energy Landscapes

The ELL

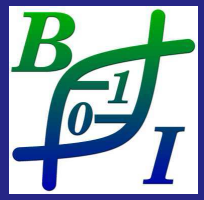
Martin Mann

Available so far:

- Multitudes of models (from biology, physics, . . .)
- Lots of algorithms for landscape investigations
- Most of them model independent (e.g. barrier trees) but only available for some models

What would be nice:

- Fast and easy landscape model creation or extension
- Algorithm design independent from landscape models
- A pool of basic algorithms to focus on new ideas
- A huge tool set for standard investigations of new models
- Everything for free . . . ☺



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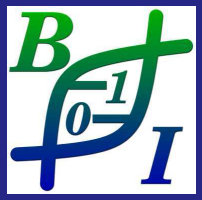

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The Energy Landscape Library
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The ELL

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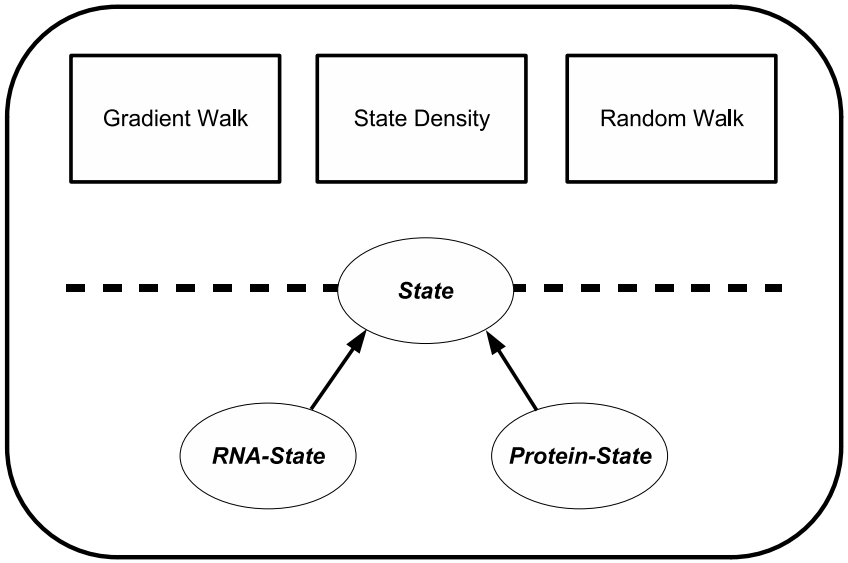

What do we have ?

- An abstract state 'thing' of a landscape model
- A variaty of such models
- Algorithms are independent of the concrete instance
- . . . well suited for 'Object oriented programming' ! ☺

The ELL

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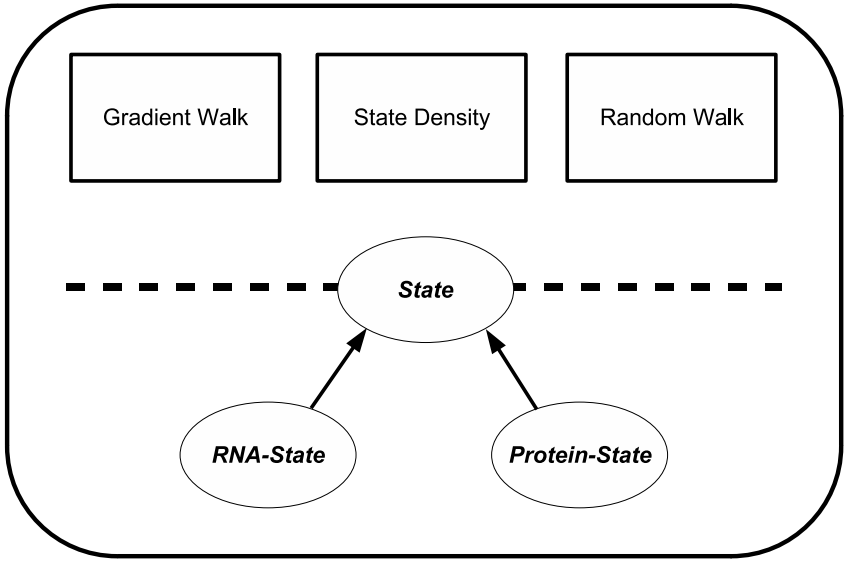

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The Energy Landscape Library - Programmers View

- C++ library for discrete state landscape models
- Object oriented and highly modular
- Strict partition of landscape state model and algorithm layer
- Free available online
- Well documented API online

The Energy Landscape Library - Modellers View

- States for RNA (port to Vienna RNA lib) and Lattice Proteins
- Neighbor iteration (successive and random)
- Compressed state representations (space reduction)
- Algorithms: gradient walk, flooder, barrier tree (sampling), . . .

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The ELL

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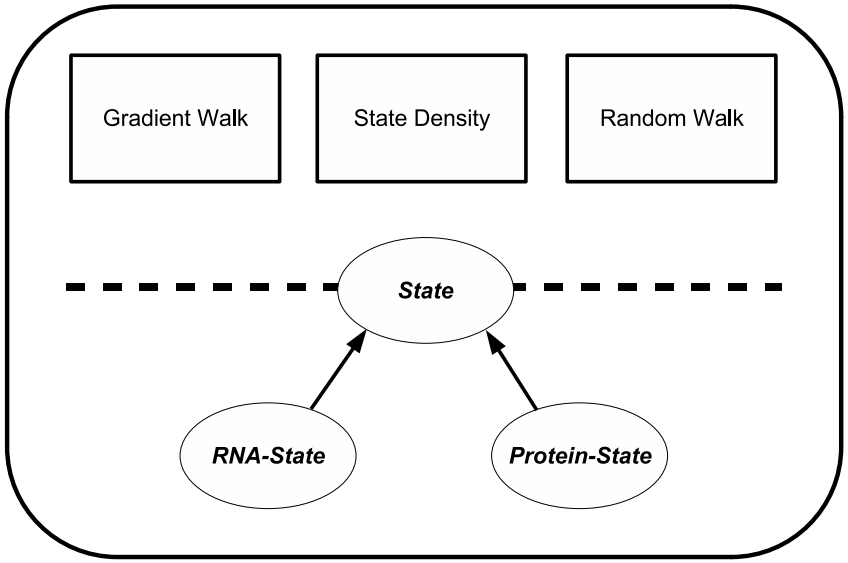
What is a state ?

- An abstract representation of a 'thing' in the landscape model
- The interface between landscape model and generic algorithms
- An abstract class in the library



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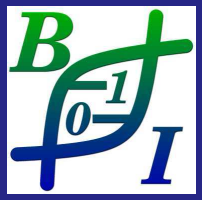
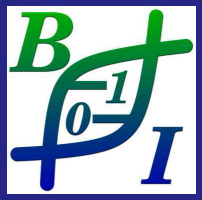


What we want . . .

What we want is . . .

- more models,
- new algorithms (e.g. Wang Landau method),
- bigger tool collection,
- tutorials and examples,
- visualization support,
- . . .

and . . . USER . . . ☺



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Summarizing . . .

The Energy Landscape Library
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Summarizing

- Object oriented C++ lib for landscape investigation
- Strict partition of landscape model and algorithm
- Both independently developable
- Pool of methods provided
- Freely available and still under construction . . .