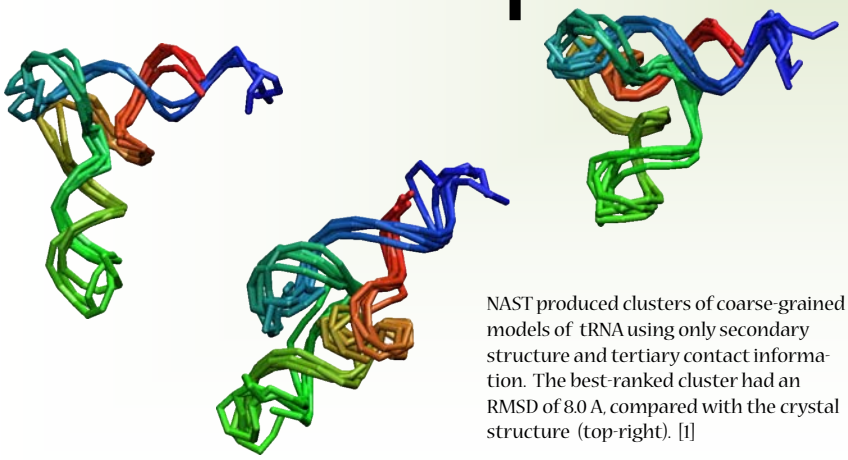
3D RNA Modeling Workshop



NAST produced clusters of coarse-grained models of tRNA using only secondary structure and tertiary contact information. The best-ranked cluster had an RMSD of 8.0 A, compared with the crystal structure (top-right). [1]

When: June 19, 2009

Where: Clark Center
Stanford University

How: Free to attend but registration is required

http://simbios.stanford.edu/RNAWorkshop.htm

The structure and dynamics of molecules is central to understanding biological function, and yet most experimentalists find existing structural modeling tools excessively limited in scope and difficult to use. In Simbios' 3D RNA Modeling Workshop, you will learn new tools that enable you to generate structures and dynamical trajectories based on your hypotheses, limited experimental information, and/or initial coordinates. The presented molecular modeling tools are designed to be easily applied by experimentalists to problems of current biological interest.

- ***Nucleic Acid Simulation Tool (NAST)*** generates a large number of conformationally diverse coarse-grained 3D structures that satisfy user-provided secondary and tertiary contacts. [1]
- ***RNABuilder*** constructs structural models of RNA by enforcing user-provided base pairing interactions and other structural constraints. Key to the algorithm's effectiveness is its ability to enforce a folding pathway that is automatically computed or provided by the user.
- ***OpenMM Zephyr*** generates a full atomic simulation using a version of the GROMACS molecular dynamics package that runs on GPUs, producing speed-ups of over 700X in some cases.

The "Introduction to 3D RNA Modeling and Simulation" lecture for the workshop will be given by Dr. Russ Altman, Chairman of the Department of Bioengineering and Director of the Biomedical Informatics Training Program at Stanford University.

The software tools presented in the workshop are freely available for downloading

NAST
http://simtk.org/home/nast

RNABuilder
http://simtk.org/home/rnatoolbox

OpenMM Zephyr
http://simtk.org/home/zephyr

simbios

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[1] Jonikas, MA, et al., "Coarse-grained modeling of large RNA molecules with knowledge-based potentials and structural filters," RNA, 2009, 15:189-199