

Center for Applied Mathematics and
Interdisciplinary Center for the Study of
Biocomplexity Colloquium

Samuel Coulbourn Flores

Altman Lab

Department of Bioengineering

Stanford University

“RNA Structure and Dynamics in Internal Coordinates”

Monday March 23, 2009

4:00pm

Location 127 Hayes-Healy Center

Tea at 3:30pm in 257 Hurley

We are soon to release RNABuilder, which folds RNA from base pairing contacts. The code can enforce all base pair types catalogued by Leontis and Westhof, in addition to base stacking. The base pairing forces can be applied in a time-order specified by the user, or according to an automatically generated co-transcriptional folding sequence. It detects helical regions and enforces the appropriate backbone geometry. Sterics and Coulomb interactions are treated approximately using Simbody's very efficient Contact subsystems. The loop backbone is subject to the knowledge-based Nucleic Acid Simulation Tool (NAST) potential. The tool can handle multiple-chain structures, and optionally use known structures as starting points for modeling conformational change. The algorithm recovers the correct topology, approximate overall geometry, and most structural features of tRNA and the Tetrahymena Ribozyme P4/P6 domain as I will demonstrate. Movies will be shown.