# Multi-Scale Modeling of RNA Structure Using Hierarchical Graph Sampling Approach

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## ABSTRACT

Mathematical modeling and simulation have been applied to and impacted in the field of chemistry and biology of proteins and nucleic acids. With increased interests in the expanded biological roles of RNA (Ribonucleic Acids), computational structure prediction of RNA shows great challenges for mathematical and computational biologists. One of these mathematical challenges is to predict RNA helical arrangements, i.e., 3D topologies, given an RNA sequence and secondary structure. To tackle this problem, we develop a hierarchical Monte Carlo sampling approach by a coarse-grained sampling of 3D graphs guided by knowledge-based potentials derived from geometrical measures based on experimentally-solved structures. The coarse-grained model using newly developed 3D RNA graphs accelerate global sampling of candidate RNA topologies. Monte Carlo results are compared to reference graphs from both solved structures and predicted structures using current available computational tools. The comparison indicates promise for our graph-based sampling approach for characterizing 3D global helical arrangements in large RNA from a given secondary structure and offer reasonable candidate for further refinement. This is joint work with the RNA group at the Schlick lab at New York University.

## REFERENCES

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