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Abstract for an Invited Paper
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Ensembles of AMBER biomolecular simulations on GPUs for assessment and validation of RNA models

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Ensembles of molecular dynamics simulations, using methods including multi-dimensional replica exchange on large-scale GPU clusters such as Blue Waters, provide a fast and efficient means to explore the conformational ensembles of biomolecules such as RNA. Enabling exploration of models in days to weeks instead of months to years we are able to better explore, assess, validate and improve the molecular mechanical force fields for RNA. We will describe our experiences modeling RNA on the large-scale resources and also outline the problems with and improvements in the AMBER suite of programs for simulation and analysis of biomolecules on heterogeneous computing platforms.