SYNCHRONOUS SAMPLING OF ORTHOGONAL SPACE IN FREE ENERGY CALCULATIONS. Wei Yang, Department of Chemistry and Biochemistry, Florida State

University, Institute of Molecular Biophysics, Tallahassee, FL 32306.

Free energy calculation is a central topic of biomolecular simulation. A bottleneck issue in free energy calculations is to efficiently sample the orthogonal space vertical to the direction of the pre-defined order parameters. In this talk, orthogonal space sampling techniques will be reviewed and the related progress will be presented.