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Chuanbin Du* (cdu@uncc.edu), 505 Barton Creek Dr. Apt J, Charlotte, NC 28262, **Hui Wang**, Charlotte, NC 28262, **Dennis Livesay**, Charlotte, NC 28262, and **Donald Jacobs**, Charlotte, NC 28262. *A Heterogeneous Adaptive Sparse Grid Method For Representing High Dimensional Free Energy Landscape in Proteins.*

The free energy landscape (FEL) is very important for quantitatively studying and understanding the relationships between structure, dynamics, stability, and functional behavior of proteins. However, the free energy landscape of a protein is a high-dimension hyper surface and is difficult to rationalize. Here, we developed an adaptive sparse grid method, which can detect important dimensions, identify and resolve singularities and local non-smooth variations in high dimensional functions. This method provides an accurate and efficient approach for the computation of the representation of the free energy landscape of proteins. (Received September 23, 2010)