1056-65-1125 **Mazen George Zarrouk*** (mzarrouk@uwm.edu), University of Wisconsin - Milwaukee, PO Box 413, Milwaukee, WI 53201, and **Dexuan Xie** (dxie@uwm.edu). *Truncated Incomplete Hessian Newton Minimization with Application to Biomolecular Potential Energy Function.*

In a recently published paper, we proposed and analyzed a new type of a modified Newton linesearch method, called the truncated incomplete Hessian Newton (T-IHN), for minimizing a twice continuously differentiable real-valued function whose Hessian matrix is dense but can be well approximated by a sparse incomplete Hessian matrix. We proved that T-IHN is globally convergent even with an indefinite incomplete Hessian matrix or an indefinite preconditioner, which may happen in practice. We also proved that when the T-IHN iterates are close enough to a minimum point, T-IHN admits a steplength of one that satisfies the Wolfe's conditions and that T-IHN has a Q-linear rate of convergence. As an important application, we constructed a particular T-IHN algorithm for minimizing a biomolecular potential energy function, and numerically tested it for a protein model problem based on a widely used molecular simulation package, CHARMM. Numerical results confirm the theoretical results, and demonstrate that T-IHN can have a better performance than most CHARMM minimizers. In this talk, we will describe the T-IHN method, show its major convergence results, describe the construction of the incomplete Hessian matrix, and present some of the promising numerical results of T-IHN. (Received September 21, 2009)