Coil-globule transition of macromolecules in mixed solvent: A semi-grand canonical molecular dynamics approach DEBASHISH MUKHERJI, KURT KREMER, Max-Planck Institute for Polymer Research — Conformational transition of macromolecules in mixed solvents are intimately linked to large local concentration fluctuations of solvent components. The numerical studies in the field are limited to the closed boundary schemes, which, however, suffer from severe system size effects. To overcome this discrepancy, we have developed a semi-grand canonical molecular dynamics scheme for complex fluids [1]. Our method makes use of the adaptive resolution scheme (AdResS) [2] with a metropolis particle exchange criterion. In AdResS, an all-atom region, containing macromolecule, is coupled to a coarse-grained (CG) reservoir. The semi-grand canonical particle exchange is performed in the CG region. As the applications of the method, we study the concentration driven reentrant collapse and swelling transition of poly(N-isopropylacrylamide) (PNIPAm) and poly(N,N-diethylacrylamide) (PDEAm) in aqueous methanol and demonstrate the role of the delicate interplay of the different intermolecular interactions. [1] D. Mukherji and K. Kremer, Macromolecules, DOI:10.1021/ma401877c (2013). [2] M. Praprotnik, L. Delle Site, and K. Kremer, J. Chem. Phys. 123, 224106, (2005).