

1014-Q1-1754 **Ignatios Vakalis*** (ivakalis@capital.edu), Dep. of Math/CS, Capital University, 1 College and Main, Columbus, OH 43209. *Connecting Mathematics, Computing and Chemistry: An Undergraduate Computational Science Program.*

Computational Science is an emerging and rapidly growing interdisciplinary field defined as the intersection of math, computing and science. It is considered as the third methodology in the development of scientific knowledge alongside theory and experimentation. Funded by grants from NSF (DUE, CCLI-EMD), W.M. Keck Foundation and Battelle, Capital University has designed a comprehensive undergraduate program in Computational Science. The program is primarily for mathematics, and science majors. Since modeling is an integral part of any computational experiment all courses have a mathematical component. The presentation will outline developed materials and curriculum structure along with specific modules on: enzyme kinetics, molecular mechanics, molecular orbitals. (Received September 29, 2005)