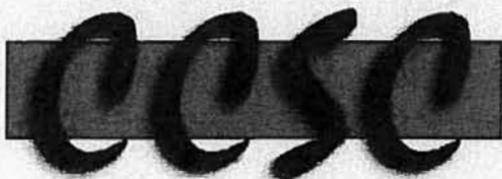


The Journal of Computing Sciences in Colleges



*The Consortium for Computing
Sciences in Colleges*

INFORMATICS*

TUTORIAL PRESENTATION

Xinlian Liu

*Department of Computer Science
Hood College, Frederick, MD 21701*

Phone: 301-696-3981, FAX: 815-371-4121, liu@hood.edu

Sarangan Ravichandran

*Advanced Biomedical Computing Center
National Cancer Institute, SAIC/Frederick, Frederick, MD 21702*

Phone: 301-846-1991, FAX: 301-846-5762, sravi@ncifcrf.gov

ABSTRACT

Fitting scientific computing into a small liberal arts college curricula has always been a challenge, and even more so when new hardware and architecture remain as moving targets. When video game consoles are commanded by the 'supercomputing on a chip' multiprocessor Cell, and multi-core CPUs become the mainstream of desktop solution, we are witnessing a renewed demand from students to offer a course in parallel computing. This tutorial attempts to address these challenges by weighing in the interest of students, the efficiency of various parallel programming models as well as the resource factor of a small college. In a progressive way, we present a pragmatic approach of teaching scientific computing and applications in small colleges with limited resources.

After presenting some principles and elements of parallel computing methods, including commonly used architectures, programming models such as message-passing interface (MPI), OpenMP, desk-side supercomputing on Cell and general purpose computing on GPU, we will continue to discuss some high-performance molecular simulation applications.

Molecular modeling is a term that is often collectively represents wide range of theoretical methods and techniques used for modeling molecules (proteins, DNA, RNA, small molecules etc.) and simulating their function. Molecular modeling is nowadays an often used tool along with experiments in research projects. The importance of this area became evident when the Nobel Prize for 1998 was awarded to Profs John Pople and Walter Kohn for the development of novel computational methods. Molecular Modeling is used in a wide range of areas including space research, Drug discovery, structural bioinformatics and several branches of engineering among others. With the recent

improvements in computer hardware and software, *in-silico* experiments that were not even imaginable before have become a reality. Even more, long simulations that had been usually carried out on main-frame computers can be easily done today on a desktop. In this tutorial we will introduce the basic concepts of molecular modeling and focus our attention on a couple of real-world applications such as protein-ligand docking and molecular dynamics simulations. Some of the popular, free high-performance molecular modeling and simulation software such as AMBER, AutoDock, and NAMD will be introduced. We will discuss how parallel programming, message-passing methods have advanced computing capability to simulate realistic environments (more number of atoms, longer time) in molecular biology and biochemistry.

Abunawass, A	9	Lobo, A	166
Allen, R	163	Marion, B	9
Anewalt, K	134	Martens, J	161
Babcock, D	151	McGeoch, C	5
Bailie, F	9	McGuire, H	53
Baker, D	166	Meinke, J	viii
Balsim, I	11	Mitchell, S	166
Barnes, T	125	Mohammed, T	99
Barr, V	109	Mollah-Hardy, N	166
Bell-Watkins, K	125	Montante, R	19
Benokraitis, V	161	Motahar, E	109
Bizot, B	161	Mullins, P	136, 164
Black, M	32	Murphy, D	25
Brown, R	161	Murtagh, T	160
Butler, M	111	Oh, J	56
Butler, T	166	Olan, M	72
Chang, E	1	Rajaravivarma, V	85
Conlon, M	136, 164	Ravichandran, S	83
Donley, P	166	Reese, K	93, 166
Dougherty, J	5	Salem, A	93
Eckhardt, R	11	Shelton, R	161
Elzer, S	65	Sheybani, E	144
Feder, E	11	St. Clair, C	9
Frey, B	166	Stewart-Gambino, H	109
Garrido, J	81	Talaga, P	56
Gillard, G	1, 81	Thomas, N	125
Guiffre, H	118	White, L	163, 166
Haiduk, H	6	Whitfield, D	9, 136
Henderson, P	159	Workman, K	65
Hiestand-Tupper, D	166	Yarmish, G	11
Hovemeyer, D	151		
Huyser, K	166		
Jahangir, S	11		
Javidi, G	144		
Klappholz, D	106		
Klingelsmith, W	166		
Lambert, L	118, 159		
Lawler, J	132		
Leitherer, B	166		
Li, C	39, 99		
Li, P	99		
Liao, W	46, 166		
Liew, C	109		
Liu, X	83		

Muhlenberg College
2400 Chew Street
Allentown, PA 18104-5586

**NON-PROFIT ORG.
U.S. POSTAGE**

PAID
ALLENTOWN, PA
PERMIT #759