Computational Science at The University of Montana
Saturday, Nov. 18th, UC Room 330

ABSTRACTS

Speaker: Andrew Ware (Physics and Astronomy)
Title: Computational Physics Research at UM
Abstract: In this talk, I’ll present an overview of computational physics research at the University of Montana. The research is in plasma physics, studying the behavior of high-temperature, ionized gasses. Our research examines the equilibrium and stability of magnetically-confined plasmas and transport of energy and particles by turbulence in plasmas. The computational aspects of our research range from small codes running on local workstations to parallel codes running on supercomputers, with an emphasis on visualization of the data from the full range of codes. Our parallel codes are run on the supercomputers at the National Energy Research Scientific Computing Center that include a 6,656-processor IBM SP and an 888-processor IBM POWER 5 system. I’ll finish up with a discussion on the future directions of our research and the computational challenges ahead.

Speaker: Rebecca Bendick (Geology)
Title: Numerical Models of Crustal Flow During Mountain Building
Abstract: Both analytical and numerical models can be used to investigate the dynamics of the solid earth in a range of tectonic settings. These techniques combine advancements in earth sciences, physics, mathematics, and computing methods.

Speaker: John Gerdes (Biomed. Pharm. Sci.)
Title: TBA

Speaker: Elizabeth Crone (Wildlife Biology)
Title: Computational Sciences in Population Ecology
Abstract: The advent of powerful, inexpensive computers has allowed ecologists to ask new kinds of questions, and increased the pace of both data availability and data collection. I present examples of computational projects in my research group, which sits at the intersection of biology with applied mathematics, statistics and database management: (1) understanding patterns of population dynamics and seed production by perennial plants, based on observations of individuals over time; (2) analyzing and predicting animal movement in heterogeneous environments, based on repeated observations of location over time; and (3) developing a web-searchable database of the vascular flora of Montana. Rather than discussing any project in detail, I briefly outline the goals, constraints and computational needs of each.
Computational Science Meeting 11/18/06, cont.

Speaker: Woodam Chung (College of Forestry and Conservation )
Title: Decision Support Systems for Forest Management Planning
Abstract: This presentation will describe several computational decision support systems that have been developed for timber transportation and forest management planning. Decision-making in forest management becomes more and more complex because not only economic efficiency, but also social, ecological, and environmental aspects of management activities need to be considered in management decision-making. In addition, advanced technologies in geographic information system (GIS) have enabled us to simultaneously analyze a variety of spatial data at a landscape scale, which makes forest planning problems larger and more complicated. This presentation will discuss needs of computational decision support systems in forest management and present applications of such systems.

Speaker: Xi Chu (Chemistry )
Title: Numerical Developments for Calculating Molecular Processes in Intense Laser Fields
Abstract: Recent advancement of attosecond ($10^{-18}$) lasers offers the possibility of probing the electron dynamics of a molecule. It demands theoretical study of the electronic structure and dynamics of molecules in the presence of intense ultrashort pulsed external fields, which cannot be performed using traditional approaches.

For accurate numerical treatment, we developed a generalized pseudospectral method (GPS). It involves optimal non-uniform spatial grid discretization of the Hamiltonian. This method is computationally more efficient and accurate than the conventional basis-set expansion variational techniques. A complex scaling procedure is combined with GPS to calculate the energies and lifetimes of resonance states. We also developed a new time-dependent GPS for solving time-dependent Schrödinger like equations. It is applied to the calculation of the tunneling ionization (TL) rates and the high-order harmonic generation (HHG) spectra.

Speaker: Anna Klene (Geography ) and Don Morton (CS )
Title: Computational Weather Forecasting for Research and Operational Activities
Abstract: The Departments of Geography and Computer Science are leading the deployment and verification of numerical weather models on high-end computational resources. The models provide forecast guidance to NOAA’s National Weather Service offices in Missoula and Fairbanks, and are additionally used in various studies of meteorological phenomena in the Northern Rockies and Alaska, including a Department of Interior project to study mesoscale meteorology in the Beaufort Sea and adjacent coastal areas. This presentation highlights some of our cutting-edge activities that would be impossible to pursue without substantial support from supercomputing centers.
Computational Science Meeting 11/18/06, cont.

Speaker: Leonid Kalachev (Mathematical Science)  
Title: Reduced Model of Neurotransmitter Transport in the Presence of Generic Receptors and Transporters  
Abstract: A system of equations describing concentrations of free glutamate, transporters and receptors in a synaptic cleft (spatially three dimensional linear diffusion equation coupled with nonlinear kinetics equations through boundary conditions) may be reduced to one nonlinear diffusion equation in two spatial dimensions under certain conditions on rate constants of forward and reverse binding reactions. Explicit expressions for effective diffusion (that depends nonlinearly on the local glutamate concentration) and effective kinetic term are derived. Reduction procedure works for any finite number of types of transporters and receptors. The results are illustrated by comparison of solutions of the full model and the reduced model in the case where only one type of transporters is present in the system.

Speaker: Alden Wright (Computer Science)  
Title: Computational PhD Proposal  
Abstract: A proposal for a Computational Science Ph.D. program is currently under consideration by the Graduate Council. This would be a broad-based interdisciplinary program for students desiring to study computer science, applied mathematics, and enough of a companion science so that they can apply their computational and mathematical skills to significant scientific problems. I will describe the program in more detail and lead a discussion about how we can make this a high-quality program.

Speaker: Jesse Johnson (Computer Science)  
Title: From geoscience to disease ecology: models, methods, resources and computational demands.