High Performance Computing Project Report

March 20, 2003

Table of Contents:

1. Introduction

The Scientific Computing Facility for Modelling, Simulation and Visualization was acquired through funding from Canada Foundation for Innovation, the BC Knowledge Development Fund, Silicon Graphics Inc. and UNBC. It provides essential tools for research aimed at understanding the function of physical and natural systems (terrestrial, aquatic, atmospheric, and extra-terrestrial) from molecular to global scales. Research ranges from: molecular interactions, microorganisms, soils, plants and wildlife, to forests, landscapes, the atmosphere, and their interactions with society.

The purpose of this report is to document the research activity involving the HPC Facility at UNBC since it was established during 2000. This report is being submitted for information purposes to the College Councils of the College of Science and Management and the College of Arts, Social and Health Science; to the Senate via the Senate Committee on Research and Graduate Studies; and to the Vice Presidents and President at UNBC. The report is available on-line at: http://web.unbc.ca/hpc/HPC-Report-March-2003.pdf.

The impact of the infrastructure on UNBC researchers includes:

a) Enhanced computational facilities for research projects.

A number of projects have been greatly facilitated through the use of this infrastructure (see Section 4).

b) Enhanced research training for researchers at UNBC.

The Scientific Computing Facility has provided new opportunities and has enhanced the previous ability of UNBC to educate UNBC researchers in areas of great importance both regionally and nationally such as: the environment, natural resource management, computing science, chemical, fluid dynamics, and physical sciences.

c) Improved recruitment and retention of personnel.

For example, Patrick Montgomery is a new faculty in Applied Mathematics who was attracted to UNBC, in part due to the presence of the HPC infrastructure.

d) Increased opportunity for collaborations and partnerships.

As an example, the facility has made it possible for Elie Korkmaz to collaborate with scientists from UNBC, TRIUMF, University of Alberta, and Ohio University to finish a high-profile experiment on data analysis.

2. The infrastructure

2.1 Hardware

The facility has two components:

a) A High-Performance Computer Server for computationally intensive applications - those requiring a very large number of computing cycles. This is a SGI Origin 34000 with 28 processors and 14 GB of memory.

b) Scientific Visualization / Data Analysis Laboratory (the HPC Lab located in room 5-151) to visualize and analyze large datasets and models. The HPC Lab is comprised of 8 SGI Intel-based Linux workstations and one SGI dual processor IRIX (Unix) workstation, Octane.

2.2 The software

The High Performance Computing facility is for faculty and graduate students as well as other UNBC members doing applicable research. A partial list of software installed in the lab includes:

a) Atmospheric models (RAMS, mc2, HYPACT);

b) Data analysis and visualization packages (IDL, R, Tecplot, OpenDX);

c) Molecular and Chemical modelling tools (Gaussian 98, HyperChem);

d) Flow modelling software (FLUENT);

e) The Portable Batch System (PBS Pro 5.2);

f) Fortran Numerical Library (NAG SMP Library);

g) GIS/Remote Sensing packages (PCI);

2.3 Personnel

Dr. Jean Wang has been hired as a Research Associate to support UNBC researchers using the facility. Her basic duties include:

a) Assisting users of the HPC Lab one-on-one in learning to use the facility, training them in using software, solving their problems, and enabling them to make the best use of the facility.

b) Assisting the Unix Administrator in system maintenance and update including ordering and installing new software, obtaining evaluation licenses for new software, and some general system administration duties such as adding new users, monitoring the system etc.

c) Promoting HPC Lab including organizing open houses, seminars, and maintaining the HPC web page.

The CTS Unix administrator is responsible for system administration.

3. Management

The HPC facility is managed by a Management Board. The Management Board presently consists of :

- Peter Jackson (Chair)
- Todd Whitcombe
- Waquar Haque
- Tim Phaneuf (Graduate Student Representative)
- Patrick Mann (non voting)
- Tom Armstrong (non voting)

4. Projects

The projects listed below are arranged alphabetically by faculty member.

4.1 Project leader: Josef Ackerman

Title: **Modelling the fluid dynamics of tandem substrates in bounded flow**
Project Description: They are using FLUENT, a commercial computational fluid dynamics software, to model the fluid dynamics of tandem substrates (three spheres, three hemispheres, and a flat plate) in bounded flow. They are using the same configuration as in a field experiment in which we examined the growth of periphyton (stream algae) on the substrates. They are examining the efficacy of riparian reserve strips in protecting the streambeds and hence the primary productivity in streams. The substrates basically represent a series of bed forms that become more embedded in time.
Use of HPC facility for project: This work could not have been possible without the use of the Origin 3400 and FLUENT, a CFD software package. Jean Wang is helping in using FLUENT to run the simulations.
Project Funding Source(s): The project is funded by FII (formerly FRBC).
Project Outputs: One paper regarding the simulation of the turbulence in open-channels is in preparation.

4.2 Project leader: Stephen Dewhurst

Title: **Lurch** (Lurch is a tool used to develop and evaluate sustainable forest management plans)
Researchers Involved: Stephen Dewhurst (UNBC Faculty) M. Karjala (M. Sc. Student) M. MacGregor (M. Sc. Student) Moshi Charnell (M. Sc. Student)
Project Description: The Lurch decision support system for sustainable forest management planning was developed with the support of the HPC facilities. Lurch, a Java application, is open source and public domain. Lurch has been used to conduct timber supply analysis in support of management plan development for UNBC's two research forests, and has been validated by the BC Ministry of Forests. Lurch is currently being made available to consulting companies, forestry companies, and interest groups for royalty-free use. Some interest is developing in adopting Lurch for operational use. Workshops and training courses in its use will be delivered at UNBC during the spring and summer of 2003. An open source model is being used for development and deployment of Lurch. Lurch has been granted a Canadian copyright and released under the GNU public license. Performance of Lurch has exceeded all expectations, and it has proven to be a robust, flexible, and high-performance application with state-of-the-art capabilities. A parallel-distributed version of Lurch is currently under development, using an innovative "pure Java" MPI implementation. This will enable the use of Lurch in larger, more complex applications while maintaining its real-time, highly interactive properties. This "Parallel Lurch" has undergone testing on a 40 CPU distributed computing cluster in February 2003. Additional work is currently under way in a 3D visualization extension, and this should be completed in 2003.
Use of HPC facility for project: Two M. Sc. students, M. Karjala and M. MacGregor, have used Lurch and the HPC facilities as part of their graduate research projects. Both of these students have been in the area of forest management, developing applications and databases for use with Lurch. In addition, M. Sc. student Moshi Charnell made extensive use of the HPC facilities in conducting research in support of his thesis on water temperature trends in response to timber harvesting and other forest management activities.
Project Outputs: *Peer Reviewed Papers*:

MacGregor, M.K. and S.M. Dewhurst. (submitted). Using Land Use Patterns to Guide Ecological Restoration in Sub-Boreal British Columbia. Restoration Ecology.

Karjala, M.K., E.E. Sherry and S.M. Dewhurst. (in Press). Criteria and Indicators for Sustainable Forest Planning: A Framework for Recording Aboriginal Resource and social Values. Forest Policy and Economics.

Karjala, M.K. and S.M. Dewhurst. (in Press). Including Aboriginal Issues in Forest Planning: a case study in central interior British Columbia, Canada. Landscape and Urban Planning.

Conference Presentations:

Dewhurst, S.M. and O. Garcia. A Stochastic Heuristic Object-Oriented Approach to Satisfying Multiple-Objective Forest Management Problems. Symposium on Models And Systems in Forestry, March 2002, Santiago Chile.

Thesis:

Charnell, M. Master of Science, 2001. Thesis Title: Spatial and Temporal Responses of Temperature in the Horsefly River.

Karjala, M.K. Masters of Natural Resources and Environmental Studies, 2001. Thesis Title: Integrating Aboriginal Values Into Strategic-Level Forest Planning on The John Prince Research Forest.

MacGregor, M.K. Master of Science, 2002. Thesis Title: Developing Reference Conditions For Ecological Restoration in Sub-Boreal British Columbia.

4.3 Project leader: Art Fredeen

Title: **Quantification of Carbon Pools in Relation to Land-use in Sub-Boreal British Columbia**
Researchers Involved: Jennifer Waughtal (M. Sc. Student) Morgan Galpin (M. Sc. Student) Art Fredeen (UNBC Faculty) Bob Madill
Project Description: Measurement of aboveground carbon pools, below ground soil carbon pools, below ground respiration, and net growing season flux was performed to determine the difference between mature forests, regenerating forests, and pastures near Hixon, BC. The values for the carbon pools and fluxes in these areas were applied to a map of land types generated by using a land type classifier program to determine the relative amounts of carbon present on the landscape.
Use of HPC facility for project: The land type classifier program was built by mostly using the HPC lab with the help of HPC consultant services and run on the SGI server. The server was accessed through both the HPC facilities and remotely using telnet. The assistance of HPC staff on troubleshooting and other problems associated with building and running the program were especially important.
Project Funding Source(s): A research grant from NSERC funded the project.
Project Outputs: M. Sc. Thesis (April 2003) plus several papers in preparation.

4.4 Project leader: Waqar Haque

Title: **Real-Time Transaction Processing Simulator**
Researchers Involved: Waqar Haque(UNBC Faculty) Blair Tennessy (Research Assistant) Kiranjit Sidhu (Research Assistant)
Project Description: For the first project, the usage had been limited to the front-end machines because of the poor performance of Java under SGI. However, they used one of Intel-based Linux workstations in the HPC Lab and the peripherals to their fullest potential.
Use of HPC facility for project: This work could not have been possible without the use of this facility. For both of these projects (the other one listed below), we will continue to use this facility on a regular basis.
Project Outputs: ASI Exchange display (March 2002); The Modelling and Simulation 2003 Conference in Palm Springs (Feb. 24-26, 2003)

Title: **MPI Deadlock Detection Tools**
Researchers Involved: Waqar Haque(UNBC Faculty) Kevin Brammer (Research Assistant) Da Hu Wang (Research Assistant) Conan Woods (Research Assistant)
Project Description: They used the HPC node to run our deadlock detection tool and compared results with other platforms. There were significant initial difficulties in porting the Detector primarily because of lack of documentation and some SGI specific parameters. SGI personnel and Jean Wang were of immense help to finally port the code over. Currently, they are expanding the simulator to a distributed environment that will be a very computationally intensive simulation. Similarly, the work on MPI is now moving towards deadlock prevention and avoidance in parallel programs.
Project Outputs: The results from this study were presented at the International Conference on Networks, Parallel and Distributed Computing in October (Tsukuba, Japan).

4.5 Project leader: Alex Hawley

Title: **Computing the capacity of the human brain for distinct neuronal cascades**
Project Description: A model of brain function and a method for calculating the number of neuronal cascades was developed. The model demonstrated that the capacity of the brain for distinct neuronal cascades was functionally infinite (in excess of 10 to the 700 power) in even small clusters of cells.
Use of HPC facility for project: Jean Wang helped in computer programming for the model calculations.
Project Outputs: One paper is in preparation.

4.6 Project leader: Peter Jackson

Title: **COSTEX Data Analysis**
Researchers Involved: Sara Reifer (Research Assistant) Peter Jackson (UNBC Faculty) Chris Reason (University of Cape Town Faculty, collaborator)
Project Description: Produce Graphs and preliminary analysis of meteorological data (from the COastal STratus EXperiment conducted on the West coast of Vancouver Island.
Use of HPC facility for project: HPC lab computers were used for data analysis and processing.
Project Funding Source(s): The following grants to P. Jackson supported the project: HRDC/MSC Science Horizons grant, NSERC Research Grant.
Project Outputs: The work is still in progress, but will result in one or more publications over the next few years.

Title: **Mesoscale Alpine Program Sodar data optimization**
Researchers Involved: Vanessa Egginton (NSERC USRA recipient) Peter Jackson (UNBC Faculty)
Project Description: Optimize the sodar data collected by P. Jackson during the Mesoscale Alpine Program field experiment conducted in the Alps during the Fall of 1999.
Project Funding Source(s): NSERC USRA, NSERC Research Grant.
Project Outputs: Jackson, P.L., and G. Geier, 2002: Case study of the North Foehn in the Eisaktal during MAP. Preprints, Tenth Conference on Mountain Meteorology. Amer. Meteor. Soc., Park City, Utah, June 17-21, pp 356-359. Other publications in preparation.

Title: **High Resolution Simulation of the Atmosphere over Complex Terrain**
Researchers Involved: Peter Jackson (UNBC Faculty) Bryan McEwen (Research Assistant) Brendan Murphy (Research Assistant) April Gibbons (NSERC USRA) Ben Burkholder (RA - Atmospheric Modelling Technician) Dustin Hudyma (RA - Computer Programming Support)
Project Description: The goal of this project is to simulate the atmosphere over BC and adjacent coastal areas at high resolution (< 1 km horizontal resolution) over a period of 5 years in hind-cast mode. The model will be optimized and fields validated through comparison with surface and upper-air observations. The generated fields will create a high resolution database to be used for a series of projects including: transport and dispersion of air pollutants and Mountain Pine Beetles, assessment of areas prone to high wind in support of forest windthrow studies, and marine safety, etc.
Project Funding Source(s): NSERC Research Grant to P. Jackson BC Ministry of Water, Land and Air Protection
Project Outputs: Work has recently started (2002) so there are no publications to-date.

Title: **The use of high Resolution Mesoscale Model Fields with the Calpuff Dispersion Modelling System in Prince George B.C.**
Researchers Involved: Peter Jackson (UNBC Faculty) Bryan McEwen (M. Sc. student)
Project Description: As a master's student, Bryan McEwen used the High Performance Computing (HPC) lab to run a mesoscale atmospheric model to support graduate research. This model was used to generate meteorological fields over Northern B.C. for use in dispersion modelling.
Use of HPC facility for project: The model requires considerable computing power and data storage and would have been very difficult to perform without the SGI Origin. Jean Wang, the HPC Consultant, helped with model installation issues and data visualization tools.
Project Funding Source(s): Grant from the Oil and Gas Commission.
Project Outputs: Master thesis, University of Northern British Columbia, November 2002. One journal publication to be submitted in March 2003 to Journal of the Air and Water Management Association.

Title: **Mesoscale atmospheric modelling**
Researchers Involved: Peter Jackson (UNBC Faculty) Bryan McEwen (Research Assistant)
Project Description: This project investigates two different ways of running a mesoscale model in 'hind-cast' mode to produce high resolution meteorological fields. This modelling concentrates on the Okanagan region and its output will be used for future studies and decisions made by the Ministry.
Use of HPC facility for project: Use of the HPC is of major importance in undertaking the project. Jean Wang has been helping with model optimization and data visualization.
Project Funding Source(s): A financial award from the B.C. Ministry of Water, Land and Air Protection.
Project Outputs: Paper in preparation.

Title: **CFD modelling of wind flow through forested environments**
Researchers Involved: Peter Jackson (UNBC Faculty) Tim Phaneuf (Master Student)
Project Description: Air flow modelling using the FLUENT package of Computation Fluid Dynamics (CFD) software. Have performed basic three-dimensional simulations of airflow past a cube, for use in validating the software. Three-dimensional modelling of wind through forested environments to understand the forces acting upon trees and how it pertains to windthrow.
Use of HPC facility for project: All components of the HPC facility (lab, Origin 3400, and consultant) have been utilized.
Project Outputs: Master Thesis in the future, plus journal publications.

Title: **Feasibility of Modeling Mountain Pine Beetle Transport and Dispersion with Mesoscale Atmospheric Models**
Researchers Involved: Peter Jackson (UNBC Faculty) Brenda Moore (M. Sc. Candidate)
Project Description: RAMS/HYPACT will be used to first produce the meteorological fields (which will be statistically validated) and then to insert a passive tracer (mountain pine beetle) and model the resultant spatial variability in concentration.
Use of HPC facility for project: Access to the HPC facility is of vital importance to my research. The model output is highly complex and requires significant computing strength to produce, which can only be done within the server Origin 3400. The component of the HPC used is the server, accessed remotely from lab 4-215 (atmospheric measurement and prediction lab). HPC consultant services may be requested at a later date.
Project Outputs: Master Thesis in the future, plus journal publications.

4.7 Project leader: Elie Korkmaz

Title: **Measurement of charge symmetry breaking in inelastic nucleon-nucleon collisions - TRIUMF experiment 704**
Researchers Involved: Elie Korkmaz (co-spokesperson, UNBC), Tracy Porcelli (Research Associate, UNBC), Grant O'Rielly (Research Asociate, UNBC), Plus 3 summer students. Allena Opper (co-spokesperson) and collaborators (Ohio), Plus 1 PhD student (Ohio). David Hutcheon and collaborators (TRIUMF). Gordon Greeniaus and collaborators (University of Alberta).
Project Description: This is a high-profile experiment which was finished at TRIUMF by a collaboration of scientists from UNBC, TRIUMF, University of Alberta, and Ohio University. The analysis, now completed, required extensive GEANT monte carlo simulations carried out over two years using the UNBC HPC facility and two other facilities of similar power at Ohio and Alberta.
Use of HPC facility for project: Use of the HPC was of major importance in undertaking the project. They used the 28 processor SGI server which allowed the simulations to be completed in a timely fashion. Typically, they used 10-15 CPU's for several months during each of 2000, 2001, and 2002.
Project Funding Source(s): Project was funded by NSERC (Dr. Korkmaz's individual research grant and other collaborative project grants) and by NSF in the USA.
This is a partial list from the last two years only: Diane Rietzner, PhD thesis, Ohio University, December 2001. A. Opper et al, Nucl. Phys. A663-664 (2001) 505-508. D. Hutcheon et al, Nucl. Inst. Meth. A459 (2001) 448-458. E. Korkmaz et al, Bull. Amer. Phys. Soc. 46 (2001) 144. A. Opper and E. Korkmaz, TRIUMF 2001 annual report (2002) 38-41.

A. Opper and E. Korkmaz, TRIUMF 2000 annual report (2001) 35-39.
E. Korkmaz, A. Opper, et al, in preparation, to be submitted to Phys. Rev. Lett. (2003).

4.8 Project leader: Margot Mandy

Title: **Energy Transfer and Dissociation in molecular hydrogen**.
Researchers Involved: UNBC: Dr. Mirjana Ticeric (Research Assistant) Timothy Rothwell (Research Assistant, Fourth year project student) Glenn McNamara (Fourth year project student to start May 2003) Collaborators at Oxford: Dr. Sergei K. Pogrebnya Professor David C. Clary Collaborators at the Canadian Institute for Theoretical Astrophysics: Professor Peter G. Martin Dr. Arnold Boothroyd
Project Description: The project encompasses detailed calculations on energy transfer and dissociation behavior in molecular hydrogen as the result of collisions with hydrogen molecules, hydrogen atoms, or helium atoms using classical and quantum mechanical methods. Classical calculations have been benchmarked with the corresponding quantum calculations for the H2 + H2 system. Currently, classical calculations are ongoing to characterize the role of internal energy in a collider molecule in causing energy transfer in target molecules. Using a new ab initio potential energy surface developed by Boothroyd and Martin, calculations will commence shortly on improved state-to-state transition probabilities for the He+H2 system.
Use of HPC facility for project: This work would not have been possible without the HPC. It used all cycles of the 28 processor SGI Origin 3400 that were not required by other users.
Project Funding Source(s): NSERC Operating Grant. Personnel costs partially covered with funding from First Jobs in Science and Technology and Human Resources and Development Canada programs.
Project Outputs: Published: S. K. Pogrebnya, M. E. Mandy, and D. C. Clary, 2002.

Vibrational relaxation in H2 + H2: Full dimensional quantum dynamical study.
International Journal of Mass Spectrometry. Vol. 223-224. pp 335-343.

M. E. Mandy, T. A. Rothwell, and P. G. Martin, 2001.
A Restricted Dimensionality Quasiclassical Trajectory Study of H2(v,0) + H2(v',0).
Journal of Chemical Physics. Vol.114, pp.10780-10790.

In Press:

M. E. Mandy, 2003.
Energy Transfer in Molecular Hydrogen: Does the Collider Matter?
Proceedings of the Conference: Star Formation 2002: Chemistry as a
Diagnostic of Star Formation.
C. L. Curry and M. Fich, Editors. National Research Council Press.

About to be submitted (within a month):

M. E. Mandy, S. K. Pogrebnya, and D. C. Clary, 2003.
Inelastic collisions of molecular hydrogen: A comparison of results from quantum and classical mechanics
Journal of Chemical Physics.

Papers in preparation:

M. E. Mandy, 2003
Collisions of molecular hydrogen with molecular hydrogen: the role of internal energy of the collider in promoting dissociation and energy transfer.
Journal of Chemical Physics.

M. E. Mandy and P. G. Martin, 2003.
Collisional excitation of H2 molecules by H2 molecules.
Astrophysical Journal.

M. E. Mandy, 2004
The role of the collider in molecular energy transfer and dissociation.
Recent Research Developments in Chemical Physics. Transworld Research
Network. (This is an invited review article.)

4.9 Project leader: Patrick Mann

Title: **Stellar Core Collapse and Black Hole Formation**
Time: Continuing
Researchers Involved: Patrick Mann
Project Description: Patrick Mann has been developing parallel versions of two relativistic hydrodynamics codes. An initial FEM version is now running using the OpenMP parallelization options available on the Origin 3400. Test with multiple processors is in progress, but it is already clear that far better resolution can be obtained with the Origin 3400. In particular a very nasty instability has been shown to be an artifact of the coarse grids used previously.
Use of HPC Facility: This project makes extensive use of the parallel processing hardware and software available on the SGI Origin 3400.
Project Outputs: Project is in development. Journal publications should result.

4.10 Project leader: Patrick Montgomery

Title: **Gravity Currents over non-horizontal bottom topography**
Time: May-August, 2001
Researchers Involved: Patrick Montgomery (faculty) and J. Arocena (undergraduate RA funded jointly by the Student Summer Works Program NSERC)
Project Description: Previous research code to calculate numerical solutions for a system of four equations representing the time dependent motion of a two-layer system after lock-release initial conditions (traditional gravity currents) was modified to include spatial variation in the frictional drag term and non-horizontal bottom topography. The resulting equations were solved to produce simulations of two-layer gravity current flow.
Use of HPC facility for project: The Origin 3400 was used, but probably in a minor way (i.e., most of the code could have been run on a simpler machine, but would increase the time from 30 min to 12 hours). The use of the HPC lab was major, in that without the software and workstations present, Dr. Montgomery would not have been able to conduct the same quality of research. The use of the HPC consultant services was of major use as this saved time to concentrate on the research.
Project Funding Source: NSERC and BC Government (Student Summer Works)
Project Outputs: Generalization of a relaxation scheme for systems of forced nonlinear hyperbolic conservation laws with spatially dependent flux functions (Studies in Applied Mathematics, volume 110 p. 1-19, 2003).

Title: **Simulation of mountain pine beetle dispersion in a reactive forest**
Time: May-August, 2001
Researchers Involved: Patrick Montgomery (faculty) and B. Burkholder (undergraduate RA)
Project Description: A system of nonlinear integer-differential equations was solved numerically using a standard finite-difference method, and solutions were displayed graphically.
Use of HPC facility for project: The SGI processor was used, but probably in a minor way (simulation time of minutes). The use of the HPC lab was minor, as the visualization was probably sufficiently simple to complete on a PC,: However the output was enhanced with the workstations and Tecplot. The use of the HPC consultant services was minor as the computing portion of the project was approximately 20% of the entire project.
Project Funding Source: NSERC
Project Outputs: Poster presentation at a national conference (Canadian Applied and Industrial Mathematics Society, Calgary AB, June 2002). Title: Global Stability for a coupled spatially independent mountain pine beetle and pine forest growth model. A coupled differential equation model for forest growth and mountain pine beetle infestation (in preparation for journal submission.)

Title: **Flow of a Stratified Fluid in a Rotating Cylinder**
Time: May-August, 2003
Researchers Involved: Patrick Montgomery (faculty) and A. Summers (undergraduate RA)
Project Description: Previously developed numerical code was used to model the flow of a fluid stratified by thermal forcing in a rotating cylinder.
Use of HPC facility for project: The Origin 3400 was used, but probably in a minor way (i.e., most of the code could have been run on a simpler machine, but would increase the time required). The use of the HPC lab was major, in that without the software and workstations present, Dr. Montgomery would not have been able to conduct the same quality of research. The use of the HPC consultant services was minor as the computing portion was a small part of the project.
Project Funding Source: NSERC
Project Outputs: Poster presentation at a national conference (Canadian Applied and Industrial Mathematics Society, Montreal, June 2003). Title: Slow Fluid Circulation in a Cylinder.

4.11 Project leader: Tomson Ogwang

Title: **A Monte Carlo Study of the Bounds of Inequality Measures**
Researchers Involved: Tomson Ogwang (UNBC faculty) Baotai Wang (UNBC faculty)
Project Description: In this project, Monte Carlo methods are used to assess the reliability of the bounds of several income inequality measures. Large random samples are generated from relevant probability distributions and then used to form grouped frequency distributions which are, in turn, used to construct bounds of the inequality measures of interest. For each distribution, thousands of replications are made. This is a very computationally intensive approach that requires extensive use of HPC facilities. The study involves extensive use of NAG FORTRAN subroutines that are currently available only on the SGI servers.
Use of HPC facility for project: Since the study is very computer intensive, access to UNBC HPC facility is crucial. They have been using mainly the 28 processor SGI server. They have also been consulting regularly, with Jean Wang, the HPC Consultant, regarding programming and other technical aspects. The project would not have been possible without the use of HPC facilities.
Project Outputs: They hope to submit the full paper for consideration for possible publication in a refereed journal by the end of April 2003. The first part of the project, which involved limited use of HPC facilities but formed the theoretical basis for the Monte Carlo study, resulted in a paper entitled ABounds of the Gini Index Using Sparse Information on Mean Incomes,@ *UNBC Economics Program Working Paper No. 0202*, July 2002. This paper is currently under consideration for possible publication in a refereed journal.

4.12 Project leader: Mark Shegelski

Project #1 Description:

Study of reconstruction of object imaged in "low energy electron point source" (LEEPS) holograms (theoretical simulations): electrons emerge from a sharp tip of a metal as nearly spherical electron waves, some of which scatter off an object to be imaged, while others are unscattered; these electrons combine on a screen to give an electron hologram. Their work is to continue to develop methods which will ultimately give atomic resolution of the object in practical situations.

Project #2 Description:

Time development of state function initially localized within a well, and numerical determination of time taken for state to decay, or escape, or tunnel, outside the inner well.

Project #3 Description:

Study of tunneling of 1-dimensional chains.

Project #4 Description:

Numerical study of trajectories of sliding, rotating cylinders.

Project Outputs:

Published:

Mark R.A. Shegelski and Roman Holenstein, "The Motion of rapidly Rotating Sliding Cylinders: Trajectories with Large Lateral Displacements", Canadian Journal of Physics, volume 80, pages 141-147 (2002).

Roman Holenstein, Timothy Rothwell, and Mark R.A. Shegelski, "Reconstruction of Composite In-line Holograms Using a Small Emission Cone", Ultramicroscopy, volume 94, pages 99-107 (2003).

Mark R.A. Shegelski and Erik V. Kozijn, “Quantum Mechanical vs. Quasi-classical Tunneling Times For Smooth Potential Barriers”, accepted for publication in the Canadian Journal of Physics on December 10, 2002.

In preparation:

Dino Gigliotti and Mark R.A. Shegelski, "The motion of curling rocks: experimental and theoretical results", Canadian Journal of Physics.

5. HPC Events

High Performance Computing Open House **Friday April 20, 2001 11:00 - 13:00**
It was the first HPC lab open house. The lab had been opened for hands-on demonstration of the hardware and some of the software we had available (e.g. SGI Developer package, Splus, Tecplot, PCI, ArcInfo, etc.).

HPC software demo - invited eight 4-th year undergraduate students. **Dec. 3rd, 2001**
Computer facilities at UNBC, includes the introduction of Origin 3400. Software source at HPC lab.

HPC Open house / software demo **January 11, 2002 10:00 am - 12:00 noon.**
Gaussian98 - by Prof. Todd Whitcombe. OpenDX - by Dr. Patrick Mann. Tecplot - by Jean Wang FLUENT - by Jean Wang Splus - by Dieter Ayers. Develop Magic - by Jean Wang.

HPC Seminar Series, Splus demo by Dieter Ayers: **January 24 – February 21, 2002**
January 24, Thursday 1:30 pm to 3:00 pm Introduction to data analysis with Splus. February 7, Thursday 1:30 pm to 3:00 pm Modern regression techniques with Splus.

February 21, Thursday 1:30 pm to 3:00 pm
Graphical displays with Splus.

High Performance Computing May 2002 Open House
Friday May 10, 2002 10:00 am - 12:00 noon.

SGI Developer Magic;
PGI CDK Development Kit;
RAMS - Regional Atmospheric Modelling System;
FLUENT - flow modelling;
R - statistics software;
Tecplot - plot tool.

One week mc2 Workshop
Tuesday May 28, 2002 to Monday June 3, 2002

The course was funded externally, taught by a research scientist from Recherche en Prevision Numerique of Environment Canada, to 12 researchers of whom 5 were from UBC, 1 from BC WLAP and 6 from UNBC.

DAY 1: INTRODUCTION

Background

An introduction to numerical weather models (Jackson)
The role and special issues surrounding mesoscale models
The Mesoscale Compressible Community model (Chamberlain)
Community for Mesoscale Modelling (COMM)
Recherche en Prevision Numerique (RPN/MRB)
Resources: How to find and use documentation

MC2 Architecture and Overview

Pre-processor
Prognostic model
Post-processor

Installing and Running MC2

Installation

File system structure
Managing file system (Etagere)
Running benchmark case
Viewing output (Xrec)
Log files and trouble shooting

Prelude to Running Your Own Test Case

Input files required
How to generate or obtain input files
Location of input files
Managing a file system (Etagere)
Planning nested runs
Modifying source code

DAY 2-3: DATA PREPARATION and UTILITIES

RPN/FST Format

Description
Utilities
GRIB_CVT
EDITFST

Worked Examples
Creating RPN/FST files
Changing map projections
Data format conversion (gdecode/gencode)
Editing FST files

Data Preparation: Pilot files

Description and purpose
Interpolating data onto model grid (champs, tape1 and PGSM)
Scripts
Worked Examples

DAY 4-5 PUTTING IT ALL TOGETHER

Worked Examples

Working Example 1A: Single grid run with CMC Analysis
Working Example 1B Nested run with CMC Analysis
Working Example 2: Nested run with Eta Forecast Initialization

(By Brendan Murphy)

Special Topics: How to do non-standard things like

Use different geophysical datasets
Hi-res topography
Output special variables at each time step, etc.

HPC seminar: FLUENT Demo by Jean Wang.
July 04 2002 2:00 pm - 3:00 pm.

Training interested researchers to use FLUENT.

High Performance Computing September 2002 Open House
Friday September 27 2002 10:00 am - 12:00 noon.

HPC Lab Introduction - by Peter Jackson.
PBS Introduction - by Jean Wang.
Introduction of the Origin 3400 - by Patrick Mann.
Tecplot - by Jean Wang.

6. Summary and Statistics

In the past two years, HPC facility has been used by a variety of researchers at UNBC. Publications resulting from projects involving the HPC facility, based on the uncompleted information, are summarized below:

Journal:	
Published or in Press	13
Submitted	3
In preparation	13
Reports:	3
Conference:	6
Theses: (Completed or in preparation):	
Ph. D.	1
Master of Science	7
Total:	46

Many projects are in progress and have not yet reached the publication stage. There are approximately 22 projects had or have been involved in using HPC facility, as listed in Section 4. Among them, over 60% of the projects have obtained the HPC consultant's help. The important access to the HPC facility in undertaking the projects are summarized below:

Origin 3400	
Major	9
Minor	3
HPC Lab	
Major	11
Minor	3

Information regarding HPC user account is summarized below:

Total users	85	
Active users	44	
Among Active users		
Faculty and Staff	14	32%
Graduate Students	13	30%
Undergraduate Students	17	38%

Averaged total CPU usage on the 28 processor SGI server is 99%.