



ATLANTIC COMPUTATIONAL EXCELLENCE NETWORK

Introduction to ACEnet

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What is ACEnet?

Consortium of Atlantic Canada universities

Canada Foundation for Innovation (CFI) is the principal funding source

High-performance computing facility

- * Hardware

Computing – visualization – communication

- * Software

- * Expertise

Where is ACEnet?

Member institutions



Where is ACEnet?

Member institutions



Cluster name: Glooscap

Current compute nodes
hosting institutions



Cluster name: Fundy/Courtenay



Cluster name: Placentia



Cluster name: Brasdor



Cluster name: Mahone

Hardware:

Processors - 2.6 GHz dual-core Opteron 285 SE

	Available Cores	Operating System	RAM per core (GB)	Node connection
Brasdor	1080	Linux	2	GigE
Fundy	640	Linux	4 or 8	GigE and Infiniband
Courtenay	52	Linux	4	GigE
Mahone	564	Linux	4	GigE and 2K
Placentia	940	Linux	4	GigE and 10G and Infiniband
Glooscap	232	Linux	1	GigE

Linux - Red Hat Enterprise Linux 4 & 5

GigE - Gigabit Ethernet

2K - Myrinet 2000

10G - Myrinet 10G

Cluster Layout

- ▣ Clusters are structured with a single head node controlling access
- ▣ A job submission system (N1GE) controls access to the compute nodes
- ▣ A single username / password provides access to all clusters

Hardware:

Processors - 1.5 GHz Itanium2 (intel)

	Available Cores	Operating System	RAM per core (GB)	Node connection
Urdur	10	Linux	1	NUMAlink SMP
Skuld	16	Linux	1	NUMAlink SMP
Verdandi	16	Linux	1	NUMAlink SMP

Primary Usage: Gaussian, Fluent
and Quad Precision Computations



Storage:

	User quota in /main	/home/username/ scratch	/scratch/tmp
Brasdor	47 Gb	238 Gb	40 Gb
Fundy	47 Gb	238 Gb	38 Gb
Mahone	13 Gb	238 Gb	42 Gb
Placentia	13 Gb	238 Gb	31 Gb
Glooscap	13 Gb	48 Gb	13 Gb



Across the nodes



On each local node

NQS – No Quota Scratch

- ▣ Some jobs require even more storage
- ▣ NQS provides unlimited temporary storage
- ▣ No guarantee that files will remain there

Mahone	Brasdor	Placentia	Glooscap	Courtenay	Fundy
13TB	12TB	10TB	2.7TB	2TB	13TB

Software:

http://wiki.ace-net.ca/index.php/Available_Software

Scientific computing	Scientific Libraries	Parallel APIs	Compilers & Languages	Debuggers & Profilers
Star Lab	FFTW	MPICH	C/C++	gdb
Octave	ACML	CRE	Fortran 77/90	dbx
Gaussian	LAPACK	OpenMP	Java	Sun Studio
Gromacs	GSL	pyMPI	Perl/Python	TotalView

Software requests at:

http://wiki.ace-net.ca/index.php/Software_Requests

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Available Software

NOTE: Software versions in these tables indicate the highest version available on any ACEnet resource. Older versions may also be available. More information is available by clicking the software titles.

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Scientific Computing Packages

[\[edit\]](#)

software	version	brasdor	mahone	placentia	fundy	glooscap	courtenay	other
ABINIT	5.6.3	Y	Y	Y	Y	Y	Y	-
BIMr	--	Y	Y	Y	Y	Y	Y	-
CPMD	3.13.2	Y	Y	Y	Y	Y	Y	-
DiVinE	0.8.3	Y	Y	Y	Y	Y	Y	-
DL_POLY	3.08	Y	Y	Y	Y	Y	Y	-
DL_MESO	2.2	Y	Y	Y	Y	Y	Y	-
elmer-fem	5.4.1	Y	Y	Y	Y	Y	Y	-



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Compilers & Languages

[\[edit\]](#)

software	version	brasdor	mahone	placentia	fundy	glooscap	courtenay	other
Portland Group compilers (C, C++, Fortran)	8.0-6	Y	Y	Y	Y	Y	Y	-
Sun Studio 12 Compilers (C, C++, Fortran)	12.0	Y	Y	Y	Y	Y	Y	-
GNU compilers (C, C++, Fortran, Java)	3.4.6	Y	Y	Y	Y	Y	Y	-
Java, 64-bit VM	6u7	Y	Y	Y	Y	Y	Y	-
Mono (.NET)	2.2	Y	Y	Y	Y	Y	Y	-
Perl	5.8.5	Y	Y	Y	Y	Y	Y	-
Python	2.6.2	Y	Y	Y	Y	Y	Y	-
Ruby	1.8.1	Y	Y	Y	Y	Y	Y	-

Debuggers & Profilers

[\[edit\]](#)

software	version	brasdor	mahone	placentia	fundy	glooscap	courtenay	other
gdb	6.2.1	Y	Y	Y	Y	Y	Y	-
dbx	7.5	Y	Y	Y	Y	Y	Y	-
pgdbg	same as PGI	Y	Y	Y	Y	Y	Y	-
pgprof ↗	same as PGI	Y	Y	Y	Y	Y	Y	-
Sun Studio	12.0	Y	Y	Y	Y	Y	Y	-
TotalView	8.6.2-2	-	Y	Y	Y	Y	Y	-
Valgrind	3.1.1-1	-	Y	Y	Y	-	Y	-

Unix Shells

[\[edit\]](#)

software	version	brasdor	mahone	placentia	fundy	glooscap	courtenay	other
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Compilers

Several compiler suites are currently available:

- Portland Group compilers (preferred compilers)
- Sun Studio 12 compilers
- GNU compilers (gcc 3 and gcc 4)

PGI compilers

[\[edit\]](#)

Description

Portland Group compilers 8.0-6 for Fortran, C, C++ and [High-Performance Fortran](#)

Resources

[Vendor website](#)

[Documentation, Tips & Techniques, etc.](#)

[PGI Support](#)

Commands

```
pgcc  
pgCC  
pgf77  
pgf90  
pgf95  
pghpf
```

All available versions can be found in `/opt/pgi/linux86-64/`

Help for any command

```
man pgf90
```

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Other Facilities

Internet videoconferencing (inSORS / Access Grid)

Located Dalhousie, Memorial, Mount Allison, Saint Mary's, Saint Francis Xavier, Acadia and New Brunswick.



Other Facilities

Data cave **new!**

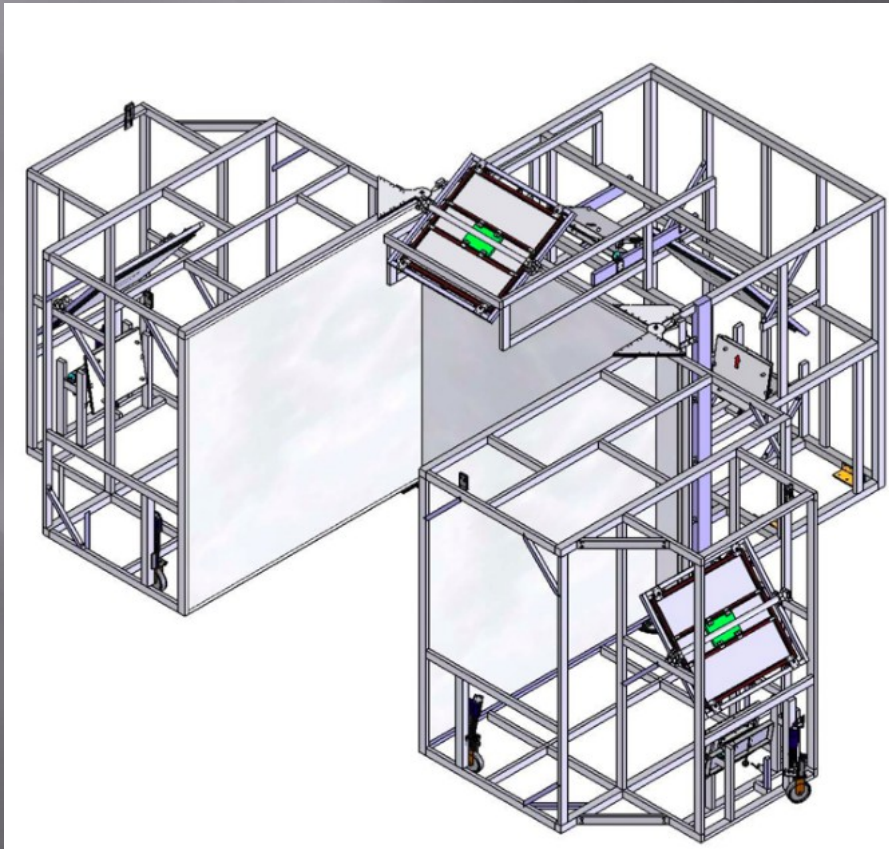
3D immersive data exploration facility (SMU)



Other Facilities

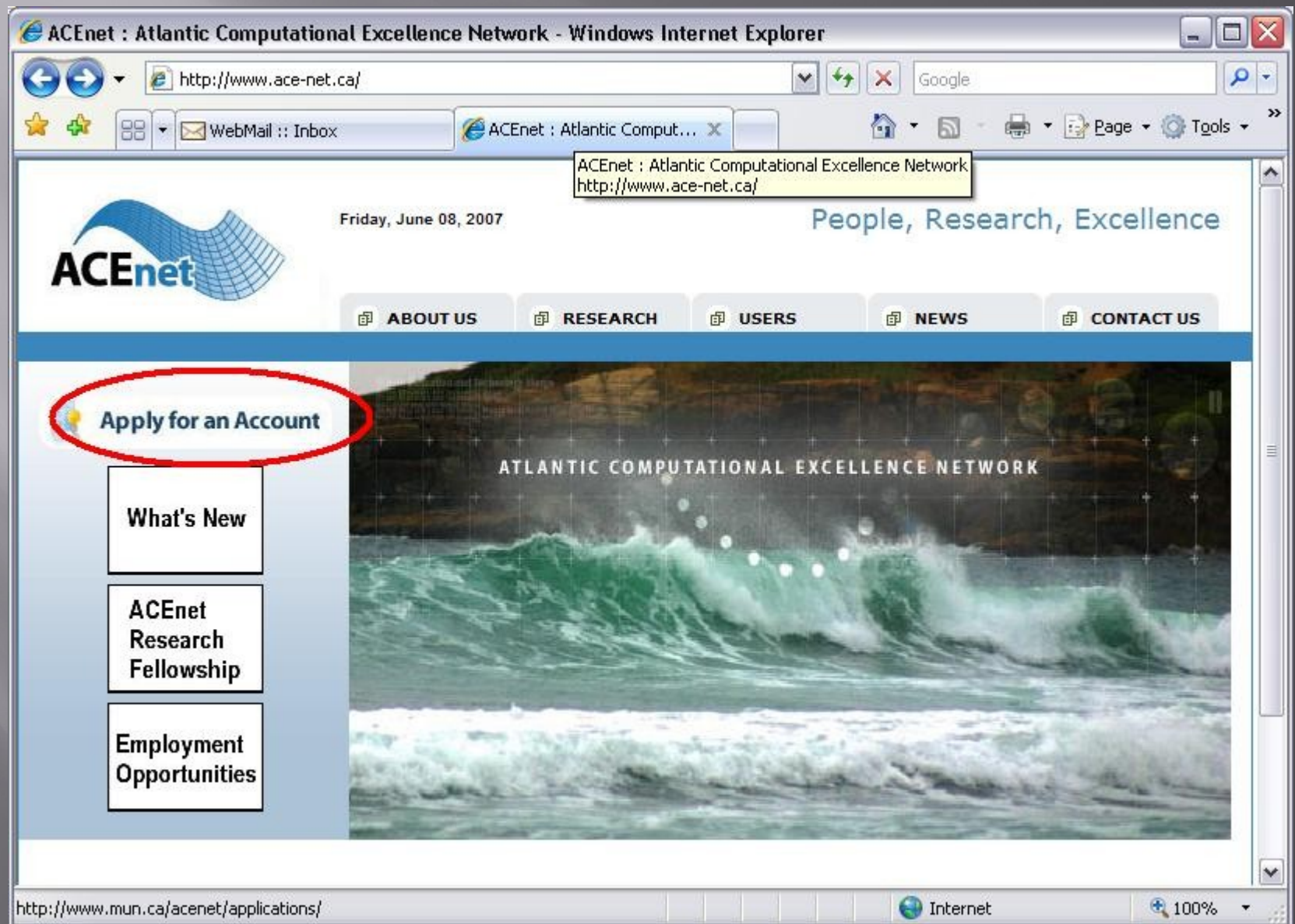
Data cave **new!**

3D immersive data exploration facility (SMU)



How do I get started?

Getting an account: <http://www.ace-net.ca/>





Friday, June 08, 2007

People, Research, Excellence

ABOUT US

RESEARCH

USERS

NEWS

CONTACT US

- [Categories of Accounts](#)
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- [User Account Application](#)

Categories of Accounts

ACEnet issues two types of accounts, **Primary Project Accounts** and **User Accounts**. Primary Project Accounts are held by the Research Project Leader who is typically the principal investigator for a project or the head of a research group. A project Leader is responsible for all other user accounts associated with the project.

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[Project Account Application](#)

User accounts will only be issued on the authority of the Research Project Leader for a particular project.

[User Account Application](#)

How Do I get Connected?

- Logging in
 - ssh *Secure Shell*
- Moving Data Around
 - sftp *Secure File Transfer Protocol*
 - scp *Secure CoPy*
- both provided with Mac OSX or Linux
 - ssh -X username@brasdor.ace-net.ca
 - sftp username@placentia.ace-net.ca
- Windows? Use PuTTY and PSFTP:
 - <http://www.chiark.greenend.org.uk/~sgtatham/putty/download.html>
 - or better yet, google 'putty psftp'



PuTTY Configuration



Category:

- Session
 - Logging
- Terminal
 - Keyboard
 - Bell
 - Features
- Window
 - Appearance
 - Behaviour
 - Translation
 - Selection
 - Colours
- Connection
 - Data
 - Proxy
 - Telnet
 - Rlogin
 - + SSH
 - Serial

Basic options for your PuTTY session

Specify the destination you want to connect to

Host Name (or IP address)

Port

brasdor.ace-net.ca

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Connection type:

☐ Raw

☐ Telnet

☐ Rlogin

☒ SSH

☐ Serial

Load, save or delete a stored session

Saved Sessions

brasdor

Default Settings

brasdor

fundy

mahone

mahone2

placentia

placentia2

Load

Save

Delete

Close window on exit:

☐ Always

☐ Never

☒ Only on clean exit

About

Open

Cancel

Taking turns

The job queue

- Login nodes are for file management, compiling, testing – small stuff
- “Production” work is distributed using queue management system
 - Sun Grid Engine (N1GE)
- Relevant commands:
 - qsub – qstat – qdel – man

Types of Jobs

Serial versus Parallel

- multiple serial jobs can be run in parallel
- parallel jobs can be run in multiple configurations
- the aim is to complete a calculation in the shortest amount of time.
- should all existing serial codes be made parallel?

Upcoming Workshops

- ACEnet workshops

- Introduction to ACEnet
- Introduction to Linux
- Introduction to Grid Engine
- Introduction to Shell Scripting
- etc.

- There is also the possibility of customized workshop material (e.g. MPI programming, GAUSSIAN, etc.)

Where to go for help

- ACEnet User Guide
 - https://wiki.ace-net.ca/index.php/User_Guide
- ACEnet User Wiki
 - <http://wiki.ace-net.ca>
- Research/user support personnel
 - email: support@ace-net.ca