

ATLANTIC COMPUTATIONAL EXCELLENCE NETWORK

ACEnet: Free Cluster Computing For Researchers

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What is ACEnet?

- Atlantic Computational Excellence Network
- Shared regional resource for ...
 - ... high-performance computing (HPC)
 - ... remote collaboration
 - ... visualization
- Hardware, software, and personnel

Remote Collaboration



Internet videoconferencing - VisiMeet software

Dalhousie - Memorial - Mount Allison - Saint Mary's - Saint Francis Xavier
Acadia - New Brunswick + **other sites across Canada & the world**

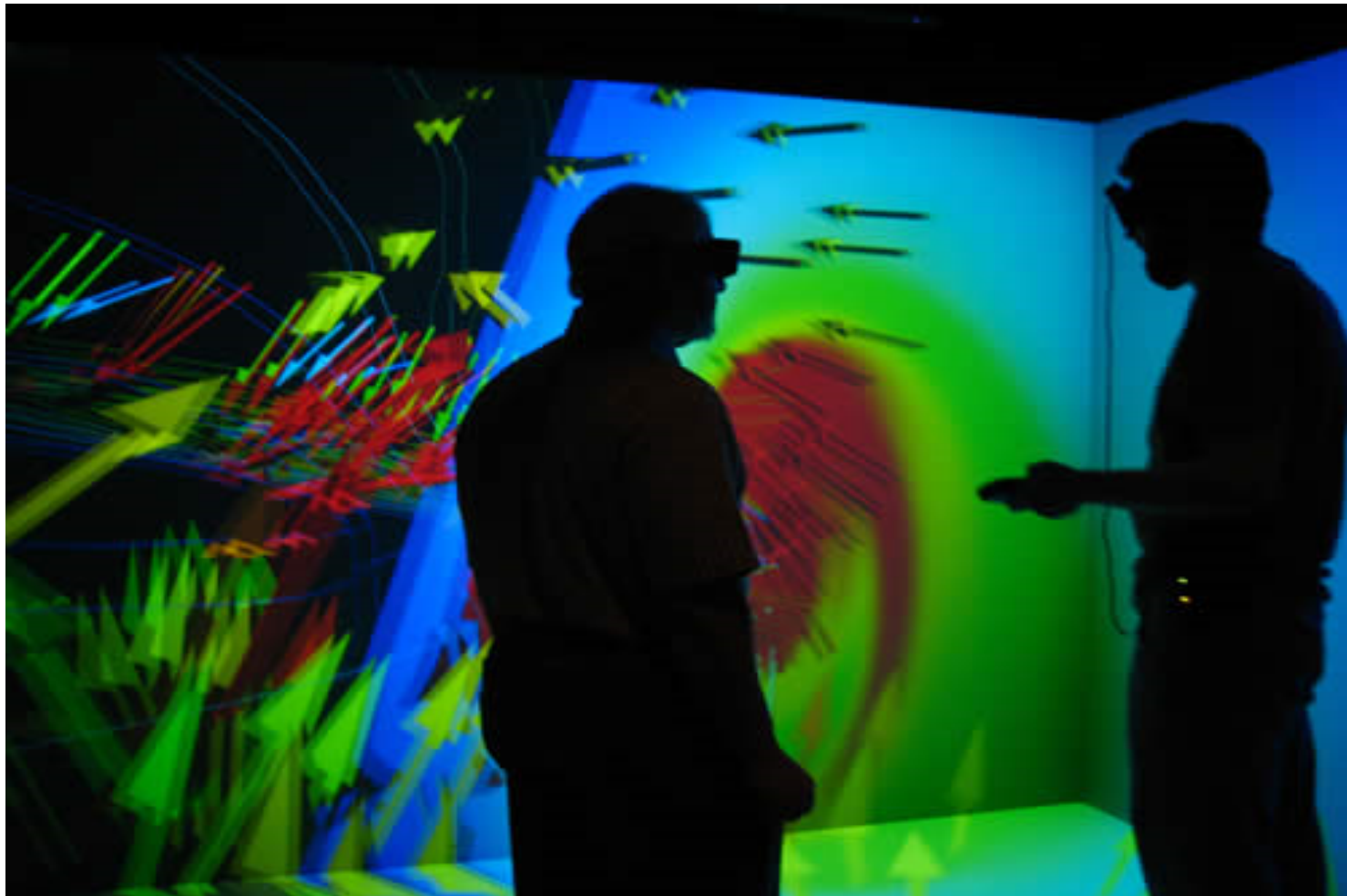


Advanced Visualization



Data cave

3D immersive data exploration facility @ Saint Mary's

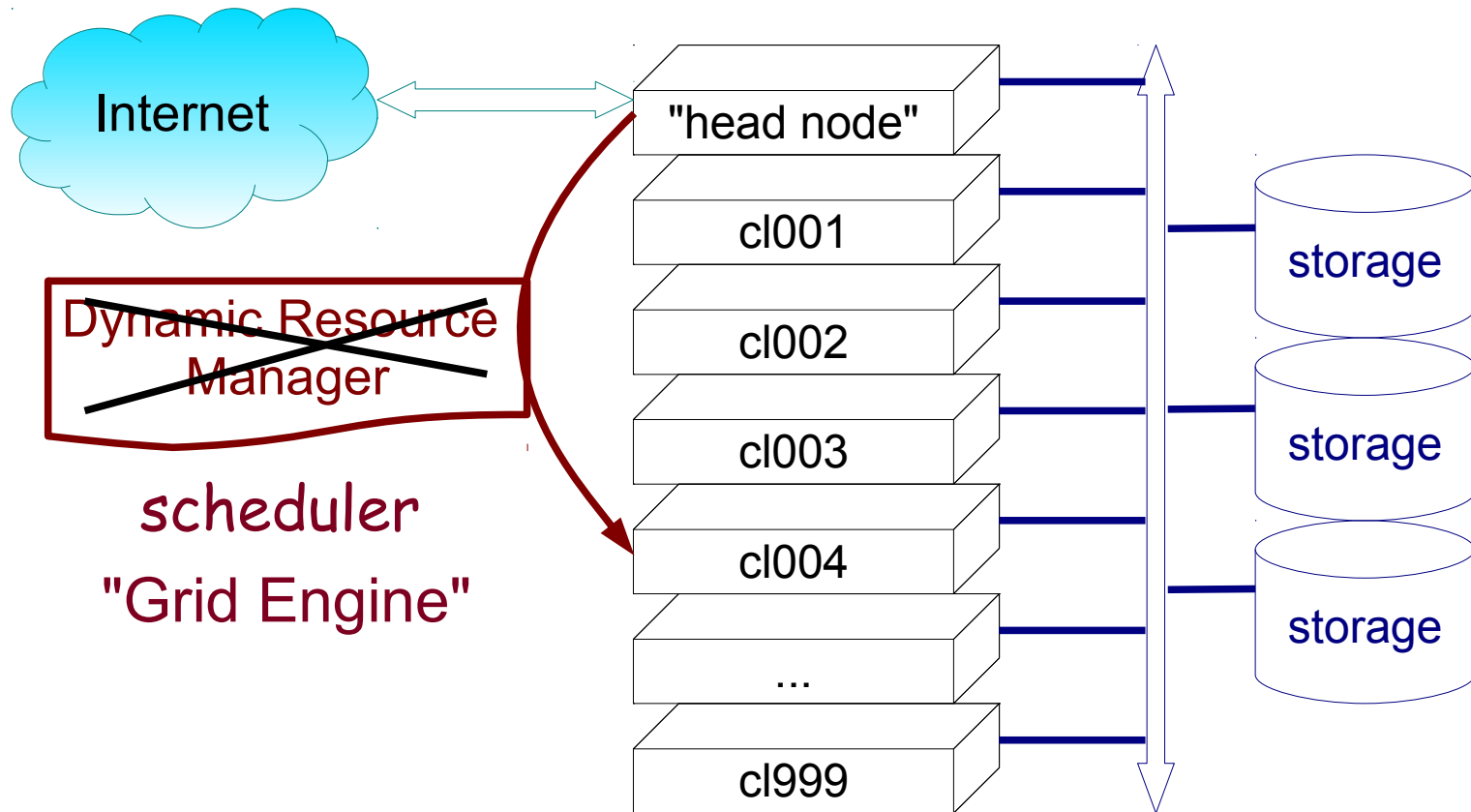


What's “High Performance Computing”?

- Many CPUs working on one problem
 - Many “serial” jobs running at once, or
 - many CPUs working in close coordination.
 - Communication between CPUs is key!
- Advantages
 - Faster results
 - Larger problems or more detailed simulations
- Principal tool: Computer **cluster**
 - Racks of regular computers, networked



What's a cluster?



ACEnet computers

- Four clusters
- 7000 CPU cores
- 20 TB RAM
- 500 TB disk storage
 - plus tape
- plus software
- remember: Shared resources!
 - about 400 active users

*aggregated
numbers*

Applications

<http://www.ace-net.ca/wiki/Software>

<u>Molecular</u>	<u>Math&CS</u>	<u>Engineering</u>	<u>Earth &Ocean</u>	<u>Bio</u>
Gaussian	Sage	ANSYS		AbySS
Gromacs	GAP	(Fluent)	CDO	Bowtie
CPMD	DiVinE	CFX	NCO	mpiBlast
Abinit	...	LS-DYNA*	GMT	MrBayes
NAMD	<u>Astro</u>	OpenFOAM	MM5	Migrate-n
WebMO	StarLab		...	PhyML
VMD	IRAF			PLINK
...	...			...

Software requests to:

support@ace-net.ca

Software Development

<http://www.ace-net.ca/wiki/Software>

<u>Languages</u>	<u>Compiler</u>	<u>Parallel</u>	<u>Libraries</u>	<u>Tools</u>
C/C++	<u>Suites</u>	<u>APIs</u>	LAPACK	TotalView
Fortran	GCC	MPI	FFTW	dbx, gdb
Perl	Intel	OpenMP	GSL	Valgrind
Python	PGI	...	ACML	make
R	SunStudio		netCDF	cvs, svn
Java			HDF	git
...			Boost	...
			...	

Software requests to:

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Data Analysis



<http://www.ace-net.ca/wiki/Software>

R

Rmpi

Octave

Matlab*

*Distributed Computing Server

Python

Numpy

SciPy

Sage

pyMPI

pylab

matplotlib

Software requests to:

support@ace-net.ca

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

A screenshot of a web browser window displaying the ACEnet website. The browser is Firefox, and the address bar shows the URL "http://www.ace-net.ca/wiki/Get_an_Account". The page title is "Get an Account - ACEnet". The main content area is titled "Get an Account" and contains sections for "Eligibility", "How to Get an Account", and "Step 1. Get a Compute Canada ID". A sidebar on the left contains a navigation menu with links such as "Cluster Status", "Ask Support", "Get an Account", "Resources", "User Support", "News and Events", and "Organization". The "Get an Account" link in the sidebar is circled in red. The "compute+calcul CANADA" logo is visible in the main content area. The footer of the page states "This page was last modified on April 4, 2011, at 14:26."

Firefox

Get an Account - ACEnet

http://www.ace-net.ca/wiki/Get_an_Account

Search

ACEnet

Cluster Status
Ask Support
Get an Account

Resources
Compute Resources
Videoconferencing
Visualization
Software

User Support
User Guide
Job Control
Ask Support

News and Events
Cluster Status
Wavelets
Events

Organization
Partners
Governance
Personnel
ACEnet Institutes

Get an Account

Eligibility

ACEnet facilities are designated for Canadian researchers or those collaborating on Canadian research projects. Any academic researcher from a Canadian research institution who needs high performance computing to support his or her research may apply for an account on ACEnet.

Note: If you are a researcher with an organization other than a Canadian University, click [here](#) .

If you are at a Canadian university, continue with the procedure below.

How to Get an Account

Please read [Conditions of Use](#) before you decide to apply for an account.

Step 1. Get a Compute Canada ID

All eligible ACEnet users must [register with Compute Canada](#) , obtaining a Compute Canada Identifier (CCI). Faculty members must obtain a CCI before any non-faculty members of their research group (graduate students, post docs, research assistants, etc.) can register.

Step 2. Get an ACEnet Account

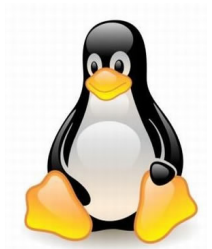
Once you have your CCI (usually takes 24-48 hours) log into the [Compute Canada Database](#)  (CCDB) and click the 'Apply' button next to ACEnet.

This page was last modified on April 4, 2011, at 14:26.

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 OS X** or **Linux**
 - ssh -X username@mahone.ace-net.ca
 - sftp username@placentia.ace-net.ca
- **Windows?** Try MobaXterm
or PuTTY and WinSCP
just google for them



Command-Line Interface



```
mahone.ace-net.ca - PuTTY
login as: rdickson
rdickson@mahone.ace-net.ca's password:
Last login: Fri Jan 11 10:58:59 2013 from rdickson-2.ucis.da

IMPORTANT: Jobs running on the head node must be less than 1
and have small memory and CPU requirements. Jobs violating t
terminated without warning. Better options for test jobs at:
http://www.ace-net.ca/wiki/Test_Jobs

rdickson@mahone: ~ $ passwd
Changing password for user rdickson.
Enter login(LDAP) password: █
```

Environment modules

```
$ module list
```

```
Currently Loaded Modulefiles:
```

```
  1) pgi/8.0-6      2) openmpi/pgi/1.2.9 ...
```

```
$ module avail
```

```
...long list...
```

```
$ module load package
```

```
$ module help
```

More at <http://www.ace-net.ca/wiki/Modules>

Where to go for help

- ACEnet web site
 - <http://www.ace-net.ca>
- ACEnet User Guide
 - http://www.ace-net.ca/wiki/User_Guide
- Research/user support personnel
 - email: support@ace-net.ca



Spring Training 2014

Basics Seminars

All same location as today. Registration requested.
<http://acenet-workshops.eventbrite.ca/>

- Intro to the Command Line
 - Thursday May 8, 12:30
- Shell Scripting
 - Tuesday May 13, 12:30
- Grid Engine
 - Thursday May 15, 12:30

Certificate of completion for those who come to all four of these basic seminars

Spring Training 2014

Focus seminars

All same location as today. Registration requested.
<http://acenet-workshops.eventbrite.ca/>

- Managing Many Jobs – May 20
- Parallel programming – May 22
 - MPI – May 27
 - OpenMP – May 29
- Make and Makefiles – June 3

A few exercises

- Change your **password**.
 - The command is **passwd**
- Find a program at ACEnet relevant to your research and load the corresponding **module**.
 - You can use either
www.ace-net.ca or
module avail
 - What version of the program do you get?
- www.surveymonkey.com/s/TXJ5Q9C