

HPC at W&M / VIMS

June 17, 2015

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HPC at W&M and VIMS is active and in constant development

About 150 total users / 50 active users in the last month

Active Departments: Physics, VIMS/CCRM, Applied Science, Math,
Biology, Psychology, Chemistry, Computer Science, ...

Consists of three clusters:

SciClone – at W&M

Storm – at Applied Research Center (Jefferson Lab)

Chesapeake – VIMS

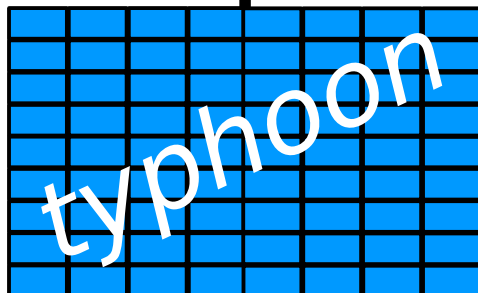
Outline

- Overview of each cluster
- Help / resources available
- Filesystems / Backup
- Linux Permissions

SciClone

.sciclone.wm.edu

Typhoon



4 cores / node
72 nodes -> 288 cores
2 or 6 GB mem / core
Opteron Santa-Rosa
DDR Infiniband

Hurricane

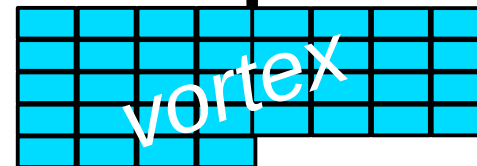


8 cores / node
12 nodes -> 96 cores
6 GB mem / core
Intel Westmere
QDR Infiniband



8 cores / node
52 nodes -> 416 cores
8 or 24 GB mem / core
Intel Westmere
QDR Infiniband

Vortex



12 cores / node
36 nodes -> 432 cores
2.7 or 10.7 GB mem / core
Opteron Seoul
FDR Infiniband

Other servers for
filesystems / backup etc.

Tornado

Gale

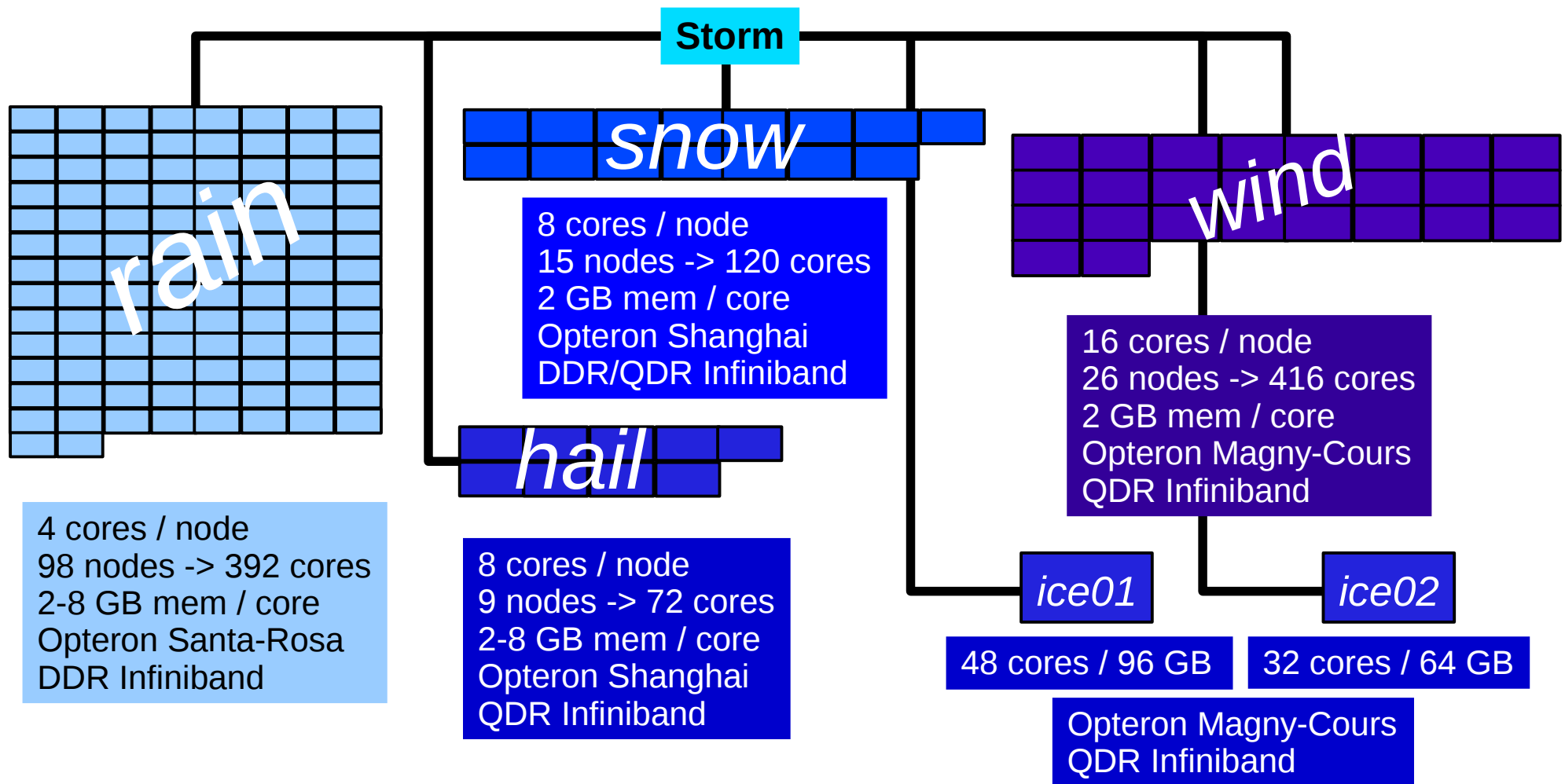
Gulfstream

Twister

- SciClone has 1232 cores total
- 2 Intel & 2 Opteron clusters
- Typhoon uses SLES 10 – rest RHEL 6.2
- Total usage for May 2015 : 74%
- *hurricane* cluster has 2xM2075 GPUs (Fermi)
- **change all passwords on Hurricane**

Storm

.hpc.wm.edu



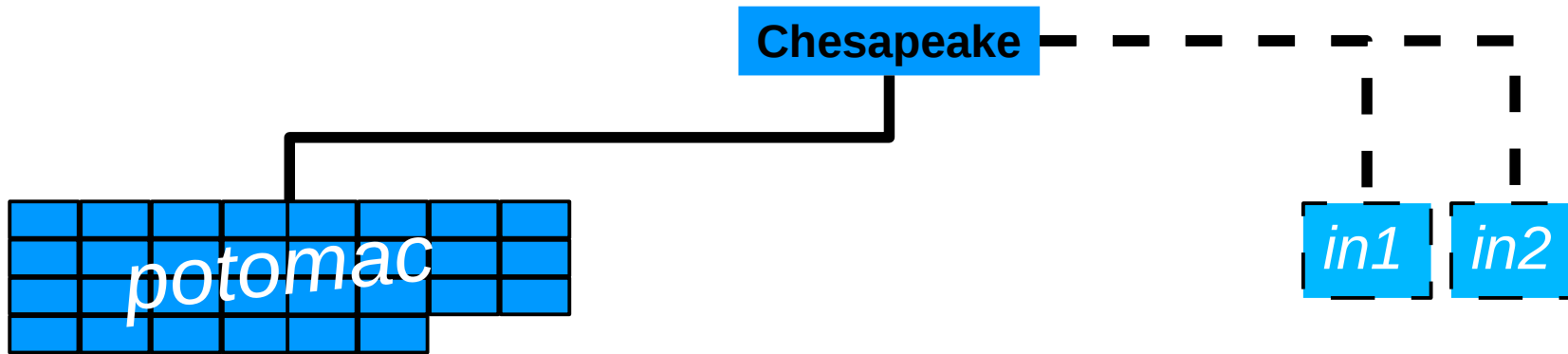
Other servers for
filesystems / backup etc.

gust

- Storm has 1080 cores total
- All Opteron
- RHEL 6.2
- Total usage for May 2015 : 67%
- Has Lustre filesystem

Chesapeake

.hpc.vims.edu



12 cores / node
30 nodes -> 360 cores
2.7 GB mem / core
Opteron Seoul
QDR Infiniband

Other servers for
filesystems / backup etc.

Rappahannock

York

Chickahominy

- Chesapeake has 380 cores total
- All Opteron
- RHEL 6.2
- Total usage for May 2015 : 32%
- Still need to incorporate Indian nodes

hpc gateway to all clusters: hpc.wm.edu

Help @ HPC

The screenshot shows a web browser window with the URL 'http://hpc.wm.edu/support'. The page title is 'it/hpc/SUPPORT ticket tracking' and it is identified as a 'SUPPORT TICKET SYSTEM'. The navigation menu includes 'Home', 'New Ticket', and 'Ticket Status'. A welcome message states: 'Welcome to the HPC support center. This is the support center for the SciClone and Storm clusters at the College of William and Mary and the Chesapeake cluster at VIMS. Please use this ticket system to submit all trouble reports, inquiries, and requests for assistance for the HPC systems only. You may also generate a support request via email to help@hpc.wm.edu. Every support request is assigned a unique ticket number which you can use to track the progress and responses online. For your reference we provide complete archives and history of all your support requests. A valid email address is required in order to access the system.'

There are two main sections:

- Open A New Ticket:** Includes a plus icon and text: 'Please provide as much detail as possible so we can best assist you. To update a previously submitted ticket, please use the form to the right.' Below this is an 'Open New Ticket' button.
- Check Ticket Status:** Includes an information icon and text: 'We provide archives and history of all your support requests complete with responses.' Below this are input fields for 'Email:' and 'Ticket#:', followed by a 'Check Status' button.

At the bottom, there is a copyright notice: 'Copyright © osTicket.com. All rights reserved' and a logo for 'osTicket Powered'.

Can submit a ticket via web or email
Used extensively by HPC group
<http://hpc.wm.edu/support>
email: help@hpc.wm.edu

Wiki

W&M IT/HPC | SciClone / SciClone Computing Complex - Mozilla Firefox

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W&M IT/HPC | SciClone / ... x W&M IT/HPC | SciClone / ... x IT/HPC Support x +

www.hpc.wm.edu/SciClone/Home

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it/hpc/SciClone

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edit SideBar

SciClone / SciClone Computing Complex



<h4>Getting Started</h4> <ul style="list-style-type: none">IntroductionAccount Request FormFrequently Asked QuestionsTutorials	<h4>Support</h4> <ul style="list-style-type: none">Help DeskUser's GuideLocal Docshpc-users Archive
<h4>Hardware</h4> <ul style="list-style-type: none">Major ComponentsCabling	<h4>Software</h4> <ul style="list-style-type: none">HPC Software Matrix
<h4>Research</h4> <ul style="list-style-type: none">HighlightsCitationsAttribution	<h4>System Status</h4> <ul style="list-style-type: none">Jobprobe: Web Start AppletNodeprobeEnvironment Power ServersIT System Status

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Page last modified on May 18, 2015, at 01:44 PM

URL: www.hpc.wm.edu/SciClone/Home

Software

W&M IT/HPC | SciClone / HPC Software Matrix - Mozilla Firefox

W&M IT/HPC | SciClone / ... x W&M IT/HPC | SciClone / ... x IT/HPC Support x

www.hpc.wm.edu/SciClone/Software

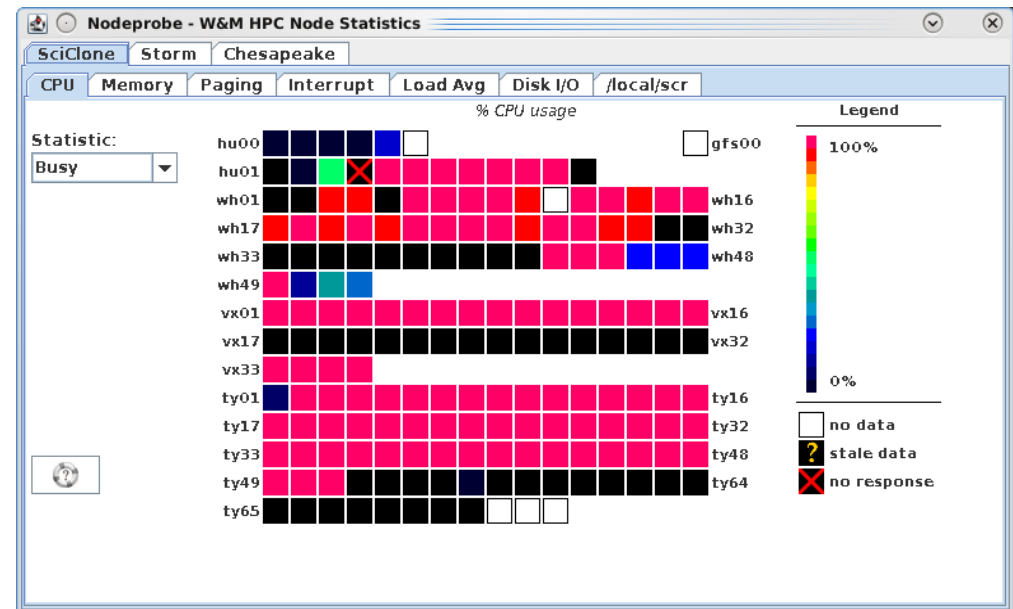
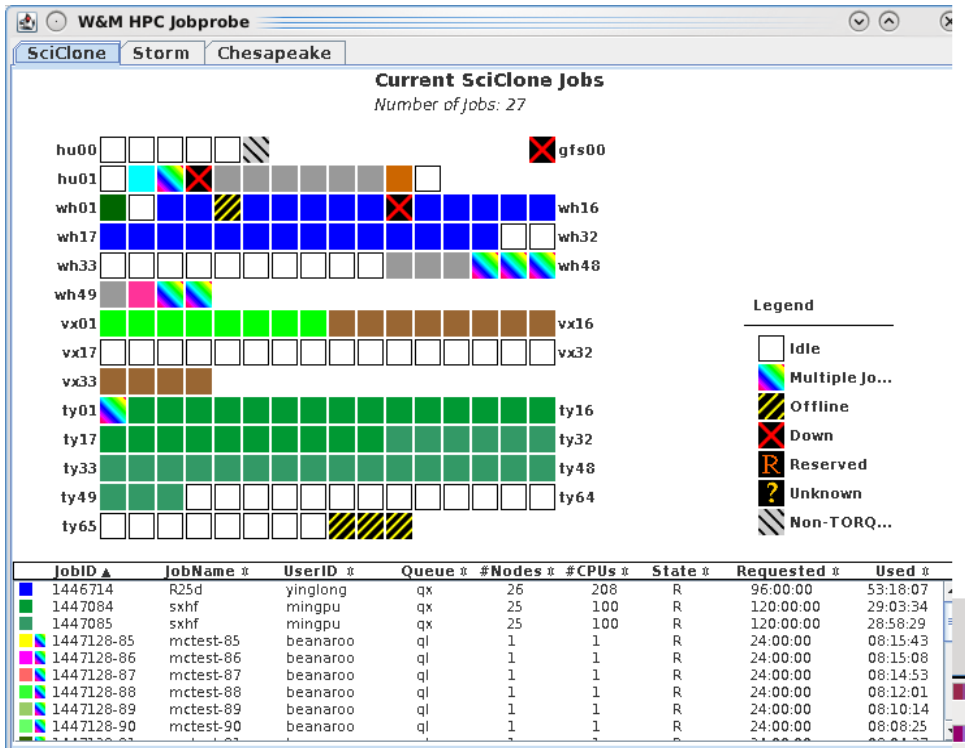
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Note: Some software packages encompass several categories; for the sake of compactness, only the most descriptive category is listed in the table.

Name/Version	Compiler	Category	typhoon	hurricane	whirlwind	vortex	potomac	rain, snow, hail, wind, ice
ACML 4.1.0	PGI	Math	X					
ACML 4.1.0	GCC	Math	X					
ACML 5.1.0	PGI	Math		X				
ACML 5.1.0	GCC	Math		X				
ACML 5.3.1	PGI	Math					X	X
ACML 5.3.1	GCC	Math					X	X
ACML 5.3.1	Open64	Math					X	X
ACRO-PICO 1.3	GCC	Math	X					
ALLPATHS-LG 4.7.0.17	GCC	Bio		X	X			
AMOS 3.1.0	GCC	Bio		X	X			
AMD APP SDK 2.9-1	GCC	Developer						(ice only)
AMPL 20090926	-	ModSim	X					
AMPL 20101125	-	ModSim	X					
Armadillo 3.920.1	GCC	Math		X	X			
ARPACK96	PGI	Math	X	X	X			
ARPACK96	GCC	Math	X	X	X			
ATLAS 3.8.3	GCC	Math	X					
AUTO-07p 0.9	GCC	Math	X	X	X			
binutils 2.19.1	-	Developer	X					
Bowtie 2.2.1.0	GCC	Bio	X	X	X			
Cairo 1.2.6	GCC	Graphics	X					
Cairo 1.10.2	GCC	Graphics	X	X	X			
Canopy 1.4.0	-	Developer						
CBLAS 03/04/2010	GCC	Math	X	X	X			
Charm++ 6.5.0	PGI	Comm		X	X			
Charm++ 6.5.0	GCC	Comm	X	X	X			
CHomP 2010-02-13	GCC	Math	X					
Circonspect 0.2.6	-	Bio		X	X			
CLoog-PPL 0.15.11	GCC	Math		X	X			
CMake 2.6.4	-	Developer		X	X			

FACT: Software is requested and installed more quickly than documentation can be written
 Submit a ticket for any software requests. Please make sure you need the software.

Jobprobe / Nodprobe



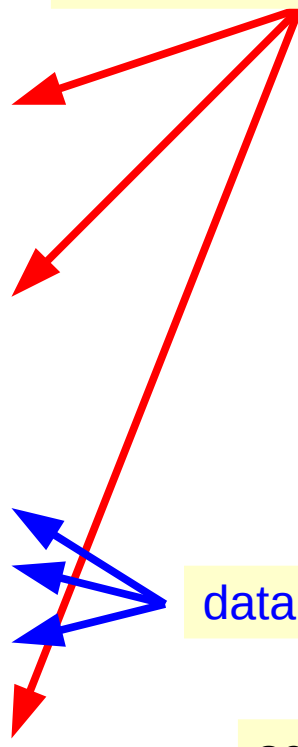
Jobprobe shows states of jobs on all three clusters
Nodeprobe show states of nodes on all three clusters
Needs java and must be run within hpc.wm.edu, hpc.vims.edu, or sciclone.wm.edu

HPC Filesystems / Backup

```
146 [hurricane] df -h
```

Filesystem	Size	Used	Avail	Use%	Mounted on
/dev/mapper/VolGroup00-LogVol00	7.9G	4.8G	2.8G	64%	/
tmpfs	7.8G	76K	7.8G	1%	/dev/shm
/dev/sda1	485M	76M	384M	17%	/boot
/dev/mapper/VolGroup00-LogVol03	7.9G	147M	7.4G	2%	/tmp
/dev/mapper/VolGroup00-LogVol02	14G	5.5G	7.7G	42%	/usr
/dev/mapper/VolGroup00-LogVol04	7.9G	1.7G	5.9G	23%	/var
/dev/mapper/VolGroup00-LogVol06	413G	7.0G	385G	2%	/sciclone/scr01
/dev/mapper/VolGroup30-LogVol31	917G	482G	390G	56%	/sciclone/home00
tn00:/usr/local	134G	113G	15G	89%	/usr/local
tn00:/export	46G	15G	30G	33%	/import
mh00:/var/spool/mail	7.9G	4.3G	3.3G	57%	/var/spool/mail
gfs00:/sciclone/home04	591G	429G	157G	74%	/sciclone/home04
ty00:/sciclone/scr02	273G	81M	273G	1%	/sciclone/scr02
tn00:/sciclone/scr10	7.9G	2.3G	5.3G	31%	/sciclone/scr10
tn00:/sciclone/scr30	17T	13T	4.7T	72%	/sciclone/scr30
gfs00:/sciclone/data10	16T	15T	1.9T	89%	/sciclone/data10
gfs00:/sciclone/vims20	26T	19T	6.7T	74%	/sciclone/vims20
tw00-i8:/sciclone/data20	73T	57T	16T	79%	/sciclone/data20
/dev/md1	8.1T	5.0T	2.8T	65%	/sciclone/scr20
vx00:/sciclone/home10	2.7T	202M	2.6T	1%	/sciclone/home10
vx00:/sciclone/scr00	318G	4.8G	297G	2%	/sciclone/scr00

home – nightly backup



data – weekly backup

scr – not backed up

Sharing Files & Folders : Permissions I

see

<https://www.nersc.gov/users/storage-and-file-systems/unix-file-permissions>
for more information

```
33 [hurricane] pwd
/sciclone/home04/ewalter
```

print working directory

```
34 [hurricane] ls -ld results
drwx----- 2 ewalter hpcf 512 Jun 16 14:37 results
```

list directory

↑
directory

┌	┌	┌	┌	┌
user	group	other	associated	associated
r-read			user	group
w-write				
x-execute				

****directories need to be 'x' to be entered/passed through**

```
35 [hurricane] ls -l results
total 3
```

list files in directory

```
-rw----- 1 ewalter hpcf 194 Jun 16 14:37 ww.dat
-rw----- 1 ewalter hpcf 194 Jun 16 14:37 yy.dat
-rw----- 1 ewalter hpcf 194 Jun 16 14:37 zz.dat
```

Sharing Files & Folders : Permissions II

I want to share my results directory and files with those in the *seadas* group:

Am I in the seadas group?:

```
46 [hurricane] groups ewalter
ewalter : hpcf wmall hpcstaff www seadas vasp wm sysadmin hpcadmin hpsmh
```

Change the group for the directory and all files below:

```
47 [hurricane] chgrp -R seadas results/
```

```
49 [hurricane] ls -ld results/
drwx----- 2 ewalter seadas 512 Jun 16 14:37 results/
```

```
50 [hurricane] ls -l results/
total 3
-rw----- 1 ewalter seadas 194 Jun 16 14:37 ww.dat
-rw----- 1 ewalter seadas 194 Jun 16 14:37 yy.dat
-rw----- 1 ewalter seadas 194 Jun 16 14:37 zz.dat
```

Make:
files group readable
folders group readable **and** executable

```
51 [hurricane] chmod g+rX -R results/
```

```
52 [hurricane] ls -ld results/
drwxr-x--- 2 ewalter seadas 512 Jun 16 14:37 results/
```

```
53 [hurricane] ls -l results/
total 3
-rw-r----- 1 ewalter seadas 194 Jun 16 14:37 ww.dat
-rw-r----- 1 ewalter seadas 194 Jun 16 14:37 yy.dat
-rw-r----- 1 ewalter seadas 194 Jun 16 14:37 zz.dat
```

Sharing Files & Folders : Permissions III

What happens when a new file is created?

```
78 [hurricane] cd results/
80 [hurricane] touch newfile
81 [hurricane] ls -l
total 3
-rw----- 1 ewalter hpcf      0 Jun 16 15:13 newfile
-rw-r----- 1 ewalter seadas 194 Jun 16 14:37 ww.dat
-rw-r----- 1 ewalter seadas 194 Jun 16 14:37 yy.dat
-rw-r----- 1 ewalter seadas 194 Jun 16 14:37 zz.dat
```

This is bad since the new file isn't in the seadas group!

```
88 [hurricane] chmod g+s results/   add "setgid" to folder only
89 [hurricane] cd results/
```

```
91 [hurricane] touch newfile
92 [hurricane] ls -l
total 3
-rw----- 1 ewalter seadas    0 Jun 16 15:14 newfile
-rw-r----- 1 ewalter seadas 194 Jun 16 14:37 ww.dat
-rw-r----- 1 ewalter seadas 194 Jun 16 14:37 yy.dat
-rw-r----- 1 ewalter seadas 194 Jun 16 14:37 zz.dat
```

file group inherits the group from the folder it is in

Sharing Files & Folders : Permissions IV

The user's **umask** controls what permissions files and folders are given when created:

```
93 [hurricane] umask
77

135 [hurricane] touch file077
136 [hurricane] ls -l file077
-rw----- 1 ewalter seadas 0 Jun 16 15:24 file077

137 [hurricane] umask 022
138 [hurricane] touch file022
139 [hurricane] ls -l file0*
-rw-r--r-- 1 ewalter seadas 0 Jun 16 15:24 file022
-rw----- 1 ewalter seadas 0 Jun 16 15:24 file077

140 [hurricane] umask 027
141 [hurricane] touch file027
142 [hurricane] ls -l file0*
-rw-r--r-- 1 ewalter seadas 0 Jun 16 15:24 file022
-rw----- 1 ewalter seadas 0 Jun 16 15:24 file027
-rw----- 1 ewalter seadas 0 Jun 16 15:24 file077
```

HPC default umask is **077**

Can be changed in your startup file (.cshrc etc.)

QUESTIONS?