Scarf

Guide to running simulations for DLS Spectroscopy

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Access to Scarf

Login: ssh -Y fedid@ui1.scarf.rl.ac.uk

- ssh: secure shell, log in to a remote machine (scarf)
- -Y: X11 forwarding, access graphical interfaces
- fedid: Federal ID and username to access scarf
- ui1.scarf.rl.ac.uk: host address

Places on SCARF

Name	Location	Description
Home	$HOME	80 GB, weekly back up
Scratch	/scratch/	Area for simulations (not recommended, randomly purged)
	/scratch21/	Area for simulations (not recommended, randomly purged)
Work	/work4/dls/	Area for simulations (recommended not backed up)

Useful Commands 1

Bash

Command	Description
Files	
ls -ltrh	list directory, list format
cat	display contents of file
cd	change to home directory
cd ../	change to upper directory
cd */path/*	change to specific directory path
cp.	copy file a to b
cp -r	copy recursively a to b (folders)
mkdir	make a directory
mv	move folder a to b
rm	remove a file
rm -r	remove recursively (deleting folders)
Batch Jobs	
sbatch job.sh	submit job.sh to scheduler
squeue	display full queue
squeue -u scarfxxxx	display user xxxx queued jobs
scancel xxxxx	cancel job xxxxx
Modules	
module list	list loaded modules
module avail	list available modules
module load	load module
module purge	clear all loaded modules
module show	display module information
Git	
git add	add files/folders to committed
git branch	display all branches
git checkout	checkout a branch
git checkout -b	create a branch and checkout
git clone	clone a repository
git commit -m	package changes
git pull	update local branch
git push --set-upstream origin	update remote branch
git status	show changes

Useful Commands 2

vim

Getting Started with Quantum Espresso 1

Steps to running Quantum Espresso on SCARF for the first time

Make directory for simulations

Make a directory under work4 and create a symbolic link in home directory to access.

- cd /work4/dls
- mkdir $fedid
- cd
- ln -s /work4/dls/$fedid .

Obtain example files

Create a folder for example simulations and download the example files directly from the github repository.

- cd $fedid
- mkdir test
- cd test
- git clone https://github.com/jodaelliott/XSpectra-CONEXSworkshop2022.git
- cd XSpectra-CONEXSworkshop2022

Getting Started with Quantum Espresso 2

Steps to running Quantum Espresso on SCARF for the first time

Load modules for simulations and plotting

Search and load Quantum Espresso (pw.x, xspectra.x) and xmgrace modules for simulations and plotting the results.

- module avail espresso
- module load contrib/dls-spectroscopy/quantum-espresso/6.5-intel-18.0.3
- module avail grace
- module load xmgrace/5.1.25
- module list

Run first calculations

Execute diamond.scf.in and diamond.xspectra.in by editing job.sh file and using upf2core.sh script

- cd 01_Diamond
- sbatch job.sh
- squeue -u scarfxxxx
- vi job.sh; edit input=diamond.xspectra and mpirun command to xspectra.x
- ../tools/upf2plotcore.sh ../pseudopotentials/C_PBE_TM_2pj.UPF > C.wfc
- sbatch job.sh
- xmgrace xanes.dat