MBB KI

PSF Xray Newsletter 6

Quarter 3, 2015

Martin Moche

8/31/2015

Contents

How to save wall time and core hours at NSC Triolith 2

Max IV and NSC collaboration 3

PSF software updates 2015 4

MiTeGen in-Situ-1 available at PSF 4

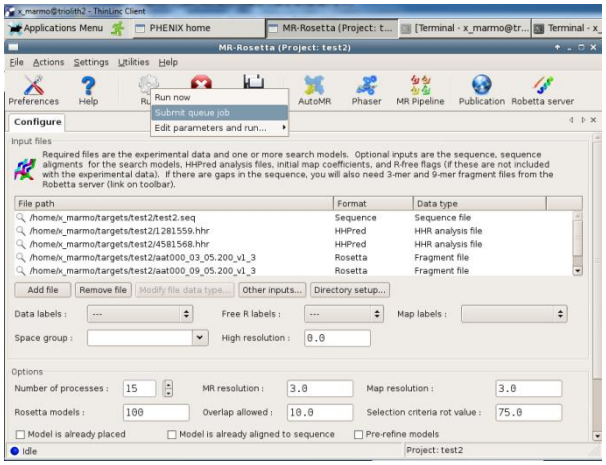
The ambition of this newsletter is to create a simple summary of current actions and issues taking place at PSF Xray instead of sending out several emails.

How to save wall time and core hours at NSC Triolith

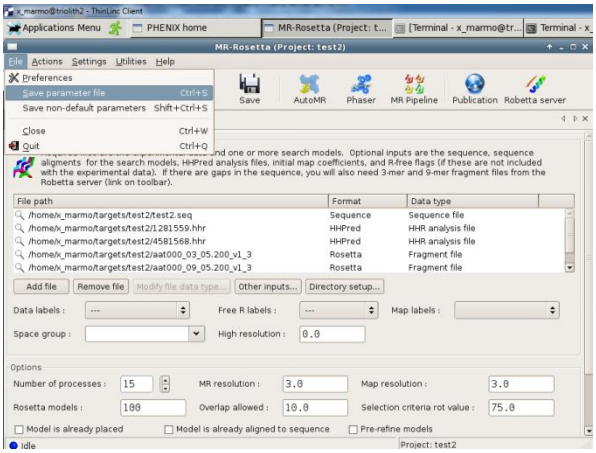
Please share your ideas on how to housekeep/optimize NSC Triolith usage and find some startup tips below:

A) When possible use phenix instead of ccp4 since the phenix-GUI can be run at the login node and all jobs submitted to compute nodes using “submit queue job” or sbatch followed by automatic “exit” from the compute node saving compute time. In contrast when using ccp4 we are forced to estimate some “extra time” on an interactive node to enable our jobs to finish followed by manual “exit” in the terminal window to save compute time – not efficient.

B) Frequently many phenix GUI wizards do not enable “submit queue job” for instance “MRage-automated pipeline” and “Rosetta refinement (alpha)”. In these instances you can save a parameter file and execute a sbatch to submit jobs to the Triolith queue. Examples for MRage and rosetta_refine are given below. The drawback with the sbatch command is that logfiles does not enter the phenix GUI.



Submit queue job not always possible



Save parameter file instead for sbatch

Example rosetta_refine

%sbatch rosetta_refine.script

where rosetta_refine.script is:

#!/bin/bash
#SBATCH -t 168:00:00
#SBATCH -N 1
#SBATCH --mail-type=ALL
module load proj/xray
module load phenix/1.10-2148
phenix.rosetta_refine rosetta_refine_1.eff

Example MRage

%sbatch MRage.script

where MRage.script is:

#!/bin/bash
#SBATCH -t 168:00:00
#SBATCH -N 1
#SBATCH --mail-type=ALL
module load proj/xray
module load phenix/1.10-2148
phenix.mrage mr_pipeline_1.eff

C) Use parallel software such as phenix.MRage for phaser molecular replacement and xds_par for data processing.

Package	phenix	phenix	ccp4
Phaser variant	phenix.mrage	phenix.phaser	phaser
Start job from GUI	No -> sbatch Mrage.script	Yes -> submit queue job	Yes
Resource allocation where?	within Mrage.script	Preferences-Processes	In terminal window
Allocation example	sbatch -N1 -t 96:00:00 --mail-type=ALL	sbatch -N1 -t 96:00:00 --mail-type=ALL	interactive -N1 -t 96:00:00
Time allocated above	96 hours	96 hours	96 hours
Allocation auto-terminated	Yes => compute time saved	Yes => compute time saved	No => manual exit required
# processors allocated	16	16	16
# processors used	16	2	2
# processors not used	0	14	14
Comment	Good – fast & no waste	Bad - 14 proc. not used	Worst - 14proc&time lost

Table 3. Good and bad ways of running phaser at NSC Triolith

Unfortunately we are frequently using the most wasteful way of running phaser at NSC Triolith today being phaser started from an interactive node running ccp4i. When allocating an entire node with 16 processors and then use only 2 for phaser, we waste 7 times the computing time used for each phaser job submitted and additional compute time if using ccp4 on an interactive node not performing "exit" once finished.

We collectively need to learn how to housekeep computing resources at NSC Triolith since overspending as now (July 2015) make it difficult to acquire an interactive node and low priority for all our jobs in the queue https://www.nsc.liu.se/support/batch-jobs/triolith/

Our pilot allocation is unfortunately too small for molecular dynamics simulations and research groups that want to perform molecular dynamics simulations such as Chemistry II and Medical Inflammation Research have already applied or being instructed to apply for their own NSC Triolith allocation at https://supr.snic.se/ while the pilot project limits itself to MX calculations.

Max IV and NSC collaboration

Max IV has shown interest in collaborating with SNIC regarding user authentication and data management at the upcoming beamlines. NSC wrote an application to make this pilot project a MaxIV satellite, the application was granted and negotiations are currently ongoing regarding the details. Max IV is now supporting NSC with some financial resources with in-kind contribution from the MX community.

PSF software updates 2015

PSF recently upgraded its computers into 64-bit Scientific Linux 6 (nemo and donald) and 32-bit Scientific Linux 6 (daffy). Nemo and Donald computers now require 64-bit software settings available under "Protein crystallography software" at http://ki.se/en/mbb/protein-crystallography-platform.

The new 64-bit settings file https://kiedit.ki.se/node/44211 could be copied into settings.txt and sourced after login to PSF computers ($ source settings.txt) and you are then ready to use the following software at PSF donald and nemo computers: https://kiedit.ki.se/node/44212 .
The old 32-bit settings files currently hold by PSF software users are no longer functional except at the daffy computer and the 32-bit software platform http://psf.ki.se/Xray/PSF_Xray_Software_2013.html will not be further updated.

MiTeGen in-Situ-1 available at PSF

In request from Joseph Brock at Chemistry 2 we are now started to define MiTeGen in-Situ-1 at PSF robotic setup. MiTeGen in-Situ-1 can be directly mounted at synchrotron beamlines such as Diamond i03, i24 and i04-1 (http://www.diamond.ac.uk/Beamlines/Mx/Equipment-on-Demand/In-situ-Data-Collection.html) and more information regarding the plate is found at MiTeGen homepage (http://www.mitegen.com/mic_catalog.php?c=insituplates).

MiTeGen in-Situ-1 appears to be a sitting drop plate, however can be used as a hanging drop plate as well simply by inverting it, i.e. turning it upside-down, as indicated in the figure 1 below. The sitting and hanging drop MiTeGen in-Situ-1 plate have separate names in RockMaker as

- 96 MiTeGen 2 drop In-Situ-1 (sitting drop)
- i96 MiTeGen 2 drop In-Situ-1 (hanging drop)

For imaging of MiTeGen in-Situ-1 we use "drop location" instead of a fixed drop since the drop well is flat and drop position might vary.

A1.....A12 Sitting drop
.....
.....
H1.....H12

should become

H1.....H12 Hanging drop
.....
.....
A1.....A12

Figure 1. For imaging to work properly the plate need to be rotated along the row when flipped over into hanging drop mode. For the hanging drop plate imagers are calibrated to find A1 drop 1 in the bottom left corner instead of top left during sitting drop.
The barcode should be placed at the column 12-side for the inverted hanging drop plate as for sitting drop plates.

From a single MiTeGen 2 drop In-Situ-1 plate filled with JCSG+ screen and Lysozyme protein two example experiments called “96 MiTeGen 2 drop In-Situ-1” (sitting drop) and “i96 MiTeGen 2 drop In-Situ-1” (hanging drop, inverted) was made available in RockMaker under: SGC Core Xray/Moche/TestExpe to show that the same drops were imaged in both sitting and hanging drop mode.

The first Phoenix and Mosquito “standard protocol” and plates created with this plate are called:

- Phoenix: Mosquito 1 MiTeGen In-Situ-1
- Mosquito: 96 well MiTeGen in-Situ-1

In the standard Phoenix protocol the default volume transfer to the well is 35 ul since MiTeGen in-Situ-1 holds maximum 40 ul well solution. In the standard Mosquito protocol the default drop volumes have been set to:

- drop 1: 0.15 + 0.15 ul (well + protein)
- drop 2: 0.20 + 0.10 ul (well + protein)

Changes to the initial “standard protocols” will occur once we know how to run this plate optimally.