

CCPEM computational needs workshop, and review of computational needs survey – by Alan Roseman

All are encouraged to attend. (Friday 29th May, 1pm-2pm)

Background:

As Tom explained, CCP-EM is developing a software framework. It is assimilating existing software packages and accepting contributions from developers (the CCP4 model).

e.g. MRC suite packages, mrc image software library, FlexEM, DockEM, FindEM.

Provide tools to link-up existing packages.

Exchange of “jiffy” / glue programs,

e.g. transform angles coordinates from one program’s convention to another.

We do have a good idea of what is needed, but would like a community view, not to leave something out.

What needs to be linked up?

Therefore the survey:

Present survey results:

All use computers,

Linux o/s

Clusters are big a feature

Identifying computational needs

Panel discussion

Identify topics where CCP-EM can help.

Might have some answers.

Aim: Identify a few topics for online user community discussion forum.

Any suggestions....

CCP-EM activities

1. Community: meetings etc.
2. Education and training
3. Support for developers
4. Software suite

Possible topics for CCP-EM forums/discussions

Ideas for projects:

Database for tomography and/or subtomogram averages

Virtual machine/iso/some delivery of working software system.

Keep track of workflows.

Specific software issues:

Graphic cards problems. Problems with drivers or Cuda versions.

General topics and ideas for ccpem to help on:

General/specific advice

Contact point

Packages need frequent updating in this fast moving field.

Advise on hardware purchases.

Advice on negotiating with local IT departments on computing requirements, hardware and configuration.

Training courses

Wiki workshops, downloadable guides/primers.

Specify a recommended OS and standard set up for a new lab. i.e. similar to a ccpem local system so best support can be provided.

Cloud computing advice and help. Forums. Scripts exchange?

Possible topics for primers, notes or introduction courses

Setting up group working

Background of file systems

Mounting external file systems

Remote working tools

Data Security

Intro to sys admin, or how to talk "sys admin language".

3D screens

Python scripting course

Conclude with panel discussion