The CCP1GUI

NWGrid Training Event
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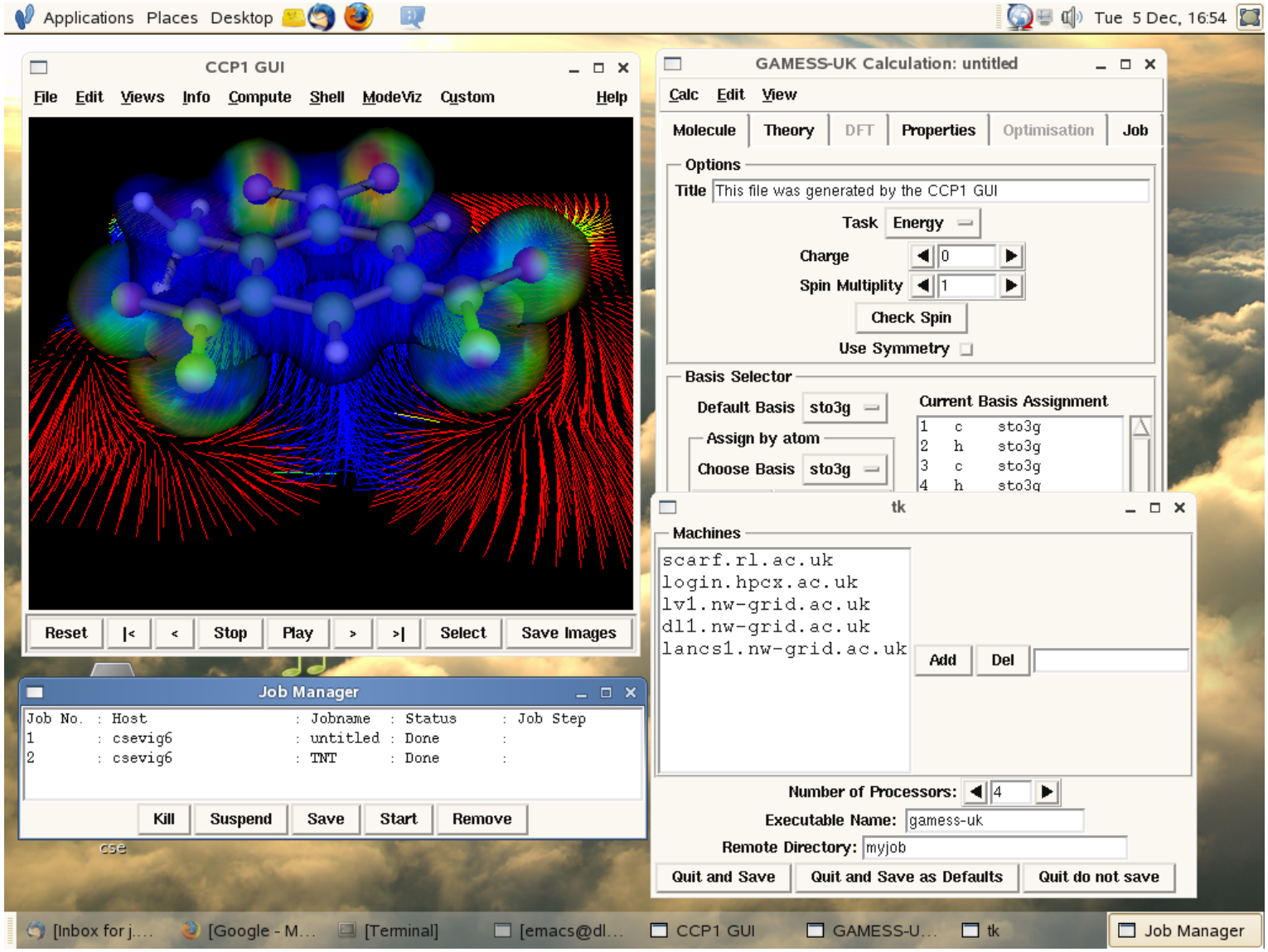
Overview

- A free graphical interface for a range of Computational Chemistry codes (GAMESS-UK, Dalton, Molpro, etc.)
- Written in Python so a very quick development cycle, and the code can be customised by the users.
- Powerful visualisation capabilities based on VTK (viewers for molecules, scalar and vector data – some in 3D!).
- Runs on any operating system that supports Python/VTK, which is pretty much anything (even AIX!).
- Recent developments allow the to CCP1GUI to submit remote jobs to Grid resources. Have centred on NW-Grid, but can also submit to Nordugrid or an eMinerals setup.

The CCP1GUI in action



Aims

- Provide a single environment to run multiple codes.
- High-quality graphics to enable expert and novice users to easily extract as much information from their calculations as possible.
- Encourage external groups and developers to get involved and develop functionality that is useful to them and others in their field.
- Released under the GPL and hosted on Sourceforge:

  http://sourceforge.net/projects/ccp1gui

CCP1GUI and the Grid

- Grid computing resources are becoming increasingly available and have the potential to deliver powerful computing resources to a user's desktop.
- The CCP1GUI provides a reasonably transparent and consistent way of accessing a range of local and remote resources.
- We have interfaces to Globus (VDT,Growl…), Nordugrid and eMinerals infrastuctures.
- This is very much developmental software – please let us know what you think and how we could make this more useful for you.

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