

The CCP1GUI



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



The screenshot displays the CCP1 GUI interface on a Linux desktop. The main window, titled "CCP1 GUI", shows a 3D molecular model of a complex organic molecule with isosurface electron density plots. Below the model are controls for "Reset", navigation arrows, "Stop", "Play", "Select", and "Save Images".

The "GAMESS-UK Calculation: untitled" window is open, showing calculation parameters:

- Task: Energy
- Charge: 0
- Spin Multiplicity: 1
- Check Spin button
- Use Symmetry checkbox (unchecked)

The "Basis Selector" section shows:

- Default Basis: sto3g
- Current Basis Assignment table:

Atom No.	Element	Basis
1	c	sto3g
2	h	sto3g
3	c	sto3g
4	h	sto3g

The "tk" window shows a list of machines for job distribution:

- scarf.rl.ac.uk
- login.hpcx.ac.uk
- lv1.nw-grid.ac.uk
- dl1.nw-grid.ac.uk
- lanes1.nw-grid.ac.uk

Additional controls include "Add", "Del", "Number of Processors" (set to 4), "Executable Name" (gamsess-uk), and "Remote Directory" (myjob).

The "Job Manager" window displays a table of running jobs:

Job No.	Host	Jobname	Status	Job Step
1	csevig6	untitled	Done	
2	csevig6	TNT	Done	

Buttons for "Kill", "Suspend", "Save", "Start", and "Remove" are available at the bottom of the Job Manager window.

- 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 infrastructures.
- This is very much developmental software – please let us know what you think and how we could make this more useful for you.