Computational chemistry with ECCE on EGEE grids

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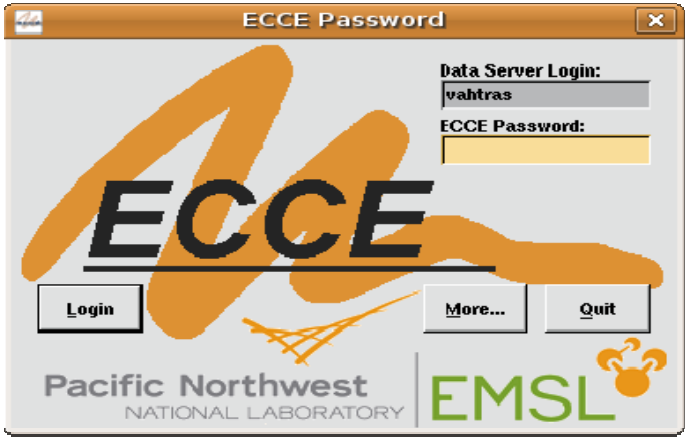
KTH

www.eu-egee.org

e-infrastructure

- **Extensible Computational Chemistry Environment**
  - A complete environment for defining, submitting, storing and analyzyng computational chemistry calculations
    - GUI
    - Compute servers
    - Data servers



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e-infrastructure

About ECCE

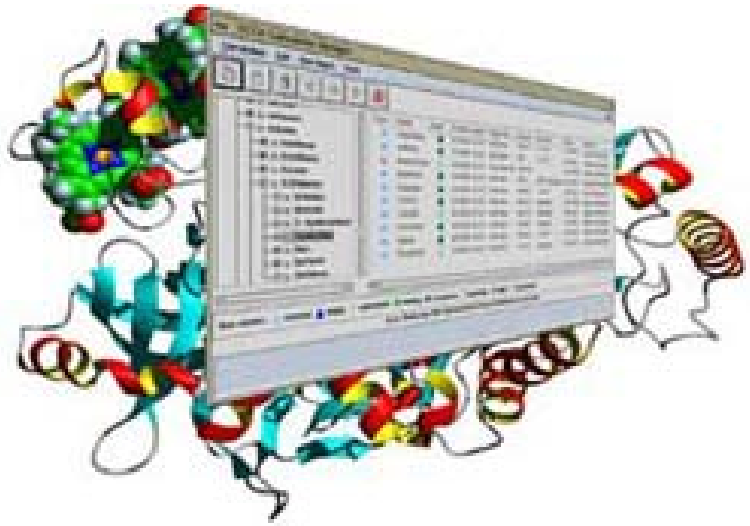
- Developed by PNNL
- Supported on Linux, SGI, Sun
- Free of use for academic users
- Support for NWChem, Gaussian98, Gaussian03, Gamess-UK,Amica
- Written in C++
- X Windows Motif toolkit
- OPENGL graphics

Main panel

- **Organizer**
- **Builder**
- **Viewer**
- **Machine browser**
- **Periodic table**

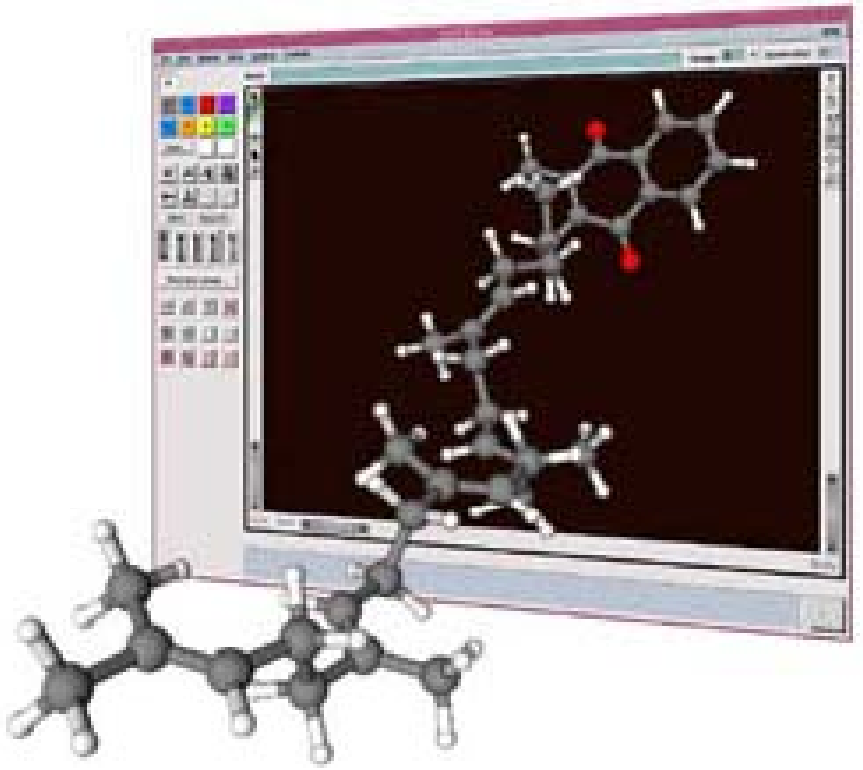
Organizer

- Organizer summarizes projects and calculations in a “file manager” view
- Information is stored on a data server (apache server with a Web-DAV) interface
- Color-coded status of calculations (ready, running, finished, error)



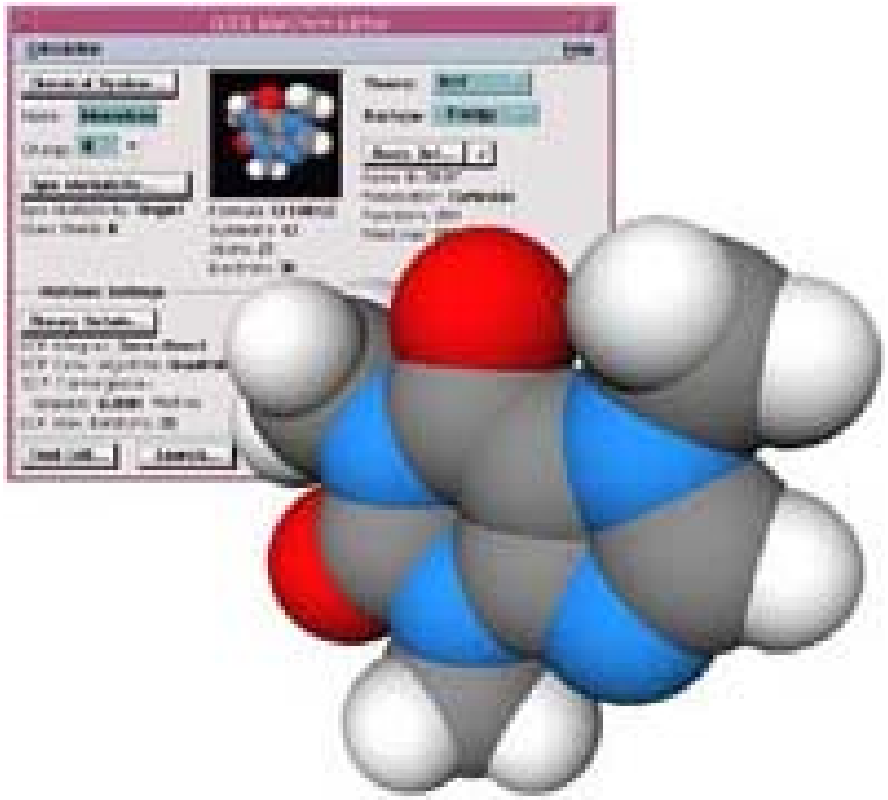
Builder

- **Builder: compose molecular system from atoms or molecular building blocks from the Structure library**
- **Initial structure from simple molecular mechanics or user input**
- **Gaussian and NWChem calculations can be imported**



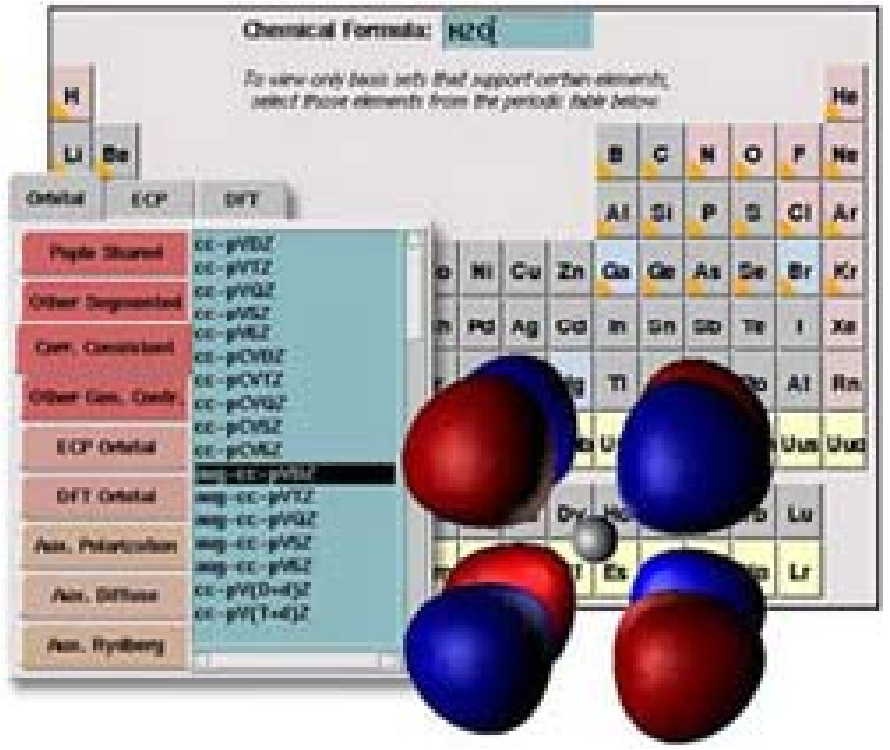
Editor

- Define charge, multiplicity basis set
- Choose basis set from a basis set library
- Define method (HF, DFT)
- View generated input file
- Launch calculation



Basis set library

- **Choose basis set for all atoms or different basis set for different atom types**

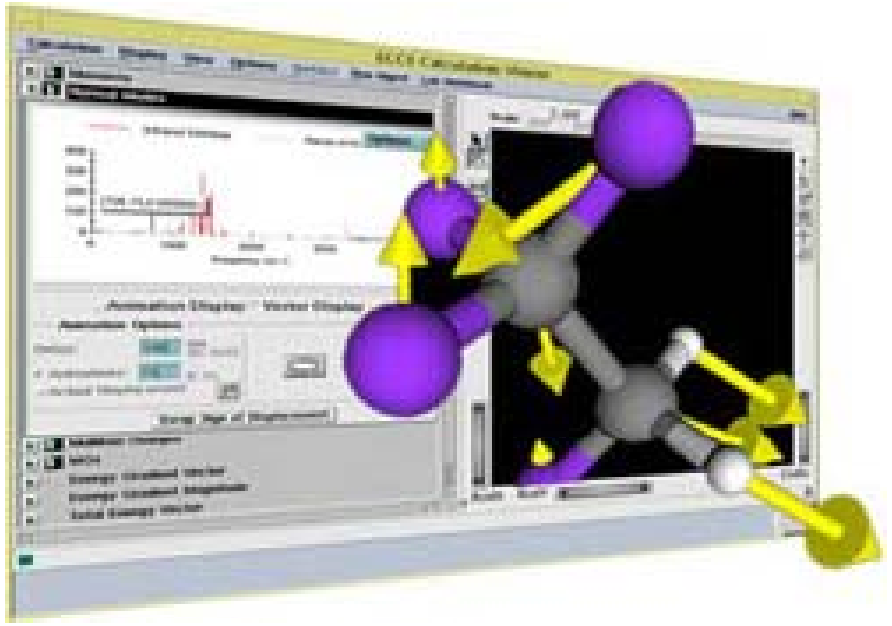


Launcher

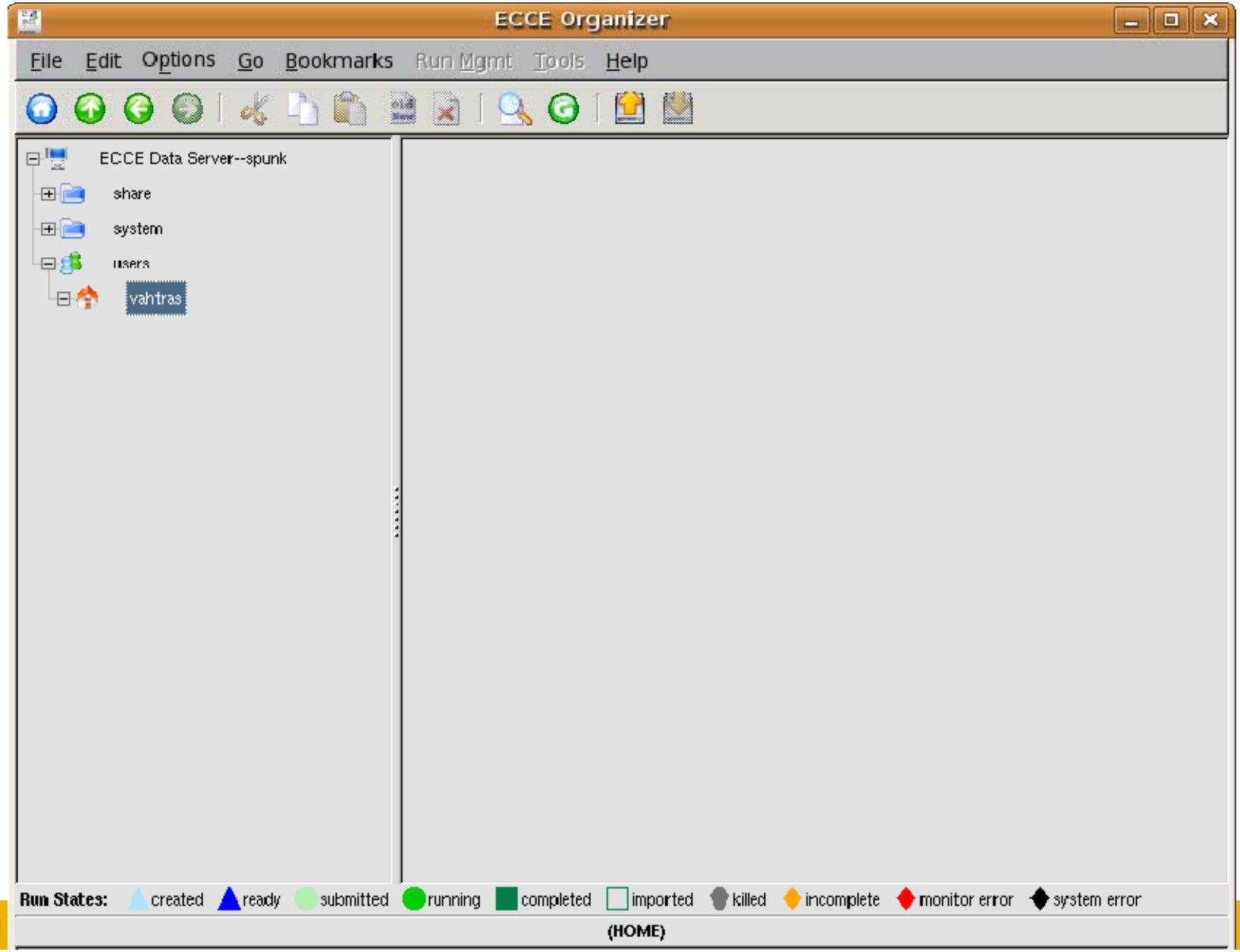
- **Select machine where the calculation is to run**

Viewer

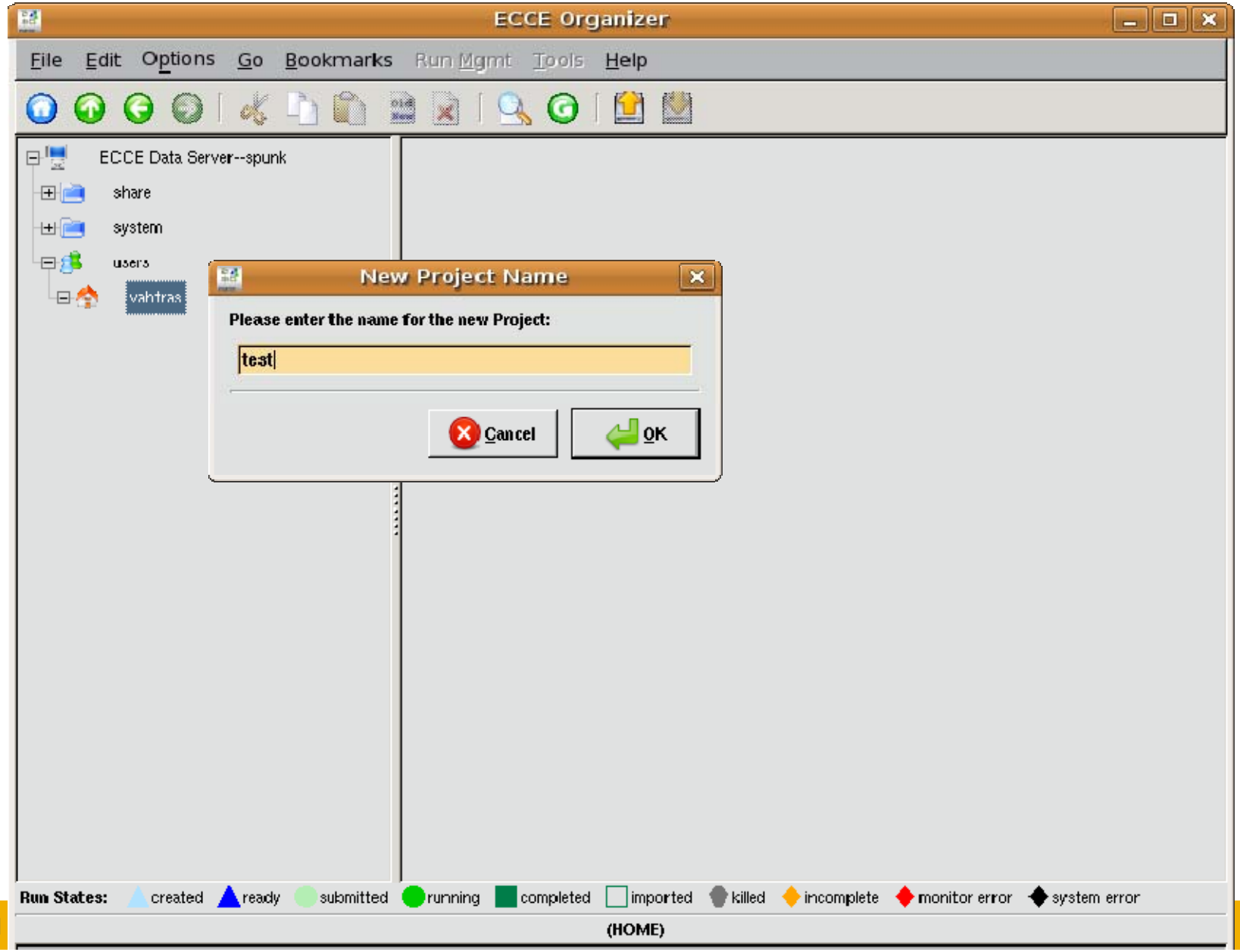
- Graphical presentation of final result
- Geometry
- Forces
- Electron density
- Orbitals
- Convergence graph



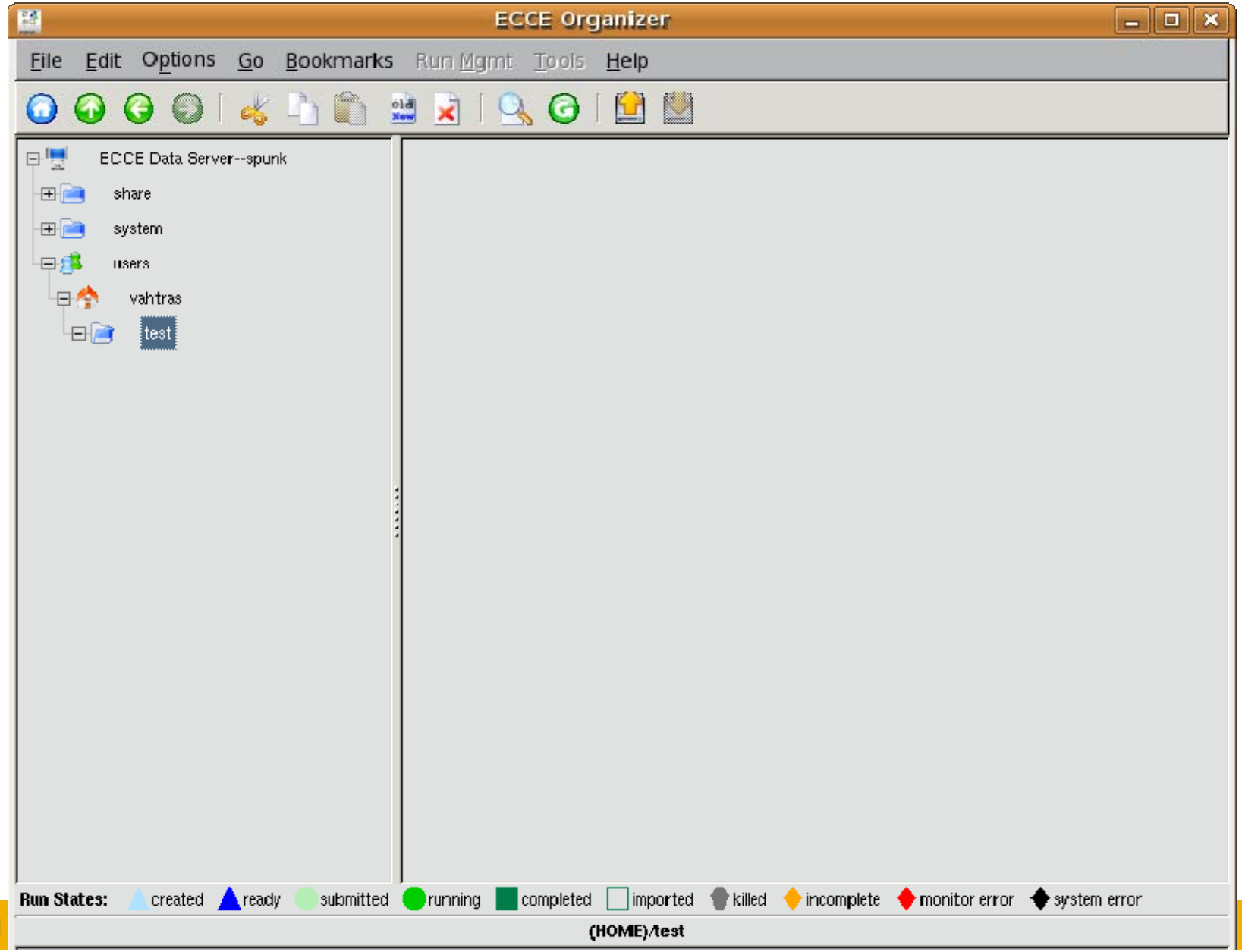
Example


ECCE Organizer
File Edit Options Go Bookmarks Run Mgmt Tools Help
ECCE Data Server--spunk
share
system
users
vahtras
Run States: created ready submitted running completed imported killed incomplete monitor error system error
(HOME)

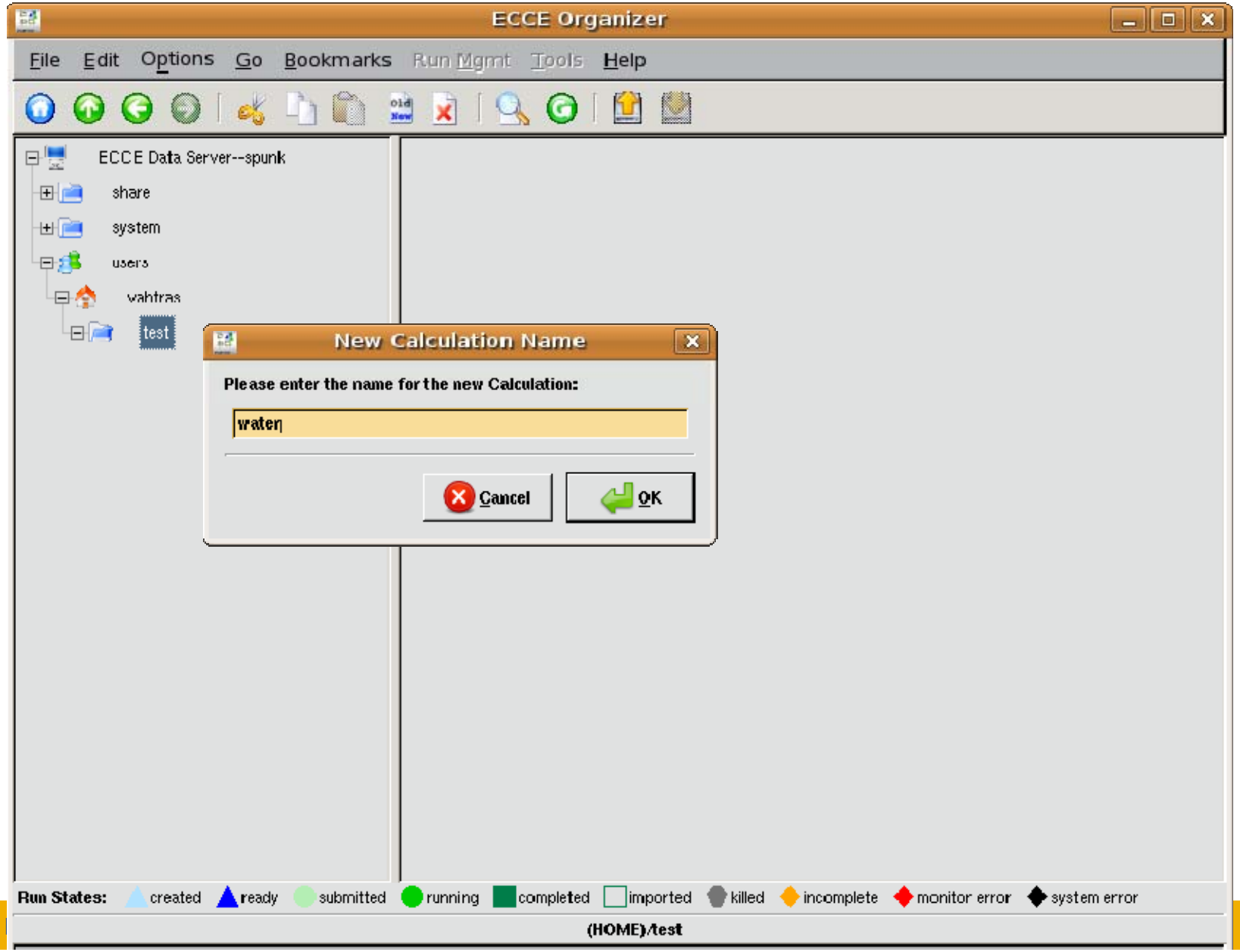
Example


ECCE Organizer
File Edit Options Go Bookmarks Run Mgmt Tools Help
ECCE Data Server--spunk
share
system
users
vahtras
New Project Name
Please enter the name for the new Project:
test
Cancel
OK
Run States: created ready submitted running completed imported killed incomplete monitor error system error
(HOME)

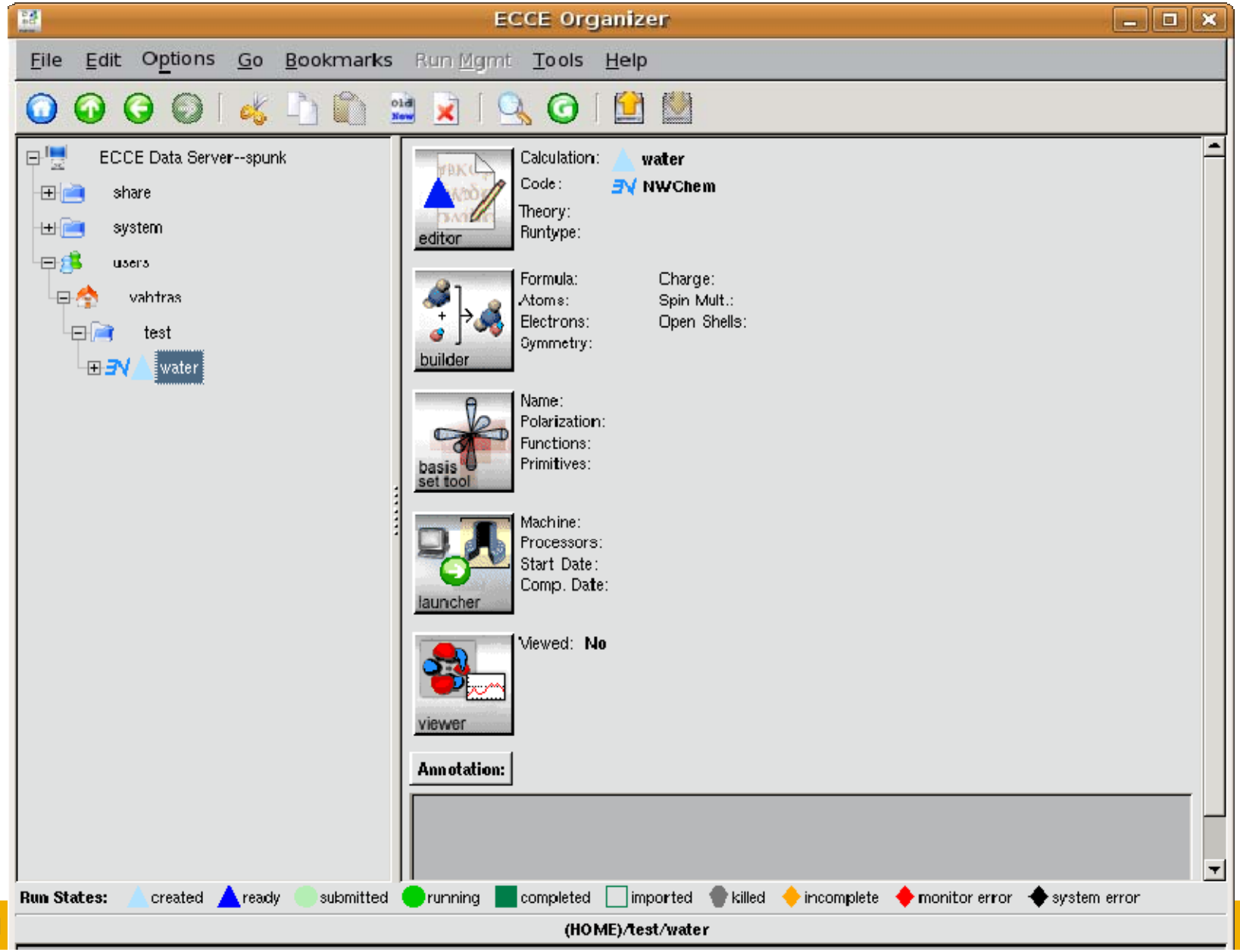
Water


ECCE Organizer
File Edit Options Go Bookmarks Run Mgmt Tools Help
ECCE Data Server--spunk
share
system
users
vahtras
test
Run States: created ready submitted running completed imported killed incomplete monitor error system error
(HOME)/test

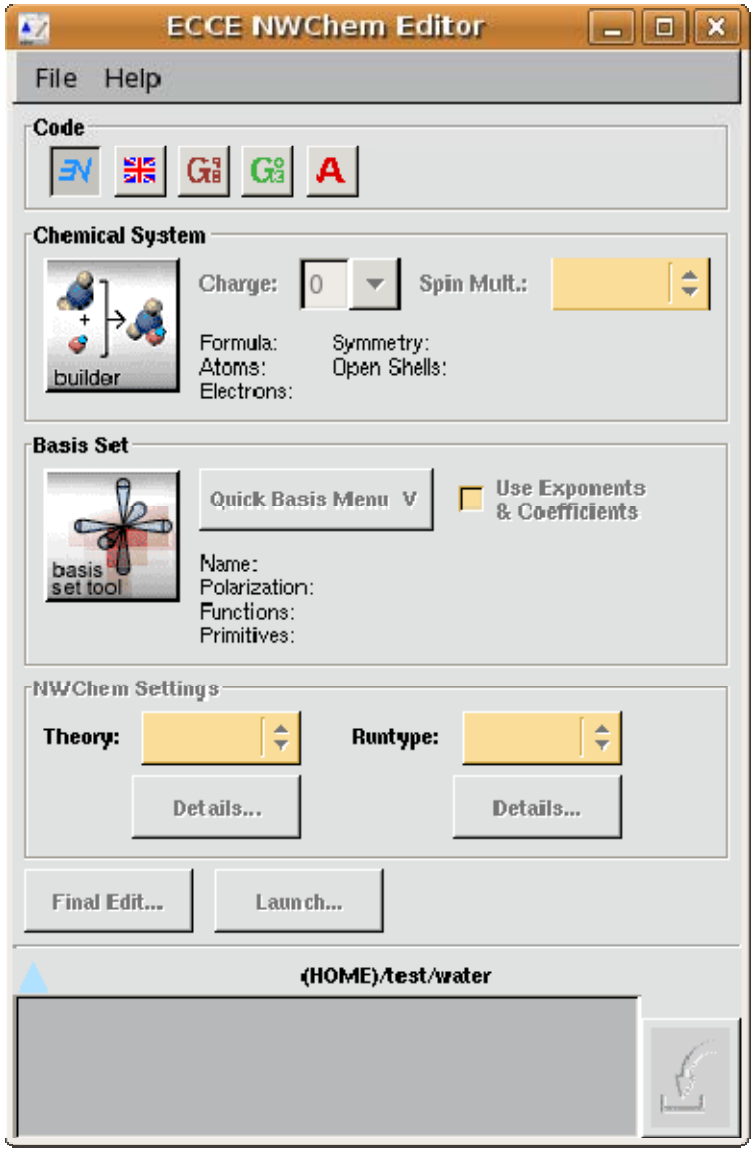
Water


ECCE Organizer
File Edit Options Go Bookmarks Run Mgmt Tools Help
ECCE Data Server--spunk
share
system
users
vahtras
test
New Calculation Name
Please enter the name for the new Calculation:
water
Cancel
OK
Run States: created ready submitted running completed imported killed incomplete monitor error system error
(HOME)/test

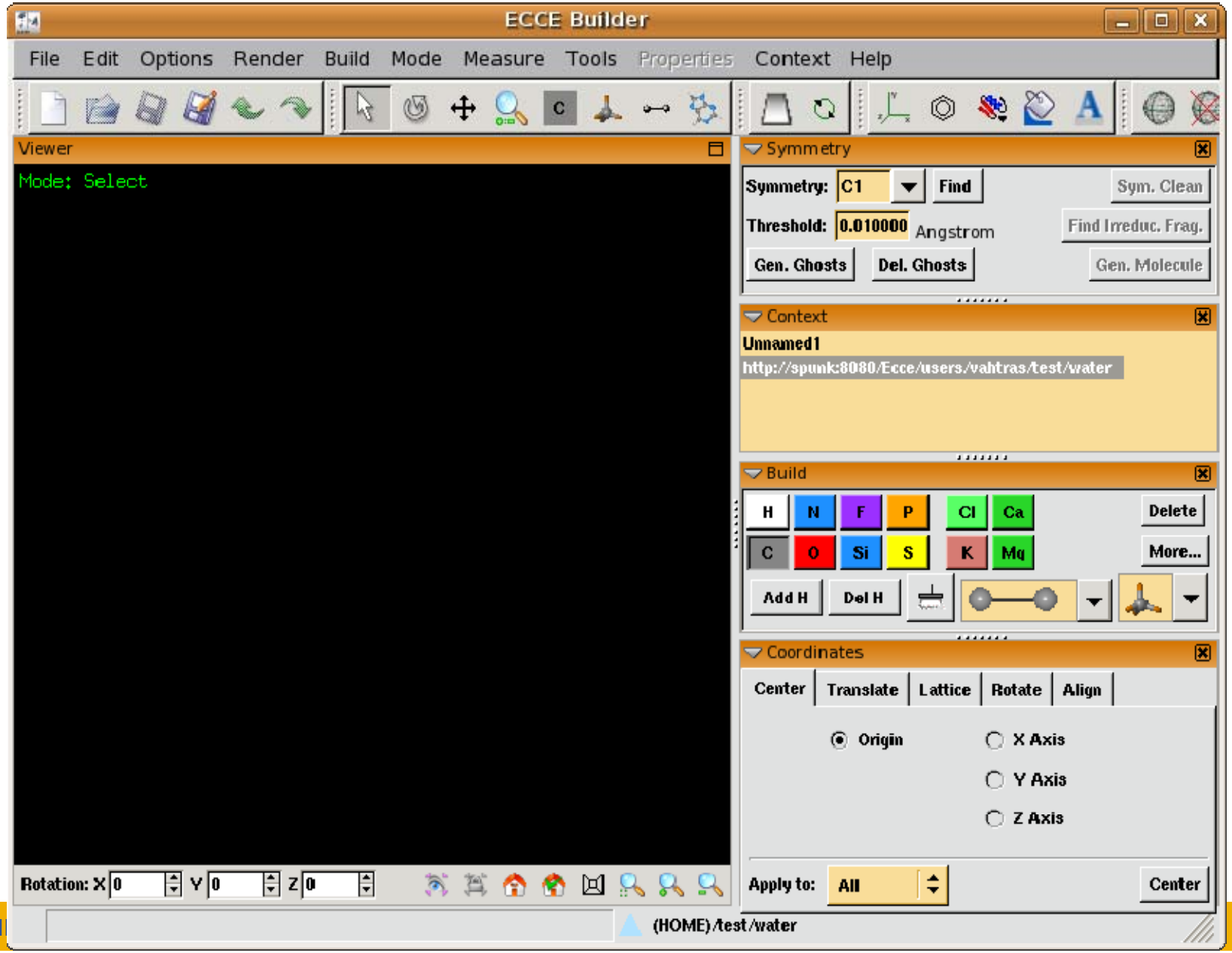
Water


ECCE Organizer
File Edit Options Go Bookmarks Run Mgmt Tools Help
ECCE Data Server--spunk
share
system
users
vahtras
test
water
editor
Calculation: water
Code: NWChem
Theory:
Runtype:
builder
Formula:
Atoms:
Electrons:
Symmetry:
Charge:
Spin Mult.:
Open Shells:
basis set tool
Name:
Polarization:
Functions:
Primitives:
launcher
Machine:
Processors:
Start Date:
Comp. Date:
viewer
Viewed: No
Annotation:
Run States: created ready submitted running completed imported killed incomplete monitor error system error
(HOME)/test/water

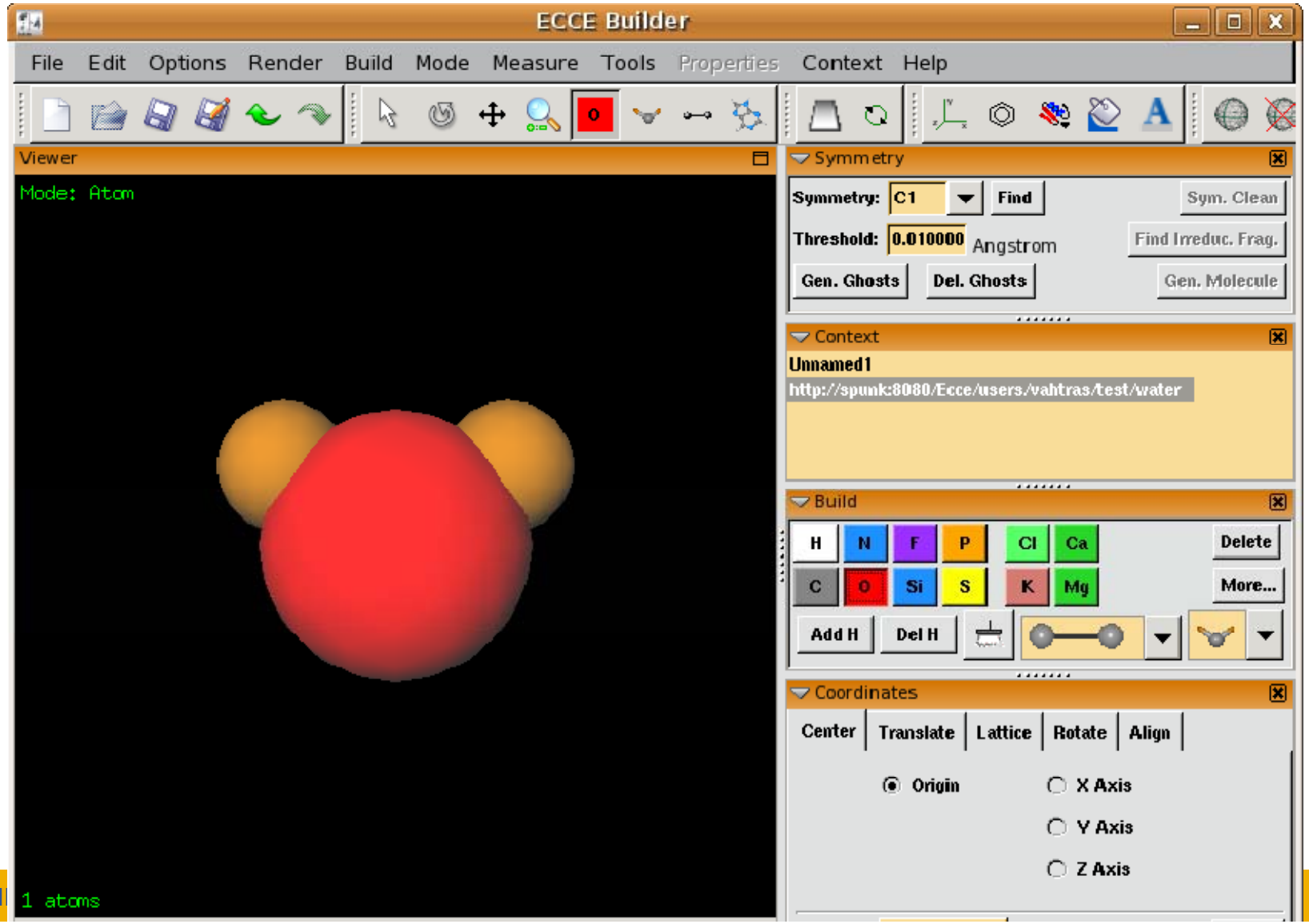
Editor


ECCE NWChem Editor
File Help
Code
Chemical System
Charge: 0
Spin Mult.:
builder
Formula:
Atoms:
Electrons:
Symmetry:
Open Shells:
Basis Set
Quick Basis Menu
Use Exponents & Coefficients
basis set tool
Name:
Polarization:
Functions:
Primitives:
NWChem Settings
Theory:
Runtype:
Details...
Details...
Final Edit...
Launch...
(HOME)/test/water

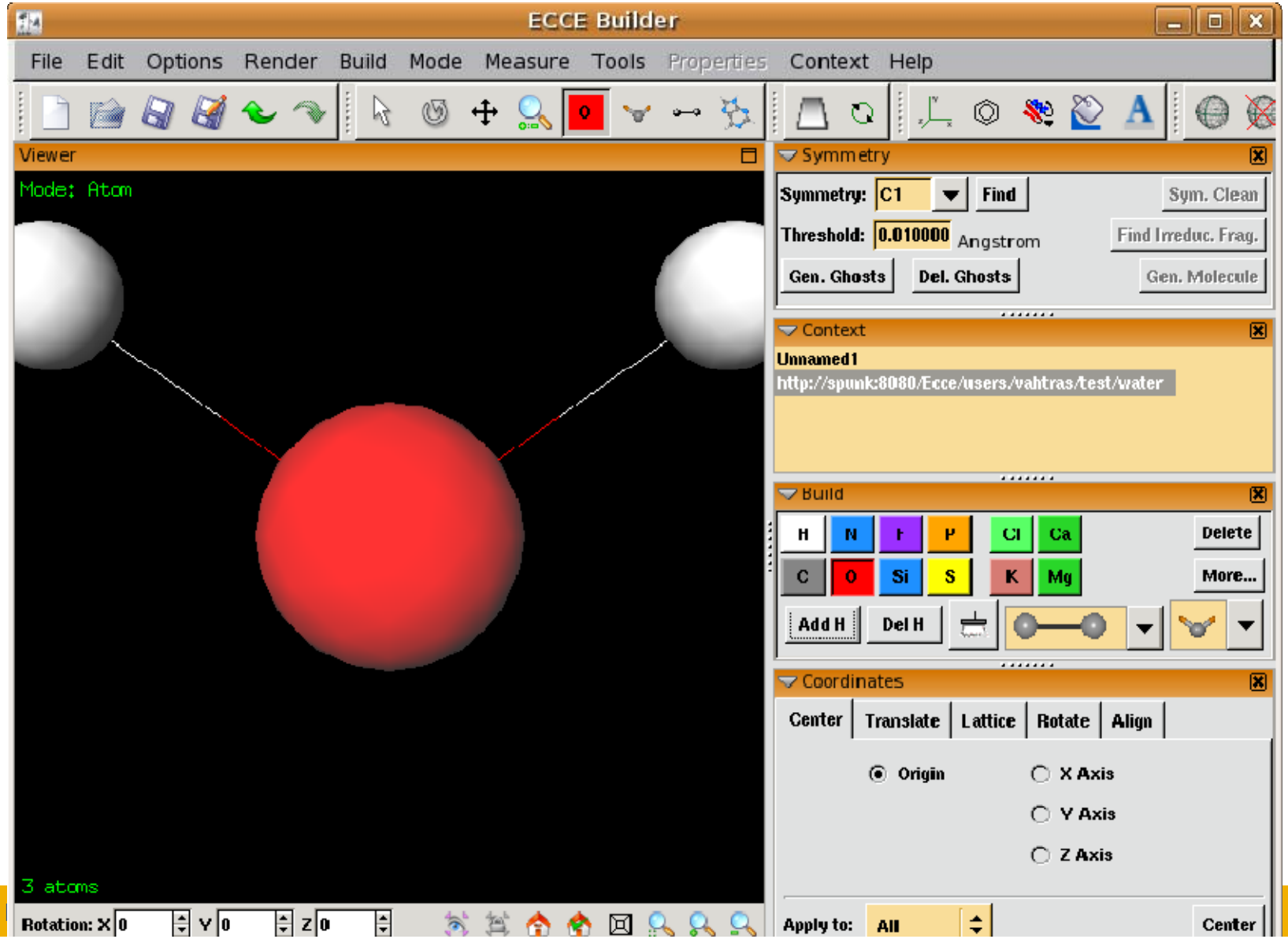
Builder


ECCE Builder
File Edit Options Render Build Mode Measure Tools Properties Context Help
Viewer
Mode: Select
Rotation: X 0 Y 0 Z 0
Symmetry
Symmetry: C1 Find Sym. Clean
Threshold: 0.010000 Angstrom Find Irreduc. Frag.
Gen. Ghosts Del. Ghosts Gen. Molecule
Context
Unnamed1
http://spunk:8080/Ecce/users/vahtras/test/water
Build
H N F P Cl Ca Delete
C O Si S K Mg More...
Add H Del H
Coordinates
Center Translate Lattice Rotate Align
Origin X Axis
Y Axis
Z Axis
Apply to: All Center
(HOME)/test/water

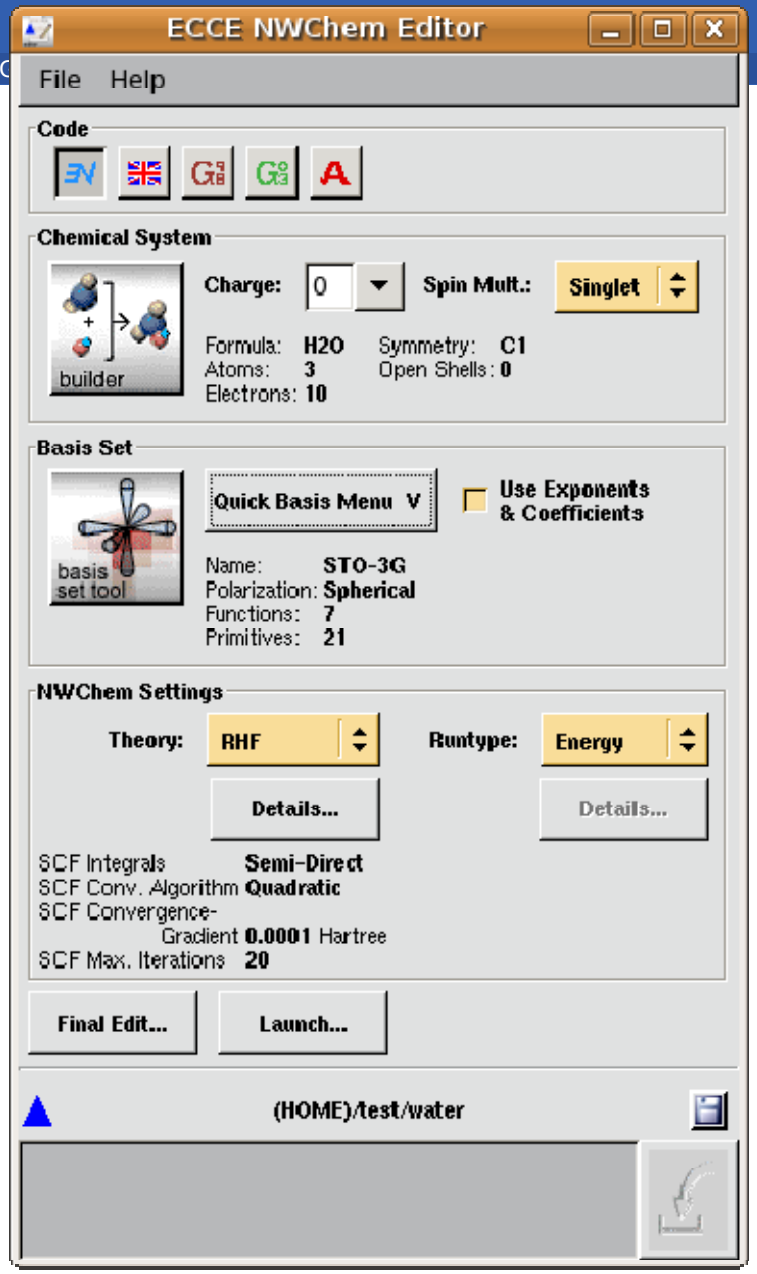
Oxygen


ECCE Builder
File Edit Options Render Build Mode Measure Tools Properties Context Help
Viewer
Mode: Atom
1 atoms
Symmetry
Symmetry: C1 Find Sym. Clean
Threshold: 0.010000 Angstrom Find Irreduc. Frag.
Gen. Ghosts Del. Ghosts Gen. Molecule
Context
Unnamed1
http://spunk:8080/Ecce/users/vahtras/test/water
Build
H N F P Cl Ca Delete
C O Si S K Mg More...
Add H Del H
Coordinates
Center Translate Lattice Rotate Align
Origin X Axis
Y Axis
Z Axis

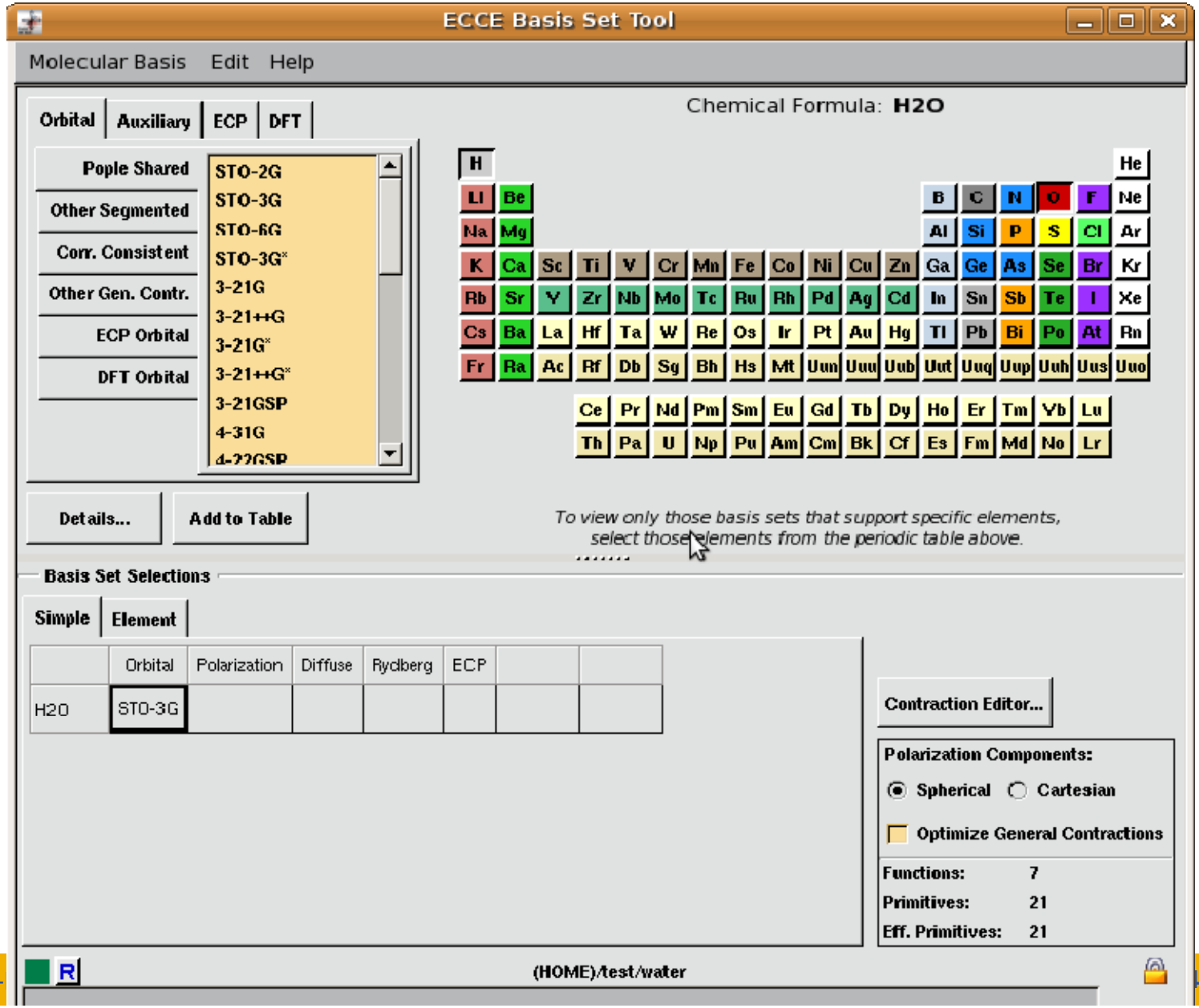
Add hydrogens



Editor


ECCE NWChem Editor
File Help
Code
Chemical System
builder
Charge: 0
Spin Mult.: Singlet
Formula: H2O
Atoms: 3
Electrons: 10
Symmetry: C1
Open Shells: 0
Basis Set
basis set tool
Quick Basis Menu
Use Exponents & Coefficients
Name: STO-3G
Polarization: Spherical
Functions: 7
Primitives: 21
NWChem Settings
Theory: RHF
Runtype: Energy
Details...
Details...
SCF Integrals Semi-Direct
SCF Conv. Algorithm Quadratic
SCF Convergence-
Gradient 0.0001 Hartree
SCF Max. Iterations 20
Final Edit...
Launch...
(HOME)/test/water

Basis set tool

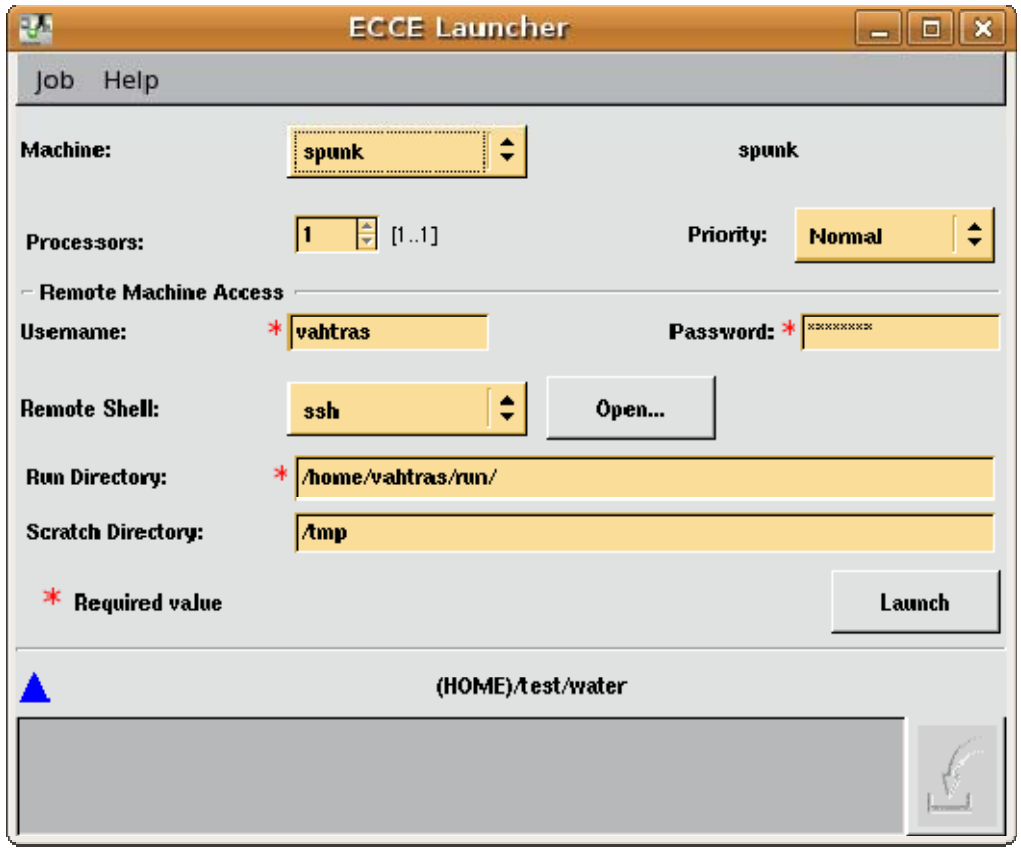


Final Edit

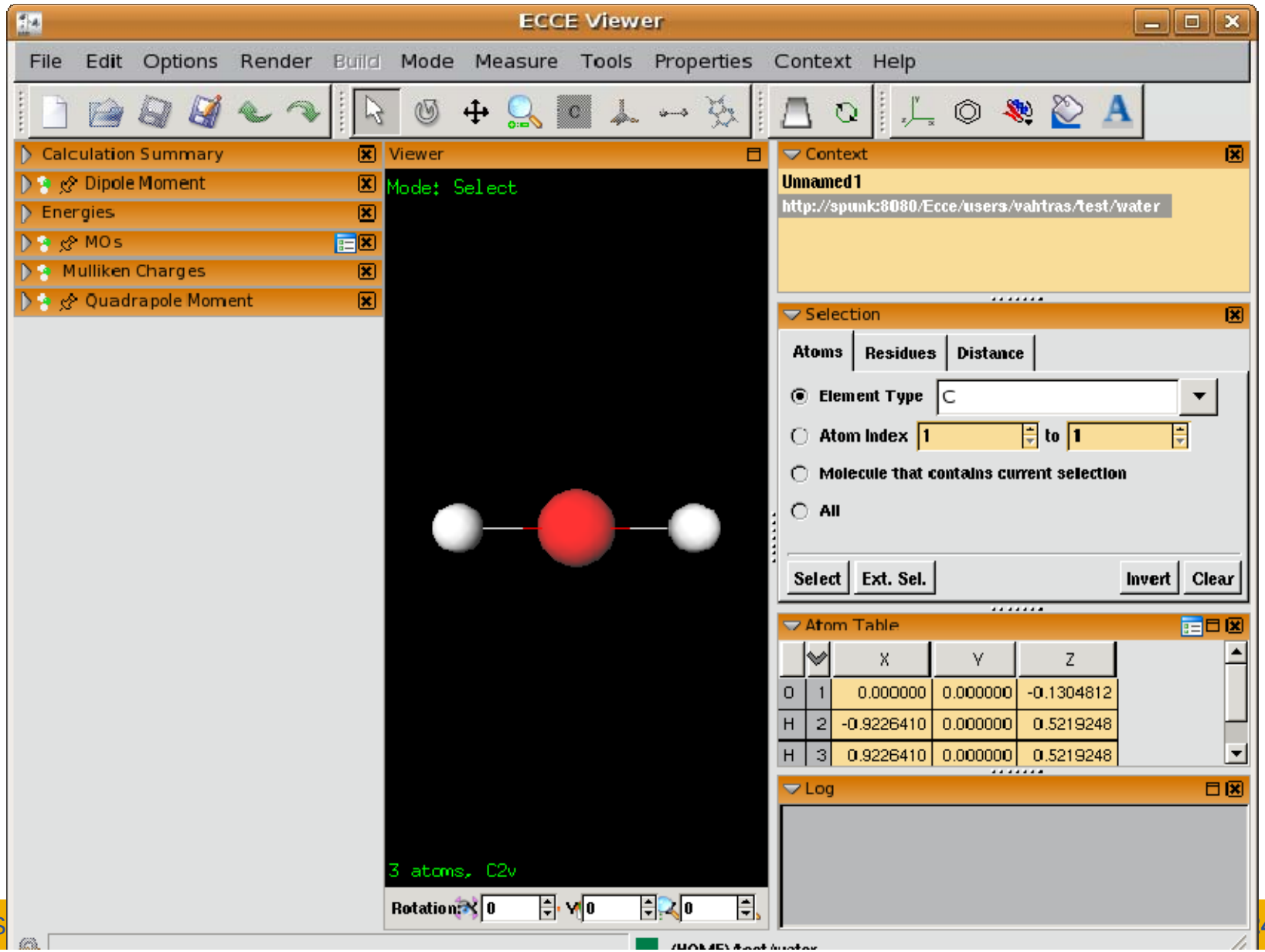
ECCEalkGgE (/tmp/ecce_vahtras) - VIM

```
title "water"

Start  water

echo

charge 0

geometry autosym units angstrom
 O      0.00000     0.00000     0.00000
 H      0.922641     0.652406     0.00000
 H     -0.922641     0.652406     0.00000
end

ecce_print ecce.out

basis "ao basis" spherical print
  H library "STO-3G"
  O library "STO-3G"
END

scf
  RHF
  nopen 0
end

task scf energy
~
~
~
~
~
~
~
~
~
~
~
~
"/tmp/ecce_vahtras/ECCEalkGgE" 27L, 546C                    1,1           All
```

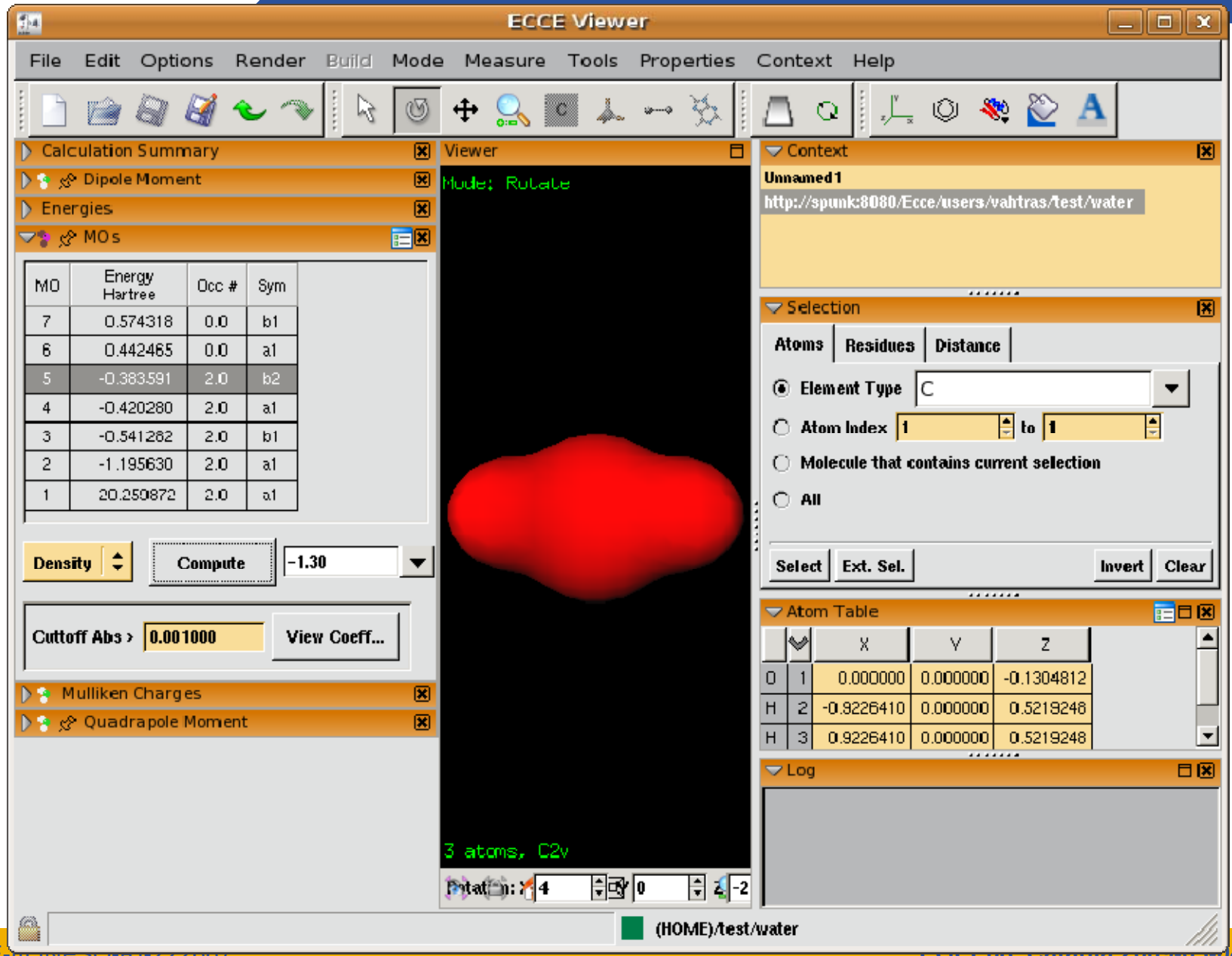
Launch


ECCE Launcher
Job Help
Machine:
spunk
spunk
Processors:
1
[1..1]
Priority:
Normal
Remote Machine Access
Username:
vahtras
Password:
Remote Shell:
ssh
Open...
Run Directory:
/home/vahtras/run/
Scratch Directory:
/tmp
Required value
Launch
(HOME)/test/water

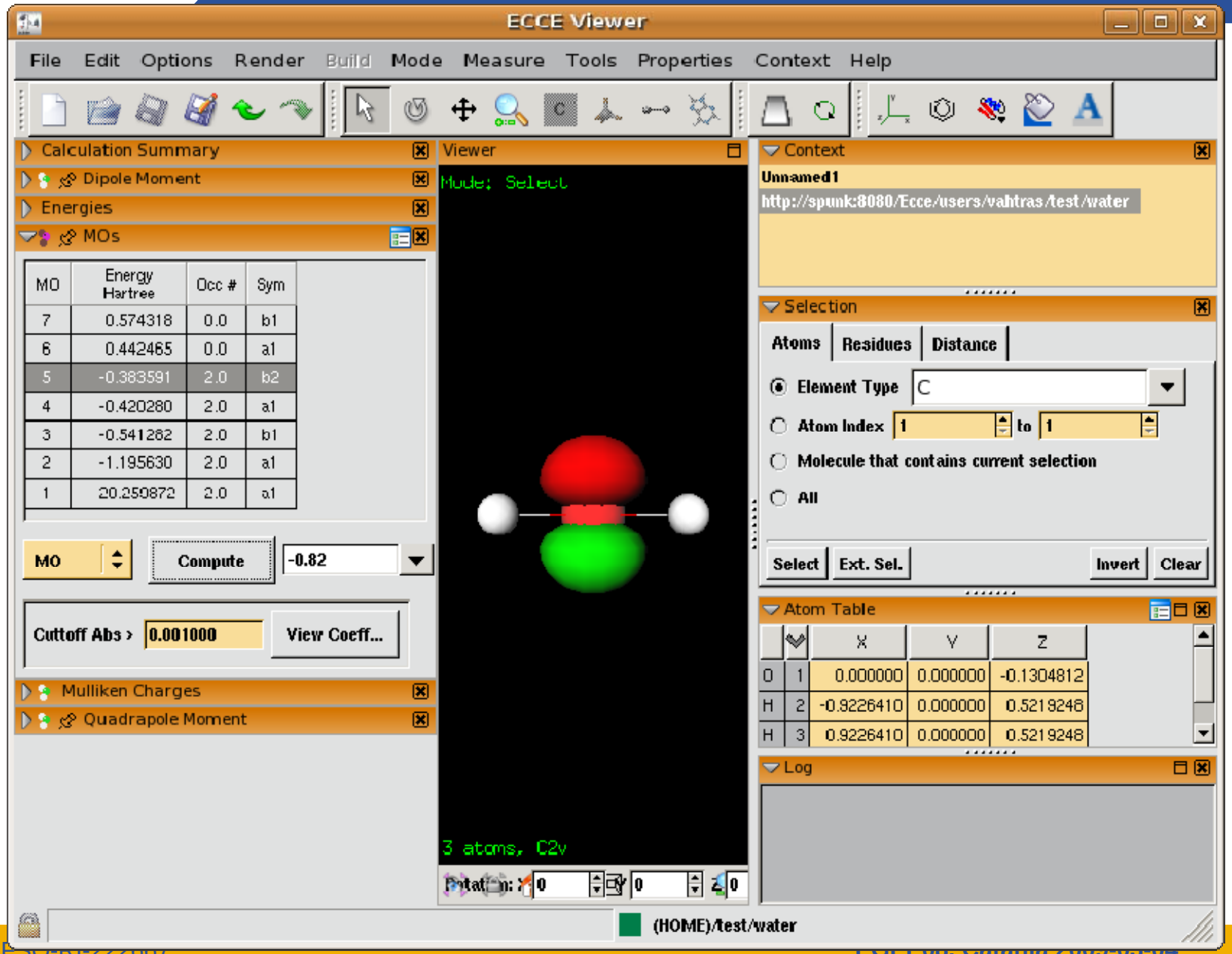
Viewer


ECCE Viewer
File Edit Options Render Build Mode Measure Tools Properties Context Help
Calculation Summary
Dipole Moment
Energies
MOs
Mulliken Charges
Quadrapole Moment
Viewer
Mode: Select
3 atoms, C2v
Rotation: X 0 Y 0 Z 0
Context
Unnamed1
http://spunk:8080/Ecce/users/vahtras/test/water
Selection
Atoms Residues Distance
Element Type C
Atom Index 1 to 1
Molecule that contains current selection
All
Select Ext. Sel. Invert Clear
Atom Table
X Y Z
0 1 0.000000 0.000000 -0.1304812
H 2 -0.9226410 0.000000 0.5219248
H 3 0.9226410 0.000000 0.5219248
Log

View density



View HOMO


ECCE Viewer
File Edit Options Render Build Mode Measure Tools Properties Context Help
Calculation Summary
Dipole Moment
Energies
MOs
MO | Energy Hartree | Occ # | Sym
7 | 0.574318 | 0.0 | b1
6 | 0.442465 | 0.0 | a1
5 | -0.383591 | 2.0 | b2
4 | -0.420280 | 2.0 | a1
3 | -0.541282 | 2.0 | b1
2 | -1.195630 | 2.0 | a1
1 | 20.259872 | 2.0 | a1
MO
Compute
-0.82
Cutoff Abs >
0.001000
View Coeff...
Mulliken Charges
Quadrapole Moment
Viewer
Mode: Select
3 atoms, C2v
Rotation:
Context
Unnamed1
http://spunk:8080/Ecce/users/vahtras/test/water
Selection
Atoms
Residues
Distance
Element Type
C
Atom Index
1
to
1
Molecule that contains current selection
All
Select
Ext. Sel.
Invert
Clear
Atom Table
X
Y
Z
0 1 0.000000 0.000000 -0.1304812
H 2 -0.9226410 0.000000 0.5219248
H 3 0.9226410 0.000000 0.5219248
Log
(HOME)/test/water

ECCE on grids

- **Tasks**
  - Make ECCE talk to g-lite
    - Submitting
    - Monitoring
      - *Job status*
      - *Job progress*
    - Retrieving
  - Options
    - Text configuration files
    - Perl communication scripts
- **All work in progress**

Adapting ECCE

- **Define a queue manager in siteconfig/QueueManagers**
  - GLITE|submitCommand: glite-job-submit
  - GLITE|cancelCommand: glite-job-cancel
  - GLITE|queryJobCommand: glite-job-status
- **Define a submit host where glite is installed (could be the same as the ECCE client host**
  - Configuration files glitehost.Q, Machines,Queues
- **Define ecce states in relation to glite job states (running,queued,completed)**
  - Perl script eccejobmonitor

- **Summary**
  - A chemists “project management” software
  - ECCE GUI hides details from the user
  - Collects results from a variety of computational resources in a single database
  - ECCE has a high pedagogical value for students of chemistry
  - Lower threshold for computational chemists to turn to grid resources

Acknowledgment

- **Acknowledgement**
  - Gary Black, PNNL