



Enabling Grids for E-science

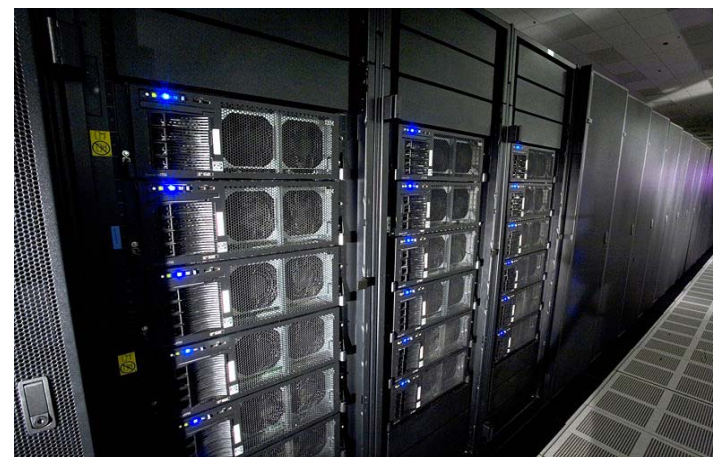
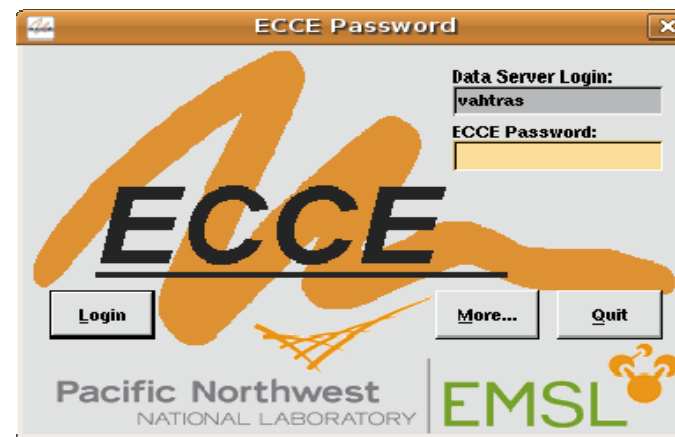
Computational chemistry with ECCE on EGEE grids

Olav Vahtras
KTH

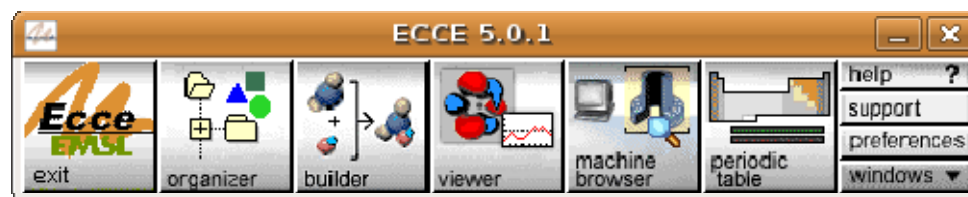
www.eu-egee.org



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

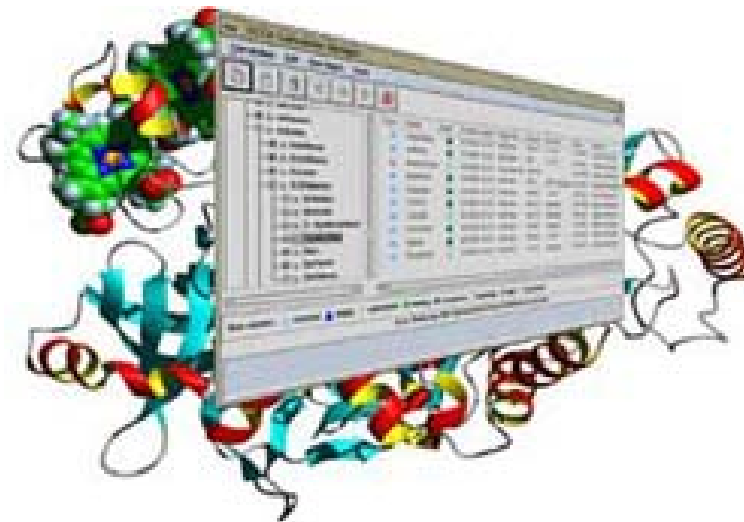


- **Developed by PNNL**
- **Supported on Linux, SGI, Sun**
- **Free of use for academic users**
- **Support for NWChem, Gaussian98, Gaussian03, Gamess-UK,Amica**
- **Written in C++**
- **X Windows Motif toolkit**
- **OPENGL graphics**

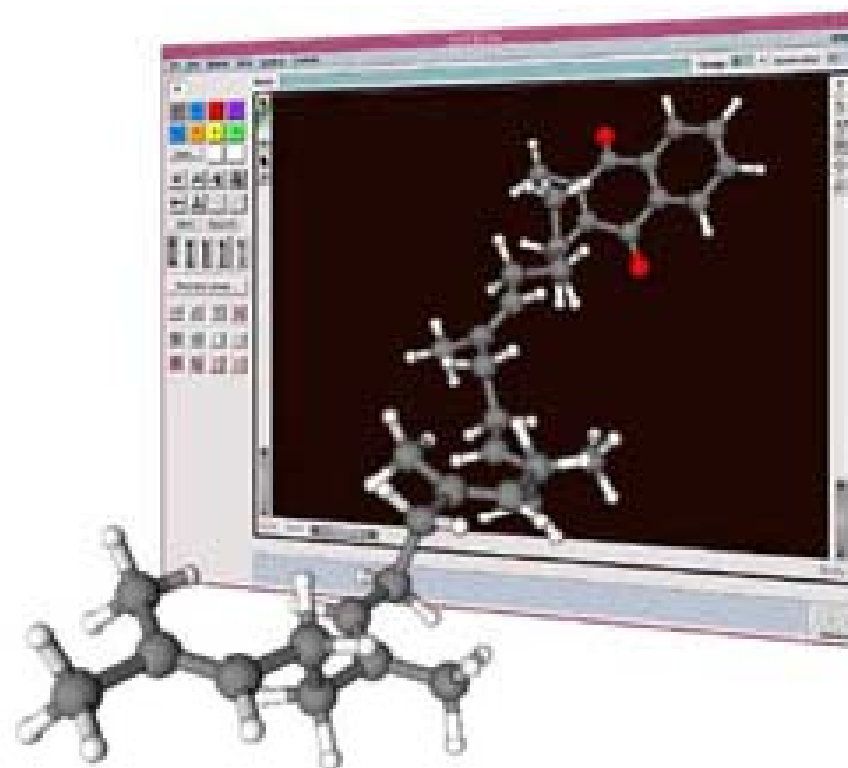


- Organizer
- Builder
- Viewer
- Machine browser
- Periodic table

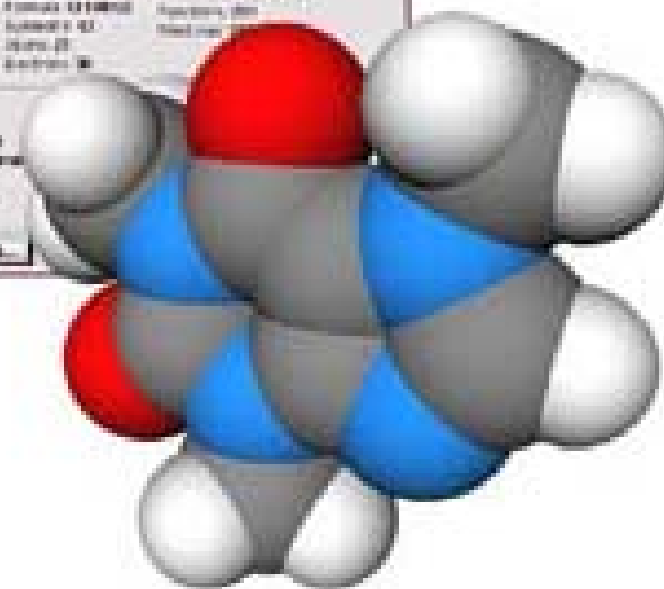
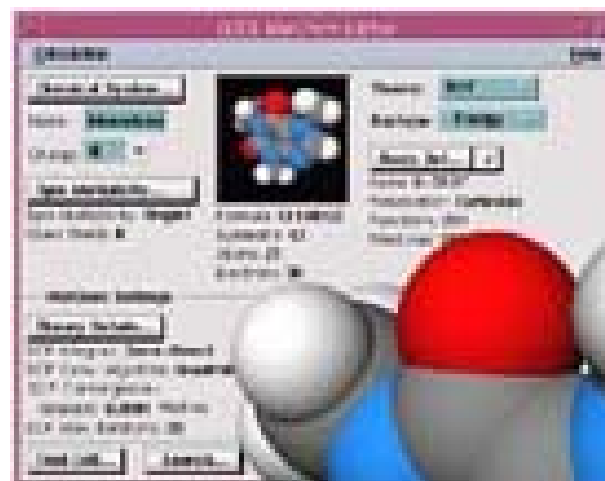
- **Organizer summarizes projects and calculations in a “file manager” view**
- **Information is stored on a data server (apache server with a Web-DAV) interface**
- **Color-coded status of calculations (ready, running, finished, error)**



- **Builder: 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**



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

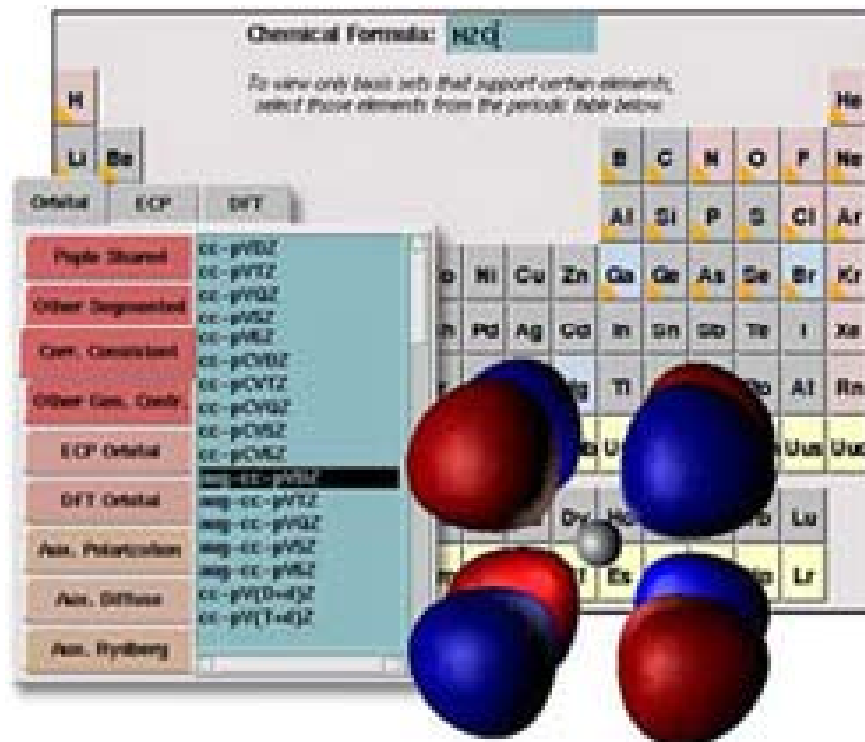


- Choose basis set for all atoms or different basis set for different atom types

Chemical Formula:

To view only basis sets that support certain elements, select those elements from the periodic table below.

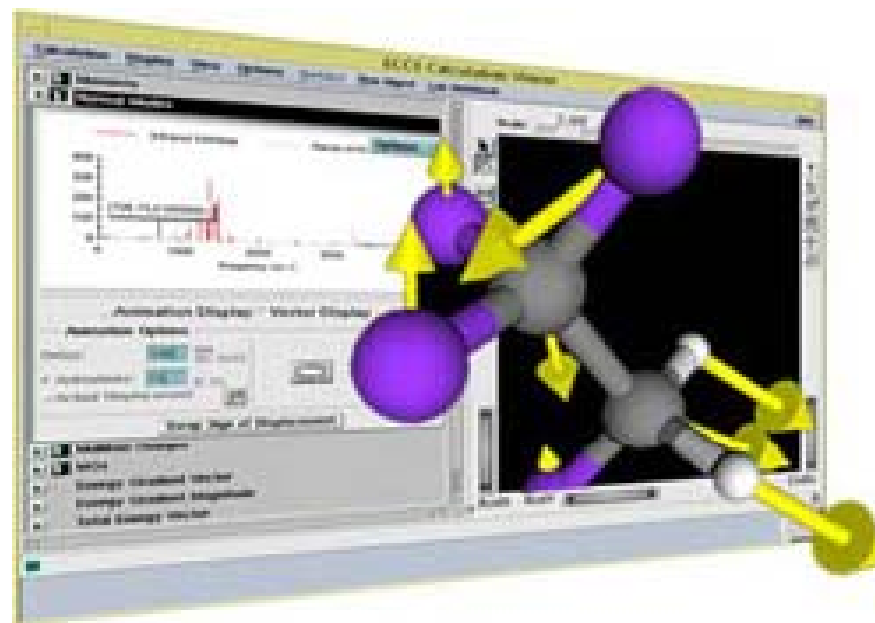
Orbital	ECP	DFT
Triple Shared	cc-pVTZ	
Other Segmented	cc-pVTZ	
Other Segmented	cc-pVTZ	
Core Contracted	cc-pVTZ	
Other Core, Condy	cc-pVTZ	
ECP Orbital	cc-pVTZ	
DFT Orbital	aug-cc-pVTZ	
Ass. Polarization	aug-cc-pVTZ	
Ass. Diffuse	cc-pVTZ+d	
Ass. Rydberg	cc-pVTZ+d	

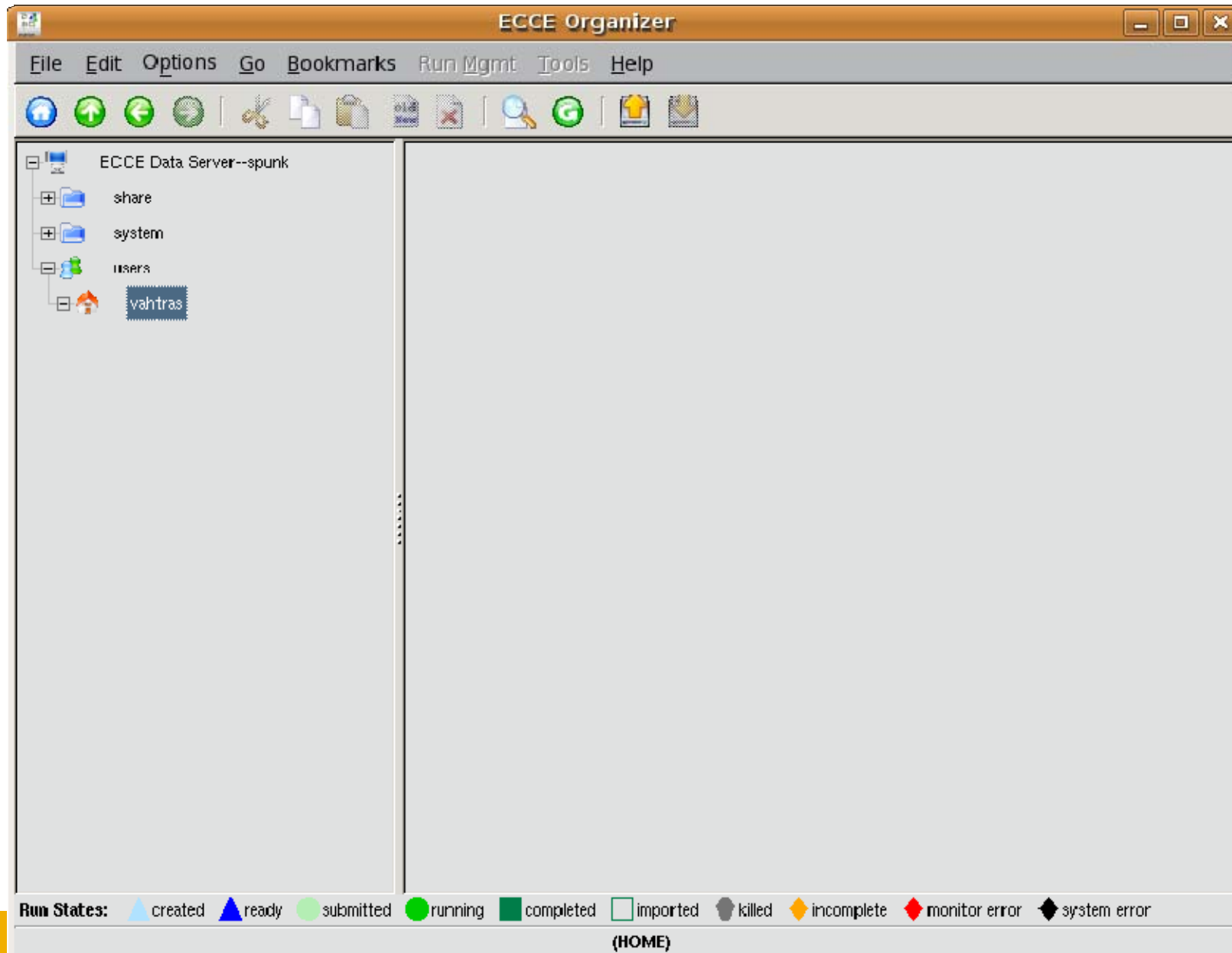


- **Select machine where the calculation is to run**



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





ECCE Organizer

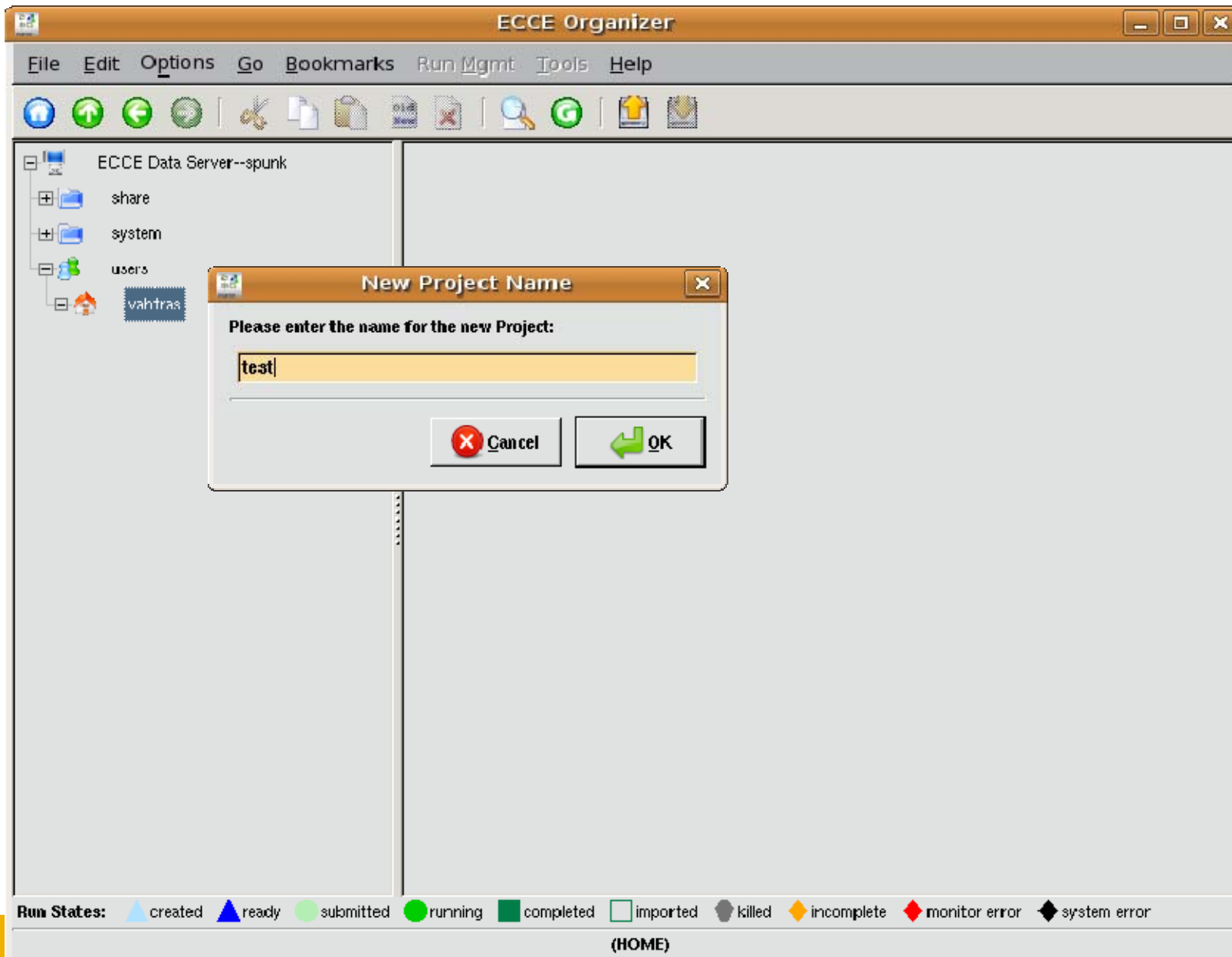
File Edit Options Go Bookmarks Run Mgmt Tools Help

ECCE Data Server--spunk

- share
- system
- users
 - vahtras

Run States: ▲ created ▲ ready ● submitted ● running ■ completed □ imported ● killed ◆ incomplete ◆ monitor error ◆ system error














(HOME)



The screenshot shows the ECCE Organizer application window. The title bar reads "ECCE Organizer". The menu bar includes "File", "Edit", "Options", "Go", "Bookmarks", "Run Mgmt", "Tools", and "Help". Below the menu bar is a toolbar with various icons. The main window area is divided into two panes. The left pane shows a tree view of the "ECCE Data Server--spunk" with sub-items: "share", "system", "users", and "vahtras". The right pane is currently empty. A "New Project Name" dialog box is open in the center, containing the text "Please enter the name for the new Project:" and a text input field with "test" entered. Below the input field are "Cancel" and "OK" buttons. At the bottom of the application window, there is a "Run States" legend with the following items: created (light blue triangle), ready (dark blue triangle), submitted (light green circle), running (dark green circle), completed (dark green square), imported (light green square), killed (grey diamond), incomplete (orange diamond), monitor error (red diamond), and system error (black diamond). The text "(HOME)" is centered at the bottom of the window.

ECCE Organizer

File Edit Options Go Bookmarks Run Mgmt Tools Help

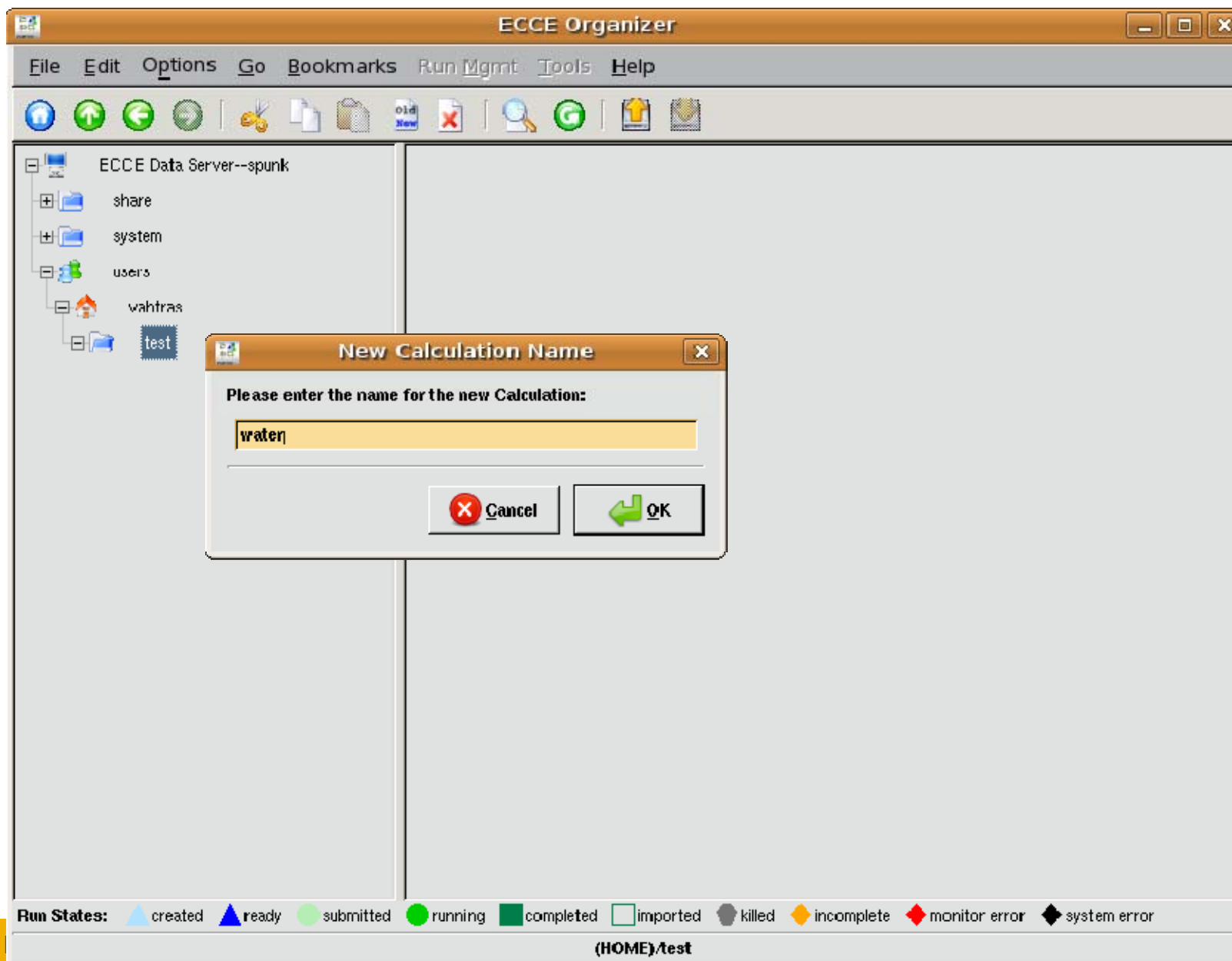














ECCE Data Server--spunk

- share
- system
- users
 - vahtras
 - test

Run States:
▲ created
 ▲ ready
 ● submitted
 ● running
 ■ completed
 imported
 ■ killed
 ◆ incomplete
 ◆ monitor error
 ◆ system error

(HOME)/test



The screenshot shows the ECCE Organizer application window. The title bar reads "ECCE Organizer". The menu bar includes "File", "Edit", "Options", "Go", "Bookmarks", "Run Mgmt", "Tools", and "Help". Below the menu bar is a toolbar with various icons. The main area is split into two panes. The left pane shows a tree view of the "ECCE Data Server--spunk" with folders for "share", "system", "users", "vahtras", and a "test" folder. A dialog box titled "New Calculation Name" is open in the foreground, containing the text "Please enter the name for the new Calculation:" and a text input field with "water" typed in. Below the input field are "Cancel" and "OK" buttons. At the bottom of the application window, there is a "Run States" legend with icons for created, ready, submitted, running, completed, imported, killed, incomplete, monitor error, and system error. The status bar at the bottom right shows "(HOME)/test".

ECCE Organizer

File Edit Options Go Bookmarks Run Mgmt Tools Help

ECCE Data Server--spunk

- share
- system
- users
 - vahtras
 - test
 - water

Calculation: ▲ **water**
 Code: **NWChem**
 Theory:
 Runtime:

Formula: Charge:
 Atoms: Spin Mult.:
 Electrons: Open Shells:
 Symmetry:

Name:
 Polarization:
 Functions:
 Primitives:

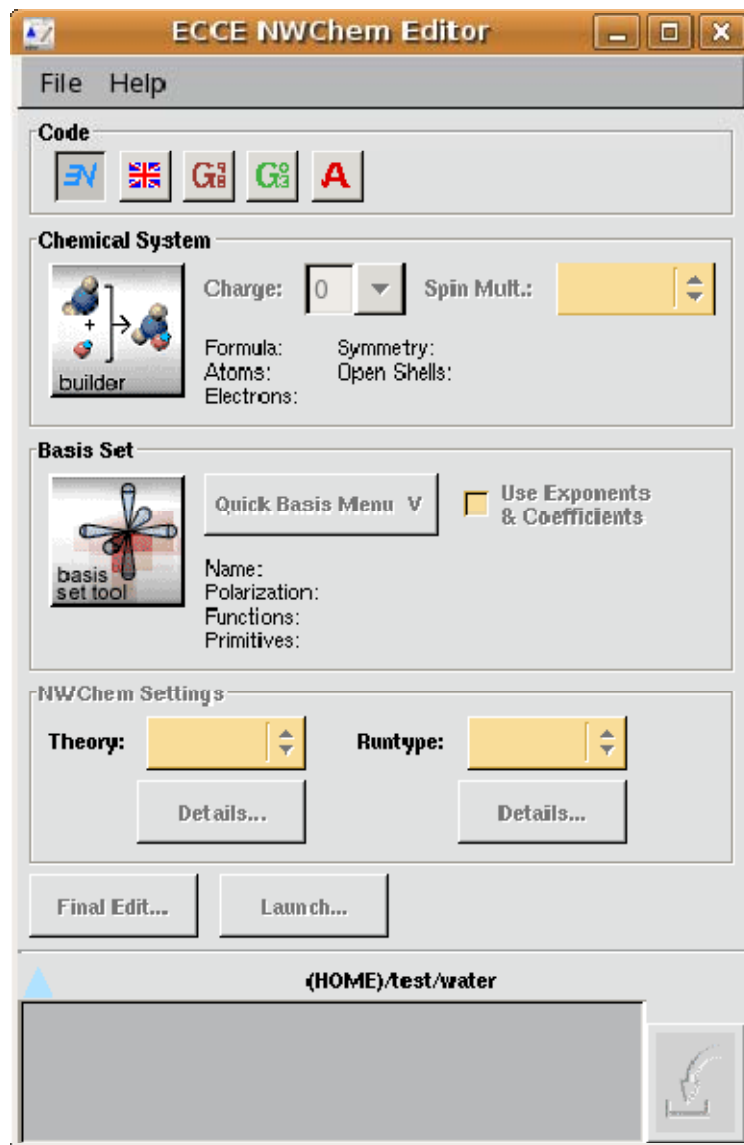
Machine:
 Processors:
 Start Date:
 Comp. Date:

Viewed: **No**

Annotation:

Run States: ▲ created ▲ ready ● submitted ● running ■ completed □ imported ● killed ◆ incomplete ◆ monitor error ◆ system error

(HOME)/Test/water



ECCE Builder

File Edit Options Render Build Mode Measure Tools Properties Context Help

Viewer
Mode: Select

Symmetry

Symmetry: C1 Find Sym. Clean

Threshold: 0.010000 Angstrom Find Irreduc. Frag.



Gen. Ghosts Del. Ghosts Gen. Molecule

Context

Unnamed 1
<http://spunk:8080/ECce/users/vahtras/test/water>

Build

H	N	F	P	Cl	Ca	Delete
C	O	Si	S	K	Mg	

Add H Del H  

Coordinates

Center Translate Lattice Rotate Align

Origin X Axis

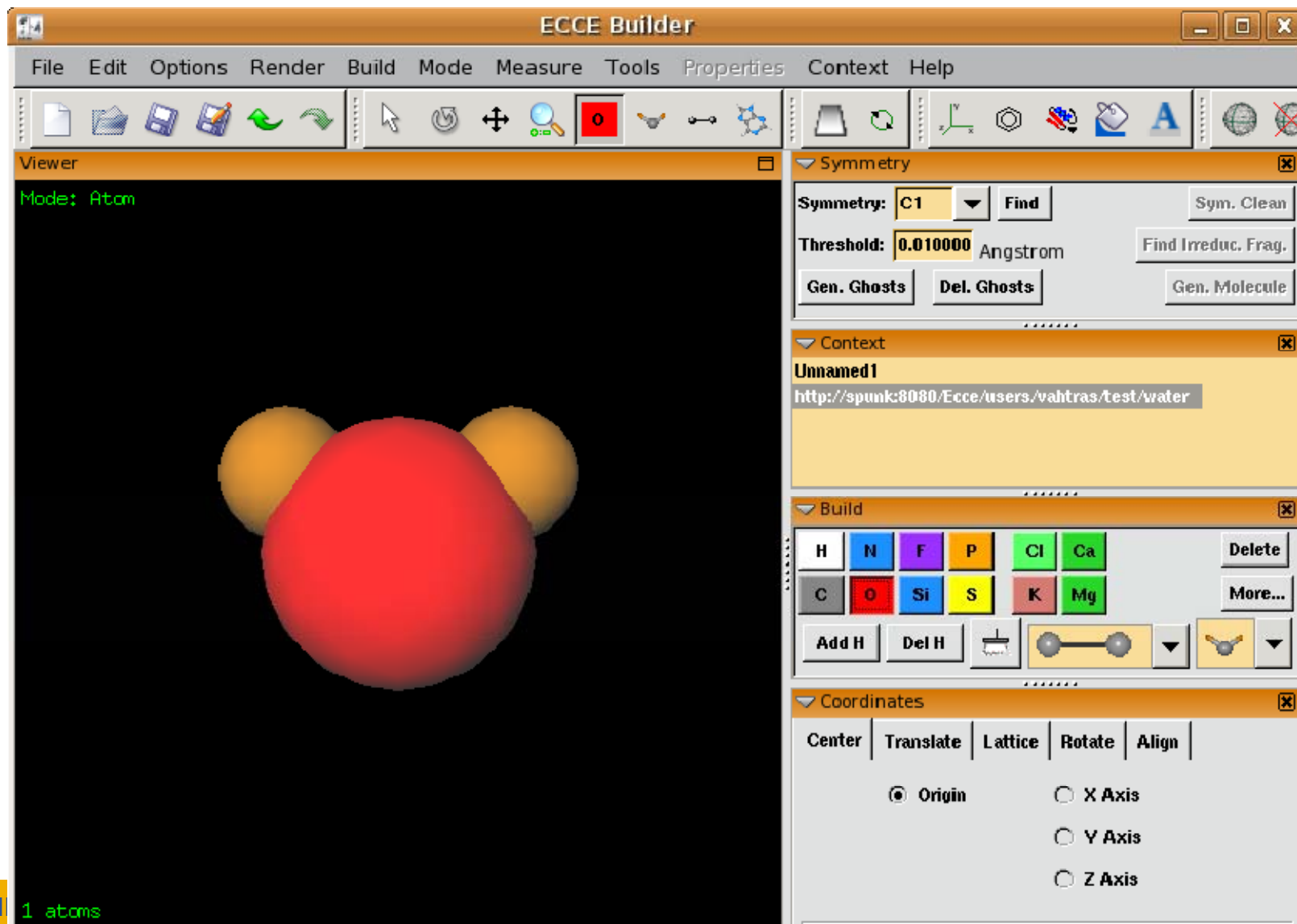
Y Axis

Z Axis

Apply to: All Center

Rotation: X 0 Y 0 Z 0

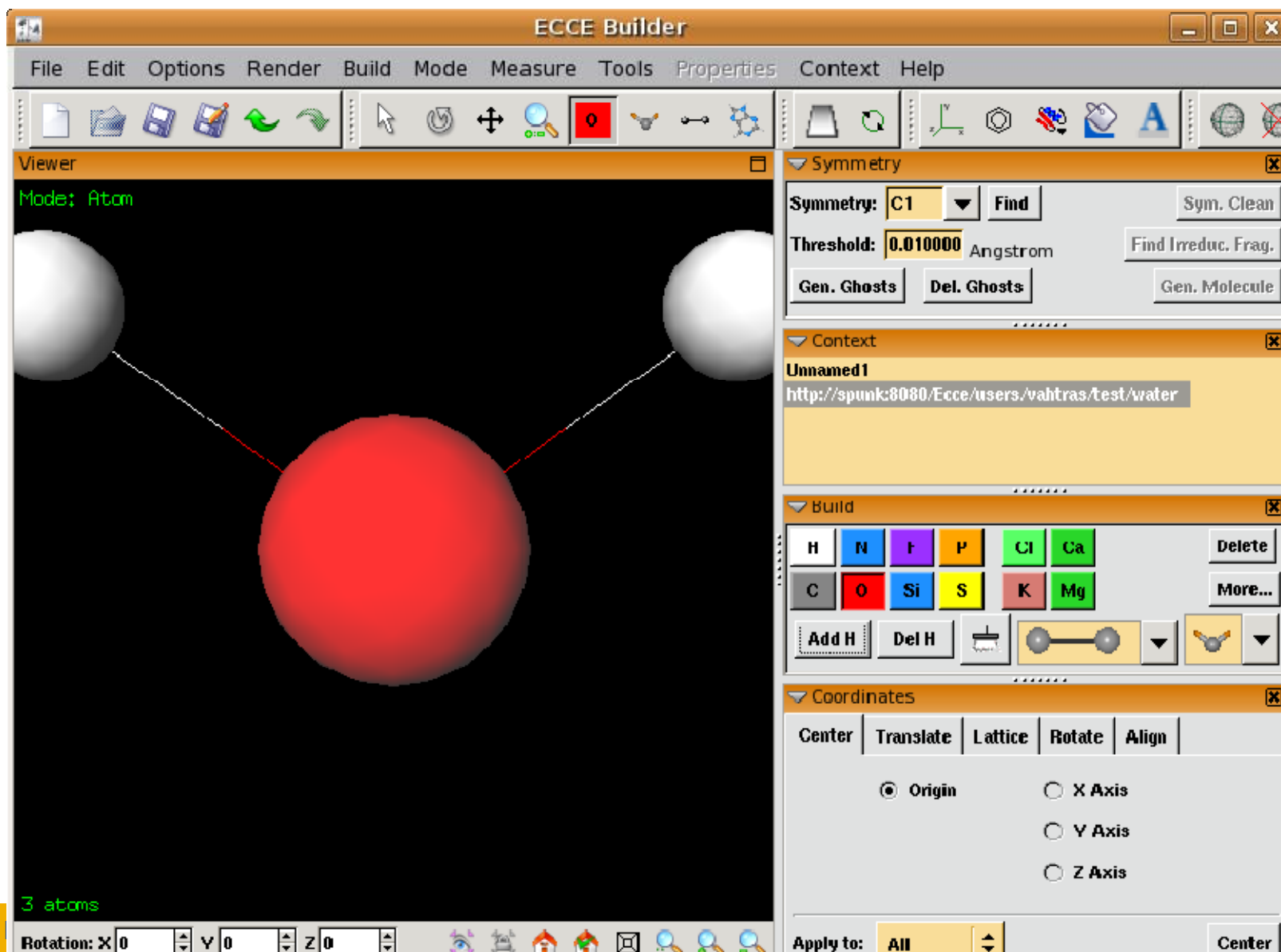
(HOME)/test/water



The screenshot displays the ECCE Builder application window. The main viewer shows a 3D ball-and-stick model of a water molecule (H₂O) with a large red oxygen atom and two smaller yellow hydrogen atoms. The interface includes a menu bar (File, Edit, Options, Render, Build, Mode, Measure, Tools, Properties, Context, Help) and a toolbar with various icons. On the right side, there are several panels:

- Symmetry:** Symmetry: C1, Find, Sym. Clean, Threshold: 0.010000 Angstrom, Find Irreduc. Frag., Gen. Ghosts, Del. Ghosts, Gen. Molecule.
- Context:** Unnamed 1, <http://spunk:8080/Ecce/users/vahtras/test/water>
- Build:** H, N, F, P, Cl, Ca, C, O, Si, S, K, Mg, Delete, More..., Add H, Del H, and bond type selection tools.
- Coordinates:** Center, Translate, Lattice, Rotate, Align, Origin (selected), X Axis, Y Axis, Z Axis.

At the bottom left of the viewer, the text "Mode: Atom" is visible. At the bottom left of the entire slide, a yellow box contains the text "EGEE-III IN 1 atoms". At the bottom right of the slide, a yellow box contains the number "18".



The screenshot shows the ECCE Builder application window. The main viewer displays a molecular model with three atoms: a large red sphere in the center and two smaller white spheres on either side, connected by thin lines. The text "Mode: Atom" is visible in the viewer area, and "3 atoms" is shown at the bottom left. The interface includes a menu bar (File, Edit, Options, Render, Build, Mode, Measure, Tools, Properties, Context, Help) and a toolbar with various icons. On the right side, there are several panels: "Symmetry" (set to C1, Threshold: 0.010000 Angstrom), "Context" (showing "Unnamed 1" and a URL), "Build" (with buttons for H, N, F, P, Cl, Ca, C, O, Si, S, K, Mg, and "Add H", "Del H"), and "Coordinates" (with options for Center, Translate, Lattice, Rotate, Align, and radio buttons for Origin, X Axis, Y Axis, Z Axis). The bottom status bar shows rotation values for X, Y, and Z axes.

ECCE NWChem Editor

File Help

Code

Chemical System

builder

Charge: 0 Spin Mult.: Singlet

Formula: H2O Symmetry: C1
 Atoms: 3 Open Shells: 0
 Electrons: 10

Basis Set

basis set tool

Quick Basis Menu V Use Exponents & Coefficients

Name: STO-3G
 Polarization: Spherical
 Functions: 7
 Primitives: 21

NWChem Settings

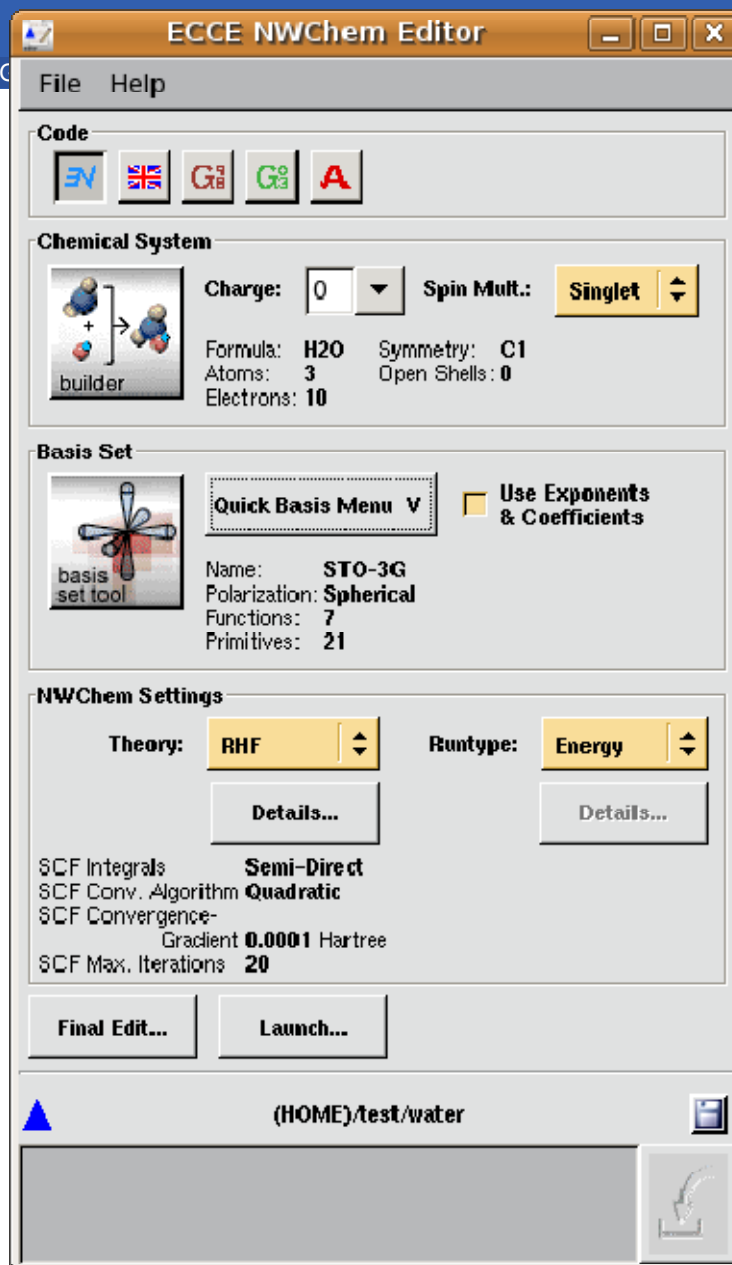
Theory: RHF Runtype: Energy

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



ECCE Basis Set Tool
_ □ ×

Molecular Basis
Edit
Help

Orbital	Auxiliary	ECP	DFT
Pople Shared			
	STO-2G		
Other Segmented			
	STO-3G		
	STO-6G		
Corr. Consistent			
	STO-3G*		
Other Gen. Contr.			
	3-21G		
	3-21++G		
ECP Orbital			
	3-21G*		
DFT Orbital			
	3-21++G*		
	3-21GSP		
	4-31G		
	4-??GSP		

Chemical Formula: **H2O**

H																		He
Li	Be									B	C	N	O	F				Ne
Na	Mg									Al	Si	P	S	Cl				Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br		Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I		Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At		Rn
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Uun	Uuu	Uub	Uut	Uuq	Uup	Uuh	Uus		Uuo

To view only those basis sets that support specific elements, select those elements from the periodic table above.

Details...
Add to Table

Basis Set Selections

Simple	Element	Orbital	Polarization	Diffuse	Rydberg	ECP		
H2O	STO-3G							

Contraction Editor...

Polarization Components:

Spherical Cartesian


Optimize General Contractions

Functions: 7


Primitives: 21

Eff. Primitives: 21

EGEE-III INFSO-



(HOME)/test/water



21

```

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" 2/L, 546L 1,1 All
    
```



ECCE Viewer

File Edit Options Render Build Mode Measure Tools Properties Context Help

Viewer

Mode: Select

3 atoms, C2v

Rotation: X 0 Y 0 Z 0

Context

Unnamed 1

<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
O	1	0.000000	0.000000	-0.1304812
H	2	-0.9226410	0.000000	0.5219248
H	3	0.9226410	0.000000	0.5219248

Log

ECCE Viewer

File Edit Options Render Build Mode Measure Tools Properties Context Help

Viewer

Mode: Rotate

Context

Unnamed 1

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
O 1	0.000000	0.000000	-0.1304812
H 2	-0.9226410	0.000000	0.5219248
H 3	0.9226410	0.000000	0.5219248

Log

3 atoms, C2v

Rotation: 4 0 -2

(HOME)/test/water

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	-0.541262	2.0	b1
2	-1.195630	2.0	a1
1	20.250872	2.0	a1

Density Compute

Cutoff Abs > View Coeff...

Mulliken Charges

Quadrupole Moment

ECCE Viewer

File Edit Options Render Build Mode Measure Tools Properties Context Help

Viewer

Mode: Select

Context

Unnamed 1

<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
O 1	0.000000	0.000000	-0.1304812
H 2	-0.9226410	0.000000	0.5219248
H 3	0.9226410	0.000000	0.5219248

Log

3 atoms, C2v

MO

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	-0.541262	2.0	b1
2	-1.195630	2.0	a1
1	20.250872	2.0	a1

Compute -0.82

Cutoff Abs > 0.001000 View Coeff...

Mulliken Charges

Quadrupole Moment

(HOME)/test/water

- **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**

- **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

- **Acknowledgement**
 - Gary Black, PNNL