Qbox tutorial

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MICCoM Tutorial

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MICCoM

Qbox code: main features

- C++/MPI implementation of First-Principles Molecular Dynamics
- DFT/GGA, meta-GGA and hybrid DFT exchange-correlation
- Plane-wave, norm-conserving pseudopotentials
- NVT, NpT molecular dynamics
- Wannier functions, constrained MD, electric field, IR, Raman ...
- Client-server interface (coupling to SSAGES, WEST, i-PI)
- Installed on bebop.lcrc.anl.gov
- http://qboxcode.org
- Documentation: http://qboxcode.org/doc/html
- Qbox forum: http://qboxcode.org/qbox-list

Using Qbox on bebop.lcrc.anl.gov

- Login on bebop using the ssh -Y option to enable X11 graphics:

  ssh -Y <username>@bebop.lcrc.anl.gov

- Qbox tutorial files are located at

  /lcrc/project/MICCoM-train/qbox_tutorial

- Make a copy of **qbox_tutorial** to your home directory:

  ```
  $ cd
  $ cp -ra /lcrc/project/MICCoM-train/qbox_tutorial .
  ```

- Setup Qbox environment variables and paths:

  ```
  $ cd qbox_tutorial
  $ source qbsetup.sh
  ```

Using Qbox on bebop.lcrc.anl.gov

- Qbox interactive session example:

```
$ cd qbox_tutorial/examples/ch4
$ runqbox.sh
[qbox] ...(interactive session)
```

- Qbox batch job example:
  - uses input file **gs.i**
  - writes output on **gs.r**

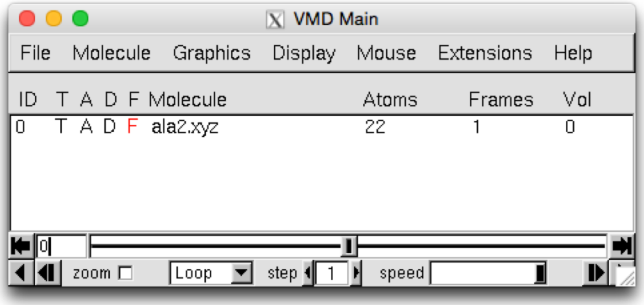
```
$ cd qbox_tutorial/examples/ch4
$ sbatch -J gs ../../qbox.job
```

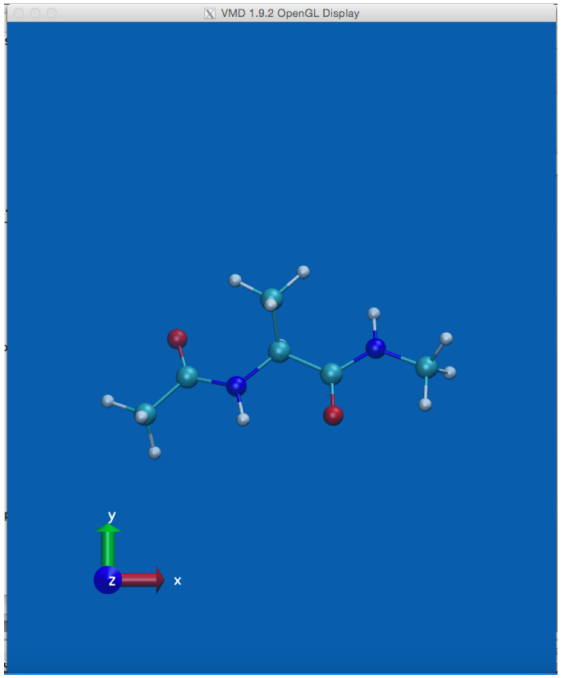
Test visualization with VMD

Use the VMD program to visualize a molecule

```
$ cd qbox_tutorial/vmdtest
$ vmd –e cpk.vmd ala2.xyz
```

These windows should appear:





Use the File->Quit option to exit.

Qbox basic operation

- interactive mode
  - $ qb
  - Qbox prompt: [qbox]
- reading from an input script
  - $ qb input.i
- using an input script, writing on an output file
  - $ qb input.i > output.r
- output.r is an XML document

Qbox commands

- Qbox reads commands from input and executes them sequentially
- Examples
  - define the plane wave energy cutoff (Ry)

```
[qbox] set ecut 35
```

  - define an atom at a given position

```
[qbox] atom C carbon 0.123 0.456 0.789
```

  - position in atomic units (Bohr)

Qbox commands

- Get more details using “help <*command*>”

```
[qbox] help move

 move

 syntax: move atom_name {to|by} x y z

   The move command displaces an atom to a new position.
   The new position is defined by absolute coordinates (to) or
   by a relative displacement (by).
   When using 'to', if one or more of the arguments is '*',
   the corresponding component of the velocity is unchanged.
```

- A detailed description of all commands is given in the documentation page
  - http://qboxcode.org/doc/html

Qbox variables

- Qbox variables can be set using the “set” command.
- Variable values are printed using the “print” command
- Examples
  - set the ecut variable

```
[qbox] set ecut 35
```

  - print the value of the ecut variable

```
[qbox] print ecut
```

qbox_tutorial/examples

- **/lcrc/project/MICCoM-train/qbox_tutorial/examples**
  - **ch4** CH_4 molecule
  - **h2o** H_2O molecule
  - **h2ofield** H_2O molecule with electric field
  - **c60** C_{60} molecule
  - **h2o32** Liquid water
  - **heliq** Liquid helium
  - **o2gs** Oxygen molecule
  - **silicon** Silicon crystal
  - **si64liq** Liquid silicon at 2000 K
  - **dce** Dichloroethane free energy profile
  - **qbdriver** Client-server mode
  - **ssages** Example Qbox-SSAGES simulation

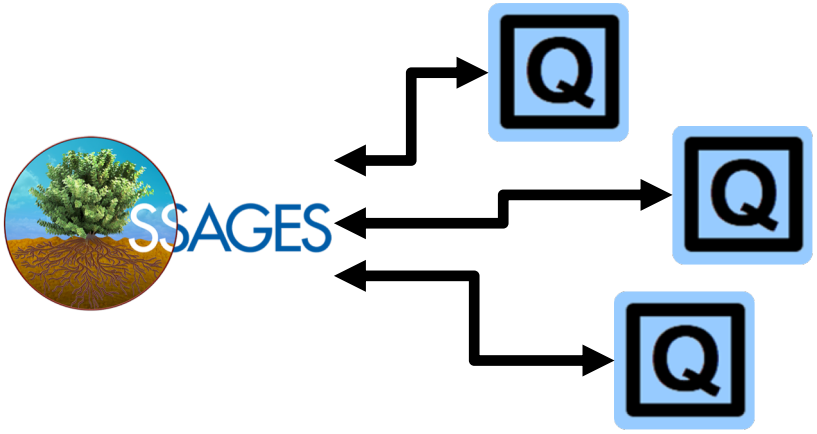
Each example directory includes a README file with detailed instructions

Coupling Qbox with other codes: client-server mode

- Qbox can be used as a "DFT engine" driven by another simulation code
- Example: Free energy surface calculations
  - SSAGES "driver" code generates biasing forces for advanced sampling
  - Qbox provides DFT energy and forces
- Example: Path Integral simulations (http://ipi-code.org)
  - i-PI "driver" generates configuration for Path Integral sampling
  - Qbox provides DFT energy and forces
- Details: http://qboxcode.org/doc/html/usage/client-server.html#client-server-operation

Qbox+SSAGES client-server mode

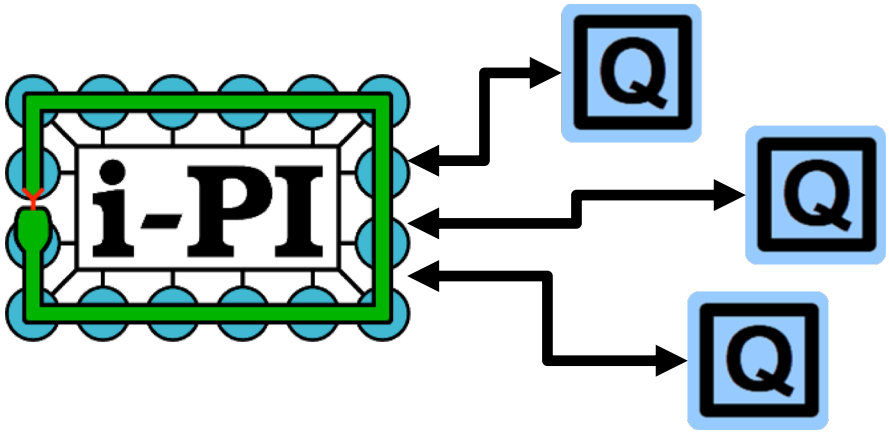
- Advanced sampling algorithms implemented in SSAGES https://ssagesproject.github.io/



H. Sidky *et al*, SSAGES: software suite for advanced general ensemble simulations, *J. Chem. Phys.* **148** 044104 (2018).

Qbox+i-PI client-server mode

- Path-integral sampling and quantum thermostats implemented in i-PI http://ipi-code.org



Ceriotti M *et al*, i-PI: A Python interface for ab initio path integral molecular dynamics simulations, *Comput. Phys. Comm.* **185** 1019-26, (2014).

Kapil et al., Comp. Phys. Comm. 236, 214–223 (2018)

Analyzing Qbox output: Qbox tools

- in /lcrc/project/MICCoM-train/qbox_tutorial/qbox/util
- Simple x-y plots (uses Gnuplot)
  - **`etotal.plt`** Kohn-Sham energy
  - **`econste.plt`** Check energy conservation
  - **`temp_ion.plt`** Temperature
  - **`force.plt`** Ionic forces
  - **`volume.plt`** Unit cell volume
- Analysis scripts
  - **`qbox_xyz.py`** Make xyz file for visualization
  - **`qbox_distance.py`** Distance between two atoms
  - **`qbox_angle.py`** Angle defined by three atoms
  - **`qbox_torsion.py`** Dihedral angle defined by four atoms
  - **`qbox_maxforce.py`** largest ionic forces

Extracting elements from Qbox output: XML parsers

- The “xml_grep” command can be used to extract elements from Qbox output

```
$ xml_grep sysname output.r

<?xml version="1.0" ?>
<xml_grep version="0.7" date="Tue Jul 28 10:59:52 2009">
<file filename="output.r">
  <sysname> Linux </sysname>
</file>
</xml_grep>


$ xml_grep --nowrap sysname output.r
<sysname> Linux </sysname>
```

- Using XML and XML parsers is safer than using plain text and grep

Tutorial

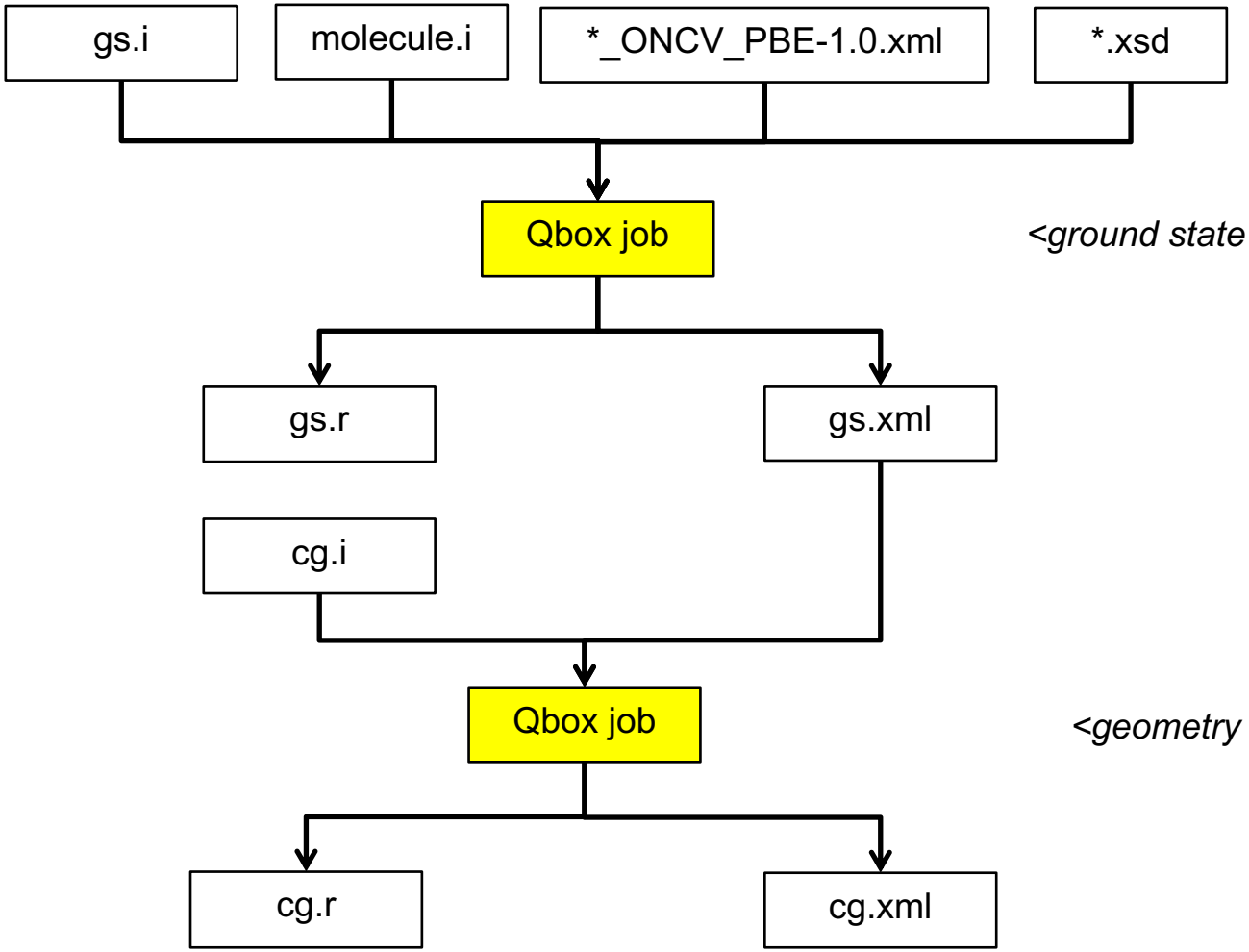
Qbox commands

- List all commands using the “help” command

```
[qbox] help
 valid commands are:

 angle            atom             bisection        compute_mlwf
 constraint       distance         extforce         fold_in_ws
 help             kpoint           list_atoms       list_species
 load             move             partial_charge   plot
 print            quit             randomize_r      randomize_v
 randomize_wf     rescale_v        reset_rotation   reset_vcm
 response         rseed            run              save
 set              set_velocity     species          spectrum
 status           strain           torsion
```

Workflow


gs.i
molecule.i
*_ONCV_PBE-1.0.xml
*.xsd
Qbox job
<ground state calculation>
gs.r
gs.xml
cg.i
Qbox job
<geometry optimization>
cg.r
cg.xml

Extracting elements from Qbox output: XPath syntax

- XPath is a WWW standard for referring to fragments of XML documents

```
$ xml_grep 'atom[@name="Si2"]/position' cg1.r

<?xml version="1.0" ?>
<xml_grep version="0.7" date="Tue Jul 28 11:09:34 2009">
<file filename="cg1.r">
  <position> 0.00000000 2.00000000 0.00000000 </position>
  <position> 0.00000000 2.10021981 0.00000002 </position>
  <position> 0.00000000 2.12916202 0.00000002 </position>
  <position> 0.00000000 2.16991837 0.00000003 </position>
  <position> 0.00000000 2.19074911 0.00000004 </position>
  . . .
```

- World Wide Web Consortium (W3C) http://www.w3.org
- XPath: http://www.w3.org/TR/xpath

The Qbox sample file

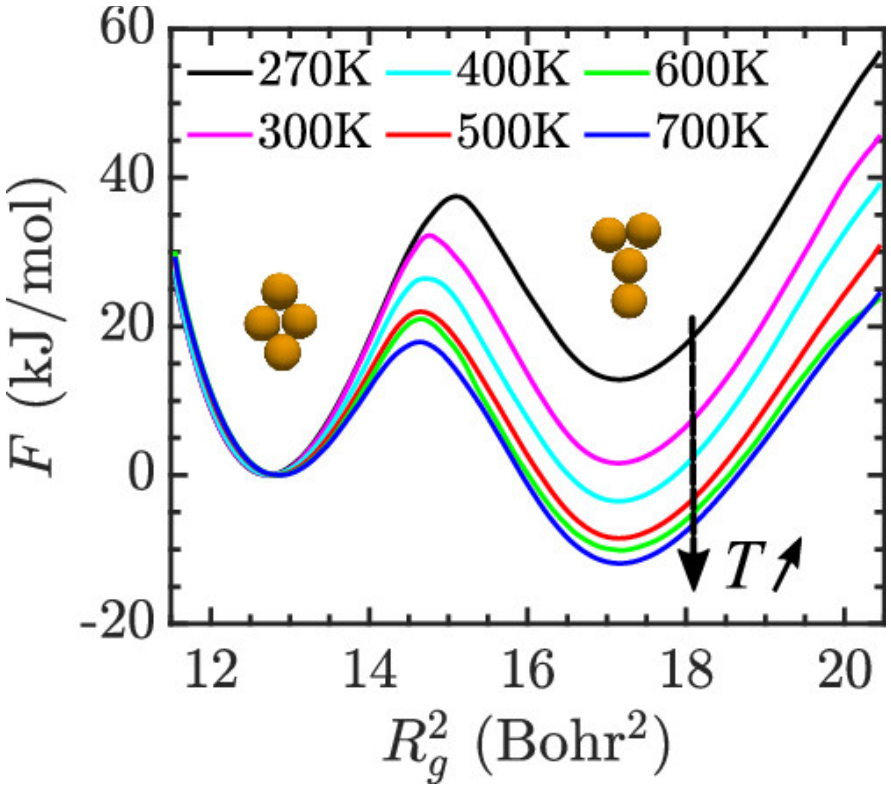
- Qbox saves its current state in a sample file (restart file) using the **`save`** command.
- Sample files can be reloaded later using the **`load`** command
- Qbox sample files conform to the XML schema specified at

  http://www.quantum-simulation.org
- Sample files are portable across platforms

Encoding binary data

- Part of the information in restart files consists of large arrays of floating point data
- Could be saved in binary form in a separate file (but would not be portable)
- Keeping track of multiple files lead to confusion and errors
- Qbox uses base64 little-endian encoding
  - inflates data by 30%
  - portable
- Keep a single-file model: One sample, one file.

Free energy simulation of Au_4



J. Shi, S. Huang, F. Gygi, J.K. Whitmer, "Free-Energy Landscape and Isomerization Rates of Au_4 Clusters at Finite Temperatures", J. Chem. Phys. A 126, 3392-3400 (2022).

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qbox_tutorial/examples/dce
Free energy barriers

- The example in **qbox_tutorial/examples/dce** includes the calculation of the free energy profile of 1,2 dichloroethane as a function of the Cl-C-C-Cl dihedral angle