Qbox tutorial

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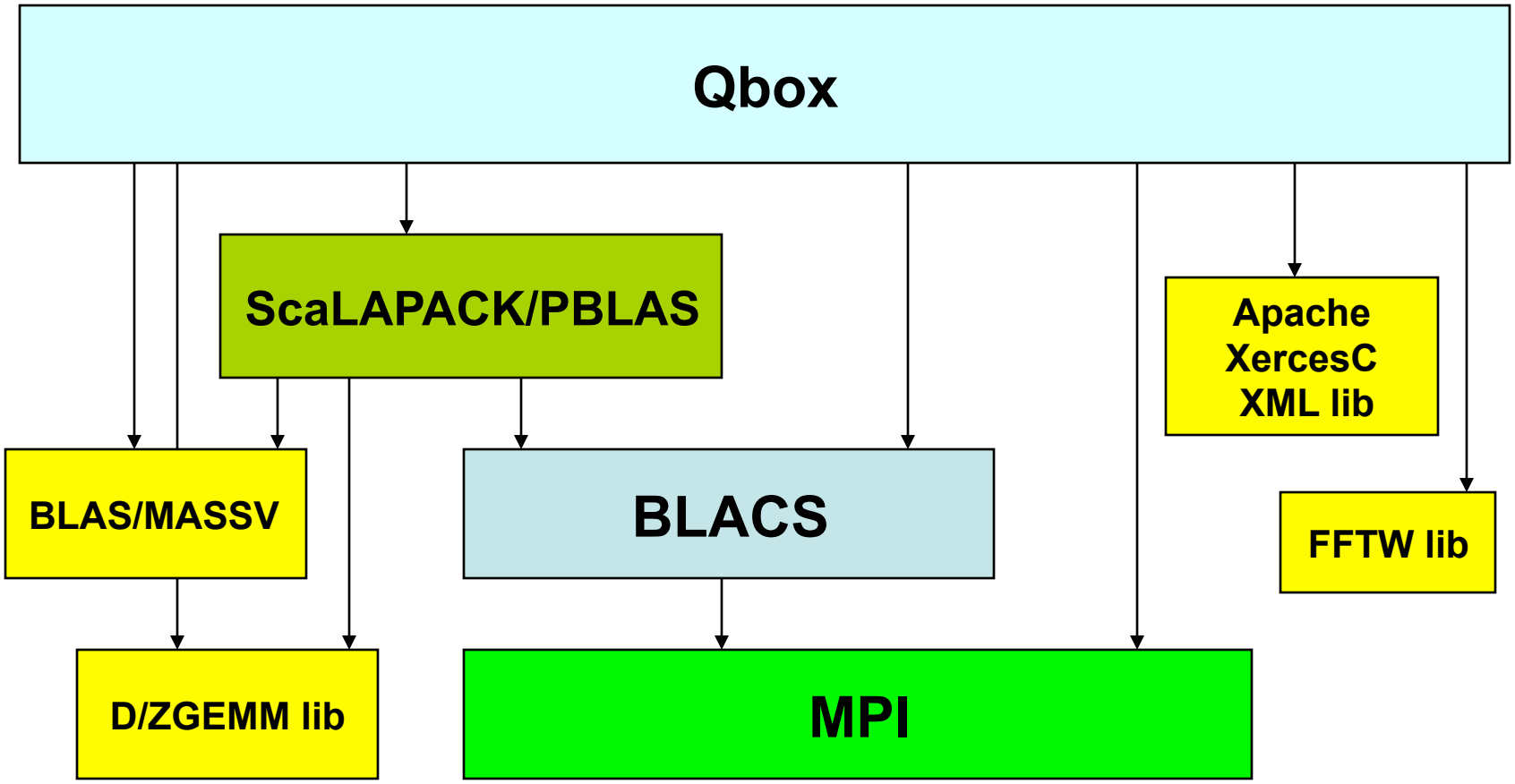
Qbox code: main features

- C++/MPI implementation of First-Principles Molecular Dynamics
- DFT/GGA and hybrid DFT exchange-correlation
- Plane-wave, norm-conserving pseudopotentials
- Designed for large-scale parallel platforms
- Built on optimized parallel libs: PBLAS, ScaLAPACK
- XML interface
- Installed on BlueGene/Q, Cray XC40, …, MacBook
- http://qboxcode.org

Qbox code architecture



F.G., IBM J. Res. Dev. **52**,137 (2008)

Downloading Qbox

- Downloading:
  - http://qboxcode.org/download

```
$ svn export http://qboxcode.org/svn/qb/tags/rel1_63_7
$ git clone https://github.com/qboxcode/qbox-public.git
```

- MacOS X precompiled version:

http://qboxcode.org/download/qbox-1.63.5-OSX-Yosemite.tgz

- Compiling:
  - http://qboxcode.org/build

Qbox basic operation

- Start Qbox in interactive mode (serial version)
  - $ qb
  - Qbox prompt: [qbox]
- Start Qbox reading from an input script
  - $ qb input.i
- Start Qbox 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

angle	compute the angle formed by three atoms
atom	define an atom
bisection	apply recursive subspace bisection to wave functions
compute_mlwf	compute maximally localized Wannier functions
constraint	manage constraints on atomic positions
distance	compute the distance between two atoms
extforce	add external forces on atoms
fold_in_ws	fold atoms into the Wigner-Seitz cell
help	print a short message about the use of a command
kpoint	add or remove k-points
list_atoms	print a list of currently defined atoms
list_species	print a list of currently defined atomic species
load	load a sample from a file previously saved
move	move atoms
partial_charge	compute the amount of charge in atom-centered spheres.
plot	generate a plot file with atoms and/or charge density

Qbox commands

print	print the value of a Qbox variable
quit	exit Qbox
randomize_r	add random noise to the atomic positions
randomize_v	initialize velocities with a Maxwell Boltzmann distribution
randomize_wf	add random noise to the wavefunction coefficients
rescale_v	rescale all atomic velocities
reset_vcm	set the velocity of the center of mass to zero
rseed	initialize the random number generator
run	run MD or electronic optimization steps
save	save a sample on a file for later use
set	assign a value to a Qbox variable
set_velocity	set the velocity of an atom
species	define a new atomic species
status	print a summary of the current state
strain	impose a strain on the sample
torsion	compute the dihedral angle defined by four atoms
!(shell escape)	execute a shell command

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_vcm        rseed
 run              save             set              set_velocity
 species          status           strain           torsion

[qbox]
```

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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 user guide: QboxUserGuide.pdf
  - http://qboxcode.org/QboxUserGuide.pdf

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 variables

alpha_PBE0	coefficient of HF exchange in PBE0
atoms_dyn	ionic dynamics control variable
blHF	bisection levels in Hartree-Fock exchange
btHF	bisection threshold in Hartree-Fock exchange
cell	dimensions of the unit cell
cell_dyn	unit cell dynamics control variable
cell_lock	control of allowed unit cell motions
cell_mass	fictitious mass of the unit cell
charge_mix_coeff	mixing coefficient for charge density update
charge_mix_ndim	Anderson dimension for charge density mixing
charge_mix_rcut	Kerker screening for charge density update
debug	debug parameters (not for normal use)
dt time	step (a.u.)
ecut	plane wave energy cutoff (Ry)
ecutprec	energy cutoff of the preconditioner (Ry)
ecuts	energy cutoff of the confinement potential

Qbox variables

e_field	applied electric field
emass	fictitious electronic mass (for CP dynamics)
ext_stress	externally applied stress
fermi_temp	Fermi temperature (K)
iter_cmd	script executed every iter_cmd_period steps
iter_cmd_period	number of steps between iter_cmd executions
nempty	number of empty states
net_charge	net charge of the system
nrowmax	maximum size of process grid columns
nspin	number of spin degrees of freedom
polarization	algorithm used to compute dipole and quadrupole
ref_cell	dimensions of the reference unit cell
scf_tol	tolerance criterion for SCF iterations
stress	stress control variable

Qbox variables

thermostat	thermostat control variable
th_temp	thermostat temperature (K)
th_time	thermostat time constant (a.u.)
th_width	thermostat width (K)
wf_diag	wavefunction diagonalization control variable
wf_dyn	wavefunction dynamics control variable
xc	exchange-correlation control variable

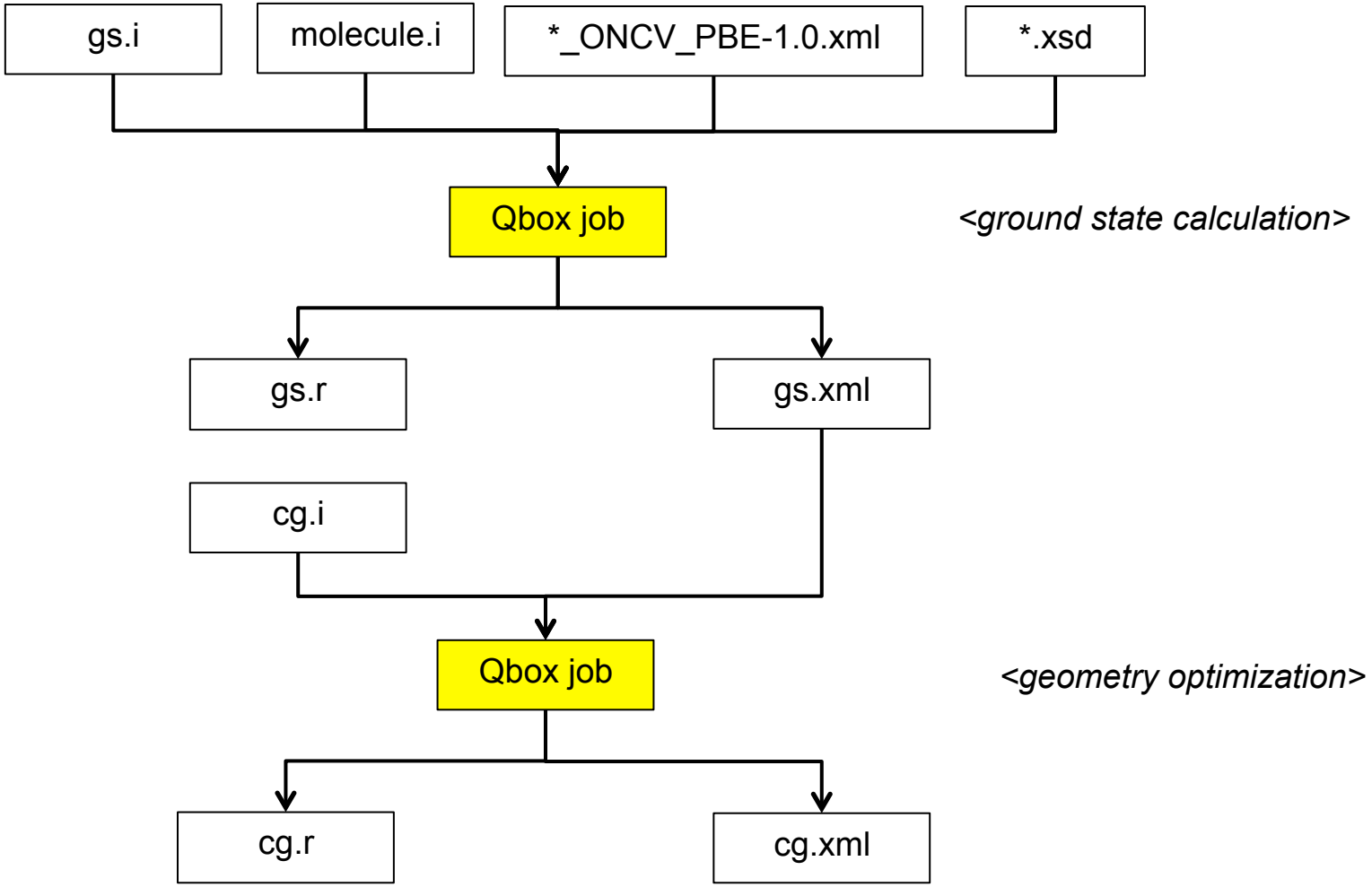
A simple Qbox input script

```
# optimization of the geometry of Si4
set cell 20 0 0  0 20 0  0 0 20
species silicon http://fpmd.ucdavis.edu/potentials/Si/Si_HSCV_LDA-1.0.xml
atom Si1 silicon  3.500  0.000  0.000
atom Si2 silicon  0.000  2.000  0.000
atom Si3 silicon -3.500  0.000  0.000
atom Si4 silicon  0.000 -2.000  0.000
set ecut 6

# compute the electronic ground state
# select wavefunction optimization algorithm
set wf_dyn PSDA
# randomize wavefunctions to avoid high symmetry saddle points
randomize_wf
# run 200 SCF iterations
run 0 200

# optimize the geometry, running 50 ionic steps with 5 SCF steps
set atoms_dyn CG
run 50 5
. . .
```

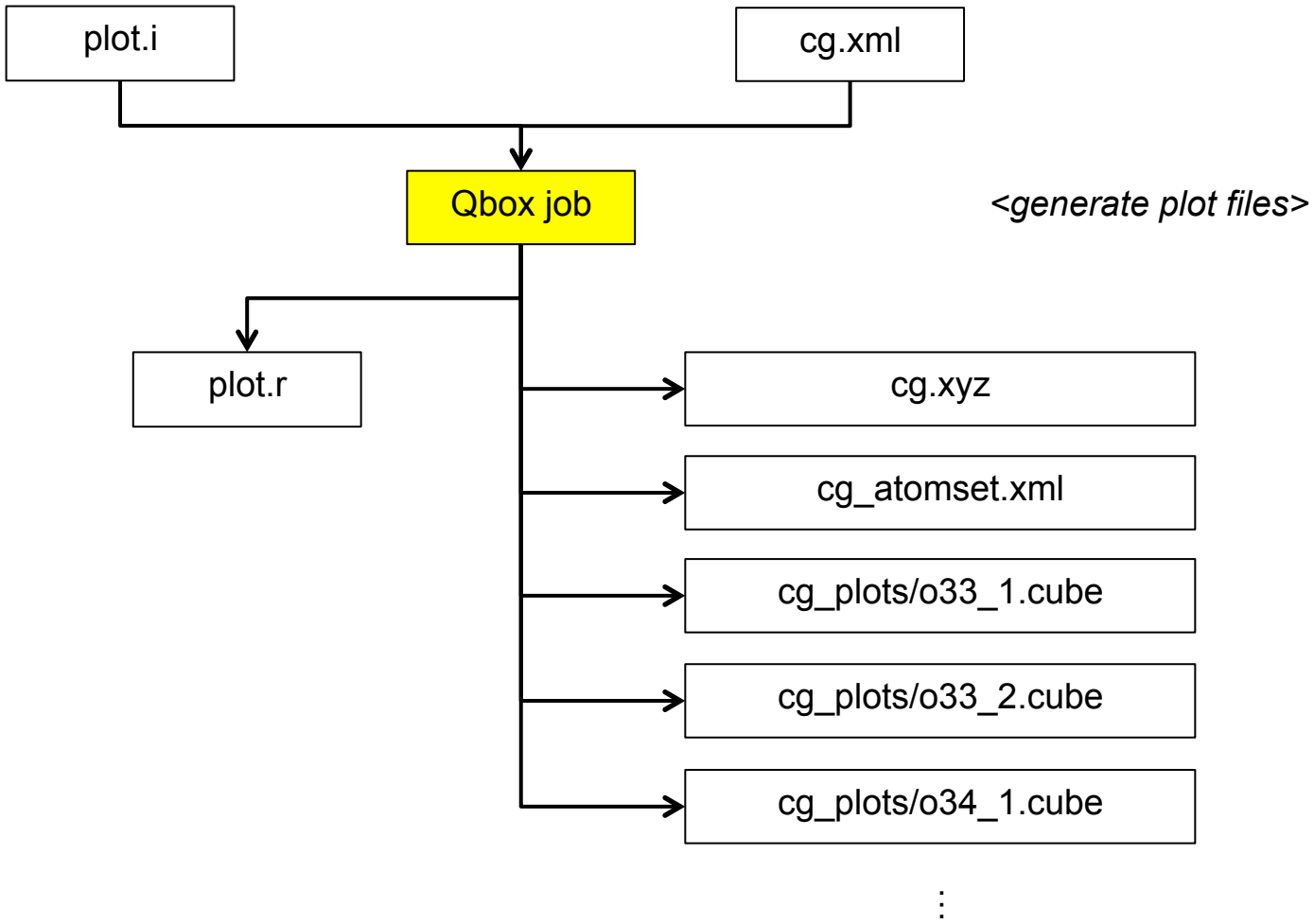
A simple Qbox input script

```
. . .

# displace one atom
move Si2 by 0.2 0 0

# recalculate the ground state
run 0 20

# run MD simulation
set atoms_dyn MD
set dt 40
run 100 5

# save sample for later use
save md.xml
```

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

Workflow


plot.i
cg.xml
Qbox job
<generate plot files>
plot.r
cg.xyz
cg_atomset.xml
cg_plots/o33_1.cube
cg_plots/o33_2.cube
cg_plots/o34_1.cube
⋮

Qbox output: an XML document

```
<?xml version="1.0" encoding="UTF-8"?>
<fpmd:simulation xmlns:fpmd="http://www.quantum-simulation.org/ns/fpmd/fpmd-1.0">

                    ============================
                    I qbox 1.63.5              I
                    I                          I
                    I                          I
                    I                          I
                    I                          I
                    I                          I
                    I                          I
                    I                          I
                    I                          I
                    I                          I
                    I                          I
                    I                          I
                    I                          I
                    I http://qboxcode.org      I
                    ============================

<release> 1.63.5 midway </release>
<user> fgygi </user>
```

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Qbox output: an XML document

```
. . .
<sysname> Linux </sysname>
<nodename> midway088 </nodename>
<start_time> 2017-07-16T23:37:16Z </start_time>
<mpi_processes count="1">
<process id="0"> midway088 </process>
</mpi_processes>
[qbox]
```

Analyzing Qbox output: Qbox tools

- http:/qboxcode.org/tools
- Simple x-y plots
  - **`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`** 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

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
- We use base64 little-endian encoding
  - inflates data by 30%
  - portable
- Keep a single-file model: One sample, one file.

The Qbox sample file

```
<?xml version="1.0" encoding="UTF-8"?>
<fpmd:sample xmlns:fpmd="http://www.quantum-simulation.org/ns/fpmd/fpmd-1.0"
 xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
 xsi:schemaLocation="http://www.quantum-simulation.org/ns/fpmd/fpmd-1.0
sample.xsd">
<description>  Created 2017-07-08T23:19:03Z by qbox-1.63.5  </description>
<atomset>
<unit_cell
    a=" 16.00000000   0.00000000   0.00000000"
    b="  0.00000000  16.00000000   0.00000000"
    c="  0.00000000   0.00000000  16.00000000" />
<species name="silicon" href="silicon.xml"/>
  <atom name="Si1" species="silicon">
    <position>   3.78993440  -0.05782115  -0.00028353   </position>
    <velocity>  6.481116e-05 -7.347506e-05 -5.581231e-08 </velocity>
  </atom>
  <atom name="Si2" species="silicon">
    <position>   0.05373812   2.25793417   0.00133574   </position>
  . . .
```

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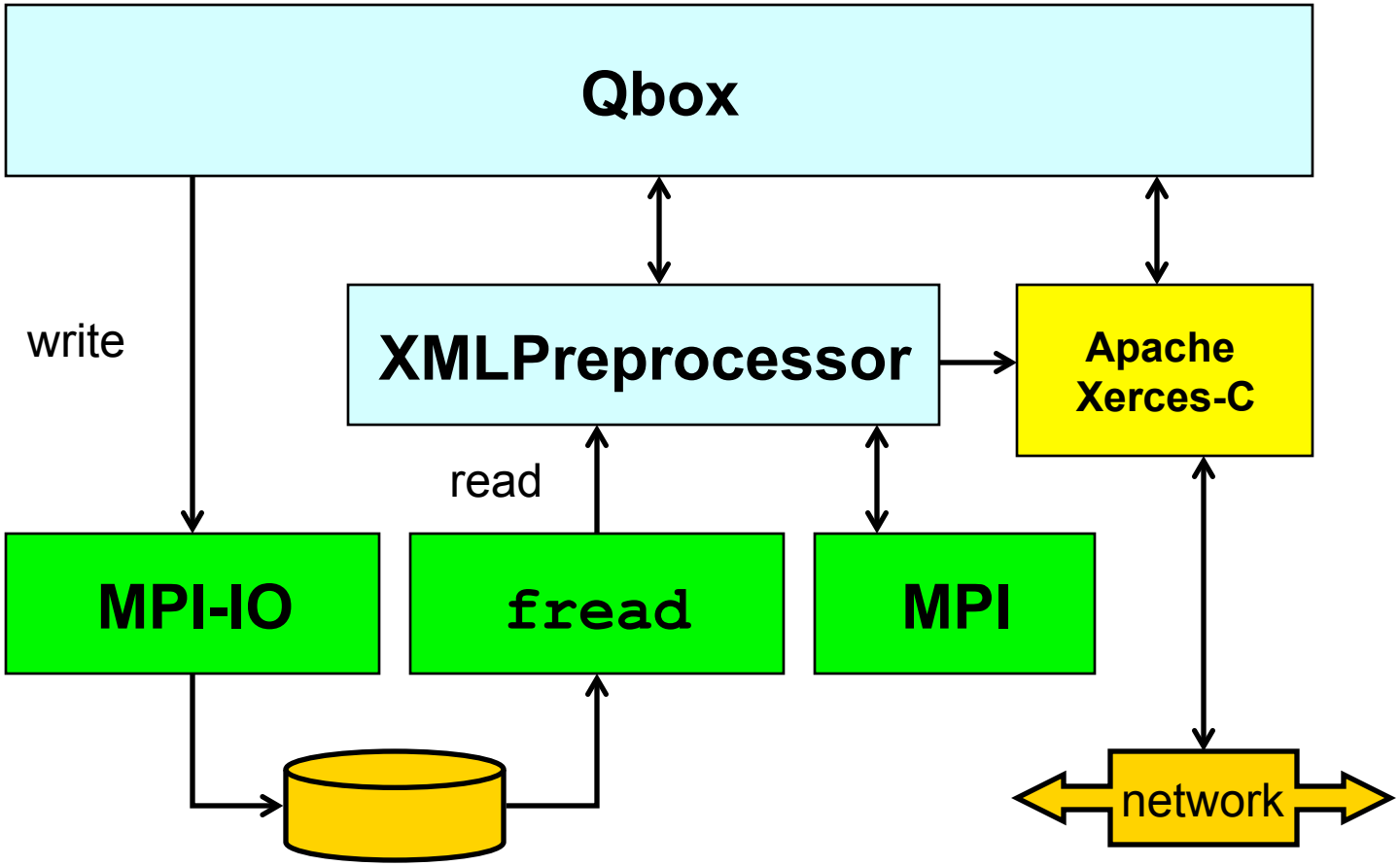
The Qbox sample file (cont'd)

```
. . .
<wavefunction ecut="3" nspin="1" nel="16" nempty="0">
<domain a="16 0 0"
        b="0 16 0"
        c="0 0 16"/>
<grid nx="14" ny="14" nz="14"/>
<slater_determinant kpoint="0 0 0"
  weight="1" size="8">
<density_matrix form="diagonal" size="8">
 2.00000000 2.00000000 2.00000000 2.00000000 2.00000000 2.00000000 2.00000000
2.00000000
</density_matrix>
<grid_function type="double" nx="14" ny="14" nz="14" encoding="base64">
JOKp5mfU7j8lTFHumHAZwGswARq/giHA4ZbowT3hFMBArxDWNAnWv2OdQWQ4qO8/hnpXb9Ys
4z/iCe2p/wLaP7CA2Fsl48g/JyPLTVjOtz+YesKvbXq3Pzz795WF18o/lh9MpNXF8D9PE2Sa
omQEQDsgdtEK5xBAjjyqjXY/IEBcCDauHK8oQBGbSjqfJSNAjfWgJxuC/D86W50+3NoQwKJW
T16svxbAXBamLa3zB8AsgTTCugPRPxGpsQzMuu4/vtv7o04r5D/G3xkZWfLaPyBgoXndC8Y/
9TVNRHx/tT8IdDgiFui0P17fmNFDdMM/PhR12ITj6T9ScaluessCQHW7UqHpLhFApFUza8LG
H0BKfH+Z26QnQGo7CljS7yJAftATNO8dCECLXX2o0h3zvwLD7E54sgDAqEOt93M58b+m9D5g
. . .
```

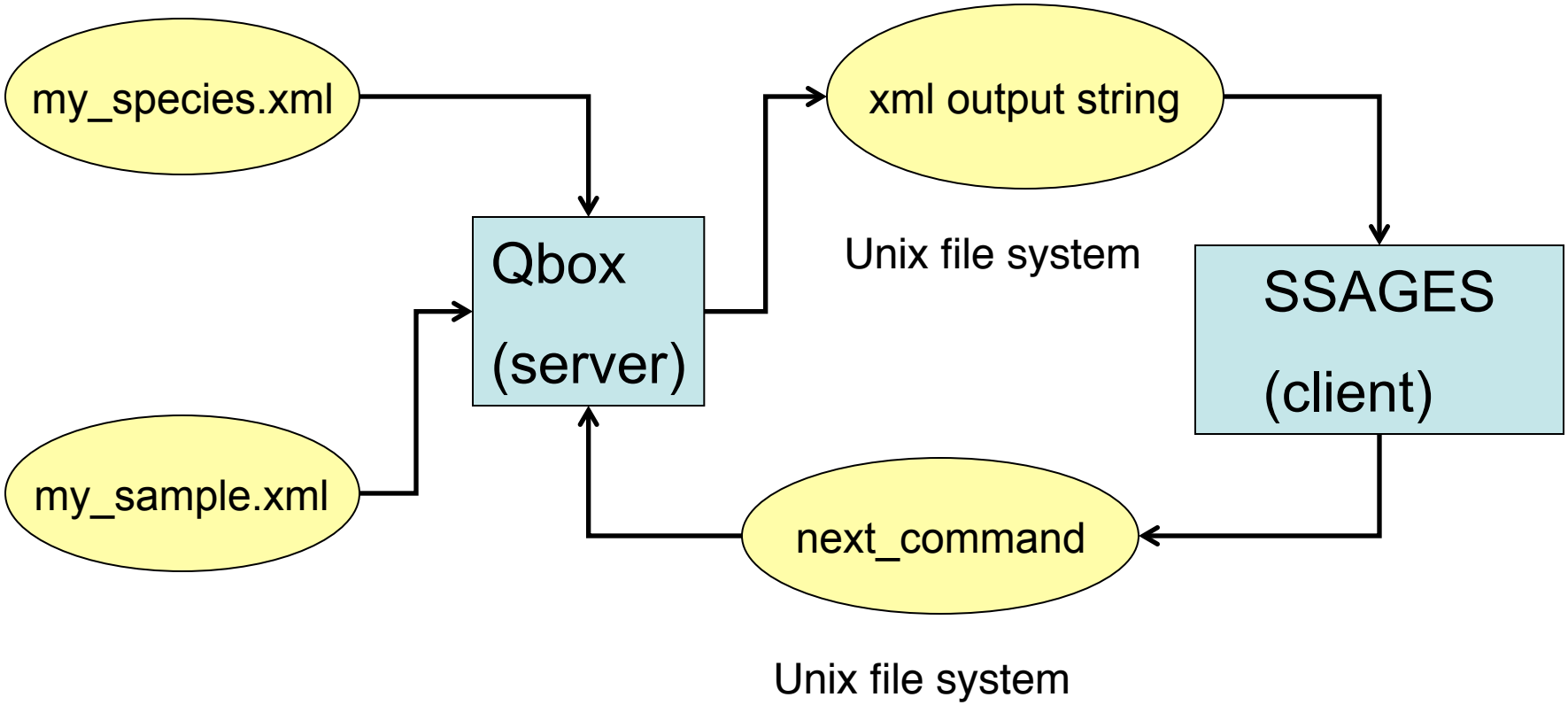
Qbox I/O


Qbox
write
XMLPreprocessor
Apache
Xerces-C
read
MPI-IO
fread
MPI
network

Coupling Qbox with other codes: a client-server model

- In some applications, it is useful to have quantum simulations “driven” by another simulation code
- Example: Free energy surface calculations
  - SSAGES "driver" code generates biaising forces
  - Qbox updates positions and velocities using DFT forces
- Requires two-way communication between the driver and Qbox
- File-based Client-server model

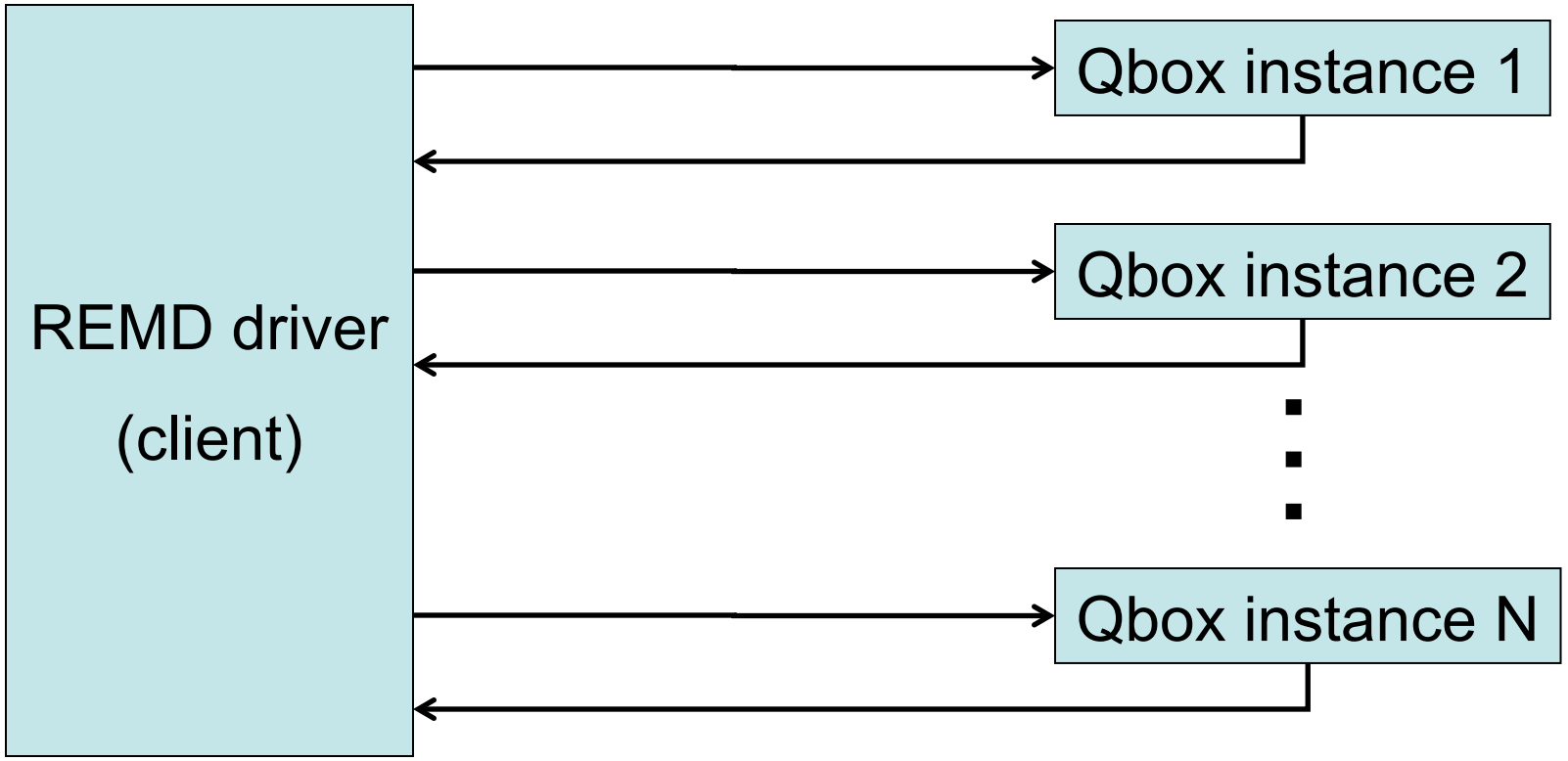
Qbox client-server implementation



Client and server may run on separate platforms

(must share an NFS file system)

Qbox client-multiple server (e.g. replica exchange MD)

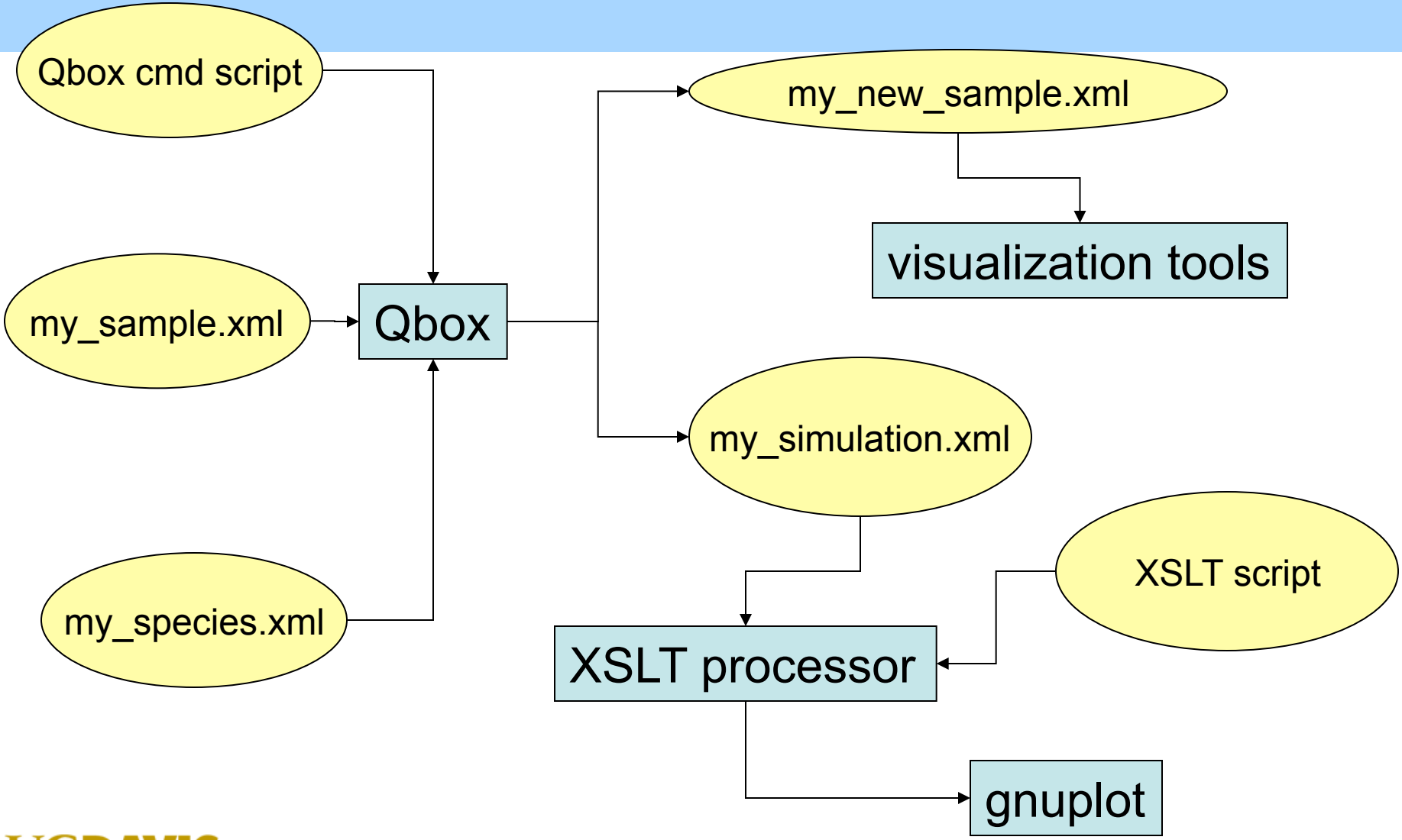


Also applies to: Nudged Elastic Band, Swarm of Trajectories, etc.

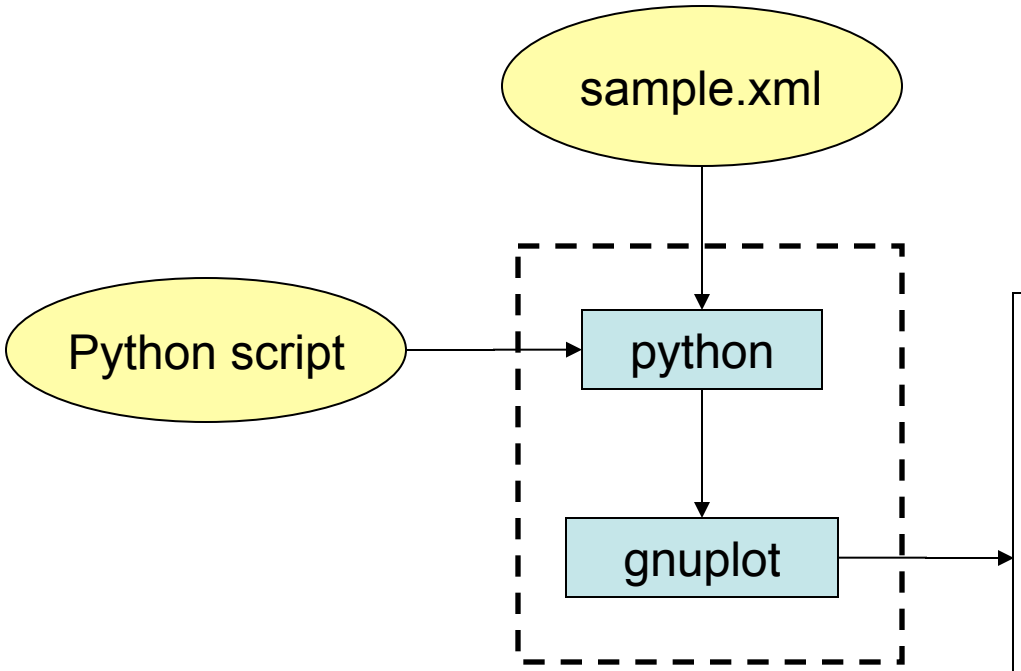
Post-processing

- Users build post-processing pipelines
- **`xsltproc`** XSLT processor
  - namespace-aware
  - web-aware (can post-process web-based samples)
- **`xml_grep`** (Perl Twig toolkit)
  - easy to use in scripts (uses the XPath language)
- Some applications based on libxml2
- Python scripts: **`xml.sax, etree`**

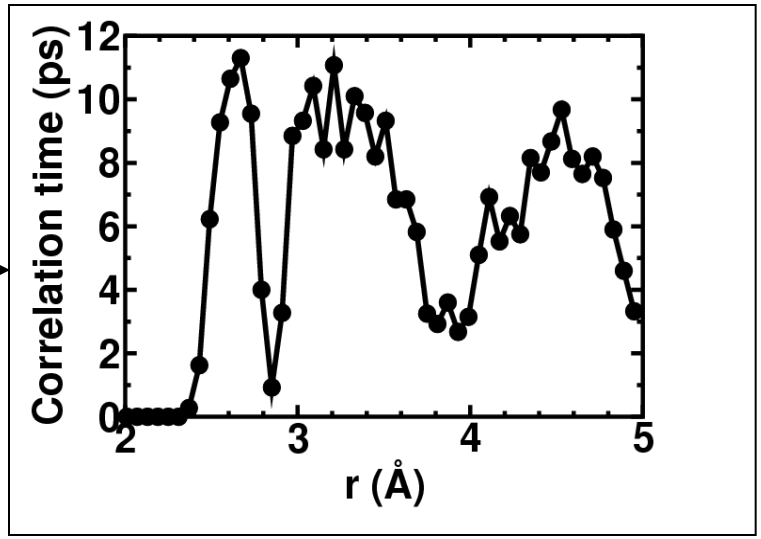
Post-processing pipelines



Data analysis using mixed scripts



- Python and gnuplot scripts embedded in a bash shell script



Qbox examples on **midway.rcc.uchicago.edu**

- **/project2/miccom-school/qbox/examples**
  - **ch4** CH_4 molecule
  - **c60** C_{60} molecule
  - **h2o** H_2O molecule
  - **h2ofield** H_2O molecule with electric field
  - **h2o32** Liquid water
  - **heliq** Liquid helium
  - **o2gs** Oxygen molecule
  - **silicon** Silicon crystal
  - **si64liq** Liquid silicon at 2000 K
  - **glycol** Ethylene glycol isomerization