

Modulization of Quantum Theories for Web Platform

PRAGMA 36

April 25, 2019

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Quantum Mechanics

- “*The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.*” by Dirac in 1929.

Quantum Mechanical Software

The Nobel Prize in Chemistry 1998

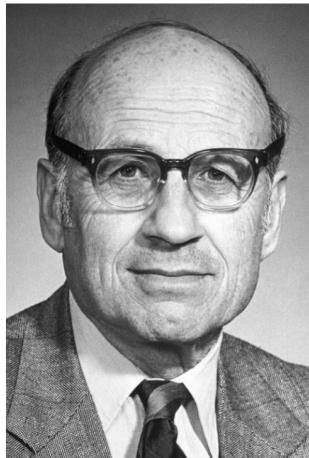


Photo from the Nobel Foundation archive.

Walter Kohn

Prize share: 1/2

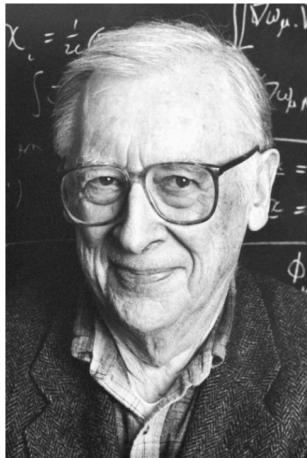
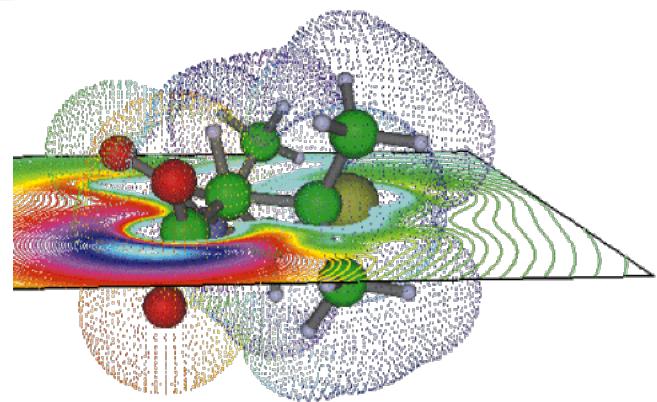


Photo from the Nobel Foundation archive.

John A. Pople

Prize share: 1/2

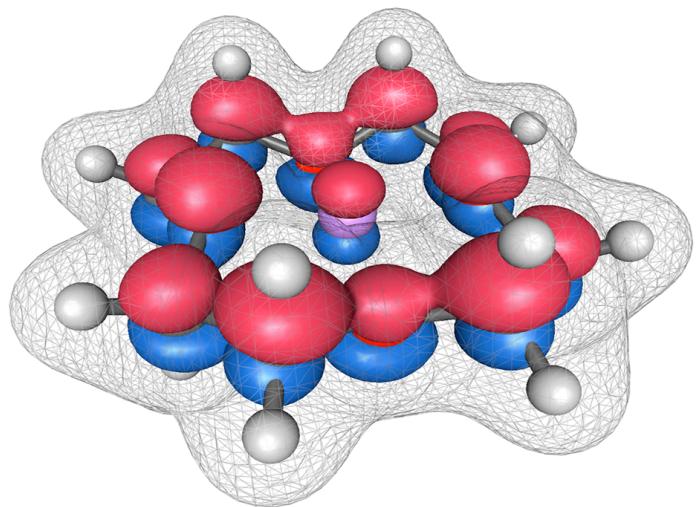


Gaussian
GAMESS
ACES
MolPro
COLUMBUS
NWChem
Qchem
etc

The Nobel Prize in Chemistry 1998 was divided equally between Walter Kohn "for his development of the density-functional theory" and John A. Pople "for his development of computational methods in quantum chemistry."

Closed Community

- Limited Developers
- Closed Development Environments
- Legacy Codes ~ 60 yrs old
- No Interoperability
- Difficult Maintenance



Modulization Movements

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Home > Volume 92 Issue 34 > Quantum Chemistry's Modular Movement

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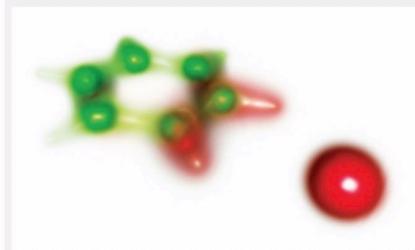
Volume 92 Issue 34 | p. 26
Issue Date: August 25, 2014

Quantum Chemistry's Modular Movement

ACS Meeting News: Software developers seek to reduce redundancy by writing reusable code

By Elizabeth K. Wilson

[+Enlarge]



SUSTAINABLE SIMULATION

Software developed with the PANACHE library created this model of benzene being polarized by a sodium cation.

Credit: Robert Parrish

Modern chemists who want to use computers to predict molecular structures or probe the dynamics of chemical reactions have a wealth of quantum chemistry software packages from which to choose.

That's great for the scientists using the software. But for academic researchers who develop quantum chemistry software packages, it can mean months of code-writing drudgery.



No more
reinventing
wheel!

C&EN, 2014, v94(34), p26

But how?

Science with IT

- Science Software with the Help of IT
- Web Platform
- Modularization at App Level
- Decentralized Control by Community

Basic Modules

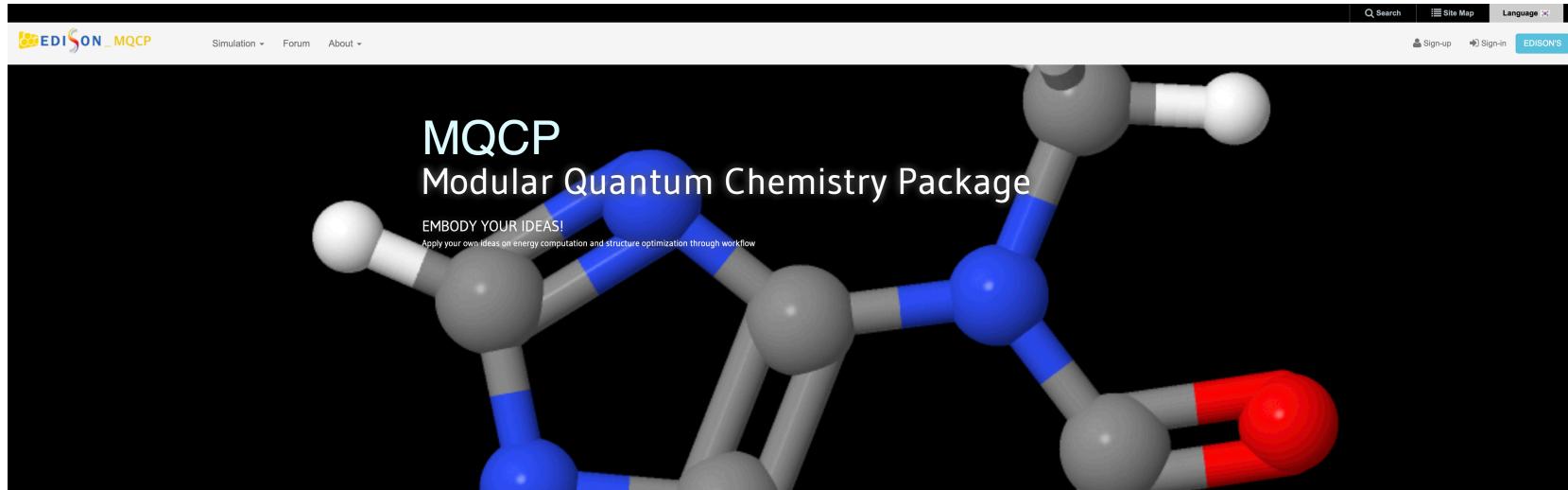
- Inputs
- Parameter Settings
- Initial Orbital Guess
- Integrals
- SCF: Self-consistent field
- Energy Calculations
- Gradient Calculations
- Geometry Optimizer
- Hessian Calculations

Intermediate Files and Data Types

- IR = 5 : INPUT
- IW = 6 : OUTPUT
- IVU = 9 : VECU
- IFU = 10 : FOCK MATRIX
- IOU = 11 : ORBITAL
- XYZ = 12 : Geometry
- INF = 13 : Information
- SHL = 14 : SHELLS
- HST = 15 : H, S and T matrices
- DMT = 16 : Density matrices
- MOE = 17 : Energy, MO energy and orbitals

데이터타입명	버전
mqcp_counter	V1.0.0
mqcp_dmt	V1.0.0
mqcp_fcm	V1.0.0
mqcp_Geom_Cvged	V1.0.0
mqcp_hst	V1.0.0
mqcp_ifl	V1.0.0
mqcp_inf	V1.0.0
mqcp_inp	V1.0.0
mqcp_log	V1.0.0
mqcp_moe	V1.0.0
mqcp_shl	V1.0.0
mqcp_xyz	V1.0.0

MQCP



The image shows the MQCP logo. It features a 3D molecular model composed of grey spheres (representing carbon) and blue spheres (representing nitrogen). A red sphere (representing oxygen) is also present. The text "MQCP" and "Modular Quantum Chemistry Package" is overlaid on the molecule. Below the molecule, the tagline "EMBODY YOUR IDEAS!" and the subtext "Apply your own ideas on energy computation and structure optimization through workflow" are displayed.

EDISON MQCP

Simulation ▾ Forum About ▾

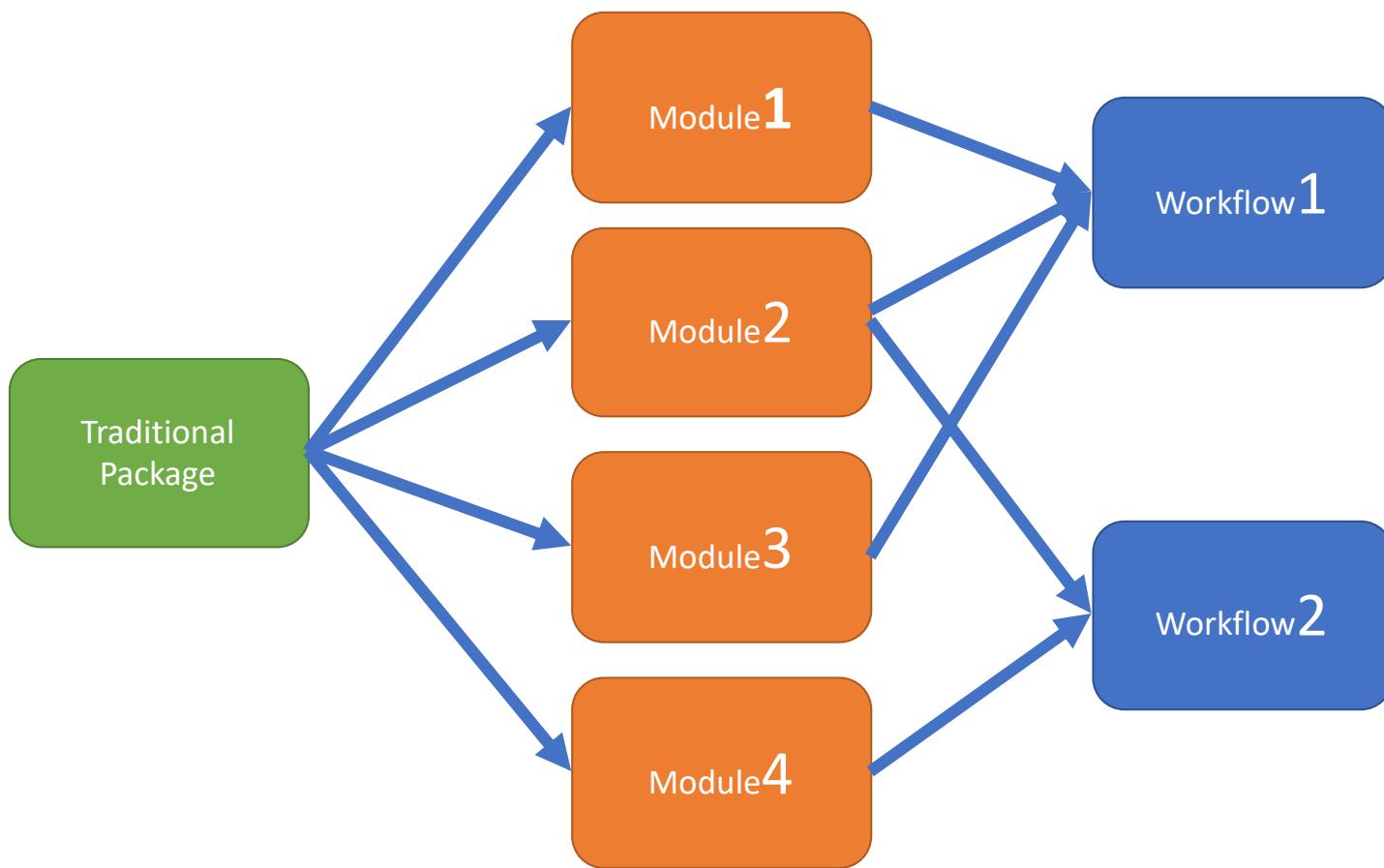
Search Site Map Language

Sign-up Sign-in EDISON

MQCP
Modular Quantum Chemistry Package

EMBODY YOUR IDEAS!
Apply your own ideas on energy computation and structure optimization through workflow

SO How does it work?



The Modules

ScienceApp Search

ScienceApp v

Paths > MQCP > Quantum Chemistry

ScienceApp (22 Found)

Latest

new_coordinates
New Coordinates for Modular Quantum Chemistry Package (MQCP)
version : 1.0.0 / Owner : chchoi

HF' initial_hessian
Initial Hessian Guess for Modular Quantum Chemistry Package (MQCP)
version : 1.0.0 / Owner : chchoi

HF $\left(\frac{\partial E}{\partial x}\right)$ rhf_gradient
RHF Gradient Calculation for Modular Quantum Chemistry Package (MQCP)
version : 1.0.0 / Owner : chchoi

E_{HF} rhf_energy
RHF Energy Calculation for Modular Quantum Chemistry Package (MQCP)
version : 1.0.0 / Owner : chchoi

B3LYP B3LYP_RHF_Gradient
Gradient Calculation with B3LYP for Modular Quantum Chemistry Package (MQCP)
version : 1.0.0 / Owner : chchoi

E_{B3LYP} B3LYP_Energy
Main SCF with B3LYP for Modular Quantum Chemical Package(MQCP)
version : 1.0.0 / Owner : chchoi

Hückel_Guess
Initial Huckel Guess for Modular Quantum Chemistry Package
version : 1.0.0 / Owner : chchoi

1e⁻ HSandT
H, S and T matrices for Modular Quantum Chemistry Package(MQCP)
version : 1.0.0 / Owner : chchoi

6-31G basis_631g
6-31G basis set for Modular Quantum Chemical Package(MQCP)
version : 1.0.0 / Owner : chchoi

6-31G(d) basis_631gd
6-31G(d) basis set for Modular Quantum Chemical Package
version : 1.0.0 / Owner : chchoi

1 2 3

Module: Details



[Manual](#) [Run](#)

App Name	uChem
Version	4.0.2
App Type	Solver
Developer	Cheol Ho Choi
Date	2017-10-29
Rating	0.0 (0 vote)
Bookmark	☆

Category

[PRAGMA](#) [PRAGMA](#)
[Computational Chemistry](#)
[Quantum chemistry](#) [QMCP](#)
[Quantum Chemistry](#)

Statistics

👤 Simulation Users : 1,161
⌚ Simulation Runs : 23,236

Relate Info

📅 ScienceApp : 0
📁 Content : 0
💻 Simulation Project : 0
🌐 Community : 0

Detailed Info Relate Data Relate Info Review Statistics

Quantum Chemical Package with RHF and B3LYP Theories

Detailed Info

- Both RHF and B3LYP theories
- Energy as well as gradient calculations
- Geometry Optimizations
- 6-31G and 6-31G(d) basis sets

Input Port

#	Port Name	Datatype	Editor	Sample
1	-inp	uchem_4_input	FILE_SELECTOR,TEXT_EDITOR	-

Log Port

#	Port Name	Datatype	Editor	Analyzeer
1	Log	OSPText	-	OSPTextViewer

Output Port

#	Port Name	Datatype	Editor	Analyzeer
1	xyz	xyz	TEXT_EDITOR,KMOL	JSMol,OSPTextViewer,NGLViewer

Module: UChem

uChem
Ver 4.0.2

Simulations New Copy Delete Log Download Open Data Manual

tst

H2 molecule

#0002

input -inp log Log output xyz

#0001

2019-03-15-28-06.700/inp

natoms:11
6.0 -0.2814116433 -0.0914064155 0.0569146050
6.0 -0.0108420173 1.3451955938 -0.4302553427
6.0 -1.5164903822 -0.7099985842 -0.6138764961
1.0 0.5652250728 -0.7142140575 -0.1449089075
1.0 -0.3980187758 -0.0846805453 1.1288285918
1.0 0.2402967369 1.3696657263 -1.4851529300
1.0 -0.9033547396 1.9429289671 -0.2719580118
1.0 0.8176724903 1.7961170180 0.1140239055
1.0 -1.9541584238 -1.15030395028 -0.1071310512
1.0 1.212953834 -1.1336105793 -1.5855662126
1.0 -2.2652494650 0.0377688194 -0.7774286105
Hamilton: dft
Basis=6-31G(d)
charge=0
runtype=energy

coordinate.xyz

</>

JSmol

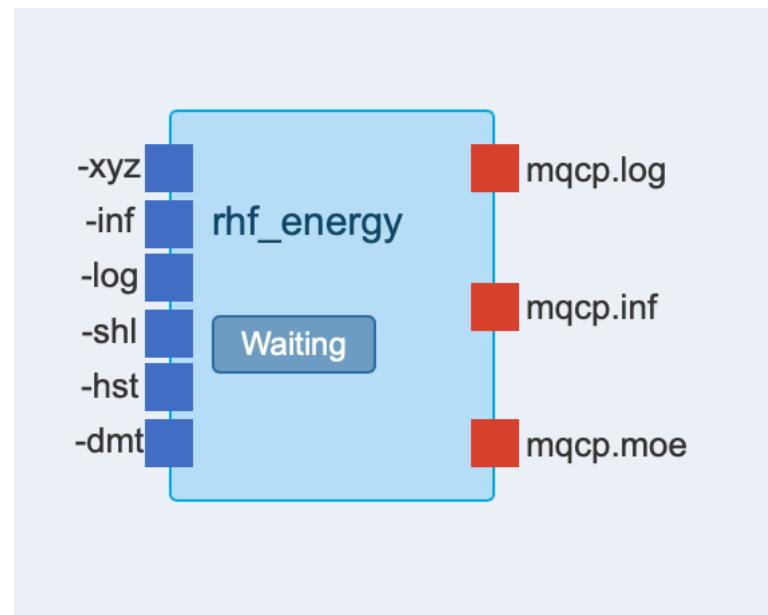
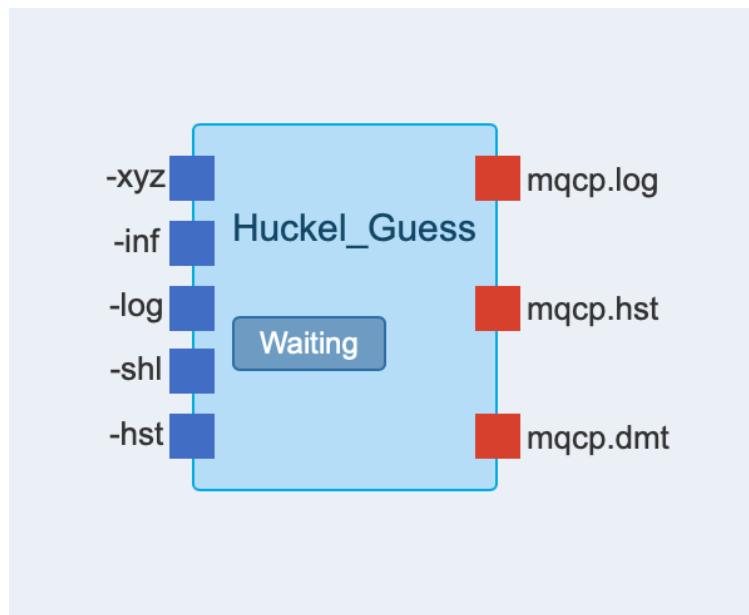
uchem.log

Execution of UChem begin at Tue Mar 5 15:28:10 2019

UChem is a pilot program initiated by Cheol Ho Choi
at Kyungpook National University on Aug. 2012
Geometry Optimization Included on Feb. 2015.

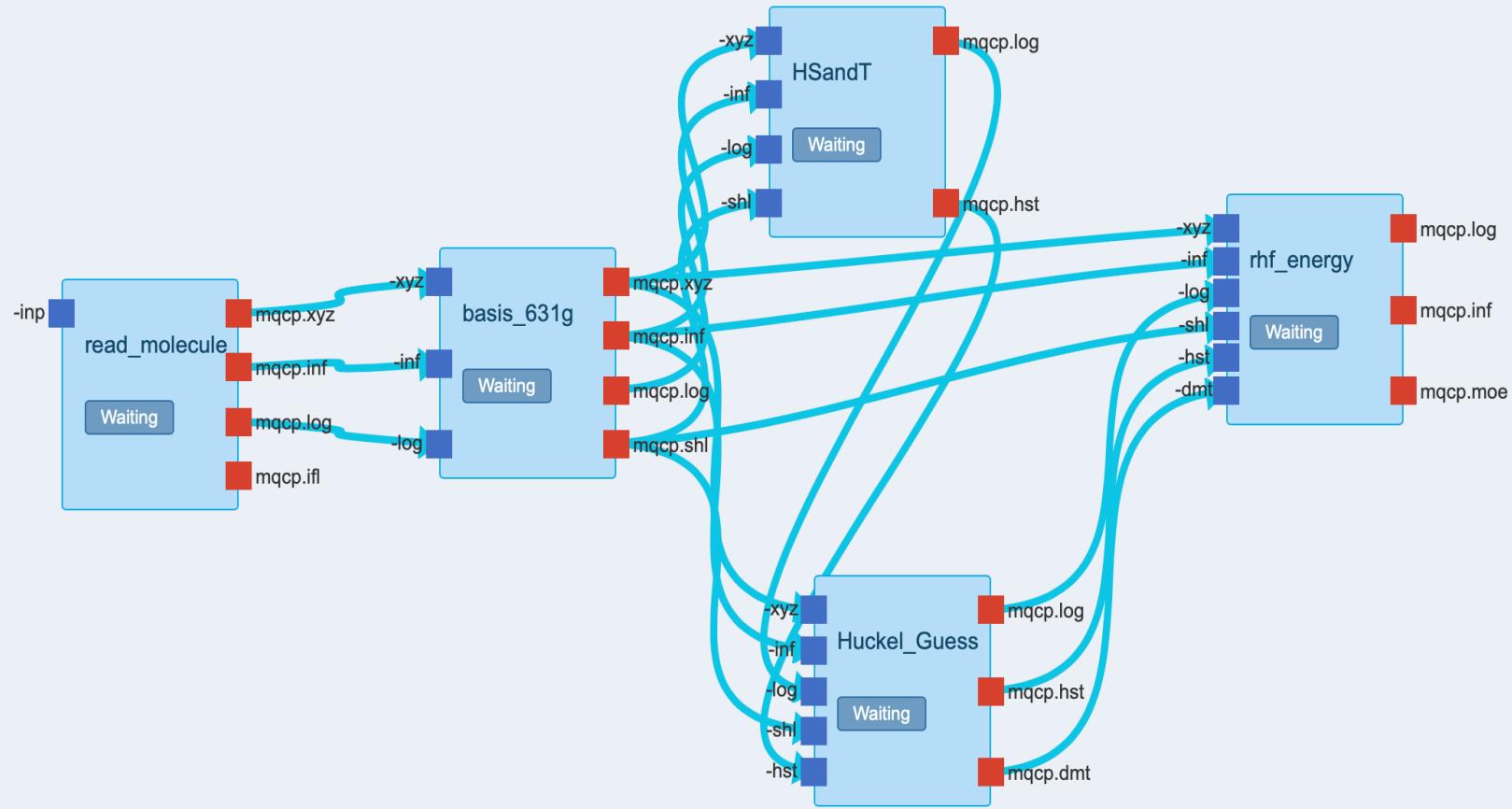
===== Atomic numbers and Cartesian Coordinates =====
Atom Name X Y Z
1 C -0.2814116433 -0.0914064155 0.0569146050
2 C -0.0108420173 1.3451955938 -0.4302553427
3 C -1.5164903822 -0.7099985842 -0.6138764961
4 H 0.5652250728 -0.7142140575 -0.1449089075
5 H -0.3980187758 -0.0846805453 1.1288285918
6 H 0.2402967369 1.3696657263 -1.4851529300
7 H -0.9033547396 1.9429289671 -0.2719580118

Module: The format

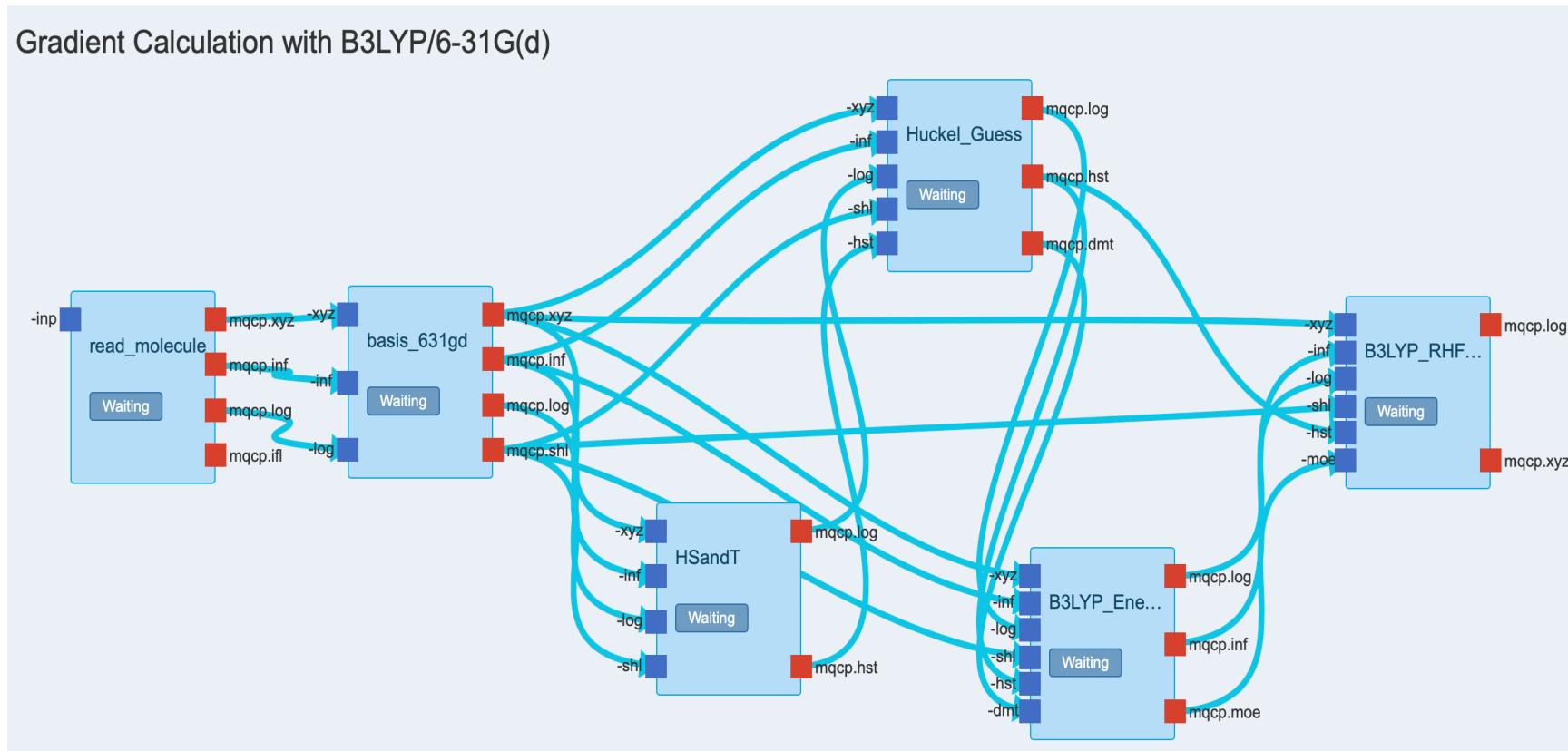


Workflow: Energy Calculation with HF/6-31G

Energy Calculation with HF/6-31G



Workflow: Gradient Calculation with B3LYP/6-31G



Advantages

- Open Development Environments
- Easy to add new modules
- Easy to create workflows
- Easy to maintain modules



Accelerating
Development Speed
of Scientific
Software

Acknowledgements

- Dr. Jung Heon Seo at KISTI
- Korea Institute of Science and Technology Information
- Samsung Science & Technology Foundation for financial supports

Science + IT → SIT

Thanks Much!