Master projects in Molcas group, Computational Chemistry

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https://www.molcas.org/VV/master_projects.html

Code development and research driven by code development

Large (50Mb of source code) computational package

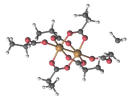
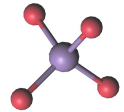
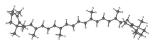
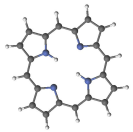
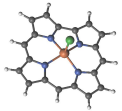
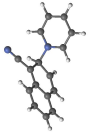
In Past: many PhD and postdoc projects

Tools	Symmetry adapted SCF orbitals. Basis set tools.
GUI	Point group recognition. Optimization in internal coordinates.
Data	Structure models for C-S-H. Energy profiles in ionic crystals.

Master projects in Past:

Present and future: Master projects in chemistry but with an optional knowledge of chemistry itself

Ex. 1. Benchmark suite: small large huge

								
BFs	388	540	244	90	840	406	429	312
CSF	3	15	226512	$2*10^6$	113456	$2*10^6$	1497	$2*10^6$
Time CAS	49’	1h53’	1h8’	4h	1h46’	1h16’	10’	2h28’
Time DGEMM $\alpha A^T B+\beta C$	49%	39%	86%	90%	38%	86%	36%	97%

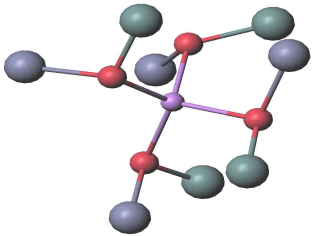
Problems: What are the sizes of these matrices, used in 10 000 000 DGEMM calls?
Can these calls be combined? What is the best CPU/GPU balance?

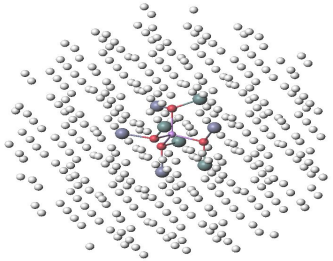
Ex 2. Tools

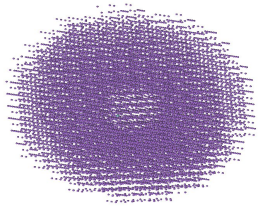
Used together with the main code. Small codes (mostly written in C/Julia/Python instead of FORTRAN). More easy to learn and to modify.

Typical examples: code to optimize basis sets, model potentials, charges, etc.

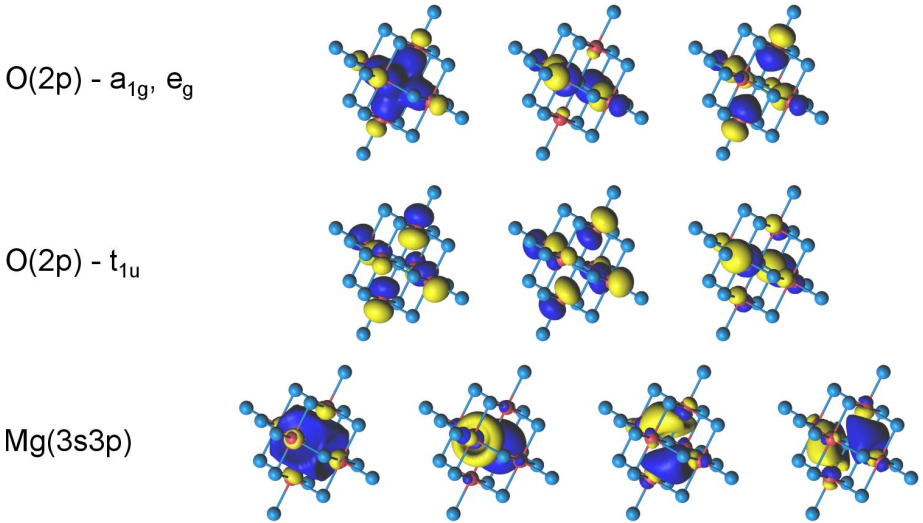
Typical problems: working prototype: no optimization, ugly interface, no GUI.







Ex 3. Visualization

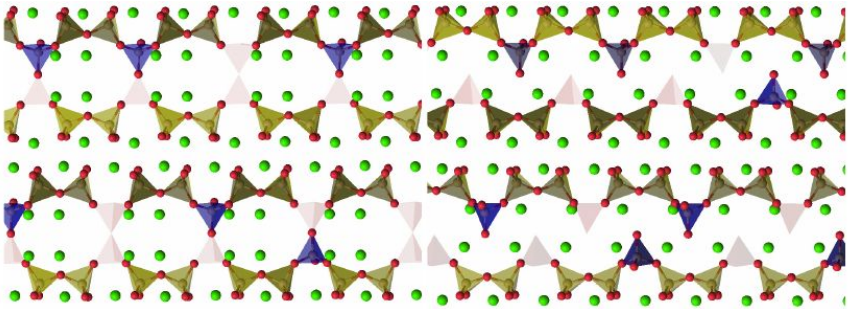


Homemade GUI (OpenGL, GTK+), to visualize orbitals: GV/LUSCUS

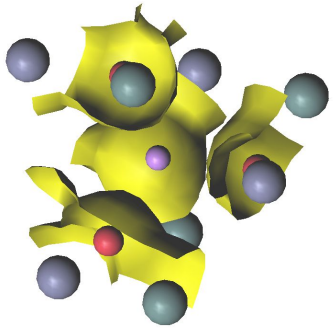
New features are needed: for example, 3D potential energy surfaces, tools to build clusters

Compact form of files with visualization data

Ex 4. Data analysis and databases



Structure of concrete >10^{30} possible variants



Mobility of Li atom in LISICON.
3D grid of points

Initial setup (of one calculation) requires ‘computational chemistry’ knowledge.

How to handle, 1000 (10000) similar calculations? How to store and present the results?