HOW TO USE ALL THOSE SCRIPTS AND ALIASES YOU JUST SET UP

HOW TO RUN ES2K

To run es2k jobs use the command 'runes2k' followed by the name of the folder of your project.
This is done from outside of it, contrary to how 'runes2k' works on Bovisa.
Upon succesful submission of a job to the scheduler, a one-liner confirmation message will be printed and also saved onto the ACTIVITY LOG.
G100 nodes carry 48 cores and about 350Gb of memory each: good values for 'numprocll' and 'gmemll' are 48 and 800MW.

HOW TO RUN G16

To run g16 jobs use the command 'rung16' followed by the name of the input (*.com) file with no extension.
So to submit 'geom.com' you type 'rung16 geom' from within the working directory and press ENTER.
Upon succesful submission of a job to the scheduler, a one-liner confirmation message will be printed and also saved onto the ACTIVITY LOG.
Special lines at the beginning of the g16 input file require a specific formatting, as per the following example:
%chk=tmp
%mem=350Gb
%nproc=48

HOW TO USE THE ACTIVITY LOG

A new line is added to the ACTIVITY LOG any time a job is successfully submitted to the scheduler via 'runes2k' or 'rung16' commands (most recent jobs at the top).
The ACTIVITY LOG can be summoned or filtered using the following commands:
vL --- opens the ACTIVITY LOG into VIM.
hL --- prints the 10 most recent jobs. add '-n' followed by an integer number to print an arbitrary number of lines.
cL --- must be followed by a string-type argument (quotation marks not needed). greps the ACTIVITY LOG for that string.
supports regular expressions. supports any keyword the regular 'grep' command would.
Each ACTIVITY LOG line uses the following formatting:

---

submission time jobID project folder for es2k jobs, input file path for g16 jobs procs mem account

---

Tue 31.Jan.2023 12:44:18
7396917 /g100_work/IscrB_autoVTST/ab/Bist/pople_plus_for_fig2/bt02 (nproc:48|mem:317Gb|acc:IscrB_autoVTST)

HOW TO MANAGE JOBS

Submitted jobs can be handled via the following commands:
Coda --- shows the standard scheduler output of the 'squeue' command, grepped for your username.
coda --- shows status and running time for jobs followed by the corresponding info from the ACTIVITY LOG.
scancel --- must be folloewed by a jobID. deletes that job.
saldo -b --- shows the standard accounting message, with all recent active and expired projects and corresponding info.
Saldo --- shows a verbose accounting log listing the daily activity of each user for each day, limited to one project (currently IscrB_autoVTST)

ES2K OUTPUT VISUALIZATION UTILITIES
A few 'smart' commands to quickly browse es2k output are provided via the following commands:
Molden --- followed by the path of an es2k project folder. opens a g16 file into molden following a natst > ts_l1 > reac1_l1 priority list.
if 'pop=full' is used, the corresponding xyz file is opened instead to avoid long loading times.
a missing argument will be interpreted as '.' or 'current folder'.
Grep --- followed by the path of an es2k project folder. prints info following a ts_l1 > reac1_l1 priority list.
these are, in order: L1 energy (Ha), L1 zpe (Ha), number of imaginary frequencies (if any), HL energy (Ha)
a missing argument will be interpreted as '.' or 'current folder'.
KNOWN BUG: only works correctly for DFT jobs, no MP methods and double-hybrids such as B2PLYP.
Thermo --- followed by the path to a g16 output file. prints the following info:
molar mass (g/mol), last energy (Ha), zpe (Ha), rotational constants (GHz), vibrational frequencies.
KNOWN BUG: only works correctly for DFT jobs, no MP methods and double-hybrids such as B2PLYP.

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l --- lists files and directories much like 'll' does, shows hidden files, no user or group, uses a personalized time string such as 'Fri 10-Jun-2022 18:41:27'
lt --- lists files and directories in the 'l' format, sorted by modification time, recent first.
molden --- opens molden, no shader, no automatic atom number reordering
python --- alias for 'python3'
ci --- alias for 'vi'
gerp --- alias for 'grep'
grp --- alias for 'grep'
MOlden --- alias for 'Molden'