

Practical session #1: Basic use of CASINO

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In this practical session we aim at familiarising ourselves with CASINO, running the most common types of calculations and playing around with the most important parameters.

Before you start

The command line:

You will be working in a UNIX-style command line. Some of you will be experts, while others may have little or no experience with this environment. We are happy to help with any problems that you encounter, but please try to follow the instructions in these sheets as closely as possible (pay special attention to the presence or absence of spaces in the commands!).

Conventions:

- Keys to be pressed will be enclosed in a grey box, for example: `Enter`.
- Commands to type at the command line are enclosed in yellow boxes. For example: `cd ~/CASINO`. You are supposed to type the commands verbatim and press `Enter` at the end of each line.
- Other text (text to add to a file, a command's output, etc.) will be enclosed in a `blue box`.
- Any text that you need to replace inside a box will be in italics, for example: `cd directory`.

The GEDIT editor:

The instructions below assume that you are going to use the GEDIT editor. The basics of GEDIT are:

- To open a file, type `gedit file`.
- To save the file, click on the “save” button and close the editor window.

You are welcome to use any other editor that is available on the computer. For example, you may replace any occurrence of `gedit file` in this tutorial with `vi file`, `emacs file` or `kate file`.

Running CASINO:

- In these tutorials, when instructed to run CASINO you should type `runqmc -B`. This will run CASINO in the background using all cores available on the machine.
- Then type `tail -f out` to see the progress of the calculation as it goes. If you want to return to the command line, hold `Ctrl` and press `C`. This will not stop CASINO, you will just stop seeing its output in real-time. To resume seeing the output, type `tail -f out` again.
- If you realise you have made a mistake, you can stop CASINO if you type `killall casino`. Then type `cleanup` to delete the by-products of the failed run, fix the mistake you made, and you are ready to re-run.
- You should also use `cleanup` when you want to run a new calculation after a successful run. However, we recommend keeping a copy of (at least) the `out` file for successful runs. To do this, type `mv out out.n`, where n is 1 for the first file you save, 2 for the second, and so on (or use your own convention!).

Abbreviated error bars:

In case you didn't know, when you encounter a number like $-37.843(2)$, the “2” in parentheses represents the standard error in the last figure of -37.843 . That is, $-37.843(2)$ means -37.843 ± 0.002 .

1 Activity 1: VMC calculations

VMC runs are flagged using `runtype : vmc`. In input files you can find a section called “VMC”, which include the most important VMC-related keywords.

- Copy the files for the lithium atom example to a working directory by typing

```
mkdir -p ~/your-name/tuesday/act1
cd ~/your-name/tuesday/act1
cp ~/CASINO/examples/atom/lithium/* .
gunzip *gz
```

- Edit the input file by typing `gedit input`. Set

```
vmc_nstep      : 1000000
vmc_nblock     : 10
vmc_decorr_period : 1
```

(NB, you will have to add `vmc_decorr_period` to the input file, e.g., at the bottom of the “VMC” section. This instructs CASINO to collect 1,000,000 local energies, arranged in 10 blocks (these are for reporting purposes, nothing to do with reblocking; the value of `vmc_nblock` does not change the results), performing a single configuration move between energy evaluations.

Now run CASINO.

- A couple of new files will have been generated. Typing `ls` should produce the following:

```
[2x64 tti10 act1] ls
config.out  correlation.data  gwfn.data  input  out  vmc.hist
```

The file called `out` is the main output file. Open it and look through it. After the initial setup reports there is information about the outcome of the VMC calculation, arranged in ten blocks as requested.

The correlation time reported for each block is quite a bit larger than unity, meaning there is a significant amount of serial correlation. Exit the editor and type `envmc`. This will extract the energy from the output file and correct for serial correlation using the correlation time information. Take note of the reported values of the total energy and variance (with error bars).

- Let’s reblock the VMC data in `vmc.hist`. To do this, type `reblock` at the command line. Type `1` `Enter` when asked for the units, and press `Ctrl` `C` (i.e., hold the former while pressing the latter) when prompted for a block size, since we do not know it yet. A new file called `reblock.plot` will have been created.

Type `plot_reblock` to visualise the reblocking transformation. Choose a “reblock transformation number” r that you think corresponds to the x -coordinate of the onset of the plateau, and close the plotting program. Now run REBLOCK again following the same steps as before, but this time when you are asked for the block length enter 2^r (whatever number is the result of this operation). Take note of the reported values of the total energy and variance (with error bars) after processing.

- Questions:
 - Do the correlation-corrected error bars given by ENVMC and REBLOCK agree?
 - The variance of a set of independent local energies should equal `vmc_nstep` times the square of the error in the mean energy.
 - The standard error in the mean of a set of independent data is the square root of the variance over the square root of the number of data (`vmc_nstep` in this case). Does this hold for the energies read off the output of ENVMC? Why?
- (Optional) Play with the parameters in the VMC block, e.g.:

- CASINO automatically optimises the VMC time step so that the acceptance ratio is of about 50% (that's why we haven't worried about setting the VMC time step). Turn this feature off by setting `opt_dtvmc : 0`. Does the acceptance ratio behave as you would expect when you increase/decrease the value of the VMC time step (`dtvmc`)?
- Set `vmc_decorr_period : 10` and re-run the calculation. Does the reblocking curve look any different? Why?

2 Activity 2: optimising a wave function

Wave-function optimisation requires prior accumulation of VMC data. Alternate VMC → optimisation runs are flagged in CASINO by setting `runtype : vmc_opt`. There is a section of the input file called “OPTIMIZATION” with parameters controlling the optimisation procedure.

- Copy the files for the lithium atom example to a working directory by typing

```
mkdir -p ~/your-name/tuesday/act2
cd ~/your-name/tuesday/act2
cp ~/CASINO/examples/atom/lithium/* .
gunzip *gz
```

- We will now remove the Jastrow factor to perform an optimisation from scratch. Edit the `correlation.data` file and remove the linear parameters of the u , χ , and f terms, leaving e.g.,

```
...
Cutoff (a.u.)      ; Optimizable (0=NO; 1=YES)
  2.01531066662296      0
Parameter values  ; Optimizable (0=NO; 1=YES)
END SET 1
END CHI TERM
...
```

CASINO will interpret this as “start by running a HF-VMC calculation”. Also change the expansion orders to $N_u = N_\chi = 8$ and $N_{f,ee} = N_{f,eN} = 3$.

- Edit the input file. Set

```
runtype : vmc_opt
vmc_nstep : 100000
vmc_nblock : 10
vmc_nconfig.write : 10000
opt_cycles : 4
```

This instructs CASINO to run a VMC calculation sampling 100,000 configurations, dividing the output in 10 blocks for monitoring, and to store 10,000 of the 100,000 configurations for use in the optimisation stage.

Now run CASINO.

- Once the calculation has finished, type `envmc` in the command line to how the optimisation has gone (you can also do this while it is running to monitor the optimisation). You will see one line for each VMC run. Between every two consecutive VMC runs there has been a parameter optimisation, therefore the energies and variances should be slightly different. You should now locate the best VMC energy and take note of the `correlation.out.x` to which it corresponds.
- Questions:
 - Which is the best Jastrow factor among those you generated?
 - The first VMC result corresponds to HF-VMC (i.e., using no Jastrow factor). How good is it?

- Repeat the optimisation process using `vmc_nconfig_write : 200`. What happens?
- (Optional) Play with the parameters, e.g.:
 - Set `opt_method : emin` and re-run. Is the optimal energy lower or higher? Is the optimal variance lower or higher?

3 Activity 3: running DMC

DMC runs start from VMC configurations, and have an equilibration stage and an accumulation stage. VMC → DMC equil. → DMC accum. runs are flagged in CASINO by setting `runtype : vmc_dmc`. There is a dedicated section of the input file labelled “DMC” to control DMC calculations.

- Copy the files for the lithium atom example to a working directory by typing

```
mkdir -p ~/your-name/tuesday/act3
cd ~/your-name/tuesday/act3
cp ~/CASINO/examples/atom/lithium/* .
gunzip *gz
```

- Edit the input file. Set

```
runtype           : vmc_dmc
vmc_nstep         : 1024
vmc_nconfig_write : 64
dmc_equil_nstep   : 8000
dmc_equil_nblock  : 10
dmc_stats_nstep   : 100000
dmc_stats_nblock  : 50
dmc_target_weight : 64.d0
dtdmc            : 0.01
```

This instructs CASINO to produce 64 VMC configurations and store them for DMC. Then CASINO will run a DMC equilibration of 8,000 steps and a DMC statistics-accumulation of 100,000 steps, with a target population of 64 configurations (NB, this should generally match the number of configurations written in VMC). The DMC time step is 0.01 a.u.

Now run CASINO.

- Once the run is finished, run `reblock` as we did in the VMC exercise, only this time you have to provide the length of the equilibration stage when prompted. Discard 8,000 steps in this case. Take note of the processed energy (with error bar).
- Repeat this for a time step of 0.04, taking note of the final energy and error bar that you get.
- Edit a new file by typing `gedit dmc.dat`, and write two lines, in each of which you should put the time step, energy and error bar (in this order) of each of the runs. For example,

```
0.01  -7.47828  0.00024
0.04  -7.47857  0.00013
```

- Type `extrapolate_tau`, enter `dmc.dat`, press `Enter`, and then type `2` `Enter` `0` `Enter` `1` `Enter` (this asks for a linear extrapolation of the DMC energies to zero time step). Take note of the energy labelled as “DMC energy at zero time step”, which is the final result.
- (Optional) Re-run one of the individual DMC runs with `use_jastrow : F`. This forces the use of a HF wave function, which is poorer—what differences do you see in the `graphdmc` plot?