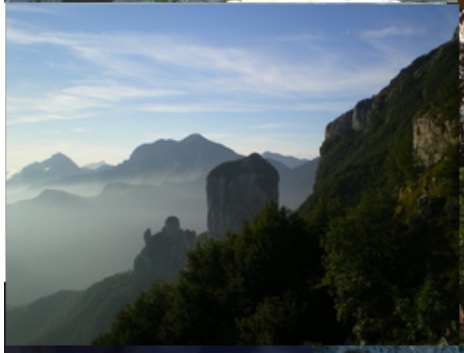
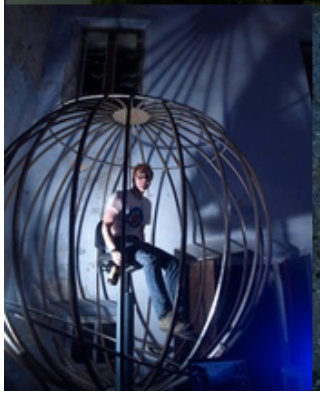







The Towler Institute

2016 International Summer School

Quantum Monte Carlo and the CASINO program X

Vallico Sotto, Tuscany, Italy 23rd - 30th July 2016

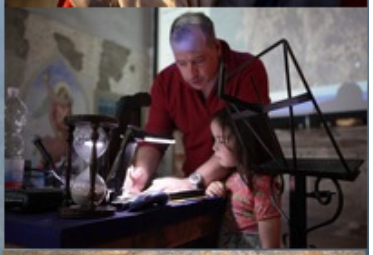
vallico.net/tti/tti.html

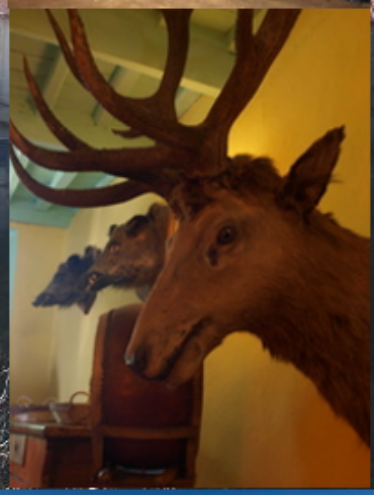
email : mdt26 at cam.ac.uk





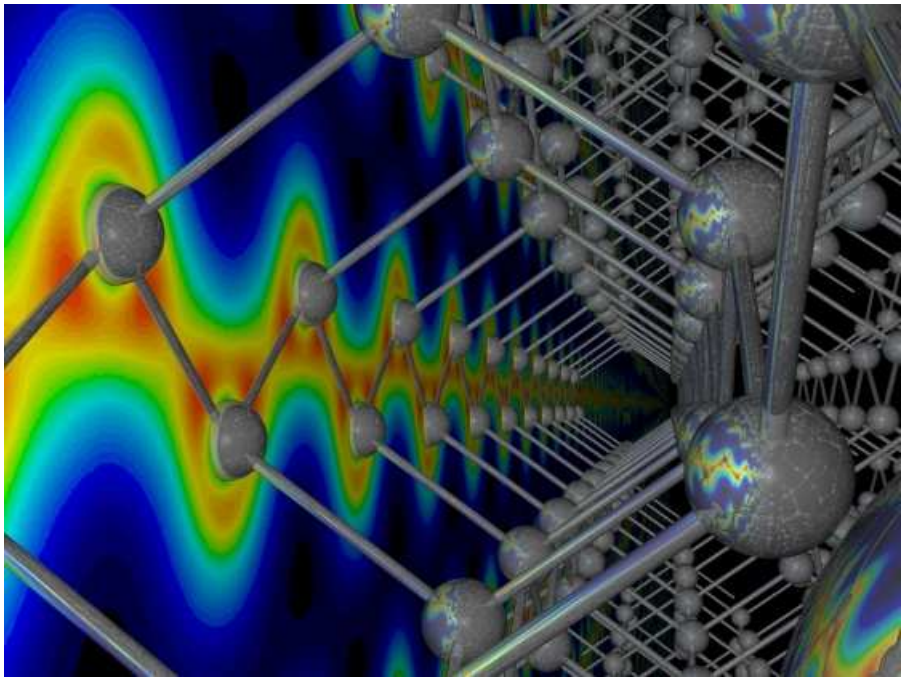






The CASINO program

Basic introduction to functionality and input/output



Mike Towler

TCM Group, Cavendish Laboratory, University of Cambridge

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Email: `mdt26@cam.ac.uk`

History of CASINO

- QMC research in Cambridge began in the early 1990s with the writing of a Fortran77 development code (known simply as 'the QMC code') by Richard Needs and Guna Rajagopal, assisted by helpful discussions with Matthew Foulkes. This was later extended by Andrew Williamson up to 1995 and then by Mike Towler and Paul Kent up to 1998. Various different versions of this program were able to treat *fcc* solids, single atoms and the homogeneous electron gas.
- By the late 1990s it was clear that a modern, general code capable of treating arbitrary systems (at least atoms, molecules, polymers, slabs, crystals and model systems) was required, not only for the Cambridge QMC group, but for public distribution. So, beginning in 1999, a new Fortran90 code - CASINO - was gradually developed in the group of Richard Needs initially by Mike Towler, with important contributions from 2002 by Neil Drummond and from 2004 by Pablo López Ríos (all now considered to be the principal authors of the code).
- Other contributions: Andrew Porter, Randy Hood, Andrew Williamson, Dario Alfè, Gavin Brown, Chris Pickard, Rene Gaudoin, Ben Wood, Zoltan Radnai, Andrea Ma, Ryo Maezono, John Trail, Paul Kent, Nick Hine, Alex Badinski, John Jumper, Robert Lee, Norbert Nemec, Lucian Anton, Priyanka Seth, Jonathan Lloyd-Williams, Pascal Bugnion, Elaheh Mostaani, Albert Defusco, Mike Deible, Blazej Jaworowski

`vallico.net/casinoqmc`

CASINO

The Cambridge Quantum Monte Carlo Code

R.J Needs, M.D. Towler, N.D. Drummond, P. López Ríos

CASINO

The Cambridge Quantum Monte Carlo Code

R.J Needs, M.D. Towler, N.D. Drummond, P. López Ríos

casino m. **1** brothel, whorehouse **2** noise . . . **3** mess, $\langle volg \rangle$ cock-up

CASINO

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R.J Needs, M.D. Towler, N.D. Drummond, P. López Ríos

casino m. **1** brothel, whorehouse **2** noise . . . **3** mess, $\langle volg \rangle$ cock-up

casinò m. casino

CASINÒ

The Cambridge Quantum Monte Carlo Code

R.J Needs, M.D. Towler, N.D. Drummond, P. López Ríos

casino m. **1** brothel, whorehouse **2** noise . . . **3** mess, $\langle volg \rangle$ cock-up

casinò m. casino

CASINO

A general QMC electronic structure software package for finite and periodic systems

Generality

VMC/DMC for systems with 'arbitrary' system size (given enough computing power) and arbitrary geometry, including atoms; molecules; systems periodic in 1/2/3 dimensions (polymers, slabs, crystalline solids); various electron and electron-hole phases ; generalized quantum particles with arbitrary charge/mass/spin. Choice of basis sets (plane waves/Gaussians/blips/Slaters) or grids. Interfaces to wide-range of electronic structure codes for generating trial wave functions.

Portability

Strict Fortran95. Modern software design. Runs on 'any' parallel (MPI with occasional OpenMP) and serial hardware. Automatic, user customizable compilation/setup.

Ease-of-use

Shell script automation. Full documentation: internal help system, comprehensive manual, on-line material including pseudopotential library. Wide range of examples included. Discussion forum: `vallico.net/tti/casino-forum`. Helpful interactive website: `vallico.net/casinoqmc`.

Speed

As far as possible uses the most efficient algorithms optimized for speed including best possible scaling with system size and with number of processors.

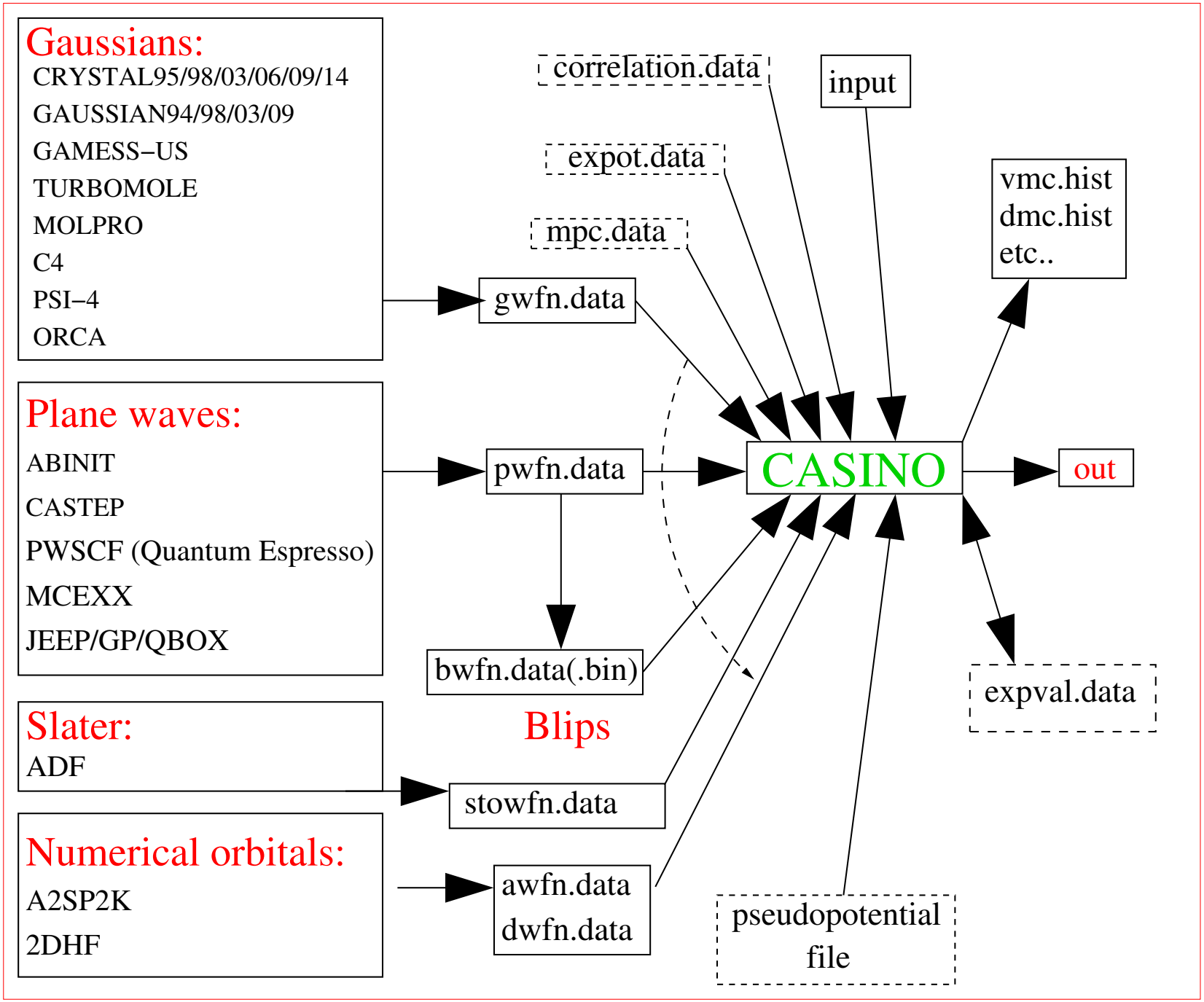
Memory efficient

Fully capable of exploiting all types of shared memory (System V/Posix/Blue Gene Posix).

CASINO : additional capabilities

- VMC and DMC (branching or with weights).
- Various algorithms for wave function optimization through variance or energy minimization, including highly efficient algorithm for linear parameters.
- Uses Slater-Jastrow wave functions where the Slater part may consist of (possibly spin-polarized) multiple determinants.
- Homogeneous and inhomogeneous backflow transformations to give highly accurate trial wave functions.
- Orbital expansions in plane-waves, blips, atom-centred Gaussians (s, sp, p, d, f, g) with cusp corrections, or atom-centred Slater functions. Numerical orbitals on grids for atoms and molecular dimers.
- Calculation of periodic electron-electron interactions with Ewald, MPC or structure factor methods.
- Excited states from promotion, addition, or subtraction of electrons.
- Computation of expectation values other than the total energy : density, spin density, spin density matrix, pair correlation function, localization tensor, structure factor, one-electron density matrix, two-electron density matrix, electric dipole moment, momentum density plus atomic charges, spins, and covariances.
- Automatic stopping algorithms for high-throughput.

Interface to other packages



CASINO distribution

```
tti_laptop1% ls -F
arch/          CHANGES  doc/       install*  manual/          src/
bin_qmc/       data/    examples/  lib/      README           utils/
build-tools/   DIARY    FAQ        Makefile  README_INSTALL   VERSION
```

Files

CHANGES	Summary of major changes to the code
DIARY	Detailed list of all changes to the code
FAQ	Frequently-asked questions
README	General introduction to CASINO
README_INSTALL	Instructions for installing CASINO
VERSION	File containing automatically-generated version number
Makefile	File used by *make* to compile CASINO and utilities
install	Clever automatic installation/compiling script

Directories

arch	Architecture-dependent configuration files
bin_qmc	Where executable programs are placed by the Makefiles
build-tools	Various utilities used for building CASINO
data	Illustrative results from real QMC calculations
doc	Miscellaneous things to read
examples	Large number of examples and test cases
manual	CASINO manual in PDF format
src	CASINO source files (may be obfuscated)
utils	Source code for CASINO utility programs

input file

```
#------------------#
# CASINO input file #
#------------------#

# Hydrogen atom (Gaussian basis)

# SYSTEM
neu                 : 1      #*! Number of up electrons (Integer)
ned                 : 0      #*! Number of down electrons (Integer)
periodic            : F      #*! Periodic boundary conditions (Boolean)
atom_basis_type     : blip   #*! Basis set type (Text)

# RUN
runtype             : vmc    #*! Type of calculation (Text)
newrun              : T      #*! New run or continue old (Boolean)
testrun             : F      #*! Test run flag (Boolean)

# VMC
vmc_equil_nstep     : 1000   #*! Number of equilibration steps (Integer)
vmc_nstep           : 10000  #*! Number of steps (Integer)
etc..
```

What do the input keywords mean?

You can look in the manual, or – once you have compiled and setup the code – you can type '`casinohelp [keyword]`' or '`casinohelp search [searchword]`'.

```
2x64:ttilaptop18% casinohelp dmc_stats_nstep
CASINO HELP SYSTEM
==================

Keyword : dmc_stats_nstep
Title   : No of steps in DMC stats accum
Type    : Integer

DESCRIPTION
-----------
Number of DMC steps performed on each processor in the statistics accumulation phase,
and consequently, the total number of local energy samples (averaged over configs and
processors) written to the dmc.hist file. The accumulation phase may be partitioned into
DMC_STATS_NBLOCK blocks, but this does not affect the total number of steps (just how
frequently stuff is written out). However, if DMC_STATS_NSTEP is not divisible by the
number of blocks, then it will be rounded up to the nearest multiple of DMC_STATS_NBLOCK.
Furthermore, DMC_AVE_PERIOD consecutive local energies may be averaged together in DMC
before writing them to the dmc.hist file (hence reducing its size), but again, if
DMC_STATS_NSTEP is not divisible by DMC_AVE_PERIOD, it will be rounded up to the nearest
multiple of it. Note the difference in parallel behaviour compared to VMC_NSTEP, which is
not a per processor quantity; this is because the DMC phase is parallelized over configs.
```

Note: a major point of confusion is what the keywords mean on *parallel machines*. If I say **vmc_nstep** = 1000 and there are 10 processor cores, does each core do 1000 steps of VMC, or do the 10 cores each do 100 steps to make a total of 1000? The answer depends on what keyword you are talking about. Make sure you read carefully and understand the precise definitions of at least the following keywords: **vmc_equil_nstep**, **vmc_nstep**, **vmc_nblock**, **vmc_decorr_period**, **vmc_ave_period**, **vmc_nconfig_write**, **dmc_equil_nstep**, **dmc_equil_nblock**, **dmc_stats_nstep**, **dmc_stats_nblock**, **dmc_target_weight**, **dmc_ave_period**.

`xwfn.data` file

Communication between external programs and CASINO

- This data file contains the geometry and the orbital and determinant data produced by the wave-function generating code. It also contains a specification of the basis set used to represent the orbitals; this may be a set of Gaussian functions (`gwfn.data`), plane-waves (`pwfn.data`), blip functions (`bwfn.data`) or Slater functions (`stowfn.data`). Instead of a basis set, the `awfn.data` file contains the specification of a radial grid at whose points the orbitals for a single-atom wave function are given explicitly (`dwfn.data` for dimers).
- These files are produced by routines embedded within the external program (if the developers allow us to do so, e.g. ABINIT, PWSCF) or from various utilities which read the output of the external program (e.g. GAUSSIAN09 or CRYSTAL14) and transform it into a format understandable by CASINO .
- The file is not necessary if the trial wave function can be specified without the use of an external program (e.g. the homogeneous electron gas). In such cases, the state of the system is specified in the input file through the **free_particles** block.

`correlation.data` file

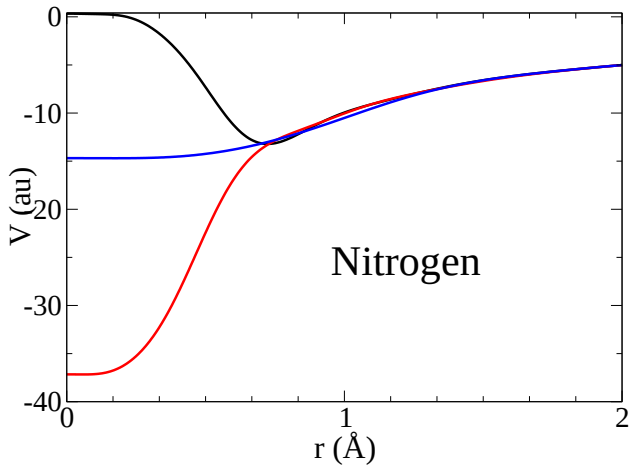
The `correlation.data` file contains all the *optimizable* parameters in the trial wave function. CASINO may improve upon the wave function produced by the generating code by optimizing these parameters. Specifically, the file may contain any of the following:

- A Jastrow factor
- A backflow function
- The determinant expansion coefficients (if more than one determinant)
- Parameters modifying the shape of the given DFT/HF orbitals
- Parameters relating to electron gases and pairing wave functions

The most common practice is to use only a Jastrow factor; the last four are typically used in more advanced work.

Note that optimization of the `correlation.data` file will generally lead to the generation of a `correlation.out` file, which should be renamed `correlation.data` when you actually want to use it.

`x_pp.data` file



- This file contains a specification of a non-local (angular-momentum-dependent) *pseudopotential* V for element `x`. Contains a radial grid r and data for $r \times V$ for (usually) s, p and d angular momentum channels (f and g also possible).
- With CASINO each atom can be treated either as all-electron or the core electrons can be replaced with a pseudopotential. To specify the former simply omit the pseudopotential file.
- Visualize the contents of the files using the PTM utility.
- Get pseudopotentials for particular elements from the pseudopotential library accessible from the CASINO home page (click the periodic table at top right) :

`vallico.net/casinoqmc/pplib/`

Other input files

`config.in/out` (produced in normal operation, but can be turned off)

The `config.out` checkpoint file stores the current state of the calculation (e.g. the particle positions and associated energy data of all active walkers/configs; the state of the random number generator ; etc.). This allows one to 'continue' the run later (see the **newrun** keyword; rename the checkpoint file to `config.in`) or to run the next step of a multi-stage calculation such as optimization or DMC after VMC. By default `config.out` is automatically written after every block of moves. The input keyword **checkpoint** may be used to control the frequency of this, even to the extent of preventing all use of checkpoint files (Type '*casinohelp checkpoint*').

`mpc.data` (optional)

This file contains the Fourier components of the charge density corresponding to the Slater wave function and the Fourier components of the $1/r$ Coulomb interaction treated within the minimum-image convention. Required for the *model periodic Coulomb* (MPC) interaction used in periodic systems to reduce finite-size effects.

`expot.data` (optional)

Contains specification of an external potential (e.g. potential for inhomogeneous electron-gas calculation, or the potential due to an external electric field) together with any data defining the orbitals associated with the potential.

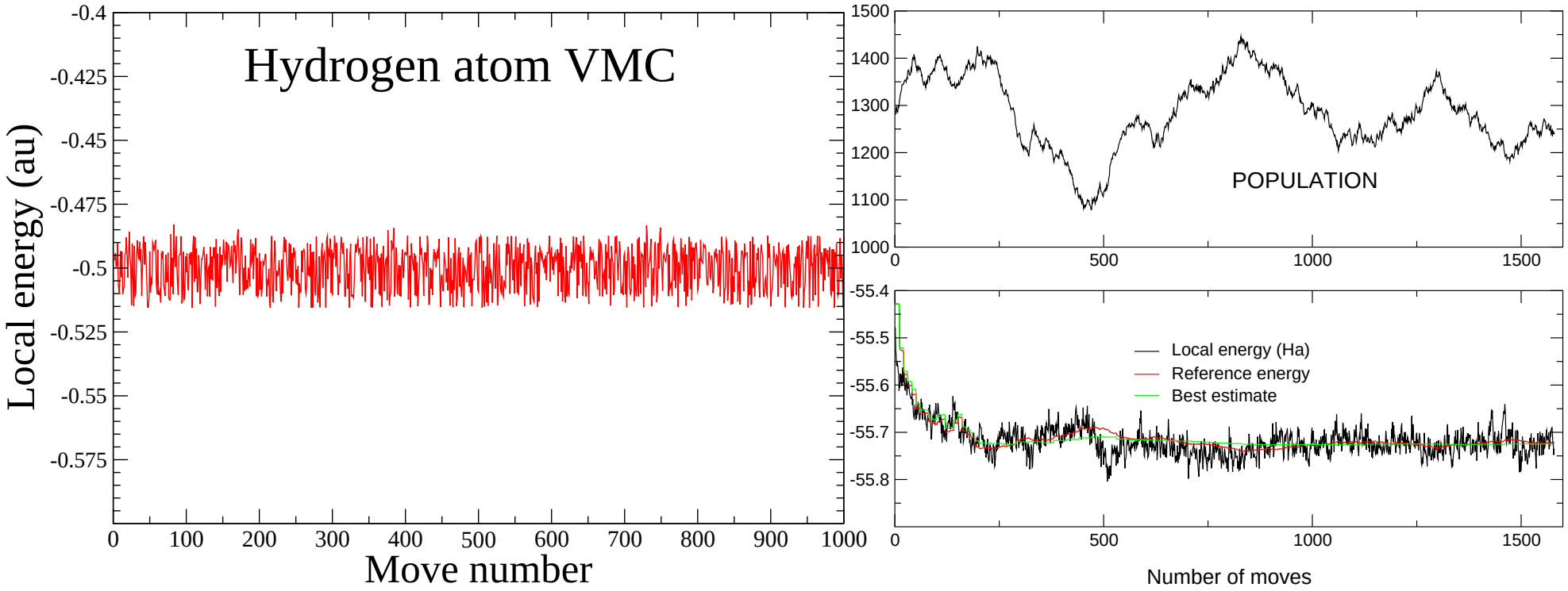
out file

```
CASINO v2.13.390 [Mike Towler] (8 July 2014)
Running on titan [linuxpc-gcc-pbs-parallel.titan]
Binary compiled in opt mode
Job started: Sun  3 Aug 10:10:42 BST 2014
------------------------------------------------------------------------

 #####
##   ##    ##     ####   ##  #   ##   ####
##        ####   ##      ##  ##  ##  ##  ##
##       ##  ##   ####   ##  ### ##  ##  ##
##       ######      ##  ##  ## ###  ##  ##
##   ##  ##  ##  ##  ##  ##  ##  ##  ##  ##
 #####   ##  ##   ####   ##  ##   #   ####

   The Cambridge Quantum Monte Carlo Code
CASINO v2.13.390 [Mike Towler] (8 July 2014)

Main Authors : R.J.Needs, M.D.Towler, N.D.Drummond and P.Lopez Rios
     Theory of Condensed Matter Group, Cavendish Laboratory,
         University of Cambridge, Cambridge, CB3 0HE, UK.
              CASINO web page: vallico.net/casinoqmc
               Current contact: mdt26 at cam.ac.uk

 Started 2014/08/03 10:10:43.209
 Running in parallel using 224356 MPI processes.
```

out file

```
Starting VMC.
 ================================================================
 In block : 1
 Acceptance ratio <level 1>         (%)  =  53.9326
 Acceptance ratio <levels 1-2>      (%)  =  50.0875
 Diffusion constant           (Bohr^2)  = 5.1031E-02
 Correlation time              (steps)  = 2.5659E+00 +- 4.8777E-02
 Efficiency                (au^-2 s^-1)  = 8.4262E+03
 No. of VMC steps per process            = 10000
  Block average energies (au)
  Total energy                                (au) =          -6.299284243152
  Standard error                                +/-           0.002175524045
  Kinetic energy KEI (used in Total)          (au) =           3.949186541390
  Standard error                                +/-           0.006860781971
  <lines deleted>
 Time taken in block    : : :        9.7200
 ================================================================
 FINAL RESULT:
  VMC energy (au)    Standard error      Correction for serial correlation
 -6.299284243152 +/- 0.002175524045      No correction
 -6.299284243152 +/- 0.003484863685      Correlation time method
 -6.299284243152 +/- 0.003659126872      On-the-fly reblocking method
 ================================================================
 Total CASINO CPU time  : : :       10.0400
 Total CASINO real time : : :       10.0470
```

`vmc.hist`/`dmc.hist` files



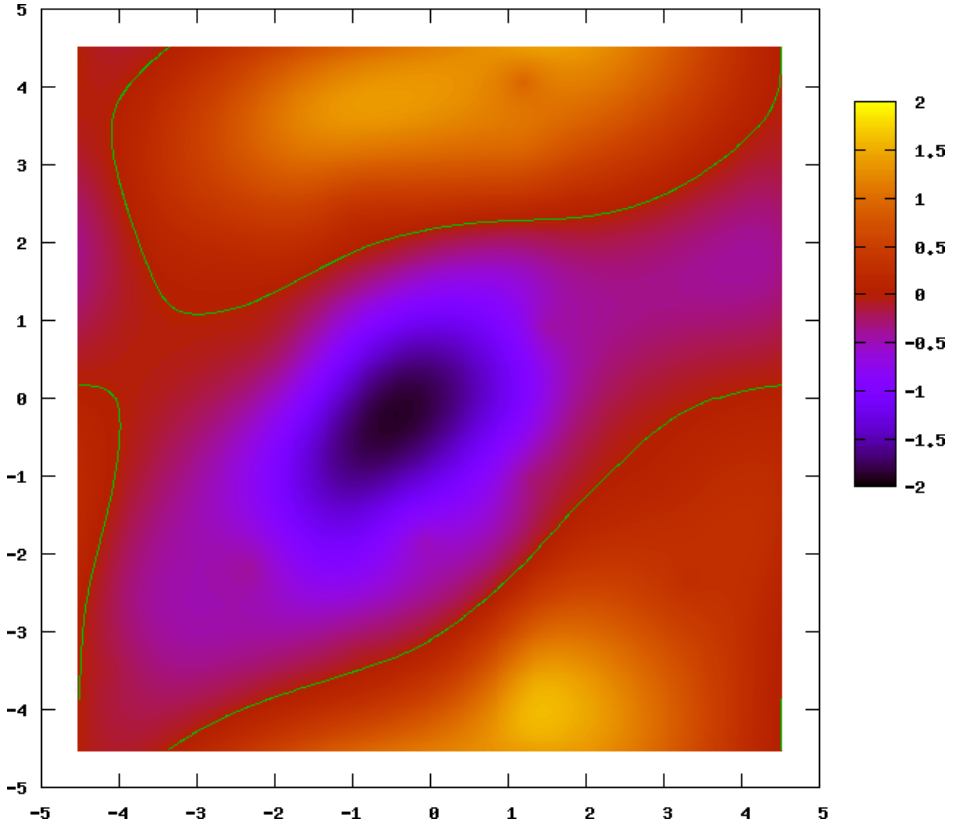
- The `vmc.hist` file contains the energy components calculated during a VMC run (each number is an average over processors). It can be plotted using the PLOT_HIST utility (above left).
- The `dmc.hist` file contains the energy components and important simulation parameters at each iteration of a DMC simulation (each number is an average over processes and configurations). Selected components can also be plotted using the PLOT_HIST utility, although a better picture including population fluctuations can be obtained with the GRAPHDMC utility (above right).
- Statistical analysis/reblocking of the data in both files can be done after the calculation using the REBLOCK utility (see stats lecture). However the reblocking is also done 'on the fly' by CASINO and the results written to the *out* file, so use of the utility is normally unnecessary.

`expval.data` file

Expectation values other than the energy

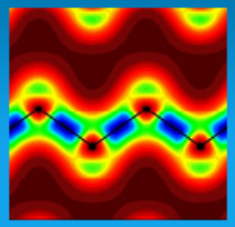
- The `expval.data` file may contain a large variety of data sets describing any of the following quantities : density, spin density, spin-density matrix, reciprocal-space pair-correlation function, spherically averaged pair-correlation function, structure factor, spherically-averaged structure factor, localization tensor, momentum density, one- and two-electron density matrices, ionic populations and (soon) spin moments, fluctuations etc..
- The `expval.data` file also acts as an input file. If a data set is already present and CASINO is asked to accumulate data for that particular set then the newly accumulated data will be added to the existing data.

Other output files



- Visualization of data is handled through the `lineplot.dat`, `2Dplot.dat` and `3Dplot.dat` files for data in one, two or three dimensions respectively. One-dimensional plots are best visualized through the XMGRACE software, while 2D/3D can be visualized quickly through the CASINO utility `plot_2D` which provides a user-friendly interface to the GNUPLOT software.
- Many other files can be produced by CASINO but these are generally for logging or obscure visualization purposes that are only likely to be of interest to developers.

Any problems, ask the discussion forum..!



The CASINO forum

A forum for discussing quantum Monte Carlo and the Cambridge QMC code CASINO
[*Online since June 2013*]
CASINO home page
CASINO events
CASINO FAQ
CASINO manual
CASINO development log

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[Moderator Control Panel]

Last visit was: Wed Jul 23, 2014 10:54 am

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FORUM	TOPICS	POSTS	LAST POST
General announcements How to use these forums. Announcements of new versions of CASINO, summer schools and workshops, etc.	8	8	by **Mike Towler** Thu Feb 20, 2014 10:12 pm
The CASINO program General discussion of the Cambridge quantum Monte Carlo code CASINO; how to install and setup; how to use it; what it does; applications.	51	326	by Mdeible Sun Aug 03, 2014 1:35 am
Quantum Monte Carlo General discussion of quantum Monte Carlo in electronic structure theory	2	3	by **Mike Towler** Mon Mar 17, 2014 11:33 pm
Computational electronic structure Any other relevant topic not directly about QMC, including DFT, quantum chemistry, etc..	1	8	by Cyrus_Umrigar Thu Feb 20, 2014 1:55 pm
Jobs QMC job adverts; careers advice	5	5	by pfloos Mon Mar 03, 2014 9:09 am

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In total there are **2** users online :: 1 registered, 0 hidden and 1 guest (based on users active over the past 5 minutes)
Most users ever online was **28** on Tue Mar 04, 2014 9:23 pm

Registered users: **vallico**
Legend: Administrators, Global moderators

STATISTICS

Total posts **350** • Total topics **67** • Total members **515** • Our newest member **Xiaojie_Zhang**

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Next...

- Distribution, setup, and compilation of the CASINO program.
- Local and remote computer resources
- How to apply for computer time on big parallel computers..
- Web resources

But first.. lunch!