Remarks on Vconstr code interfaced with GAMESS-US

basic information, compilation and use

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1 General Information

The dsfun code is available for users that have acces to the bitbucket repository at ???.

The code requires the follwing input information to run

- 3D grid (x, y, z, w) for numerical integration,
- system and basis set information,
- one and two electron integrals

The infomation is usually provided in the form of files

```
echo Files used on the master node master were:
ls -lF
```

1.1 Grid

The numerical grid can be calculated using the fortran code written by M. Franchini [1] that is included as a standalone program in the dsfun repository. Firs the the grid program needs to be compiled which can be done using `foray` [2] utility by typing `foray` comman in the `generate_grid` directory:

```
cd Source/generate_grid
foray
```

2 dbrain.f requires the following data

- `hmatx` core hamiltonian matrix
- `tsmat` kinetic energy operator integrals
- `vnmat` electron-nuclear attraction operator integrals
- `vmopao` molecular orbitals in primitive ao basis
- `vmoao` moelcular orbitals in mo basis
- `pmo` mo density matrix in mo basis
- `pnomo` ci density matrix in mo basis

3 dsfun.x input

Table 1: dsfun input parameters

name	type	comment
`title`	character(len=8)	
`nmos`	integer	number of molecular orbitals
`occ`	real(1:nmos)	occupation numbers
`df`	real	shift
`nppr`	integer	pprint, intermediate storage of Vxc at every iteration
`scfdmp`	real	damping
`lrfun`	logical	linear response
`dvdmp`	real	linear response procedure damping
`lfield`	logical	electric field
`fzyx`	real(1:3)	components of the electric field
`nvpr`	integer	vprint
`lsym`	logical	symmetrize the orbitals
`lintsm`	logical	determine symmetry using orbitals(if false h-matrix)
`ismo`	integer	mo section in the atmol dumpfile
`isno`	integer	no section in the atmol dumpfile
`isao`	integer	adapt section in the atmol dumpfile from which the Vmopao matrix is res

4 iPrint

0 - minimal printing, standard dsfun printing (this option is the default),

1 - print one electron integrals (kinetic and nuclear-electron attraction) over AO's and nuclar repulsion energy read from Gamess-US dictionary file,

2 - same as `iPrint=1` plus orbitals (HF MO's in AO, NO's in AO), NO occupation numbers - read from Gamess-US dictionary file and calculates in the program (NO's in MO) and densities (CI-NO density in MO, HF-MO density in MO),

3 - same as `iPrint=2` plus basis set information as read from the Gamess-US basinfo file,

4 - same as `iPrint=3` plus Hartree potential at every iteration of KS potential,

5 - same as `iPrint=4` plus values, gradients, and laplacians for every AO and grid point, Warning! for large numbers of AO and grid points this will create very big files!

References

[1] M. Franchini, P. H. T. Philipsen and L. Visscher. *J. Comput. Chem.*, **34**, no. 21, 1819–27 (2013).

[2] D. McCormack. foraytool, An advanced build tool for Fortran developers. (2010). URL http://code.google.com/p/foraytool/.