Graphics Processing Units for Atoms and Molecules GPUAM

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The Graphics Processing Units for Atoms and Molecules was designed to evaluate efficiently scalar and vectors fields defined within the quantum chemistry. This code needs of orbitals expressed in terms of local functions like Gaussian type functions (GTF) or Slater type functions (STF).

1 Input files

GPUAM manipulates GTFs from wfn or wfx files. You can obtain these files if use G09, NWChem of GAMESS codes. Also, GPUAM uses STFs from mgf files, such files are obtained from MOPAC.

2 Running GPUAM

GPUAM has been optimized by using Intel compilers. Thus, you need these compilers or the libiomp5.so library.

2.1 GTFs

By executing the command
`./Gpuam_GPU.x < input_wfx > output`
where `input_wfx` has the information:
`agua.wfx`
`agua`
`K`
`A`
you will obtain the critical points of the molecule defined in the wfx file since in this case we use the option `K`. For GTFs, GPUAM has several options:

```
(A) ith Molecular orbital
(B) Electron density
(C) Laplacian of the electron density
(D) Module gradient density
(E) Reduced density gradient
(F) Gradient of ith molecular orbital
(G) Gradient electron density
(H) Kinetic energy density
(I) Electron localization function
(J) Localized orbital locator
```

```
(K) Search critical points of electron density
(L) Search critical points of laplacian of the electron density
(M) Electrostatic potential
(N) Non-covalent interactions index
(O) Localized electrons detector
(P) Non-covalent interactions and critical points
(Q) Electron density of the basins
```

2.2 STFs

For STFs, the options are:

```
(A) ith Molecular orbital
(B) Electron density
(C) Laplacian of the electron density
(D) Module gradient density
(E) Reduced denisty gradient
(F) Search critical points of electron density
(G) Non-covalent interactions index
(H) Localized electrons detector
(I) Gradient of electron density
```

If you use `./Gpuam_GPU.x` then you can explore the options provided by GPUAM, you will see that this is very intuitive.

2.3 Results

Except for the critical points searching, all options give as result properties evaluated over a mesh and the results are reported in a file with CUBE format. For the option related to the critical points searching you will find all information in a file with extension log and the coordinates of nuclei and critical points are reported in a file with extension xyz.

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