

Examples

bef2.fchk

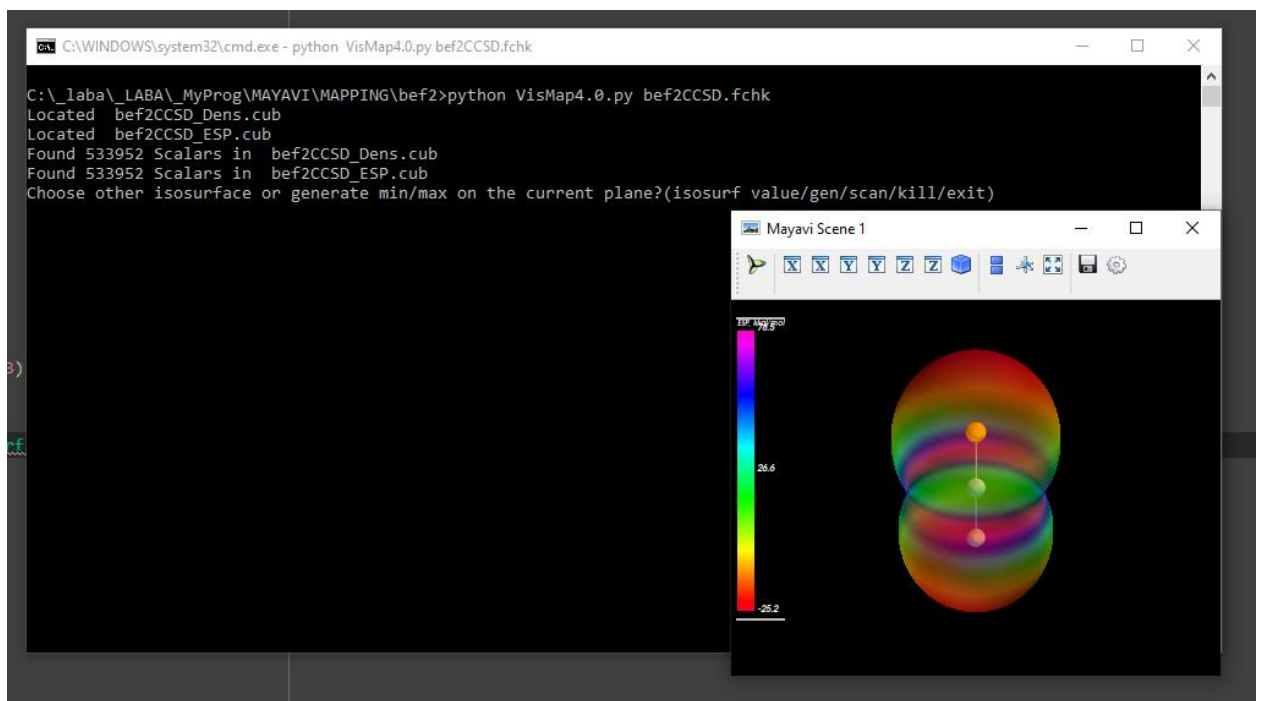
```
C:\WINDOWS\system32\cmd.exe
C:\_laba\_LABA\_MyProg\MAYAVI\MAPPING\bef2>dir
Том в устройстве с метку Windows
Серийный номер тома: 584C-5CDD

Содержимое папки C:\_laba\_LABA\_MyProg\MAYAVI\MAPPING\bef2
19.04.2021 18:05 <DIR> .
19.04.2021 18:05 <DIR> ..
18.09.2020 12:20      483 311 bef2CCSD.fchk
19.04.2021 17:23       18 559 VisMap4.0.py
                2 файлов      501 870 байт
                2 папок    452 176 900 096 байт свободно

C:\_laba\_LABA\_MyProg\MAYAVI\MAPPING\bef2>python VisMap4.0.py bef2CCSD.fchk_
```

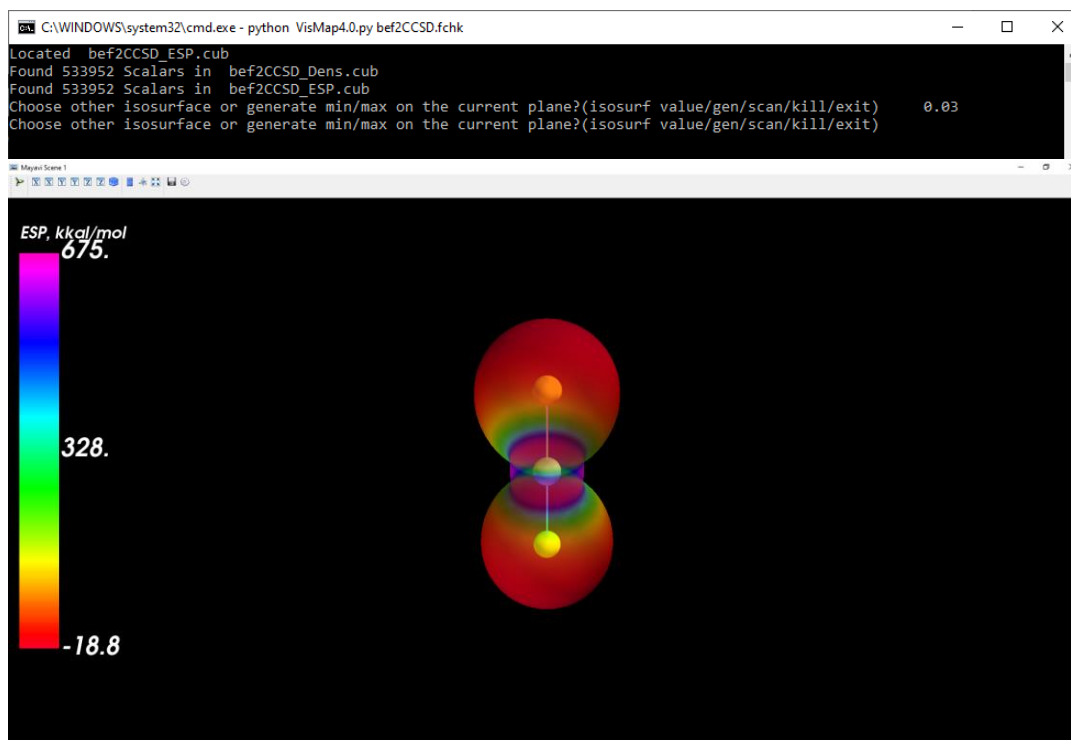
There are no cubes, so the script accesses the Multiwfn and generates them.

After generation, the Mayavi window appears, and the "interactive" mode is enabled in the command line.



For example, I am not satisfied with an isosurface of 0.001, I want 0.03

I write *0.03*



To find all the critical points of ESP on the surface, I write *gen*

```

C:\WINDOWS\system32\cmd.exe - python VisMap4.0.py bef2CCSD.fchk
Located bef2CCSD_ESP.cub
Found 533952 Scalars in bef2CCSD_Dens.cub
Found 533952 Scalars in bef2CCSD_ESP.cub
Choose other isosurface or generate min/max on the current plane?(isosurf value/gen/scan/kill/exit) 0.03
Choose other isosurface or generate min/max on the current plane?(isosurf value/gen/scan/kill/exit) gen
Searching surfanalysis.txt file with points
File not found. Calling Multiwfn for min/max locating

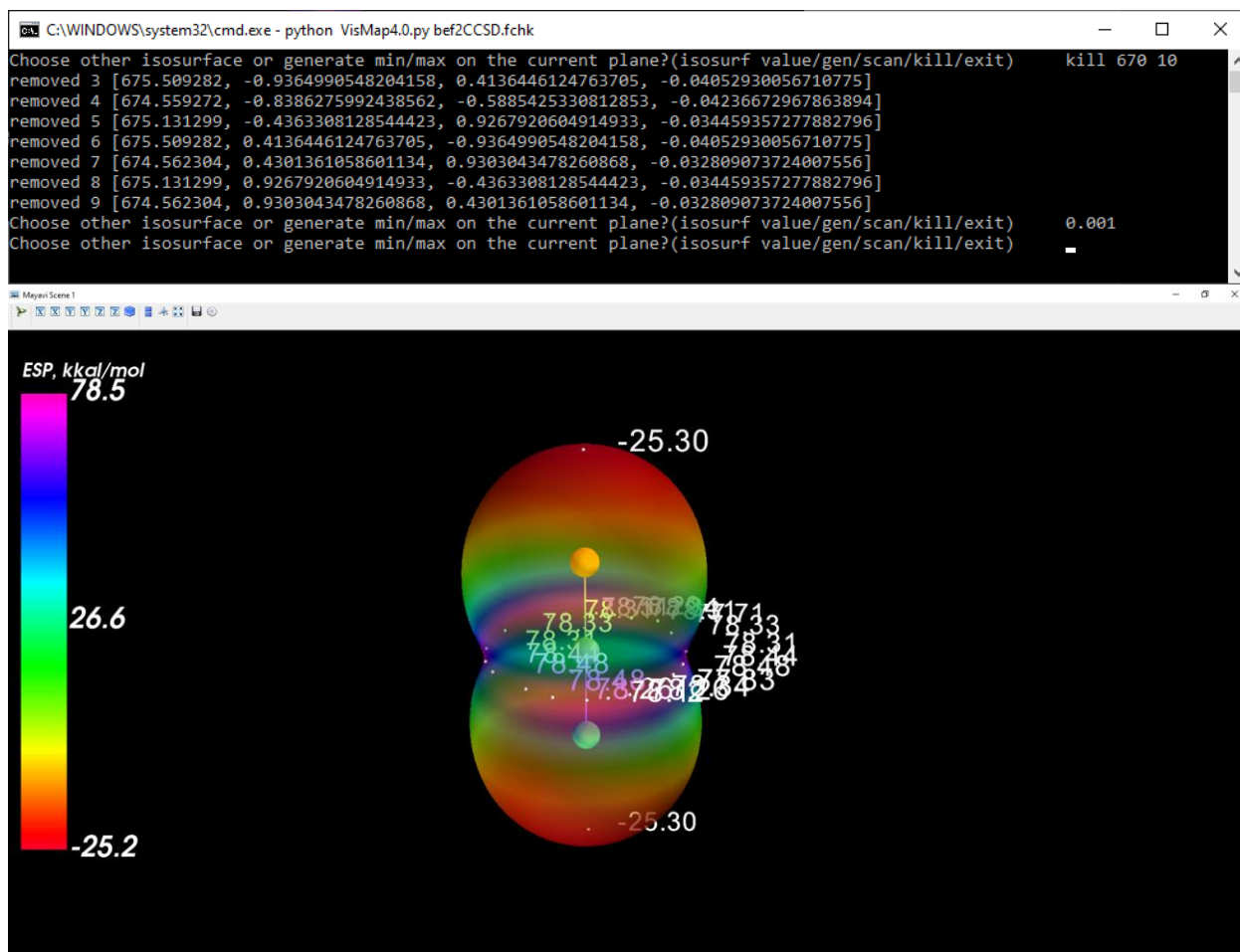
```

The file was not found – the script accesses the Multiwfn to generate it. After generation, the points are added to the visualizer.

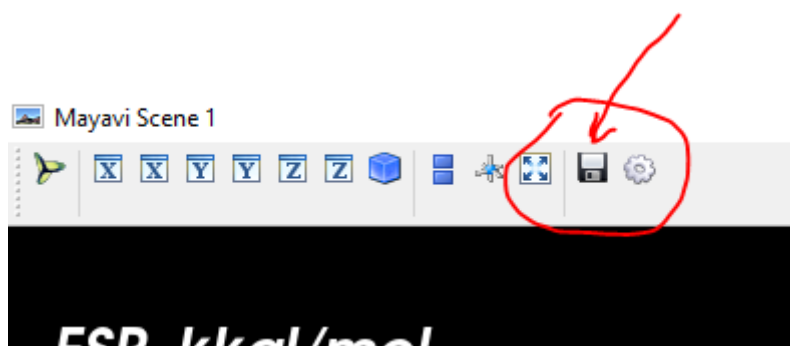
```

C:\WINDOWS\system32\cmd.exe - python VisMap4.0.py bef2CCSD.fchk
Multiwfn.exe      00007FF7A3F94462 Unknown      Unknown Unknown
Multiwfn.exe      00007FF7A425E614 Unknown      Unknown Unknown
KERNEL32.DLL      00007FFD14C07034 Unknown      Unknown Unknown
ntdll.dll         00007FFD16BE2651 Unknown      Unknown Unknown
Located 10 extremum points on the surface
Choose other isosurface or generate min/max on the current plane?(isosurf value/gen/scan/kill/exit)

```

To save the picture, click



To exit the “interactive” mode, I write exit

```
C:\WINDOWS\system32\cmd.exe - python VisMap4.0.py bef2CCSD.fchk
Multiwfn.exe      00007FF7A368A998 Unknown Unknown Unknown
Multiwfn.exe      00007FF7A364E7A6 Unknown Unknown Unknown
Multiwfn.exe      00007FF7A337698A Unknown Unknown Unknown
Multiwfn.exe      00007FF7A32FFF1D Unknown Unknown Unknown
Multiwfn.exe      00007FF7A3F94462 Unknown Unknown Unknown
Multiwfn.exe      00007FF7A425E614 Unknown Unknown Unknown
KERNEL32.DLL     00007FFD14C07034 Unknown Unknown Unknown
ntdll.dll        00007FFD16BE2651 Unknown Unknown Unknown
Located 22 extremum points on the surface
Choose other isosurface or generate min/max on the current plane?(isosurf value/gen/scan/kill/exit) exit
```

Only then I close the visualizer window.

CpMnCO2C2H2I2_zora_pbe0_tzvp_en.wfn

I have pre-generated all the files I am interested in

```
C:\WINDOWS\system32\cmd.exe
C:\_laba\_LABA\_MyProg\MAYAVI\MAPPING\bef2>dir
Том в устройстве C имеет метку Windows
Серийный номер тома: 584C-5CDD

Содержимое папки C:\_laba\_LABA\_MyProg\MAYAVI\MAPPING\bef2

19.04.2021  18:51    <DIR>          .
19.04.2021  18:51    <DIR>          ..
16.04.2021  19:26           1 662 548 CpMnCO2C2H2I2_zora_pbe0_tzvp_en.wfn
16.04.2021  19:42           6 997 599 CpMnCO2C2H2I2_zora_pbe0_tzvp_en_Dens.cub
16.04.2021  20:23           6 997 599 CpMnCO2C2H2I2_zora_pbe0_tzvp_en_ESP.cub
19.04.2021  16:10              1 221 CpMnCO2C2H2I2_zora_pbe0_tzvp_en_sa_0.001.txt
19.04.2021  18:45              19 113 VisMap4.0.py
               5 файлов             15 678 080 байт
               2 папок             452 137 242 624 байт свободно

C:\_laba\_LABA\_MyProg\MAYAVI\MAPPING\bef2>_
```

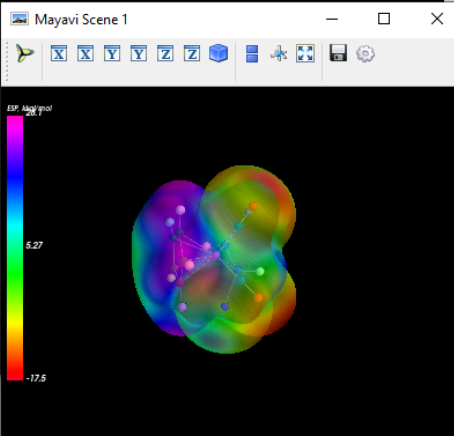
Launching

```
C:\WINDOWS\system32\cmd.exe - python VisMap4.0.py CpMnCO2C2H2I2_zora_pbe0_tzvp_en.wfn
Серийный номер тома: 584C-5CDD

Содержимое папки C:\_laba\_LABA\_MyProg\MAYAVI\MAPPING\bef2

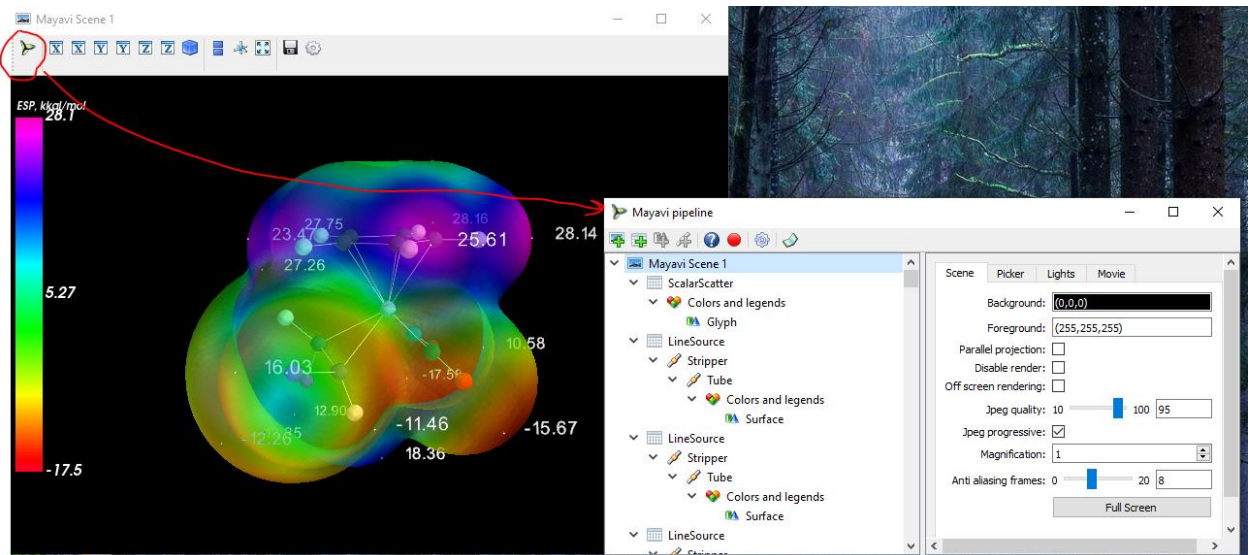
19.04.2021  18:51    <DIR>          .
19.04.2021  18:51    <DIR>          ..
16.04.2021  19:26           1 662 548 CpMnCO2C2H2I2_zora_pbe0_tzvp_en.wfn
16.04.2021  19:42           6 997 599 CpMnCO2C2H2I2_zora_pbe0_tzvp_en_Dens.cub
16.04.2021  20:23           6 997 599 CpMnCO2C2H2I2_zora_pbe0_tzvp_en_ESP.cub
19.04.2021  16:10              1 221 CpMnCO2C2H2I2_zora_pbe0_tzvp_en_sa_0.001.txt
19.04.2021  18:45              19 113 VisMap4.0.py
               5 файлов             15 678 080 байт
               2 папок             452 137 242 624 байт свободно

C:\_laba\_LABA\_MyProg\MAYAVI\MAPPING\bef2>python VisMap4.0.py CpMnCO2C2H2I2_zora_pbe0_tzvp_en.wfn
Located CpMnCO2C2H2I2_zora_pbe0_tzvp_en_Dens.cub
Located CpMnCO2C2H2I2_zora_pbe0_tzvp_en_ESP.cub
Found 531196 Scalars in CpMnCO2C2H2I2_zora_pbe0_tzvp_en_Dens.cub
Found 531196 Scalars in CpMnCO2C2H2I2_zora_pbe0_tzvp_en_ESP.cub
Choose other isosurface or generate min/max on the current plane?(isosurf value/gen/scan/kill/exit)
```

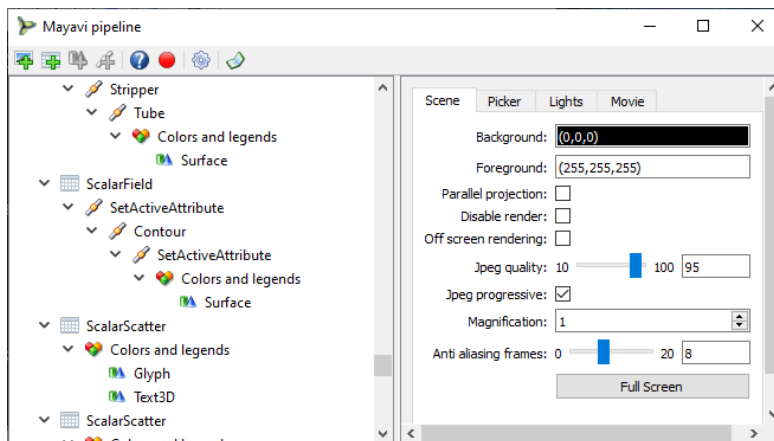


It finds all the cubes, I write *scan* to find the critical points of ESP on the surface closest to the atoms we are interested in.

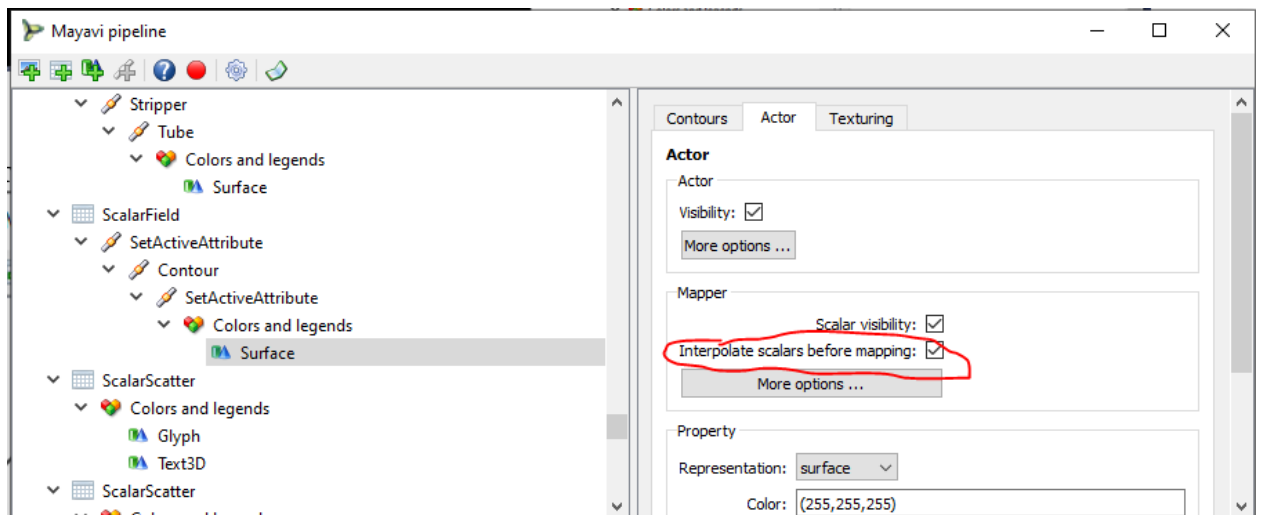
```
C:\_laba\_LABA\_MyProg\MAYAVI\MAPPING\bef2>python VisMap4.0.py CpMnCO2C2H2I2_zora_pbe0_tzvp_en.wfn
Located CpMnCO2C2H2I2_zora_pbe0_tzvp_en_Dens.cub
Located CpMnCO2C2H2I2_zora_pbe0_tzvp_en_ESP.cub
Found 531196 Scalars in CpMnCO2C2H2I2_zora_pbe0_tzvp_en_Dens.cub
Found 531196 Scalars in CpMnCO2C2H2I2_zora_pbe0_tzvp_en_ESP.cub
Choose other isosurface or generate min/max on the current plane?(isosurf value/gen/scan/kill/exit) scan
Searching surfanalysis.txt file with points
Located 17 extremum points on the surface
Choose other isosurface or generate min/max on the current plane?(isosurf value/gen/scan/kill/exit) _
```

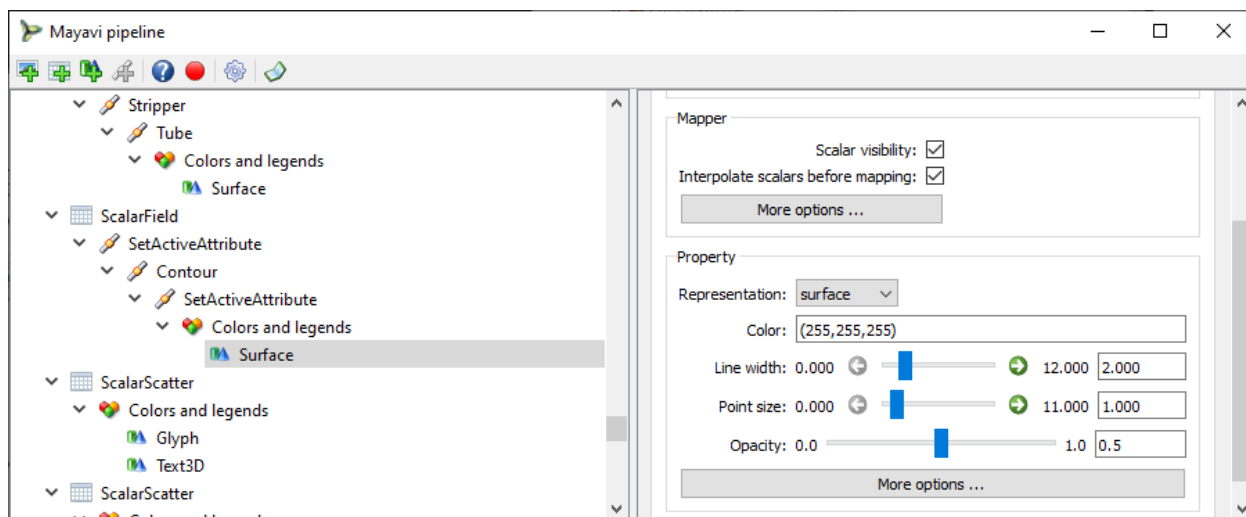
Scroll down to ScalarField



In the Surface → Actor tab, you can enable interpolation to remove the "ribbing"



Just below, the Opacity slider changes the transparency of the surface



In the colors tab, you can select your Lut mode, for example, I poked a jet

