DCACP2TM.sh includes the dispersion corrected atom centered potential (DCACP) as the f channel in Troullier-Martins (TM) pseudopotentials (format adapted in the CPMD code).

1 Derivation

ionic pseudopotential operator:

$$\hat{V}_{\text{ion}}^{\text{PP}}(r) = V_{\text{ion,local}}^{\text{PP}}(r) + \sum_{l} V_{\text{nonlocal},l}(r)\hat{P}_l$$

$V_{\text{ion,local}}^{\text{PP}}(r)$ is the local potential and $V_{\text{semi-local},l}(r)\hat{P}_l = \Delta V_l(r) = V_{\text{ion},l}^{\text{PP}}(r) - V_{\text{ion,local}}^{\text{PP}}(r)$ is the semi-local potential for the angular momentum component l. $\hat{P}_l$ projects out the lth angular momentum component from the wave function.

The semi-local form can be transformed into a nonlocal one using a procedure suggested by Kleinman and Bylander (KB).

$$V_{\text{nonlocal},l}^{\text{KB}}(\mathbf{r},\mathbf{r}') = \sum_{m=-l}^{l} Y_{lm}(\hat{\mathbf{r}}) \frac{|\Delta V_l(r)\,\phi_l(r)\rangle\,\langle\Delta V_l(r')\,\phi_l(r')|}{\langle\phi_l(r'')\,|\Delta V_l(r'')|\,\phi_l(r'')\rangle} Y_{lm}(\hat{\mathbf{r}}')$$

$$V_{\text{DCACP}}(\mathbf{r},\mathbf{r}') = \sum_{m=-l}^{l} Y_{lm}(\hat{\mathbf{r}})\, p_{l1}(r)\, h_{11} p_{l1}(r')\, Y_{lm}(\hat{\mathbf{r}}')$$

so...

$$p_{l1}(r)\, h_{11} p_{l1}(r') = \frac{|\Delta V_l(r)\,\phi_l(r)\rangle\,\langle\Delta V_l(r')\,\phi_l(r')|}{\langle\phi_l(r'')\,|\Delta V_l(r'')|\,\phi_l(r'')\rangle}$$

One choice: $\Delta V_l(r)$ is a constant; then

$$p_{l1}(r)\, h_{11} p_{l1}(r') = \phi_l(r) \frac{\Delta V_l(r)}{\langle\phi_l(r'')\,|\phi_l(r'')\rangle} \phi_l(r')$$

Thus we can select

$$p_{l1}(r) = \phi_l(r)$$
$$h_{11} = \frac{\Delta V_l(r)}{\langle\phi_l(r'')\,|\phi_l(r'')\rangle}$$

$$p_{l1}(r) = \frac{\sqrt{2} r^l \exp\left(-\frac{r^2}{2r_l^2}\right)}{r_l^{l+3/2}\sqrt{\Gamma(l+3/2)}}$$

Γ denotes the gamma function.

The projectors satisfy the normalization condition:

$$\int_0^\infty p_{l1}(r)\, p_{l1}(r)\, r^2 dr = 1$$

2 Script

Example 1: H_MT_BLYP.psp

```
&POTENTIAL
   511
  .62500000E-02      -.76586836E+01 -.56929400E+01
  .63593750E-02      -.76586835E+01 -.56929400E+01
...

&WAVEFUNCTION
   511 CHANNELS=1
  .62500000E-02       .30730264E-02  .21382580E-04
  .63593750E-02       .31268044E-02  .22137519E-04
...
```

Example 2: N_MT_BLYP.psp

```
&POTENTIAL
   624
  .89285714E-03      -.67725706E+01 -.20208424E+02 -.16542135E+02
  .90848214E-03      -.67725706E+01 -.20208424E+02 -.16542135E+02
...

&WAVEFUNCTION
   624 CHANNELS=1
  .89285714E-03       .21376395E-03  .96690717E-06  .56480573E-10
  .90848214E-03       .21750482E-03  .10010450E-05  .59497997E-10
...
```

we have to write in the TM pseudopotential (PP) file

- as the "wave function" $r\,p_{l1}$
- as the "potential"

$$\begin{aligned} & h_{11}\langle\phi_l|\ \phi_l\rangle + V_{\text{loc}}\,(r) \\ & \quad \rightarrow h_{11} + V_{\text{loc}}\,(r) \end{aligned}$$

The script: (DCACP2TM.sh)

```
#!/bin/bash
## input from command line
# TM PP file name
file_M="$1"
# SG DCACP PP file name
file_G="$2"
# local potential channel in number! s=0, p=1, d=2
vloc=$3
...
```

As an example, to generate a DCACP-included TM PP using H_DCACP_BLYP_H2_CI (DCACP-included Goedecker *et al.* PP) and H_MT_BLYP.psp (original TM PP) using p channel as the local potential, one executes:

```
./DCACP2TM.sh H_MT_BLYP.psp H_DCACP_BLYP_H2_CI 1
```

It produces an output file, which might be useful if something seems to be wrong...

```
input TM PP = H_MT_BLYP.psp
input DCACP SG PP = H_DCACP_BLYP_H2_CI
local channel = 1
LMAX in DCACP SG PP = 4; GAMMA = 11.6317283966
r_l = 2.706646438534561; h_11 = -4.0558298753945934E-004
constant in projector = 4.6962476603e-03
```

When choosing the local channel, one should bear in mind that in the code CPMD, one can only SKIP ONE channel at a time. Please consult the keyword SKIP in the CPMD manual for further information (http://www.cpmd.org/manual/node46.html).

Example 1: DCACP_H_MT_BLYP.psp

```
&POTENTIAL
   511
.62500000E-02   -7.6586836E+00  -5.6929400E+00  0.0000000E+00   -5.6933456E+00
.63593750E-02   -7.6586835E+00  -5.6929400E+00  0.0000000E+00   -5.6933456E+00
...

&WAVEFUNCTION
   511 CHANNELS=1
.62500000E-02   3.0730264E-03   2.1382580E-05   0.0000000E+00   7.1658861E-12
.63593750E-02   3.1268044E-03   2.2137519E-05   0.0000000E+00   7.6808191E-12
...
```

In the input file for CPMD...

```
&ATOM
*DCACP_H_MT_BLYP.psp KLEINMAN-BYLANDER
LMAX=F LOC=P SKIP=D
...
```

Example 2: DCACP_N_MT_BLYP.psp

```
&POTENTIAL
   624
.89285714E-03   -6.7725706E+00  -2.0208424E+01  -1.6542135E+01  -1.6542740E+01
.90848214E-03   -6.7725706E+00  -2.0208424E+01  -1.6542135E+01  -1.6542740E+01
...

&WAVEFUNCTION
   624 CHANNELS=1
.89285714E-03   2.1376395E-04   9.6690717E-07   5.6480573E-11   2.1540102E-15
.90848214E-03   2.1750482E-04   1.0010450E-06   5.9497997E-11   2.3087953E-15
...
```

In the input file for CPMD...

```
&ATOM
*DCACP_N_MT_BLYP.psp KLEINMAN-BYLANDER
LMAX=F LOC=D
...
```