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:

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

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

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

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

so...

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

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

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

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

$\Gamma$ 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
 .9084214E-03 -.67725706E+01 -.20208424E+02 -.16542135E+02
... 

&WAVEFUNCTION
624 CHANNELS=1
 .89285714E-03 .21376395E-03 .96690717E-06 .56480573E-10
 .9084214E-03 .21750482E-03 .10010450E-05 .59497997E-10
... 

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

• as the “wave function” $r \rho_1$
• as the “potential”

\[ h_{11} \langle \phi_1 | \phi_1 \rangle + V_{\text{loc}} (r) \]
\[ \rightarrow h_{11} + V_{\text{loc}} (r) \]

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...

```plaintext
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_1 = 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 -2.020824E+01 -1.6542135E+01 -1.6542740E+01
.90848214E-03 -6.7725706E+00 -2.020824E+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
...