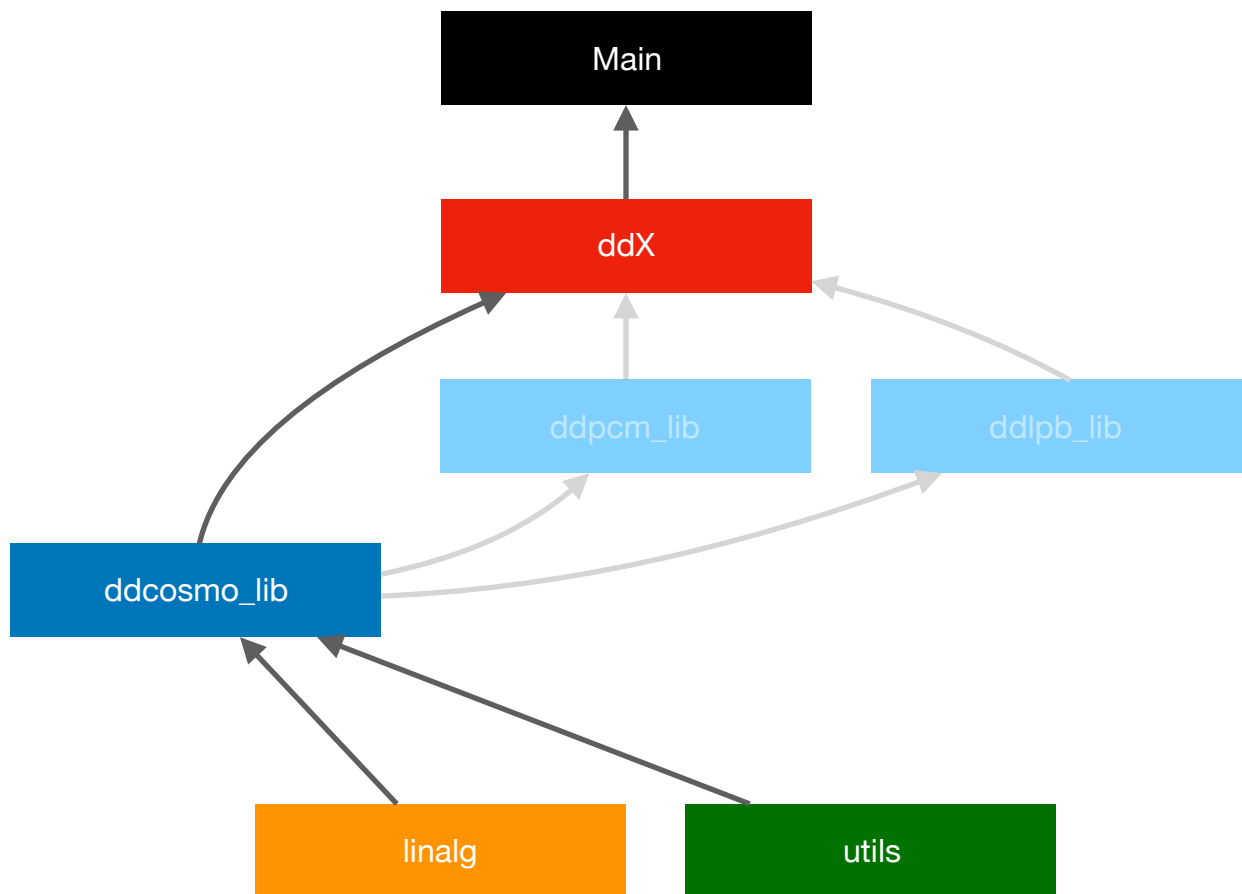


ddX

Modules:

- ddX
- ddcosmo_lib
- ddpcm_lib
- ddlpb_lib
- linalg
- utlis



Main

File name: Main.f90

Use: ddX

Variables:

- phi, psi, gradphi
- x, y, z, ncav, nsphere
- ccav
- nbasis
- rvdw, charge
- energy
- fx
- (for QM: Fock-matrix, dnudmuPsi, dnudmuPhi)

Subroutines:

- mkrhs
- paraminit (new)

Content:

- call ddmain
- mkrhs: copy-paste from existing
- paraminit: read parameter file and initialise utility variables

Module name: ddX

File name: ddX.f90

Use: ddcosmo_lib, ddpcm_lib, ddlpb_lib, linalg, utils

Variables:

- none

Subroutines:

- ddinit
- ddmain
- ddfree (former memfree)

Content:

- ddinit: copy-paste from existing
- ddmain: call ddcosmo, ddpcm or ddlpb depending on model
- ddfree: copy-paste from memfree

Module name: ddcosmo_lib

File name: ddcosmo.f90

Use: linalg, utils

Variables:

- X
- s
- g

Subroutines:

- ddcosmo
- intlmp
- ddmkxi
- calcv
- adjrhs
- fdoka, fdokb, fdoga
- lx, lstarx, ldm1x

Module name: utils
File name: utils.f90
Use: none

Variables:

- todo

Subroutines:

- sprod, fsw, dfsw
- ptcart, prtsph
- intrhs
- ylmbas, dbasis, polleg, trgev
- wghpot
- hsnorm, hnorm
- header