Ab-initio molecular dynamics and geometry optimization, new developments

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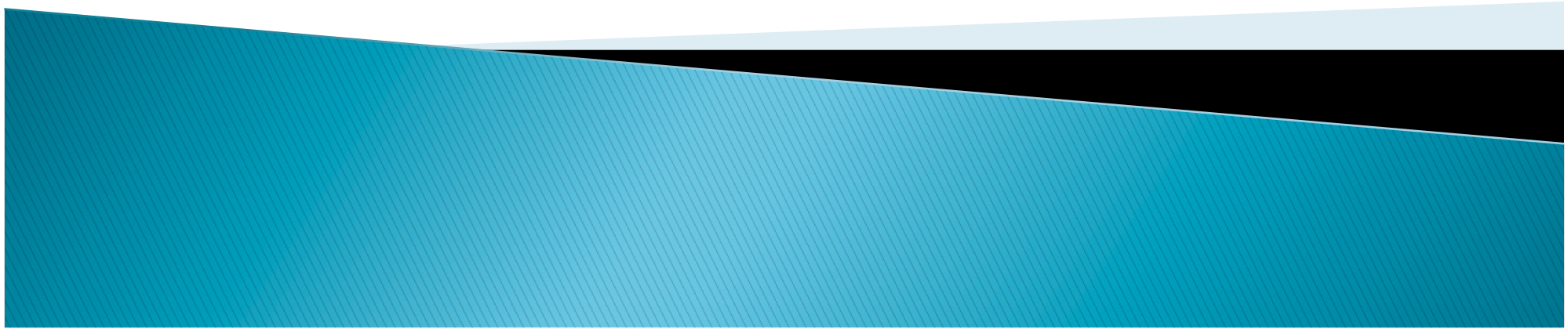
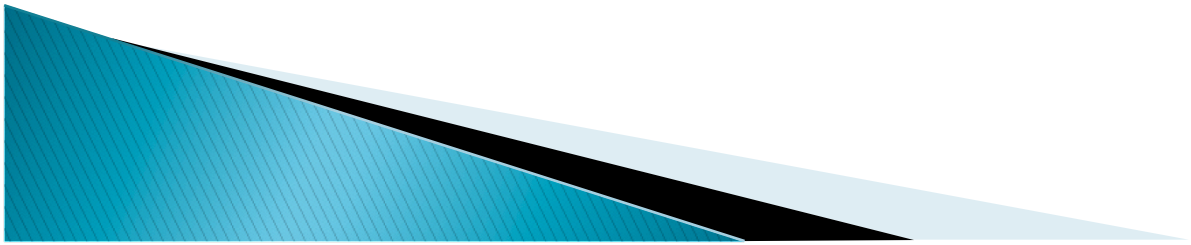
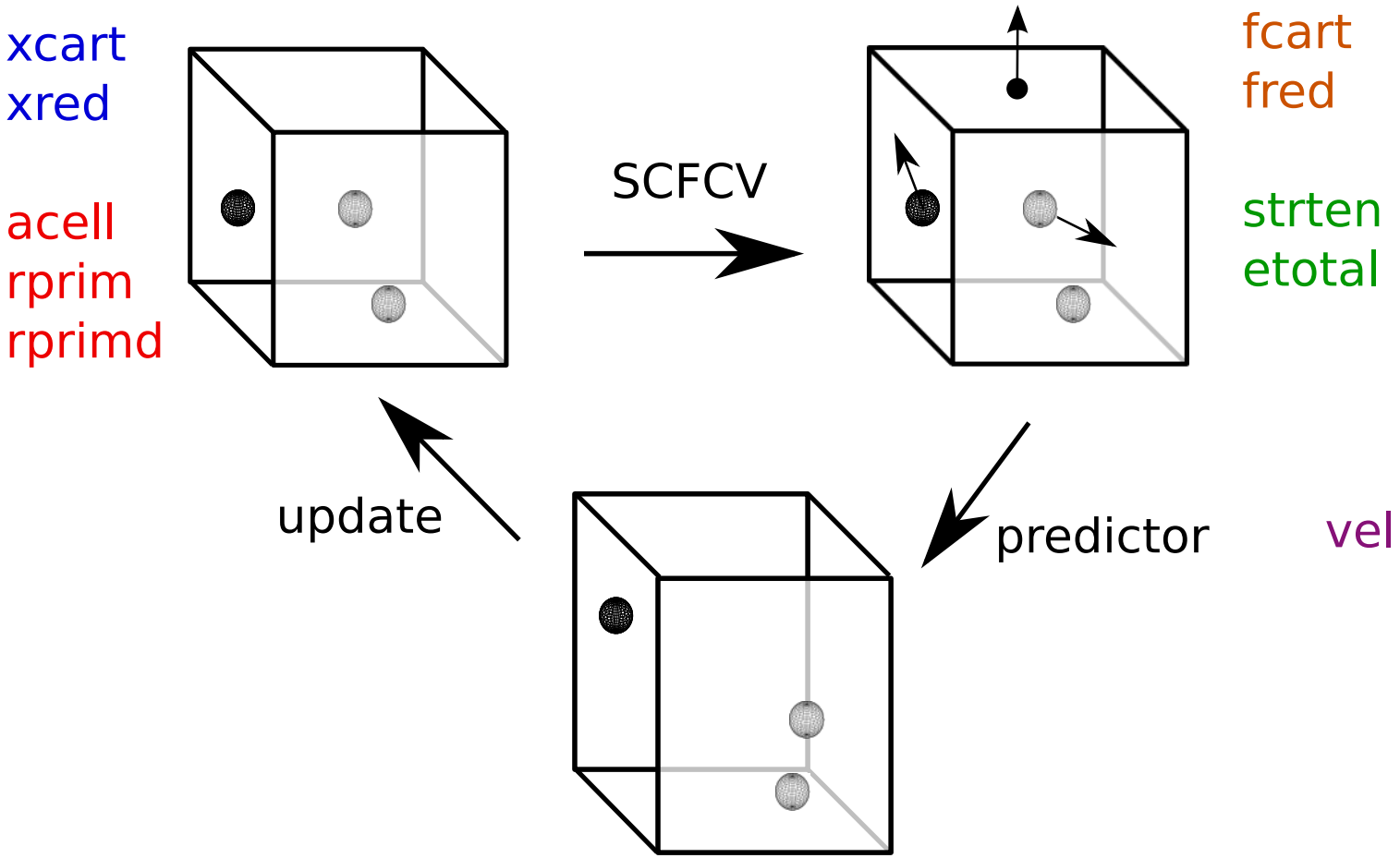


What is all about?

- Molecular dynamics
  - Preserve quantities (energy, temperature, etc…)
  - **Born–Oppenheimer approximation**
- Geometry optimization
  - Minimization problem
  - Local minima?
  - Critical points



How to compute that

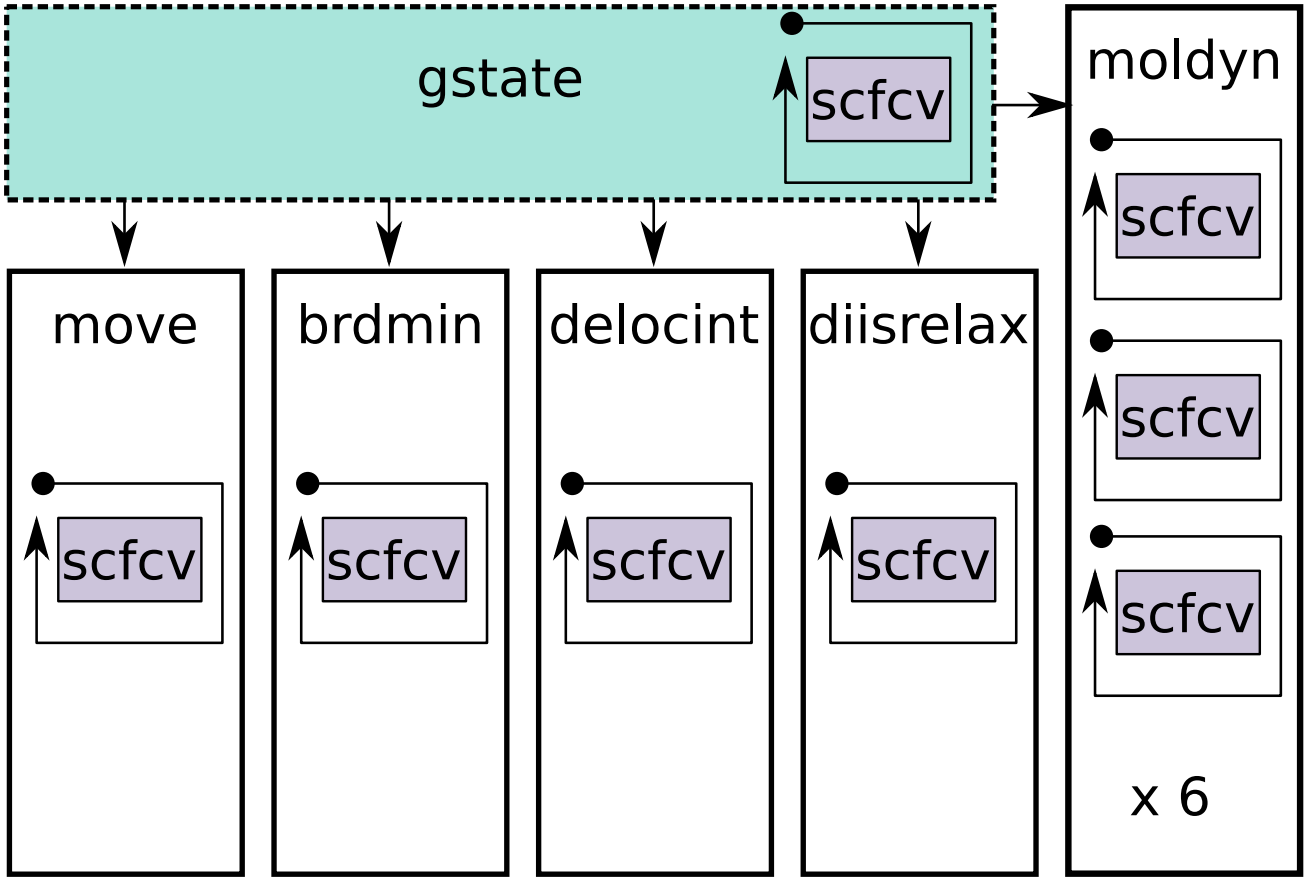


Predictors implemented

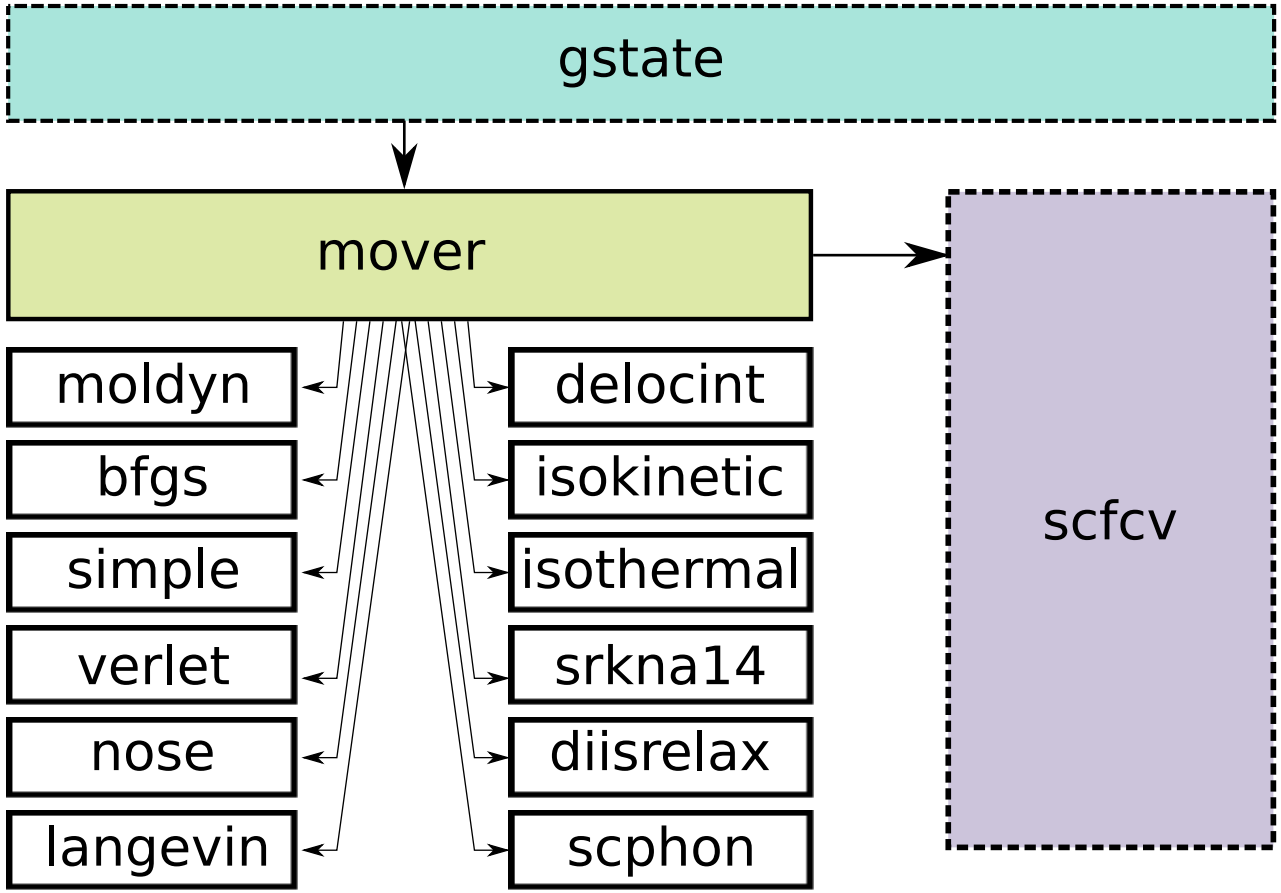
ionmov	predictor	Purpose	optcell ≠ 0	var. related
1	pred_moldyn	MD – GO	NO	vis, dtion
2 and 3	pred_bfgs	GO	YES	
4 and 5	pred_simple	GO	NO	
6 and 7	pred_verlet	MD – GO	NO	dtion
8	pred_nose	MD	NO	*, noseinert
9	pred_langevin	MD	NO	*, friction
10 and 11	pred_delocint	GO	NO	
12	pred_isokinetic	MD	NO	*, friction
13	pred_isothermal	MD	YES	*, nnos, qmass
14	pred_srkna14	MD	NO	
20	pred_diisrelax	GO	NO	diismemory

* = dtion, mditemp, mdftemp

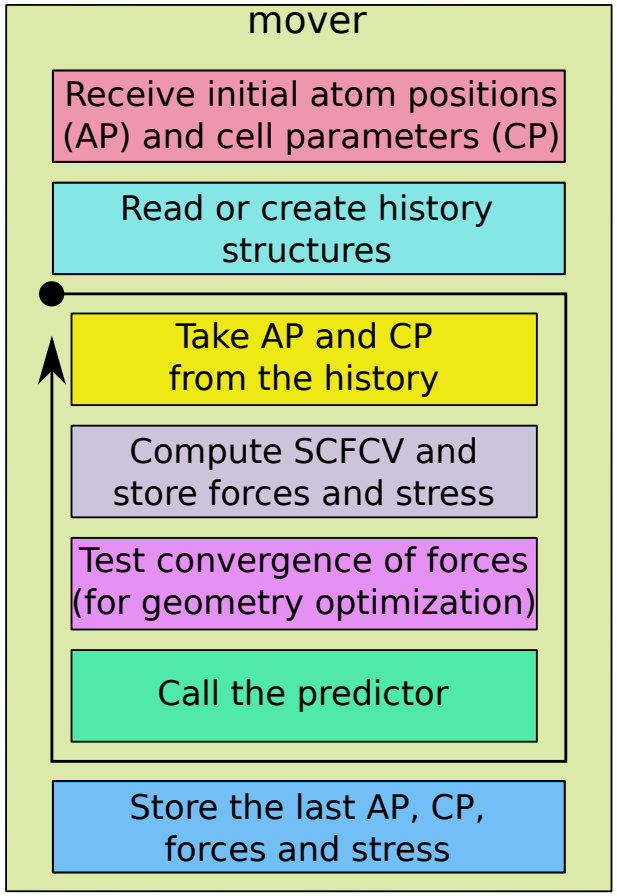
MD-GO (old structure)



MD-GO (new structure)

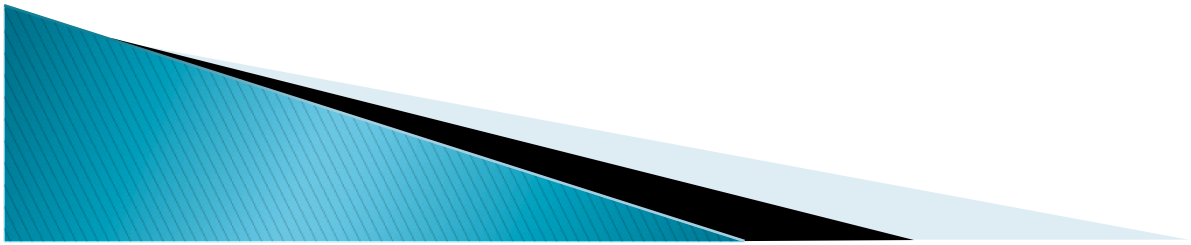


MD-GO (new structure)



Advantages

- The function SCFCV is called in only one place
- The history of previous configurations is stored in a NetCDF file and some predictors can take advantage of this.
- The restart procedure is generalized for all the predictors
- Text and XML output could be generated for all the predictors in a centralized way.



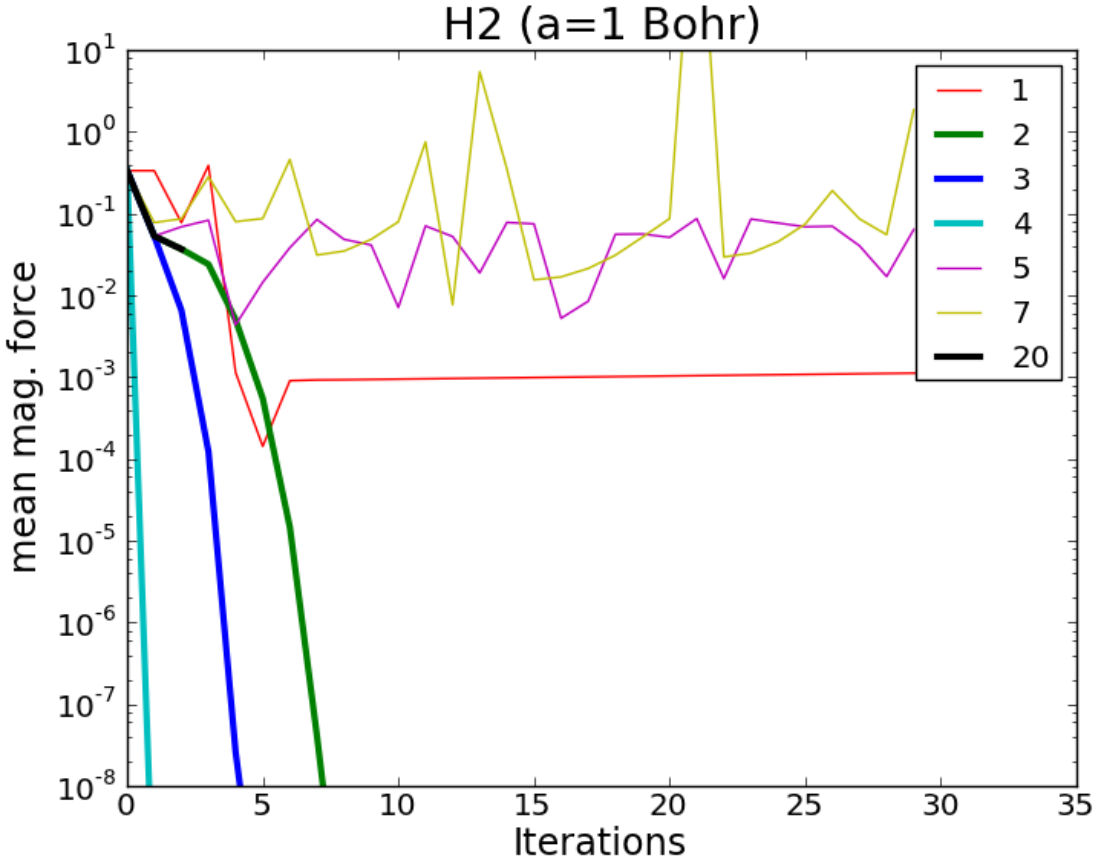
Restarting a MD-GO calculation

- `restartxf -1`: Complete restart using the HIST file
- `restartxf -2`: For restart a calculation taking the configuration with the lowest value of energy and forgeting the history.

- You can set `restartxf` even if you don't have a HIST file, it will start from the values inside the input file.

Some cases of study: (H2)

- H-H=1.4355 Bohr



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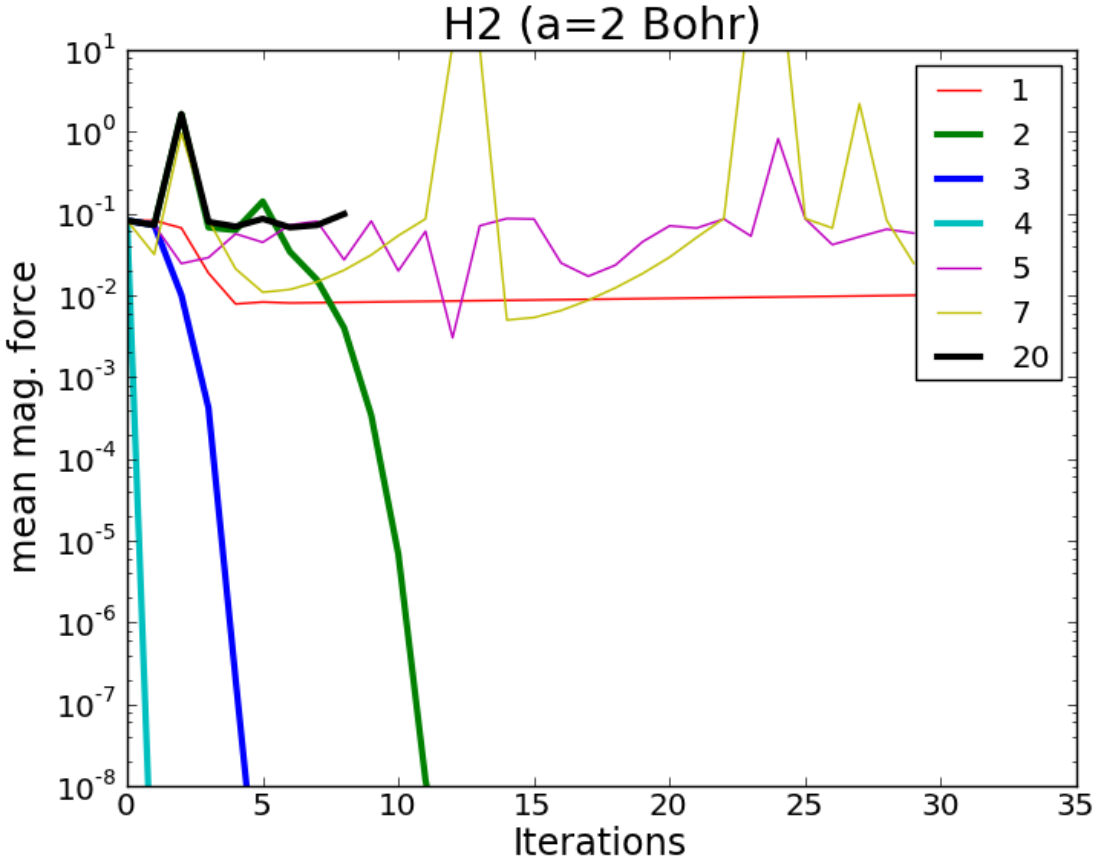
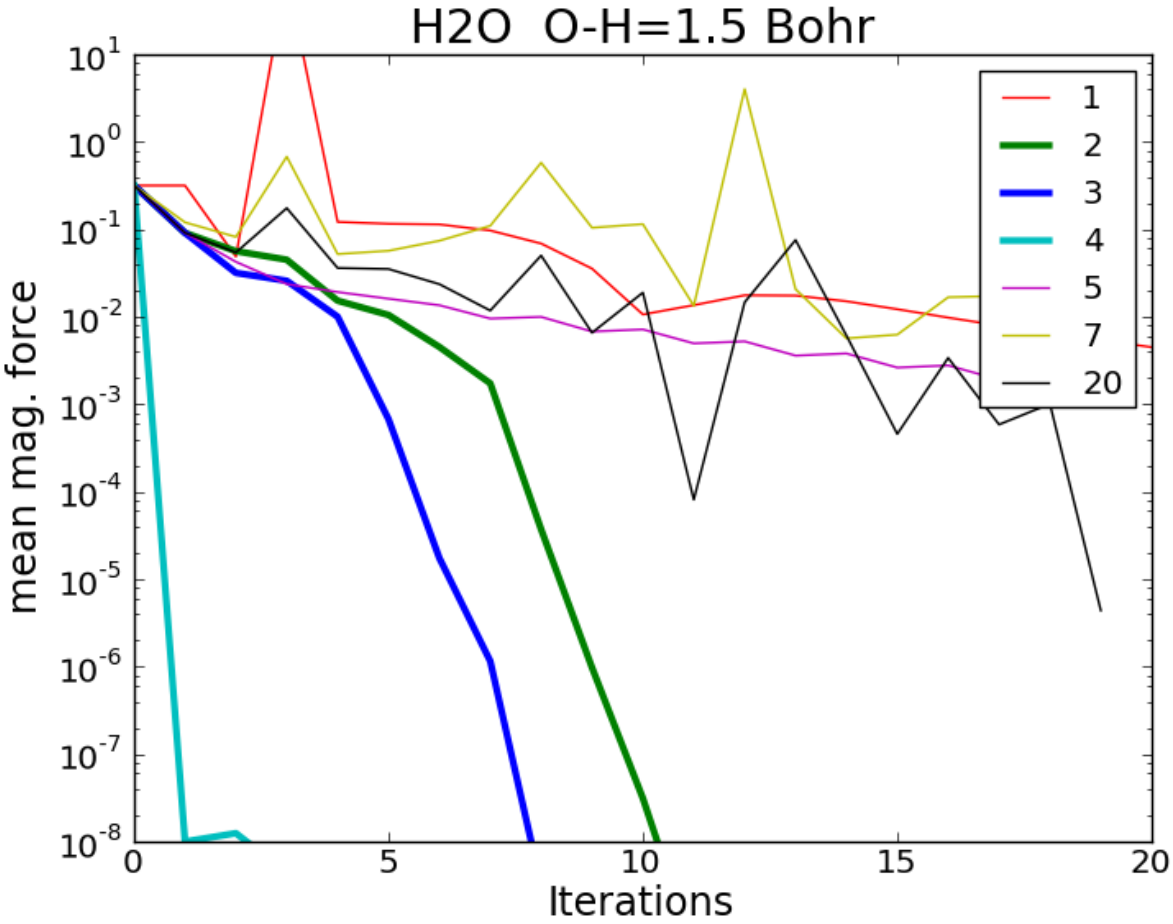


Some cases of study: (H2O)



O–H = 1.8245 Bohr

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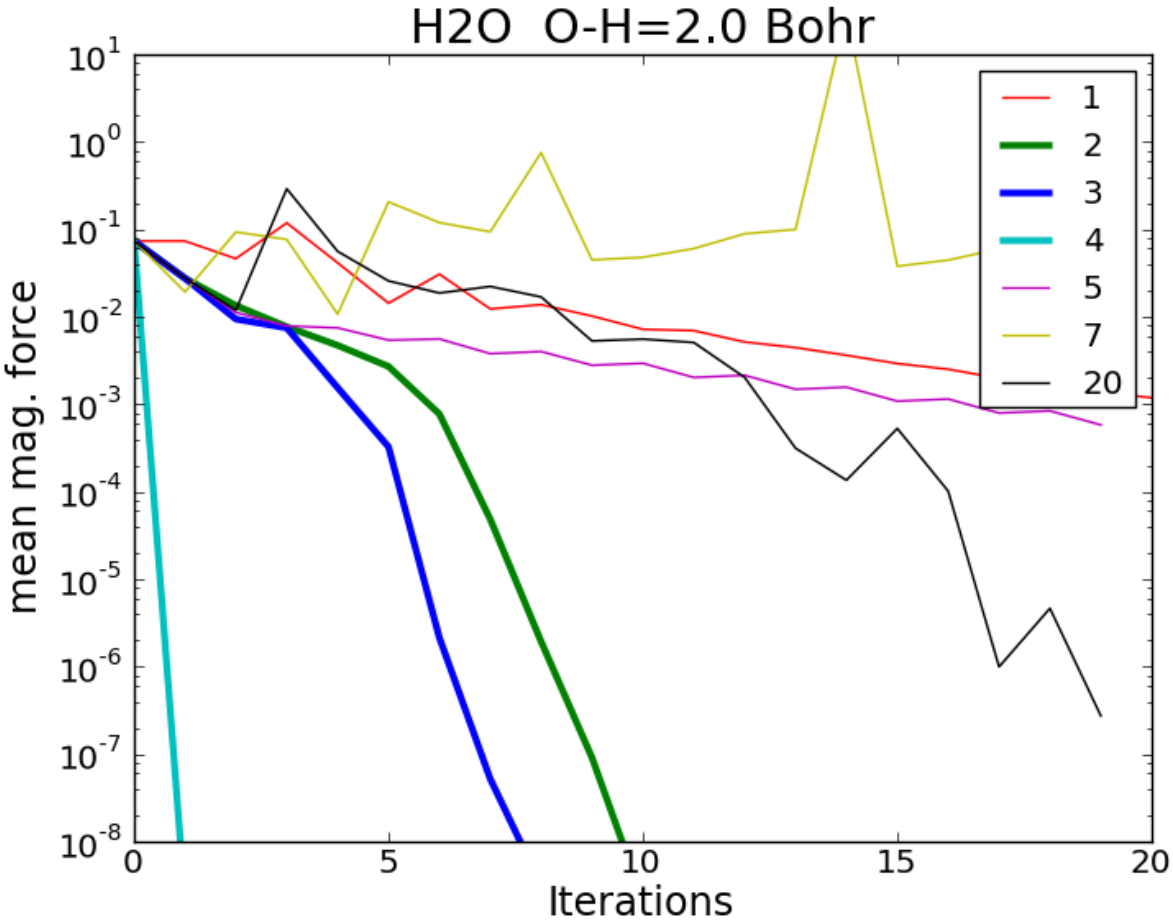

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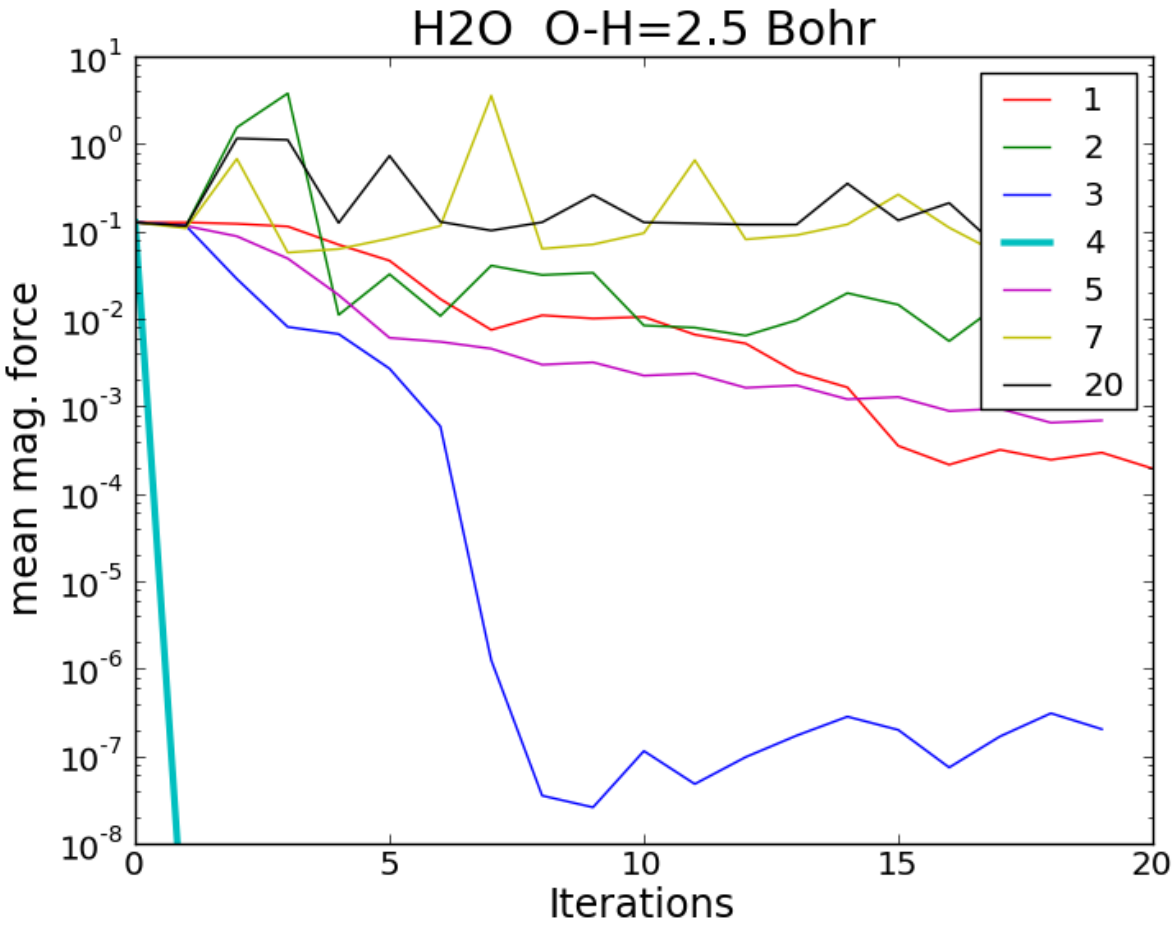
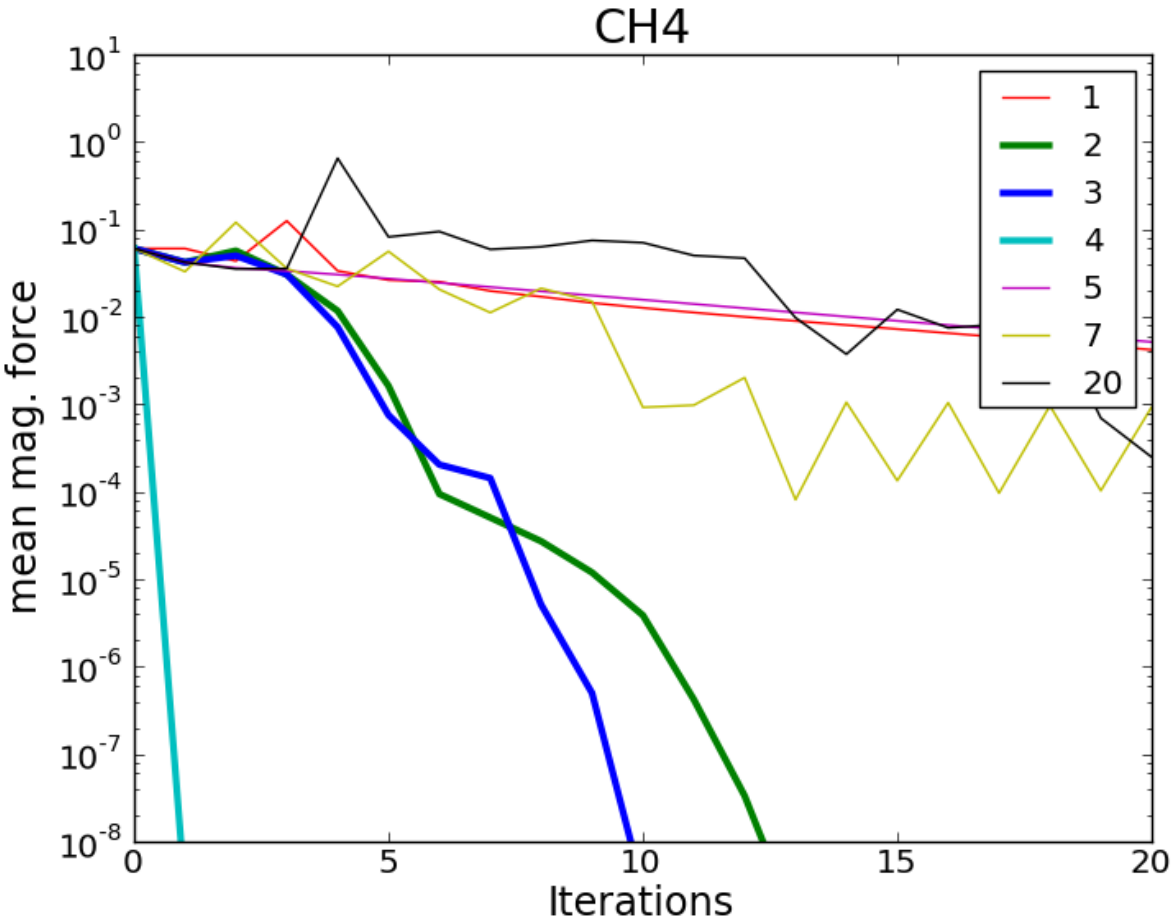


O-H = 1.8245 Bohr

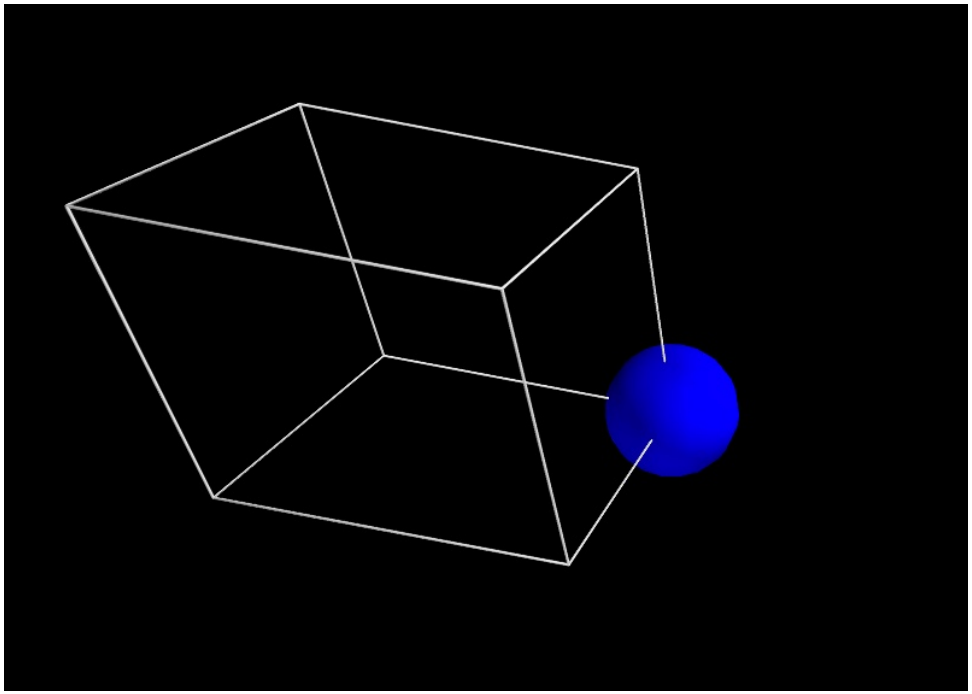
Some cases of study: (CH4)



Some cases of study: (Al)

- FCC
- Typical `rprim`

```
0  1  1
1  0  1
1  1  0
```



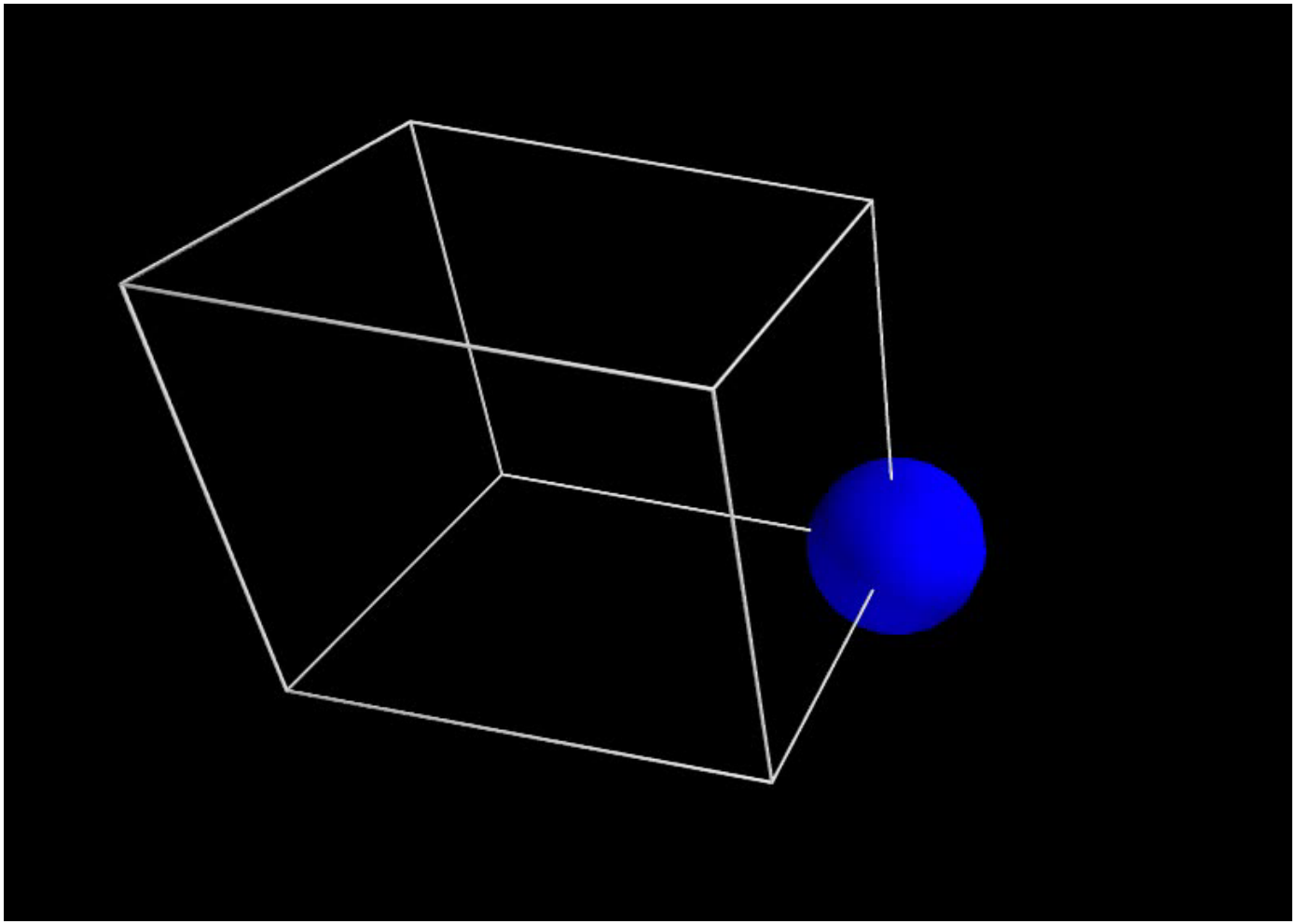
Some cases of study: (Al)

- optcell 2
- dilatmx 1.1
- acell 3*1
- Optimal rprim
  (a, b)=(4.89, 0.79)

$$rprim = a\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + b\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

(a, b)	(5.1, 0.6)	(5.0, 0.6)	(5.1, 0.7)	(5.2, 0.7)
ionmov 2	11	10	9	10
ionmov 3	28	10	10	23

Some cases of study: (Al)

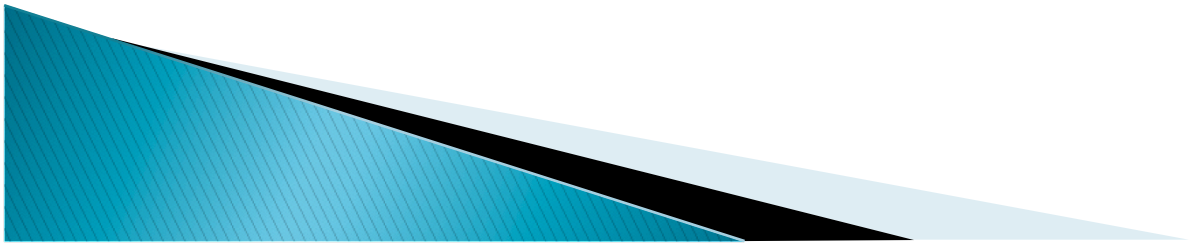


Modularization

- SCFCV plays an essential role for the movement of ions.

- ```
  subroutine scfcv( atindx, atindx1, cg, cpus,&
  & dtefield, dtfil, dtpawuj, dtset, ecore,&
  & eigen, electronpositron, fatvshift, hdr,&
  & iapp, indsym, initialized, irrzon, kg,&
  & mpi_enreg, nattyp, ndtpawuj, nfftf, npwarr,&
  & occ, paw_dmft, pawang, pawfgr, pawrad,&
  & pawrhoij, pawtab, phnons, psps, pwind,&
  & pwind_alloc, pwnsfac, rec_set, resid,&
  & results_gs, rhog, rhor, rprimd, scf_history,&
  & symrec, taug, taur, wffnew, wffnow, wvl,&
  & xred, xred_old, ylm, ylmgr)
  ```

- 52 arguments

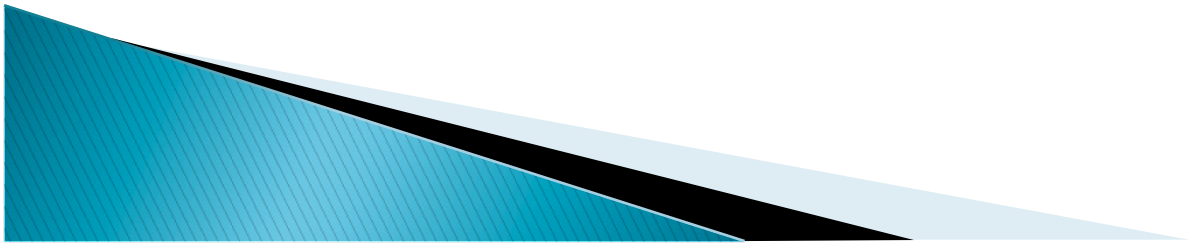

  ```

Modularization

- ```
  subroutine scfcv_new( ab_scfcv_in, cg, dtefield,&
  & dtfil, dtpawuj, dtset, eigen, electronpositron,&
  & hdr, initialized, irrzon, mpi_enreg, nfftf,&
  & occ, paw_dmft, pawfgr, pawrhoij, rec_set,&
  & resid, results_gs, rhog, rhor, rprimd,&
  & scf_history, symrec, taug, taur, wffnew,&
  & wffnow, wvl, xred, xred_old)
  ```

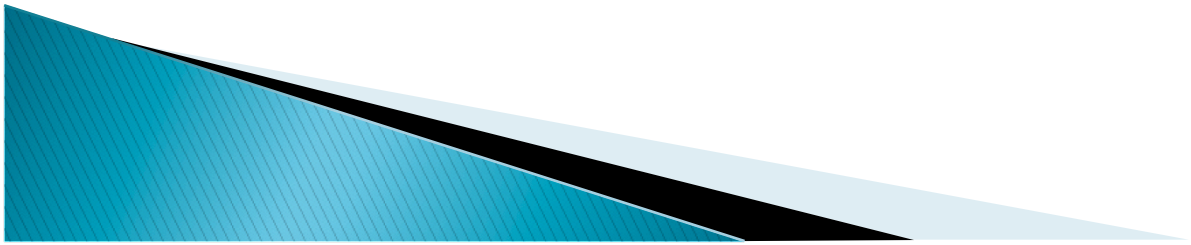
- 32 arguments

- ```
  type(ab_scfcv_args_in),intent(in) :: ab_scfcv_in
  ```



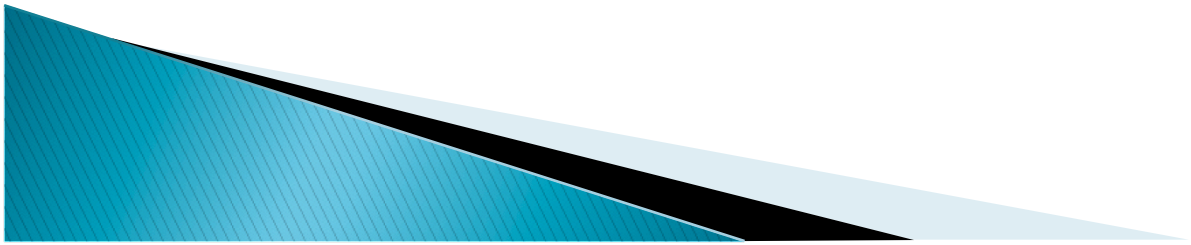
Modularization (ab_movetype)

- All the variables relevant for movement of ions are stored inside the `ab_mover` datatype
- `type(ab_movetype) :: ab_mover`
- It contains 33 variables representing a subset of `dtset` and `dtfil`.



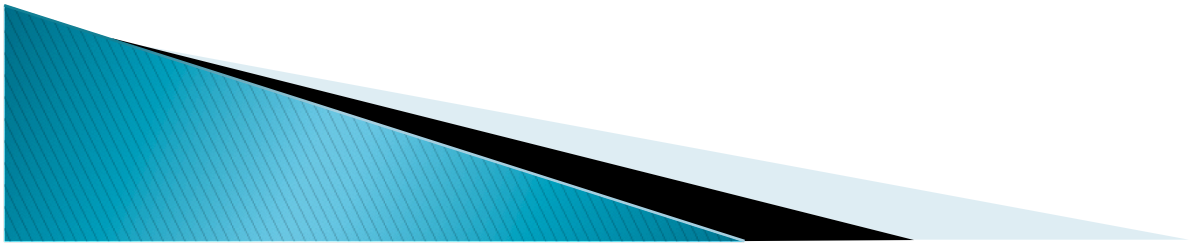
Modularization (ab_movehistory)

- `real(dp), pointer :: histA(:,:)`
- `real(dp), pointer :: histE(:)`
- `real(dp), pointer :: histR(:,:,:)`
- `real(dp), pointer :: histS(:,:)`
- `real(dp), pointer :: histV(:,:,:)`
- `real(dp), pointer :: histXF(:,:,:,:)`



The Future

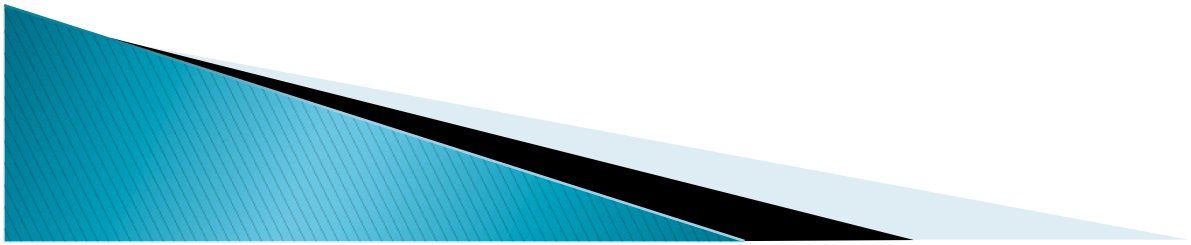
- Implement a set of preconditioners
- Increase the robustness of some predictors.
- Preconditioners
- Convert it into a library



Off Topic…

- Output variables in NetCDF format
  - Use ncdump to visualize the contents

```
netcdf MD-GO-o_OUT {
dimensions:
   one = 1 ;
   acell = 3 ;
   ngfft = 3 ;
...
variables:
   double acell(acell) ;
   double amu(one) ;
   double diemac(one) ;
...
xcart1 = -0.5, 0, 0, 0.5, 0, 0 ;
xcart2 = -16.2933031711595, 0, 0, 16.2933031711595, 0, 0 ;
xcart3 = -0.717744974279991, 0, 0, 0.717744974279991, 0, 0 ;
```



Off Topic…

- abi_python library:
  - Read input files, output in NetCDF format
  - Post-processing
  - Visualization