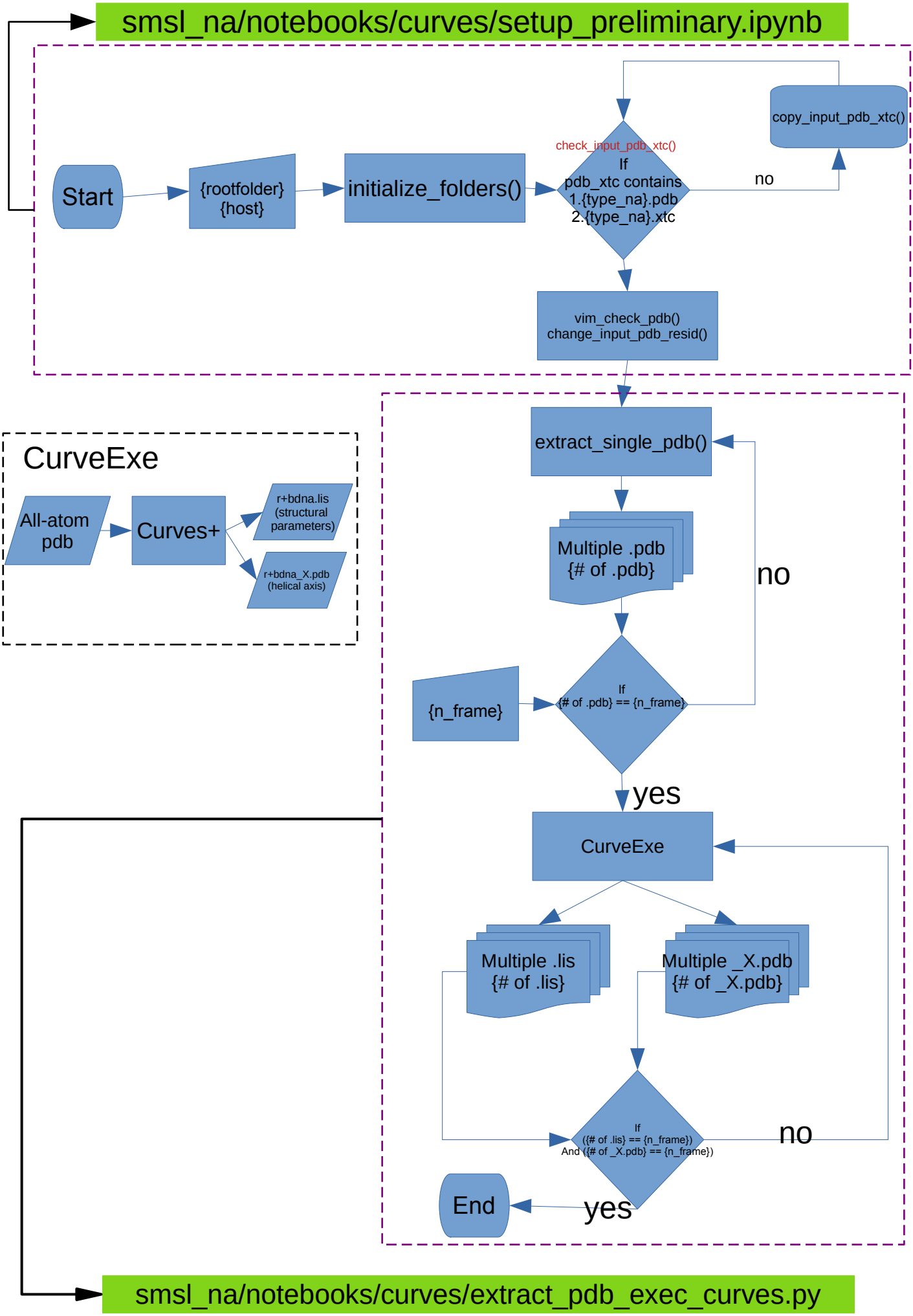
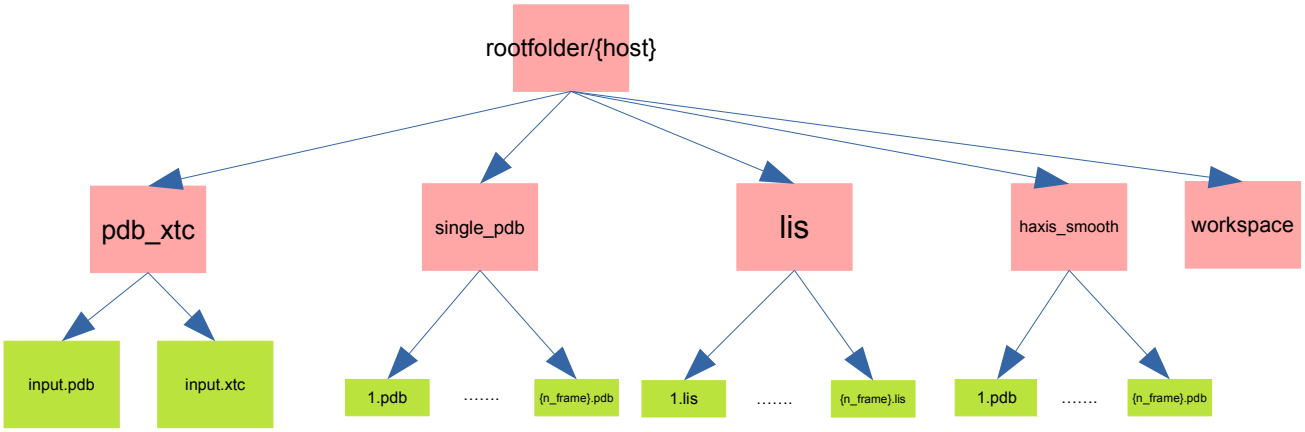

smsl_na/notebooks/curves/setup_preliminary.ipynb
Start
{rootfolder}
{host}
initialize_folders()
check_input_pdb_xtc()
If
pdb_xtc contains
1.{type_na}.pdb
2.{type_na}.xtc
no
copy_input_pdb_xtc()
vim_check_pdb()
change_input_pdb_resid()
CurveExe
All-atom
pdb
Curves+
r+bdna.lis
(structural
parameters)
r+bdna_X.pdb
(helical axis)
extract_single_pdb()
Multiple .pdb
{# of .pdb}
no
{n_frame}
If
{# of .pdb} == {n_frame}
yes
CurveExe
Multiple .lis
{# of .lis}
Multiple _X.pdb
{# of _X.pdb}
If
({# of .lis} == {n_frame})
And ({# of _X.pdb} == {n_frame})
no
End
yes
smsl_na/notebooks/curves/extract_pdb_exec_curves.py

Directory Tree