CombiFF

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1 CombiFF Workflow

The CombiFF workflow is illustrated in Figure 1

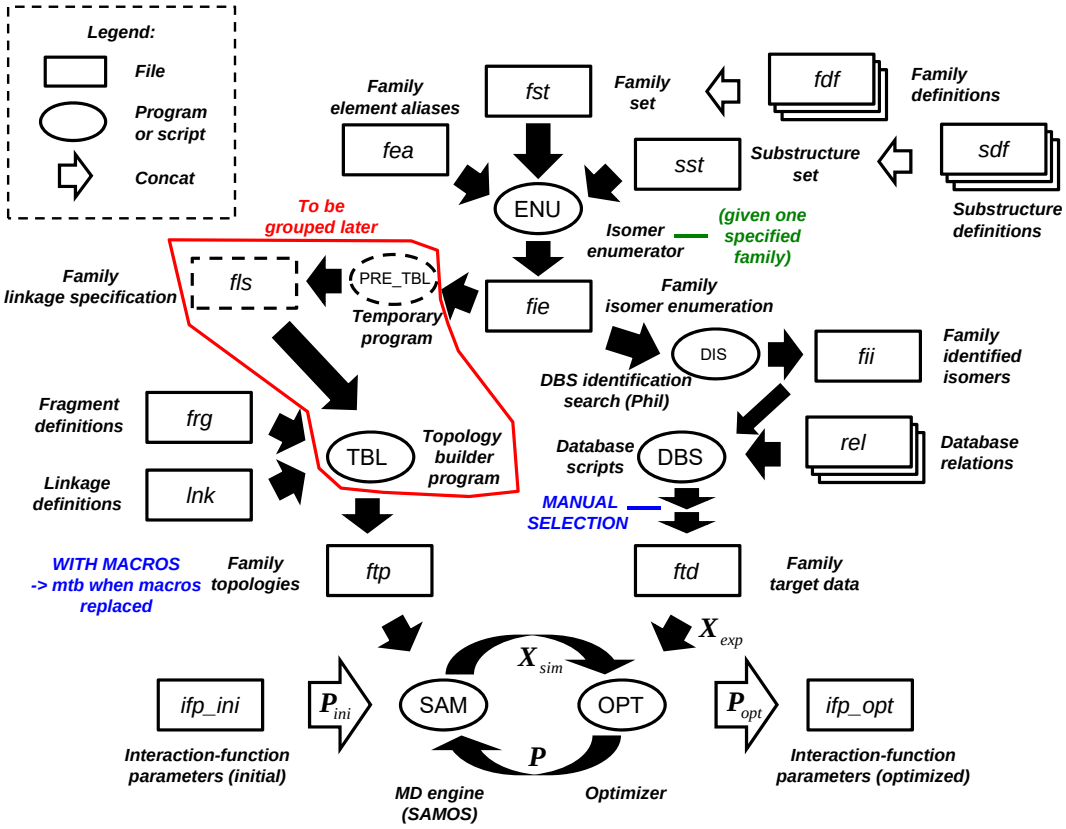

Figure 1: XXX

2 CombiFF Programs

The programs/scripts involved in CombiFF summarized in Table 1 and described in the following subsections.

3 CombiFF File Types

The file types involved in CombiFF summarized in Table **??** and described in the following subsections. For the labelling of the files, we will refer to a version number (v%%) and to family numbers (####). The family number is a four-digit number that refers to a given family of compounds.

Programs/scripts involved in CombiFF	
enu	isomer enumerator
tbl	topology builder
DIS	(Phil-to-write) scans DBS to map
DBS	scripts of the experimental database
SAM	MD engine (SAMOS)
OPT	parameter optimizer
cnv	converter and canonicalization program

Table 1

3.1 Family definition file

- Format: xml
- Location: CombiFF/use/input_files/family_definitions
- Content: specification of one or more compound families for enu
- Output of: Generated/edited manually
- Input of: enu

A fdf file defines a given compound family with the number #### within the CombiFF version v%%. These files are created/edited manually to define/modify families.

3.1.1 Format

see Combiff/use/input_files/family_definitions/README and Combiff/use/input_files/family_definitions

3.2 Substructure files

- Format: xml
- Location: CombiFF/use/input_files/substructures
- Content: substructures that can be included/excluded in the definition of families
- Output of: Generated/edited manually
- Input of: enu

3.2.1 Format

see Combiff/use/input_files/substructures/README and Combiff/use/input_files/substructures/substruct

3.3 Alias files

- Format: xml
- Location: CombiFF/use/input_files/aliases
- Content: aliases for sets of atom types (e.g. Hal for {Br, Cl, F, I}) that can be used in family definitions
- Output of: Generated/edited manually
- Input of: enu

3.3.1 Format

see Combiff/use/input_files/aliases/README and Combiff/use/input_files/aliases/aliases.dtd

3.4 Pseudoatom files

- Format: xml
- Location: `CombiFF/use/input_files/aliases`
- Content: definition of pseudoatoms that can be used for family definitions
- Output of: Generated/edited manually
- Input of: `enu`

3.4.1 Format

see `Combiff/use/input_files/pseudoatoms/README` and `Combiff/use/input_files/pseudoatoms/pseudoatoms.d`

It is important to note that all atoms in a pseudoatom must be fully bonded, except for the atom in the first position of the ATOMS list. For example C-O-OH would be a valid pseudoatom, since only the carbon can form any bonds outside of the pseudoatom, but C-O-O would *not* be a valid pseudoatom, since both the carbon and the 2nd oxygen can form bonds outside of the pseudoatom.

3.5 Fragment files

- Format: xml
- Location: `CombiFF/use/input_files/fragments`
- Content: definition of fragments to use to assemble molecules
- Output of: Generated/edited manually
- Input of: `tbl`

3.5.1 Format

see `Combiff/use/input_files/fragments/README` and `Combiff/use/input_files/fragments/fragments.dtd`

3.6 Family isomer enumeration files

- Format: xml
- Location: `CombiFF/use/output_files/family_isomer_enumerations`
- Content: list of constitutional isomers for a given family
- Output of: `enu`
- Input of: `tbl`

3.7 Family stereoisomer enumeration files

- Format: xml
- Location: `CombiFF/use/output_files/family_isomer_enumerations_stereo`
- Content: list of stereoisomers (from tetrahedral centers and double bonds) for a given family
- Output of: `enu`
- Input of: –

3.8 molecule decomposition files

- Format: xml
- Location: `CombiFF/use/output_files/molecule_decompositions`
- Content: specifies how to assemble the molecules of a family with given fragments
- Output of: `tbl` or manual creation
- Input of: `tbl`

3.9 molecules with macros files

- Format: xml
- Location: `CombiFF/use/output_files/molecules_with_macros`
- Content: molecular topologies with macro parameters for parameters (i.e. bond types, charges, etc.)
- Output of: `tbl`
- Input of: `tbl`

3.10 GROMOS mtb files - with macros

- Format: xml
- Location: `CombiFF/use/output_files/mtb`
- Content: GROMOS mtb files for given families with macros
- Output of: `tbl`
- Input of: `tbl`

3.11 GROMOS mtb files - with parameters

- Format: xml
- Location: `CombiFF/use/output_files/mtb`
- Content: GROMOS mtb files for given families with FF parameters
- Output of: `tbl`
- Input of: `GROMOS/SAMOS`