Working with projects

(visit Getting started pictogram for a summary on the Project creation workflow)

The pyMDMix project consists of different macromolecules to be studied (the systems) and individual simulation set ups (Replicas). Once a project is started, all program commands should be issued inside the project folder.

Creating an empty project

```
> mdmix create project -n MyProject
```

This will write a new folder under the current working directory with name **`MyProject`**. This new folder is considered the PROJECT FOLDER from now on and across all documentation. To work with the project, we should move to the recently created directory.

The **project folder** contains a file named **`MyProject.mproj`**. This file is internally used by the project and should never be removed.

Adding systems

The project is prepared for dealing with more than one system. This option has been implemented thinking in different states of a same macromolecule that could be simulated independently applying restraints. In the majority of situations, we will be interested in adding just one system. Check System preparation section for details and examples on how to create the system. This system is a macromolecule prepared for a simulation *in vacuo*. Solvent will be added when creating replicas.

In this example, we have created a system identified with name `SystemA` inside configuration file `mysystem.cfg`. To add it to current project:

```
> mdmix add system -f mysystem.cfg
```

This command will save a file `SystemA.msys` in the project folder for internal use. Don't remove this file. Remember this command should be executed inside the project folder.

Creating replicas

Once a system is added to the project, we can start creating Replicas of the system. To do so, we have to prepare a **Settings configuration file**. This file contains the set of parameters needed to create the solvated system and the MD input files. `NREPL` option allows you to create several replicas sharing the same settings at once. Check The Replicas and MD Settings for details on default parameters and examples.

We have decided the replicas to create and saved all the settings in `replicas_settings.cfg` file. To finally create the MD inputs needed to run the simulations, execute:

```
> mdmix add replicas -f replicas_settings.cfg -sys SystemA
```

New folders will be created inside MD folder. Each folder corresponds to one of the replicas. **Take now these folders to run the simulation!**

Creating projects in one step

A more comfortable way of creating a project from scratch when you already decided the system and what replicas to simulate is to join Settings configuration file and System configuration file sections into one unique file (e.g. joining previous two example cfg files into `SystemA_replicas.cfg`). The project would be created with:

```
> mdmix create project -n MyProject -f SystemA_replicas.cfg
```

The separate method of creation is interesting when you decide to add more replicas to an already created project.

Print project information

By calling the following command inside a project folder, a summary of the project status will be printed. Information on the systems linked, the replicas created or groups defined will be printed. More over, a summary of the different replica parameters and the simulation status will be checked and printed (that is, the program will check if all simulation steps are complete and the trajectory has been aligned).

```
> mdmix info project
------------------------------
PROJECT pep_project INFO
------------------------------
SYSTEMS:
========
SYSTEM:pep

REPLICAS
========
REPLICA:ETA_1 system:pep_ETA nanos:1 restrMode:HA restrForce:0.010 Min:True Eq:True Prod:TrueAlign:True
REPLICA:WAT_1 system:pep_WAT nanos:1 restrMode:HA restrForce:0.010 Min:True Eq:True Prod:TrueAlign:True

GROUPS
======
project_group: ETA_1, WAT_1
------------------------------
```

Project folder structure

The project folder contains a folder called `MD` where all replica folders are saved once a replica is created. Apart from this folder, several files might be present:

- Project file: a file with same name of the project and extension **`mproj`**. Internally used by pyMDMix.
- System files: When adding systems to the project, two files will be written with system name as prefix: a **PDB file** with a reference structure that can be loaded with the grids generated after analysis to visualize results, and a file with extension **`msys`** internally used by pyMDMix. This file can be moved across projects and will still be valid (e.g. copy systems between projects would be as easy as copying this file to the destination project folder).

After energy analysis is completed, a new folder **`PROBE_AVG`** might be created which will contain resulting grids. The following diagram summarizes this folder content and the replica folder content.