http://miccom-center.org

2017 Summer School

Topic: Setting up your SSAGES Workflow

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COMPILING THE CODE

- Minimum requirements:
  - openmpi/1.8
  - cmake/3.4
  - gcc/4.9

- Clone
  - git clone https://github.com/MICCoM/SSAGES-public.git

- Specify engine
  - cmake .. –DLAMMPS=yes
  - cmake .. –DGROMACS=yes
  - cmake .. –DLAMMPS_SRC=/path/to/lammps/src
  - cmake .. –DGROMACS_SRC=/path/to/gromacs/

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CODE

```
[ycolon@midway-login2 SSAGES]$ ls
build           doc        hooks     LICENSE.txt  schema  test
CMakeLists.txt  Examples   include   README.md     src     Tools
```

- build
  - Contains executable
- doc
  - Contains documentation
- examples
  - Contains examples for all the methods in SSAGES
- schema
  - Contains .json templates for methods and CVs
- src
  - Contains .cpp and .h files for methods and CVs

.JSON FILE

```
{
        "type" : "object",
        "varname" : "ParticleCoordinateCV",
        "properties" : {
                "type" : {
                        "type" : "string",
                        "enum" : ["ParticleCoordinate"]
                },
                "dimension" : {
                        "type" : "string",
                        "enum" : ["x", "y", "z"]
                },
                "atom_ids" : {
                        "type" : "array",
                        "minItems" : 1,
                        "items" : {
                                "type" : "integer",
                                "minimum" : 0
                        }
                },
                "bounds" : {
                        "type" : "array",
                        "minItems" : 2,
                        "maxItems" : 2,
                        "items" : {
                                "type" : "number"
                        }
                },
                "name" : {
                        "type" : "string"
                }
        },
        "required": ["type", "atom_ids", "dimension"],
        "additionalProperties": false
}
```

```
"CVs" :
[
        {
                "type" : "ParticleCoordinate",
                "atom_ids" : [1],
                "dimension" : "x"
        }
]
```

RUNNING A SIMULATION WITH SSAGES

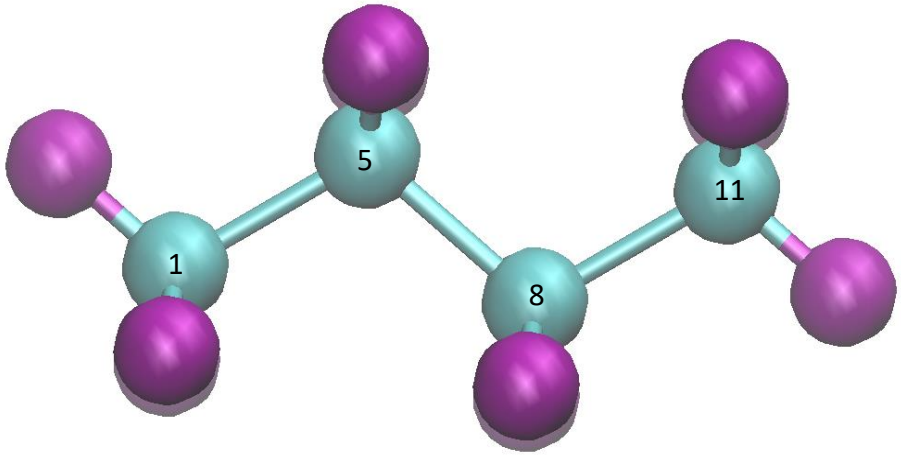
- Each engine SSAGES is coupled to requires its own executable
- Slightly different input files
- mpirun -np x /path/to/SSAGES/build/ssages MyInputFile.json

LAMMPS

```
# Model system
units           real
atom_style      full
boundary        p p p
p
d
p
b
a
d
k
s
n
n
r
g
t
thermo_style    custom etotal ke temp press vol
thermo_modify   line multi
thermo          1
thermo_modify   flush yes
timestep 1
fix 1 all nvt temp 300 300 100# iso 1.0 1.0 1000.0

fix ssages all ssages

run 10000
```




```
{
    "input" : "in.butane"
    "walkers" : 1,
    "methods" : [
        {
            "type" : "Umbrella",
            "ksprings" : [100],
            "output_file" : "ulog.dat",
            "centers" : [1.0],
            "cvs" : [0]
        }
    ],
    "CVs" : [
        {
            "type" : "Torsional",
            "atom_ids" : [1,5,8,11]
        }
    ]
}
```

Units consistent with engine:
LAMMPS real [=] kcal/mol

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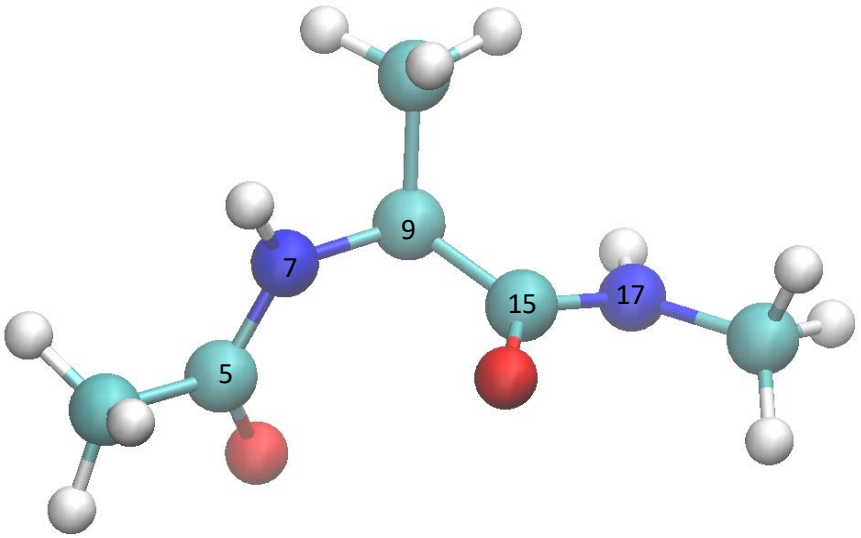
GROMACS

```
{
    "args" : ["-v", "-deffnm", "example_adp"],
    "walkers" : 1,
    "methods" : [
        {
            "type" : "Umbrella",
            "ksprings" : [100],
            "output_file" : "ulog.dat",
            "centers" : [1.0],
            "cvs" : ["foo"]
        }
    ],
    "CVs" : [
        {
            "type" : "Torsional",
            "atom_ids" : [5,7,9,15],
            "name" : "foo"
        }
    ]
}
```

New input line



Units consistent with engine:
GROMACS [=] kJ/mol

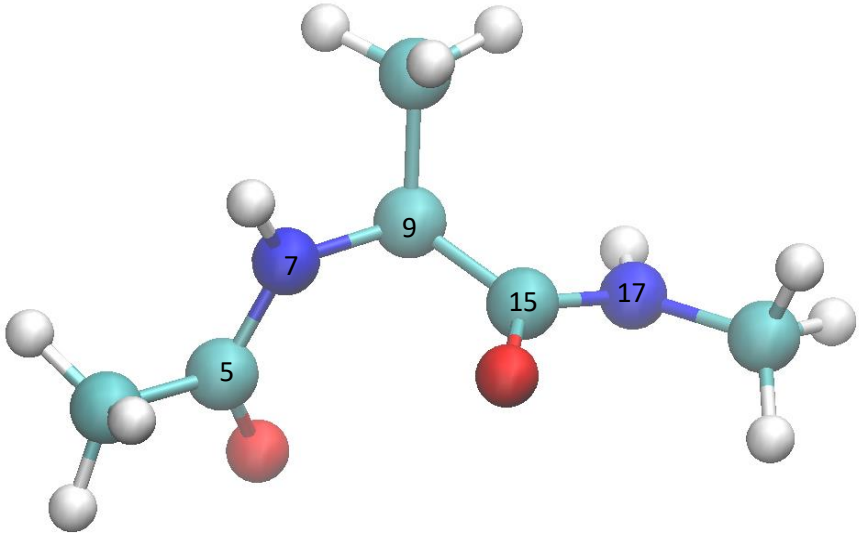
ADAPTIVE BIASING FORCE: ADP IN GROMACS

```
[ycolon@midway-login2 SSAGES]$ ls
build           doc       hooks    LICENSE.txt  schema  test
CMakeLists.txt  Examples  include  README.md    src     Tools
```

- cd Examples/User/ABF/Example_AlanineDipeptide/ABF_ADP_Gromacs_Example/
- Provided .tpr and .json file
- To run:
  - /path/to/SSAGES/build/ssages ADP_ABF_1walker.json

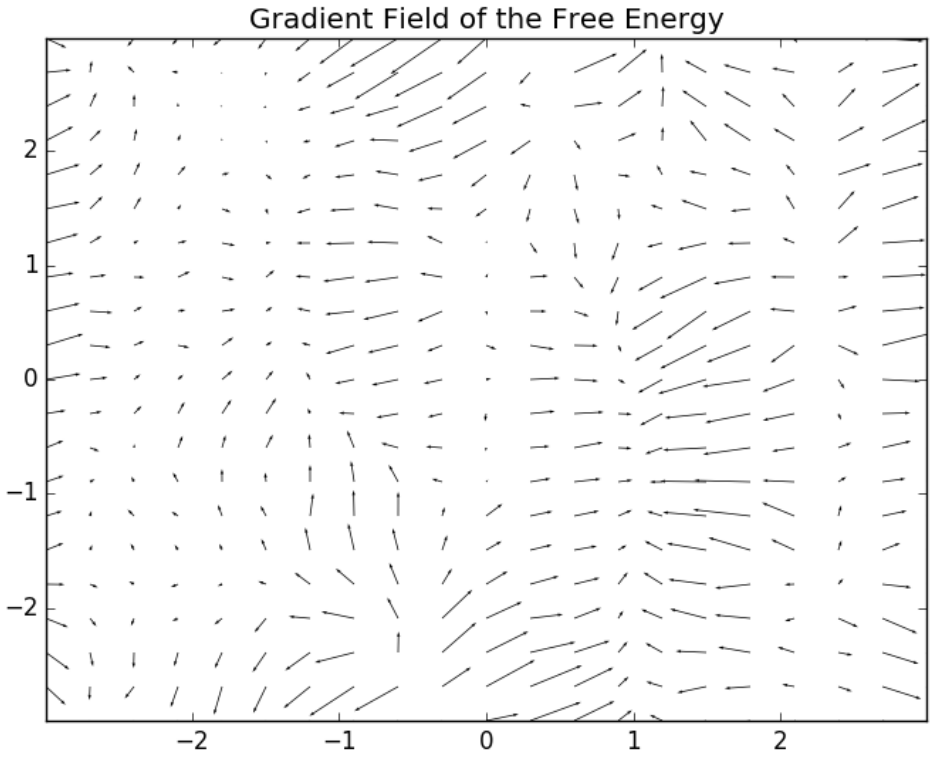
ABF: ADP IN GROMACS

- .json file

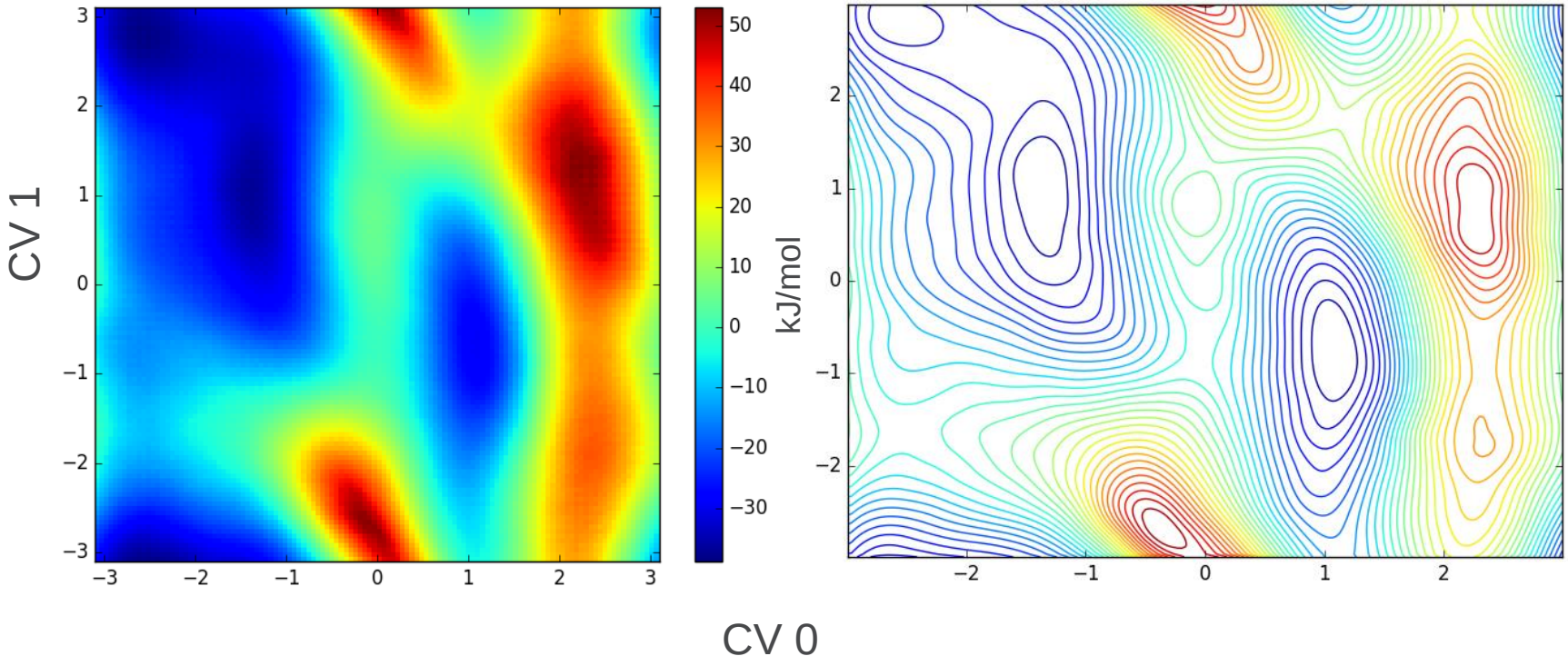


SAMPLE OUTPUT

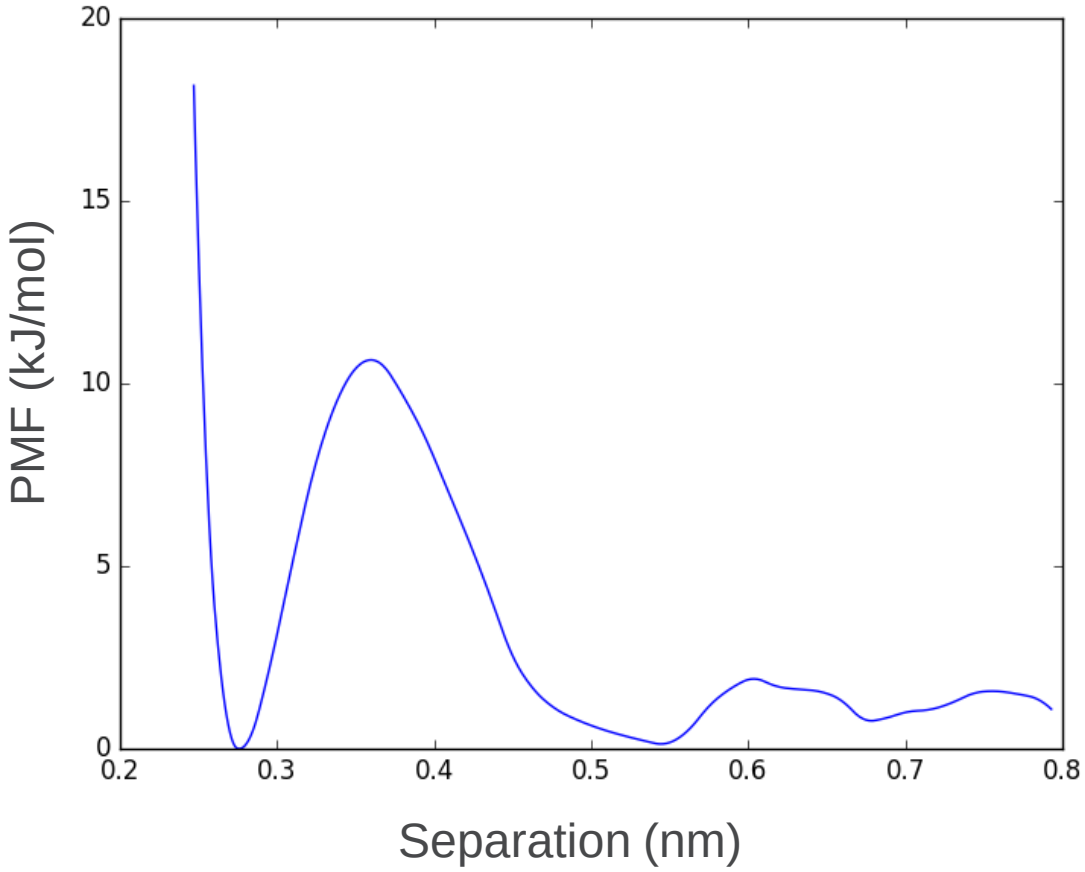
- Examples/User/ABF/Example_AlanineDipeptide/Sample_Outputs/



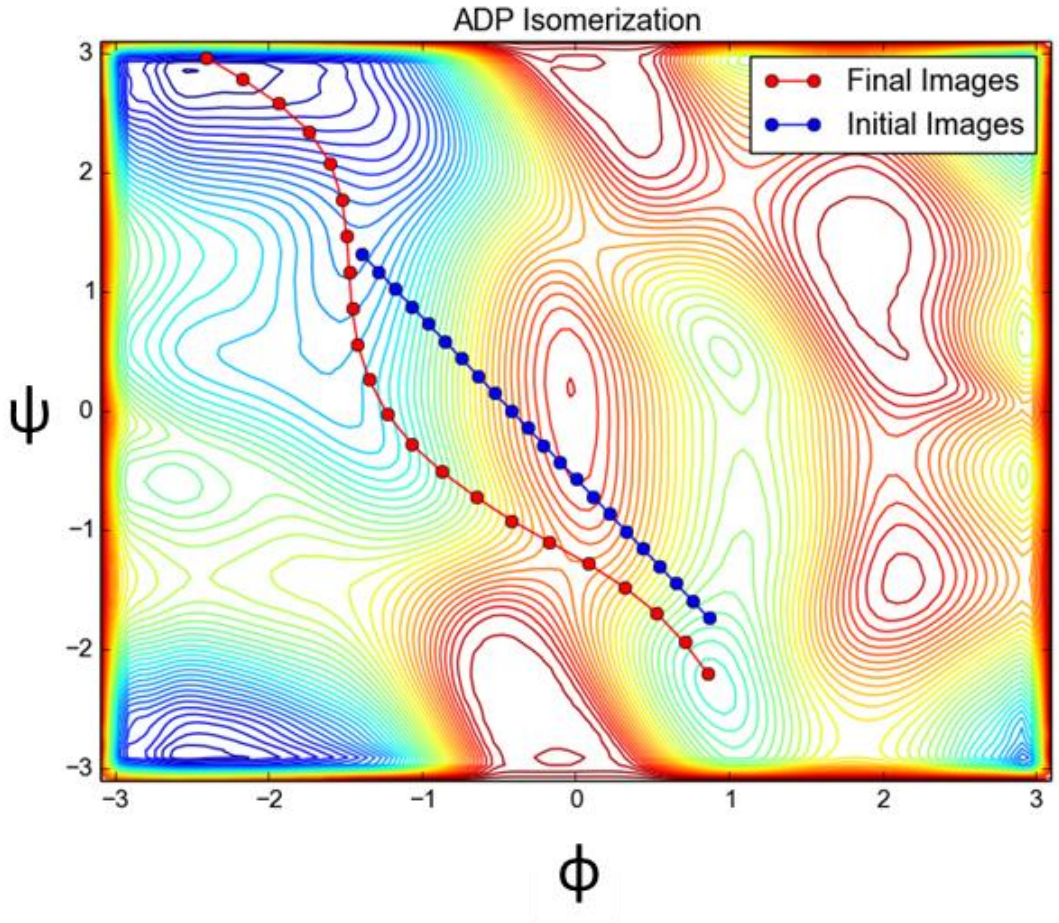
SAMPLE OUTPUT

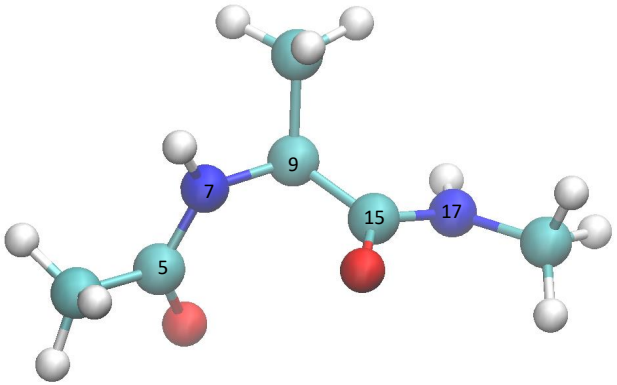


ABF NACL



FTS ADP LAMMPS





SUMMARY

- Different engines require different executables.
- .json input files to SSAGES are simple.
- There are examples for all methods in SSAGES.
- Use free energy and string methods.
- git clone https://github.com/MICCoM/SSAGES-public.git

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