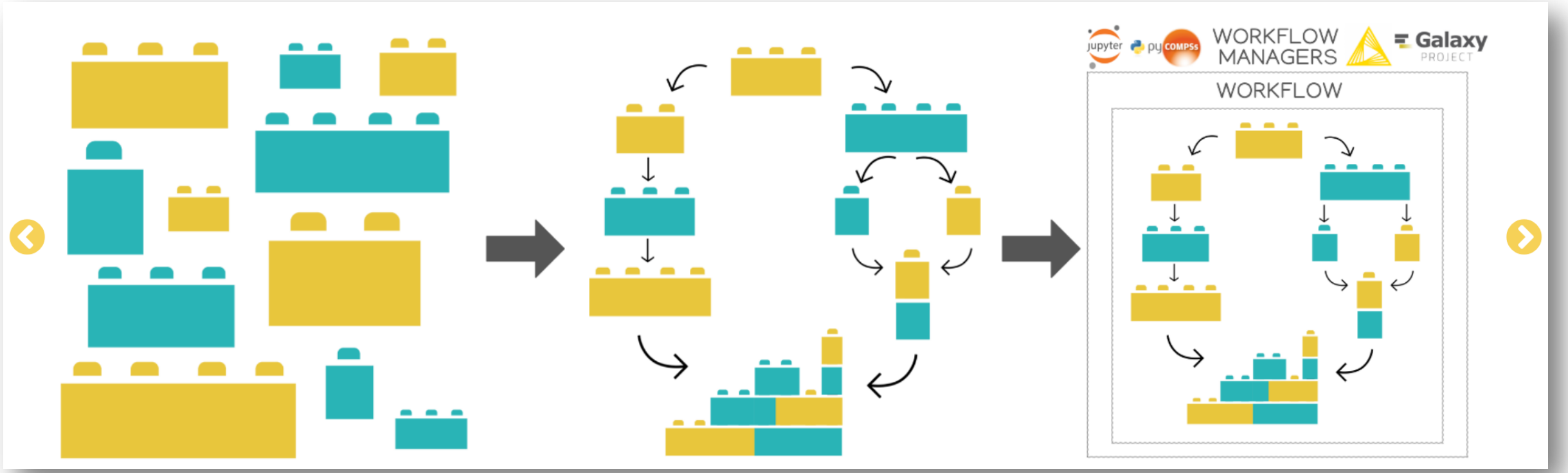
bioexcel
Centre of Excellence for Computational Biomolecular Research

Horizon 2020
European Union Funding
for Research & Innovation

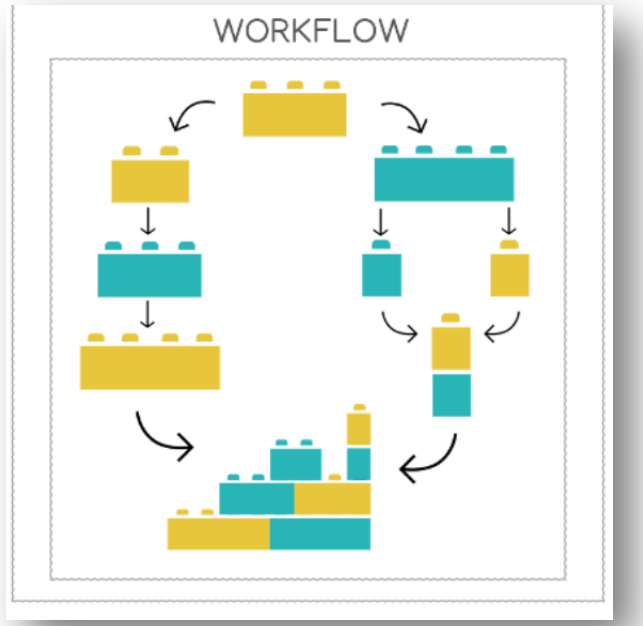
BioExcel Building Blocks (BioBB) and HPC

credit: Adam Hospital (IRB)

BioExcel Building Blocks, a software library for interoperable biomolecular simulation workflows



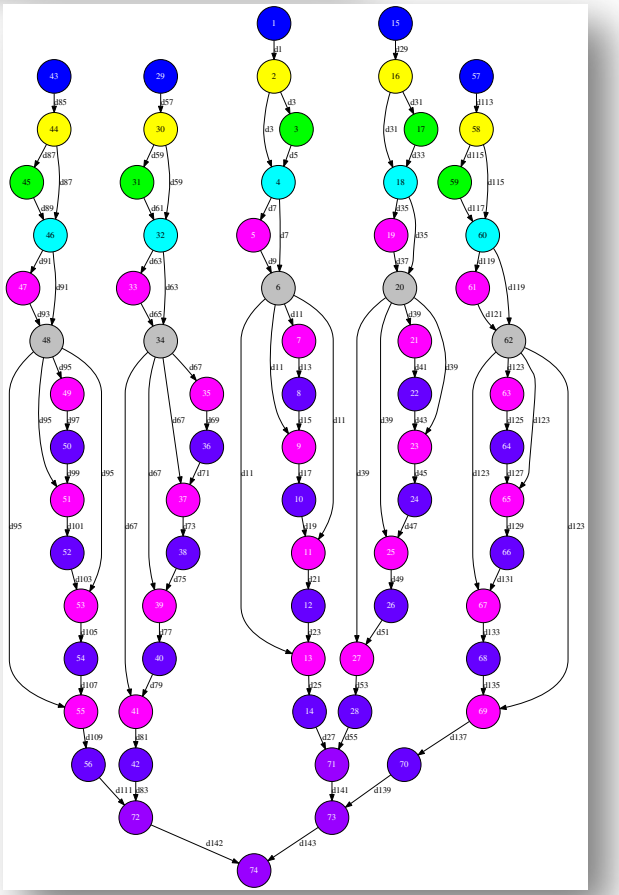
Building Blocks ***Workflows*** ***Execution***

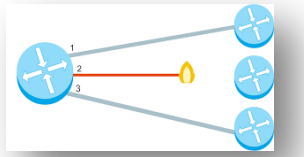


- **Biomolecular simulation workflows:** e.g. MD, free energy, Virtual Screening
- **Prepared for the pre-exascale:** efficient use of thousands of cores in one single job:
  - Highest number used: 40,000 cores
  - Common use: ~2,000 cores
- **Flexible and easy to adapt:** custom biomolecular workflows

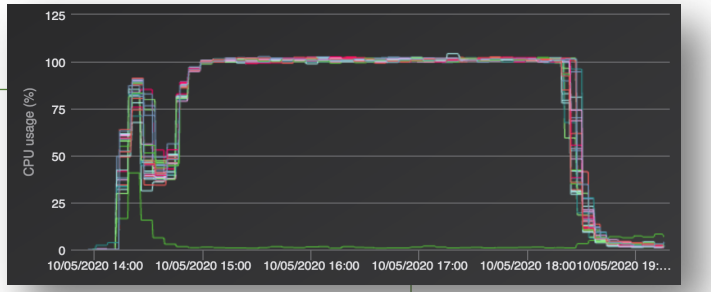
```
print 'step2: mmbuniprot -- Get mutations'
mmbuniprot = uniprot.MmbVariants(prop['pdb_code'])
mutations = mmbuniprot.fetch_variants()

for mut in mutations:
    mut_path = cdir(wd, mut)

    print 'step3: scw -- Model mutation'
    scw_path = cdir(mut_path, 'step3_scw')
    scw_pdb = opj(scw_path, prop['mutated_pdb'])
    scw = scwrl.Scwrl4(mmbpdb_pdb, scw_pdb, mut, scwrl_path=scwrl_path)
    scw_pdb2 = scw.launchPyCOMPSs()
```

"Embarrassingly parallel" executions





Fault tolerance



How it works

```python
global_log.info("step1_pdb: Download the initial Structure")
Pdb(**global_paths["step1_pdb"], properties=global_prop["step1_pdb"]).launch()

global_log.info("step2_fixsidechain: Modeling the missing heavy atoms in the structure side chains")
FixSideChain(**global_paths["step2_fixsidechain"], properties=global_prop["step2_fixsidechain"]).launch()

global_log.info("step3_pdb2gmx: Generate the topology")
Pdb2gmx(**global_paths["step3_pdb2gmx"], properties=global_prop["step3_pdb2gmx"]).launch()

global_log.info("step4_editconf: Create the solvent box")
Editconf(**global_paths["step4_editconf"], properties=global_prop["step4_editconf"]).launch()

global_log.info("step5_solvate: Fill the solvent box with water molecules")
Solvate(**global_paths["step5_solvate"], properties=global_prop["step5_solvate"]).launch()

global_log.info("step6_grompp_genion: Preprocess ion generation")
Grompp(**global_paths["step6_grompp_genion"], properties=global_prop["step6_grompp_genion"]).launch()

global_log.info("step7_genion: Ion generation")
Genion(**global_paths["step7_genion"], properties=global_prop["step7_genion"]).launch()

global_log.info("step8_grompp_min: Preprocess energy minimization")
Grompp(**global_paths["step8_grompp_min"], properties=global_prop["step8_grompp_min"]).launch()

global_log.info("step9_mdrun_min: Execute energy minimization")
Mdrun(**global_paths["step9_mdrun_min"], properties=global_prop["step9_mdrun_min"]).launch()

global_log.info("step10_energy_min: Compute potential energy during minimization")
GMXEnergy(**global_paths["step10_energy_min"], properties=global_prop["step10_energy_min"]).launch()
```

Workflow script

Python code
Building blocks
Loops / conditionals
Global log
Output folders hierarchy

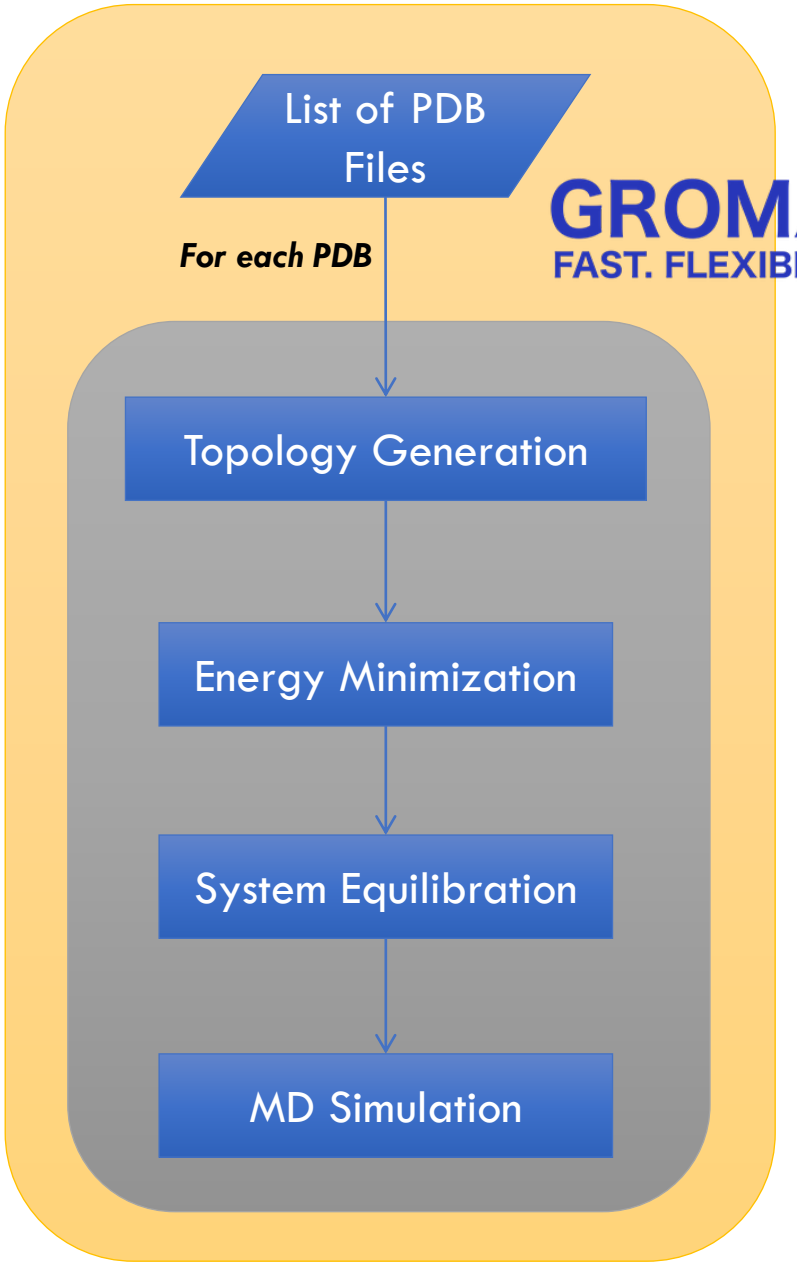

```yaml
# Example of a YAML configuration file for a BioExcel building blocks workflow

working_dir_path: md_tutorial     # Folder to write i/o files of the workflow steps
can_write_console_log: False      # Verbose writing of log information
restart: False                     # Skip steps already performed
remove_tmp: True

step1_pdb:
  paths:
    output_pdb_path: structure.pdb
  properties:
    pdb_code: 1aki

step2_fixsidechain:
  paths:
    input_pdb_path: dependency/step1_pdb/output_pdb_path
    output_pdb_path: fixsidechain.pdb

step3_pdb2gmx:
  paths:
    input_pdb_path: dependency/step2_fixsidechain/output_pdb_path
    output_gro_path: pdb2gmx.gro
    output_top_zip_path: pdb2gmx_top.zip

step4_editconf:
  paths:
    input_gro_path: dependency/step3_pdb2gmx/output_gro_path
    output_gro_path: editconf.gro

step5_solvate:
  paths:
    input_solute_gro_path: dependency/step4_editconf/output_gro_path
    output_gro_path: solvate.gro
    input_top_zip_path: dependency/step3_pdb2gmx/output_top_zip_path
    output_top_zip_path: solvate_top.zip
```

Workflow parameters

Steps Inputs / Outputs
Steps Dependencies
Steps Properties
Workflow inputs
Workflow parameters

Example:

MD setup and run for a list of structures



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```python
for structure in conf.properties['input_structures'].split(','):

    prefix_str = os.path.basename(structure)
    prefix_str = prefix_str.replace('.','_')

    mut_prop = conf.get_prop_dic(prefix=prefix_str)
    mut_paths = conf.get_paths_dic(prefix=prefix_str)

    global_log.info("Starting setup process for PDB: " + prefix_str)
    mut_paths['step1_pdb2gmx']['input_pdb_path'] = structure

    global_log.info("step1_pdb2gmx: Generate the topology")
    pdb2gmx_pc(**mut_paths["step1_pdb2gmx"], properties=mut_prop["step1_pdb2gmx"])

    global_log.info("step2_editconf: Create the solvent box")
    editconf_pc(**mut_paths["step2_editconf"], properties=mut_prop["step2_editconf"])

    global_log.info("step3_solvate: Fill the solvent box with water molecules")
    solvate_pc(**mut_paths["step3_solvate"], properties=mut_prop["step3_solvate"])
```

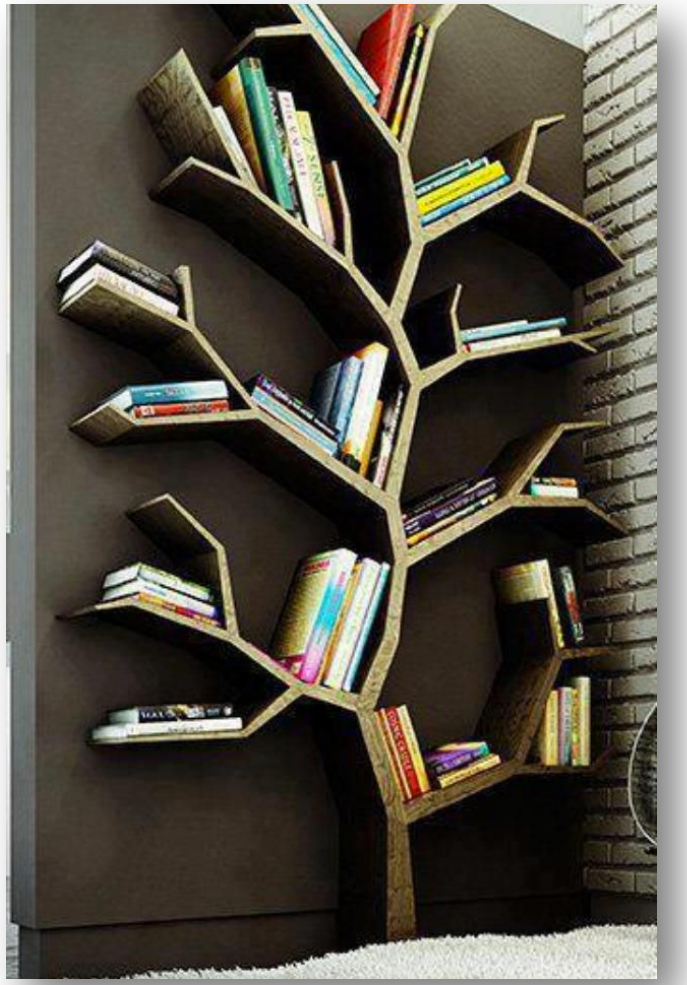
```yaml
# List of structures to be simulated
input_structures: ['/home/bscxxxx/str.pdb','/home/bscxxxx/str2.pdb',
                   '/home/bscxxxx/str3.pdb','/home/bscxxxx/str4.pdb']

step1_pdb2gmx:
  paths:
    output_gro_path: mut_gmx.gro
    output_top_zip_path: mut_gmx.top.zip
  properties:
    force_field : amber99sb-ildn

step2_editconf:
  paths:
    input_gro_path: dependency/step1_pdb2gmx/output_gro_path
    output_gro_path: editconf.gro
  properties:
    box_type: octahedron
    distance_to_molecule: 1.2

step3_solvate:
  paths:
    input_solute_gro_path: dependency/step2_editconf/output_gro_path
    output_gro_path: solvate.gro
    input_top_zip_path: dependency/step1_pdb2gmx/output_top_zip_path
    output_top_zip_path: solvate_top.zip
```

Workflow Templates: Library



MD setup + run for a list of structures

python YAML

Model + MD setup + run for a set of protein mutations

python YAML

Free energy calculations with fast-growth TI

python YAML

Virtual Screening

python YAML

And many more...

Workflow Launcher

 # BioExcel Building Blocks
module load ANACONDA/2019.10
module load biobb/covid_dev

 # [Py]COMPSs release
module load COMPSs/2.6.4

 # Singularity
module load singularity

 # GROMACS 2019
module load gromacs/2019.1

 # Specific Run Parameters

Environment Modules

Welcome to the Environment Modules open source project. The Environment Modules package provides for the dynamic modification of a user's environment via modulefiles.

pmx: generate hybrid protein structure and topology
Computational Biomolecular Dynamics Group

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```
enqueue_compss
--job_name=mds_pmx_covid
--num_nodes=8
--exec_time=2800
--worker_in_master_cpus=48
--base_log_dir=$PWD
--qos=bsc_ls
wf.py  --config wf.yaml
```

Workflow Launcher

 # BioExcel Building Blocks
module load BioBB/2.6

 # [Py]COMPSs release
module load COMPSs/2.6

 # PCoCC
module load PCoCC

 # GROMACS 2019
module load gromacs/2019.4

 # Specific Run Parameters

Environment Modules

Welcome to the Environment Modules open source project. The Environment Modules package provides for the dynamic modification of a user's environment via modulefiles.

HPC HIGH PERFORMANCE COMPUTING

pmx: generate hybrid protein structure and topology
Computational Biomolecular Dynamics Group

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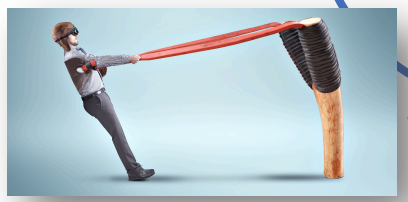
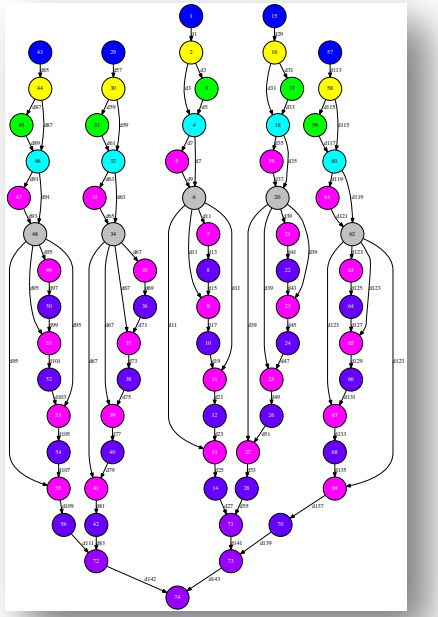
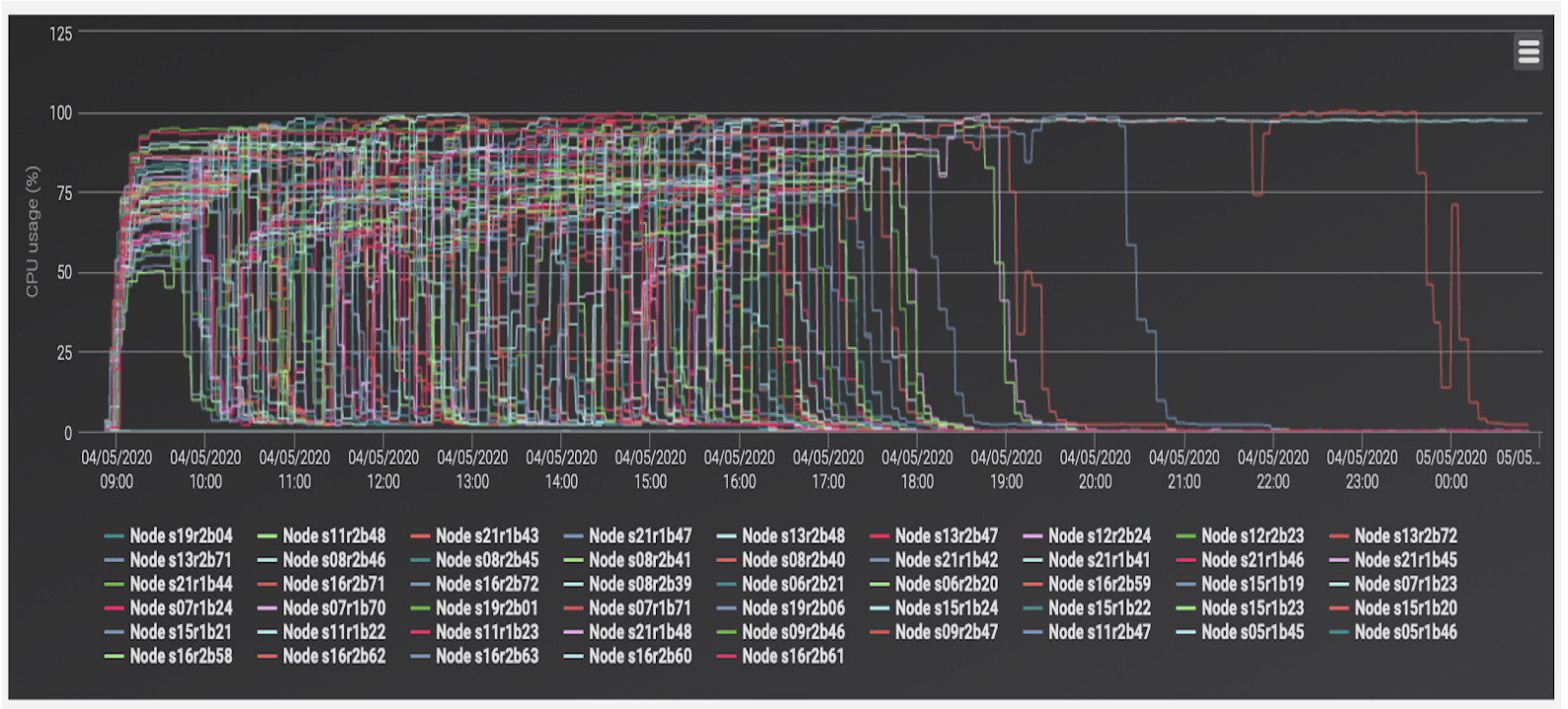
```
enqueue_compss
--job_name=mds_pmx_covid
--num_nodes=8
--exec_time=2800
--worker_in_master_cpus=128
--base_log_dir=$PWD
--qos=bsc_ls
wf.py  --config wf.yaml
```



Examples



Efficient usage of resources



n° nodes < n° executions

Protein-protein benchmark
200 HADDOCK executions

BSC MareNostrum 50 nodes (2400 cores)
1 execution x node

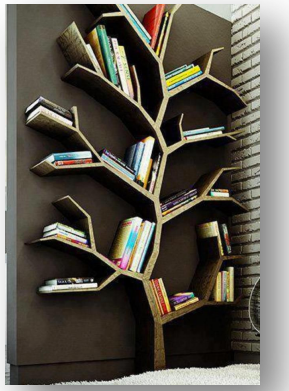
BioExcel Building Blocks (BioBB) High Performance Computing (HPC) Workflow repository

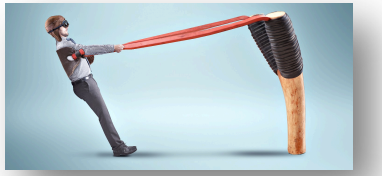
GitHub

https://github.com/bioexcel/biobb_hpc_workflows

We are working on some new workflows that will be added to the current list of workflows and launchers:

- Workflows for MD:
  - md_list: Performs a system setup and runs a molecular dynamics simulation on each one of the structures listed in the YAML properties file.
  - md_muts_sets: Performs a system setup and runs a molecular dynamics simulation for each one of the listed mutations in a given structure.
  - md_add_muts_wt: Applies a list of mutations over the initial structure obtaining a set of structures (initial structure + one mutation, initial structure + two mutations, initial structure + three mutations, ...). Finally performs a system setup and runs a molecular dynamics simulation for each of the structures in the set.
- Workflows for Free Energy Calculation (PMX):
  - pmx_cv_cufix_term: Performs a fast-growth mutation free energy calculation from two equilibrium trajectories.
- Launchers:
  - md_launch: Launcher for the md_list workflow.
  - mdmut_launch: Launcher for the md_muts_sets and md_add_muts_wt workflows.
  - pmx_launch: Launcher for the pmx_cv_cufix_term.





```
bscxxxxx@login1:~>/apps/BIOBB/workflows/MN4/md_launch.py  -h
usage: md_launch.py [-h] -i INPUT_STRUCTURES [-s SYSTEM] [-f FORCE_FIELD]
                    [-bs BOX_SIZE] [-bt BOX_TYPE] [-c CONCENTRATION]
                    [-q QUEUE] [-t TIME] [-nn NUM_NODES] [-cv COMPSS_VERSION]
                    [-d] [-l MD_LENGTH] [-mpi MPI_NODES] [--base_dir BASE_DIR]
                    [-o OUTPUT_DIR] [-jn JOB_NAME] [-gl GROMACS_LIB]
```

Workflow to setup and run MD simulations for a set of **PDB structures.**

```
/apps/BIOBB/workflows/md_launch.py
        -i structures.list
        -l 100
        -nn 16
        -mpi 4
        -o MDs
        -q bsc_ls
        -t 2800
        -jn biobb_mds
```

Structures.list file:

/home/bscxxxx/PDBs/str1.pdb
/home/bscxxxx/PDBs/str2.pdb
/home/bscxxxx/PDBs/str3.pdb
/home/bscxxxx/PDBs/str4.pdb

Table S1. DNA sequences in the miniABC library.

Seq. number	Watson strand (5'-3' direction)
1	GCAACGTGCTATGGAAGC
2	GCAATAAGTACCAGGAGC
3	GCAGAAACAGCTCTGCGC
4	GCAGGCGCAAGACTGAGC
5	GCATTGGGGACACTACGC
6	GCGAACTCAAAGGTTGGC
7	GCGACCGAATGTAATTGC
8	GCGGAGGGCCGGGTGGGC
9	GCGTTAGATTAAAATTGC
10	GCTACGCGGATCGAGAGC
11	GCTGATATACGATGCAGC
12	GCTGGCATGAAGCGACGC
13	GCTTGTGACGGCTAGGGC

https://mmb.irbbarcelona.org/miniABC/

The static and dynamic structural heterogeneities of B-DNA: extending Calladine–Dickerson rules

Pablo D Dans ✉, Alexandra Balaceanu, Marco Pasi, Alessandro S Patelli, Daiva Petkevičiūtė, Jürgen Walther, Adam Hospital, Genís Bayarri, Richard Lavery, John H Maddocks ... Show more

Author Notes

Nucleic Acids Research, Volume 47, Issue 21, 02 December 2019, Pages 11090–11102, https://doi.org/10.1093/nar/gkz905

/apps/BIOBB/workflows/MN4/md_launch.py

1. **13 MDs with Na ions –** 4,992 cores (8 MareNostrum nodes x each MD)
2. **13 MDs with K ions –** 4,992 cores (8 MareNostrum nodes x each MD)
3. **13 MDs with Na + K ions –** 4,992 cores (8 MareNostrum nodes x each MD)

parmBSC0* / *parmBSC1

```
/apps/BIOBB/workflows/MN4/md_launch.py
-i structures.list
-q class_a
-nn 104 –mpi 8
-jn miniABC –t 3800 –l 1000
-o ~/miniABC/Na_MDs
-f amber99bsc1
```

MENU SCIENTIFIC DATA

Article | Open Access | Published: 10 September 2019

BioExcel Building Blocks, a software library for interoperable biomolecular simulation workflows

Pau Andrio, Adam Hospital, Javier Conejero, Luis Jordá, Marc Del Pino, Laia Codo, Stian Soiland-Reyes, Carole Goble, Daniele Lezzi, Rosa M. Badia, Modesto Orozco & Josep Ll. Gelpi

Scientific Data **6**, Article number: 169 (2019) | Cite this article

biobb http://mmb.irbbarcelona.org/biobb/

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BioExcel Building Blocks, a software library for interoperable biomolecular simulation workflows

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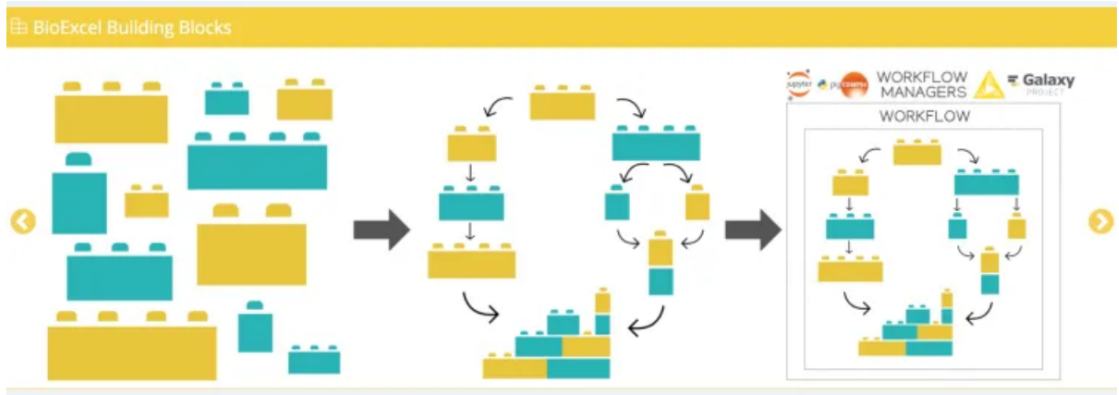
BioExcel Building Blocks

Enabling real science

Building biomolecular simulation workflows to solve scientific problems

Webinar: Computational biomolecular simulation workflows with BioExcel building blocks

August 7, 2020 Arno Proeme



BioExcel's webinar series continue with a presentation by Adam Hospital

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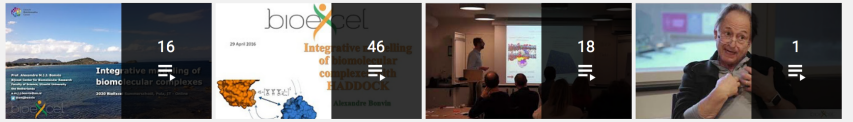

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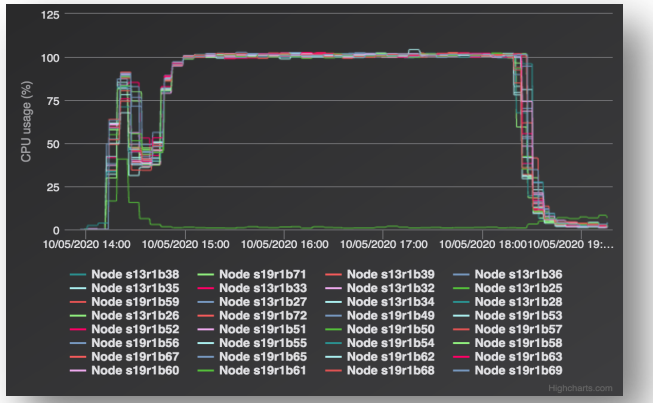
Try it!

- Openly available on BSC MareNostrum 4 supercomputer
  1. module load python/3.6.1
  2. /apps/BIOBB/workflows/md_launch.py
  3. /apps/BIOBB/workflows/mdmut_launch.py
  4. /apps/BIOBB/workflows/pmx_launch.py



- European supercomputers:
  - MareNostrum 4 supercomputer (BSC – Spain)
  - Irene Rome (CEA – France)
  - Hawk (HLRS – Stuttgart)

- If interested to try, contact
  - adam.hospital@irbbarcelona.org