

ER-flow Application Description Template

Application Name:

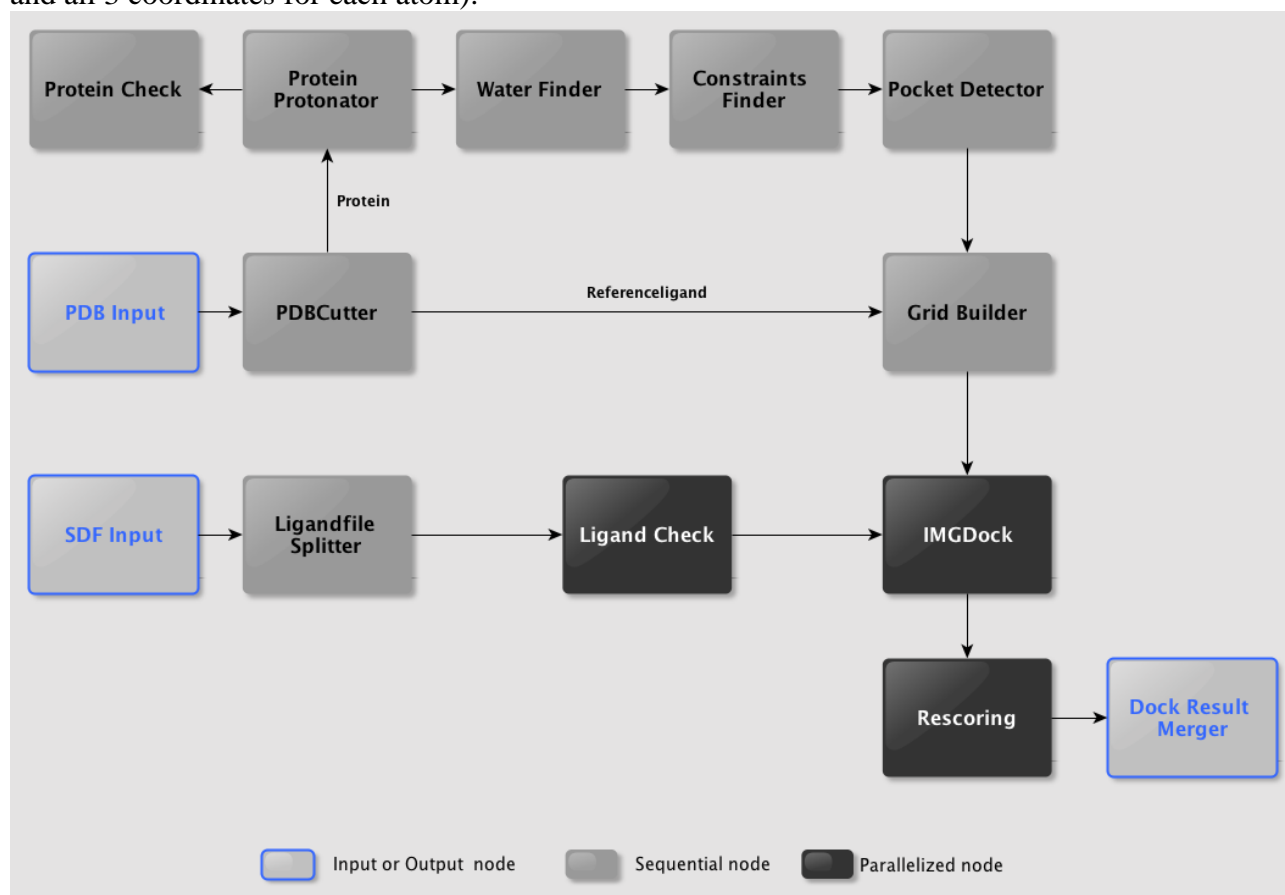
CADDSuite – Docking without ligand generation

Application domain:

Docking

Brief description of application

This workflow performs a docking procedure of ligands into a protein. This version allows more advanced user input and is thus suitable for users who have performed docking before. The actual docking process includes splitting of the receptor-file into protein and reference ligand, grid building, docking and rescoring of the dock results. For this workflow a protein structure file containing a protein in complex with a referenceligand and a file with the screening library (i.e., ligands that are to be docked into the protein) is required. The imported screening library will be checked, but no 3D coordinates will be created for the ligands - thus it is the user's responsibility to make sure the ligand input is correctly formatted (sdf MUST contain all hydrogens of each molecule and all 3 coordinates for each atom).



data:

input data format: PDB and SDF input data value range

output data format: PDB and SDF output data value range

sample data: <https://mosgrid.de/help/docking>

application: <http://www.ball-project.org/caddsuite>

documentation <http://www.ballview.org/Support/caddsuite-tutorial-1>

publication: <http://link.springer.com/article/10.1186%2F1758-2946-4-S1-O2>

Execution environment

DCI: UNICORE, MoSGrid VO (computing, data, VO, etc)

middleware: gUSE/UNICORE

workflow system: ws-pgrade

Execution characteristics

data size (per unit, typical number of units):

input 1-10 MB receptor; 10 kB per ligand temporary output 100 MB

processing time (per unit): 10 seconds per ligand

memory usage: 8-16 GB disk usage: low

Target users

Community, projects: MoSGrid (mosgrid.de), SCI-BUS (sci-bus.eu)

number of users: 10

user type: end-user

Usage scenario for workflow in the ER-FLOW (how workflow will be reused, metaworkflow, how expected to contribute to project indicators, etc.).

Contact information (author)

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