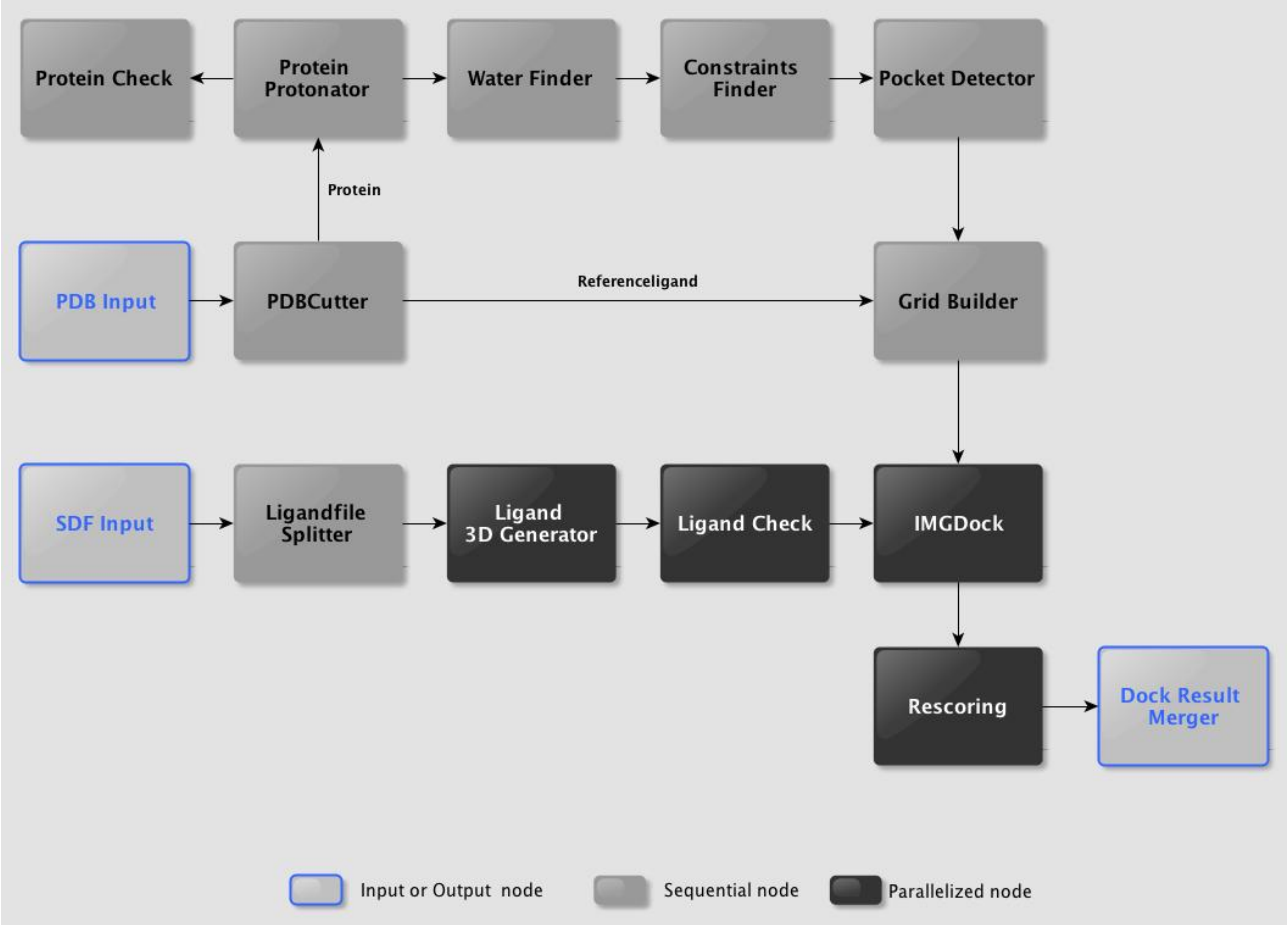
ER-flow Application Description Template

Application Name:
CADDSuite – Docking with ligand generation

Application domain:
Docking

Brief description of application

This workflow performs a docking procedure of ligands into a protein. This version is simplified so that only minimal user input is needed and thus is aimed at the novice user. 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 reference ligand and a file with the screening library (ligands) is required.



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.).

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