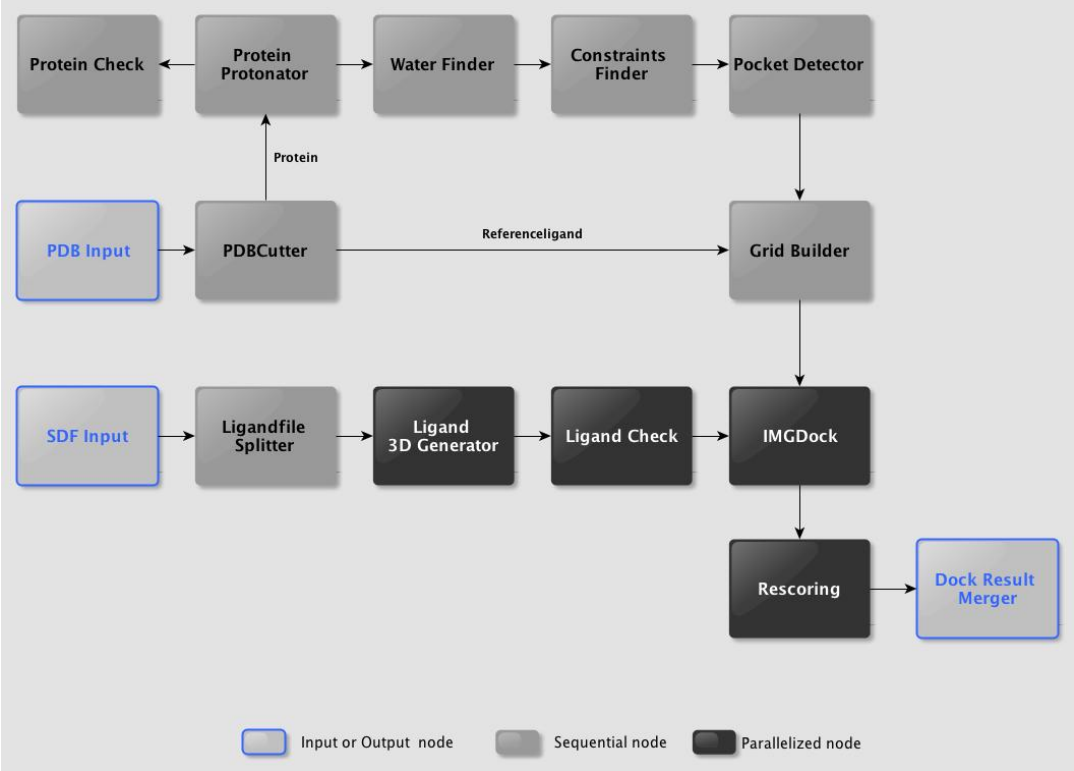
ER-flow Application Description Template

Application Name:
AutoDockVinaFull

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, docking with AutoDock Vina, and export of the dock results. AutoDock Vina creates a grid on the fly and thus no separate grid-building step is performed. For this workflow a protein structure file containing a protein in complex with a reference ligand and a file with the screening library (i.e., ligands that are to be docked into the protein) is required.



data:
input data format: PDBQT input data value range
output data format: PDBQT output data value range
application: http://vina.scripps.edu/
documentation: http://vina.scripps.edu/manual.html
publication: http://onlinelibrary.wiley.com/doi/10.1002/jcc.21334/abstract

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: 20 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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