RosettaScripts

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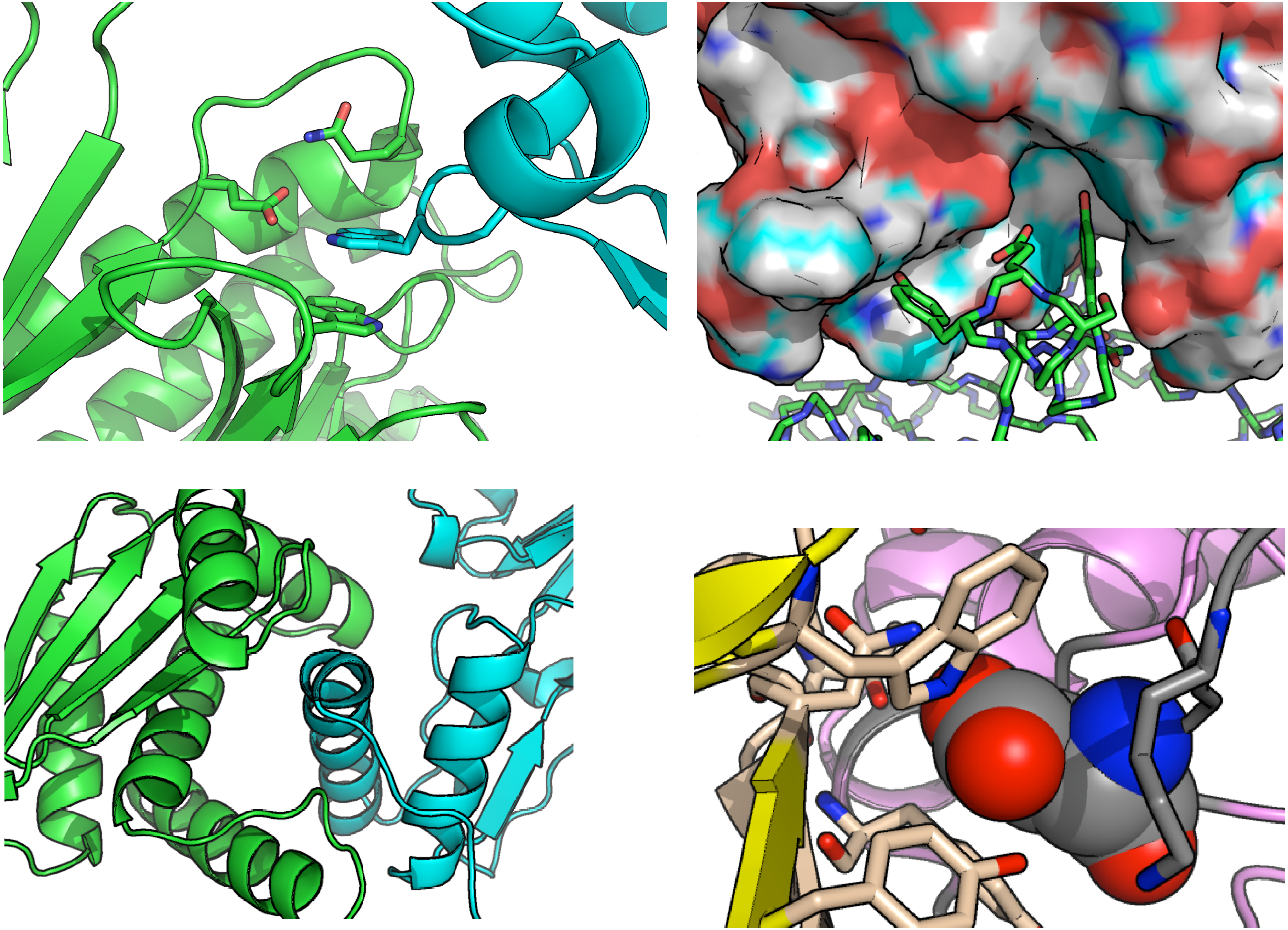
“Easy things should be easy, difficult things should be possible”

-Larry Wall



Objectives of the RosettaScripts

- Separate protocol writing from programming
- Provide control over internal functionality
- Facilitate code sharing within and between the design and prediction groups
- Speedup the learning, testing and fine-tuning of new functionalities

Architecture

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void Mover(pose&)

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Filter
bool apply(Pose const)

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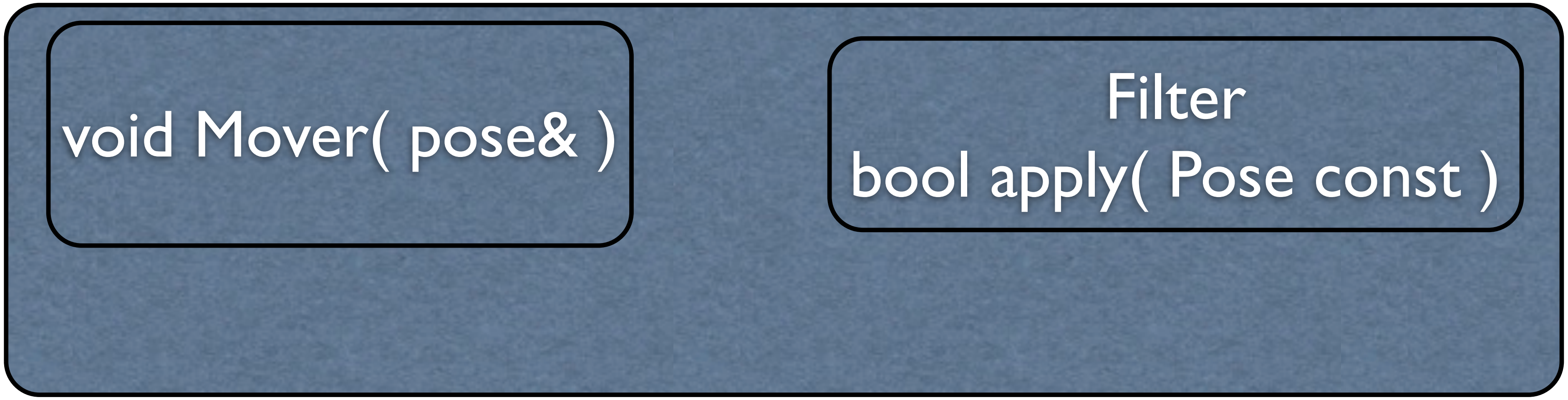
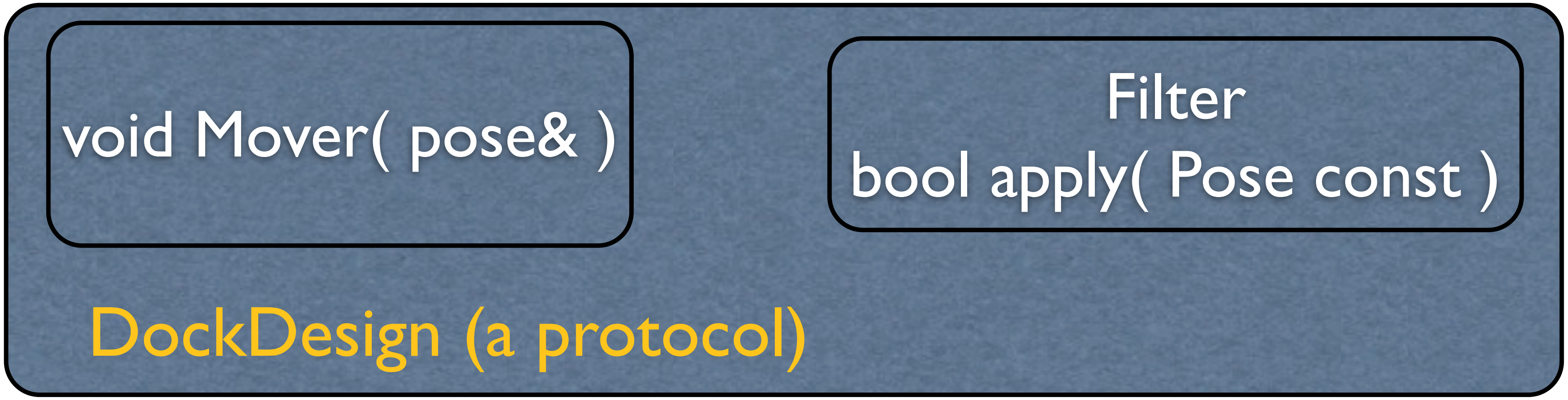


void Mover(pose&)

Filter
bool apply(Pose const)

Architecture

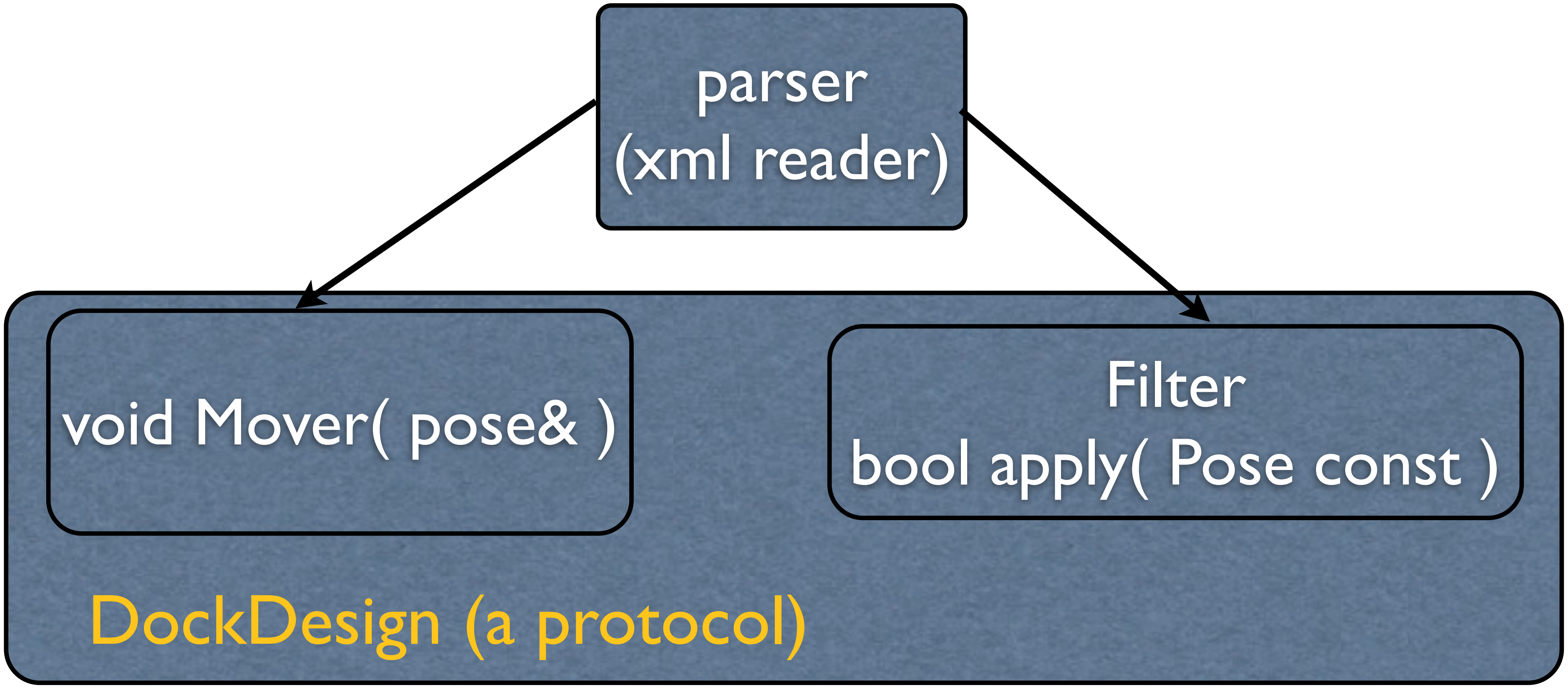


void Mover(pose&)

Filter
bool apply(Pose const)

DockDesign (a protocol)

Architecture



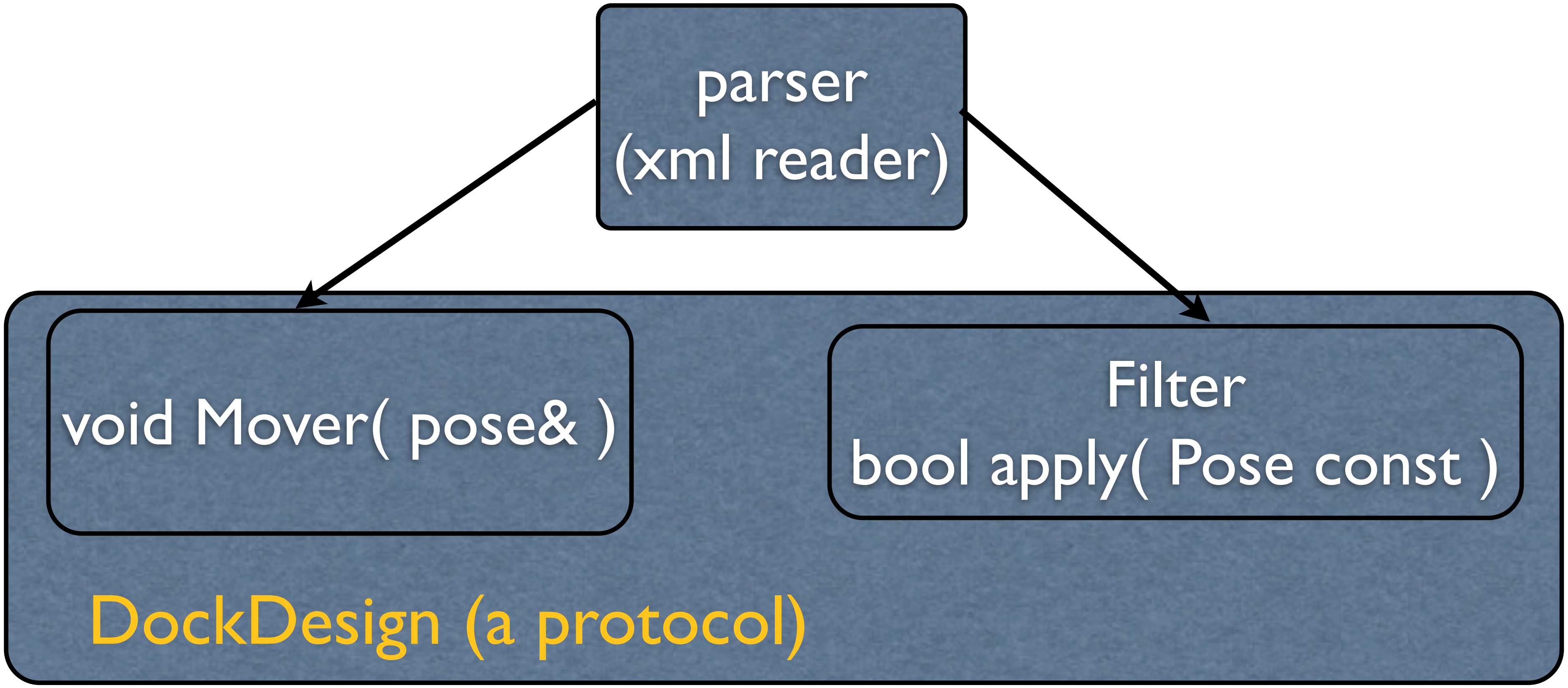
parser
(xml reader)

void Mover(pose&)

Filter
bool apply(Pose const)

DockDesign (a protocol)

Architecture



parser
(xml reader)

void Mover(pose&)

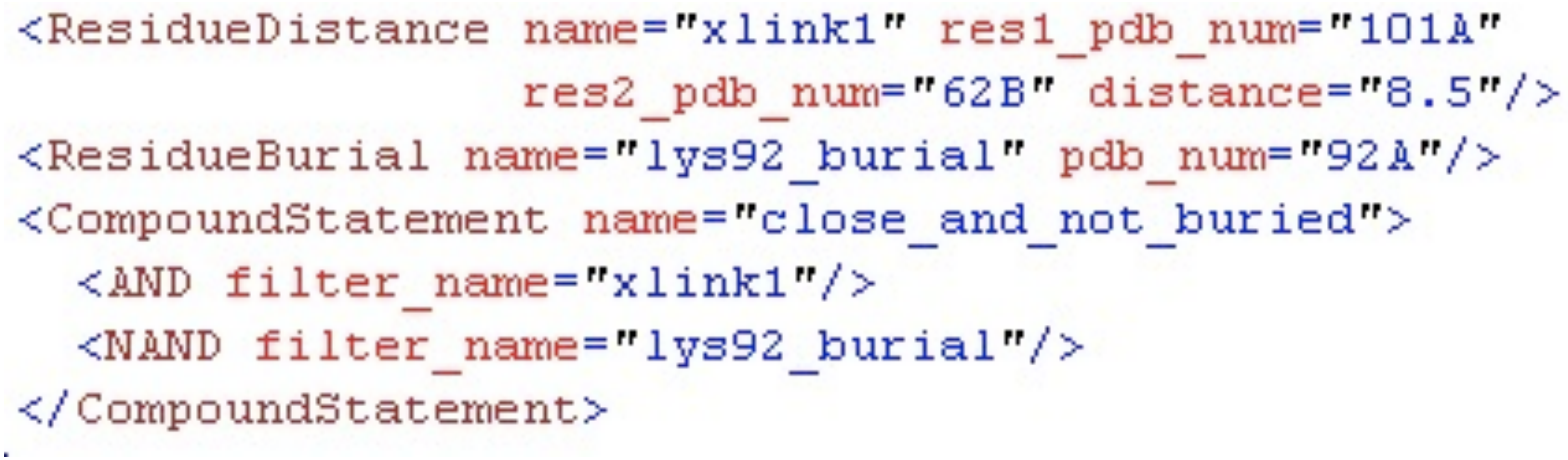
Filter
bool apply(Pose const)

DockDesign (a protocol)

Run examples

Filters

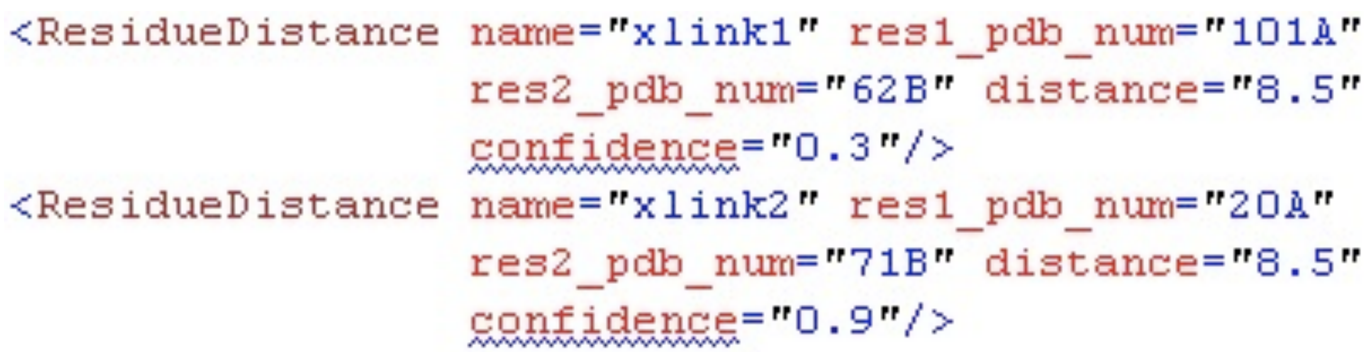
- Filters can be combined into boolean statements that are functionally complete (OR, AND, XOR, NAND, NOR).



```
<ResidueDistance name="xlink1" res1_pdb_num="101A"
                 res2_pdb_num="62B" distance="8.5"/>
<ResidueBurial name="lys92_burial" pdb_num="92A"/>
<CompoundStatement name="close_and_not_buried">
  <AND filter_name="xlink1"/>
  <NAND filter_name="lys92_burial"/>
</CompoundStatement>
```

Filters

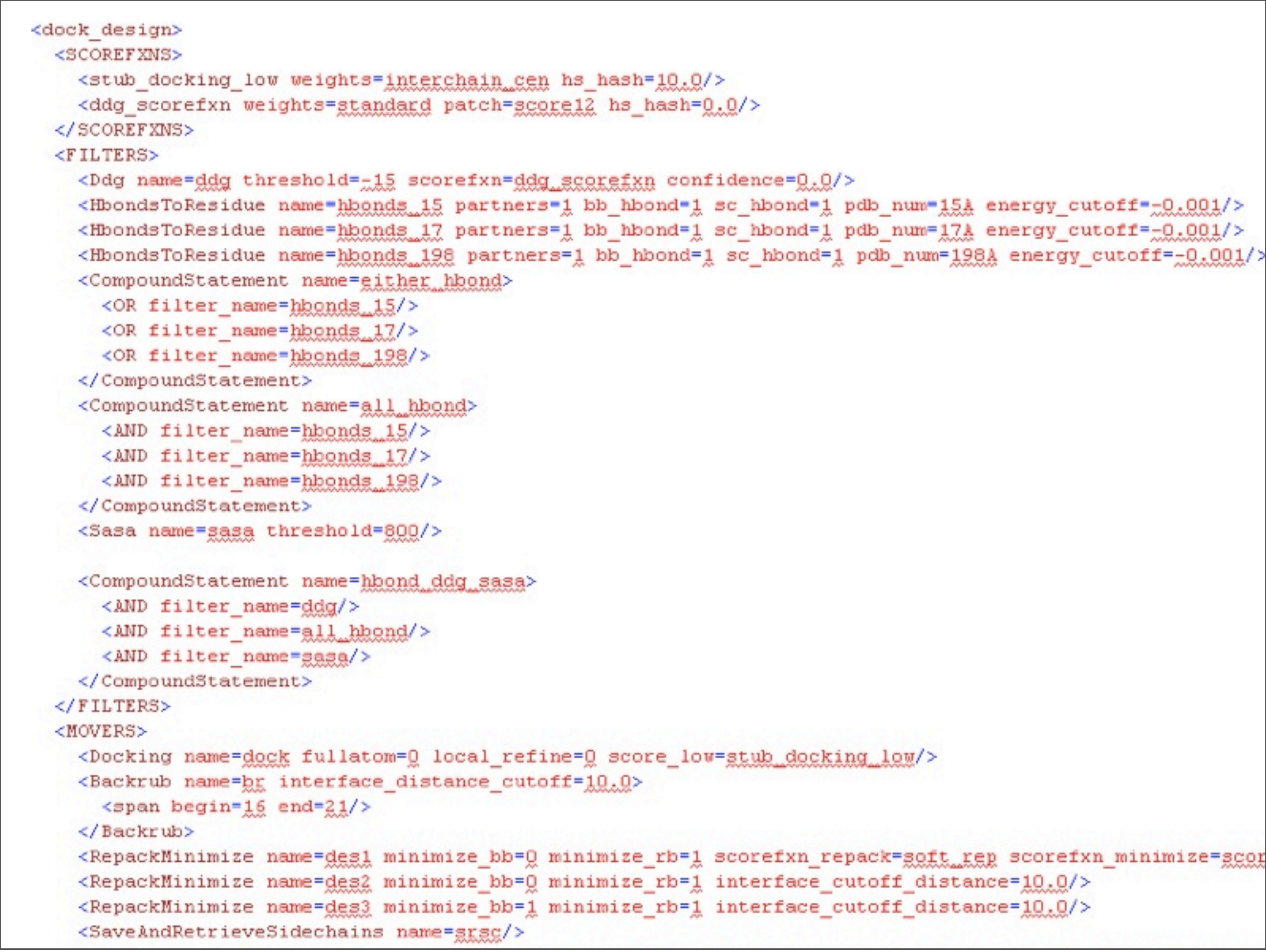
- Filters' internals are added to score & silent files.
- Fuzzy logic support.



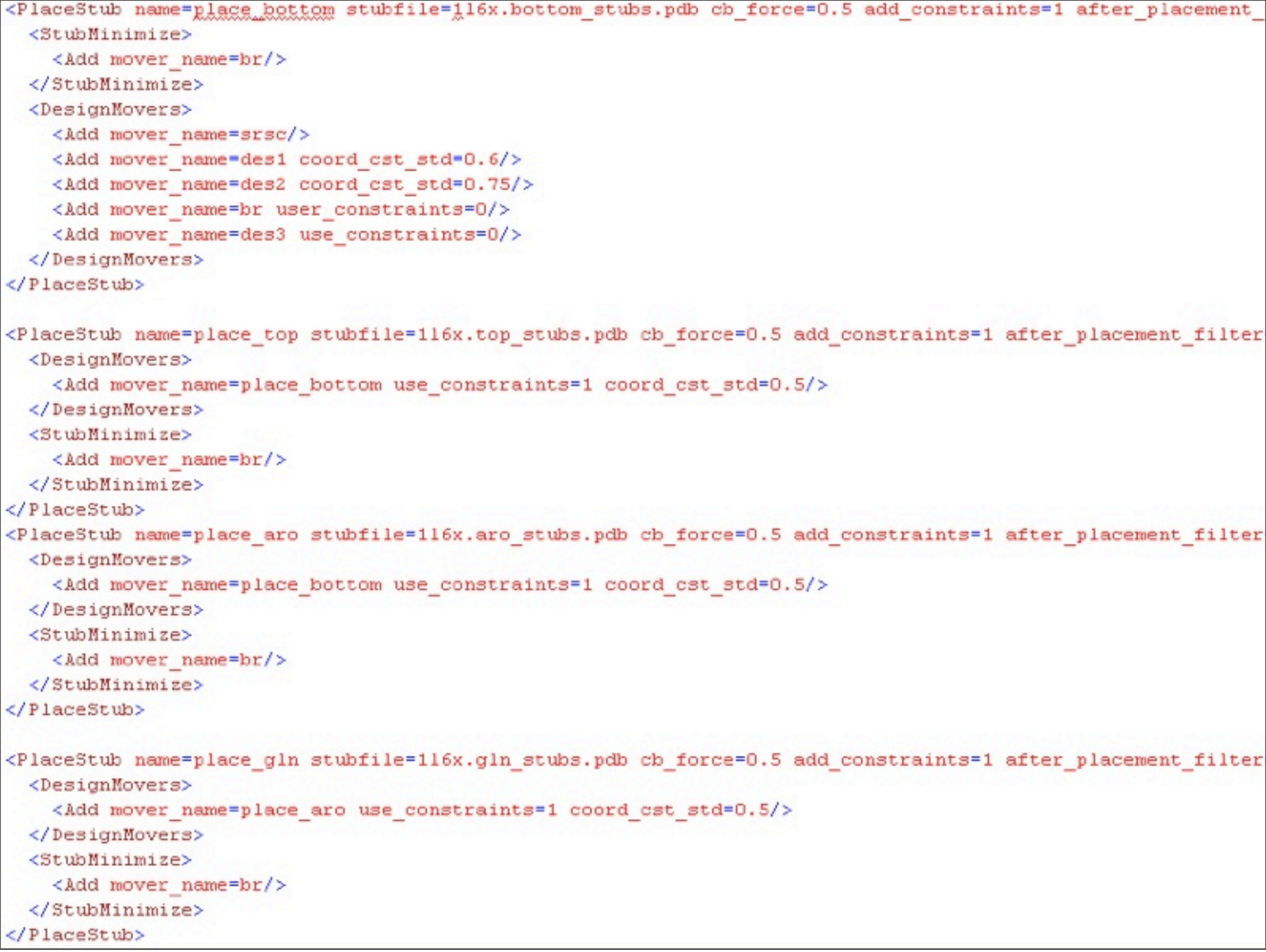
```
<ResidueDistance name="xlink1" res1_pdb_num="101A"
                 res2_pdb_num="62B" distance="8.5"
                 confidence="0.3"/>
<ResidueDistance name="xlink2" res1_pdb_num="20A"
                 res2_pdb_num="71B" distance="8.5"
                 confidence="0.9"/>
```

Loops of movers

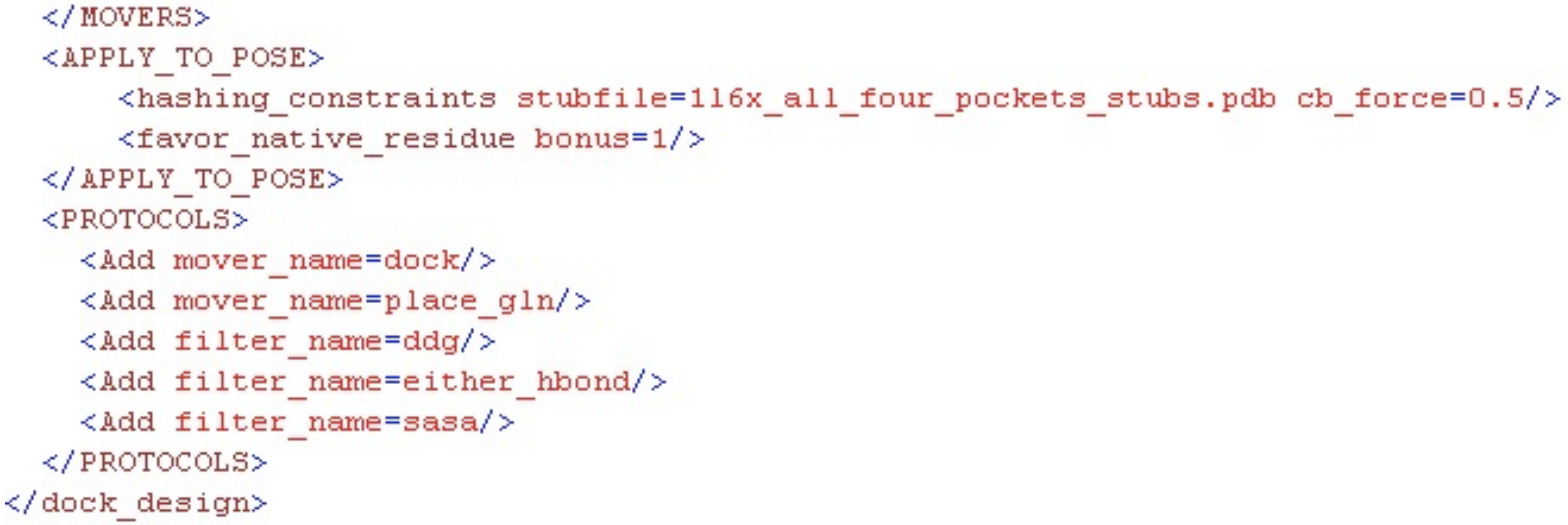
```
<dock_design>
  <SCOREFXNS>
  </SCOREFXNS>
  <FILTERS>
    <Ddg name="ddg" threshold="-10"/>
  </FILTERS>
  <MOVERS>
    <Docking name="dock" score_high="score12" fullatom="0" local_refine="1"/>
    <Backrub name="br"/>
    <RepackMinimize name="design" minimize_bb="1" minimize_rb="1" interface_cutoff_distance="10"/>
    <DockDesign name="single_trajectory">
      <Add mover_name="dock"/>
      <Add mover_name="design"/>
      <Add mover_name="br"/>
    </DockDesign>
    <LoopOver filter_name="ddg" name="loop" iterations="50" mover_name="single_trajectory"/>
  </MOVERS>
  <APPLY_TO_POSE>
  </APPLY_TO_POSE>
  <PROTOCOLS>
    <Add mover_name="loop"/>
    <Add filter_name="sasa"/>
  </PROTOCOLS>
</dock_design>
```



```
<dock_design>
  <SCOREFXNS>
    <stub_docking_low weights=interchain_cen hs_hash=10.0/>
    <ddg_scorefxn weights=standard patch=score12 hs_hash=0.0/>
  </SCOREFXNS>
  <FILTERS>
    <Ddg name=ddg threshold=-15 scorefxn=ddg_scorefxn confidence=0.0/>
    <HbondsToResidue name=hbonds_15 partners=1 bb_hbond=1 sc_hbond=1 pdb_num=15A energy_cutoff=-0.001/>
    <HbondsToResidue name=hbonds_17 partners=1 bb_hbond=1 sc_hbond=1 pdb_num=17A energy_cutoff=-0.001/>
    <HbondsToResidue name=hbonds_198 partners=1 bb_hbond=1 sc_hbond=1 pdb_num=198A energy_cutoff=-0.001/>
    <CompoundStatement name=either_hbond>
      <OR filter_name=hbonds_15/>
      <OR filter_name=hbonds_17/>
      <OR filter_name=hbonds_198/>
    </CompoundStatement>
    <CompoundStatement name=all_hbond>
      <AND filter_name=hbonds_15/>
      <AND filter_name=hbonds_17/>
      <AND filter_name=hbonds_198/>
    </CompoundStatement>
    <Sasa name=sasa threshold=800/>

    <CompoundStatement name=hbond_ddg_sasa>
      <AND filter_name=ddg/>
      <AND filter_name=all_hbond/>
      <AND filter_name=sasa/>
    </CompoundStatement>
  </FILTERS>
  <MOVERS>
    <Docking name=dock fullatom=0 local_refine=0 score_low=stub_docking_low/>
    <Backrub name=br interface_distance_cutoff=10.0>
      <span begin=16 end=21/>
    </Backrub>
    <RepackMinimize name=des1 minimize_bb=0 minimize_rb=1 scorefxn_repack=soft_rep scorefxn_minimize=scor
    <RepackMinimize name=des2 minimize_bb=0 minimize_rb=1 interface_cutoff_distance=10.0/>
    <RepackMinimize name=des3 minimize_bb=1 minimize_rb=1 interface_cutoff_distance=10.0/>
    <SaveAndRetrieveSidechains name=srsc/>
```



```
<PlaceStub name=place_bottom stubfile=116x.bottom_stubs.pdb cb_force=0.5 add_constraints=1 after_placement_
  <StubMinimize>
    <Add mover_name=br/>
  </StubMinimize>
  <DesignMovers>
    <Add mover_name=srsc/>
    <Add mover_name=des1 coord_cst_std=0.6/>
    <Add mover_name=des2 coord_cst_std=0.75/>
    <Add mover_name=br user_constraints=0/>
    <Add mover_name=des3 use_constraints=0/>
  </DesignMovers>
</PlaceStub>

<PlaceStub name=place_top stubfile=116x.top_stubs.pdb cb_force=0.5 add_constraints=1 after_placement_filter
  <DesignMovers>
    <Add mover_name=place_bottom use_constraints=1 coord_cst_std=0.5/>
  </DesignMovers>
  <StubMinimize>
    <Add mover_name=br/>
  </StubMinimize>
</PlaceStub>
<PlaceStub name=place_aro stubfile=116x.aro_stubs.pdb cb_force=0.5 add_constraints=1 after_placement_filter
  <DesignMovers>
    <Add mover_name=place_bottom use_constraints=1 coord_cst_std=0.5/>
  </DesignMovers>
  <StubMinimize>
    <Add mover_name=br/>
  </StubMinimize>
</PlaceStub>

<PlaceStub name=place_gln stubfile=116x.gln_stubs.pdb cb_force=0.5 add_constraints=1 after_placement_filter
  <DesignMovers>
    <Add mover_name=place_aro use_constraints=1 coord_cst_std=0.5/>
  </DesignMovers>
  <StubMinimize>
    <Add mover_name=br/>
  </StubMinimize>
</PlaceStub>
```



```
  </MOVERS>
  <APPLY_TO_POSE>
      <hashing_constraints stubfile=116x_all_four_pockets_stubs.pdb cb_force=0.5/>
      <favor_native_residue bonus=1/>
  </APPLY_TO_POSE>
  <PROTOCOLS>
    <Add mover_name=dock/>
    <Add mover_name=place_gln/>
    <Add filter_name=ddg/>
    <Add filter_name=either_hbond/>
    <Add filter_name=sasa/>
  </PROTOCOLS>
</dock_design>
```

Where can I get one of those!!!!

- https://wiki.rosettacommons.org/index.php/IDDocumentation
- jd2_scripting.cc

Thanks!

- Justin Ashworth
- Andrew Leaver-fay and Steven Lewis (Kuhlman lab)
- Jacob Corn, Eva Strauch and Tim Whitehead
- Paul Murphy
- Avner Aharoni (Program Manager of Visual Studio at Microsoft)