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ProcessTrak

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4/22/2016



This material is based on work supported by the Air Force Research Laboratory under Contract #FA8650-10-D-5210, Task Order #023, and performed at Iowa State University





Motivation

- Lab data processing or analysis is easy when you can collect all steps into a single MATLAB or Python script that runs quickly.
- Once the steps are complicated enough or time consuming enough that you can't just rerun them each time, you end up with a mess.
- ProcessTrak provides a framework for avoiding/minimizing the mess



The mess

- With processing split into multiple scripts, you end up with a lot of intermediate files.
- It is often unclear which intermediates come from which script and/or which order the scripts must be run to recreate the final output
- It is often unclear that all scripts have been run in the correct order and therefore unclear that the final output is correct and meaningful.



The solution

- Based on datacollect2, represent experiment log as XML
- Processing starts by copying raw experiment log (.xlg) to processed experiment log (.xlp)
- Each processing step operates in place on the processed experiment log (.xlp).
- Processing steps defined in the .prx file, generally written in Python.
- Can be re-executed out-of-order as needed.
- Provenance-based result integrity checking.



Example .prx file

```
orcessinginstructions xmlns=
"http://limatix.org/processtrak/processinginstructions"
xmlns:xlink="http://www.w3.org/1999/xlink">
 <inputfiles>
  <inputfile xlink:href="example input.xlg"/>
 </inputfiles>
 <!-- elementmatch says what elements in the experiment log to
    Iterate over by default -->
 <elementmatch>xpath_condition</elementmatch>
 <step name="pullparams" descr="Pull in parameters from other files">
  <script xlink:href="pullparams.py">
   <!-- Parameters can be generated from other elements of the
        Experiment log, or explicitly in the .prx file: -->
   <parameter name="foo">
    <numvalue>34.5</numvalue>
   </parameter>
   <parameter name="bar">
    <strvalue>BAR</strvalue>
   </parameter>
  </script>
 </step>
```



Example script

```
import sys
import numpy as np
from limatix.dc_value import numericunitsvalue

def run(_xmldoc,_element,dc_magnitudesquared_numericunits):
    magsq=dc_magnitudesquared_numericunits.value('Volts^2')

mag=np.sqrt(magsq)

return { "dc:magnitude": numericunitsvalue(mag,'Volts') }
```

- This example script reads the 'dc:magnitudesquared' element
 - (or the dc_magnitudesquared_numvalue parameter if given in the .prx file)
- converts the value to volts², takes the square root, and stores the square root in the 'dc:magnitude' element.