Introduction to NucNet Tools

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Input data

- Input data is in eXtensible Markup Language (XML)
- "Self-describing data"
- Schemas: check that the input obeys a predefined grammar
- XSLT: output the data in a format
- XPath: select subsets of the data
- XInclude: include XML inside other XML

XML Document (from W3Schools)

- Get xml file note.xml
- Get schema file note.xsd
- Type: xmllint --schema note.xsd note.xml
- Now edit note.xml to introduce an error
- Type: xmllint --schema note.xsd note.xml

XSLT

- Get the file breakfast.xml
- Get the file breakfast.xslt
- Type: xsltproc breakfast.xslt breakfast.xml > breakfast.html
- Open breakfast.html:
 - -in linux, type: evince breakfast.html
 - -on Mac, type: open breakfast.html
 - -cygwin, type: cygstart breakfast.hml

XSLT

- Get the file lunch.xml
- Get the file lunch.xslt
- Type: xsltproc lunch.xslt lunch.xml > lunch.html
- Open lunch.html:
 - -in linux, type: evince lunch.html
 - -on Mac, type: open lunch.html
 - -cygwin, type: cygstart lunch.hml

XSLT

- Get the file menu.xml
- Get the file menu.xslt
- Type: xsltproc --xinclude menu.xslt menu.xml > menu.html
- Open menu.html:
 - -in linux, type: evince menu.html
 - -on Mac, type: open menu.html
 - -cygwin, type: cygstart menu.hml

Exercise I with libnucnet

- cd nucnet-tools-code/build
- make -f Makefile.libnucnet all_libnucnet
- make -f Makefile.libnucnet libnucnet data
- cd ../libnucnet
- ./create_nuc_xml_from_text ../data_pub/ example_nuc.txt nuc.xml

Exercise 2 with libnucnet

- ./print_nuclides nuc.xml
- ./print_nuclides ../data_pub/example_nuc.xml
- ./print_nuclides http://libnucnet.sourceforge.net/
 data_pub/2013-02-12/example_nuc.xml

Exercise 3 with libnucnet

- ./validate_nuc_xml nuc.xml
- Edit nuc.xml to add error and try again
- ./validate_nuc.xml ../data_pub/example_nuc.xml

Exercise 4 with libnucnet

- ./print_nuclides nuc.xml "[z = 1]"
- ./print_nuclides ../data_pub/example_nuc.xml "[z = 15 or a z = 20]"
- ./print_nuclides http://libnucnet.sourceforge.net/
 data_pub/2013-02-12/example_nuc.xml "[(z >= 15 and z <= 20) or z = 23]"

Limiting the Network

- Where possible, use XPath to limit your network, especially to use a small network to test your calculation before using a big network.
- If the XPath is too complicated, or you otherwise want to restrict the species in a network, see: http://sourceforge.net/u/mbradle/blog/2014/04/ selecting-an-input-network/
- Also consider using network views: https://sourceforge.net/u/mbradle/blog/2014/04/
 limiting-the-reaction-network/

Carrying on

- libnucnet (wn_matrix, libstatmech, libnuceq) examples: http://libnucnet.sourceforge.net
- blog: http://sourceforge.net/u/mbradle/blog
- NucNet Projects: http://nucnet-projects.sourceforge.net