The FUDGE translation of the TENDL-2021 library from ENDF-6 to GNDS

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Overview

- Demonstrate FUDGE installation from GitHub
- Demonstrate translation of TENDL-2021 library from ENDF6 to GNDS
- Summary of TENDL-2021 library translation from ENDF6 to GNDS

Downloading TENDL-2021 Library

In [ ]:
```
%%bash

for projectile in a d g h n p t; do
  tarFile=TENDL-${projectile}.tgz
  if [[ ! -f $tarFile ]]; then
    echo https://tendl.web.psi.ch/tendl_2021/tar_files/TENDL-${projectile}.tgz
    wget https://tendl.web.psi.ch/tendl_2021/tar_files/TENDL-${projectile}.tgz
  fi
done
```

FUDGE installation from GitHub

The following code demonstrates the installation of FUDGE to a Python virtual environment.

In [ ]:
```
%%bash

python3 -m pip install git+https://github.com/LLNL/fudge.git@6.2.0
```

Translating TENDL-2021 Library from ENDF6 to GNDS

Function to run shell commands from within python

In [ ]:
```
import pathlib
import subprocess

def runShellCommand(commandList, cwd=pathlib.Path()):
  process = subprocess.Popen(commandList, universal_newlines=True, cwd=cwd)
  process.communicate()
```

Path to FUDGE translation script

In [ ]:
```
import brownies

translationScript = pathlib.Path(brownies.__path__._path[0]) / 'bin' / 'endf2gnds.py'
```

Arguments available in processing script

In [ ]:
```
runShellCommand(['python3', translationScript, '-h'])
```

```
usage: endf2gnds.py [-h] [-v] [--skipBadData] [--skipCovariances]
                    [--verboseWarnings] [--printBadNK14]
                    [--continuumSpectraFix] [--ignoreBadDate]
                    [--acceptBadMF10FissionZAP] [--traceback]
                    [--formatVersion {1.10,2.0}] [--energyUnit ENERGYUNIT]
                    [--JENDL_stylePrimarygammas]
                    [--IDs {familiar,nucleus,nuclide}]
                    inFile [outputFile]

Translates an ENDF file to the GNDS format.

positional arguments:
  inFile                input file
  outputFile            output file

options:
  -h, --help            show this help message and exit
  -v, --verbose         enable verbose output. The more the gabbier.
  --skipBadData         skip bad data, rather than throw an exception, when
                        reading an ENDF file
  --skipCovariances     skip the covariance, if present
  --verboseWarnings     print verbose warnings
  --printBadNK14        print bad NK's if found
  --continuumSpectraFix
                        fix continuous spectra on read, if foobar
  --ignoreBadDate       ignore malformed ENDF dates
  --acceptBadMF10FissionZAP
                        allow MF=10 MT=18 IZAP=0
  --traceback           print traceback on exception
  --formatVersion {1.10,2.0}
                        Specifies the format for the outputted GNDS file.
  --energyUnit ENERGYUNIT
                        Convert all energies in the gnds file to this unit.
  --JENDL_stylePrimarygammas
                        If prsent, treat MF=6 primary gamma energies as
                        binding energy, otherwise as gamma energy.
  --IDs {familiar,nucleus,nuclide}
                        Choose between light charged particle naming
                        conversion: "nuclide" (i.e., H1, H2, H3, He3 and He4),
                        "nucleus" (i.e., h1, h2, h3, he3 and he4), or
                        "familiar" (i.e., p, d, t, h and a).
```

Shell script to run FUDGE translation script

In [ ]:
```
import stat

translateSingleProtare = [
    '#!/usr/env/sh bash',
    '',
    'if [[ "$1" == "" ]]; then',
    '  echo "USAGE ERROR: $0 endf_file"',
    '  exit 1',
    'fi',
    '',
    'endf6File=$1',
    'gndsFile=$(basename ${endf6File}).gnds.xml',
    'logFile=${gndsFile%gnds.xml}log',
    'outputFile=${gndsFile%gnds.xml}out',
    f'python3 {translationScript} $endf6File $gndsFile --verbose 2>$logFile 1>$outputFile',
    ''
]

endf2gndsScript = pathlib.Path('endf2gnds.sh')
endf2gndsScript.write_text('\n'.join(translateSingleProtare))
endf2gndsScript.chmod(endf2gndsScript.stat().st_mode | stat.S_IEXEC)
```

Translate files

In [ ]:
```
import tarfile as tarfileModule

projectileKeyMap = {"a": "alpha", "d": "deuteron", "g": "gamma", "h": "helion", "n": "neutron", "p": "proton", "t": "triton"}

for tarFile in pathlib.Path().glob('*.tgz'):
  projectileDir = tarFile.parent / projectileKeyMap[tarFile.name[-5]]
  if not projectileDir.is_dir():
    projectileDir.mkdir()
    tarfileModule.open(tarFile).extractall(path=projectileDir)

  gndsDir = projectileDir / 'gnds'
  if not gndsDir.is_dir():
    gndsDir.mkdir()

    fileList = [file.resolve() for file in projectileDir.glob('*.tendl')]
    numberFiles = len(fileList)
    for i, endf6File in enumerate(fileList):
      shellCommand = ['bash', endf2gndsScript.resolve(), endf6File]
      runShellCommand(shellCommand, gndsDir)

      if i % 10 == 0:
        print(f'{i}/{numberFiles} for {projectileKeyMap[tarFile.name[-5]]}s')
```

TENDL-2021 library translation at LLNL

Summary of translation failures

The table below gives an overview of the number of translation failures for different versions of the FUDGE brownies module and command line arguments. The first column shows the version of FUDGE used for the translations. Version 6.2 was used in the first three cases with the arguments shown in the second column. The FUDGE/Brownies module was subsequently modified to ignore the problems associated with MF 8, 10 and 40. These are associated with radioactive production cross sections but they are redundant and are not necessary for transport applications. The resulting translations are shown in the last two cases below.

FUDGE Version	Translation Script Arguments	alphas	deuterons	gammas	helions	neutrons	protons	tritons
6.2	No Arguments	194	237	71	232	306	217	269
6.2	--acceptBadMF10FissionZAP	194	236	71	232	306	217	269
6.2	--continuumSpectraFix	194	236	71	232	245	216	269
6.2 with Brownies updates	No Arguments	2	2	0	2	84	4	1
6.2 with Brownies updates	--acceptBadMF10FissionZAP --continuumSpectraFix	2	2	0	2	23	3	1

The remaining cases that failed to translate are the following:

- ^{1}H projectile: ^{2}H, ^{237}Pa and ^{238}Pa targets
- ^{2}H projectile: ^{3}H and ^{237}U targets
- ^{3}H projectile: ^{236}U targets
- ^{3}He projectile: ^{236}Pa and ^{236}Th targets
- ^{4}He projectile: ^{233}Pa and ^{233}Th targets
- n projectiles:
  - ^{2}H
  - ^{241}Am
  - ^{10}B
  - ^{9}Be
  - ^{243}Cm
  - ^{262}Db, ^{263}Db, ^{264}Db
  - ^{233}Pa
  - ^{237}Pu, ^{238}Pu, ^{239}Pu, ^{240}Pu
  - ^{272}Sg, ^{273}Sg
  - ^{232}Th
  - ^{232}U, ^{234}U, ^{235}U, ^{236}U, ^{237}U, ^{239}U, ^{240}U