Kraken workshop

Short overview of KrakenTools

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krakentools Python package

Collection of Python scripts, functionalities and definitions useful for the Kraken framework.

Examples:

- Producing water and fuel material definitions for Serpent.
- Producing material volumes for Serpent.
- Interacting with Serpent binary restarts.
- Regression testing.
- Radial reflector homogenization.
- Condensation of Serpent group constant data.

Producing water and fuel material definitions for Serpent

Producing water compositions for Serpent

krakentools.utils.write_water_composition()
krakentools.utils.write_p_t_water_composition()
krakentools.utils.write_saturated_water_composition()
Tests 01, 02, 14, 15.

Feed in basic data: (p, T, boron, …)

```
pressure = 15e6 # Pa
temperature = 550 # K
boron = 1000 # ppm (weight)
```

Get Serpent material definition:

```
mat cool_1000B_76D -0.76978 tmp 550
                   moder lw550K 1001
                   rgb 200 200 255
O-16.03c   3.323385e-01
O-17.03c   1.265963e-04
80180      6.829536e-04
H-1.03c    6.662196e-01
H-2.03c    7.662406e-05
B-10.03c   1.105860e-04
B-11.03c   4.451225e-04
```

Producing fuel compositions for Serpent

krakentools.utils.write_fuel_composition()
Krakentools/tests/17_fuel_composition/input.py

Feed in basic data: (density, enrichment, gadolinium, …)

```
density = 10.2 # g/cm3
wt_frac_U234 = 0.0002 # of U
wt_frac_U235 = 0.04 # of U
wt_frac_U236 = 0.0002 # of U
wt_frac_Gd2O3 = 0.02 # of fuel density
```

Get Serpent material definition:

```
mat fuel_20U4_40U5_20U6_20GO -10.2 tmp 800
92234.06c   -1.727707e-04
92235.06c   -3.455413e-02
92236.06c   -1.727707e-04
92238.06c   -8.289537e-01
8016.06c    -1.187942e-01
64152.06c   -3.352815e-05
64154.06c   -3.702705e-04
64155.06c   -2.530124e-03
64156.06c   -3.522011e-03
64157.06c   -2.709997e-03
64158.06c   -4.328777e-03
64160.06c   -3.857778e-03
```

Producing material volumes for Serpent

krakentools.utils.process_material_volumes()

- Serpent needs information on the volumes of each depletion zone for burnup calculation.
- Depletion zone numbering may be hard to follow.
- Clever use of symmetries increases statistics, but means that some depletion zones can have 2, 4 or 8 times the base volume.
- Serpent can estimate volumes based on Monte Carlo sampling, but that leaves statistical uncertainties.

```
% --- Material volumes:

% Produced Wed Jul 17 10:40:00 2019 by MC volume calculation routine by
% sampling 10000000 random points in the geometry.

set mvol

fuelNoGad     35 1.98263E+00 % (0.005)
fuelNoGad     34 1.96811E+00 % (0.004)
fuelNoGad     33 3.98636E+00 % (0.003)
fuelNoGad     32 1.99161E+00 % (0.005)
fuelNoGad     31 3.96966E+00 % (0.004)
fuelNoGad     30 3.98779E+00 % (0.003)
fuelNoGad     29 3.96966E+00 % (0.003)
...
```

krakentools.utils.process_material_volumes()

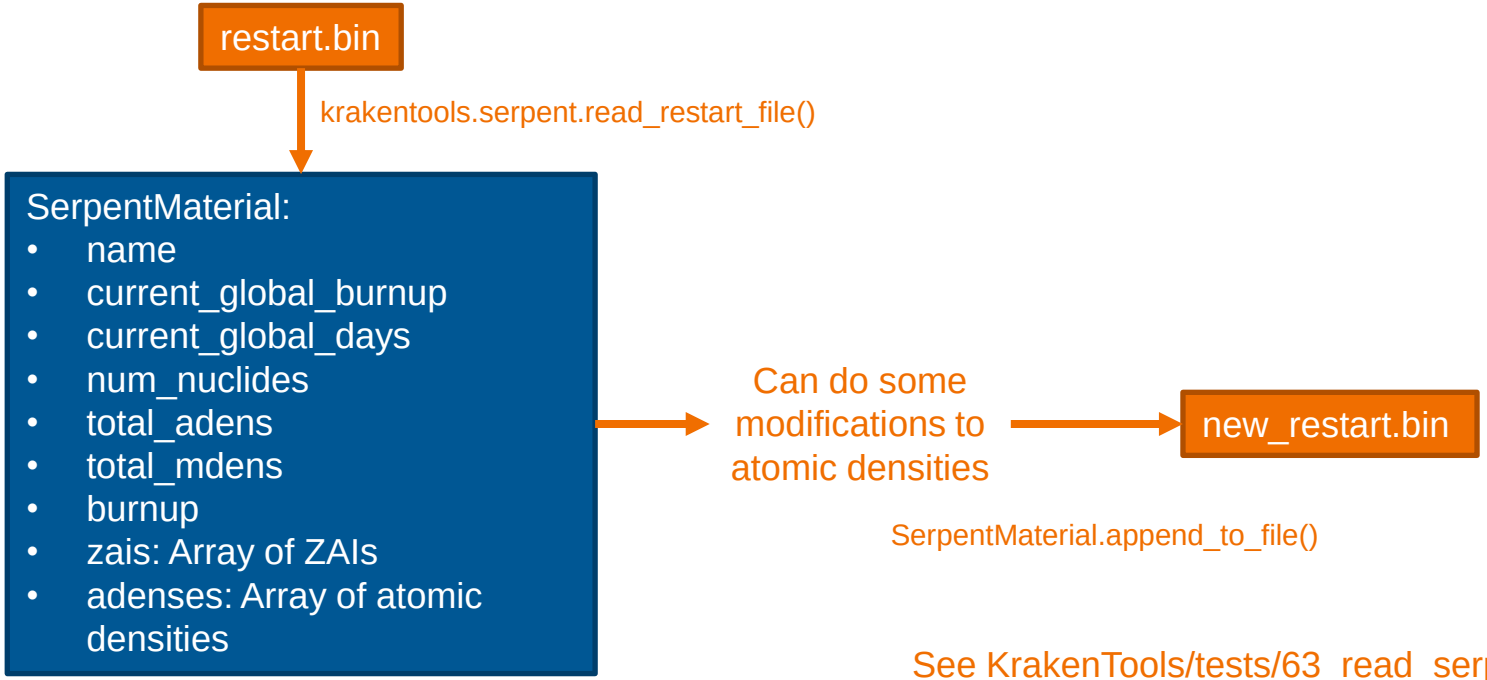
- Some clean up can be made to the Monte Carlo calculated volumes based on basic information on the depletion zone setup.
- KrakenTools/tests/06_material_volume_processing/input.py
- KrakenTools/tests/62_process_arbitrary_fuel_volumes/input.py

```
% --- Material volumes:


set mvol

fuelNoGad       35 1.98557E+00     %% original volume 1.98263E+00 was a multiple of 4 (3.994 as float)
fuelNoGad       34 1.98557E+00     %% original volume 1.96811E+00 was a multiple of 4 (3.965 as float)
fuelNoGad       33 3.97113E+00     %% original volume 3.98636E+00 was a multiple of 8 (8.031 as float)
fuelNoGad       32 1.98557E+00     %% original volume 1.99161E+00 was a multiple of 4 (4.012 as float)
fuelNoGad       31 3.97113E+00     %% original volume 3.96966E+00 was a multiple of 8 (7.997 as float)
fuelNoGad       30 3.97113E+00     %% original volume 3.98779E+00 was a multiple of 8 (8.034 as float)
fuelNoGad       29 3.97113E+00     %% original volume 3.96966E+00 was a multiple of 8 (7.997 as float)
...
```

Interacting with Serpent binary restarts

krakentools.serpent.read_restart_file()

- Serpent can be told to write material compositions into restart files (set rfw) for later utilization in restart simulations (set rfr).
- Krakentools can be used to extract the material data from such files (including all burnup points) into SerpentMaterial objects:



See KrakenTools/tests/63_read_serpent_restart

Simple regression testing module

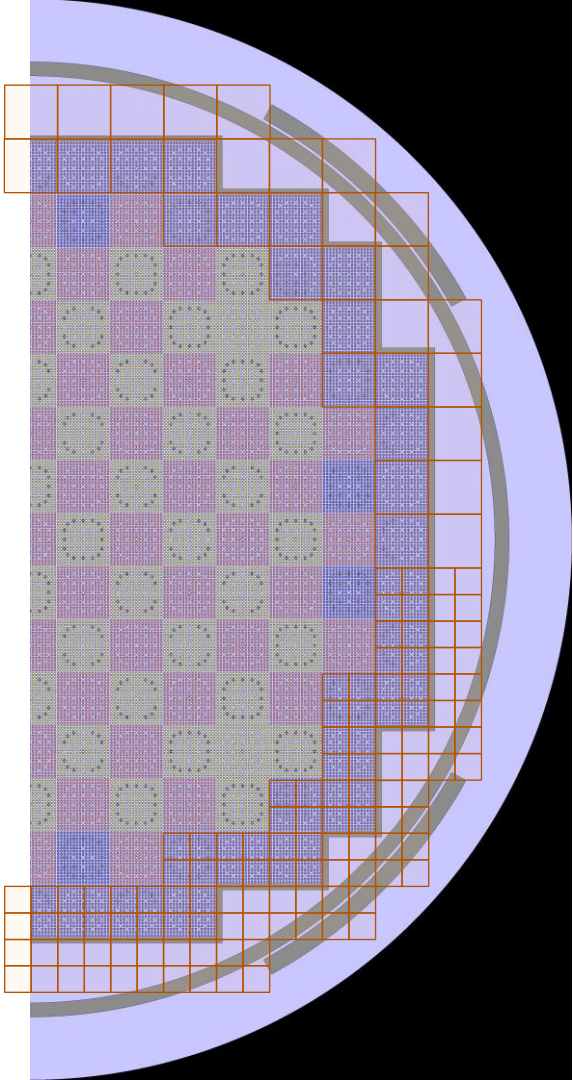
krakentools.testing

- Provides functionalities for regression testing during Kraken development.
- Runs all tests or some subset.
- Compares results to an earlier reference in three potential ways:
  1. File fully matches the reference.
  2. The reference file is a part of the new file.
     - New file is allowed to contain some additional parts.
  3. A user/developer written script checks the output to see if it is acceptable.
     - Flexible and extendable.
- Utilized in regression testing of the Kraken modules:
  - Serpent, Ants, SuperFINIX, Kharon, KrakenTools, Cerberus, …

Radial reflector homogenization

Radial reflector homogenization

- We homogenize the radial reflector for Ants from a Serpent 2D full core simulation (square or hexagonal lattice).
- The tedious parts are automated with krakentools.CoreLattice and krakentools.reflectorhg:
  - Setting up the superimposed universes to the Serpent model.
    - 1x1 or 2x2, one layer of reflector or multiple.
  - Collecting Serpent output data and averaging it over symmetry sectors.
  - Running single node Ants calculations to evaluate homogeneous surface fluxes for discontinuity factors.
  - (potentially condensing the data further)
  - Group constant fitting and library production.
- See tests 08, 11, 13, 16, 48, 49
- Also see: Evaluating the X2 Initial Core Zero Power Physics Tests with Serpent-Ants
  Ville Valtavirta *et al.*
  Tue 1:30 pm, Brighton III/IV, *Data, Methods, Code Validation: V*



Condensation of Serpent group constant data

Condensing Serpent group constant data further

- Generate group constants with Serpent into some energy group structure.
- Read the data into NodeBranch objects with
  - krakentools.serpent.read_coe_and_res()

Reading utilizes functionalities from serpentTools: Andrew Johnson, Dan Kotlyar, Stefano Terlizzi, and Gavin Ridley, “serpentTools: A Python Package for Expediting Analysis with Serpent.”, Nuclear Science and Engineering, 194 (2020)

- Each krakentools.containers.NodeBranch object contains data for a single universe/node at specific conditions (branch).

- Use NodeBranch.give_condensed_version() to obtain an energy condensed variant (both infinite spectrum and leakage corrected data if available).
- See tests 50 and 51.

NodeBranch.calculate_critical_spectra() being prepared for applying leakage correction outside Serpent.

Summary

- KrakenTools collects many functionalities for Kraken related tasks.
  - Built primarily to serve VTT internal purposes as most of the Kraken framework.
- For general Serpent purposes you may have your own scripts already:
  - Producing material compositions
  - …
- For Kraken purposes you may find the capabilities of KrakenTools invaluable:
  - Full core 2D radial reflector homogenization.
  - Group constant parametrization.
  - …

Serpent users should also consider testing out serpentTools:
https://github.com/CORE-GATECH-GROUP/serpent-tools
https://serpent-tools.readthedocs.io/en/master/overview.html

VTT

beyond
the obvious

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