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Easy_PERT: a Python tool for writing PERT cards and parsing PERT card results

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PERT card overview

- Uses differential operator method[1] to compute first- and second-order tally variations due to density, composition, and reaction cross-sections
- Can have multiple PERT cards in one MCNP input deck to study tally variations for several sets of nuclides, reactions, and energy ranges
- METHOD option tells MCNP to calculate either the perturbed tally (METHOD=-1, -2, -3) or the change in the unperturbed tally (METHOD=1, 2, 3)

1. J. A. Kulesza et al., “MCNP® Code Version 6.3.0 Theory & User Manual,” LA-UR-22-30006, Rev. 1, Section 2.12.1, (2022)

Sensitivity analysis via the PERT card

- The PERT card can be used[1] to compute tally sensitivities with respect to nuclear data
  - For each nuclide, reaction, and energy range, write one PERT card with METHOD=2
  - Parse the MCTAL file for the unperturbed tally (c_0) and tally variation (Δc_1)
  - Calculate the first-order sensitivity as $S_{c,\sigma_x} = \frac{\Delta c_1}{p \cdot c_0}$
  - p is an arbitrary perturbation size (typically choose $p = 1$)
- PERT cards can also be used[1] to calculate the statistical uncertainty of the sensitivities
  - Treating c_0 and Δc_1 as independent, only METHOD=2 is needed
  - To account for correlation between c_0 and Δc_1, need METHOD=2, -2

1. J. Favorite, "Using the MCNP Taylor series perturbation feature (efficiently) for shielding problems," EPJ Web of Conferences 153, 06030 (2017)

Difficult to use PERT card capability by hand

- User must add the following to their MCNP input deck
  - Create a “fictitious” material that is copied from an existing material
    - Multiply original nuclide fraction by $1 + p$
    - Multiply original material density by $\frac{\sum_i \omega_i'}{\sum_i \omega_i^0}$
  - Write PERT cards for all nuclides, reactions, energy ranges, and methods
- User must parse the output MCTAL file for tally results and their corresponding uncertainties to calculate
  - Tally sensitivities to nuclear data
  - Uncertainty in sensitivities due to Monte Carlo statistics

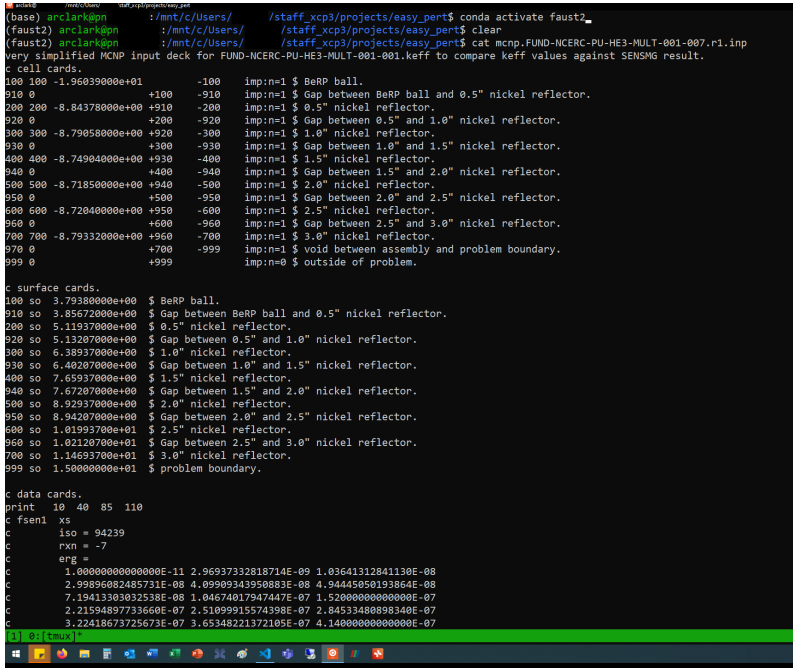
Easy_PERT simplifies the process

- Python tool that is run from the command line
  - Uses Faust[1] to modify the MCNP input deck and write outputs in a JSON format
  - Uses MCNPTools[2] to parse the output MCTAL file
- User provides an existing MCNP input deck and specifies nuclides, reactions, energy ranges, and methods
- Tool handles
  - Calculating modified fractions and material densities
  - Writing a modified MCNP input deck
  - Parsing the output MCTAL file into a JSON format

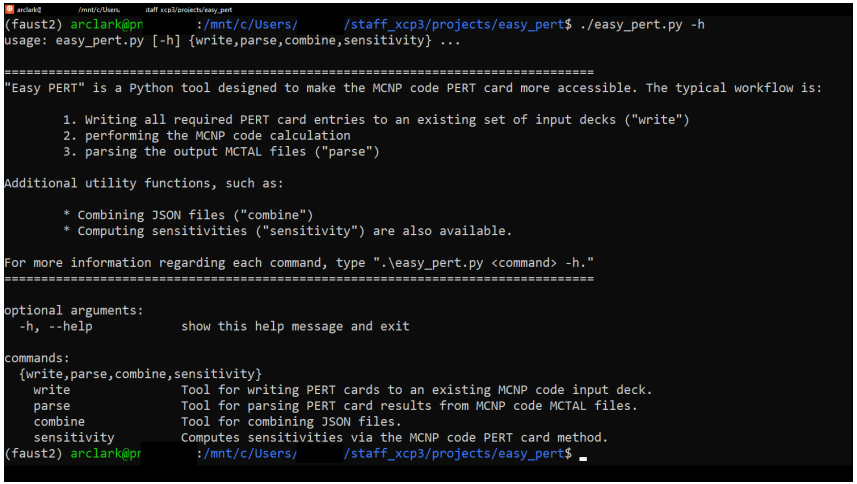
1. W. Haeck, A. R. Clark, and M. W. Herman, “Calculating the Impact of Nuclear Data Changes with Crater,” Trans. Am. Nucl. Soc., Vol. 123, No. 1, p. 723-726 (Nov. 2020)
2. C. R. Bates et al., “The MCNPTools Package: Installation and Use,” LA-UR-22-28935, (Aug. 2022)

Easy_PERT demo

- Start with an existing MCNP input deck



- Main Python script is used to perform each of the steps



Easy_PERT demo

- Use the “write” command to add required PERT card entries to your existing input deck

Easy_PERT demo

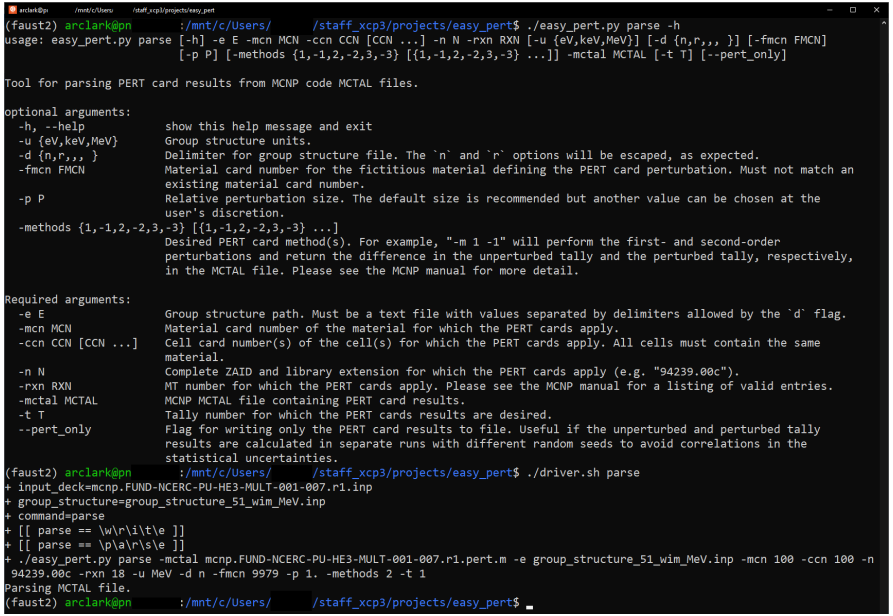
- The tool takes care of making the fictitious material, calculating the fictitious density, and writing all of the relevant PERT cards

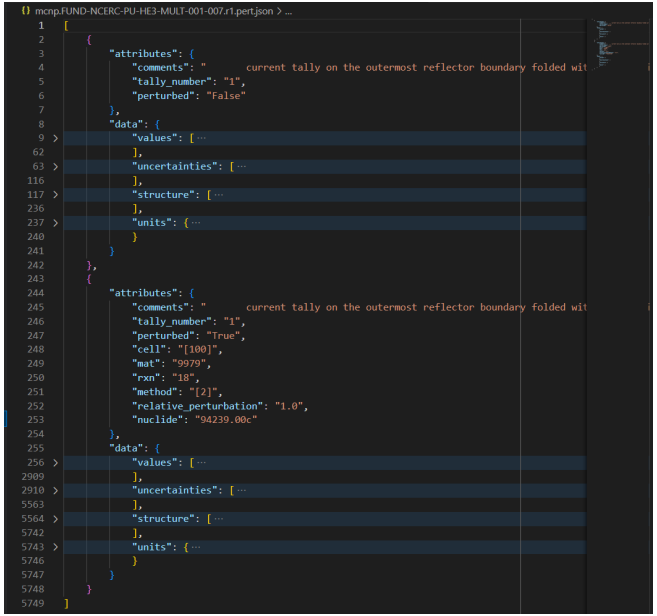
```
160 c
161 c materials cards.
162 c
163 c BeRP ball.
164 m100    6012.00c  4.54853000e-03
165         11023.00c 2.58307000e-04
166         31069.00c 6.85800000e-04
167         31071.00c 4.55256000e-04
168         73181.00c 2.33361000e-03
169         74182.00c 6.08751000e-04
170         74183.00c 3.28717000e-04
171         74184.00c 7.03705000e-04
172         74186.00c 6.53009000e-04
173         92235.00c 8.51567000e-04
174         92236.00c 1.97532000e-04
175         94238.00c 1.54199000e-04
176         94239.00c 9.26002000e-01
177         94240.00c 5.83805000e-02
178         94241.00c 5.61676000e-04
179         94242.00c 2.73395000e-04
180         95241.00c 2.52674000e-03
181 c 0.5" nickel reflector.
182 m200    5011.00c 1.30276000e-04
```

```
272 c fictitious material for use with the PERT card
273 c using p=1.0, nuclide=94239.00c
274 m9979
275      6012.00c 0.00454853
276      11023.00c 0.000258307
277      31069.00c 0.0006858
278      31071.00c 0.000455256
279      73181.00c 0.00233361
280      74182.00c 0.000608751
281      74183.00c 0.000328717
282      74184.00c 0.000703705
283      74186.00c 0.000653009
284      92235.00c 0.000851567
285      92236.00c 0.000197532
286      94238.00c 0.000154199
287      94239.00c 1.852004
288      94240.00c 0.0583805
289      94241.00c 0.000561676
290      94242.00c 0.000273395
291      95241.00c 0.00252674
292 pert1:n cell=100 mat=9979 rho=-37.76580849855271 rxn=18 erg=1.000000e-11, 2.969370e-09 method=2
293 pert2:n cell=100 mat=9979 rho=-37.76580849855271 rxn=18 erg=2.969370e-09, 1.036410e-08 method=2
294 pert3:n cell=100 mat=9979 rho=-37.76580849855271 rxn=18 erg=1.036410e-08, 2.998960e-08 method=2
295 pert4:n cell=100 mat=9979 rho=-37.76580849855271 rxn=18 erg=2.998960e-08, 4.099090e-08 method=2
296 pert5:n cell=100 mat=9979 rho=-37.76580849855271 rxn=18 erg=4.099090e-08, 4.944450e-08 method=2
297 pert6:n cell=100 mat=9979 rho=-37.76580849855271 rxn=18 erg=4.944450e-08, 7.194130e-08 method=2
```

Easy_PERT demo

- After performing the MCNP calculation to get a MCTAL file, use the “parse” command to parse the tally information into a JSON format





Summary and future work

- A powerful use-case for the MCNP code PERT card is calculating tally sensitivities to nuclear data[1]
- Writing PERT card entries and parsing output MCTAL files is tedious and error-prone
- Easy_PERT makes use of existing tools (Faust[2] and MCNPTools[3]) to handle writing PERT card entries and parsing the output MCTAL files
- Early in development process, so upcoming capabilities are
  - Calculating sensitivities
  - Combining MCTAL files from separate runs into one JSON file
- Looking forward to feedback, suggestions, and friendly testers

1. J. Favorite, “Using the MCNP Taylor series perturbation feature (efficiently) for shielding problems,” EPJ Web of Conferences 153, 06030 (2017)
2. W. Haeck, A. R. Clark, and M. W. Herman, “Calculating the Impact of Nuclear Data Changes with Crater,” Trans. Am. Nucl. Soc., Vol. 123, No. 1, p. 723-726 (Nov. 2020)
3. C. R. Bates et al., “The MCNPTools Package: Installation and Use,” LA-UR-22-28935, (Aug. 2022)

Questions?

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