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SUBJECT: (U) Release of SOURCES4D Featuring Sensitivity Capabilities

Abstract—SOURCES is a code for computing neutron source rates and spectra from spontaneous fission (including delayed neutrons) and (α,n) reactions. The first release since 2002, SOURCES4D, is now available. The main updates include new output that allows the user to calculate, in post-processing, first and second derivatives of the (α,n) source rate density and spectrum with respect to nuclide densities in a homogeneous material and first derivatives of the (α,n) source rate density and spectrum with respect to nuclide stopping powers and (α,n) cross sections (nuclear data). The value of π was made more accurate in order to eliminate negative spontaneous-fission sources. Otherwise, SOURCES4D has made no changes to the physics or data of neutron source calculations used in SOURCES4C. First and second derivatives are calculated in an example problem.

I. Introduction

SOURCES is a code for computing neutron source rates and spectra from spontaneous fission (including delayed neutrons) and (α,n) reactions in homogeneous materials and (α,n) reactions in single-interface and two-interface geometries.[1] SOURCES is a Los Alamos National Laboratory (LANL) code that is written in FORTRAN and distributed through the Radiation Safety Information Computation Center (RSICC). LANL's last release of SOURCES to RSICC was SOURCES4C in 2002.

SOURCES4D is now available. SOURCES4D includes sensitivity capabilities for (α,n) sources in homogeneous materials. Specifically, SOURCES4D writes new output that can be used to calculate, in post-processing, first and second derivatives of the (α,n) source rate density and spectrum with respect to nuclide densities in a homogeneous material[2,3] and first derivatives of the (α,n) source rate density and spectrum with respect to nuclide stopping powers and (α,n) cross sections (nuclear data).[4] These derivatives are useful for uncertainty quantification, predictive modeling, and other applications in neutron transport problems.

Several minor modifications have also been made, including a more accurate value for π that prevents negative spontaneous-fission sources.

Reference 1 remains the manual for SOURCES4D. This brief report covers only the modifications that have been made to SOURCES4C to create SOURCES4D.

This report is organized as follows. Section II describes the capabilities in SOURCES4D that assist in calculating the first derivatives of the (α,n) source rate density and spectrum with respect to nuclide densities in a homogeneous material, and Sec. III reviews the first derivative of the spontaneous-fission source rate density and spectrum with respect to nuclide densities. Section IV describes the capabilities in SOURCES4D that assist in calculating the second derivatives of (α,n) sources, and Sec. V reviews the second derivatives of spontaneous-fission sources. Section VI discusses very briefly the capability for SOURCES4D to assist in calculating the first derivatives of the (α,n) source rate density and spectrum with respect to isotopic nuclear data. Section VII discusses some more minor modifications. Section VIII is an example problem showing how to use the output to compute first and second derivatives. Section IX is a summary and conclusions.

II. First Derivatives of the (α,n) Source Rate Density and Spectrum with Respect to Nuclide and Material Densities in a Homogeneous Material

The first derivative of the (α,n) source rate density $Q_{(\alpha,n),k,i}$ due to target i and α source k with respect to the atom density N_j of nuclide j in a homogeneous material is[2]

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial N_j} = \delta_{ji}\frac{Q_{(\alpha,n),k,i}}{N(N_i/N)} + \delta_{jk}\frac{Q_{(\alpha,n),k,i}}{N_k} - \lambda_k\frac{N_k}{N}\sum_{l=1}^{L} f_{kl}^{\alpha} P_{i,j}^{(1)}(E_l), \tag{1}$$

where δ_{ab} is the Kronecker delta, satisfying

$$\delta_{ab} = \begin{cases} 1, & a = b \\ 0, & a \neq b. \end{cases} \tag{2}$$

In addition,

N = total atom density of the material in atoms/(b·cm)
λ_k = decay constant for α source nuclide k in s^{-1}
L = number of discrete α-particle energies (or levels) emitted from α source nuclide k
f_{kl}^{α} = fraction of all decays of nuclide k resulting in an α particle of energy E_l
$P_{i,j}^{(1)}(E_l)$ = a unitless quantity defined in Eq. (22) of Ref. 2.

The quantity $P_{i,j}^{(1)}(E_l)$ includes α-energy-dependent (α,n) cross sections for nuclide i, α-energy-dependent stopping cross sections for nuclide j and the entire material, and the target nuclide atom fractions N_i/N.

The derivative $\partial Q_{(\alpha,n),k,i}/\partial N_j$ shown in Eq. (1) consists of three terms. The first term on the right side of Eq. (1) applies when nuclide j is a target; the second term applies when nuclide j is an α emitter (for α beam problems, α emissions by radioactive decay are ignored); and the third term accounts for nuclide j's contribution to the material's α stopping power. (All isotopes of an element have the same value for the third term, for a given source nuclide k and target nuclide i.)

For each combination of target i and α source k, SOURCES4D outputs the atom fraction N_i/N of the target nuclide i, the atom density N_k of the α source nuclide k, the source nuclide decay constant λ_k, the source rate density $Q_{(\alpha,n),k,i}$, and, for each stopping nuclide j (that is, all nuclides in the material), the sum $\sum_{l=1}^{L} f_{kl}^{\alpha} P_{i,j}^{(1)}(E_l)$. The sum is the same for all isotopes of an element, so it is only reported for each element along with the atom fraction for each stopping element in the material. These quantities are written to a new output file, `pdata`.

The user can combine these values according to Eq. (1) to compute $\partial Q_{(\alpha,n),k,i} \big/ \partial N_j$. The user needs to provide the total material atom density N in units of atoms/(b·cm). SOURCES4D has no way of knowing N or the target nuclide densities N_i. That is why the expression $N(N_i/N)$ is used in the first term of Eq. (1). The source nuclide atom densities are given to SOURCES4D in atoms/cm^3, but they are written to the `pdata` file in atoms/(b·cm). The sum $\sum_{l=1}^{L} f_{kl}^{\alpha} P_{i,j}^{(1)}(E_l)$ is written in units of b·cm/cm^3 so that the units of the product are the same as the other terms, [neutrons/(cm^3·s)]/[atoms/(b·cm)].

The derivative of the total (α,n) neutron source rate density with respect to N_j is the sum of Eq. (1) over all sources k and targets i:

$$\frac{\partial Q_{(\alpha,n)}}{\partial N_j} = \sum_k \sum_i \frac{\partial Q_{(\alpha,n),k,i}}{\partial N_j}. \tag{3}$$

The first derivative of the (α,n) source rate density $Q_{(\alpha,n),k,i}$ due to target i and α source k with respect to the atom density N of the homogeneous material is[2]

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial N} = \frac{Q_{(\alpha,n),k,i}}{N}. \tag{4}$$

This can also be calculated from the nuclide derivatives using

$$\frac{\partial Q_{(\alpha,n),k,i}}{\partial N} = \sum_j \frac{\partial Q_{(\alpha,n),k,i}}{\partial N_j} \frac{N_j}{N}. \tag{5}$$

Using Eq. (1) in Eq. (5) yields

$$\begin{aligned} \frac{\partial Q_{(\alpha,n),k,i}}{\partial N} &= \sum_j \delta_{ji} \frac{Q_{(\alpha,n),k,i}}{N(N_i/N)} \frac{N_j}{N} + \sum_j \delta_{jk} \frac{Q_{(\alpha,n),k,i}}{N_k} \frac{N_j}{N} - \sum_j \lambda_k \frac{N_k}{N} \left(\sum_{l=1}^{L} f_{kl}^{\alpha} P_{i,j}^{(1)}(E_l) \right) \frac{N_j}{N} \\ &= \frac{Q_{(\alpha,n),k,i}}{N} + \frac{Q_{(\alpha,n),k,i}}{N} - \sum_j \lambda_k \frac{N_k}{N} \frac{N_j}{N} \sum_{l=1}^{L} f_{kl}^{\alpha} P_{i,j}^{(1)}(E_l). \end{aligned} \tag{6}$$

Comparing Eq. (6) with Eq. (4), it is evident that

$$\sum_j \lambda_k \frac{N_k}{N} \frac{N_j}{N} \sum_{l=1}^{L} f_{kl}^{\alpha} P_{i,j}^{(1)}(E_l) = \frac{Q_{(\alpha,n),k,i}}{N}. \tag{7}$$

These equations can be used for consistency checks and debugging. The atom fractions N_j/N are written to the `pdata` file for stopping elements, not nuclides (the same way they are entered into the SOURCES4D input file). The sum in Eq. (7) can be over elements or nuclides.

An approximation for the derivative of the source rate density $Q^g_{(\alpha,n),k,i}$ in neutron energy group g (g = 1,…,G) due to target i and α source k is[2]

$$\frac{\partial Q^g_{(\alpha,n),k,i}}{\partial N_j} \approx \frac{Q^g_{(\alpha,n),k,i}}{Q_{(\alpha,n),k,i}} \frac{\partial Q_{(\alpha,n),k,i}}{\partial N_j}. \tag{8}$$

The energy-dependent source rate density $Q^g_{(\alpha,n),k,i}$ is printed in the standard SOURCES4D output file `tape7`. The normalized source rate density $Q^g_{(\alpha,n),k,i} / Q_{(\alpha,n),k,i}$ is printed in the standard SOURCES4D output file `tape8`. (Reference 2 describes new outputs of the neutron spectrum averaged over target nuclides and source nuclides. These outputs are not printed in SOURCES4D.)

The derivative of the (α,n) neutron source rate density in neutron energy group *g* with respect to N_j is the sum of Eq. (8) over all sources *k* and targets *i*:

$$\frac{\partial Q^g_{(\alpha,n)}}{\partial N_j} = \sum_k \sum_i \frac{\partial Q^g_{(\alpha,n),k,i}}{\partial N_j}. \tag{9}$$

These derivatives are absolute unconstrained derivatives with respect to nuclide atom densities, as opposed to relative or constrained derivatives, meaning that if the density of nuclide *j* is perturbed to $N_j + \Delta N_j$, the density of the material is perturbed to $N + \Delta N_j$. These derivatives can be used to compute relative constrained derivatives using the formulas of Ref. 5.

III. First Derivatives of the Spontaneous-Fission Source Rate Density and Spectrum with Respect to Nuclide Densities

For comparison, the derivative of the neutron source rate density $Q_{s.f.,k}$ due to spontaneous-fissioning nuclide *k* with respect to the density of nuclide *j* in the material is

$$\frac{\partial Q_{s.f.,k}}{\partial N_j} = \delta_{jk} \frac{Q_{s.f.,k}}{N_k}. \tag{10}$$

No information is needed other than $Q_{s.f.,k}$, found in SOURCES standard output file `tape6`, and the nuclide density. Likewise, the derivative of the energy-dependent neutron source rate density $Q^g_{s.f.,k}$ in neutron energy group *g* due to spontaneous-fissioning nuclide *k* with respect to the density of nuclide *j* in the material is

$$\frac{\partial Q^g_{s.f.,k}}{\partial N_j} = \delta_{jk} \frac{Q^g_{s.f.,k}}{N_k}. \tag{11}$$

The energy-dependent source rate density $Q^g_{s.f.,k}$ is found in SOURCES standard output file `tape7`.

IV. Second Derivatives of the (α,n) Source Rate Density and Spectrum with Respect to Nuclide and Material Densities in a Homogeneous Material

The second derivative of the (α,n) source rate density $Q_{(\alpha,n),k,i}$ due to target *i* and α source *k* with respect to the atom densities N_j and $N_{j'}$ of nuclides *j* and *j'* in a homogeneous material is[3]

$$\begin{aligned}\frac{\partial^2 Q_{(\alpha,n),k,i}}{\partial N_{j'} \partial N_j} = &\left(\delta_{ji}\delta_{j'k} + \delta_{j'i}\delta_{jk}\right) \frac{Q_{(\alpha,n),k,i}}{N(N_i/N)N_k} - \frac{\lambda_k N_k}{N^2(N_i/N)} \left(\delta_{ji} \sum_{l=1}^{L} f^{\alpha}_{kl} P^{(1)}_{i,j'}(E_l) + \delta_{j'i} \sum_{l=1}^{L} f^{\alpha}_{kl} P^{(1)}_{i,j}(E_l) \right) \\ &- \frac{\lambda_k}{N} \left(\delta_{jk} \sum_{l=1}^{L} f^{\alpha}_{kl} P^{(1)}_{i,j'}(E_l) + \delta_{j'k} \sum_{l=1}^{L} f^{\alpha}_{kl} P^{(1)}_{i,j}(E_l) \right) + 2 \frac{\lambda_k N_k}{N^2} \sum_{l=1}^{L} f^{\alpha}_{kl} P^{(2)}_{i,j,j'}(E_l),\end{aligned} \tag{12}$$

where $P^{(2)}_{i,j,j'}(E_l)$, defined in Eq. (20) of Ref. 3, is unitless, like $P^{(1)}_{i,j}(E_l)$ of Sec. II. In addition to the outputs discussed in Sec. II, for each combination of target *i* and α source *k*, SOURCES4D outputs the sum $\sum_{l=1}^{L} f^{\alpha}_{kl} P^{(2)}_{i,j,j'}(E_l)$ for each pair of stopping nuclides *j* and *j′*. The sum is the same for all isotopes of an element, so it is only reported for each pair of elements. These quantities are written to the new output file, `pdata`. The sum $\sum_{l=1}^{L} f^{\alpha}_{kl} P^{(2)}_{i,j,j'}(E_l)$ is written in units of b·cm/cm^3. To see that all four terms on the right side of Eq. (12) have the same units, multiply the third term by N_k/N_k.

The second derivative of $Q_{(\alpha,n),k,i}$ with respect to the density N_j of nuclide *j* in the material is obtained by setting $j' = j$ in Eq. (12):

$$\frac{\partial^2 Q_{(\alpha,n),k,i}}{\partial N_j^2} = -\delta_{ji} 2 \frac{\lambda_k N_k}{N^2 (N_i / N)} \sum_{l=1}^{L} f^{\alpha}_{kl} P^{(1)}_{i,j}(E_l) - \delta_{jk} 2 \frac{\lambda_k}{N} \sum_{l=1}^{L} f^{\alpha}_{kl} P^{(1)}_{i,j}(E_l) + 2 \frac{\lambda_k N_k}{N^2} \sum_{l=1}^{L} f^{\alpha}_{kl} P^{(2)}_{i,j,j}(E_l). \tag{13}$$

In this case, the first term in Eq. (12) becomes zero because *j* cannot be both *i* and *k*, for physical reasons: α-particle emitters are not (α,n) targets.

The second derivative of the total (α,n) source rate density with respect to the densities of nuclides *j* and *j′* is the sum of Eq. (12) over all sources and targets:

$$\frac{\partial^2 Q_{(\alpha,n)}}{\partial N_{j'} \partial N_j} = \sum_k \sum_i \frac{\partial^2 Q_{(\alpha,n),k,i}}{\partial N_{j'} \partial N_j}. \tag{14}$$

The second derivative of the (α,n) source rate density $Q_{(\alpha,n),k,i}$ due to target *i* and α source *k* with respect to the atom density *N* of the homogeneous material is[3]

$$\frac{\partial^2 Q_{(\alpha,n),k,i}}{\partial N^2} = 0. \tag{15}$$

This can also be calculated from the nuclide derivatives using

$$\frac{\partial^2 Q_{(\alpha,n),k,i}}{\partial N^2} = \sum_j \sum_{j'} \frac{\partial^2 Q_{(\alpha,n),k,i}}{\partial N_j \partial N_{j'}} \frac{N_j N_{j'}}{N^2}. \tag{16}$$

Using Eq. (12) in Eq. (16) [and using Eq. (7)] yields

$$\begin{aligned}
\frac{\partial^2 Q_{(\alpha,n),k,i}}{\partial N^2} = & \sum_j \sum_{j'} \left(\delta_{ji} \delta_{j'k} + \delta_{j'i} \delta_{jk} \right) \frac{Q_{(\alpha,n),k,i}}{N (N_i / N) N_k} \frac{N_j N_{j'}}{N^2} \\
& - \sum_j \sum_{j'} \frac{\lambda_k N_k}{N^2 (N_i / N)} \left(\delta_{ji} \sum_{l=1}^{L} f^{\alpha}_{kl} P^{(1)}_{i,j'}(E_l) + \delta_{j'i} \sum_{l=1}^{L} f^{\alpha}_{kl} P^{(1)}_{i,j}(E_l) \right) \frac{N_j N_{j'}}{N^2} \\
& - \sum_j \sum_{j'} \frac{\lambda_k}{N} \left(\delta_{jk} \sum_{l=1}^{L} f^{\alpha}_{kl} P^{(1)}_{i,j'}(E_l) + \delta_{j'k} \sum_{l=1}^{L} f^{\alpha}_{kl} P^{(1)}_{i,j}(E_l) \right) \frac{N_j N_{j'}}{N^2} \\
& + 2 \sum_j \sum_{j'} \frac{\lambda_k N_k}{N^2} \left(\sum_{l=1}^{L} f^{\alpha}_{kl} P^{(2)}_{i,j,j'}(E_l) \right) \frac{N_j N_{j'}}{N^2} \\
= & \, 2 \frac{Q_{(\alpha,n),k,i}}{N^2} - 2 \frac{Q_{(\alpha,n),k,i}}{N^2} - 2 \frac{Q_{(\alpha,n),k,i}}{N^2} + 2 \sum_j \sum_{j'} \frac{\lambda_k N_k}{N^2} \frac{N_j N_{j'}}{N^2} \sum_{l=1}^{L} f^{\alpha}_{kl} P^{(2)}_{i,j,j'}(E_l).
\end{aligned} \tag{17}$$

Comparing Eq. (17) with Eq. (15), it is evident that

$$\sum_j \sum_{j'} \frac{\lambda_k N_k}{N^2} \frac{N_j N_{j'}}{N^2} \sum_{l=1}^{L} f_{kl}^{\alpha} P_{i,j,j'}^{(2)}(E_l) = \frac{Q_{(\alpha,n),k,i}}{N^2}. \tag{18}$$

These equations can be used for consistency checks and debugging. The atom fractions N_j/N are written to the `pdata` file for stopping elements, not nuclides (the same way they are entered into the SOURCES4D input file). The sum in Eq. (18) can be over elements or nuclides.

An approximation for the second derivative of the source rate density $Q^g_{(\alpha,n),k,i}$ in neutron energy group g (g = 1,…,G) due to target i and α source k is obtained by differentiating Eq. (8). The result is[3]

$$\frac{\partial^2 Q^g_{(\alpha,n),k,i}}{\partial N_{j'} \partial N_j} \approx \frac{Q^g_{(\alpha,n),k,i}}{Q_{(\alpha,n),k,i}} \frac{\partial^2 Q_{(\alpha,n),k,i}}{\partial N_{j'} \partial N_j}. \tag{19}$$

The second derivative of the total (α,n) source rate density in group g with respect to the densities of isotopes j and j' is the sum of Eq. (19) over all sources and targets:

$$\frac{\partial^2 Q^g_{(\alpha,n)}}{\partial N_{j'} \partial N_j} = \sum_k \sum_i \frac{\partial^2 Q^g_{(\alpha,n),k,i}}{\partial N_{j'} \partial N_j}. \tag{20}$$

Calculating and outputting the terms for second derivatives is controlled by setting a logical variable that is not exposed to users, but it can be changed in the source code. The variable is `l_2nd` at the top of subroutine `homog`. Set it to `.true.` to calculate second-derivative terms and `.false.` to skip those calculations.

V. Second Derivatives of the Spontaneous-Fission Source Rate Density and Spectrum with Respect to Nuclide Densities

For comparison, the second derivative of the neutron source rate density $Q_{s.f.,k}$ due to spontaneous-fissioning nuclide k with respect to the densities of nuclides j and j' in the material is

$$\frac{\partial Q_{s.f.,k}}{N_{j'} \partial N_j} = 0. \tag{21}$$

Likewise, the second derivative of the neutron source rate density $Q^g_{s.f.,k}$ in neutron energy group g due to spontaneous-fissioning nuclide k with respect to the densities of nuclides j and j' in the material is

$$\frac{\partial Q^g_{s.f.,k}}{\partial N_j} = 0. \tag{22}$$

VI. First Derivative of the (α,n) Source Rate Density and Spectrum with Respect to Nuclear Data

The first derivative of the (α,n) source rate density and spectrum with respect to stopping powers and (α,n) cross sections are derived in Ref. 4. Reference 4 also describes the values that are written to a new output file, `sdata`, to allow these calculations in post-processing. This information will not be repeated here.

Calculating and outputting the terms for derivatives of nuclear data is controlled by setting a logical variable that is not exposed to users, but it can be changed in the source code. The variable is `l_sdata` at the top of subroutine `homog`. Set it to `.true.` to calculate the required terms and `.false.` to skip those calculations. This feature may increase the execution time.

VII. Other Modifications

SOURCES4C sometimes prints negative spontaneous fission sources at low neutron energies. In 2019, Ruixian Fang (University of South Carolina) identified the problem as not enough digits in π. The value of π was changed from 3.14159 in SOURCES4C to 3.1415926535898 in SOURCES4D. In addition, the value of e (Napier's constant) was changed from 2.71828 in SOURCES4C to 2.7182818284590 in SOURCES4D.

The maximum number of elements in a homogeneous material was increased from 20 in SOURCES4C to 100 in SOURCES4D (except for the three-region problem). On the other hand, the maximum number of α energy groups was decreased from 4000 in SOURCES4C to 2000 in SOURCES4D. This new limit was applied to all three types of problems (homogeneous material, two region, and three region).

SOURCES4D includes more error checks for bad input, such as too many input values, that would cause SOURCES4C to crash. Also, SOURCES4D is allowed to proceed past some errors that resulted in a `stop` command in SOURCES4C.

Much of the output for homogeneous materials was changed to print more digits. This was done to improve the precision of the derivatives that use that output and also so that more accurate finite differences could be calculated to verify the various post-processed derivative calculations in Refs. 2, 3, and 4.

Some typos in output headers were corrected.

The normalized grand total neutron spectrum for a homogeneous material was inadvertently written to `tape7` in SOURCES4C; this was changed to `tape8` in SOURCES4D.

Some variables were not properly initialized in SOURCES4C.

Routines to calculate the error function were included in SOURCES4C but were not used because the intrinsic FORTRAN error function was used instead. They have been removed in SOURCES4D.

An outstanding issue with SOURCES4D, inherited from its predecessor, is that the normalized (α,n) neutron source spectra in output files `tape8` and `outp2` often do not sum strictly to unity.

The LASTCALL utility mentioned in Ref. 1, a graphical user interface for constructing SOURCES inputs, is no longer available.

VIII. Example

This example is from Ref. 3. The homogeneous material is specified in Table I. There are two α emitters (^{239}Pu and ^{242}Pu), two (α,n) targets (^{9}Be and ^{23}Na), and six stopping nuclides (all of them).

Table I. Material for Example Problem[(a)]

Nuclide	Weight Fraction	Atom Density (at/b·cm)	Atom Fraction
^{9}Be	0.02	2.619426605E-02	2.904942960E-01
^{23}Na	0.02	1.026851546E-02	1.138777916E-01
^{239}Pu	0.90	4.443823802E-02	4.928198653E-01
^{242}Pu	0.02	9.752520195E-04	1.081554063E-02
^{58}Ni	0.02	4.074654487E-03	4.518790044E-02
^{56}Fe	0.02	4.220435034E-03	4.680460607E-02

(a) The mass density is 19.6 g/cm^3 and the total atom density is 9.017136107E-02 at/b·cm.

For this report, the problem was run with 30 neutron energy groups and 400 α groups. The SOURCES4D input file is shown in Figure 1. The neutron energy group boundaries are specified, but the number of α groups is only used to set the number of equal-spaced bins in a numerical integral.[1,2]

```
M&C 2019 test problem material
1 2 -1
  5 0
     004  2.9049430E-01
     011  1.1387779E-01
     094  5.0363541E-01
     028  4.5187900E-02
     026  4.6804606E-02
 -30 1.70000E+01 1.39000E-10
     1.70000E+01 1.50000E+01 1.35000E+01 1.20000E+01 1.00000E+01
     7.79000E+00 6.07000E+00 3.68000E+00 2.86500E+00 2.23200E+00
     1.73800E+00 1.35300E+00 8.23000E-01 5.00000E-01 3.03000E-01
     1.84000E-01 6.76000E-02 2.48000E-02 9.12000E-03 3.35000E-03
     1.23500E-03 4.54000E-04 1.67000E-04 6.14000E-05 2.26000E-05
     8.32000E-06 3.06000E-06 1.13000E-06 4.14000E-07 1.52000E-07
  2
    0942390  4.4438238E+22
    0942420  9.7525202E+20
  2  400
    0040090  2.9049430E-01
    0110230  1.1387779E-01
```

Figure 1. SOURCES4D input file.

Snippets of output from the `pdata` file, showing the data needed for first-derivative calculations for all four source-target combinations, are shown in Figure 2.

```
⋮
target nuclide     1       40090
atom frac.    2.9049430E-01 (target)
source nuclide     1      942390
atom density  4.4438238E-02 (source)
lambda        9.1102900E-13 (source)

   (alpha,n) source rate density for this source and target  1.5528134E+05

   j   Z  at.frac.       sum_l {fal*dp_i/dN_j}
   1   4  2.9049430E-01  8.0350674E+17
   2  11  1.1387779E-01  1.7323560E+18
   3  26  4.6804606E-02  3.1387956E+18
   4  28  4.5187900E-02  2.9553863E+18
   5  94  5.0363541E-01  6.2037421E+18
⋮
target nuclide     1       40090
atom frac.    2.9049430E-01 (target)
source nuclide     2      942420
atom density  9.7525202E-04 (source)
lambda        5.8370300E-14 (source)

   (alpha,n) source rate density for this source and target  1.8194529E+02

   j   Z  at.frac.       sum_l {fal*dp_i/dN_j}
   1   4  2.9049430E-01  6.7333453E+17
   2  11  1.1387779E-01  1.4481334E+18
   3  26  4.6804606E-02  2.6230195E+18
   4  28  4.5187900E-02  2.4488835E+18
   5  94  5.0363541E-01  5.1669253E+18
⋮
target nuclide     2      110230
atom frac.    1.1387779E-01 (target)
source nuclide     1      942390
atom density  4.4438238E-02 (source)
lambda        9.1102900E-13 (source)

   (alpha,n) source rate density for this source and target  2.3263716E+03

   j   Z  at.frac.       sum_l {fal*dp_i/dN_j}
   1   4  2.9049430E-01  1.1799111E+16
   2  11  1.1387779E-01  2.5711220E+16
   3  26  4.6804606E-02  4.6559137E+16
   4  28  4.5187900E-02  4.5386314E+16
   5  94  5.0363541E-01  9.3078495E+16
⋮
target nuclide     2      110230
atom frac.    1.1387779E-01 (target)
source nuclide     2      942420
atom density  9.7525202E-04 (source)
lambda        5.8370300E-14 (source)

   (alpha,n) source rate density for this source and target  1.9622264E+00

   j   Z  at.frac.       sum_l {fal*dp_i/dN_j}
   1   4  2.9049430E-01  7.1179464E+15
   2  11  1.1387779E-01  1.5490646E+16
   3  26  4.6804606E-02  2.8011154E+16
   4  28  4.5187900E-02  2.7173995E+16
   5  94  5.0363541E-01  5.5792690E+16
⋮
```

Figure 2. Partial SOURCES4D output file `pdata` showing the first-order data. The entire output file is listed in Appendix A.

The application of Eq. (1) to compute $\partial Q_{(\alpha,n),k,i} / \partial N_j$ for k = 1,2, i = 1,2, and j = 1,…,6 is shown in Table II. It is interesting that ^{239}Pu is almost as important for its stopping power as for its α source, while ^{242}Pu is *more* important for its stopping power. The total derivatives for ^{9}Be and ^{58}Ni are similar to those given in Ref. 3 (in Tables II, III, and V), but the neutron and α energy groups here are different.

Table II. Calculations for $\partial Q_{(\alpha,n),k,i} / \partial N_j$

Source Nuclide	Target Nuclide	Nuclide	Target Nuclide Term	Source Nuclide Term	Stopping Nuclide/Element Term	Total
^{239}Pu	^{9}Be	^{9}Be	5.9281E+06	0	-3.6075E+05	5.5673E+06
		^{23}Na	0	0	-7.7778E+05	-7.7778E+05
		^{239}Pu	0	3.4943E+06	-2.7853E+06	7.0900E+05
		^{242}Pu	0	0	-2.7853E+06	-2.7853E+06
		^{58}Ni	0	0	-1.3269E+06	-1.3269E+06
		^{56}Fe	0	0	-1.4092E+06	-1.4092E+06
^{242}Pu	^{9}Be	^{9}Be	6.9460E+03	0	-4.2508E+02	6.5209E+03
		^{23}Na	0	0	-9.1422E+02	-9.1422E+02
		^{239}Pu	0	0	-3.2619E+03	-3.2619E+03
		^{242}Pu	0	1.8656E+05	-3.2619E+03	1.8330E+05
		^{58}Ni	0	0	-1.5460E+03	-1.5460E+03
		^{56}Fe	0	0	-1.6559E+03	-1.6559E+03
^{239}Pu	^{23}Na	^{9}Be	0	0	-5.2975E+03	-5.2975E+03
		^{23}Na	2.2655E+05	0	-1.1544E+04	2.1501E+05
		^{239}Pu	0	5.2351E+04	-4.1790E+04	1.0561E+04
		^{242}Pu	0	0	-4.1790E+04	-4.1790E+04
		^{58}Ni	0	0	-2.0377E+04	-2.0377E+04
		^{56}Fe	0	0	-2.0904E+04	-2.0904E+04
^{242}Pu	^{23}Na	^{9}Be	0	0	-4.4936E+00	-4.4936E+00
		^{23}Na	1.9109E+02	0	-9.7793E+00	1.8131E+02
		^{239}Pu	0	0	-3.5222E+01	-3.5222E+01
		^{242}Pu	0	2.0120E+03	-3.5222E+01	1.9768E+03
		^{58}Ni	0	0	-1.7155E+01	-1.7155E+01
		^{56}Fe	0	0	-1.7684E+01	-1.7684E+01
Total for Each Nuclide		^{9}Be	5.9350E+06	0	-3.6648E+05	5.5685E+06
		^{23}Na	2.2674E+05	0	-7.9025E+05	-5.6350E+05
		^{239}Pu	0	3.5467E+06	-2.8304E+06	7.1627E+05
		^{242}Pu	0	1.8857E+05	-2.8304E+06	-2.6418E+06
		^{58}Ni	0	0	-1.3488E+06	-1.3488E+06
		^{56}Fe	0	0	-1.4318E+06	-1.4318E+06

The third term in Eq. (1), the stopping term, can be computed on a nuclide or an element basis. If a nuclide basis is used, as shown in Table II, the nuclide atom fractions N_j/N are needed, but these must be provided by the user (except for target nuclides). If an element basis is used, the element atom fractions are given in the `pdata` output file. In both cases, the total material atom density N must be provided by the user.

The application of Eq. (1) to compute $\partial Q_{(\alpha,n),k,i}/\partial N$ for k = 1,2 and i = 1,2 is shown in Table III. Equations (4) and (7) are satisfied to the precision shown in the table. The total derivative for the material is similar to that given in Ref. 3 (in Table VII), but the neutron and α energy groups here are different.

Table III. Calculations for $\partial Q_{(\alpha,n),k,i}/\partial N$

Source Nuclide	Target Nuclide	Target Nuclide Term	Source Nuclide Term	Stopping Nuclide/Element Term	Total
^{239}Pu	^{9}Be	1.7221E+06	1.7221E+06	-1.7221E+06	1.7221E+06
^{242}Pu	^{9}Be	2.0178E+03	2.0178E+03	-2.0178E+03	2.0178E+03
^{239}Pu	^{23}Na	2.5799E+04	2.5799E+04	-2.5799E+04	2.5799E+04
^{242}Pu	^{23}Na	2.1761E+01	2.1761E+01	-2.1761E+01	2.1761E+01
Total		1.7499E+06	1.7499E+06	-1.7499E+06	1.7499E+06

The energy-dependent derivatives $\partial Q^{g}_{(\alpha,n),k,i}/\partial N_j$ are approximated by multiplying the source-target combination values from Table II by the normalized source spectra for each source-target combination from the `tape8` output file [Eq. (8)]. Then the energy-dependent derivative $\partial Q^{g}_{(\alpha,n)}/\partial N_j$ for each nuclide is Eq. (9), the sum of $\partial Q^{g}_{(\alpha,n),k,i}/\partial N_j$ over the source-target combinations. The derivatives $\partial Q^{g}_{(\alpha,n)}/\partial N_j$ are plotted in Figure 3. These derivatives have not been normalized by energy or lethargy bins.

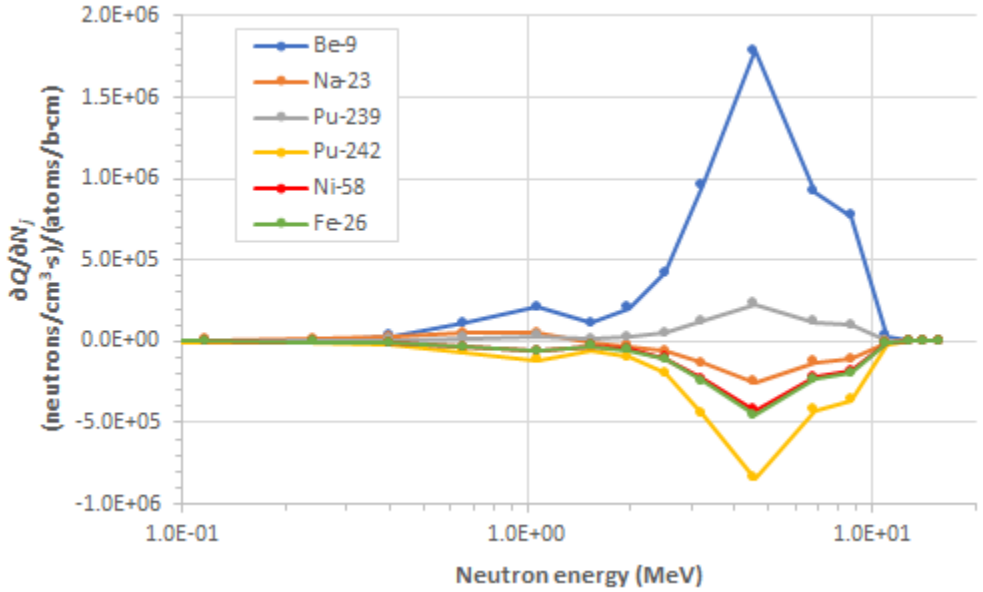

Figure 3. Spectrum of the first derivatives of the (α,n) neutron source rate density with respect to nuclide densities.

More snippets of output from the `pdata` file, showing the data needed for second-derivative calculations for the first source-target combination (^{239}Pu-^{9}Be), are shown in Figure 4.

```
⋮
target nuclide     1       40090
atom frac.    2.9049430E-01 (target)
source nuclide     1      942390
atom density  4.4438238E-02 (source)
lambda        9.1102900E-13 (source)

   (alpha,n) source rate density for this source and target  1.5528134E+05
⋮
  j1  Z1  at.frac.       j2  Z2  at.frac.       sum_l {fal*d^2p_i/dN_j1 dN_j2}
   1   4  2.9049430E-01   1   4  2.9049430E-01  1.6842068E+17
   1   4  2.9049430E-01   2  11  1.1387779E-01  3.6298276E+17
   1   4  2.9049430E-01   3  26  4.6804606E-02  6.5772108E+17
   1   4  2.9049430E-01   4  28  4.5187900E-02  6.1856201E+17
   1   4  2.9049430E-01   5  94  5.0363541E-01  1.2995709E+18
   2  11  1.1387779E-01   1   4  2.9049430E-01  3.6298276E+17
   2  11  1.1387779E-01   2  11  1.1387779E-01  7.8252277E+17
   2  11  1.1387779E-01   3  26  4.6804606E-02  1.4178085E+18
   2  11  1.1387779E-01   4  28  4.5187900E-02  1.3345631E+18
   2  11  1.1387779E-01   5  94  5.0363541E-01  2.8018950E+18
   3  26  4.6804606E-02   1   4  2.9049430E-01  6.5772108E+17
   3  26  4.6804606E-02   2  11  1.1387779E-01  1.4178085E+18
   3  26  4.6804606E-02   3  26  4.6804606E-02  2.5689452E+18
   3  26  4.6804606E-02   4  28  4.5187900E-02  2.4175216E+18
   3  26  4.6804606E-02   5  94  5.0363541E-01  5.0766751E+18
   4  28  4.5187900E-02   1   4  2.9049430E-01  6.1856201E+17
   4  28  4.5187900E-02   2  11  1.1387779E-01  1.3345631E+18
   4  28  4.5187900E-02   3  26  4.6804606E-02  2.4175216E+18
   4  28  4.5187900E-02   4  28  4.5187900E-02  2.2813338E+18
   4  28  4.5187900E-02   5  94  5.0363541E-01  4.7802053E+18
   5  94  5.0363541E-01   1   4  2.9049430E-01  1.2995709E+18
   5  94  5.0363541E-01   2  11  1.1387779E-01  2.8018950E+18
   5  94  5.0363541E-01   3  26  4.6804606E-02  5.0766751E+18
   5  94  5.0363541E-01   4  28  4.5187900E-02  4.7802053E+18
   5  94  5.0363541E-01   5  94  5.0363541E-01  1.0034106E+19
⋮
```

Figure 4. Partial SOURCES4D output file `pdata` showing the second-order data. The entire output file is listed in Appendix A.

The application of Eq. (12) to compute $\partial^2 Q_{(\alpha,n),k,i} \big/ \partial N_j \partial N_{j'}$ for the four source-target combinations ^{239}Pu-^{9}Be, ^{242}Pu-^{9}Be, ^{239}Pu-^{23}Na, and ^{242}Pu-^{23}Na is shown in Table IV, Table V, Table VI, and Table VII., respectively.

Table IV. Calculations for $\partial^2 Q_{(\alpha,n),k,i} / \partial N_j \partial N_{j'}$ for ^{239}Pu-^{9}Be

Nuclide j	Nuclide j'	Term 1	Term 2	Term 3	Term 4	Total
^{9}Be	^{9}Be	0	-2.7544E+07	0	1.6772E+06	-2.5867E+07
	^{23}Na	0	-2.9693E+07	0	3.6147E+06	-2.6078E+07
	^{239}Pu	1.3340E+08	-1.0633E+08	-8.1181E+06	1.2941E+07	3.1890E+07
	^{242}Pu	0	-1.0633E+08	0	1.2941E+07	-9.3392E+07
	^{58}Ni	0	-5.0656E+07	0	6.1598E+06	-4.4496E+07
	^{56}Fe	0	-5.3799E+07	0	6.5497E+06	-4.7250E+07
^{23}Na	^{9}Be	0	-2.9693E+07	0	3.6147E+06	-2.6078E+07
	^{23}Na	0	0	0	7.7925E+06	7.7925E+06
	^{239}Pu	0	0	-1.7503E+07	2.7902E+07	1.0399E+07
	^{242}Pu	0	0	0	2.7902E+07	2.7902E+07
	^{58}Ni	0	0	0	1.3290E+07	1.3290E+07
	^{56}Fe	0	0	0	1.4119E+07	1.4119E+07
^{239}Pu	^{9}Be	1.3340E+08	-1.0633E+08	-8.1181E+06	1.2941E+07	3.1890E+07
	^{23}Na	0	0	-1.7503E+07	2.7902E+07	1.0399E+07
	^{239}Pu	0	0	-1.2536E+08	9.9922E+07	-2.5435E+07
	^{242}Pu	0	0	-6.2678E+07	9.9922E+07	3.7244E+07
	^{58}Ni	0	0	-2.9859E+07	4.7602E+07	1.7743E+07
	^{56}Fe	0	0	-3.1712E+07	5.0555E+07	1.8842E+07
^{242}Pu	^{9}Be	0	-1.0633E+08	0	1.2941E+07	-9.3392E+07
	^{23}Na	0	0	0	2.7902E+07	2.7902E+07
	^{239}Pu	0	0	-6.2678E+07	9.9922E+07	3.7244E+07
	^{242}Pu	0	0	0	9.9922E+07	9.9922E+07
	^{58}Ni	0	0	0	4.7602E+07	4.7602E+07
	^{56}Fe	0	0	0	5.0555E+07	5.0555E+07
^{58}Ni	^{9}Be	0	-5.0656E+07	0	6.1598E+06	-4.4496E+07
	^{23}Na	0	0	0	1.3290E+07	1.3290E+07
	^{239}Pu	0	0	-2.9859E+07	4.7602E+07	1.7743E+07
	^{242}Pu	0	0	0	4.7602E+07	4.7602E+07
	^{58}Ni	0	0	0	2.2718E+07	2.2718E+07
	^{56}Fe	0	0	0	2.4074E+07	2.4074E+07
^{56}Fe	^{9}Be	0	-5.3799E+07	0	6.5497E+06	-4.7250E+07
	^{23}Na	0	0	0	1.4119E+07	1.4119E+07
	^{239}Pu	0	0	-3.1712E+07	5.0555E+07	1.8842E+07
	^{242}Pu	0	0	0	5.0555E+07	5.0555E+07
	^{58}Ni	0	0	0	2.4074E+07	2.4074E+07
	^{56}Fe	0	0	0	2.5582E+07	2.5582E+07

Table V. Calculations for $\partial^2 Q_{(\alpha,n),k,i} \big/ \partial N_j \partial N_{j'}$ for ^{242}Pu-^{9}Be

Nuclide j	Nuclide j'	Term 1	Term 2	Term 3	Term 4	Total
^{9}Be	^{9}Be	0	-3.2456E+04	0	1.9872E+03	-3.0469E+04
	^{23}Na	0	-3.4901E+04	0	4.2724E+03	-3.0629E+04
	^{239}Pu	0	-1.2453E+05	0	1.5241E+04	-1.0929E+05
	^{242}Pu	7.1223E+06	-1.2453E+05	-4.3587E+05	1.5241E+04	6.5771E+06
	^{58}Ni	0	-5.9020E+04	0	7.2174E+03	-5.1803E+04
	^{56}Fe	0	-6.3217E+04	0	7.7393E+03	-5.5478E+04
^{23}Na	^{9}Be	0	-3.4901E+04	0	4.2724E+03	-3.0629E+04
	^{23}Na	0	0	0	9.1881E+03	9.1881E+03
	^{239}Pu	0	0	0	3.2780E+04	3.2780E+04
	^{242}Pu	0	0	-9.3741E+05	3.2780E+04	-9.0464E+05
	^{58}Ni	0	0	0	1.5534E+04	1.5534E+04
	^{56}Fe	0	0	0	1.6642E+04	1.6642E+04
^{239}Pu	^{9}Be	0	-1.2453E+05	0	1.5241E+04	-1.0929E+05
	^{23}Na	0	0	0	3.2780E+04	3.2780E+04
	^{239}Pu	0	0	0	1.1696E+05	1.1696E+05
	^{242}Pu	0	0	-3.3447E+06	1.1696E+05	-3.2277E+06
	^{58}Ni	0	0	0	5.5434E+04	5.5434E+04
	^{56}Fe	0	0	0	5.9374E+04	5.9374E+04
^{242}Pu	^{9}Be	7.1223E+06	-1.2453E+05	-4.3587E+05	1.5241E+04	6.5771E+06
	^{23}Na	0	0	-9.3741E+05	3.2780E+04	-9.0464E+05
	^{239}Pu	0	0	-3.3447E+06	1.1696E+05	-3.2277E+06
	^{242}Pu	0	0	-6.6894E+06	1.1696E+05	-6.5724E+06
	^{58}Ni	0	0	-1.5852E+06	5.5434E+04	-1.5298E+06
	^{56}Fe	0	0	-1.6979E+06	5.9374E+04	-1.6386E+06
^{58}Ni	^{9}Be	0	-5.9020E+04	0	7.2174E+03	-5.1803E+04
	^{23}Na	0	0	0	1.5534E+04	1.5534E+04
	^{239}Pu	0	0	0	5.5434E+04	5.5434E+04
	^{242}Pu	0	0	-1.5852E+06	5.5434E+04	-1.5298E+06
	^{58}Ni	0	0	0	2.6326E+04	2.6326E+04
	^{56}Fe	0	0	0	2.8130E+04	2.8130E+04
^{56}Fe	^{9}Be	0	-6.3217E+04	0	7.7393E+03	-5.5478E+04
	^{23}Na	0	0	0	1.6642E+04	1.6642E+04
	^{239}Pu	0	0	0	5.9374E+04	5.9374E+04
	^{242}Pu	0	0	-1.6979E+06	5.9374E+04	-1.6386E+06
	^{58}Ni	0	0	0	2.8130E+04	2.8130E+04
	^{56}Fe	0	0	0	3.0145E+04	3.0145E+04

Table VI. Calculations for $\partial^2 Q_{(\alpha,n),k,i} \big/ \partial N_j \partial N_{j'}$ for ^{239}Pu-^{23}Na

Nuclide j	Nuclide j'	Term 1	Term 2	Term 3	Term 4	Total
^{9}Be	^{9}Be	0	0	0	2.4128E+04	2.4128E+04
	^{23}Na	0	-5.1590E+05	0	5.2577E+04	-4.6332E+05
	^{239}Pu	0	0	-1.1921E+05	1.9032E+05	7.1110E+04
	^{242}Pu	0	0	0	1.9032E+05	1.9032E+05
	^{58}Ni	0	0	0	9.2801E+04	9.2801E+04
	^{56}Fe	0	0	0	9.5206E+04	9.5206E+04
^{23}Na	^{9}Be	0	-5.1590E+05	0	5.2577E+04	-4.6332E+05
	^{23}Na	0	-2.2484E+06	0	1.1457E+05	-2.1338E+06
	^{239}Pu	5.0982E+06	-4.0697E+06	-2.5977E+05	4.1472E+05	1.1834E+06
	^{242}Pu	0	-4.0697E+06	0	4.1472E+05	-3.6550E+06
	^{58}Ni	0	-1.9844E+06	0	2.0222E+05	-1.7822E+06
	^{56}Fe	0	-2.0357E+06	0	2.0746E+05	-1.8283E+06
^{239}Pu	^{9}Be	0	0	-1.1921E+05	1.9032E+05	7.1110E+04
	^{23}Na	5.0982E+06	-4.0697E+06	-2.5977E+05	4.1472E+05	1.1834E+06
	^{239}Pu	0	0	-1.8808E+06	1.5014E+06	-3.7942E+05
	^{242}Pu	0	0	-9.4040E+05	1.5014E+06	5.6098E+05
	^{58}Ni	0	0	-4.5855E+05	7.3210E+05	2.7354E+05
	^{56}Fe	0	0	-4.7040E+05	7.5101E+05	2.8060E+05
^{242}Pu	^{9}Be	0	0	0	1.9032E+05	1.9032E+05
	^{23}Na	0	-4.0697E+06	0	4.1472E+05	-3.6550E+06
	^{239}Pu	0	0	-9.4040E+05	1.5014E+06	5.6098E+05
	^{242}Pu	0	0	0	1.5014E+06	1.5014E+06
	^{58}Ni	0	0	0	7.3210E+05	7.3210E+05
	^{56}Fe	0	0	0	7.5101E+05	7.5101E+05
^{58}Ni	^{9}Be	0	0	0	9.2801E+04	9.2801E+04
	^{23}Na	0	-1.9844E+06	0	2.0222E+05	-1.7822E+06
	^{239}Pu	0	0	-4.5855E+05	7.3210E+05	2.7354E+05
	^{242}Pu	0	0	0	7.3210E+05	7.3210E+05
	^{58}Ni	0	0	0	3.5698E+05	3.5698E+05
	^{56}Fe	0	0	0	3.6620E+05	3.6620E+05
^{56}Fe	^{9}Be	0	0	0	9.5206E+04	9.5206E+04
	^{23}Na	0	-2.0357E+06	0	2.0746E+05	-1.8283E+06
	^{239}Pu	0	0	-4.7040E+05	7.5101E+05	2.8060E+05
	^{242}Pu	0	0	0	7.5101E+05	7.5101E+05
	^{58}Ni	0	0	0	3.6620E+05	3.6620E+05
	^{56}Fe	0	0	0	3.7567E+05	3.7567E+05

Table VII. Calculations for $\partial^2 Q_{(\alpha,n),k,i} \big/ \partial N_j \partial N_{j'}$ for ^{242}Pu-^{23}Na

Nuclide j	Nuclide j'	Term 1	Term 2	Term 3	Term 4	Total
^{9}Be	^{9}Be	0	0	0	2.0582E+01	2.0582E+01
	^{23}Na	0	-4.3761E+02	0	4.4792E+01	-3.9282E+02
	^{239}Pu	0	0	0	1.6132E+02	1.6132E+02
	^{242}Pu	0	0	-4.6076E+03	1.6132E+02	-4.4463E+03
	^{58}Ni	0	0	0	7.8570E+01	7.8570E+01
	^{56}Fe	0	0	0	8.0996E+01	8.0996E+01
^{23}Na	^{9}Be	0	-4.3761E+02	0	4.4792E+01	-3.9282E+02
	^{23}Na	0	-1.9047E+03	0	9.7480E+01	-1.8072E+03
	^{239}Pu	0	-3.4301E+03	0	3.5108E+02	-3.0790E+03
	^{242}Pu	1.9594E+05	-3.4301E+03	-1.0028E+04	3.5108E+02	1.8283E+05
	^{58}Ni	0	-1.6707E+03	0	1.7099E+02	-1.4997E+03
	^{56}Fe	0	-1.7221E+03	0	1.7627E+02	-1.5459E+03
^{239}Pu	^{9}Be	0	0	0	1.6132E+02	1.6132E+02
	^{23}Na	0	-3.4301E+03	0	3.5108E+02	-3.0790E+03
	^{239}Pu	0	0	0	1.2645E+03	1.2645E+03
	^{242}Pu	0	0	-3.6116E+04	1.2645E+03	-3.4852E+04
	^{58}Ni	0	0	0	6.1588E+02	6.1588E+02
	^{56}Fe	0	0	0	6.3485E+02	6.3485E+02
^{242}Pu	^{9}Be	0	0	-4.6076E+03	1.6132E+02	-4.4463E+03
	^{23}Na	1.9594E+05	-3.4301E+03	-1.0028E+04	3.5108E+02	1.8283E+05
	^{239}Pu	0	0	-3.6116E+04	1.2645E+03	-3.4852E+04
	^{242}Pu	0	0	-7.2232E+04	1.2645E+03	-7.0968E+04
	^{58}Ni	0	0	-1.7590E+04	6.1588E+02	-1.6975E+04
	^{56}Fe	0	0	-1.8132E+04	6.3485E+02	-1.7498E+04
^{58}Ni	^{9}Be	0	0	0	7.8570E+01	7.8570E+01
	^{23}Na	0	-1.6707E+03	0	1.7099E+02	-1.4997E+03
	^{239}Pu	0	0	0	6.1588E+02	6.1588E+02
	^{242}Pu	0	0	-1.7590E+04	6.1588E+02	-1.6975E+04
	^{58}Ni	0	0	0	2.9997E+02	2.9997E+02
	^{56}Fe	0	0	0	3.0920E+02	3.0920E+02
^{56}Fe	^{9}Be	0	0	0	8.0996E+01	8.0996E+01
	^{23}Na	0	-1.7221E+03	0	1.7627E+02	-1.5459E+03
	^{239}Pu	0	0	0	6.3485E+02	6.3485E+02
	^{242}Pu	0	0	-1.8132E+04	6.3485E+02	-1.7498E+04
	^{58}Ni	0	0	0	3.0920E+02	3.0920E+02
	^{56}Fe	0	0	0	3.1874E+02	3.1874E+02

The application of Eq. (12) to compute $\partial^2 Q_{(\alpha,n),k,i} \big/ \partial N^2$ for the four source-target combinations is shown in Table VIII. Equation (18) is satisfied to the precision shown in the first five rows of the table. However, there are actually very small differences, as shown in the sixth and seventh third rows. Equation (15) does not appear to be satisfied—i.e., the total is not zero. However, the total is a very small fraction of the individual terms.

Table VIII. Calculations for $\partial^2 Q_{(\alpha,n),k,i} / \partial N^2$.

Source Nuclide	Target Nuclide	Term 1	Term 2	Term 3	Term 4	Total
^{239}Pu	^{9}Be	3.8195E+07	-3.8195E+07	-3.8195E+07	3.8195E+07	-2.4014E+00
^{242}Pu	^{9}Be	4.4754E+04	-4.4754E+04	-4.4754E+04	4.4754E+04	-8.8628E-05
^{239}Pu	^{23}Na	5.7223E+05	-5.7223E+05	-5.7223E+05	5.7223E+05	2.1241E-02
^{242}Pu	^{23}Na	4.8266E+02	-4.8266E+02	-4.8266E+02	4.8266E+02	-3.6450E-06
Total		3.8813E+07	-3.8813E+07	-3.8813E+07	3.8813E+07	-2.3803E+00
Absolute Difference from $2Q_{(\alpha,n),k,i} / N^2$		0.0000E+00	-9.2846E-01	-9.2846E-01	-5.2336E-01	-2.3803E+00
Relative Difference from $2Q_{(\alpha,n),k,i} / N^2$		0.000000%	0.000002%	0.000002%	-0.000001%	N/A

The energy-dependent derivatives $\partial^2 Q^g_{(\alpha,n),k,i} / \partial N_j \partial N_{j'}$ are approximated by multiplying the source-target combination values from Table IV through Table VII by the normalized source spectra for each source-target combination from the `tape8` output file [Eq. (19)]. Then the energy-dependent derivative $\partial^2 Q^g_{(\alpha,n)} / \partial N_j \partial N_{j'}$ for each nuclide is Eq. (20), the sum of $\partial^2 Q^g_{(\alpha,n),k,i} / \partial N_j \partial N_{j'}$ over the source-target combinations. The derivatives $\partial^2 Q^g_{(\alpha,n)} / \partial N_j^2$ are plotted in Figure 5. These derivatives have not been normalized by energy or lethargy bins.

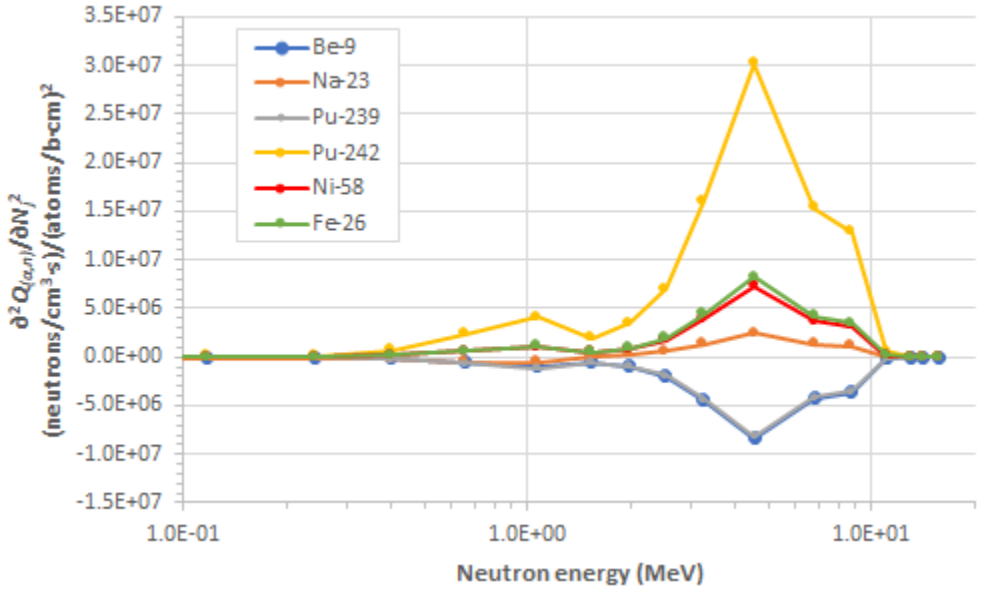

Figure 5. Spectrum of the pure second derivatives of the (α,n) neutron source rate density with respect to nuclide densities.

IX. Summary and Conclusions

SOURCES4D is an update to SOURCES4C that adds sensitivity analysis capabilities to homogeneous-material problems. The code prints out data that can be used in post-processing to compute first and second derivatives of the (α,n) source rate density and spectrum with respect to nuclide densities. The user needs to supply the total atom density of the material, which is not available to SOURCES4D.

The capability to compute first derivatives of the (α,n) source rate density and spectrum with respect to nuclide stopping powers and (α,n) cross sections (nuclear data) is also available in SOURCES4D.

SOURCES4D retains the archaic FORTRAN programming of its predecessor. An outstanding issue with SOURCES4D, inherited from its predecessor, is that the output normalized (α,n) neutron source spectra often do not sum strictly to unity.

The LASTCALL tool for writing SOURCES inputs, described in Ref. 1, is no longer available.

Acknowledgment

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XTD-RTA File

Appendix A
Output File PDATA for Example Problem

This is the `pdata` output file that SOURCES4D writes given the input file listed in Figure 1 in the main text.

```
SOURCES 4D Calculation
<<<<<<<<<<<>>>>>>>>>>>



Title: M&C 2019 test problem material
Homogeneous problem input (idd = 1)


number of stopping elems:     5
number of sources input:      2
number of targets input:      2
in this file, i is targets, j is stopping elements, k is sources, l is alpha levels

target nuclide     1       40090
atom frac.    2.9049430E-01 (target)
source nuclide     1      942390
atom density  4.4438238E-02 (source)
lambda        9.1102900E-13 (source)

   (alpha,n) source rate density for this source and target  1.5528134E+05

   j   Z  at.frac.       sum_l {fal*dp_i/dN_j}
   1   4  2.9049430E-01  8.0350674E+17
   2  11  1.1387779E-01  1.7323560E+18
   3  26  4.6804606E-02  3.1387956E+18
   4  28  4.5187900E-02  2.9553863E+18
   5  94  5.0363541E-01  6.2037421E+18

  j1  Z1  at.frac.       j2  Z2  at.frac.       sum_l {fal*d^2p_i/dN_j1 dN_j2}
   1   4  2.9049430E-01   1   4  2.9049430E-01  1.6842068E+17
   1   4  2.9049430E-01   2  11  1.1387779E-01  3.6298276E+17
   1   4  2.9049430E-01   3  26  4.6804606E-02  6.5772108E+17
   1   4  2.9049430E-01   4  28  4.5187900E-02  6.1856201E+17
   1   4  2.9049430E-01   5  94  5.0363541E-01  1.2995709E+18
   2  11  1.1387779E-01   1   4  2.9049430E-01  3.6298276E+17
   2  11  1.1387779E-01   2  11  1.1387779E-01  7.8252277E+17
   2  11  1.1387779E-01   3  26  4.6804606E-02  1.4178085E+18
   2  11  1.1387779E-01   4  28  4.5187900E-02  1.3345631E+18
   2  11  1.1387779E-01   5  94  5.0363541E-01  2.8018950E+18
   3  26  4.6804606E-02   1   4  2.9049430E-01  6.5772108E+17
   3  26  4.6804606E-02   2  11  1.1387779E-01  1.4178085E+18
   3  26  4.6804606E-02   3  26  4.6804606E-02  2.5689452E+18
   3  26  4.6804606E-02   4  28  4.5187900E-02  2.4175216E+18
   3  26  4.6804606E-02   5  94  5.0363541E-01  5.0766751E+18
   4  28  4.5187900E-02   1   4  2.9049430E-01  6.1856201E+17
   4  28  4.5187900E-02   2  11  1.1387779E-01  1.3345631E+18
   4  28  4.5187900E-02   3  26  4.6804606E-02  2.4175216E+18
   4  28  4.5187900E-02   4  28  4.5187900E-02  2.2813338E+18
   4  28  4.5187900E-02   5  94  5.0363541E-01  4.7802053E+18
   5  94  5.0363541E-01   1   4  2.9049430E-01  1.2995709E+18
   5  94  5.0363541E-01   2  11  1.1387779E-01  2.8018950E+18
   5  94  5.0363541E-01   3  26  4.6804606E-02  5.0766751E+18
   5  94  5.0363541E-01   4  28  4.5187900E-02  4.7802053E+18
   5  94  5.0363541E-01   5  94  5.0363541E-01  1.0034106E+19

target nuclide     1       40090
atom frac.    2.9049430E-01 (target)
source nuclide     2      942420
atom density  9.7525202E-04 (source)
lambda        5.8370300E-14 (source)

   (alpha,n) source rate density for this source and target  1.8194529E+02
```

j	Z	at.frac.	sum_l {fal*dp_i/dN_j}
1	4	2.9049430E-01	6.7333453E+17
2	11	1.1387779E-01	1.4481334E+18
3	26	4.6804606E-02	2.6230195E+18
4	28	4.5187900E-02	2.4488835E+18
5	94	5.0363541E-01	5.1669253E+18

j1	Z1	at.frac.	j2	Z2	at.frac.	sum_l {fal*d^2p_i/dN_j1 dN_j2}
1	4	2.9049430E-01	1	4	2.9049430E-01	1.4191915E+17
1	4	2.9049430E-01	2	11	1.1387779E-01	3.0511816E+17
1	4	2.9049430E-01	3	26	4.6804606E-02	5.5271489E+17
1	4	2.9049430E-01	4	28	4.5187900E-02	5.1544262E+17
1	4	2.9049430E-01	5	94	5.0363541E-01	1.0884864E+18
2	11	1.1387779E-01	1	4	2.9049430E-01	3.0511816E+17
2	11	1.1387779E-01	2	11	1.1387779E-01	6.5617901E+17
2	11	1.1387779E-01	3	26	4.6804606E-02	1.1885338E+18
2	11	1.1387779E-01	4	28	4.5187900E-02	1.1094100E+18
2	11	1.1387779E-01	5	94	5.0363541E-01	2.3410056E+18
3	26	4.6804606E-02	1	4	2.9049430E-01	5.5271489E+17
3	26	4.6804606E-02	2	11	1.1387779E-01	1.1885338E+18
3	26	4.6804606E-02	3	26	4.6804606E-02	2.1528829E+18
3	26	4.6804606E-02	4	28	4.5187900E-02	2.0089377E+18
3	26	4.6804606E-02	5	94	5.0363541E-01	4.2403032E+18
4	28	4.5187900E-02	1	4	2.9049430E-01	5.1544262E+17
4	28	4.5187900E-02	2	11	1.1387779E-01	1.1094100E+18
4	28	4.5187900E-02	3	26	4.6804606E-02	2.0089377E+18
4	28	4.5187900E-02	4	28	4.5187900E-02	1.8801037E+18
4	28	4.5187900E-02	5	94	5.0363541E-01	3.9588711E+18
5	94	5.0363541E-01	1	4	2.9049430E-01	1.0884864E+18
5	94	5.0363541E-01	2	11	1.1387779E-01	2.3410056E+18
5	94	5.0363541E-01	3	26	4.6804606E-02	4.2403032E+18
5	94	5.0363541E-01	4	28	4.5187900E-02	3.9588711E+18
5	94	5.0363541E-01	5	94	5.0363541E-01	8.3528258E+18

target nuclide 2 110230
atom frac. 1.1387779E-01 (target)
source nuclide 1 942390
atom density 4.4438238E-02 (source)
lambda 9.1102900E-13 (source)

(alpha,n) source rate density for this source and target 2.3263716E+03

j	Z	at.frac.	sum_l {fal*dp_i/dN_j}
1	4	2.9049430E-01	1.1799111E+16
2	11	1.1387779E-01	2.5711220E+16
3	26	4.6804606E-02	4.6559137E+16
4	28	4.5187900E-02	4.5386314E+16
5	94	5.0363541E-01	9.3078495E+16

j1	Z1	at.frac.	j2	Z2	at.frac.	sum_l {fal*d^2p_i/dN_j1 dN_j2}
1	4	2.9049430E-01	1	4	2.9049430E-01	2.4229612E+15
1	4	2.9049430E-01	2	11	1.1387779E-01	5.2797150E+15
1	4	2.9049430E-01	3	26	4.6804606E-02	9.5605724E+15
1	4	2.9049430E-01	4	28	4.5187900E-02	9.3190026E+15
1	4	2.9049430E-01	5	94	5.0363541E-01	1.9111895E+16
2	11	1.1387779E-01	1	4	2.9049430E-01	5.2797150E+15
2	11	1.1387779E-01	2	11	1.1387779E-01	1.1504741E+16
2	11	1.1387779E-01	3	26	4.6804606E-02	2.0833029E+16
2	11	1.1387779E-01	4	28	4.5187900E-02	2.0307038E+16
2	11	1.1387779E-01	5	94	5.0363541E-01	4.1646484E+16
3	26	4.6804606E-02	1	4	2.9049430E-01	9.5605724E+15
3	26	4.6804606E-02	2	11	1.1387779E-01	2.0833029E+16
3	26	4.6804606E-02	3	26	4.6804606E-02	3.7725071E+16
3	26	4.6804606E-02	4	28	4.5187900E-02	3.6773259E+16
3	26	4.6804606E-02	5	94	5.0363541E-01	7.5415690E+16
4	28	4.5187900E-02	1	4	2.9049430E-01	9.3190026E+15
4	28	4.5187900E-02	2	11	1.1387779E-01	2.0307038E+16
4	28	4.5187900E-02	3	26	4.6804606E-02	3.6773259E+16
4	28	4.5187900E-02	4	28	4.5187900E-02	3.5848073E+16
4	28	4.5187900E-02	5	94	5.0363541E-01	7.3516712E+16
5	94	5.0363541E-01	1	4	2.9049430E-01	1.9111895E+16

```
   5  94  5.0363541E-01   2  11  1.1387779E-01  4.1646484E+16
   5  94  5.0363541E-01   3  26  4.6804606E-02  7.5415690E+16
   5  94  5.0363541E-01   4  28  4.5187900E-02  7.3516712E+16
   5  94  5.0363541E-01   5  94  5.0363541E-01  1.5076804E+17

target nuclide     2      110230
atom frac.    1.1387779E-01 (target)
source nuclide     2      942420
atom density  9.7525202E-04 (source)
lambda        5.8370300E-14 (source)

   (alpha,n) source rate density for this source and target  1.9622264E+00

   j   Z  at.frac.       sum_l {fal*dp_i/dN_j}
   1   4  2.9049430E-01  7.1179464E+15
   2  11  1.1387779E-01  1.5490646E+16
   3  26  4.6804606E-02  2.8011154E+16
   4  28  4.5187900E-02  2.7173995E+16
   5  94  5.0363541E-01  5.5792690E+16

  j1  Z1  at.frac.       j2  Z2  at.frac.       sum_l {fal*d^2p_i/dN_j1 dN_j2}
   1   4  2.9049430E-01   1   4  2.9049430E-01  1.4699274E+15
   1   4  2.9049430E-01   2  11  1.1387779E-01  3.1989200E+15
   1   4  2.9049430E-01   3  26  4.6804606E-02  5.7844146E+15
   1   4  2.9049430E-01   4  28  4.5187900E-02  5.6111938E+15
   1   4  2.9049430E-01   5  94  5.0363541E-01  1.1520952E+16
   2  11  1.1387779E-01   1   4  2.9049430E-01  3.1989200E+15
   2  11  1.1387779E-01   2  11  1.1387779E-01  6.9616615E+15
   2  11  1.1387779E-01   3  26  4.6804606E-02  1.2588396E+16
   2  11  1.1387779E-01   4  28  4.5187900E-02  1.2211630E+16
   2  11  1.1387779E-01   5  94  5.0363541E-01  2.5072873E+16
   3  26  4.6804606E-02   1   4  2.9049430E-01  5.7844146E+15
   3  26  4.6804606E-02   2  11  1.1387779E-01  1.2588396E+16
   3  26  4.6804606E-02   3  26  4.6804606E-02  2.2762975E+16
   3  26  4.6804606E-02   4  28  4.5187900E-02  2.2081956E+16
   3  26  4.6804606E-02   5  94  5.0363541E-01  4.5338405E+16
   4  28  4.5187900E-02   1   4  2.9049430E-01  5.6111938E+15
   4  28  4.5187900E-02   2  11  1.1387779E-01  1.2211630E+16
   4  28  4.5187900E-02   3  26  4.6804606E-02  2.2081956E+16
   4  28  4.5187900E-02   4  28  4.5187900E-02  2.1422630E+16
   4  28  4.5187900E-02   5  94  5.0363541E-01  4.3983723E+16
   5  94  5.0363541E-01   1   4  2.9049430E-01  1.1520952E+16
   5  94  5.0363541E-01   2  11  1.1387779E-01  2.5072873E+16
   5  94  5.0363541E-01   3  26  4.6804606E-02  4.5338405E+16
   5  94  5.0363541E-01   4  28  4.5187900E-02  4.3983723E+16
   5  94  5.0363541E-01   5  94  5.0363541E-01  9.0305599E+16

(alpha,n) targets and sources
number of targets, sources     2     2
target nuclide     1       40090
target nuclide     2      110230
source nuclide     1      942390
source nuclide     2      942420
```