OAK RIDGE National Laboratory

ORIGEN Sensitivity



U.S. DEPARTMENT OF ENERGY

Learning goals



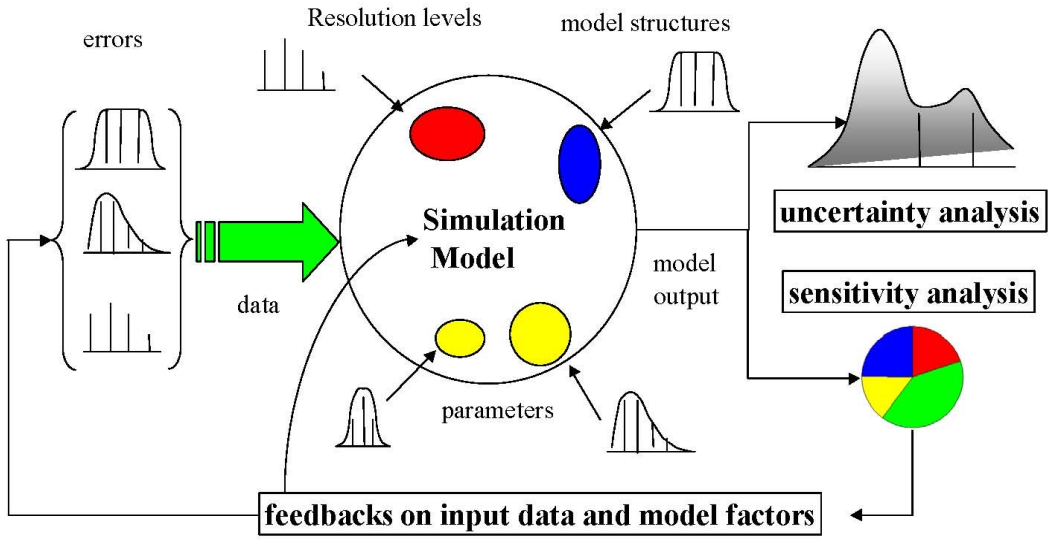
Introduce users to the new sensitivity feature in ORIGEN, enabling exploration of the impact of nuclear data changes on responses of interest.



Demonstrate through simple exercises the power of this feature in supporting a deeper understanding of the underlying physics.

Motivation for sensitivity analysis

- Sensitivity analysis provides a unique perspective on system performance by quantifying how the predicted response of the system changes when input data are modified.
- It helps identify the important decay and reaction processes in depletion, those that have the most substantial impact on reactor performance for each change in input.
- In the context of depletion SA, the general response involves an integration of both the neutron and nuclide fields

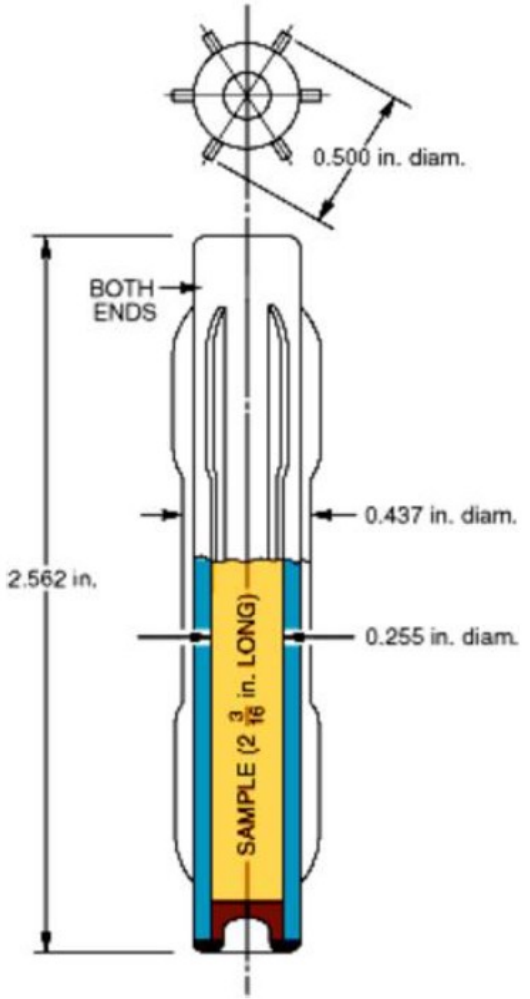


Ref: Wikipedia " sensitivity analysis"

Sensitivity capabilities in ORIGEN can answer these types of questions

1. Ra-226 is used as a target material to produce medical isotopes in HFIR (e.g., Ac-225/Bi-213 for treating leukemia). What is the sensitivity of Ra-226 after 9-day irradiation of 1 mg of Ra-226? What are the primary contributors to the build-up of certain products?

Irradiation capsule ("rabbit") in ORNL's High Flux Isotope Reactor (HFIR)

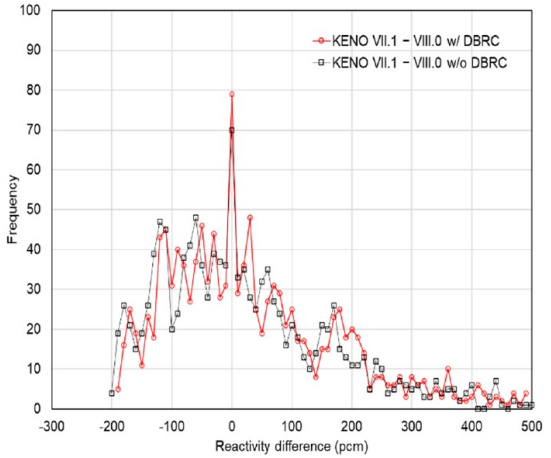


Ref) ORNL HFIR "HFIR user guide" ORNL (2015)

Sensitivity capabilities in ORIGEN can answer these questions (contd.)

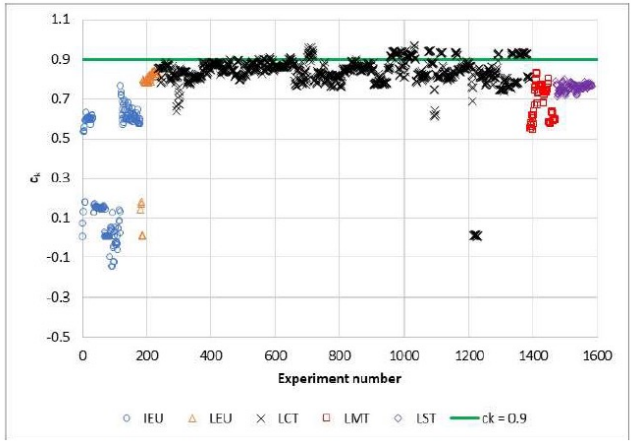
2. I have an ORIGEN depletion calculation based on ENDF/B-VII.1 nuclear data. What is the effect of the introduction of the new ENDF/VIII.0 data (released in February 2018)?

Comparison between ENDF/VII.1 and VIII.0
(Effect of nuclear data on reactivity difference for extensive PWR pin benchmark problems)



Ref) K.S Kim and W. A. Wieselquist, "Neutronic Characteristics of ENDF/B-VIII.0 Compared to ENDF/B-VII.1 for Light-Water Reactor Analysis", J. Nucl. Eng. 2021, 2(4), 318-335

3. I have two systems and want to predict the degree of similarity between them. How could I quantify this similarity?

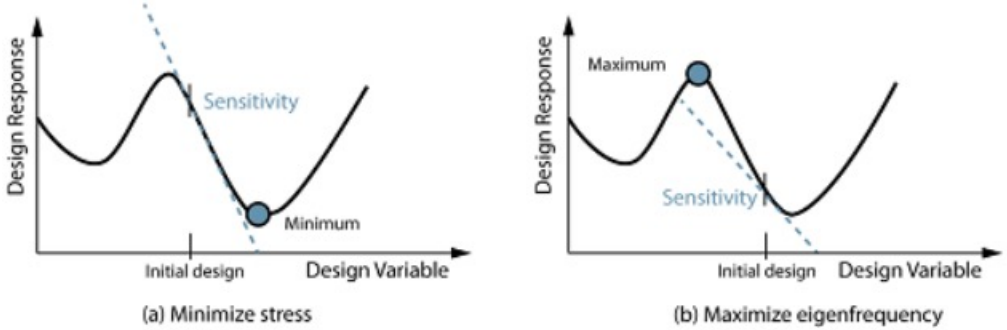


Similarity index of various transportation packages

Ref) ORNL/TM-2020/1725

Sensitivity capabilities in ORIGEN can answer these questions (contd.)

4. I found discrepancies between the measured and calculated concentrations of gadolinium, which resulted in a violation of pin peaking factor design criteria. How do I alter nuclide data or experimental values to maximize the overall consistency?



Design study using Sensitivity Coefficient

Ref: Abaqus 2022 User Manual (2022)

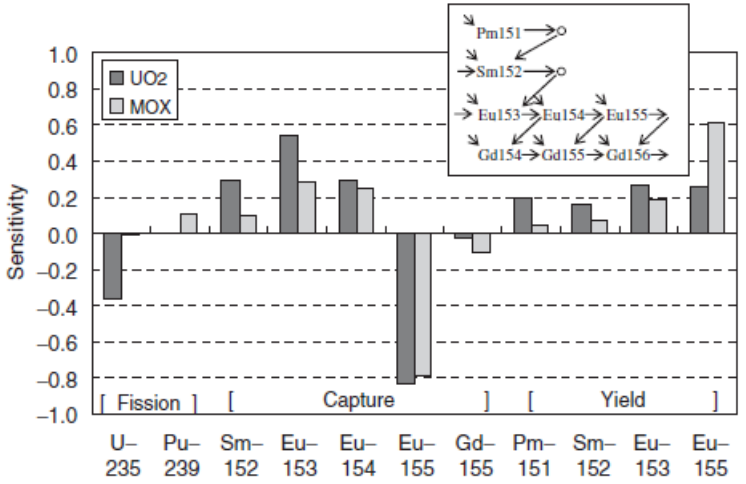


Fig. 10 Sensitivities of the Gd-155 concentration

Ref: Go Chiva et. Al., "Sensitivity analysis of fission product concentrations for light water reactor burned fuel," *J. Nucl. Sci. Technol.*, vol. 47, no. 7,pp. 652–660 (2010)

Sensitivity coefficient: relevant definitions

- Definition of response *R*

$$R = \int_0^{t_i} dt\, R(\sigma, N, \varphi_i, \varphi_i^*)$$

- Definition of sensitivity coefficient *S* for a change in input parameter α

$$R(\alpha) = R(\alpha_0) + \left.\frac{\partial R}{\partial \alpha}\right|_{\alpha_0} (\alpha - \alpha_0) + \cdots,$$

$$S \equiv \left.\frac{\partial R}{\partial \alpha}\right|_{\alpha_0} \cdot \frac{\alpha_0}{R(\alpha_0)}$$

- Sensitivity coefficient can be mathematically obtained using depletion perturbation theory (DPT) as :

$$S = \frac{\alpha}{R} \int_0^{t_i} dt N^*(t) \cdot \alpha_i \frac{\partial A}{\partial \alpha_i} \cdot N\,(t)$$

Sensitivity capabilities in ORIGEN

- ORIGEN calculates sensitivities for the following parametric changes:
  - each decay or transition channel,
  - fission yield
  - total production/loss rate

$$\frac{dN_i}{dt} = \sum_{j=1}^{m} l_{ij}\lambda_j N_j + \bar{\Phi}\sum_{k=1}^{m} f_{ik}\sigma_k N_k - (\lambda_i + \bar{\Phi}\sigma_i + r_i)N_i + F_i \quad (i = 1, \ldots m)$$

- To calculate the sensitivity coefficients, an essential requirement is the adjoint solution ($N^*(\mathrm{t})$) and its integration with the forward ($N(\mathrm{t})$) solution over time → The CRAM solver is equipped to obtain the adjoint solution!
- In SCALE 6.3, ORIGEN sensitivity supports only the nuclide concentration response

See **Section 5.1.3** of the SCALE manual for details.

Input Component: **sens**

```
=origen
case(ID){
…
}
sens{
    case = ID
    response{
        iso=[pu238=1.0 u238=1.0]
        type=NUCLIDE
        step=2
    }
    threshold = 1e-2
    dp_verify{
        nrank = 3
        nrank_pert=1.001
    }
}
end
```

See **Section 5.1.5.2.13** of the 6.3 SCALE manual for details

- **case** load from the previous case (ID) for the sensitivity calculations
- **response**
  - *iso* array: list of id=multiplier
  - *Type* : response type
    - NUCLIDE : Nuclide concentration
  - *step* : Timestep index
- **threshold** for sensitivity coefficients
- **dp_verify** direct perturbation (DP)
  - *nrank* : to limit the number of DP calculation (descending order)
  - *nrank_pert* : relative perturbed amount for DP calculation

Output file – Summary

- Summary in output (.out) file

```
552 ------------------------------------------------------------------------------
553 Sensitivity Calculation Summary (#1/1)
554 ------------------------------------------------------------------------------
555
556 Forward calculation case                              = A
557 Target step (from case)                               = 22
558 Corresponding target time (seconds)                   = 86400000.000000
559 Sensitivity coefficient report threshold              = 0.001000
560 Response type                                         = nuclide
561 Number of direct perturbation checks per group       = 3
562 Direct perturbation factor (multiplier)              = 1.001000
563 Adjoint concentration file                           = origen-sens-xe.sens1-adj.f71
564
```

Output file – Sensitivity coefficients

```
552 ------------------------------------------------------------------------------
553 Sensitivity Calculation Summary (#1/1)
554 ------------------------------------------------------------------------------
555
556 Forward calculation case                          = A
557 Target step (from case)                          = 22
558 Corresponding target time (seconds)              = 86400000.000000
559 Sensitivity coefficient report threshold         = 0.001000
560 Response type                                    = nuclide
561 Number of direct perturbation checks per group   = 3
562 Direct perturbation factor (multiplier)          = 1.001000
563 Adjoint concentration file                       = origen-sens-xe.sens1-adj.f71
564
```

Sensitivity coefficient: the relative change in response per change in a parameter α

$$S \equiv \left.\frac{\partial R}{\partial \alpha}\right|_{\alpha_0} \cdot \frac{\alpha_0}{R(\alpha_0)}$$

1. **Total decay loss** sensitivity: α = change in a nuclide's total decay constant.
2. **Decay channel** sensitivity: α = change in specific decay channels (e.g., a-decay).
3. **Decay yield** sensitivity: α = change in a decay yield; for example, the fraction of γ-decays that result in the ground state daughter versus a metastable daughter.
4. **Total reaction loss** sensitivity: α = change in a nuclide's total loss cross section.
5. **Reaction channel** sensitivity: α = change in specific reaction channels (e.g. (n,γ)).
6. **Reaction yield** sensitivity: α = change in a reaction yield (e.g., fission product yields).

Forward and adjoint nuclide inventory (f71) files

- A number of f71 files are produced as a result of the sensitivity calculation
- ${BASENAME}-sens<i>-adj.f71 contains the adjoint solution for the <i>-th sensitivity calculation
- ${BASENAME}-sens<i>-dps<k>.f71 contains the <k>-th direct perturbation solution for the <i>-th sensitivity calculation
  - Note the "Direct F71 File" column in the table indicates which one corresponds to which perturbation

TIP: Use Fulcrum to view the adjoint F71. For the current supported **nuclide** response, which is the weighted sum of a group of nuclides at some specified final time, the adjoint can be interpreted as the importance of a parent nuclide.

At the final time, only the nuclides directly involved in the response can contribute, and, therefore, the adjoint should be zero.

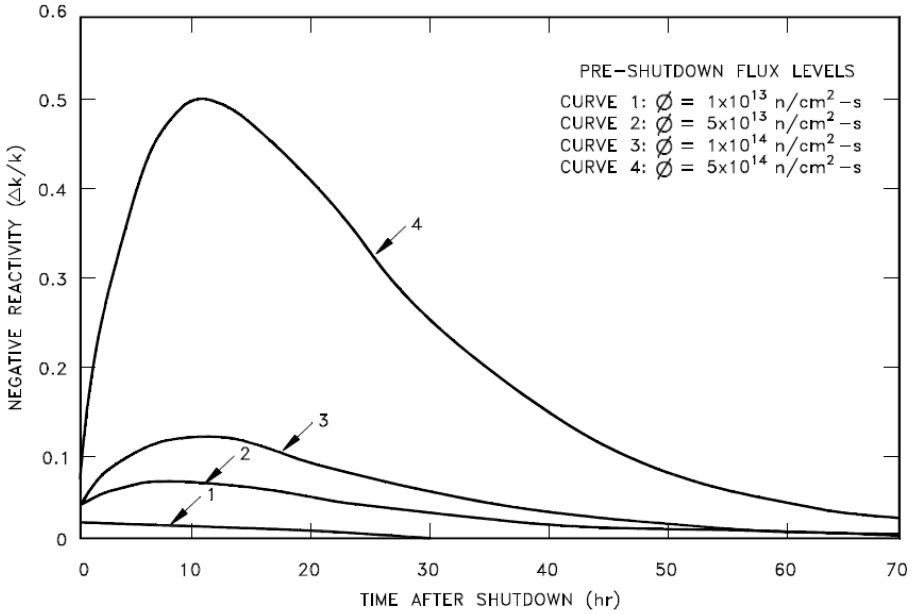
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Tutorial : Xe-135 sensitivity



A simple sensitivity calculation

- **Problem**
  - Determine the sensitivity with initial U-235 loading of the equilibrium Xe-135 concentration, after 1,000 days of reactor operation
- **Approach**
  - Start with an **xe_sens** file provided in starter folder
  - **Obiwan view –format=graphviz** can plot the relevant chains
  - Include and fill a **sens** block



Ref) DOE Fundamentals Handbook: Nuclear Physics and Reactor Theory Volume 2

OBIWAN transition plotting with graphviz

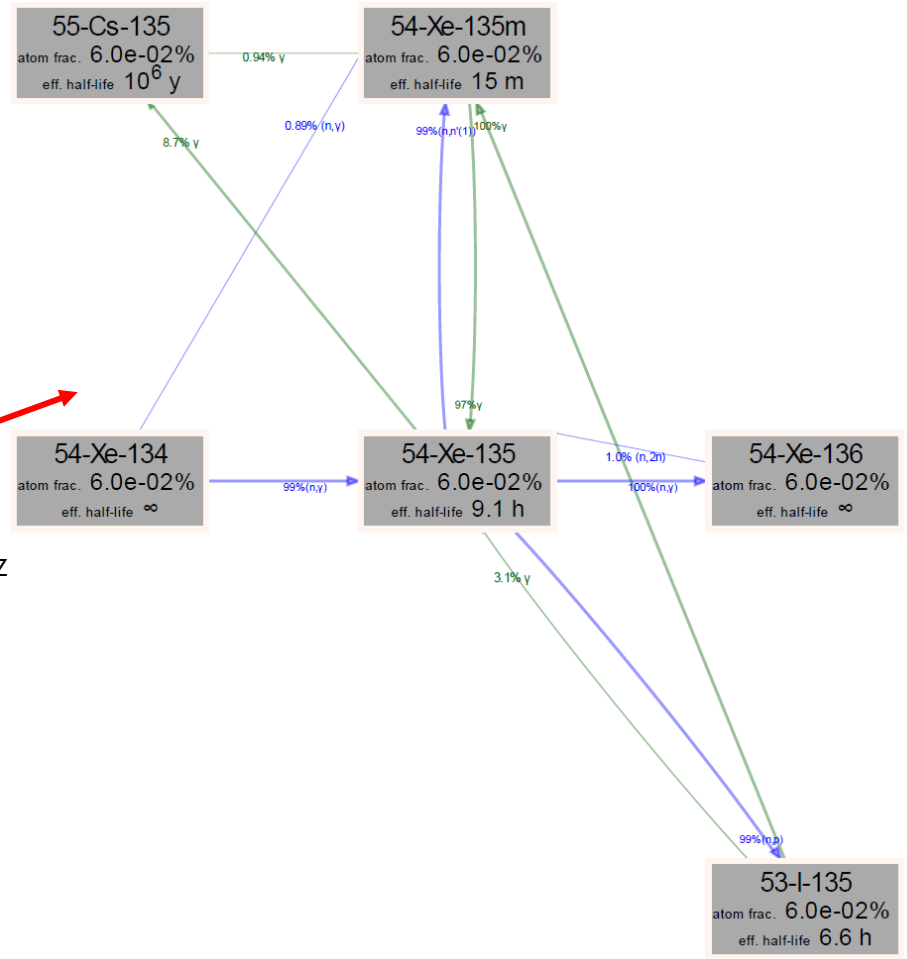
- OBIWAN includes a "**view**" command capable of producing a transition matrix output with an enhanced and visually appealing format (**graphviz**)

```
$SCALE/bin/obiwan view –format=graphviz origen.f33 > origen.dot
```

- Graphviz layout programs take descriptions of graphs in a text language (i.e., dot) and make diagrams in several useful formats such as images

```
1  digraph System {
2  edge [fontname=arial];
3  graph [fontname=arial, splines=false, truecolor=true, bgcolor="#ffffffff"];
4  node [fontname=arial, style=filled];
5  outputorder="edgesfirst"
6  53135[shape=record,rankdir=LR,fixedsize=true,label=<53-I-135<br/><FONT POINT
7  54134[shape=record,rankdir=LR,fixedsize=true,label=<54-Xe-134<br/><FONT POIN
```

"neato" in graphviz

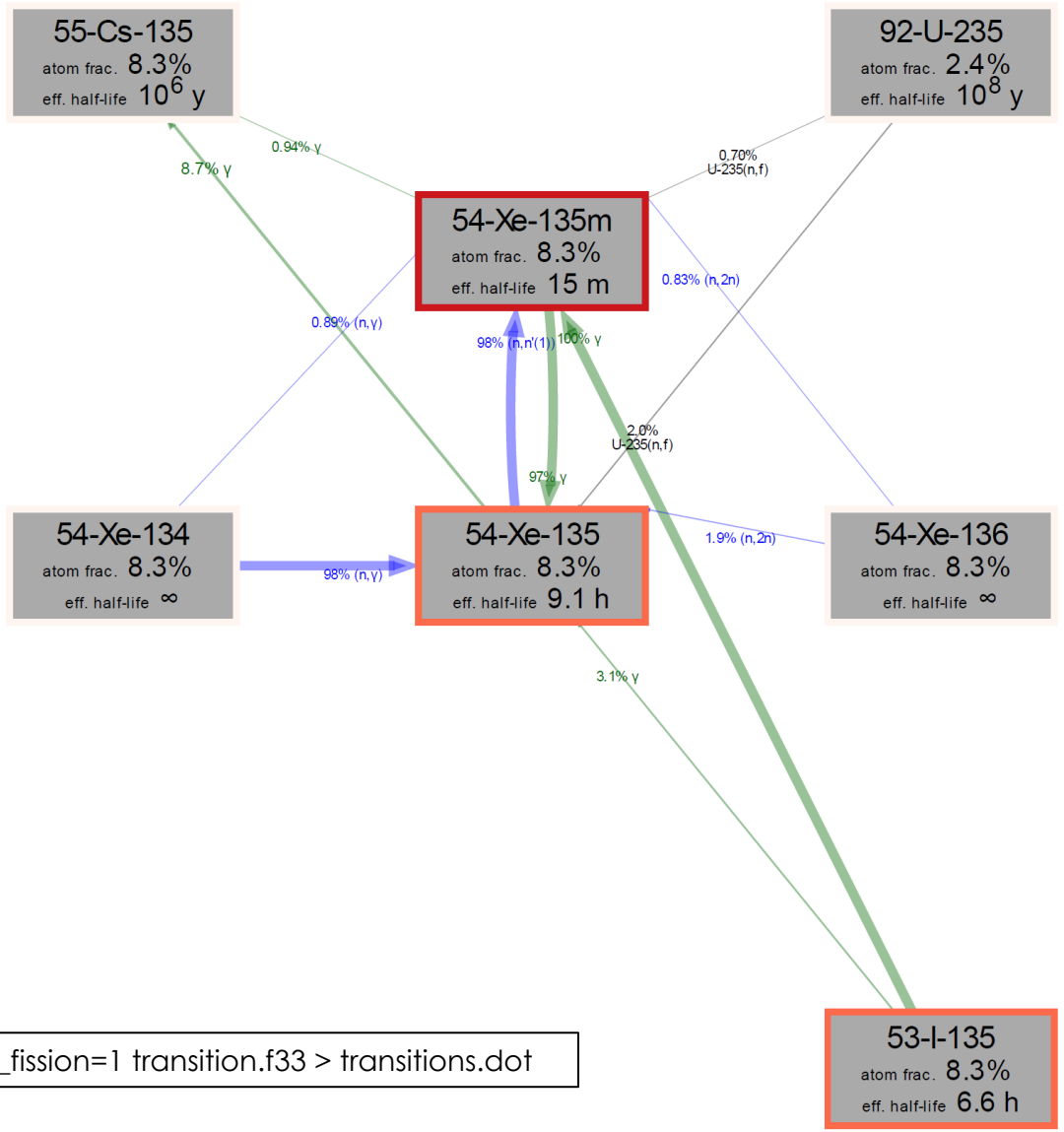


- You can install graphviz from the website on Windows or from package managers like `brew install graphviz` on Mac or `sudo apt install graphviz` on Linux

Understanding sources for Xe-135

- Xe-135 sources
  - Fission Product: 2.0% from U-235 (n,f)
  - Reaction: 1.9% from Xe-136 (n, 2n)
  - Reaction: 98% from Xe-134 (n,γ)
  - Decay: 97% I.T. from Xe-135m
  - Decay: 3.1% beta decay from I-135
- Xe-135m sources
  - Fission Product : 0.7% from U-235 (n,f)
  - Reaction: 0.83% from Xe-136 (n, 2n)
  - Reaction: 0.89% from Xe-134 (n,γ)
  - Reaction: 98% from Xe-135 (n,n')
  - Decay: 100% beta decay from I-135

U-235 irradiation problem




```
$SCALE/bin/obiwan.exe view -format=graphviz -allow_z="[54]" -allow_a="[135,235]" -allow_fission=1 transition.f33 > transitions.dot
```

Construct a **sens** block

```
=origen

% Use CRAM for forward solve so it is
consistent with adjoint solve (CRAM only
supports adjoint).
solver{ type=cram }
% Forward case with 1 gram of U235 irradiated at
constant flux for 1000 days.
case(1){
…
}
case(2){
…
}
case(A){
…
}
sens{
        % insert sens components here
}
end
```

- Each "**sens**" represents the problem "unit" corresponding to a specific case in the forward calculation
- You can have multiple **sens** blocks

Add a **case**

```
sens{
    case=A
}
```

- The name of the case to consider for the forward calculation
- Note that the default name for the first case is “1”; second case is “2”; etc.

Add a r**esponse** block for ^{135}Xe

```
sens{
    case=A
    response{
        iso=[xe135=1.0]
        type=NUCLIDE
        step=LAST
    }
}
```

- **Response** block has three components :
  - **iso=[list of key/value pairs];**
    - Key: same format as the **iso** array in the **mat** block
    - Value: user-specified multiplier
  - **type=** only "NUCLIDE" is currently supported
  - **step=** time step index at which the relative change in the response will be analyzed
- **Add 1.0 for Xe-135 concentration sensitivity**

Add a **threshold**

```
sens{
    case=A
    response{
        iso=[xe135=1.0]
        type=NUCLIDE
        step=LAST
    }
    threshold=1e-2
}
```

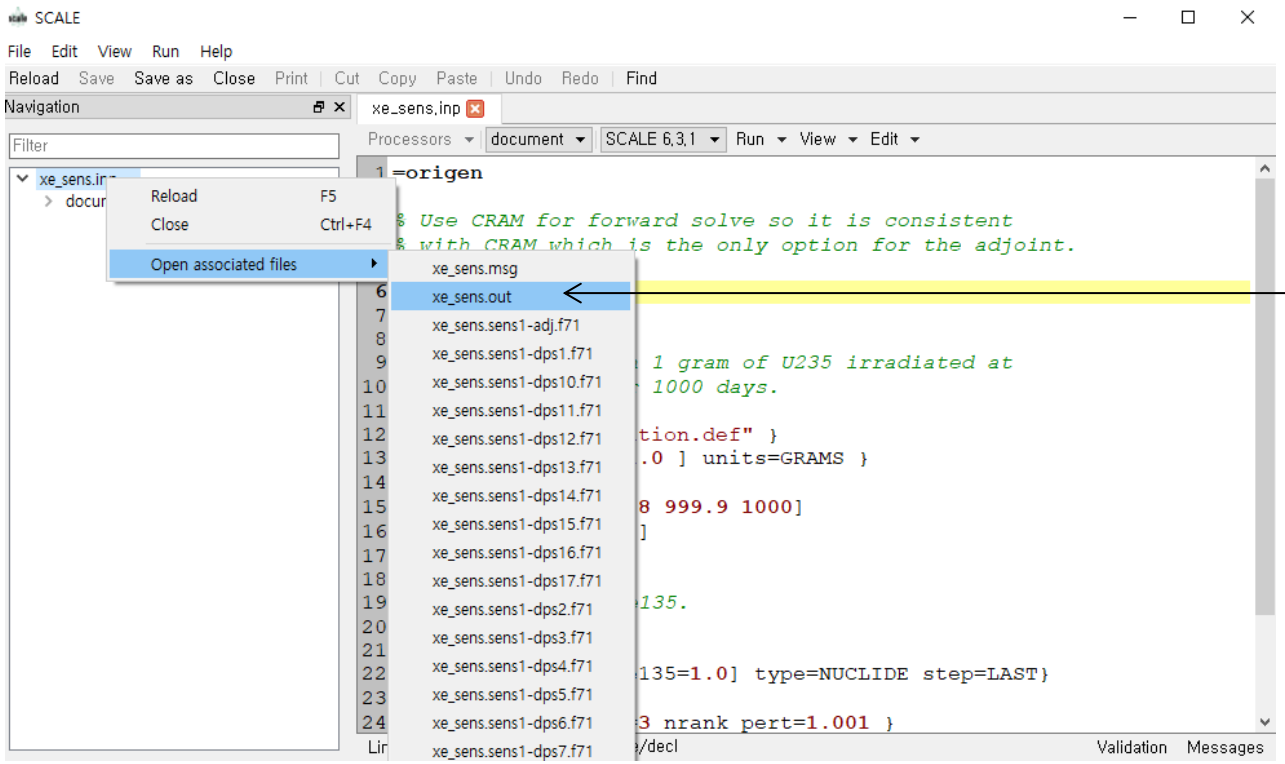
- **Threshold** = the minimum value of sensitivity coefficient to print in the output file

Add a **dp_verify** block

```
sens{
    case=A
    response{
        iso=[xe135=1.0]
        type=NUCLIDE
        step=LAST
    }
    threshold=1e-2
    dp_verify{
        nrank=3
        nrank_pert=1.001
    }
}
```

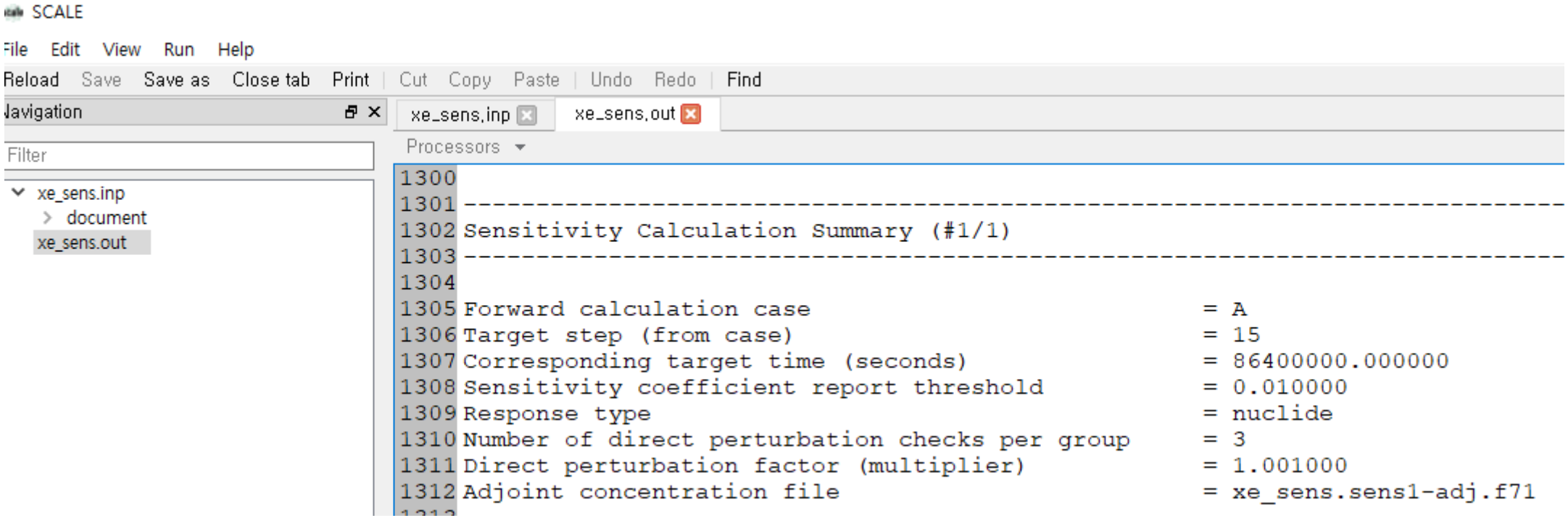
- **dp_verify** defines "direct perturbation"(DP) cases to verify the DPT-based sensitivities
- **dp_verify** block has two components :
  - **nrank=** number of DP calculations
  - **nrank_pert=** perturbation factor to assume for the dp verification: for example, "1.01" would indicate to multiply the data of interest by 1.01 (i.e., increase by 1%)
- Our problem is ready to run!

Simple sensitivity calculation: Run and open output file



- Calculation will take about one minute
- Right-click on file name in the navigation pane and "Open associated files" → xe_sens.out

Simple sensitivity calculation: Examine summary



Inspect the output files – Sensitivity coefficients

- Xe-135 decreases by 0.3% if the Xe-135 decay constant increases by 1%
- Xe-135 decreases by 0.7% if the n,gamma XS increases by 1%
- Xe-135 increases by 0.5% if either the yield of I-135 (53135) or Te-135 (52135) increases by 1%

Decay Loss Sensitivity

Nuclide ID	Decay Mode	Adjoint Sens. Coeff.	Direct Sens. Coeff.
54135	beta-	-2.89046e-01	-2.86852e-01

Reaction Loss Sensitivity

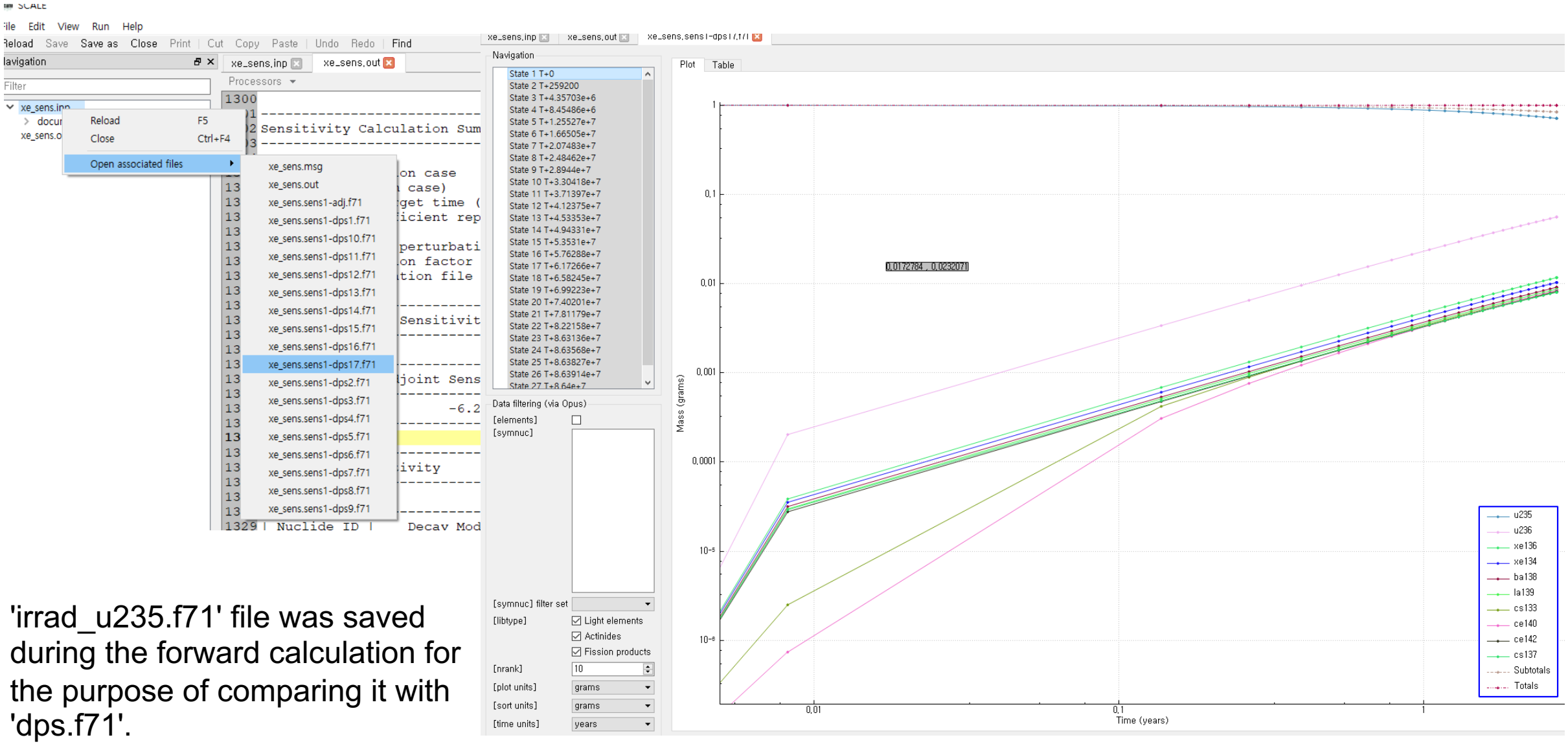
Nuclide ID	Decay Mode	Adjoint Sens. Coeff.	Direct Sens. Coeff.
54135	n,gamma	-7.18549e-01	-7.12788e-01
92235	n,gamma	-2.81529e-01	-2.81503e-01
92235	fission	-1.88686e-01	-1.98709e-01

Reaction Yield Sensitivity

Parent	Reaction	Daughter	Adjoint Sens. Coeff.	Direct Sens. Coeff.
92235	fission	52135	4.78956e-01	4.74233e-01
92235	fission	53135	4.34950e-01	4.30666e-01
92235	fission	52134	-2.98187e-02	-2.95217e-02

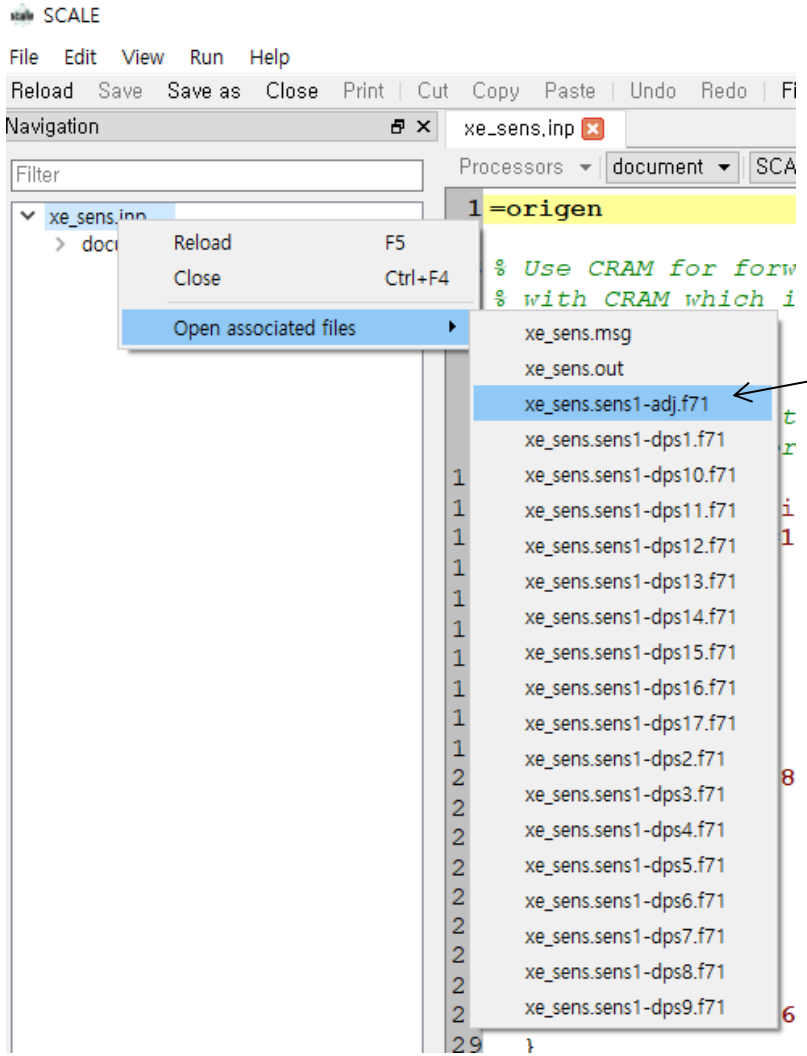
- Direct perturbations for each of the top 3 sensitivities for verification

Simple sensitivity calculations: Open dps-f71 file



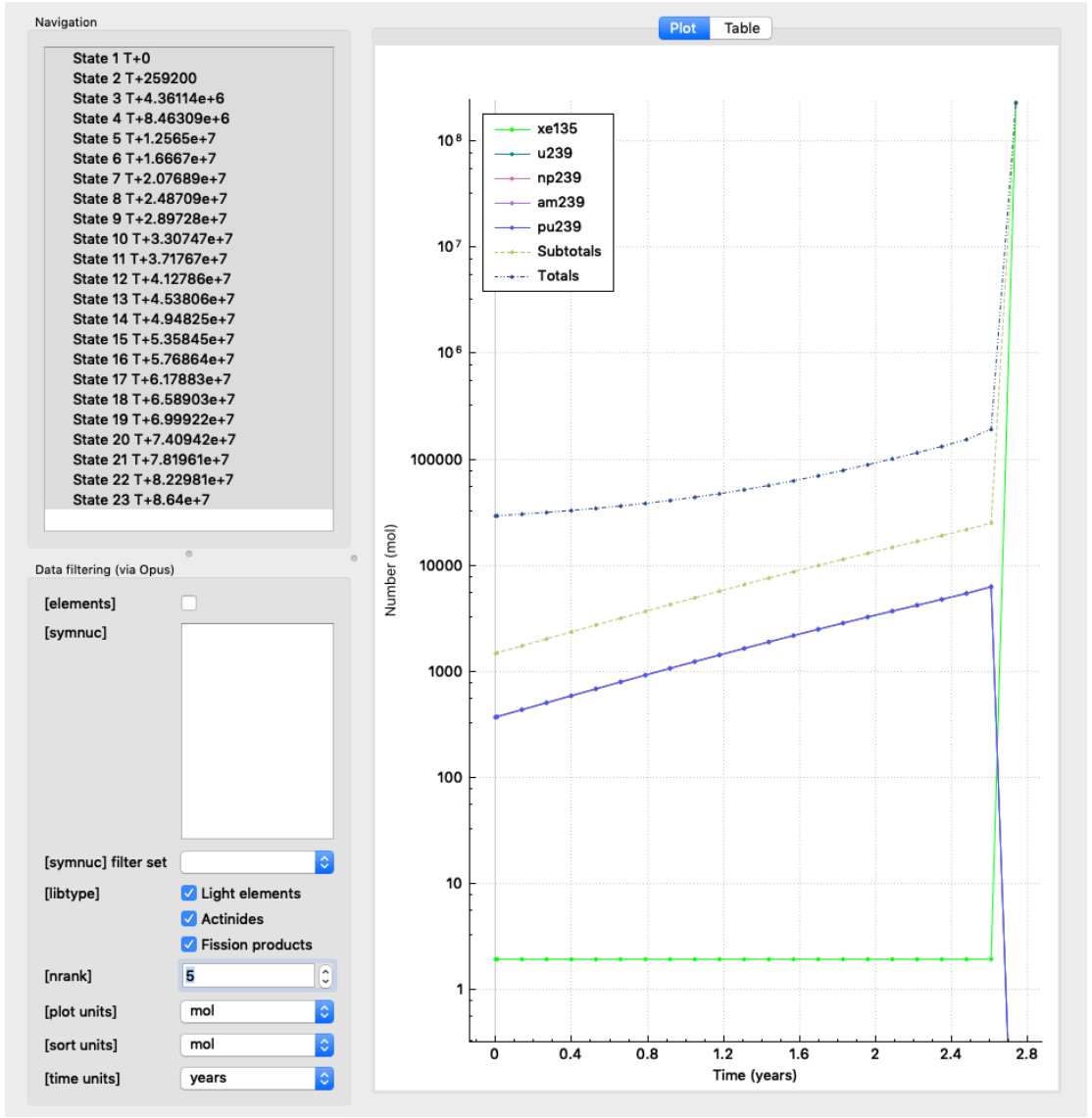
- 'irrad_u235.f71' file was saved during the forward calculation for the purpose of comparing it with 'dps.f71'.

Simple sensitivity calculations: Open adjoint f71 file



- "Open associated files" → xe_sens.sens1-adj.f71.out

Use f71 viewer to view adjoint concentration plot

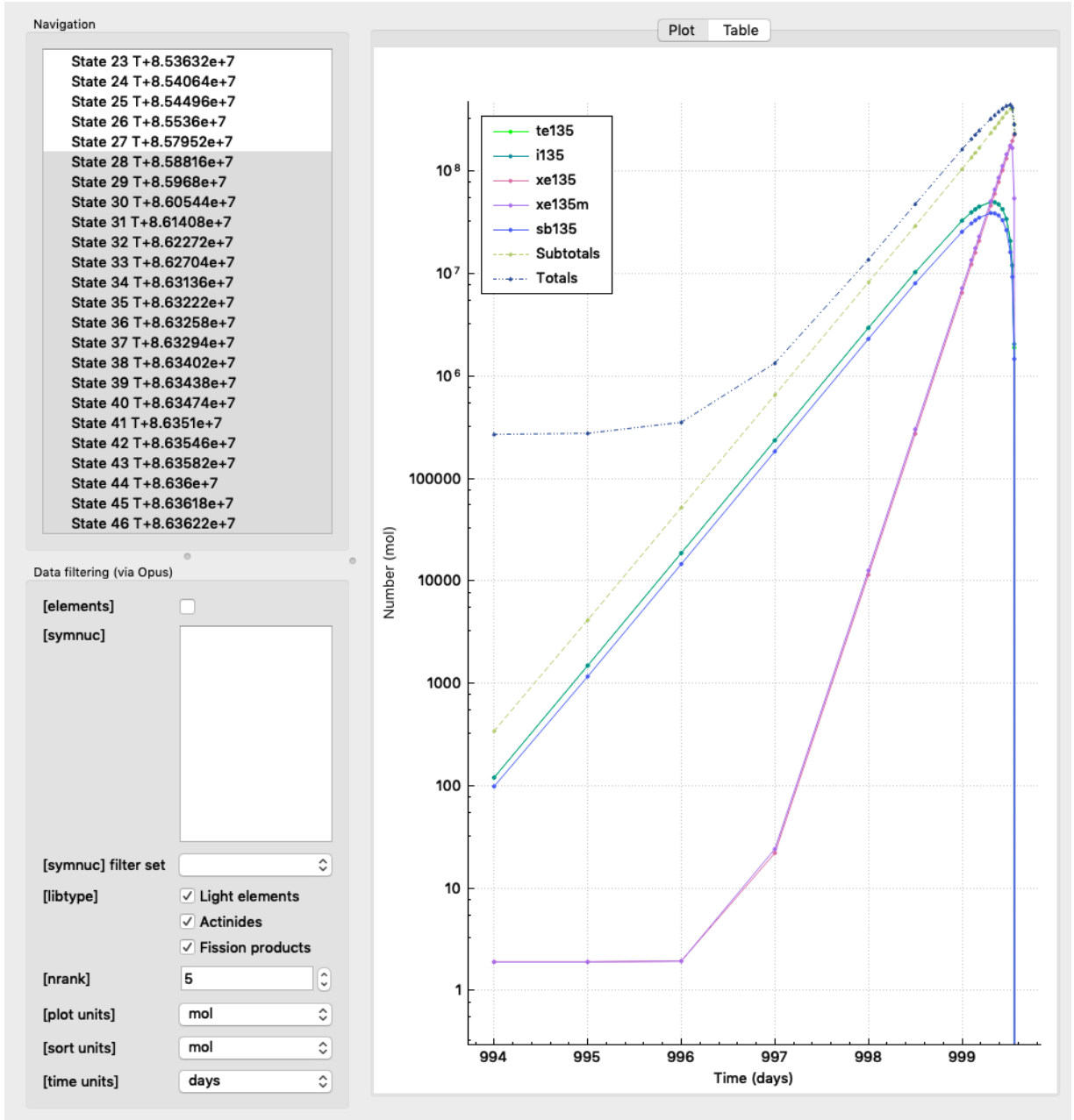


- Select all states (any of these ways)
  - Left-click and drag down
  - Hold SHIFT and select range
  - CTRL-A
- Change [plot units] and [sort units] to "grams" or "mol"
- Navigate to "**Axes→X-Axis→Scale**" and change to "**Log**"

Inspect the adjoint concentrations

- Note the huge change in adjoint concentration in the last time-step
- ORIGEN-Sensitivity assumes the linear shape of the solution between two time grid points
- You will need to update the forward time steps on the order of the effective half-life of the specific adjoints relevant for this response

$$S = \int_0^{t_i} dt N^*(t) \cdot \alpha_i \frac{\partial M}{\partial \alpha_i} \cdot N(t)$$



Solution

```
=origen
…
% Sensitivity of Xe135.
sens{
      case=A
      response{
           iso=[xe135=1.0]
           type=NUCLIDE
           step=LAST
      }
      threshold=1e-2
      dp_verify{ nrank=3 nrank_pert=1.001 }
}
 end
```

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Workshop:

Sensitivity analysis with ORIGEN



Problem 1: Deep dive into the Xe-135 sensitivity

- **Problem**
  - Simulate the behavior of a nuclear reactor that experiences an unexpected 3-day shutdown after 1,000 days of operation due to a turbine fault
- **Goal**
  - Investigate whether sensitivity coefficients change as a result of the reactor shutdown; determine whether the shutdown (zero flux) alters the importance of decay constants
  - Obtain the top decay channels/yield sensitivities and compare
- **Approach**
  - Load irrad_u235.f71 from the tutorial and add a decay case to simulate a shutdown scenario with the "end7dec" decay library
  - Use the fine time grid (e.g., unit=hours t = [34I 0.0 72.0])

Problem 2: Time grid refinement study

- **Problem**
  - We want to know whether we can use fewer time steps to simulate a 3-day reactor shutdown more efficiently and accurately
- **Goal**
  - Understand the relationship between the half-life and time grid, as well as the impact it has on the accuracy of sensitivity
  - Find the best time intervals for our simulation of Xe-135; this means using as few time steps as possible while keeping our results accurate
- **Approach**
  - Check the half-lives of the nuclides related to Xe-135
  - Plot how adjoint solutions change over time in the simulation

Problem 3: Unraveling radioactive material evolution in spent fuel

- **Problem**
  - Let's see the sensitivity change of the top 3 radioactive nuclides in a spent fuel pool at 12 hours and 3 days after shutdown
- **Approach**
  - Load composition data from "spent_fuel.f71"
  - Use Fulcrum to get radioactivity information
  - Adjust the time grid to focus on the specific 12-hour and 3-day points we're interested in here
- **Goal**
  - Find the top 3 radioactive materials in a spent fuel pool
  - Assess their decay channel sensitivities at different time points

Problem 4: Comparative analysis of ENDF data versions: Analyzing the influence of data changes on real simulation

- **ENDF VIII.0 Released in Feb 2018**

1. The photonuclear sublibrary was carried over unchanged from ENDF/B-VII.0. It contains evaluated cross sections for 163 materials (all isotopes) mostly up to 140 MeV. The sublibrary was supplied by Los Alamos National Laboratory (LANL) and it is largely based on the IAEA-coordinated collaboration completed in 2000.
2. The photo-atomic sublibrary was updated as part of the EPICS2017 project. See the EPICS2017 page for more detail.
3. The decay data sublibrary has been improved by the Brookhaven National Laboratory (BNL).
4. The spontaneous fission yields were taken over from ENDF/B-VII.1
5. The atomic relaxation sublibrary was updated as part of the EPICS2017 project. See the EPICS2017 page for more detail.
6. The neutron reaction sublibrary represents the heart of the ENDF/B-VIII.0 library. The sublibrary has been updated and extended, and it contains 557 materials, including the 6 CIELO evaluations (^{1}H, ^{16}O, ^{56}Fe, ^{235}U, ^{238}U and ^{239}Pu).
7. Neutron fission yields were taken over from ENDF/B-VII.1.

TABLE XLII: ENDF/B-VII.1 [2], ENDF/B-VIII.0, KADONIS v0.3 [169] Maxwellian-averaged neutron capture cross sections and their ratios at kT=30 keV. Comments: C-calculated from BNL-325 data [454], T-theoretical data in KADONIS v.0.3 [169]

Material	ENDF/B-VII.1 (barns)	ENDF/B-VIII.0 (barns)	KADONIS v.0.3 (barns)	ENDF/B-VII.1/ENDF/B-VIII.0	KADONIS/ENDF/B-VIII.0
92-U -235	6.930E-1±2.240E-1	7.168E-1		9.664E-1±3.238E-1	
92-U -238	4.000E-1±6.180E-3	3.950E-1		1.014E+0±1.544E-2	
94-Pu-239	5.280E-1±5.500E-2	5.434E-1		9.716E-1±1.042E-1	
94-Pu-240	6.910E-1±5.220E-4	6.747E-1±6.851E-4		1.025E+0±1.266E-3	
94-Pu-242	5.320E-1±1.660E-2	5.321E-1±1.658E-2		1.000E+0±4.407E-2	

U235 capture XS = 3.43% increase
U238 capture XS = 1.25% decrease
Pu239 capture XS = 2.92% increase
Pu240 capture XS = 2.36 % decrease

Problem 4: Comparative analysis of ENDF data versions: Analyzing the influence of data changes on real simulation

- **Problem**
  - Assess the variation in the amount of Pu in a weapon-grade plutonium system; important for nuclear safeguards applications
- **Goal**
  - Estimate the change in the total amount of Pu239 and Pu240 present after 1 cycle (200 days) of operation due to differences identified in ENDF library updates for cross-sections shown on the previous page
- **Approach**
  - Get the sensitivities of Pu239 plus Pu240 ($m_{Pu_{239}+Pu_{240}}$) concentration (define the multi-nuclides response)
  - Start with the provided file **origen_1cycle_irradiation.inp**

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Solutions



Problem 1: Deep dive into the Xe-135 sensitivity

1) Investigate whether sensitivity coefficients change because of the reactor shutdown. Determine whether the shutdown (zero flux) alters the importance of decay constants.

2) Obtain the top decay channels/yield sensitivities and compare.

ANSWER:

1) In a reactor shutdown scenario, sensitivity coefficients change, and decay constants become significantly more relevant than in normal operational scenarios.

2) Only beta decay of Xe-135 matters in the operation scenario, whereas I-135 is also important in the shutdown scenario.

Operation scenario

Nuclide ID	Decay Mode	Adjoint Sens. Coeff.	Direct Sens. Coeff.	Direct F71 File
54135	beta-	-2.89046e-01	-2.86852e-01	xe_sens.sens1-dps2.f71

Shutdown scenario

Nuclide ID	Decay Mode	Adjoint Sens. Coeff.	Direct Sens. Coeff.	Direct F71 File
54135	beta-	-3.84653e+00	-3.83881e+00	xe_sens_shutdown.sens1-dps3.f71
53135	beta-	-1.35706e+00	-1.35366e+00	xe_sens_shutdown.sens1-dps4.f71

Problem 2: Time grid refinement study

Determine the optimal time grid for Xe-135 sensitivity

ANSWER:

Your answer will be the best answer!

I used 22 steps : t=[0.1 0.2 0.5 0.7 0.9 8I 1.0 70.0 70.7 71.2 71.4 71.6 71.8 71.9 72.0] to obtain <=1% error

Uniform 34 steps time grid in Problem 1

Nuclide ID	Decay Mode	Adjoint Sens. Coeff.	Direct Sens. Coeff.	Direct F71 File
54135	beta-	-3.84653e+00	-3.83881e+00	xe_sens_shutdown.sens1-dps3.f71
53135	beta-	-1.35706e+00	-1.35366e+00	xe_sens_shutdown.sens1-dps4.f71

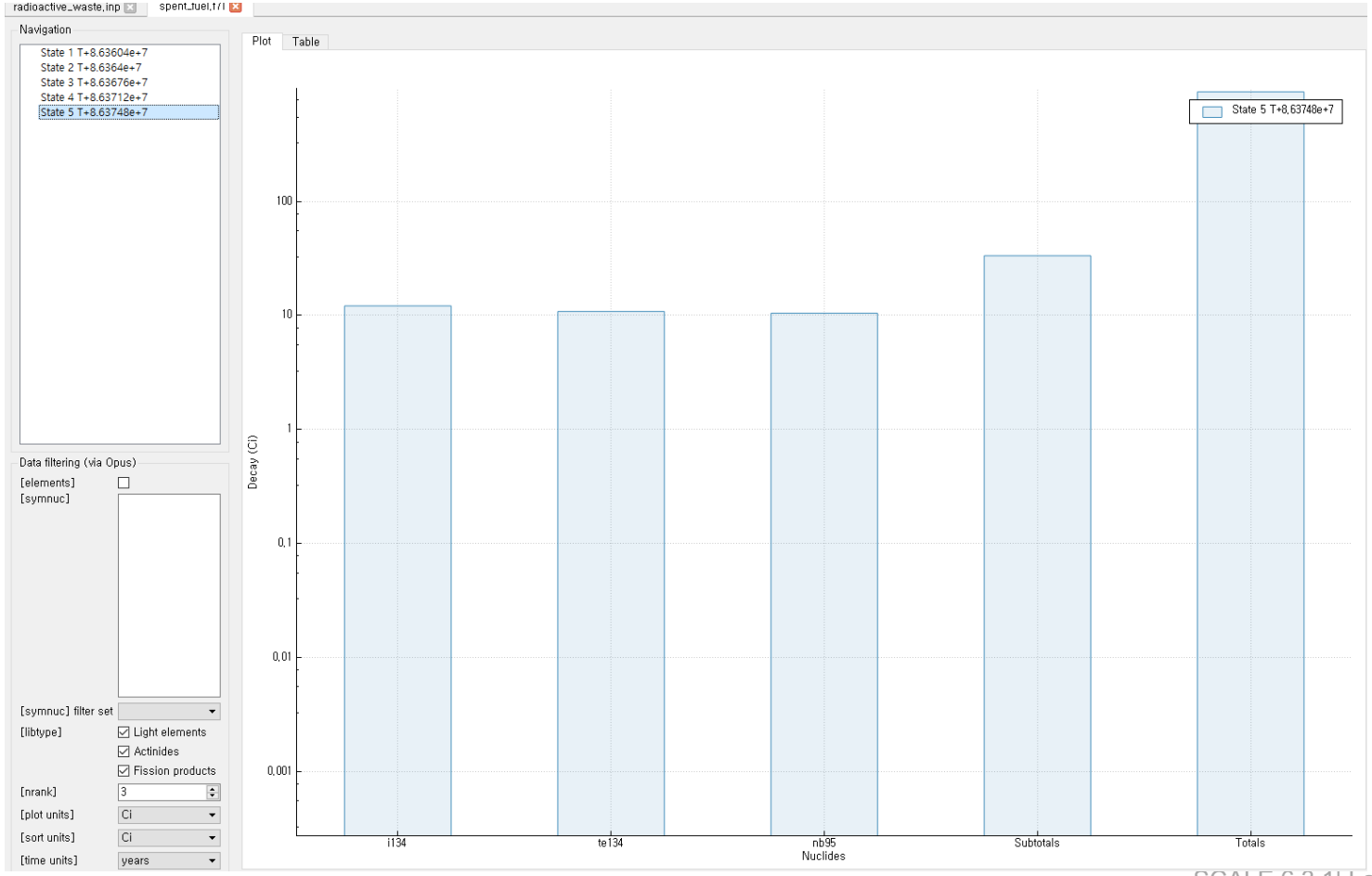
Instructor's 22 steps time grid

Nuclide ID	Decay Mode	Adjoint Sens. Coeff.	Direct Sens. Coeff.	Direct F71 File
54135	beta-	-3.83791e+00	-3.83881e+00	xe_sens_shutdown_refined.sens1-dps3.f71
53135	beta-	-1.36532e+00	-1.35366e+00	xe_sens_shutdown_refined.sens1-dps4.f71

Problem 3: Unraveling radioactive material evolution in spent fuel

1) Find the top 3 radioactive materials in a spent fuel pool.

ANSWER: I-134, Te-134, and Nb-95



Problem 3 (contd.)

2) Assess their decay channel sensitivities at different time points.

ANSWER:

I-135 and Te-134 at t=12 hours

Nuclide ID	Decay Mode	Adjoint Sens. Coeff.	Direct Sens. Coeff.	Direct F71 File
53134	beta-	-7.21219e+00	-7.20159e+00	radioactive_waste_12h.sens1-dps3.f71
52134	beta-	-2.11501e+00	-2.09117e+00	radioactive_waste_12h.sens1-dps4.f71

Nuclide ID	Decay Mode	Adjoint Sens. Coeff.	Direct Sens. Coeff.	Direct F71 File
52134	beta-	-1.19387e+01	-1.18682e+01	radioactive_waste_12h.sens2-dps2.f71

I-135 and Te-134 at t=3 days

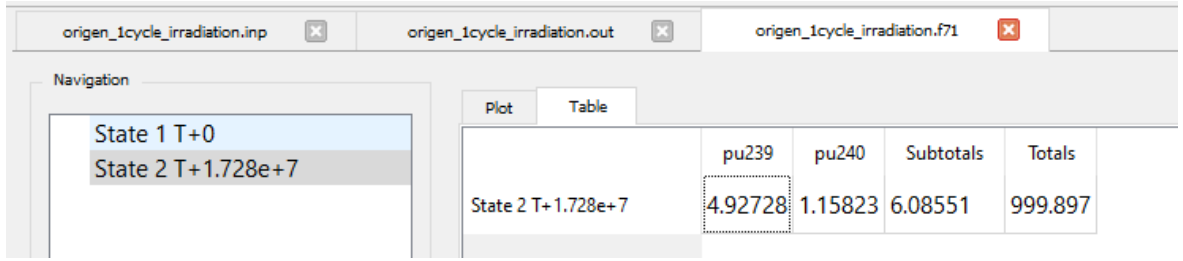
Nuclide ID	Decay Mode	Adjoint Sens. Coeff.	Direct Sens. Coeff.	Direct F71 File
53134	beta-	-5.38510e+01	-5.25612e+01	radioactive_waste_3d.sens1-dps3.f71
52134	beta-	-3.18153e+00	-3.01925e+00	radioactive_waste_3d.sens1-dps4.f71

Nuclide ID	Decay Mode	Adjoint Sens. Coeff.	Direct Sens. Coeff.	Direct F71 File
52134	beta-	-7.16330e+01	-6.91295e+01	radioactive_waste_3d.sens2-dps2.f71

Problem 4: Comparative analysis of ENDF data versions: Analyzing the influence of data changes on real simulation

- Estimate the change in the total amount of Pu239 and Pu240 present after 200 days of operation due to differences identified in library updates

- Total amount of Pu239 and Pu240 produced with ENDFVII.1 library is 6.086 kg.
- Obtained (n, gamma) channel sensitivities are <1E-3 for U-235, 9.82E-01 for U-238, -9.47E-02 for Pu-239, and -1.48E-01 for Pu-240
- The relative changes in (n, gamma) cross section between ENDFVII.1 and ENDF VIII.0 with Maxwellian-average spectrum




```
Reaction Loss Sensitivity
-------------------------------------------------------------------------------
|Nuclide ID |     Reaction     | Adjoint Sens. Coeff. | Direct Sens. Coeff. |
-------------------------------------------------------------------------------
|      92238 |         n,gamma |          9.82345e-01 |          9.90339e-01 |
|      94239 |         fission |         -4.93802e-01 |                    - |
|      94240 |         n,gamma |         -1.48035e-01 |                    - |
|      94239 |         n,gamma |         -9.46972e-02 |                    - |
-------------------------------------------------------------------------------
```

U235 capture XS = 3.43% increase
U238 capture XS = 1.25% decrease
Pu239 capture XS = 2.92% increase
Pu240 capture XS = 2.36 % decrease

Problem 4: Comparative analysis of ENDF data versions: Analyzing the influence of data changes on real simulation (contd.

- Estimate the change in the total amount of Pu present after 200 days of operation due to differences identified in library updates

ANSWER:

Under the assumption that the second-order perturbation is negligible, the relative change of Pu239 and Pu240 amounts are -1.23, -0.28, and 0.35%, respectively.

Nuclide ID	Reaction	Adjoint Sens. Coeff. (a)	XS changes [%] (b)	Relative change of Pu239 and Pu240 amount (a)×(b) [%]	Absolute difference [g]
92238	n,gamma	9.82345e-01	-1.25	-1.23	-74.7
94239	n,gamma	-9.46972e-02	2.92	-0.28	-16.8
94240	n,gamma	-1.48035e-01	-2.36	0.35	21.3
SUM	-			-1.16	-70.3

Thus, with the updated ENDF/B VIII.0 capture cross-sections of actinides, 1.16% of 6.086 kg (70.3 g) less Pu239 and Pu240 amount will be produced at the end of the cycle.

Future plans for sensitivity features

- Near term (6.3.2)
  - Improve the accuracy of sensitivity calculation for short-lived nuclides with a coarse time grid (reduce time grid dependency)
  - Manual update
- Longer term (7.0)
  - Add more response types (e.g., decay heat, fuel cycle)
  - Add the constant power condition
  - Generate Sensitivity Data File for ORIGEN (SDF)
  - Coupling with other transport codes (Polaris/TRITON)
  - Expand its usage to various analyses (decay heat analysis, depletion benchmark)

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Questions?



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Backup



Obtaining sensitivity coefficients: Two approaches

1) If you have abundant computational resources and are meticulous in your work, you may choose to manually modify data and repeatedly run ORIGEN.

- The direct stochastic sampling methods (or direct perturbation) can produce output distributions from an ensemble of coupled transport and depletion calculations with different input data sets sampled; this approach (SAMPLER/SCALE) is easy to implement, but at the expense of high computational cost

2) For those seeking efficiency and leveraging mathematical techniques, depletion perturbation theory (DPT) offers an elegant solution!

- Depletion perturbation theory (DPT) can both reduce the number of depletion calculations to obtain the sensitivity coefficients and provide nuclide-, reaction type-, branch/yield-, and flux-wise sensitivity in a single depletion calculation.

- ORIGEN utilizes the DPT to obtain the sensitivity coefficient.