ORIGEN Sensitivities in SCALE 6.3

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Depletion Perturbation Theory - background

- Sensitivity coefficients for various reactor physics parameters are important to assess a reactor's inherent safety and maintain the safety.
- In solving the depletion equation, there are uncertainties in the number densities at the beginning of each time step and in the burnup matrix (decay data and reaction cross sections). Thus, the number densities and reaction rates at the end of the time step could have uncertainties.
- The direct stochastic sampling methods 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 costs.
- Depletion perturbation theory could not only reduce the number of depletion calculations to obtain the sensitivity coefficients, but also provide nuclide-, reaction type-, branch/yield- , flux- wise sensitivity in a single depletion calculation.

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New Sensitivity Calculation Capability in SCALE 6.3

- Mark Williams employed a variational formalism to develop a Depletion Perturbation Theory (DPT) for coupled neutron and nuclide data.
- W.A. Wieselquist implemented the Mark Williams' DPT to SCALE 6.3.
- Definition of response

$$R = \int_0^{t_i} dt < R(\sigma, \mathrm{N}, \phi_i, \phi_i^* >, \quad <> \text{ indicates the integral over volume and energy}$$

- Definition of sensitivity coefficient

$$S = \frac{dR}{R} / \frac{d\alpha}{\alpha} = \frac{\alpha}{R}\Big(\underbrace{\frac{\partial R}{\partial \alpha}}_{\text{direct}} + \underbrace{\frac{\partial R}{\partial N}\frac{dN}{d\alpha}}_{\text{number density}} + \underbrace{\frac{\partial R}{\partial \phi}\frac{d\phi}{d\alpha}}_{\text{flux}} + \underbrace{\frac{\partial R}{\partial \phi^*}\frac{d\phi^*}{d\alpha}}_{\text{adjoint flux}}\Big), \quad \underbrace{\frac{\partial R}{\partial N}\frac{dN}{d\alpha}}_{\text{number density}} = < \int_0^{t_i} dt N^* \alpha_i \frac{\partial M}{\partial \alpha} N >$$

- In SCALE 6.3, ORIGEN provides the nuclide concentration response
- User can perturb each transition channel, yield or total production/loss rate.

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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
```

- `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

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Example: Equilibrium Xe-135 concentration sensitivity

Processors | document | SCALE 6.3.0 | Run | View | Edit

```
=origen

% Use CRAM for forward solve so it is consistent
% with CRAM which is the only option for the adjoint.
solver{
    type=cram
}

% Forward case with 1 gram of U235 irradiated at
% constant flux for 1000 days.
case(A){
  lib{ file="transition.def" }
  mat{ iso=[ u235=1.0 ] units=GRAMS }
  time=[ 20I 3 1000]
  flux=[ 22R 1e14  ]
}

% Sensitivity of Xe135.
sens{
  case=A
  response{ iso=[xe135=1.0] type=NUCLIDE step=22}
  threshold=1e-2
  dp_verify{ nrank=3 nrank_pert=1.001 }
}

end
```

```
case(1){
  lib{ file="transition.def" }
  mat{ iso=[ u235=1.0 ] units=GRAMS }
  time=[ 20I 3 988 ]
  flux=[ 22R 1e14  ]
}

case(2){
  time{
    start=0
    units=DAYS
    t=[0.5 1 2 5 6 7 8 9 10 10.5 11 11.1]
  }
  flux=[ 12R 1e14]
}

case(A){
  time{
    start=0
    units=HOURS
    t=[1 2 5 6 7 8 9 10 10.5 11 11.1]
  }
  flux=[ 11R 1e14]
}
```

To get the correct adjoint sensitivity coefficients for short-lived nuclides, fine time grid is required in SCALE 6.3.0

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Inspect the output files

- Summary in output (.out)file

$$S = \frac{dR}{R} / \frac{d\alpha}{\alpha}$$

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

```
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
```

```
1427 ------------------------------------------------------------------------------
1428 | Nuclide ID |    Decay Mode    | Adjoint Sens. Coeff. | Direct Sens. Coeff. |
1429 ------------------------------------------------------------------------------
1430 |      54135 |           beta- |         -2.95753e-01 |        -2.86852e-01 |
1431 |      53135 |           beta- |         -1.74595e-02 |        -4.86264e-04 |
1432 ------------------------------------------------------------------------------
```

```
1459 ------------------------------------------------------------------------
1460 | Nuclide ID |     Reaction     | Adjoint Sens. Coeff. | Direct Sens. Coeff. |
1461 ------------------------------------------------------------------------
1462 |      54135 |         n,gamma |         -7.35224e-01 |        -7.12788e-01 |
1463 |      92235 |         n,gamma |         -2.81413e-01 |        -2.81392e-01 |
1464 |      92235 |         fission |         -1.52446e-01 |        -1.98188e-01 |
1465 ------------------------------------------------------------------------
```

```
1471 ------------------------------------------------------------------------------------------
1472 |   Parent   |     Reaction     |  Daughter  | Adjoint Sens. Coeff. | Direct Sens. Coeff. |
1473 ------------------------------------------------------------------------------------------
1474 |      92235 |         fission |      52135 |          4.96308e-01 |         4.74239e-01 |
1475 |      92235 |         fission |      53135 |          4.50703e-01 |         4.30672e-01 |
1476 |      92235 |         fission |      52134 |         -3.09293e-02 |        -2.95232e-02 |
```


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Time grid dependency of sensitivity results

- Direct perturbations for each of the top 3 sensitivities with coarse Xe-135 input time grid

```
% Forward case with 1 gram of U235 irradiated at
% constant flux for 1000 days.
case(A){
  lib{ file="transition.def" }
  mat{ iso=[ u235=1.0 ] units=GRAMS }
  time=[ 20I 3 1000]
  flux=[ 22R 1e14  ]
}
```

```
-----------------------------------------------------------------
Decay Loss Sensitivity
-----------------------------------------------------------------

-------------------------------------------------------------------------------
| Nuclide ID |     Decay Mode    | Adjoint Sens. Coeff. | Direct Sens. Coeff. |
-------------------------------------------------------------------------------
|      53135 |            beta- |          1.21161e+02 |        -4.86250e-04 |
|      54135 |            beta- |         -4.32051e+01 |        -2.86852e-01 |
|    1054135 |             i.t. |          2.73021e+01 |         5.38088e-04 |
-------------------------------------------------------------------------------
```

Large differences indicate there may be a time-step/integration issue. Look at the adj.f71 in the Fulcrum viewer!

- Things to keep in mind
  - Adjoint proceeds backwards in time along the same time-grid as the forward calculation
  - Sensitivity is simple trapezoid rule integration of the forward and adjoint
  - Adjoint may vary many orders of magnitude near the time of interest, especially for a short-lived nuclide. "Short-lived" is a relative term corresponding to the input time grid

$$S = \frac{\alpha}{R}\left(\underbrace{\frac{\partial R}{\partial N}\frac{dN}{d\alpha}}_{\text{number density}}\right) = \frac{\alpha}{R}\sum_j < \int_0^t dt N^* \frac{\partial M}{\partial \alpha} N >$$

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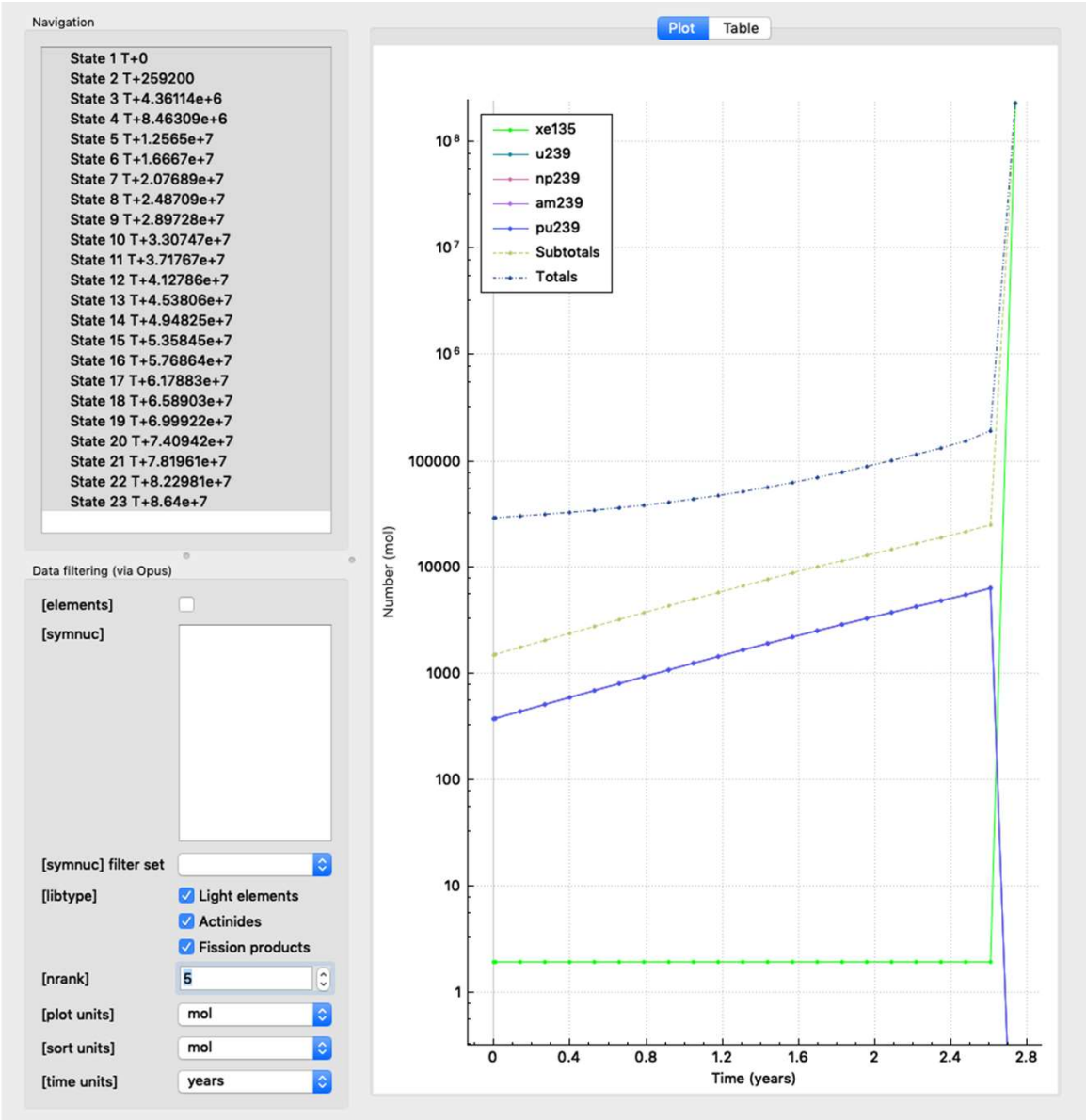
Inspect the adjoint concentrations

- Note the huge change of adjoint concentration in the last time-step
- You will need to update the forward time-steps on the order of the effective half-life of the specific adjoints which matter for this response



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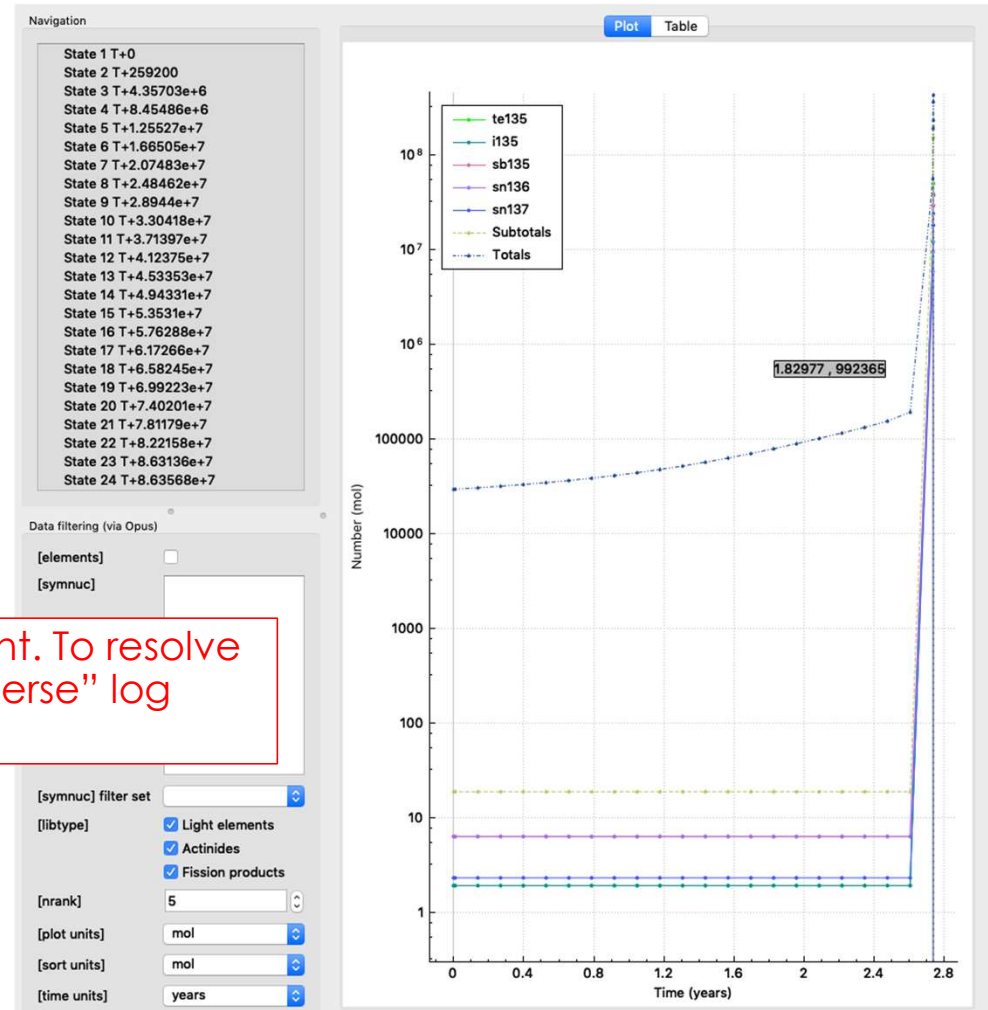
Refine the final time steps (1)

```
=origen

% Use CRAM for forward solve so it is consistent
% with CRAM which is the only option for the adjoint.
solver{
    type=cram
}

% Forward case with 1 gram of U235 irradiated at
% constant flux for 1000 days.
case(A){
  lib{ file="transition.def" }
  mat{ iso=[ u235=1.0 ] units=GRAMS }
  time=[ 20I 3 999
         999.5 999.8 999.9 1000]
  flux=[ 26R 1e14  ]
}

% 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
```

Better, but still need more refinement. To resolve exponential behaviors, need a "reverse" log time grid.

```
-----------------------
Decay Loss Sensitivity
-----------------------------------------------------------------------

-------------------------------------------------------------------------------
| Nuclide ID |    Decay Mode    | Adjoint Sens. Coeff. | Direct Sens. Coeff. |
-------------------------------------------------------------------------------
|      53135 |           beta- |        -7.06662e+00 |        -4.86250e-04 |
|      54135 |           beta- |        -3.97069e-01 |        -2.86852e-01 |
|    1054135 |            i.t. |         3.75133e-02 |         5.38088e-04 |
|      51135 |   beta-,neutron |        -3.33057e-02 |                   - |
|      51135 |           beta- |         3.32963e-02 |                   - |
|      52136 |           beta- |        -2.34964e-02 |                   - |
|      52136 |   beta-,neutron |         2.34810e-02 |                   - |
-------------------------------------------------------------------------------
```



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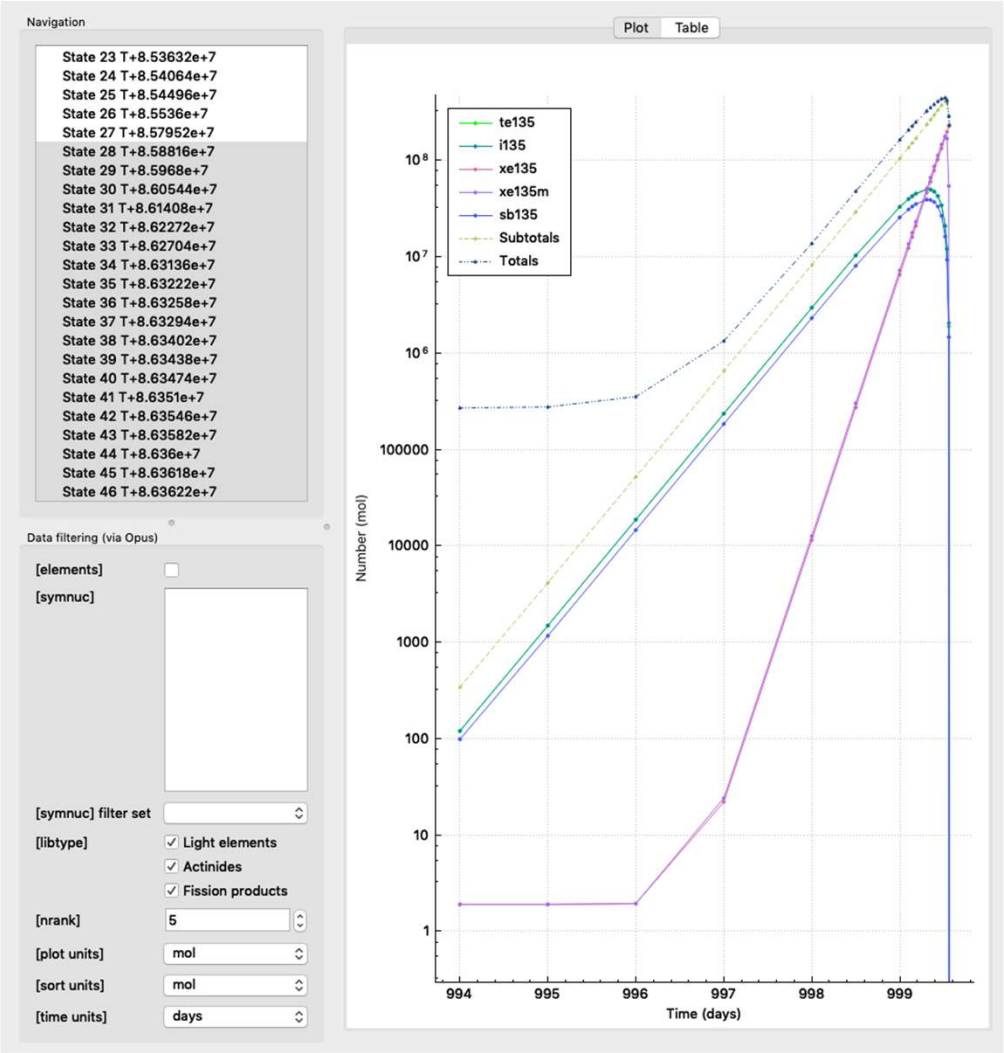
Refine the final time steps (2)

- Using a separate case with time in days or hours may be useful

```
case(1){
  lib{ file="transition.def" }
  mat{ iso=[ u235=1.0 ] units=GRAMS }
  time=[ 20I 3 988 ]
  flux=[ 22R 1e14  ]
}

case(2){
  time{
    start=0
    units=DAYS
    t=[0.5 1 2 5 6 7 8 9 10 10.5 11 11.1]
  }
  flux=[ 12R 1e14]
}

case(A){
  time{
    start=0
    units=HOURS
    t=[1 2 5 6 7 8 9 10 10.5 11 11.1]
  }
  flux=[ 11R 1e14]
}
```



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Future Plans for Sensitivity Features

- Near term (6.3.x)
  - Minor fix to handle multiple library positions of F33 (6.3.1)
  - Improve the accuracy of sensitivity calculation for short-lived nuclides with a coarse time grid (6.3.2)
  - Manual update and improving input structure
- Longer term (7.0)
  - Add more response types (e.g., Decay heat, fuel cycle)
  - Add the constant power condition
  - Coupling with transport codes (Polaris/TRITON)
  - Expand its usage to various analysis (Decay heat analysis, Depletion benchmark)

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Questions?