EXPERIENCE WITH THE SCALE CODE SYSTEM

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Outline

Application examples of the SCALE Code System in our group

- TRITON/NEWT: Modeling of Hexagonal Geometries
- KENO: Criticality Safety Calculations
- TRITON/NEWT: Spent Fuel Calculations
- MAVRIC/ORIGEN: Activation Analysis

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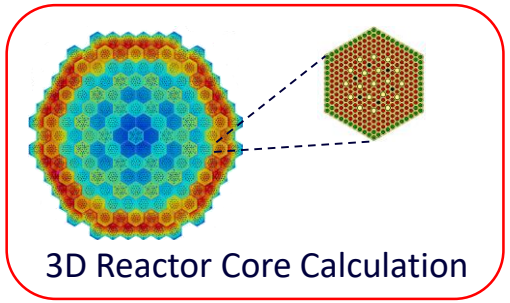
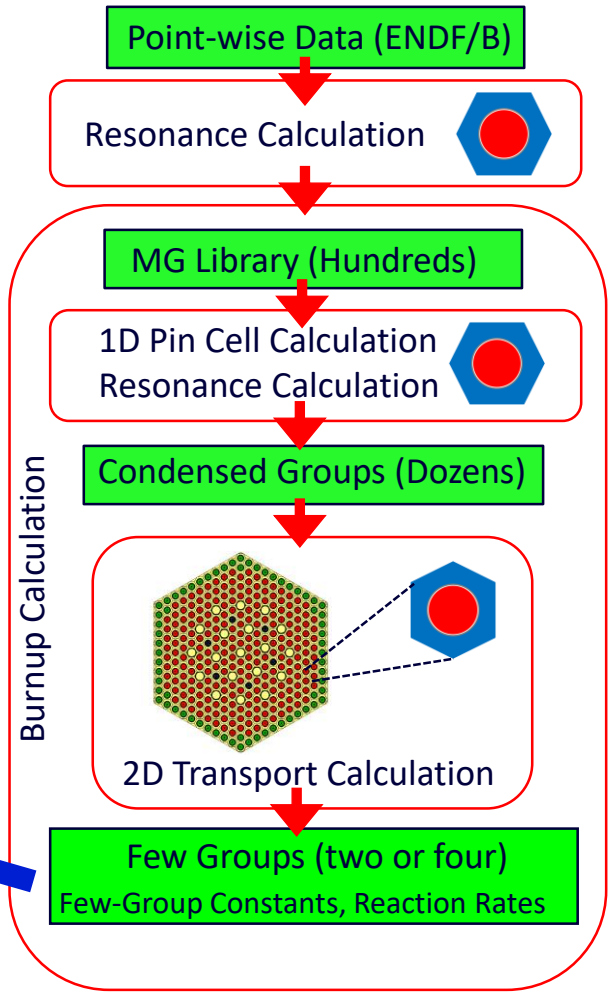
Generation of Cross Section Library for Reactor Burnup Calculations

Reactor burnup calculations are a **two-step procedure** that consists of an assembly calculation with **deterministic transport code** followed by reactor core calculation with **nodal diffusion code**.

First step – **cross section library generation**: Several branches of lattice calculations for fuel assemblies and reflectors have to be performed to generate two-energy group XS library parametrized as function of burnup and

- Moderator density
- Fuel temperature
- Boron concentration
- Rodded/unrodded situation





We use **TRITON/NEWT** from SCALE 6.2.4 for the cross section library generation.

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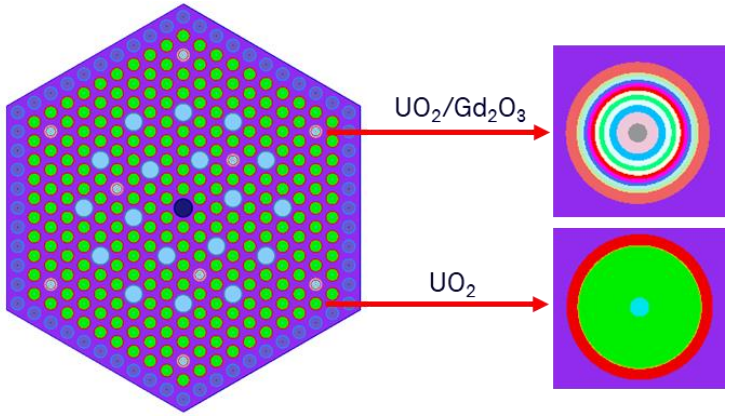
Lattice Cell Calculations with TRITON/NEWT

FA type	Number of Fuel Pins/Enrichment (wt.% of ^{235}U)	Number of Gadolinia Pins (wt.% of Gd_2O_3/ ^{235}U)	Number of FA in the Core
U13	312/1.3	--	48
U22	312/2.2	--	42
U30Y9	303/3.0	9 (8.0/2.4)	37
U39A9	243/4.0, 60/3.6	9 (5.0/3.3)	24
U39B6	240/4.0, 66/3.6	6 (5.0/3.3)	12

Due to the large absorption cross section for thermal neutrons Gd bearing fuel pellets deplete by layers from the outside to the inside (**„onion-skin“ effect**) → differences in the flux shape across the fuel pin → **manual subdivision** of the Gd region into a number of **annular zones of equal area**




```
=t-depl parm=(addnux=2)
39AU9
v7.1-252

read comp
' type_1: he
 He-3          2 0 2.68563e-11     578.0 end
 He-4          2 0 2.68563e-05     578.0 end
' type_1: uo2_enrichment_4.0
 O-16          3 0 4.57890e-02     900.0 end
 U-235         3 0 9.27010e-04     900.0 end
 U-238         3 0 2.19670e-02     900.0 end
' Type_1: he
 He-3          4 0 2.68563e-11     578.0 end
 He-4          4 0 2.68563e-05     578.0 end
' Type_1: cladding e110
 Hf-174        5 0 1.76794e-08     616.6 end
 Hf-176        5 0 5.81211e-07     616.6 end
 Hf-177        5 0 2.05523e-06     616.6 end
 Hf-178        5 0 3.01434e-06     616.6 end
 Hf-179        5 0 1.50496e-06     616.6 end
 Hf-180        5 0 3.87622e-06     616.6 end
 Nb-93         5 0 4.24567e-04     616.6 end
 Zr-90         5 0 2.20133e-02     616.6 end
 Zr-91         5 0 4.80056e-03     616.6 end
```

```
read celldata
latticecell atriangpitch pitch=1.275 6 imodr=0.06 2 fuelr=0.38 3 gapr=0.3865 4 cladr= 0.455 5 end
multiregion cylindrical right=white end
 7 0.06000
 8 0.13297
 9 0.17821
 10 0.21410
 11 0.24479
 12 0.27203
 13 0.29678
 14 0.31962
 15 0.34094
 16 0.36100
 17 0.38000
 18 0.38650
 19 0.45500
 20 0.57974 end zone
latticecell atriangpitch pitch=1.275 28 imodr=0.06 24 fuelr=0.38 25 gapr=0.3865 26 cladr=0.455 27 end
end celldata
```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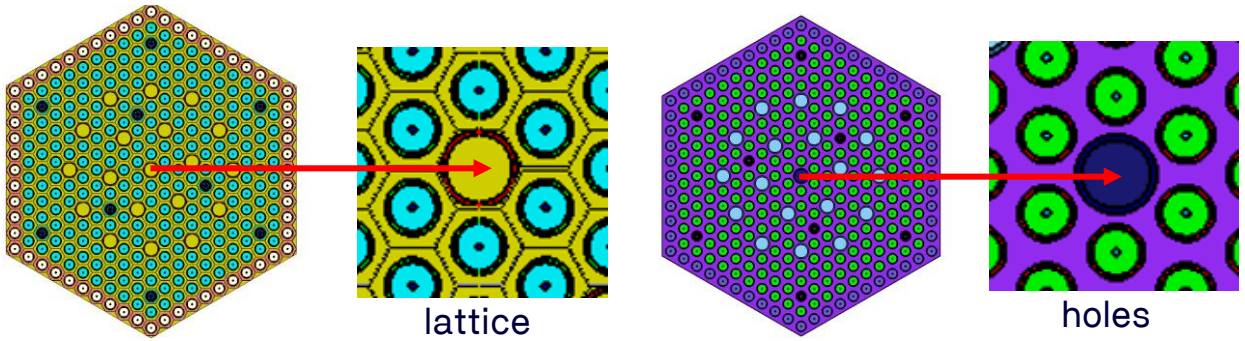
Generation of Cross Section Library for Reactor Burnup Calculations with TRITON/NEWT

To avoid geometry errors we used **holes** (**not lattice!**) in order to place individual fuel pins within the hexagonal fuel assembly → calculation of the position of each pin by a modeler → long input




```
56305 ##################################################################################################################
56306 #                                   End Section: TRITON Isotopics Summary (via ORIGEN/OPUS)                      #
56307 ##################################################################################################################
56308
56309
56310
56311 Sequence T-Depl is finished. completion code 0.
```

Pre- and post-processing of branching calculations by **self-developed programs** (e.g. IDL) necessary

```
527 global unit 6
528
529 hexprism 1 11.755
530 hole 5 origin y=-12.750 x=0.0
531 hole 5 origin y=-12.113 x=1.104
532 hole 5 origin y=-11.475 x=2.208
533 hole 5 origin y=-10.838 x=3.313
534 hole 5 origin y=-10.200 x=4.417
535 hole 5 origin y=-9.563 x=5.521
536 hole 5 origin y=-8.925 x=6.625
537 hole 5 origin y=-8.288 x=7.729
538 hole 5 origin y=-7.650 x=8.833
539 hole 5 origin y=-7.013 x=9.938
540 hole 5 origin y=-6.375 x=11.042
541 hole 5 origin y=-12.113 x=-1.104
542 hole 1 origin y=-11.475 x=0.0
543 hole 1 origin y=-10.838 x=1.104
544 hole 1 origin y=-10.200 x=2.208
545 hole 1 origin y=-9.563 x=3.313
546 hole 1 origin y=-8.925 x=4.417
547 hole 1 origin y=-8.288 x=5.521
548 hole 1 origin y=-7.650 x=6.625
549 hole 1 origin y=-7.013 x=7.729
550 hole 1 origin y=-6.375 x=8.833
551 hole 1 origin y=-5.738 x=9.938
552 hole 5 origin y=-5.100 x=11.042
553 hole 5 origin y=-11.475 x=-2.208
554 hole 1 origin y=-10.838 x=-1.104
555 hole 2 origin y=-10.200 x=0.0
556 hole 1 origin y=-9.563 x=1.104
```

312 positions

```
841 hole 1 origin y=7.012 x=-7.729
842 hole 1 origin y=7.650 x=-6.625
843 hole 1 origin y=8.287 x=-5.521
844 hole 1 origin y=8.925 x=-4.417
845 hole 1 origin y=9.562 x=-3.313
846 hole 1 origin y=10.200 x=-2.208
847 hole 1 origin y=10.837 x=-1.104
848 hole 1 origin y=11.475 x=0.0
849 hole 5 origin y=12.112 x=1.104
850 hole 5 origin y=6.375 x=-11.042
851 hole 5 origin y=7.013 x=-9.938
852 hole 5 origin y=7.650 x=-8.833
853 hole 5 origin y=8.287 x=-7.729
854 hole 5 origin y=8.925 x=-6.625
855 hole 5 origin y=9.562 x=-5.521
856 hole 5 origin y=10.200 x=-4.417
857 hole 5 origin y=10.838 x=-3.313
858 hole 5 origin y=11.475 x=-2.208
859 hole 5 origin y=12.112 x=-1.104
860 hole 5 origin y=12.750 x=0.0
861 hexprism 2 11.8
862 media 6 1 1
863 media 1 1 2 -1
864 boundary 2 44 44
865 end geometry
866
867 read bounds
868  all=white
869 end bounds
870
871 end model
872 end
```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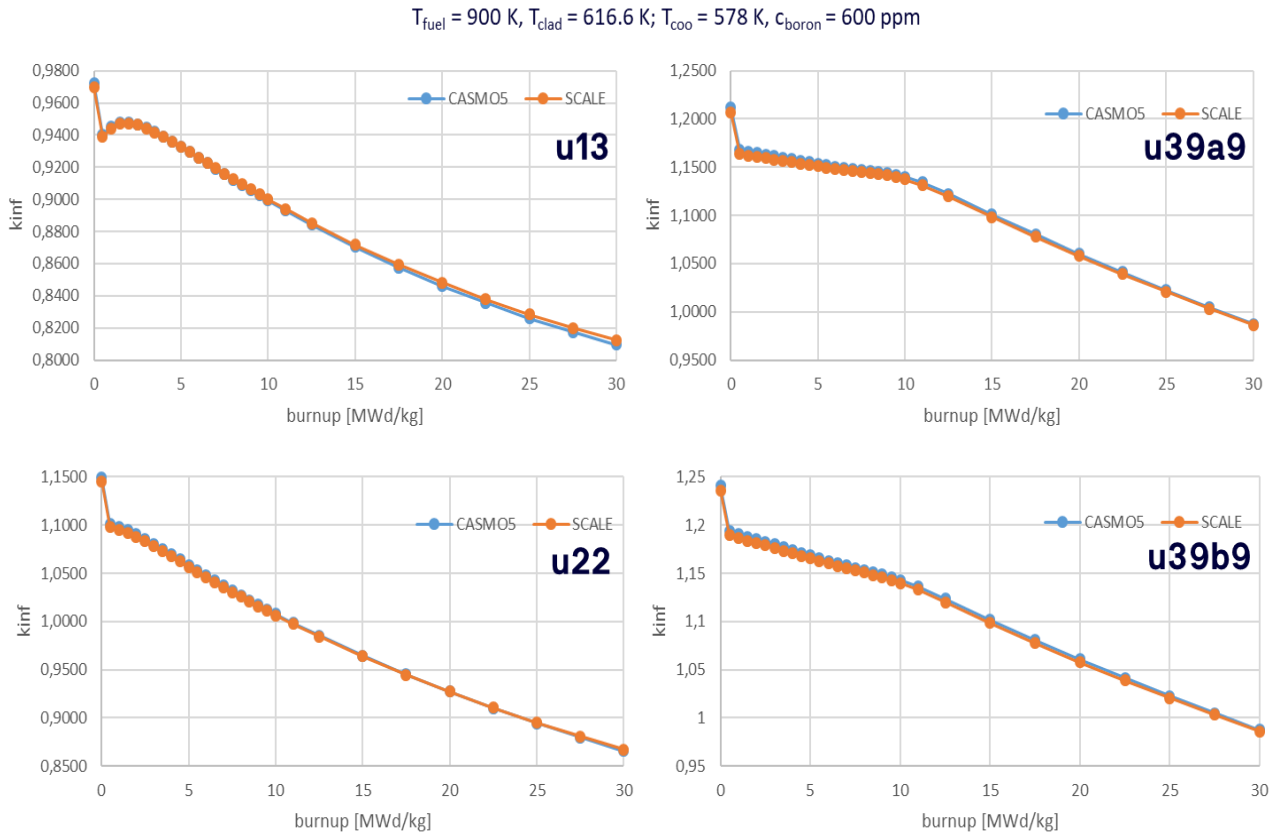
Generation of Cross Section Library for Reactor Burnup Calculations with TRITON/NEWT

We used two different computational paths for the cross section library generation: **TRITON/NEWT** from SCALE 6.2.4 and **CASMO5** (Studsvik Scandpower).

Both approaches are **appropriate** for the neutron physical description of the hexagonal fuel assemblies and provide **the necessary quality for the reactor simulation**.



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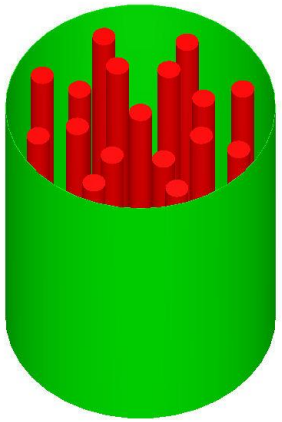
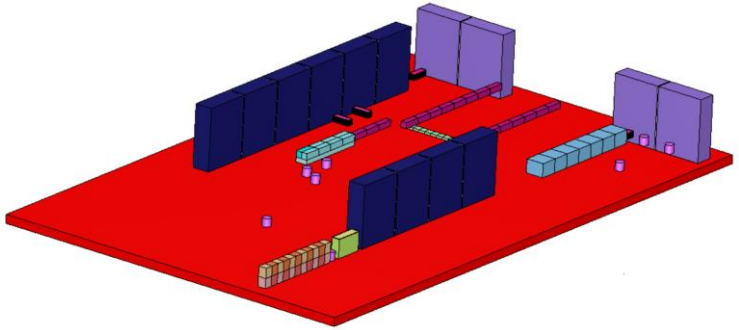
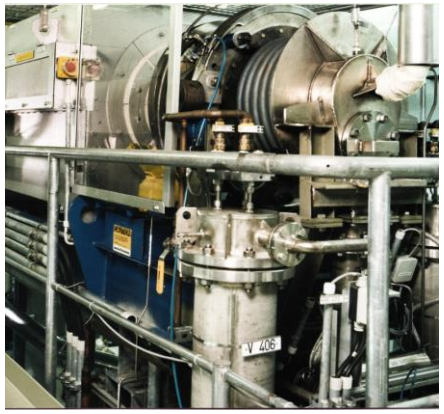
Criticality Safety Assessment in a Fuel Fabrication Plant with KENO

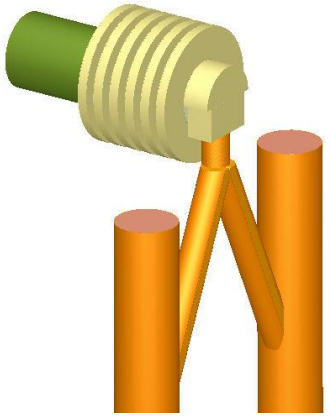
Criticality safety analyses:

- Demonstration of the compliance with the safety requirements
- Identification of ways of further reducing risk at different assembly production stages









An accurate modeling of complex structures

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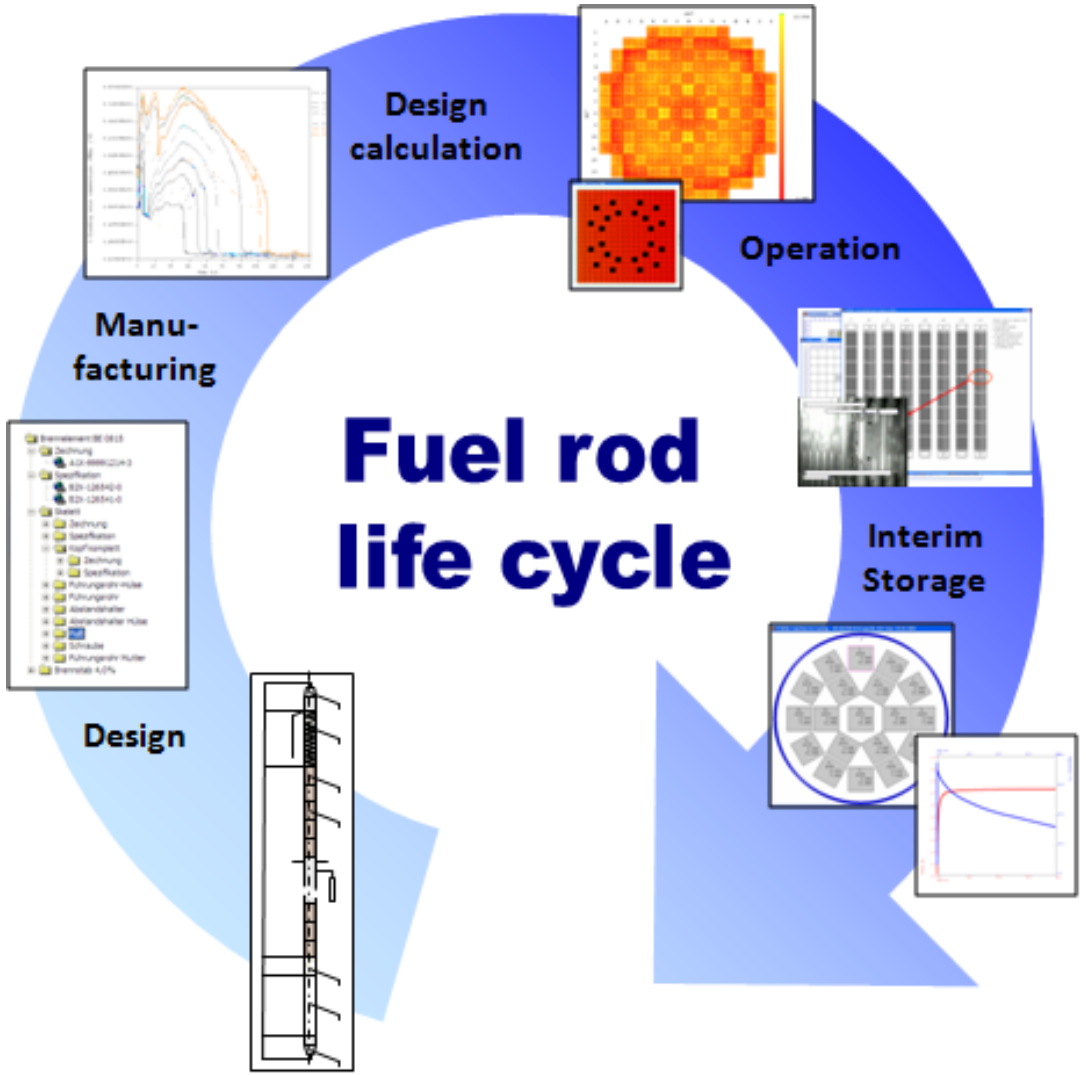
Spent fuel calculations

- At the end of their life cycle, **spent fuel assemblies** are loaded into casks for **storage**
- Calculation of relevant spent fuel **properties** (e.g. activity, decay heat) is required to assess compliance with **regulatory limits**
- **Input of data** from the fuel life cycle:
  - **Geometry** and **material composition** of fuel assemblies are based on design specification
  - **Burnup history** is based on information collected during NPP operation



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TRITON Code Sequence

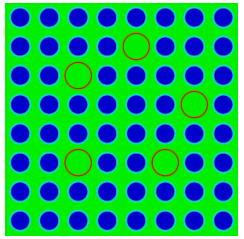
- Input of
  - fuel assembly **design parameters**
    - material composition and fuel enrichment
    - geometry and dimensions
  - **operational data** of fuel assembly type
    - average power
    - time steps until maximum burnup

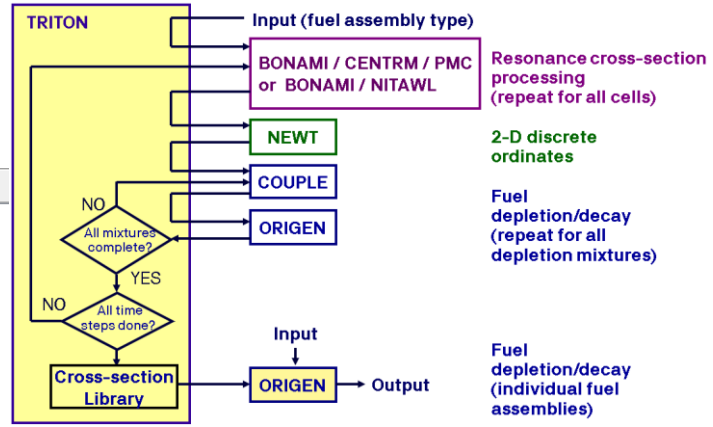
- Calculation using 252-group neutron cross section library based on ENDF/B-VII

- Output of **problem-specific cross section library**

SCALE 6.2 Run View Edit

```
read comp
' fuel
  uo2    1 den=10.4 1 873  92235  4.000
                           92238 96.000 end
' clad
  zirc4 2 1 625 end
' water
  h2o    3 den=0.702 1.000000 585 end
  boron 3 den=0.702 0.000500 585 end
end comp
' ----------------------------------------
read celldata
  latticecell squarepitch fueld=0.90 1
                          gapd= 0.95 4
                          cladd=1.10 2
                          pitch=1.45 3 end
end celldata
' ----------------------------------------
read burndata
  power=40.00  burn=90 down=0   end
  power=40.00  burn=90 down=0   end
  power=40.00  burn=90 down=0   end
  power=40.00  burn=90 down=0   end
end burndata
'
```






```
com='guide tube'
  cylinder  1 0.60
  cylinder  2 0.65
  cuboid    3 4p0.715
  media 3 1 1
  media 5 1 2 -1
  media 3 1 3 -2
  boundary 3 4 4
global unit 10
com='1/4 assembly'
  cuboid 1  12 0 12 0
  array 1 1 place 1 1 0.715 0.715
  media 3 1 1
boundary 2 32 32
end geom
'
read array
  ara=1 nux=8 nuy=8 typ=cuboidal
  fill
  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1
  1  1  2  1  1  2  1  1
  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  2  1
  1  1  2  1  1  1  1  1
  1  1  1  1  2  1  1  1
  1  1  1  1  1  1  1  1  end fill
end array
```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ORIGEN Depletion and Decay Code

- Input of
  - **cross section library** generated by TRITON
  - data of **individual fuel assembly**
    - material composition
    - irradiation history

- **Depletion** (fuel), **activation** (structures) and **decay** calculations

- Output of **spent fuel properties** (decay heat, activity, n- and γ-source terms)

- **Script-based** analysis of output files

document | SCALE 6.2 | Run | View | Edit

```
case(irrad_1){
lib {
file="ft33f001" pos=1
}

mat {
units=GRAMS
iso=[
U235=39773
U238=960227

 O=135125
Al=2750
 C=250
Ca=125
Co=70
Cr=11450
Fe=37540 ]
}

time={
units=DAYS
start=0
t=[ 8i 0 335.3 ]
}
power=[ 10r 45.20 ]
}

case(decay_1){
lib {
file="end7dec" pos=1
}
time{
units=DAYS
start=0
t=[ 0.01 0.03 0.1 0.3 1 3 10 15 ]
}
gamma{ sublib=ALL brem_medium=UO2 }
neutron{ alphan_medium=UO2 }
}

case(irrad_2){
lib {
file="ft33f001" pos=2
}
time={
```


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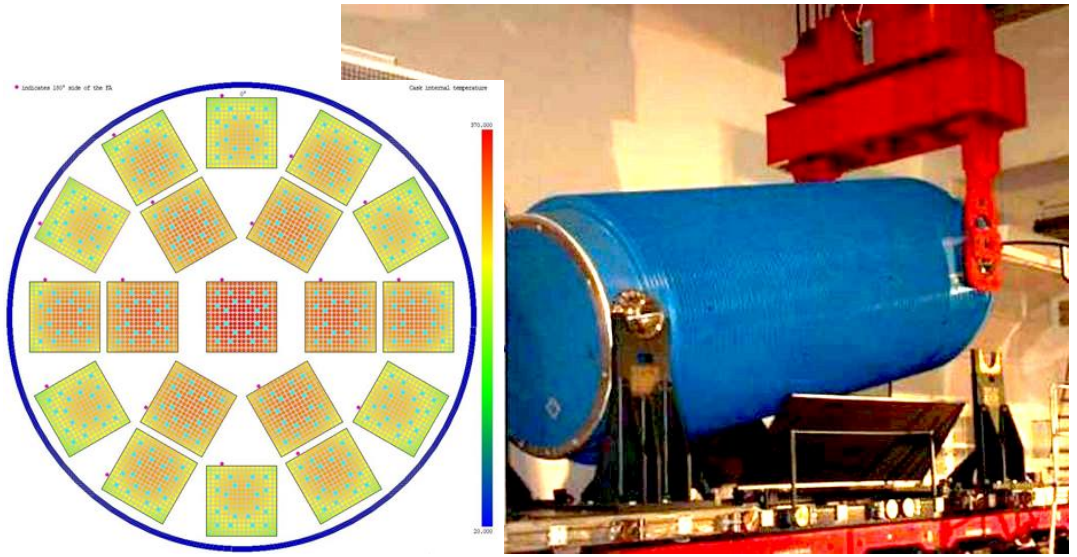
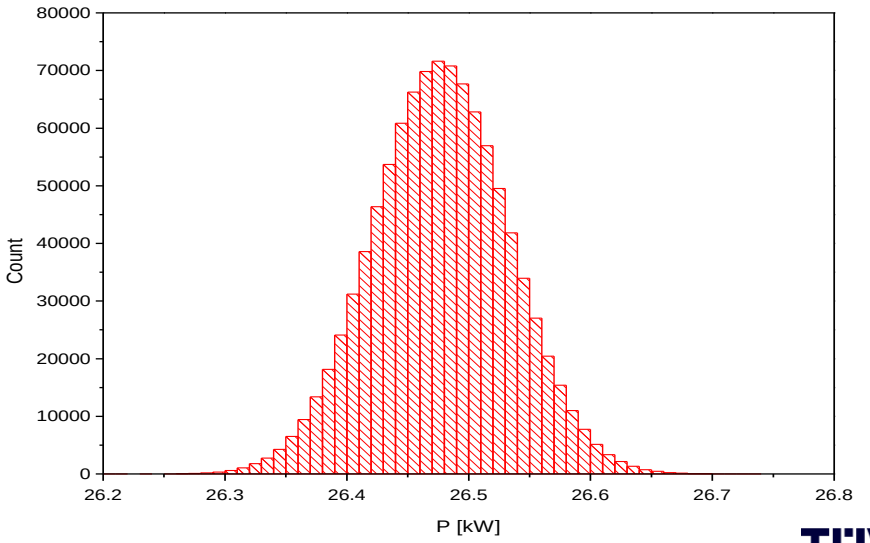
Statistics of uncertainties

- 19 fuel assemblies loaded in **cask**, individual values of each spent fuel parameter (e.g. decay heat) add up to **total value** of the cask

- Consideration of **burnup uncertainties**:
  - **Conservative addition** of maximum values for each fuel assembly results in overly conservative integral parameters, which can exceed regulatory limits
  - **Statistical analysis** of cask loading parameters
    - script-driven Monte Carlo-like **simulation** of the cask loading, combining normally distributed burnup uncertainties of each fuel assembly
    - **probability distribution** of the integral value





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Activation Calculations with SCALE

Radioactive Waste Storage

Radionuklid	Abfallbehälterklasse I						Abfallbehälterklasse II
	Abfallproduktgruppe						Abfallproduktgruppe
	01	02	03	04	05	06	01-06
H-3	2,1E+14	2,1E+14	2,1E+14	2,1E+14	4,4E+14	2,1E+14	5,4E+16
Be-10	8,6E+11	4,3E+13	1,1E+14	2,7E+14	8,6E+14	8,6E+14	2,1E+16
C-14	1,0E+12	1,0E+12	1,0E+12	1,0E+12	2,1E+15	2,1E+15	1,7E+14
S-35	2,4E+11	8,7E+12	3,1E+13	7,7E+13	2,4E+14	2,4E+14	6,1E+15
Ar-39	2,9E+16	2,9E+16	2,9E+16	2,9E+16	2,9E+16	2,9E+16	7,1E+17
Ca-41	1,6E+10	5,4E+11	2,0E+12	5,0E+12	1,6E+13	1,6E+13	4,0E+14
Ca-45	1,1E+11	3,7E+12	1,3E+13	3,4E+13	1,1E+14	1,1E+14	2,7E+15
Sc-46	1,3E+11	4,7E+12	1,7E+13	4,1E+13	1,3E+14	1,3E+14	3,3E+15
V-49	7,0E+13	2,4E+15	8,7E+15	2,1E+16	7,0E+16	7,0E+16	1,7E+18
Cr-51	1,2E+13	4,3E+14	1,6E+15	3,7E+15	1,2E+16	1,2E+16	3,0E+17
Mn-54	8,6E+10	3,0E+12	1,1E+13	2,7E+13	8,6E+13	8,6E+13	2,1E+15
Fe-55	1,4E+13	4,9E+14	1,7E+15	4,3E+15	1,4E+16	1,4E+16	3,4E+17
Co-57	7,0E+11	2,4E+13	8,7E+13	2,1E+14	7,0E+14	7,0E+14	1,7E+16
Co-58	3,1E+11	1,1E+13	3,9E+13	9,7E+13	3,1E+14	3,1E+14	7,9E+15
Fe-59	4,1E+11	1,4E+13	5,1E+13	1,3E+14	4,1E+14	4,1E+14	1,0E+16
Ni-59	7,6E+11	2,7E+13	9,3E+13	2,3E+14	7,6E+14	7,6E+14	1,9E+16
Ni-63	7,0E+11	2,4E+13	8,7E+13	2,1E+14	7,0E+14	7,0E+14	1,7E+16
Zn-65	2,3E+10	8,0E+11	2,9E+12	7,3E+12	2,3E+13	2,3E+13	5,7E+14
Kr-85	2,1E+16	2,1E+16	2,1E+16	2,1E+16	2,1E+16	2,1E+16	5,6E+17
Sr-89	3,9E+11	1,4E+13	4,9E+13	1,2E+14	3,9E+14	3,9E+14	9,7E+15
Mo-93	7,6E+10	2,6E+12	9,4E+12	2,3E+13	7,6E+13	7,6E+13	1,9E+15
Nb-93m	4,7E+11	1,7E+13	5,9E+13	1,4E+14	4,7E+14	4,7E+14	1,2E+16
Zr-93	2,4E+11	8,9E+12	3,1E+13	7,9E+13	2,4E+14	2,4E+14	6,3E+15
Zr-95	2,1E+11	7,4E+12	2,7E+13	6,7E+13	2,1E+14	2,1E+14	5,4E+15

→ Calculation of Activities with SCALE

- Germany is phasing out nuclear power
- „Requirements on Radioactive Waste for Disposal (Waste Acceptance Requirements as of December 2014) - Konrad Repository" of the „Federal Office for Radiation Protection"
- Contains limits for the activity of 197 Nuclides in a container defined for normal, accidental, thermal impact conditions

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Activation Calculations with SCALE

Procedure for Activity Calculation

First step:

Transport Calculation with **MONACO / MAVRIC** or **MCNP / ADVANTG**

Neutron Fluxes /Reaction Rates

Second step:

Construction of a One-Group-cross section-Library with **COUPLE**

1g-XS-Library

Third step:

Calculating the Activity with **ORIGEN**

SCALE

File Edit View Run Help

Reload Save Save as Close tab Print Cut Copy Paste Undo Redo Find

act_Example.inp

document SCALE 6.2 Run View Edit

```
=origen
   % Activation of steel

   % Choose the solver typ
   solver{
      type=CRAM   %MATREX
      opt{
         %terms=21
         %maxp=150
         order=16    % Orde
         % 2-4 substeps re
         substeps=3 % Numb
      }
   }

   options{
      print_xs=no
      digits=4
      fixed_fission_energy
   }
   bounds{
      neutron="origen.rev0
      alpha  = [9I 2e7 2e3
      beta   = [9I 2e7 2e3
      gamma  = [9L 5.0e7 5
   }

   case(irr){
      title="Irradiation i

      lib{
         file="${INPDIR}\E
      }
      mat{
         lib{
            file="${INPDIR}\Example.lib"
         }
         mat{
            units="GRAMS"
            iso=[ Li=3.00E-06 C=0.400 N=0.44
                  P=0.270 S=0.230 Ti=0.19 V=
                  Mn=15.0 Fe=694.1 Co=0.50 N
                  Ta=0.2 W=0.01 Pb=0.01 U-23
                  U-238=7.2000E-08
            ]
         }
         time =[
          466   500  836    890  1256  1291
         2614  2662  3055  3126  3496  3543
         4336  4370  4735  4756  5092  5124
         6193  6208  6550  6576  6977  6992
         7920  7927  8083  8110  8294  8299
         9231  9257  9595  9638  9721  9734
        10609 10634 10775 10784 10885 10898 1
        11706 11741 12008 12031 12339 ]

         flux =[ 9.44581E+09 0 1.07684E+10 0
                 1.01657E+10 0 1.01525E+10 0
                 9.95434E+09 0 9.66922E+09 0
                 1.03226E+10 0 1.07246E+10 0
                 1.10849E+10 0 1.13792E+10 0
                 1.15229E+10 0 1.13013E+10 0
                 1.11830E+10 0 1.08329E+10 0
                 1.14547E+10 0 1.12984E+10 0
                 1.12947E+10 0 1.12197E+10 0
                 1.10050E+10 0 1.02135E+10 ]

         %print{
            %nuc{ total=yes units=[GRAMS BECQ
            %gamma{ summary=yes }
            %cutoffs=[GRAMS=1E-5]
         %}
         save{
            file="Example.f71"
            steps=ALL
         }
      } % End Irradiation Case

      case(dec){
         title="Cool-down"

         % lib and mat can be omitted to cause ORIGEN to use
         % I found that end7dec gave higher gamma activities
         lib{
            file="end7dec"
         }
         % Cool-down
         time ={
           % Without start, times must be entered > 60 days b
           % start at 0. When printing the output, it will ad
           % below, with the first column being at time 0 (la
           % number of columns should be right, though.
           start = 0
           t     =[1827 2192 3288] % days
         }
         flux =[3R 0] % 0 flux means decay only

         print{
            nuc{ total=yes units=[GRAMS BECQUERELS] }
            cutoffs=[ALL=1E-16]
         }
         save{
            file="Example_cool.f71"
            steps=ALL
            time_offset=0
            time_units=DAYS
         }

         neutron=yes % options control the (alpha,n) reaction
         alpha=yes   % no options. This determines sources of
         beta=yes    % only option: pick sublibs. Like alpha,
         gamma=yes   % defaults are generally appropriate, wi
      } % End Cool-Down Case
end

=opus
data="Example_cool.f71"
title="Example"
typarams=NUCLIDES
time=DAYS
units=BECQUERELS
SORT=YES
```


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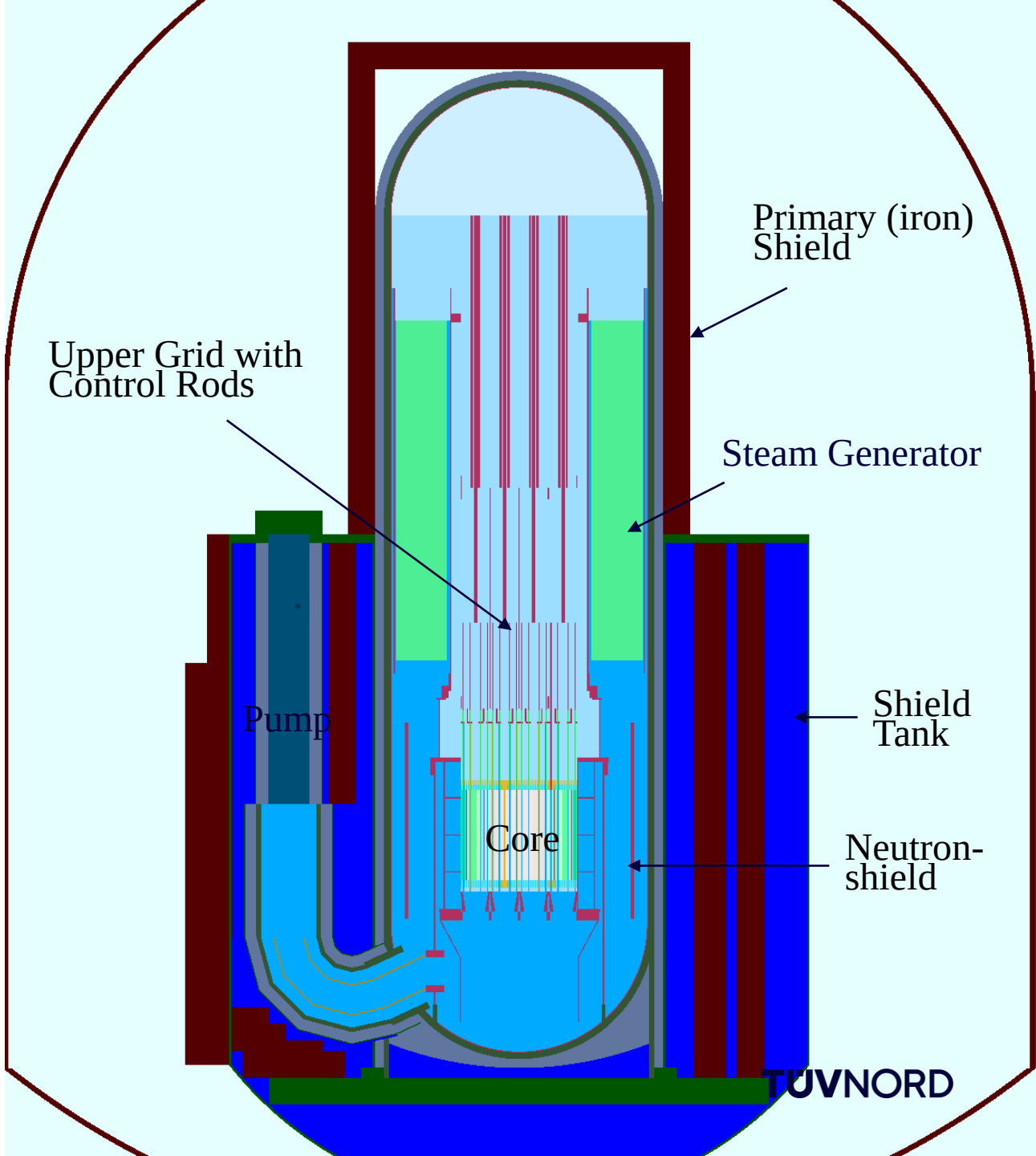
Flux Calculations with MAVRIC

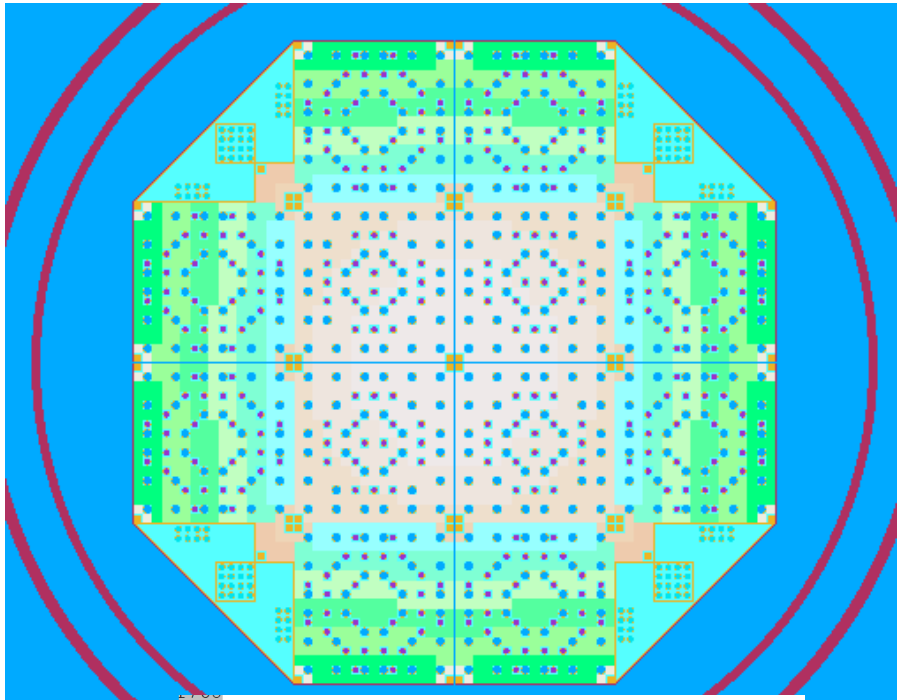
- Example of a prototype ship reactor:
  - Fuel: UO2 with 3.5% to 6% U-235
  - 12 Fuel assemblies (17x 17)
  - Active height 83 cm
  - Integral design with steam generators inside RV (homogenized)
  - 3 primary pumps (homogenized)
  - Shield tank with water and iron cask layers

- Geometry modelling (user perspective):
  - Visualization with fulcrum (3D-missing)
  - No torus as macro body
  - Careful with holes inside holes if the bounding surface is the same



Source Definition

- Activation of structure components most sensitive against outer core regions (different loading patters can lead to changes in the activation by up to a factor of ~2)
- 7 different fuel zones with power peaking factors from operational data
- Axial power profile from average axial burn up profile
- Higher burnup leads to higher total fluxes but harder spectrum
- Energy distribution from TRITON burnup calculation for average burn up (or U-235 fission Watt-spectrum)
- Energy group structure should match group structure for variance reduction and/or desired tally structure
- If not enough operational data is available the source distribution can be generated with KENO



```
read sources

 src 1
  title="Radiale Zone:1"
  neutron
  strength=2.42e+017
  cuboid 17.38 -17.38 17.38 -17.38 83.0 0.0
  mixture=101
  edistributionid=1
  zdistributionid=10
 end src

 src 2
  title="Radiale Zone:2"
  neutron
  strength=2.60e+017
  cuboid 23.7 -23.7 23.7 -23.7 83.0 0.0
  mixture=102
  edistributionid=1
  zdistributionid=10
 end src

 src 3
  title="Radiale Zone:3"
  neutron
```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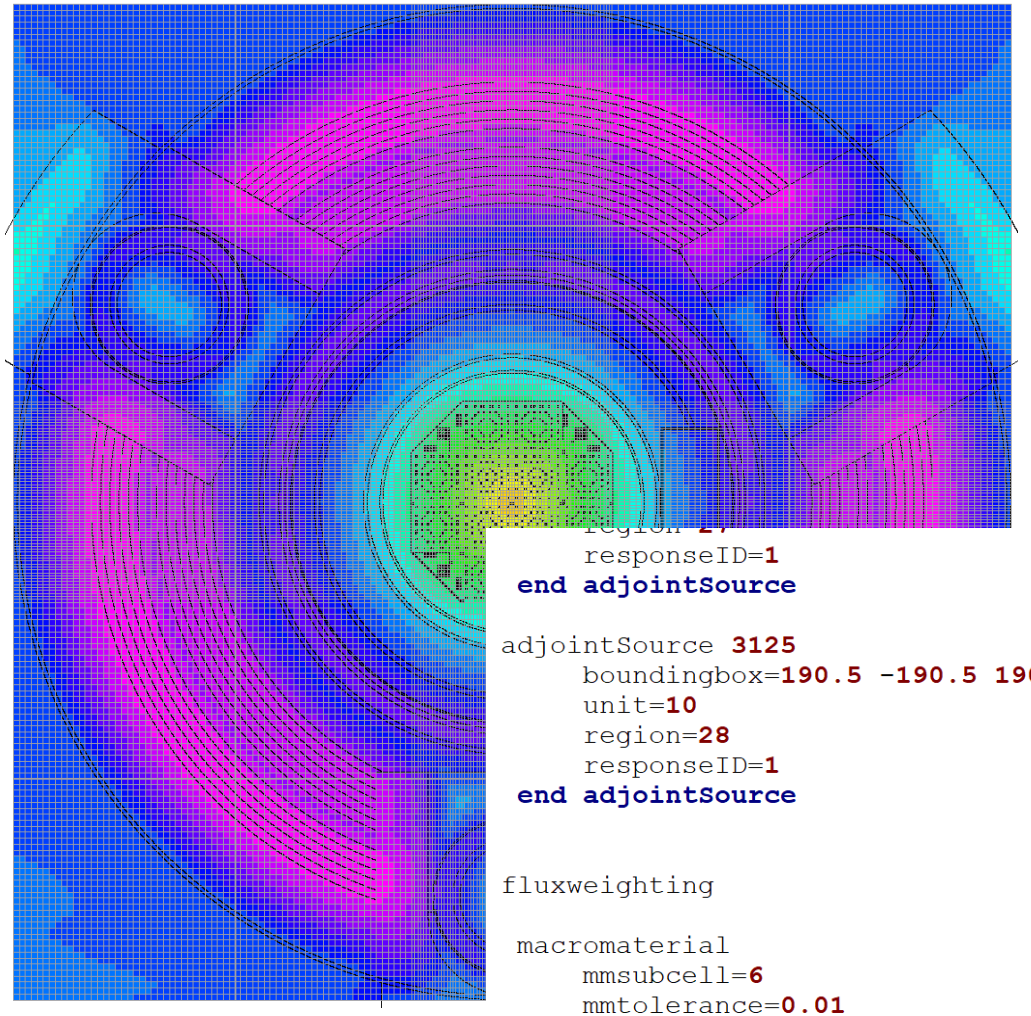
Variance reduction

- Forward CADIS
- Example: Importance map for calculating the flux in the primary shield (core midplane; epithermal)
- Usually requires several computations due to memory and time restrictions (forward and adjoint map can become larger than 1 GB)
- Grid needs to resolve source regions and important geometric boundaries
- Should cover at least the next reflecting/shielding material
- Coarser meshes require higher resolution in macro material block
- Adjoint sources placed in region of interest or behind (donkey and carrot principle)



```
    region=27
    responseID=1
end adjointSource

adjointSource 3125
    boundingbox=190.5 -190.5 190.5
    unit=10
    region=28
    responseID=1
end adjointSource


fluxweighting

 macromaterial
    mmsubcell=6
    mmtolerance=0.01
    mmRayTest
end macromaterial
```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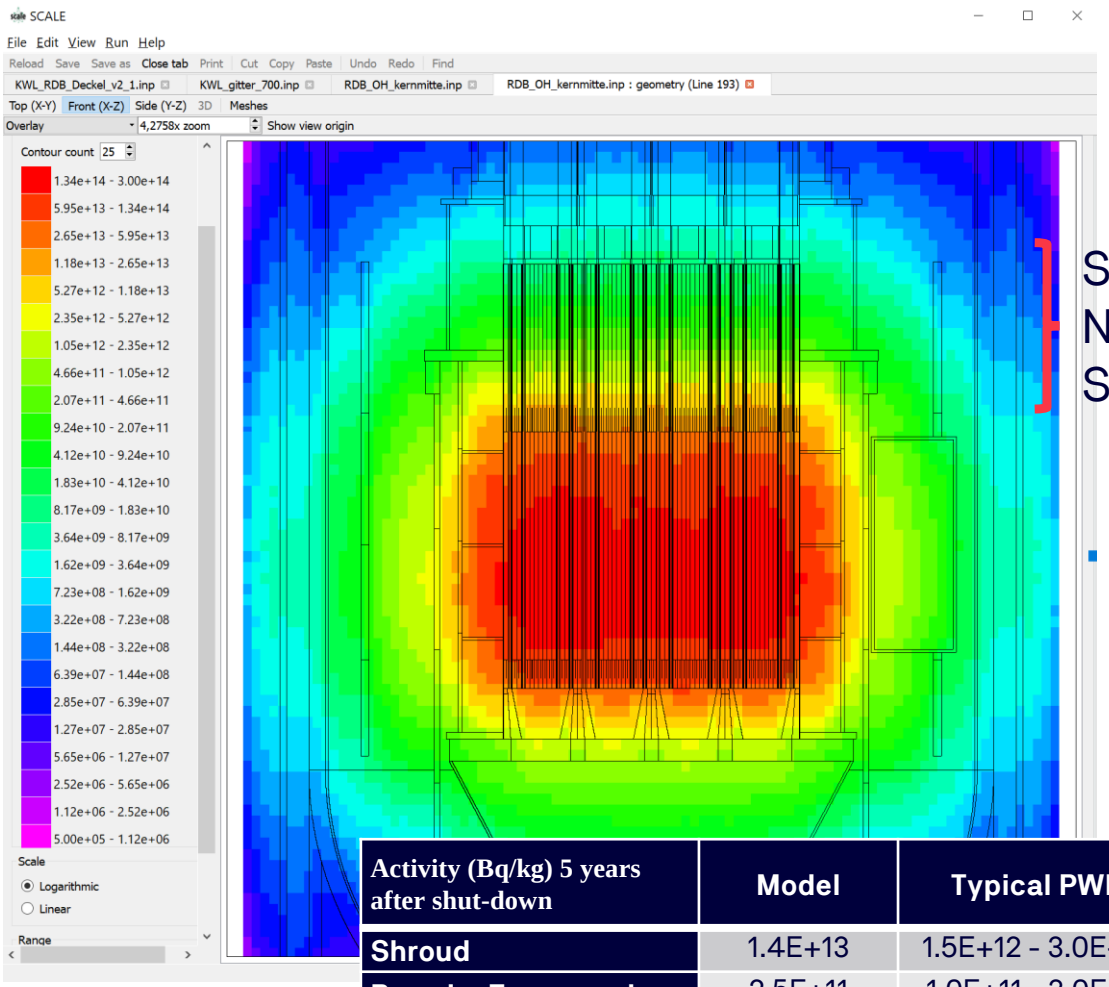
Tallies and Results

- Mesh Tallies to check flux distribution
- For large tallies use at most 3 energy groups (mesh tallies can easily reach 50 to a 100 MB)
- For the calculation of the fluxes in the components prefer region tallies due to better statistical control and simpler processing for activation calculation
- Structures need to be subdivided (rule of thumb: 10 - 50 cm axially and 3 -10 cm radially)
- Energy group structure should match group structure in COUPLE (usually 56g are sufficient)
- Uncertainty below 5% in the relevant energy groups
- Validation with measurements (or e.g. 1D-calculations in the core midplane)



Section Neutron Shield

Activity (Bq/kg) 5 years after shut-down	Model	Typical PWR
Shroud	1.4E+13	1.5E+12 - 3.0E+12
Barrel + Formers along Active Zone	2.5E+11	1.0E+11 - 3.0E+11
Upper Grid Plate	1.8E+10	5.0E+10 - 1.0E+11
Lower Grid	2.0E+10	1.5E+11 - 4.5E+11
Neutron Shield	1.7E+09	-
RV along Active Zone	1.6E+08	1.0E+08 - 3,0E+08

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Activation Calculations with SCALE

Radioactive Waste Storage

Radionuklid	Abfallbehälterklasse I						Abfallbehälterklasse II
	Abfallproduktgruppe						Abfallproduktgruppe
	01	02	03	04	05	06	01-06
H-3	2,1E+14	2,1E+14	2,1E+14	2,1E+14	4,4E+14	2,1E+14	5,4E+16
Be-10	8,6E+11	4,3E+13	1,1E+14	2,7E+14	8,6E+14	8,6E+14	2,1E+16
C-14	1,0E+12	1,0E+12	1,0E+12	1,0E+12	2,1E+15	2,1E+15	1,7E+14
S-35	2,4E+11	8,7E+12	3,1E+13	7,7E+13	2,4E+14	2,4E+14	6,1E+15
Ar-39	2,9E+16	2,9E+16	2,9E+16	2,9E+16	2,9E+16	2,9E+16	7,1E+17
Ca-41	1,6E+10	5,4E+11	2,0E+12	5,0E+12	1,6E+13	1,6E+13	4,0E+14
Ca-45	1,1E+11	3,7E+12	1,3E+13	3,4E+13	1,1E+14	1,1E+14	2,7E+15
Sc-46	1,3E+11	4,7E+12	1,7E+13	4,1E+13	1,3E+14	1,3E+14	3,3E+15
V-49	7,0E+13	2,4E+15	8,7E+15	2,1E+16	7,0E+16	7,0E+16	1,7E+18
Cr-51	1,2E+13	4,3E+14	1,6E+15	3,7E+15	1,2E+16	1,2E+16	3,0E+17
Mn-54	8,6E+10	3,0E+12	1,1E+13	2,7E+13	8,6E+13	8,6E+13	2,1E+15
Fe-55	1,4E+13	4,9E+14	1,7E+15	4,3E+15	1,4E+16	1,4E+16	3,4E+17
Co-57	7,0E+11	2,4E+13	8,7E+13	2,1E+14	7,0E+14	7,0E+14	1,7E+16
Co-58	3,1E+11	1,1E+13	3,9E+13	9,7E+13	3,1E+14	3,1E+14	7,9E+15
Fe-59	4,1E+11	1,4E+13	5,1E+13	1,3E+14	4,1E+14	4,1E+14	1,0E+16
Ni-59	7,6E+11	2,7E+13	9,3E+13	2,3E+14	7,6E+14	7,6E+14	1,9E+16
Ni-63	7,0E+11	2,4E+13	8,7E+13	2,1E+14	7,0E+14	7,0E+14	1,7E+16
Zn-65	2,3E+10	8,0E+11	2,9E+12	7,3E+12	2,3E+13	2,3E+13	5,7E+14
Kr-85	2,1E+16	2,1E+16	2,1E+16	2,1E+16	2,1E+16	2,1E+16	5,6E+17
Sr-89	3,9E+11	1,4E+13	4,9E+13	1,2E+14	3,9E+14	3,9E+14	9,7E+15
Mo-93	7,6E+10	2,6E+12	9,4E+12	2,3E+13	7,6E+13	7,6E+13	1,9E+15
Nb-93m	4,7E+11	1,7E+13	5,9E+13	1,4E+14	4,7E+14	4,7E+14	1,2E+16
Zr-93	2,4E+11	8,9E+12	3,1E+13	7,9E+13	2,4E+14	2,4E+14	6,3E+15
Zr-95	2,1E+11	7,4E+12	2,7E+13	6,7E+13	2,1E+14	2,1E+14	5,4E+15

→ Calculation of Activities with SCALE

- Germany is phasing out nuclear power
- „Requirements on Radioactive Waste for Disposal (Waste Acceptance Requirements as of December 2014) - Konrad Repository" of the „Federal Office for Radiation Protection"
- Contains limits for the activity of 197 Nuclides in a container defined for normal, accidental, thermal impact conditions

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Activation Calculations with SCALE

Procedure for Activity Calculation

First step:

Transport Calculation with **MONACO / MAVRIC** or **MCNP / ADVANTG**

Neutron Fluxes /Reaction Rates

Second step:

Construction of a One-Group-cross section-Library with **COUPLE**

1g-XS-Library

Third step:

Calculating the Activity with **ORIGEN**

SCALE

File Edit View Run Help

Reload Save Save as Close tab Print Cut Copy Paste Undo Redo Find

act_Example.inp

document SCALE 6.2 Run View Edit

```
=origen
   % Activation of steel

   % Choose the solver type. Since CR
   solver{
      type=CRAM   %MATREX
      opt{
         %terms=21
         %maxp=150
         order=16    % Order of method
         % 2-4 substeps results in la
         substeps=3 % Number time ste
      }
   }

   options{
      print_xs=no              % Outpu
      digits=4                 % high-
      fixed_fission_energy=no  % fixed
   }
   bounds{
      neutron="origen.rev01.jeff252g"
      alpha  = [9I 2e7 2e3]
      beta   = [9I 2e7 2e3]
      gamma  = [9L 5.0e7 5.0e-5]
   }

   case(irr){
      title="Irradiation in reactor--

      lib{
         file="${INPDIR}\Example.lib"
      }
      mat{
         units="GRAMS"
         iso=[ Li=3.00E-06 C=0.400 N=0.44
               P=0.270 S=0.230 Ti=0.19 V=
               Mn=15.0 Fe=694.1 Co=0.50 N
               Ta=0.2 W=0.01 Pb=0.01 U-23
               U-238=7.2000E-08
         ]
      }
      time =[
       466   500  836    890  1256  1291
      2614  2662  3055  3126  3496  3543
      4336  4370  4735  4756  5092  5124
      6193  6208  6550  6576  6977  6992
      7920  7927  8083  8110  8294  8299
      9231  9257  9595  9638  9721  9734
     10609 10634 10775 10784 10885 10898 1
     11706 11741 12008 12031 12339 ]

      flux =[ 9.44581E+09 0 1.07684E+10 0
              1.01657E+10 0 1.01525E+10 0
              9.95434E+09 0 9.66922E+09 0
              1.03226E+10 0 1.07246E+10 0
              1.10849E+10 0 1.13792E+10 0
              1.15229E+10 0 1.13013E+10 0
              1.11830E+10 0 1.08329E+10 0
              1.14547E+10 0 1.12984E+10 0
              1.12947E+10 0 1.12197E+10 0
              1.10050E+10 0 1.02135E+10 ]

      %print{
         %nuc{ total=yes units=[GRAMS BECQ
         %gamma{ summary=yes }
         %cutoffs=[GRAMS=1E-5]
      %}
      save{
         file="Example.f71"
         steps=ALL
      } % End Irradiation Case

   case(dec){
      title="Cool-down"

      % lib and mat can be omitted to cause ORIGEN to use
      % I found that end7dec gave higher gamma activities
      lib{
         file="end7dec"
      }
      % Cool-down
      time ={
        % Without start, times must be entered > 60 days b
        % start at 0. When printing the output, it will ad
        % below, with the first column being at time 0 (la
        % number of columns should be right, though.
        start = 0
        t     =[1827 2192 3288] % days
      }
      flux =[3R 0] % 0 flux means decay only

      print{
         nuc{ total=yes units=[GRAMS BECQUERELS] }
         cutoffs=[ALL=1E-16]
      }
      save{
         file="Example_cool.f71"
         steps=ALL
         time_offset=0
         time_units=DAYS
      }

      neutron=yes % options control the (alpha,n) reaction
      alpha=yes   % no options. This determines sources of
      beta=yes    % only option: pick sublibs. Like alpha,
      gamma=yes   % defaults are generally appropriate, wi
   } % End Cool-Down Case
end

=opus
data="Example_cool.f71"
title="Example"
typarams=NUCLIDES
time=DAYS
units=BECQUERELS
SORT=YES
```


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Activation Calculations with SCALE

- Surveillance of the Irradiation Behaviour of Reactor Pressure Vessel (brittle fracture)

- Irradiation of Fe-54 and Nb-93 samples

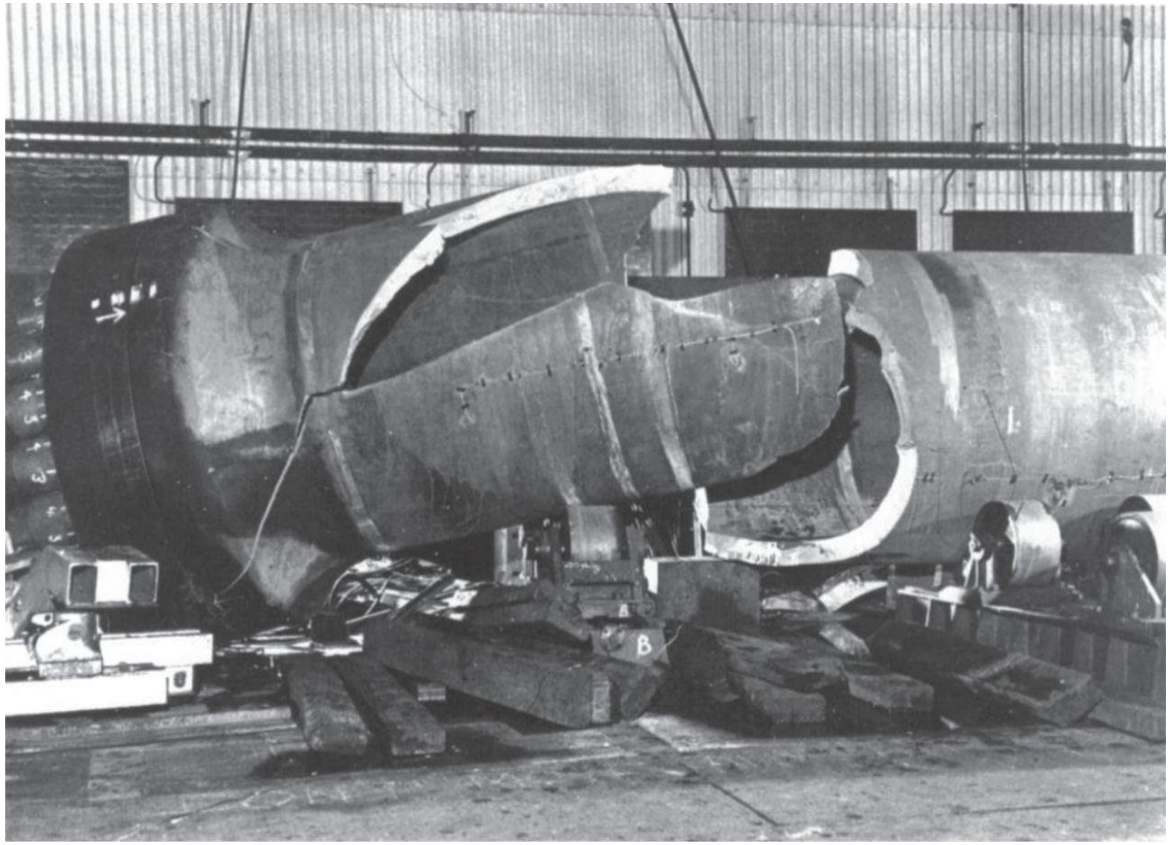
  Neutron reactions

  Fe-54 (n,p) Mn-54 & Nb-93 (n,n') Nb-93m

Comparison of Experimental Data and Calculated Data shows →

Activity Calculation with **ORIGEN** is **underestimating** the **Nb-93m-Activity**

Why?



Picture of the Vessel from: Philosophical Transactions of the Royal Society A "*Brittle fracture in structural steels: perspectives at different size-scales*" by John Knott published 28 March 2015

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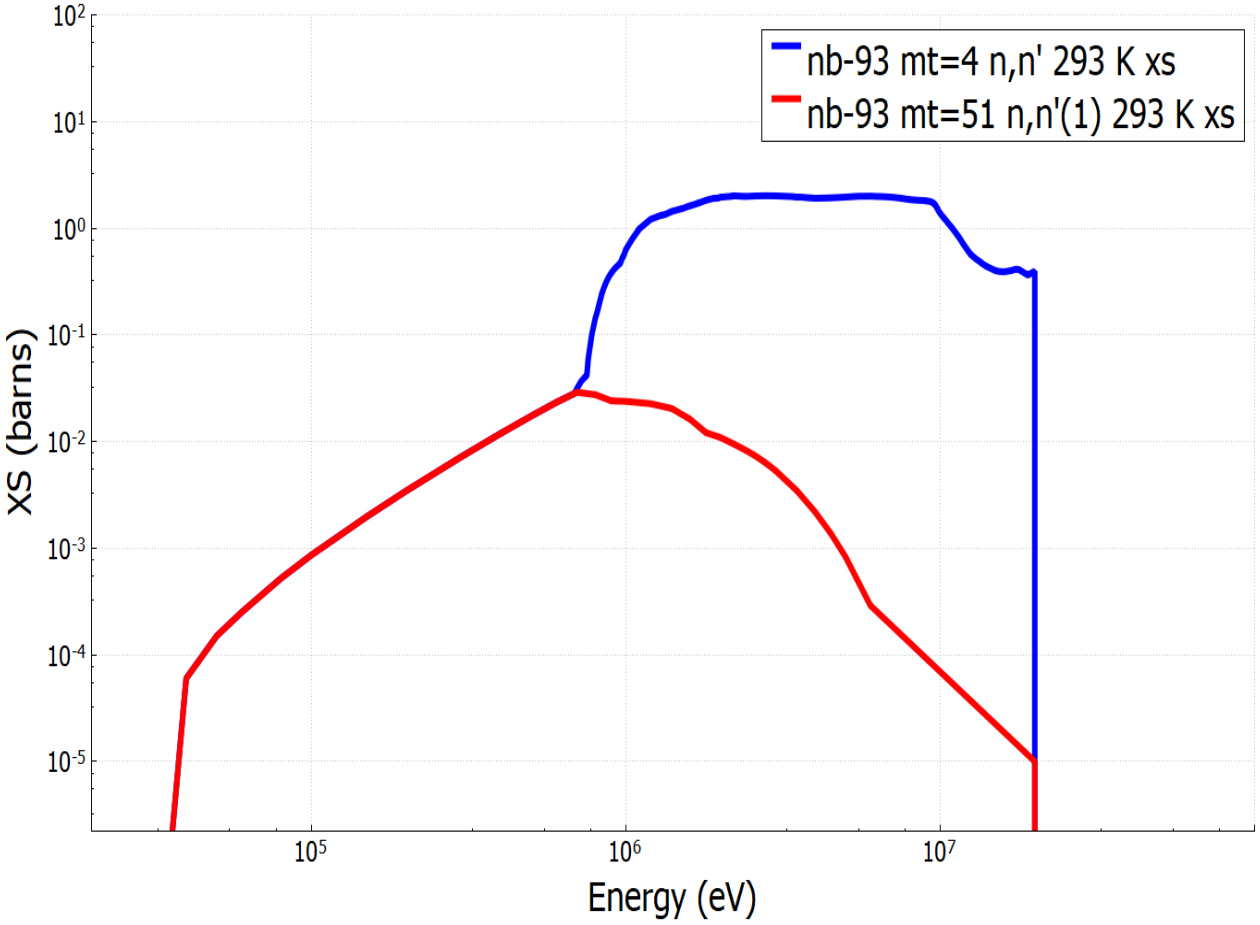
Activation Calculations with SCALE

ANSWER:



- ORIGEN considers in Activity Calculations only the **first excitation state** for Nb-93 excitation
- This can lead to an underestimation of the **Nb-93m activity** up to a factor of **10000!**
- MCNP & FISPACT II show better agreement with the Experimental data
- Maybe in future releases of SCALE this can be corrected.

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Thank you for your Attention

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