Reactor Safety and Criticality Safety analyses with SCALE at GRS

M. Behler, GRS

on behalf of the GRS SCALE Users

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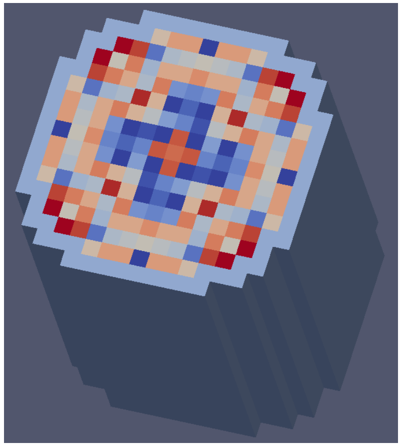
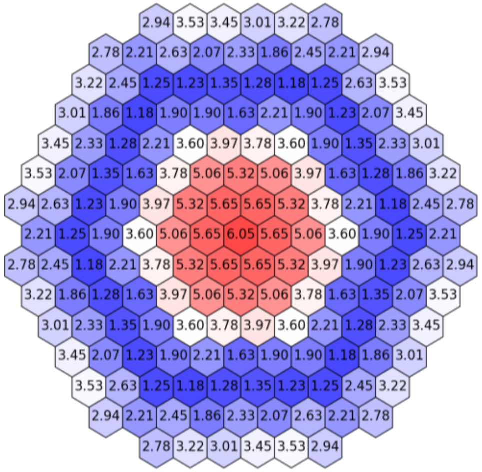
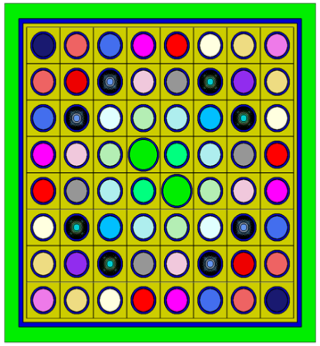
SCALE at GRS

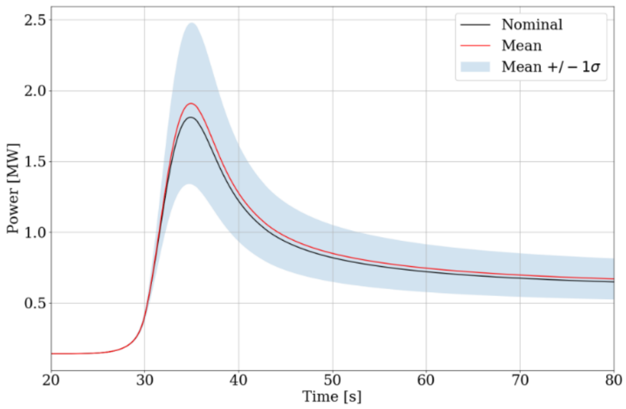
SCALE is one of the main neutronics calculation tools for reactor safety and criticality safety analyses at GRS:

- Reactor safety, e.g.
  - Core behavior, neutronics
    $\Rightarrow$ k_{eff}, control rod worth, power distributions, nuclide inventory, …
  - In combination with GRS tools:
    - S/U analyses
      $\Rightarrow$ GRS S/U analysis tool XSUSA
    - Few group XS generation
      $\Rightarrow$ GRS core simulator KMACS
    - Burn-up / depletion calculations
      $\Rightarrow$ GRS burn-up code MOTIVE





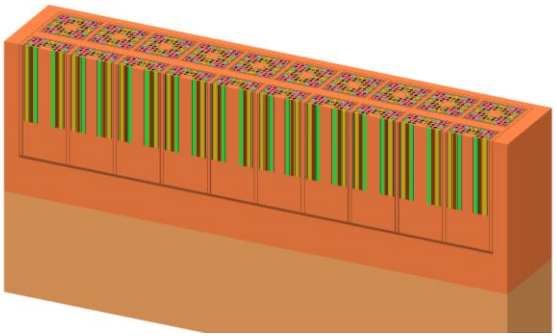


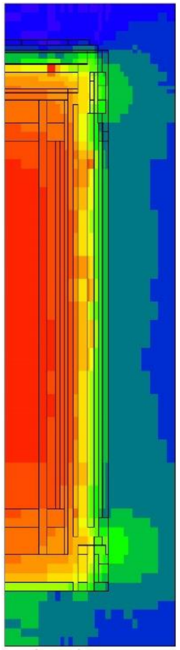


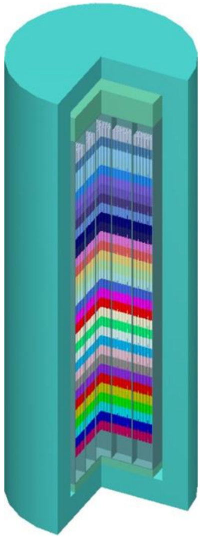
SCALE at GRS

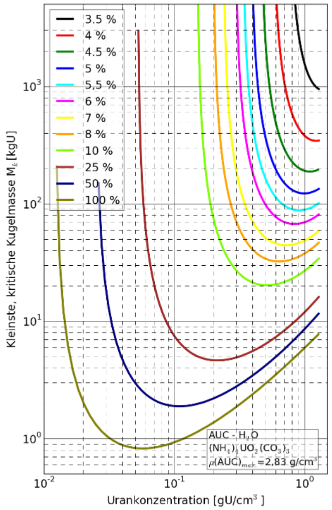
SCALE is one of the main neutronics calculation tools for reactor safety and criticality safety analyses at GRS:

- Criticality safety, e.g.
  - Criticality safety analyses
    $\Rightarrow$ k_{eff} of storage/transport casks, spent fuel pools, ...
  - Critical parameters
    $\Rightarrow$ GRS Handbook of Criticality
  - In combination with GRS tools:
    - S/U analyses
      $\Rightarrow$ GRS S/U analysis tool SUnCISTT
- Shielding, e.g.
  - Shielding analyses
    $\Rightarrow$ Dose rate calculations









Reactor Safety

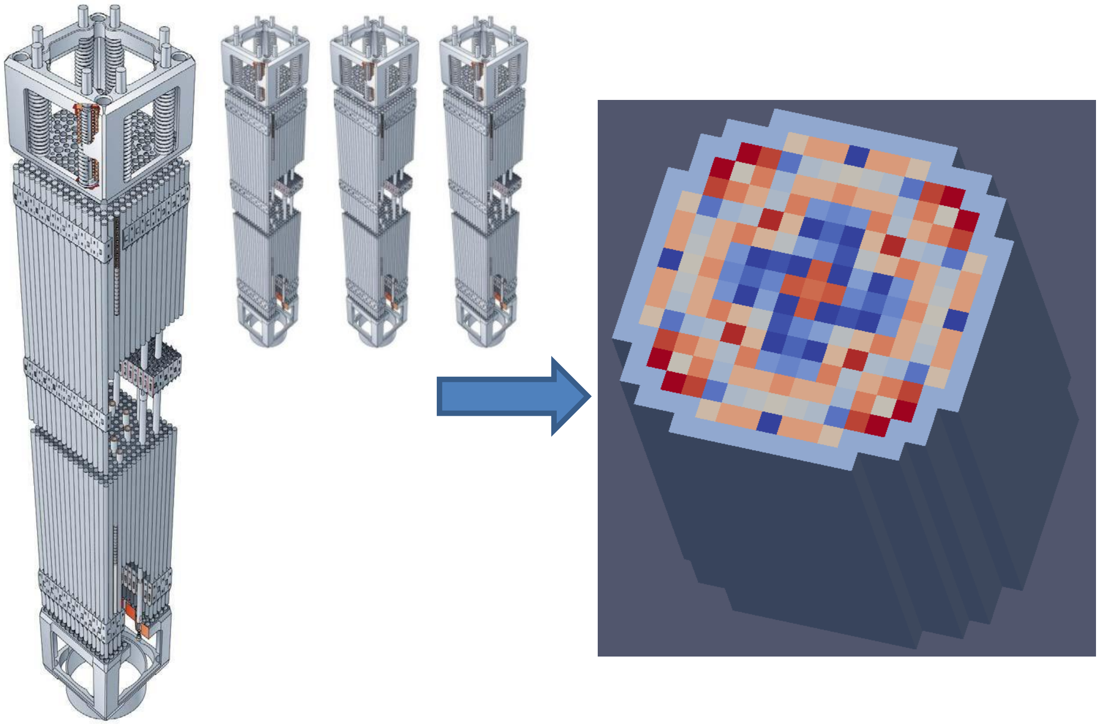
KMACS: The GRS Nodal Core Simulator Concept

1st Step:
Cross-Section Generation

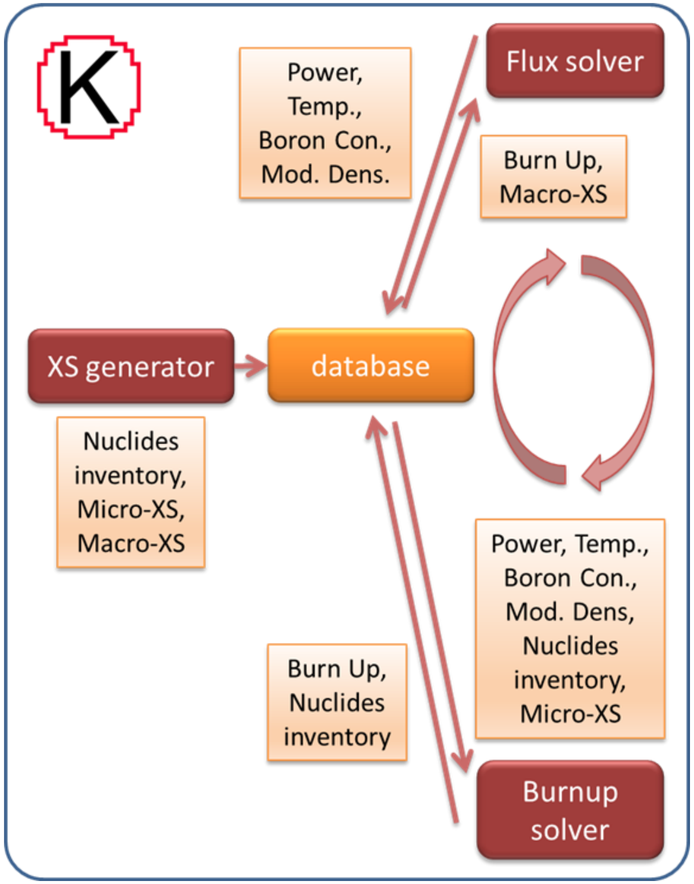
Calculation of the cross sections depending on physical properties of individual fuel assembly types

2nd Step:
Cycle calculation

Simulation of the reactor core in stationary power operation

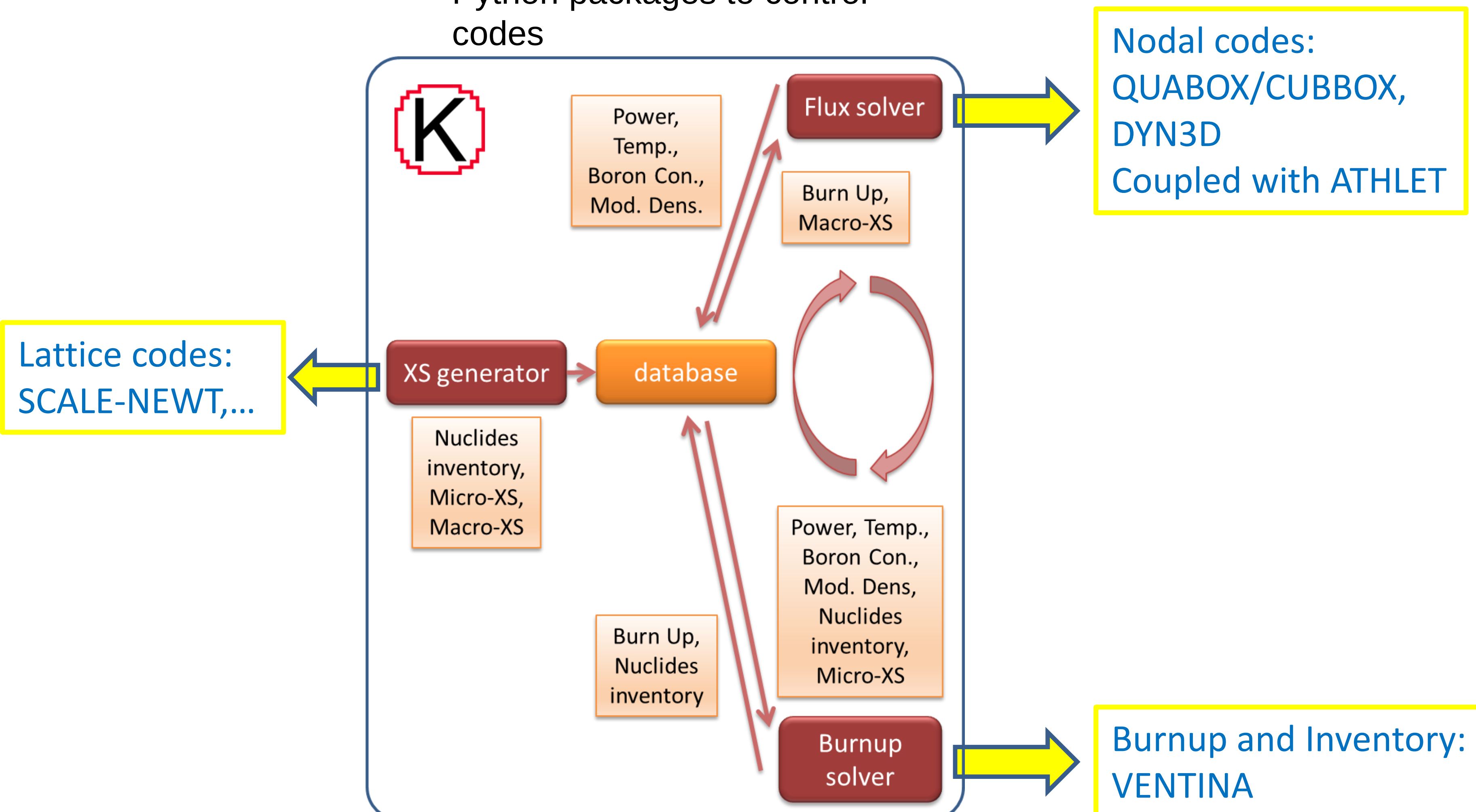


Realization in KMACS:
Python packages to control codes



KMACS: The GRS Nodal Core Simulator Concept

Realization in KMACS:
Python packages to control codes



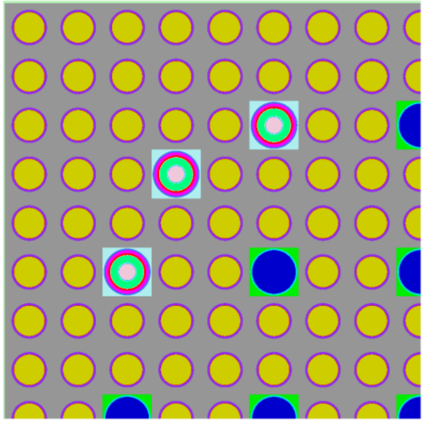
SCALE-NEWT in the GRS Core Simulator KMACS: Few-group Parameter Generation

- Wrapper around t-newt/t-depl:
  - Automated branch input generation for efficient cluster usage
    ⇒ use dumped compositions <StdCmpMix
    ⇒ perform 100s of branch jobs at once

```
U24-12:
    assemblyPitch: 21.50364

    pinTypes:
        0:
            type: guideTube
            compositions: [bypass, zirc4]
            temperatures: [moderator, cladding]
            radii: [0.56134, 0.60198]
        1:
            type: fuel
            compositions: [uox2.4, air, zirc4]
            temperatures: [fuel, gap, cladding]
            radii: [0.39218, 0.40005, 0.45720]

        2:
            type: absorberRod
            compositions: [air, ss304, air, borGlass, air, s
            temperatures: [moderator, moderator, moderator,
            radii: [0.214, 0.23051, 0.24130, 0.42672, 0.4368

    pinPitch: 1.25984
    subset: quarterOdd
    layout: |
        | 1 1 1 1 1 1 1 1 1
        | 1 1 1 1 1 1 1 1 1
        | 1 1 1 1 1 2 1 1 0
        | 1 1 1 2 1 1 1 1 1
        | 1 1 1 1 1 1 1 1 1
        | 1 1 2 1 1 0 1 1 0
        | 1 1 1 1 1 1 1 1 1
        | 1 1 1 1 1 1 1 1 1
        | 1 1 0 1 1 0 1 1 0


    spacers:
        types: [spacer,spacer,spacer]
        compositions: [inc718,ss304,zirc4]
        linearMassDensities: [!unit 1.0666 g/cm^3, 0.2187, 1
```

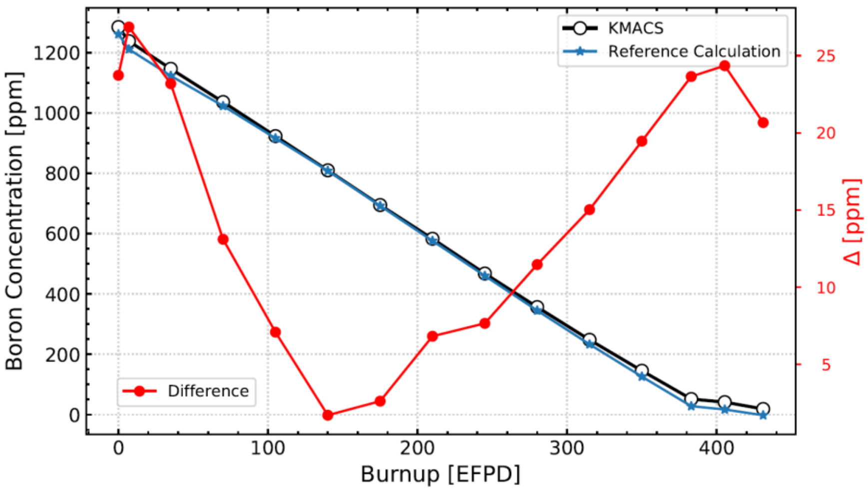
KMACS input

  - Spacers smeared into moderator
    ⇒ no change in concentrations with moderator density branch
  - Macroscopic few group data read from txtfile16
  - Nuclide-specific two-group data read from ft71f001 using paleale
    ⇒ used for 3D depletion
- Resulting few groups XS depending on burn-up, moderator density, fuel temperature, boron concentration

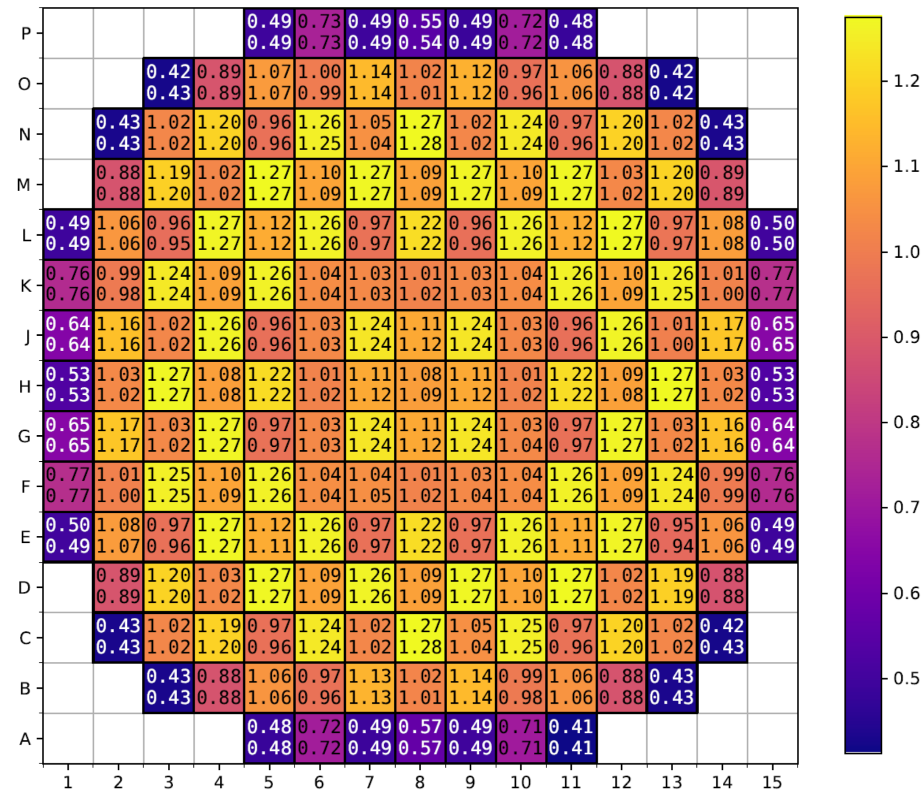


KMACS-generated NEWT input

SCALE-NEWT in the GRS Core Simulator KMACS: Results at the Core Level: German PWR Pre-KONVOI



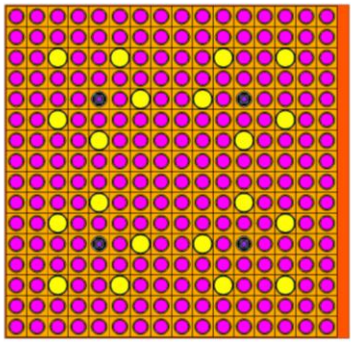
Critical boron concentrations:
$\Delta ppm \leq 30$ w.r.t. reference calculation (SIMULATE)

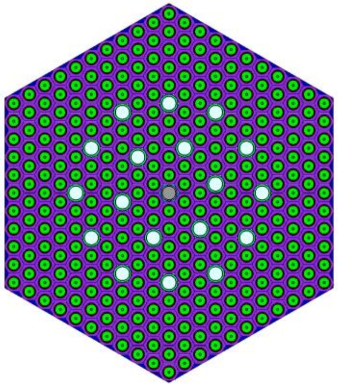


Relative assembly powers:
KMACS vs. Reference calculation (SIMULATE):
RMS = 0.37%

SCALE-NEWT in the GRS Core Simulator KMACS: Present Work & Next Steps

- Fuel assembly bowing:
  Gap-parametrized XS
- Extension to hexagonal fuel assemblies (VVER)
  - difficult to find working grid/cmfd options
  - no pin power information available
- Propagation of XSUSA nuclear data uncertainty to the core level
- Possible use of Polaris (?)





Simulating core behavior for fast reactors

- Generate **homogenized macroscopic few-group XS** using deterministic neutron transport code **NEWT** (code package from SCALE 6.2) to simulate a fast reactor system with the nodal diffusion code **PARCS**:
  - GRS is developing a core simulator KMACS using NEWT as spectral code
  - Previous works demonstrate good results using XS generated with the Monte-Carlo Code Serpent with a 3D model
    - time consumption: 100 hours CPU time for MYRRHA core but need more time for larger core (vs 10-15min/XS with NEWT)

- MG XS libraries in NEWT optimized for thermal neutron spectrum system

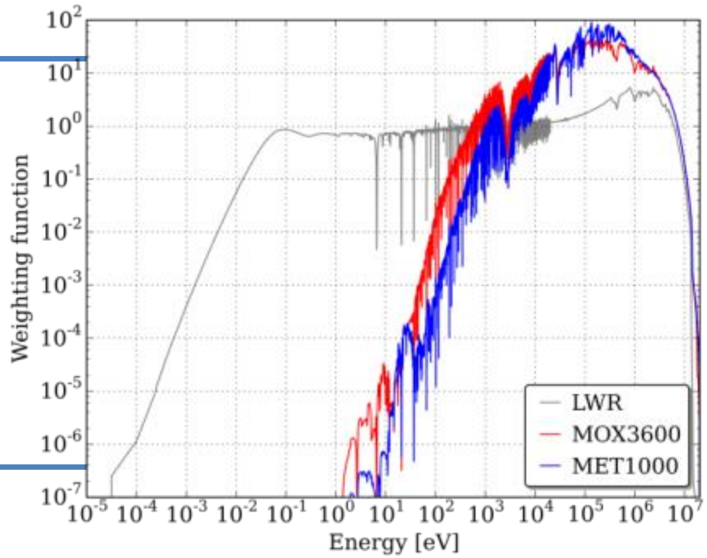
Generation of new libraries

- MG libraries **optimized for fast spectrum systems**

Simulating core behavior for fast reactors: Multi-group cross section libraries for SCALE

252 groups LWR library

- 252-group library weighted with a LWR spectrum
- fine energy group structure in the resonance region
- limited number of energy groups at fast energies



New few groups libraries adapted for fast systems:

302g MOX3600

- 302 energy groups
- Weighting spectrum: flux spectrum of a homogenized SFR fuel assembly (OECD benchmark)

302g MYRRHA

- 302 energy groups
- Weighting spectrum: flux spectrum of the homogenized MYRRHA fuel assembly

Simulating core behavior for fast reactors:
Macroscopic cross section generation with SCALE for MYRRHA

Multigroup micro XS

↓

NEWT 2D single assembly modelling

↓

Macro XS collapsed into 8 groups

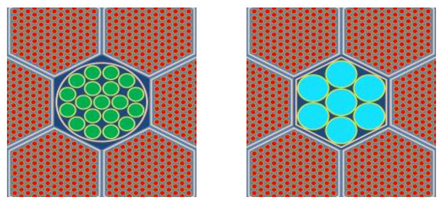
↓

PARCS

↓

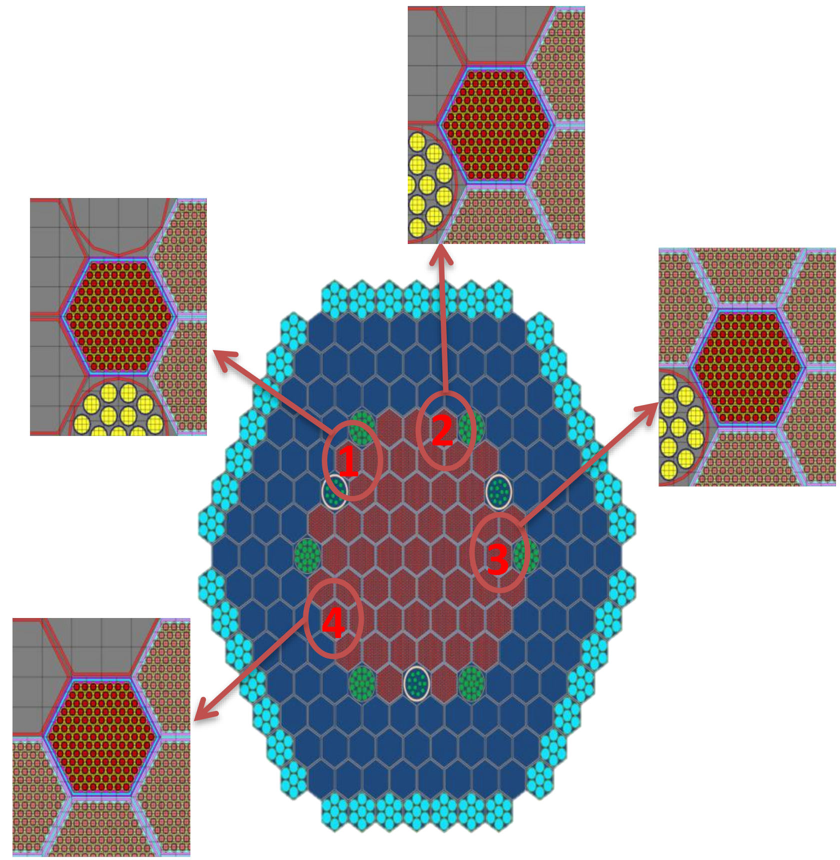
k_{eff}, Power distribution

- 2D infinite lattice
- periodic boundary condition



Group index	Lower limit [eV]
1	2.23E+06
2	8.21E+05
3	3.02E+05
4	1.11E+05
5	4.09E+04
6	1.50E+04
7	7.49E+02
8	1.00E-04

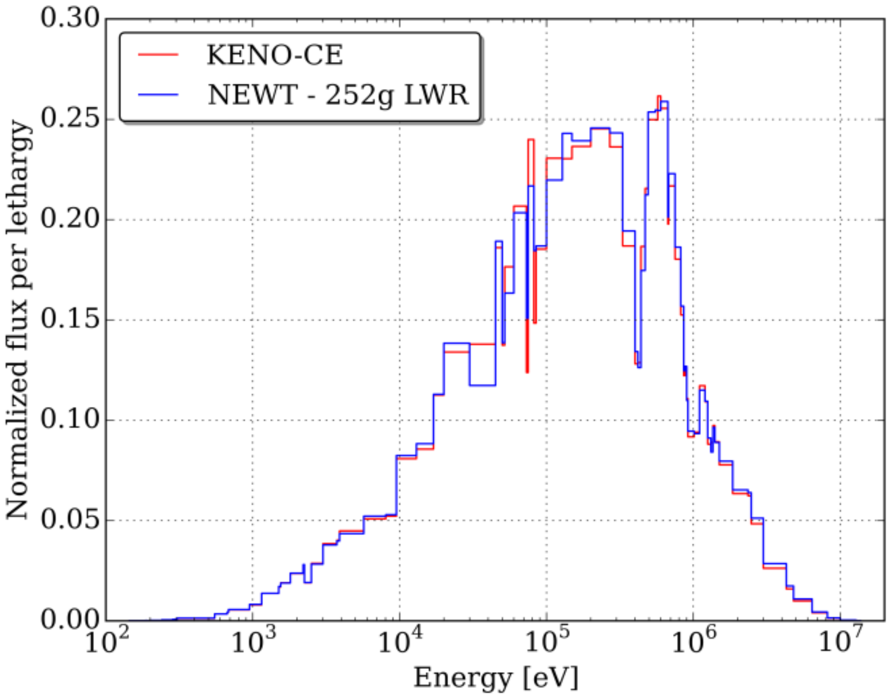
Super cell model



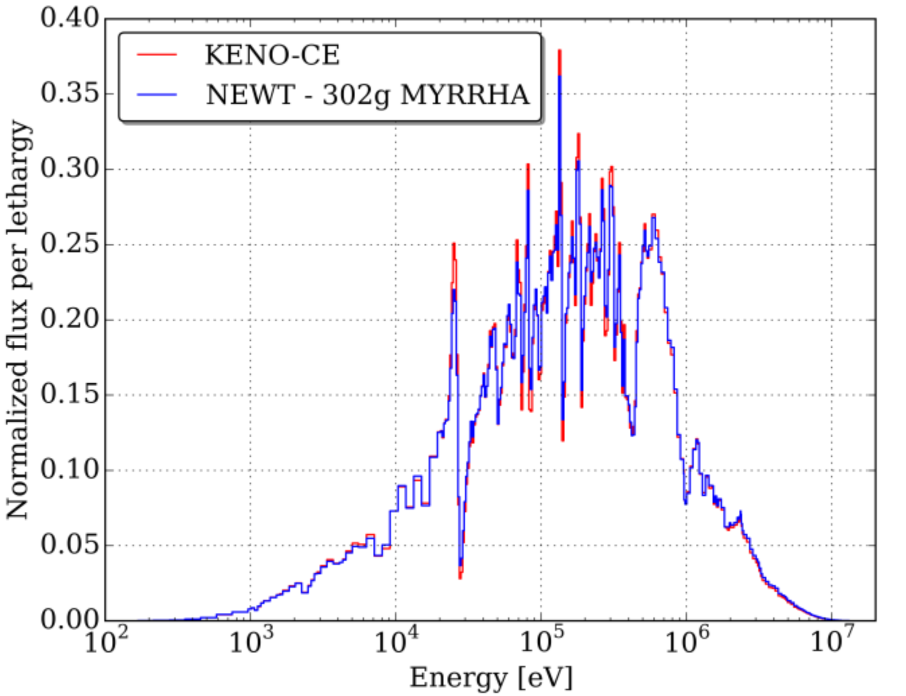
Simulating core behavior for fast reactors:
Results: Assessment of the libraries at assembly level

Code	KENO	NEWT	NEWT	NEWT
Library	CE	252g LWR	302g MOX3600	302g Myrrha
k_{inf}	1.57147	1.57517	1.57518	1.57553
$1/k_{MG}-1/k_{CE}$ [pcm]	(ref)	-150	-150	-164

252-group structure

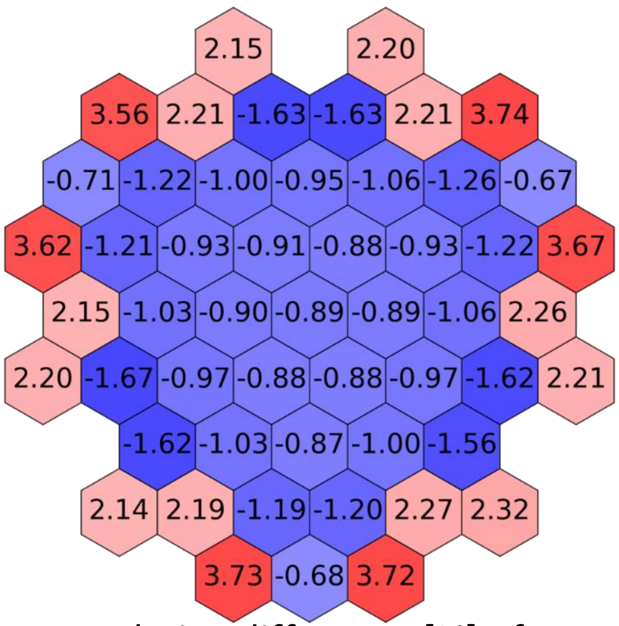


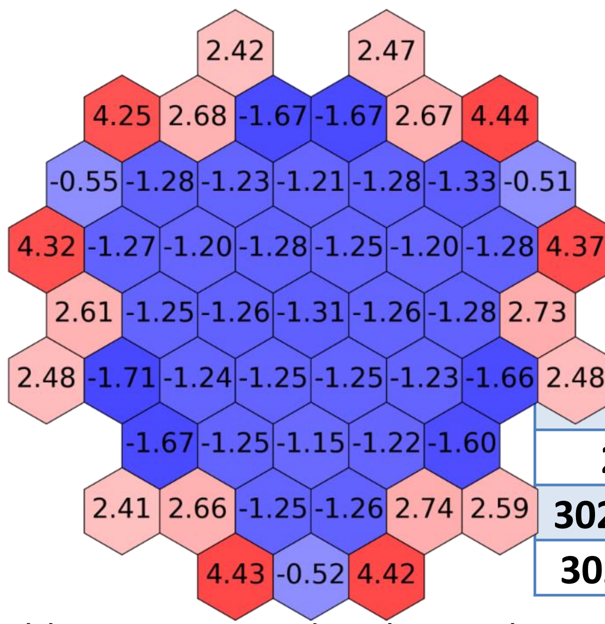
302-group structure



Simulating core behavior for fast reactors:
Results: k_{eff} and Radial Power Distribution in ARO at core level

		ARO	CR in/ SR out	CR out/ SR in	ARI
Serpent ref. solution	k_{eff}	1.01392	0.95210	0.97910	0.92853
PARCS using XS prepared with SCALE:					
252g LWR	$\Delta\rho$ (pcm)	-573	-1514	-1186	-1900
302g MOX3600	$\Delta\rho$ (pcm)	-580	-1643	-1251	-2065
302g MYRRHA	$\Delta\rho$ (pcm)	-598	-1668	-1272	-2092



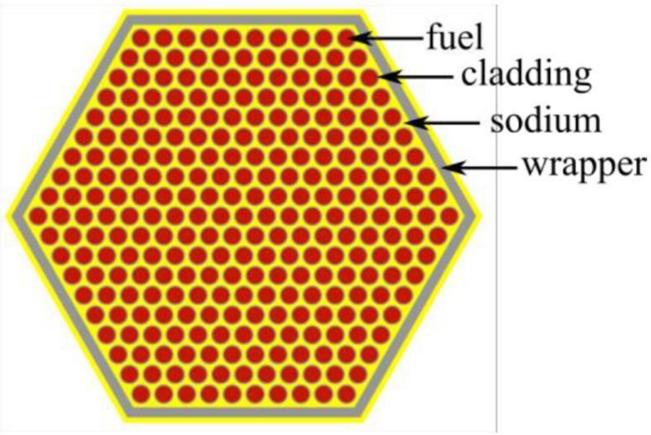


	MAX	MIN	RMS
252g LWR	3.74	-1.67	1.87
302g MOX3600	4.44	-1.71	2.20
302g MYRRHA	4.48	-1.72	2.21

Relative difference [%] of assembly-wise power distribution between Serpent and PARCS/SCALE (left: 252g LWR, right: 302g MOX3600) of the ARO configuration.

Simulating core behavior for fast reactors:
Results: Multiplication factor of SFR fuel assembly

- Analyzing SFR fuel assembly (OECD benchmark), e.g. difference in k_{eff} between KENO with continuous energy library (CE) and NEWT with multi group library (MG):



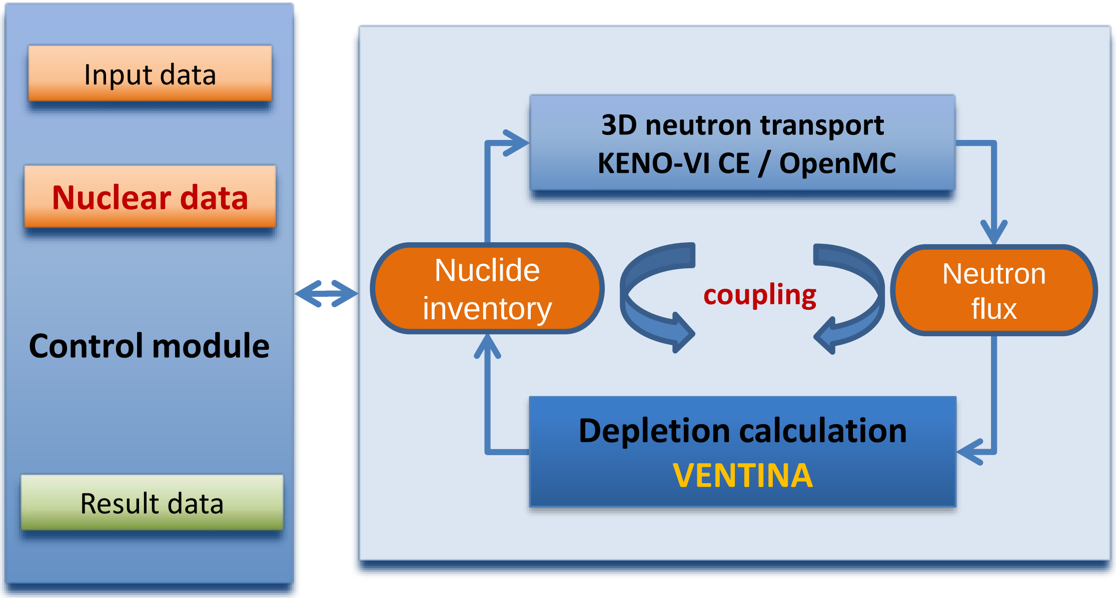
MG library	Δρ (pcm)	
	MET1000	MOX3600
252g LWR	-43	437
230g MET1000	296	394
230g MOX3600	232	377
302g MET1000	111	235
302g MOX3600	84	232
425g MET1000	95	225
425g MOX3600	66	215
2082g MET1000	(not converged)	(not converged)
2082g MOX3600	7	104

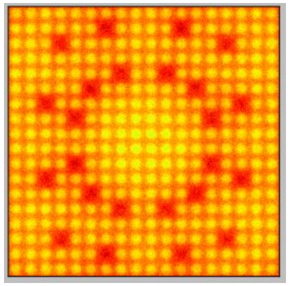
Conclusion and Outlook

- Improvements of the results in comparison with the CE reference results are depending on the considered problem
  - Generally better agreement in neutron flux compared to CE reference
- Further studies needed, e.g. focusing on the generation of macroscopic cross sections of Fuel Assemblies

GRS 3D Burn-up Code MOTIVE
Modular Tool for Inventory Calculation

- New burn-up code currently under development
- Use continuous energy Monte-Carlo codes for flux calculation
- VENTINA (PSI/GRS) for depletion calculation
- Coupling via high-resolution multi-group approach
- Flexible use of different state of the art nuclear data libraries
  - ENDF/B-VII.1
  - JEFF3.2
  - JENDL4.0 …
- Currently under validation using SFCOMPO data
- Currently only used for LWR applications (PWR, BWR, VVER)

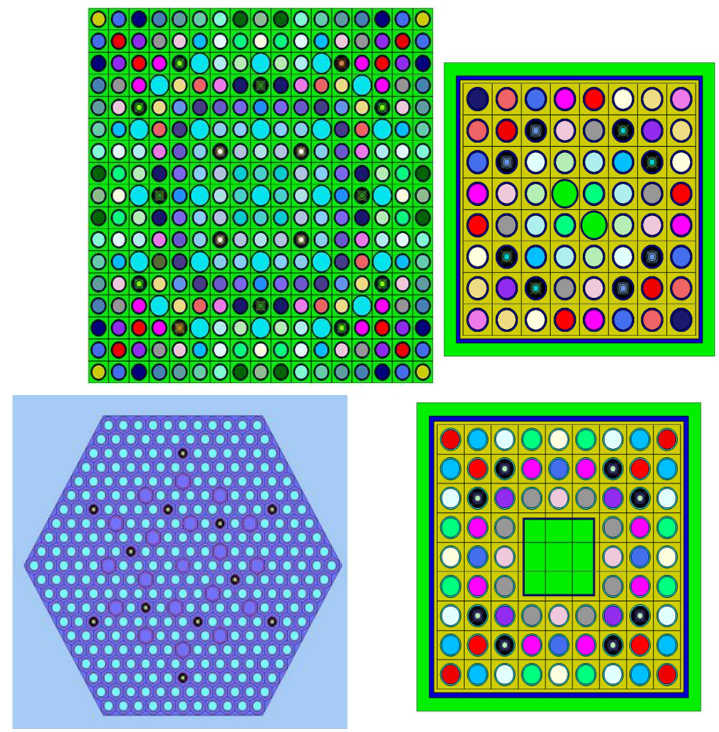




GRS 3D Burn-up Code MOTIVE

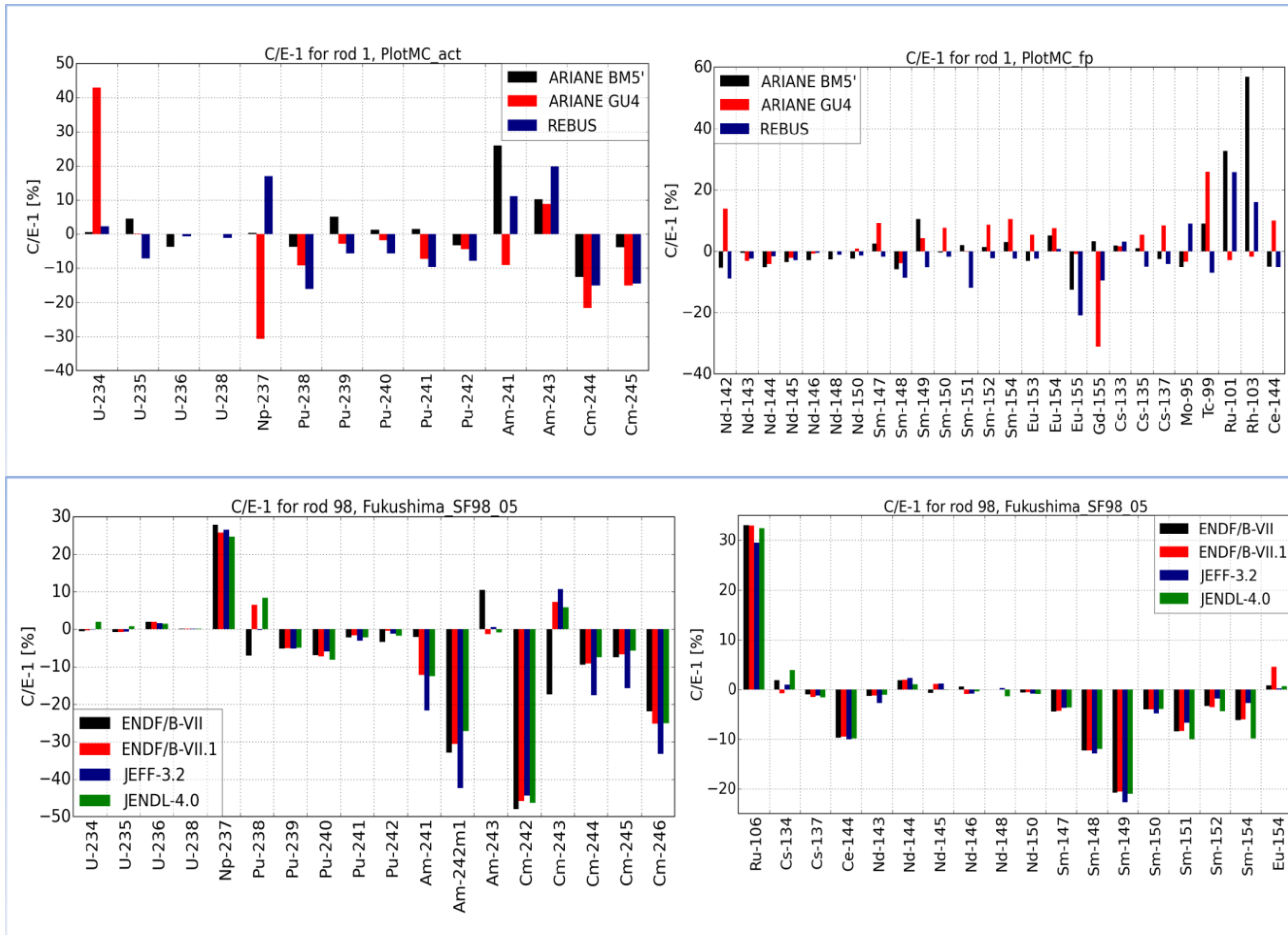
- **Basic code structure**
  - Input through keywords and parameter values
  - No complex geometry input; Specific geometry descriptions for the coupled codes implemented internally
  - Internal material property calculation: Moderator density, Fuel temperature

```
pin 1
  radii 0.4645 0.474 0.536
  materials Pu_high He clad
end
pin 11 12
  radii 0.4645 0.474 0.536
  materials Pu_low He clad
end
pin 13 to 19
  radii 0.4645 0.474 0.536
  materials Pu_medium He clad
end
[...]
fuel_assembly 1
  type=pwr
  axial_zone_nr=1
  pins_per_row 14
  pin_pitch 1.412
  assembly_pitch 19.82
  axial_zones 10.0
  axial_pin_arrays 1
  pin_array 1
     11   12   13   14   15   16   17   17   16   15   1
     12   18   19   20   21   22   23   23   22   21   2
     13   19  200   24   25  200   26   26  200   25   2
     14   20   24   27   28   29    1   30   29   28   2
     15   21   25   28  200   31   32   32   31  200   2
```



GRS 3D Burn-up Code MOTIVE
Comparison with post irradiation examination (PIE) data

- MOTIVE v0.5 using KENO-VI (SCALE 6.2.1)
- Various PIE Data taken from OECD/NEA data base SFCOMPO: Takahama-3, TMI-1, Ohi-1/2, Calvert Cliffs-1, Beznau-1, Gösgen-1, GKN-2, Fukushima Daini-2
- Mostly good agreement with experimental data; Comparable to published results of other codes

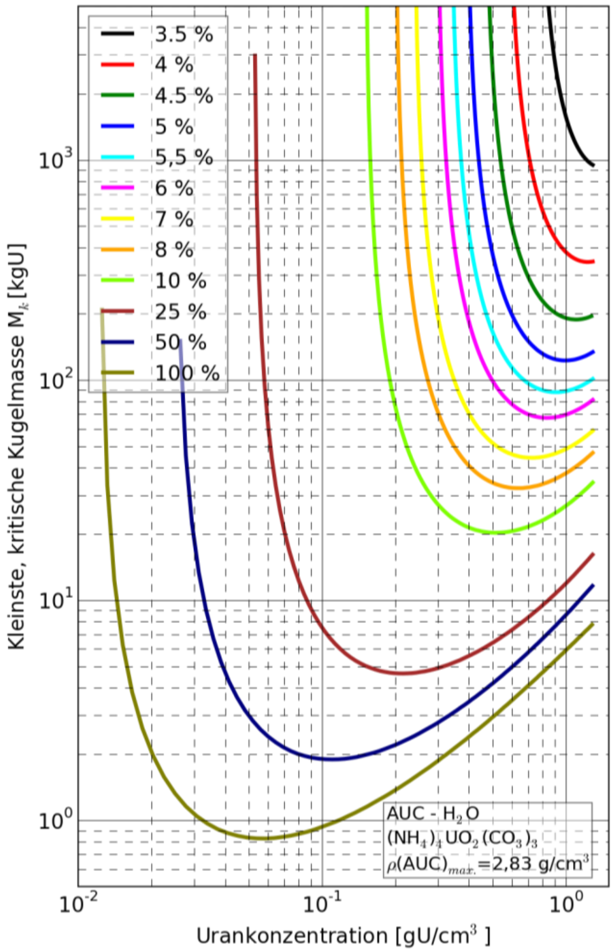


Criticality Safety

GRS Handbook of Criticality

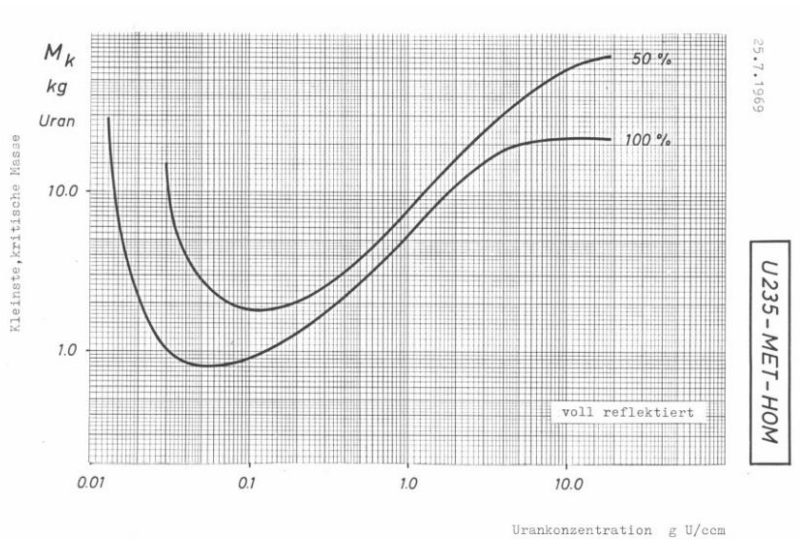
Starting at 1972s, GRS developed a Handbook of Criticality („Handbuch zur Kritikalität"):

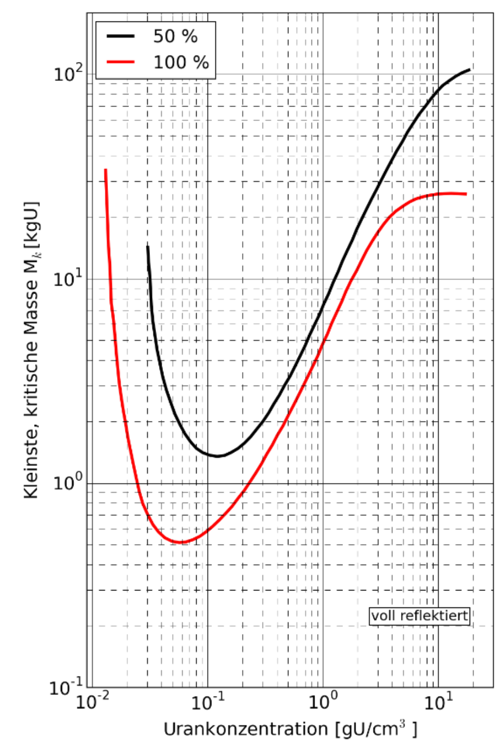
- Partially updated and enhanced from time to time over four decades
- Consists of three parts:
  - Theoretical part: Basic principles of neutron physics, criticality, nuclear safety, calculation methods, …
  - Several 100s data sheets of critical parameters:
    - ^{233}U, ^{235}U, Pu, Th, minor actinides
    - Different enrichments
    - Mainly homogeneous but also some heterogeneous systems
    - Metal, oxides, solutions
    - H_2O-, D_2O-, graphite-moderated, w/ and w/o reflector
- Critical parameter curves calculated using CSAS1
  - Search mode: search critical radius for given density/concentration
  - O(100) data points / calculations per curve



GRS Handbook of Criticality
Current and future work

- Validating critical parameter curves:
  - ICSBEP contains limited number of considered systems (e.g. solutions are mainly U/Pu Nitrates)
  - Lack of suitable experiments for many considered systems
    ⇒ S/U analyses
- Updating “on-paper-only“ parameter curves

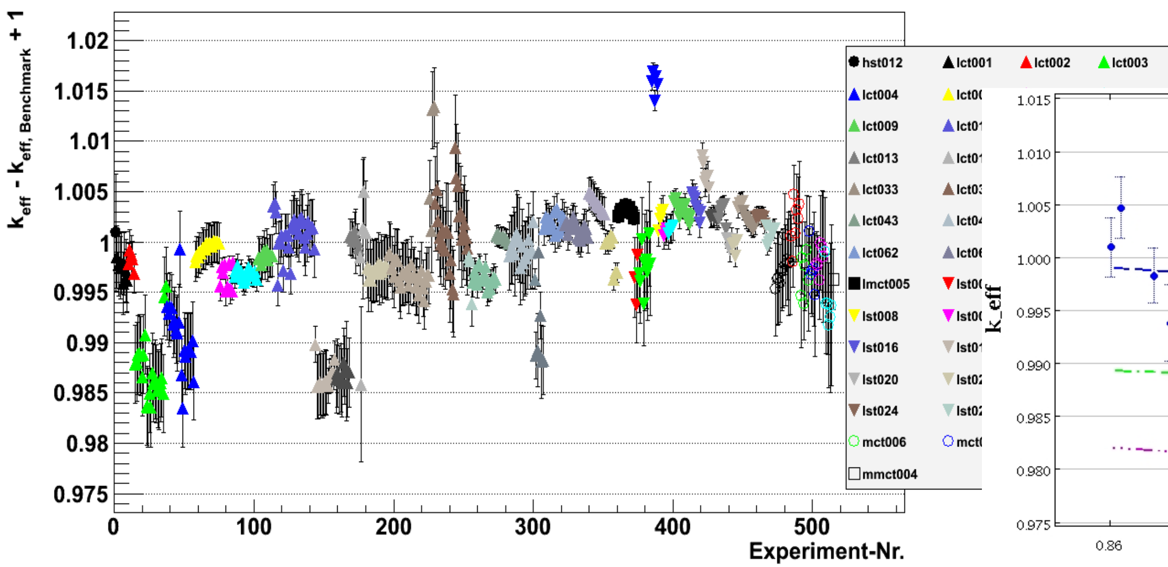


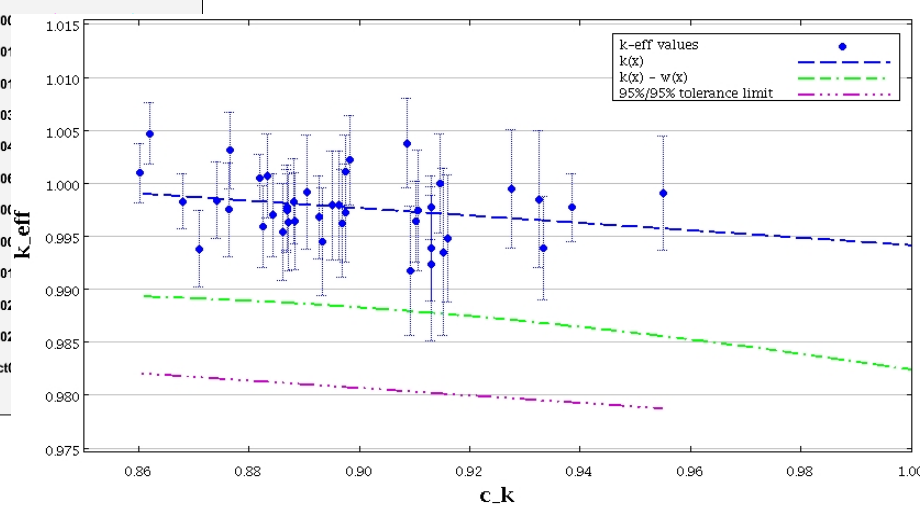


⇒ Goal: digital version of all data sheets

Validation of criticality calculations using SCALE

- Collection of CSAS5 inputs of critical experiments from ICSBEP handbook:
  - Inputs from different projects,
    Used for different purposes: validation, benchmarks, examples, …
  - About 60 different experiments, more than 600 cases (LEU-COMP-TERM, MOX-COMP-TERM, LEU-SOL-THERM, PU-SOL-THERM, …)





- But: experimental cases are correlated ⇒ needs to be considered for validation

Validation of criticality calculations using SCALE: How to handle statistical dependencies of experiments?

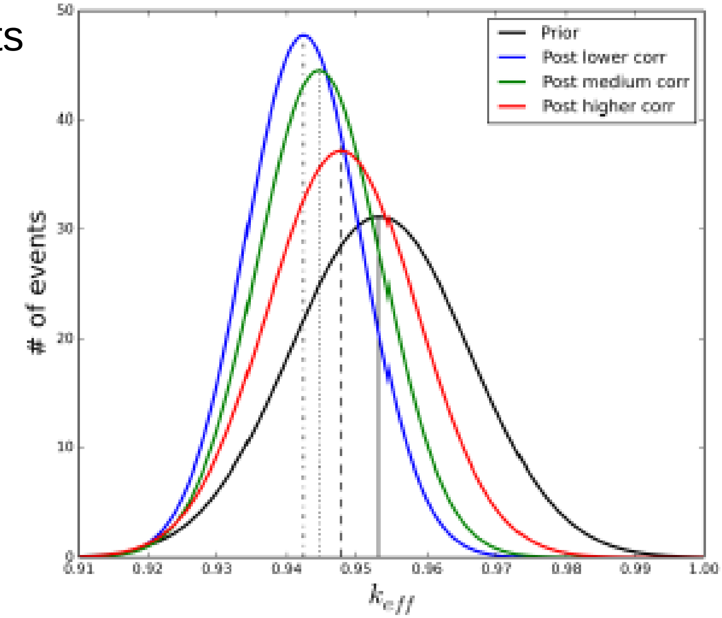
How to treat statistical dependencies of series of experiments correctly in a validation? (GRS: Bayesian Updating)

- Parameters, materials, experimental setups identical for and between series.

- Influence of integral covariance data of experimental series in validation discussed (e.g. WPNCS, OECD-NEA) and published (Ivanova et al.; Sobes et al., Hoefer et al, Peters et al.)
- How to get / derive covariance data?
  - Define statistical dependencies between experiments
  - Derive covariance (and correlation) factors

→ SUnCISTT w/ SCALE

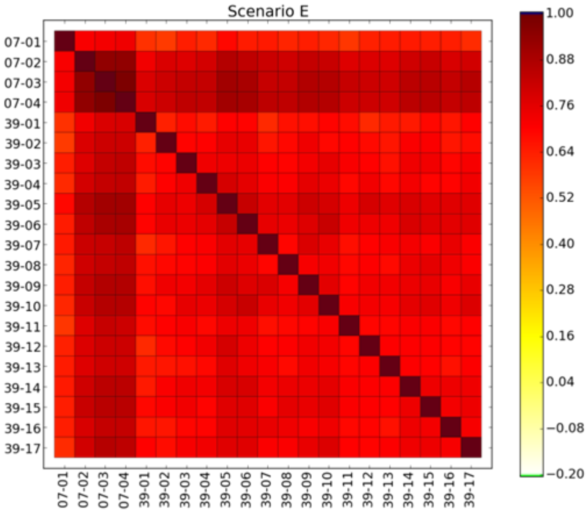
- Funded by Federal Office for the Safety of Nuclear Waste Management (BfE).
  - Guidance report for the German authority (Draft end 2018)
  - Application in licensing procedures

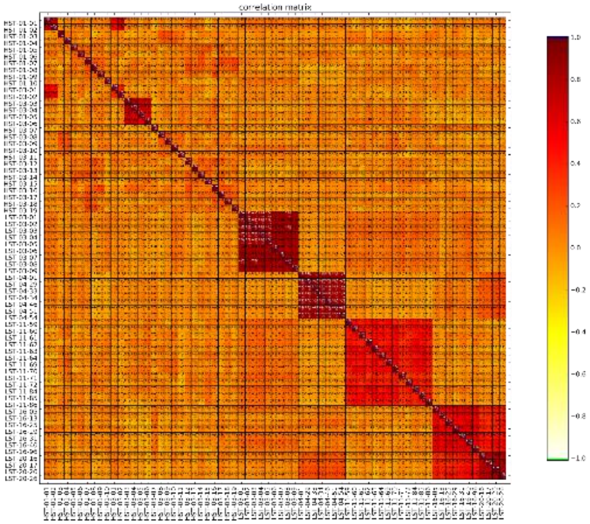


Bayesian updating of k_{eff} distribution functions for different degrees of statistical dependencies.

Validation of criticality calculations using SCALE: Determining covariances

- Determining covariances using MC sampling method ⇒ SUnCISTT
  - Leeds to extensive SCALE calculations
- Correlation Coefficients for several experimental series from ICSBEP handbook are analyzed:
  - LCT-006, -007, -035, -039, -062,
    LST-003, -004, -011, -016, -020,
    HST-001, -003,
    PST-003, -004, -005, -006, -020, -021
- Current collaborations
  - LCT-097 w/ SNL and ORNL
  - HST-001 w/ ORNL





Summary

- SCALE is and will be used for a wide variety of analyses at GRS:
  - Reactor safety
  - Criticality safety
  - Shielding analyses
  - …
- Some examples of such analyses were presented
- **SCALE is and will continue to be one of the main neutronics calculation tools for reactor safety and criticality safety analyses at GRS**