IRSN
INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

Faire avancer la sûreté nucléaire

USE OF ADVANCED OPTIMIZATION ALGORITHMS FOR THE DESIGN OF CRITICAL EXPERIMENTS

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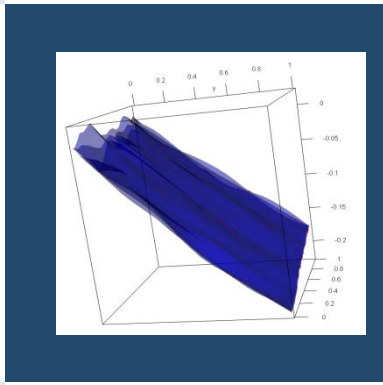
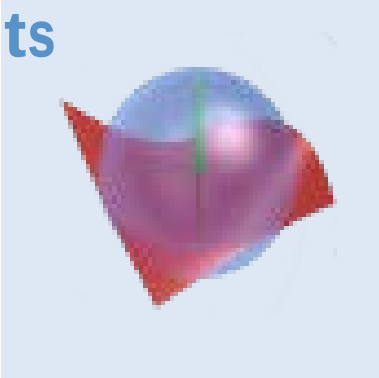
AMERICAN NUCLEAR SOCIETY
A N S

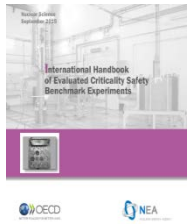
Carlsbad Section

Contents





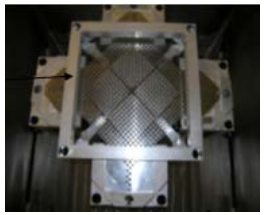
Context



- Need for validation of molybdenum in thermal and **epithermal** energy spectra

- Molybdenum elements encountered in:
  - Irradiated fuel as fission products (BUC in transport casks and storage)
  - Alloys in research, naval or space reactors
  - In reprocessing plants as UPuMoZr reprocessing plants residues

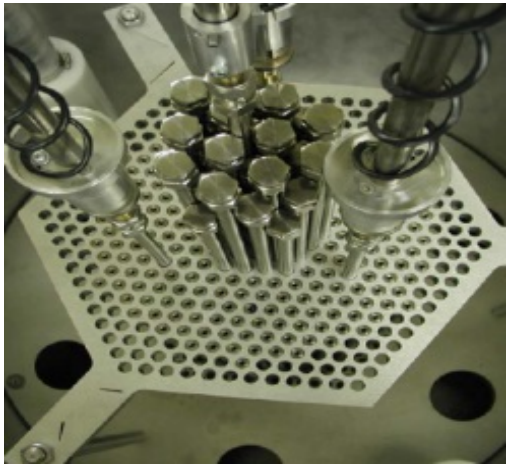
- Few experiments available in thermal energy range apart from:
  - French MIRTE program (proprietary): 4 lattices of rods separated by 10-mm Mo screen
  - French Fission Products program: Mo-CH_2 sandwich in UO_2 lattice

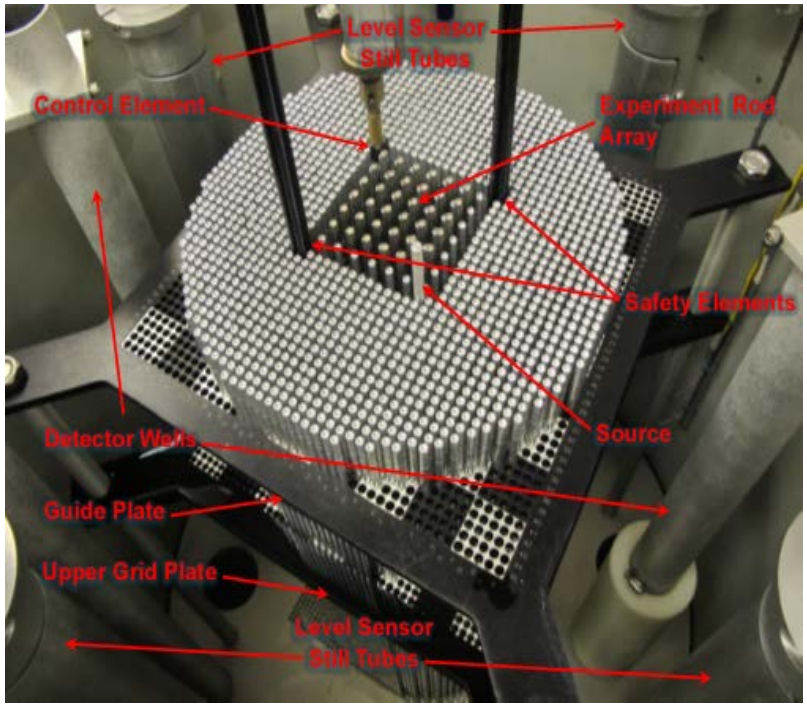


- Need of experiments uncorrelated with existing ones
  - Nuclear data issues

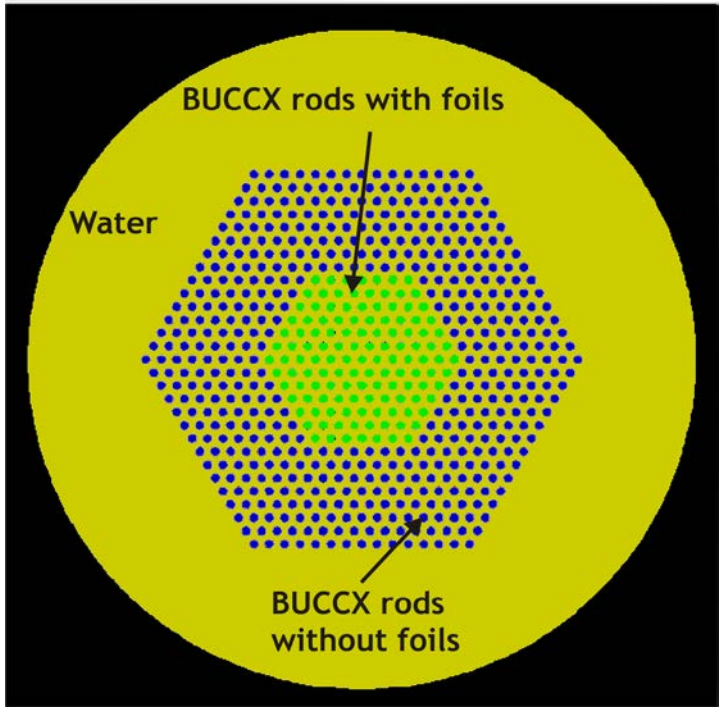
Proposed design

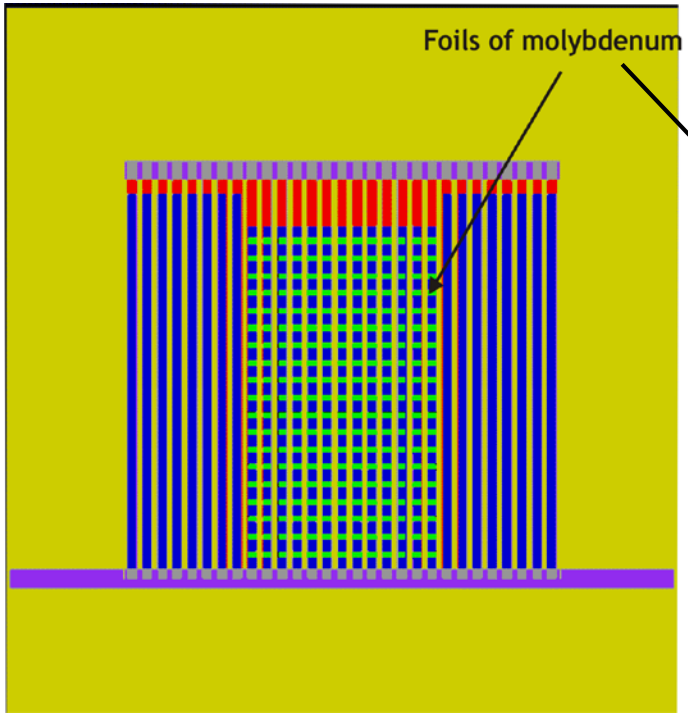
- Use of the SPRF/CX installation at SNL
  - UO_2 (BUCCX or 7uPCX) rods well characterized
    - BUCCX (4.31% ^{235}U) outer clad ϕ = 1.3818 cm
    - 7uPCX (6.9% ^{235}U) outer clad ϕ = 0.6349 cm
  - Constraints on the installation:
    - Tank dimensions
    - Number of rods:
      - 494 BUCCX rods (4.31% ^{235}U)
      - 2199 7uPCX rods (6.9% ^{235}U)

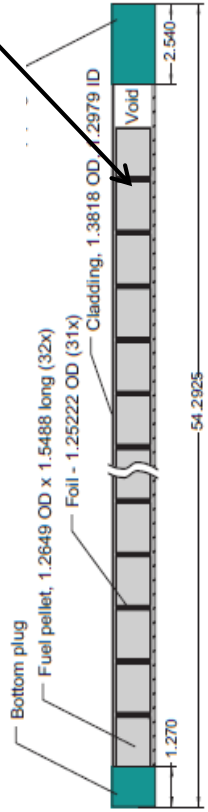




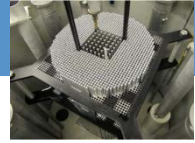
Design with BUCCX rods and foils



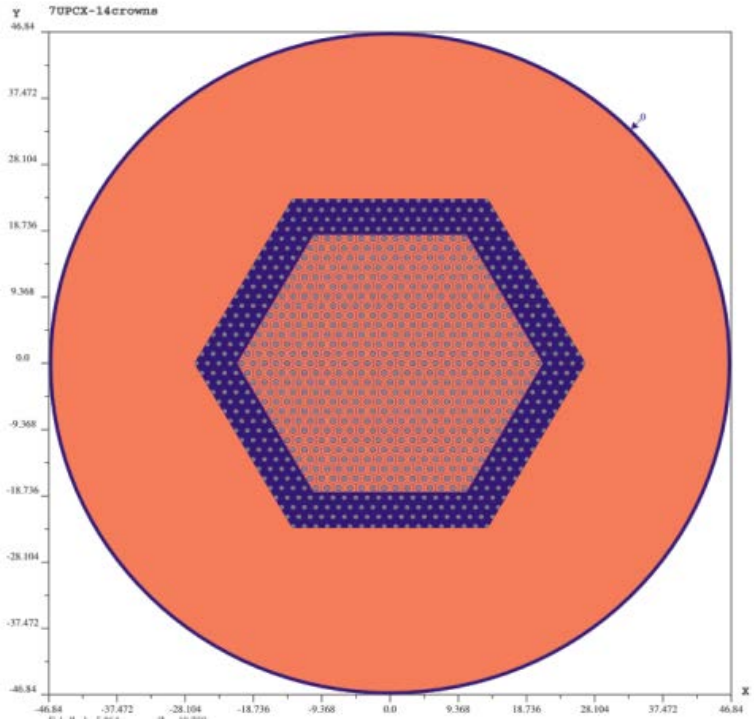


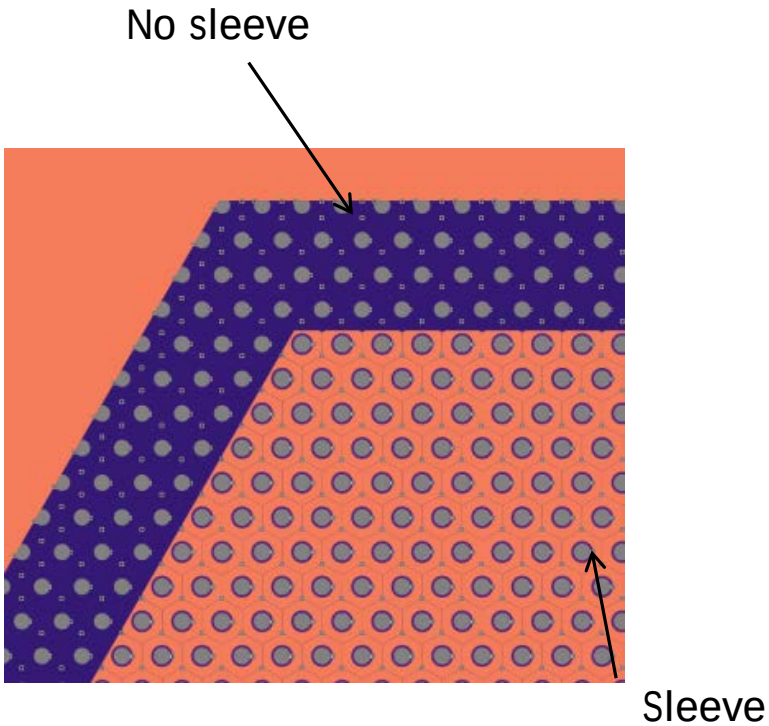


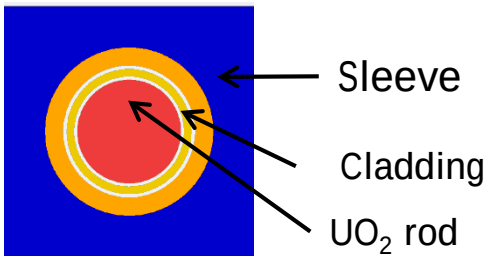
- Metallic foils incorporated in BUCCX rods (tested in LCT-079 for ^{103}Rh)
  - Improvement of sensitivity of k_{eff} to ^{95}Mo capture
- Two zones: with and without foils
- Number of foils per rod, thickness of foils: variable



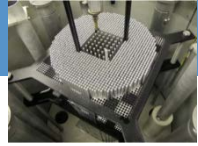
Design with 7uPCX rods and Mo sleeves



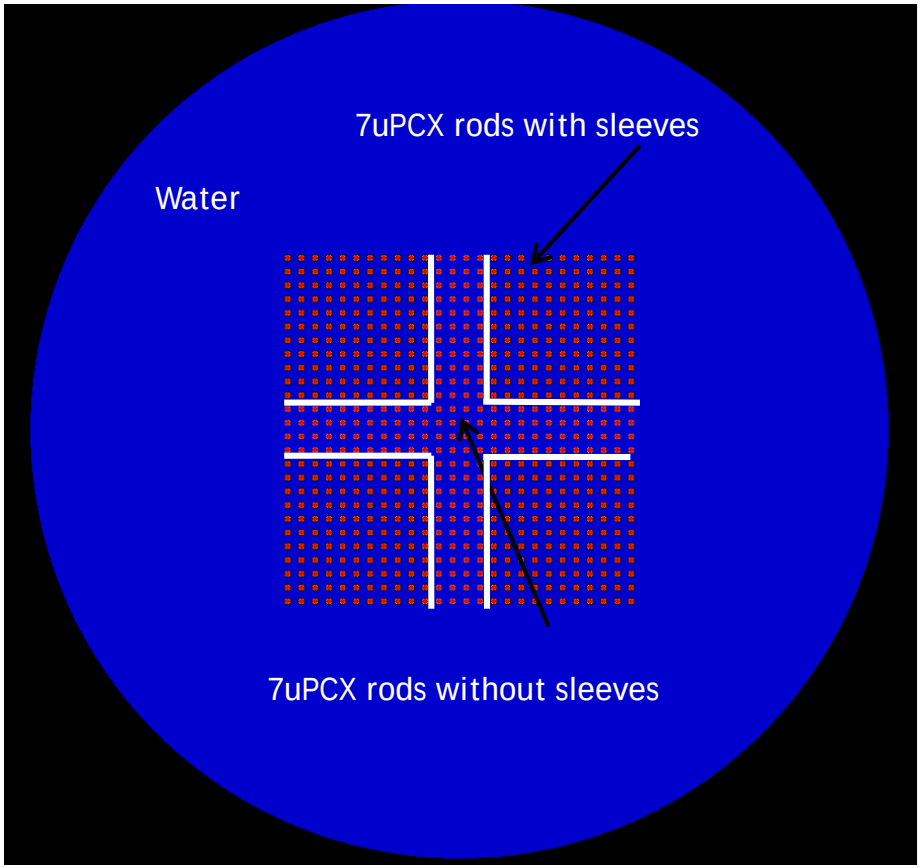




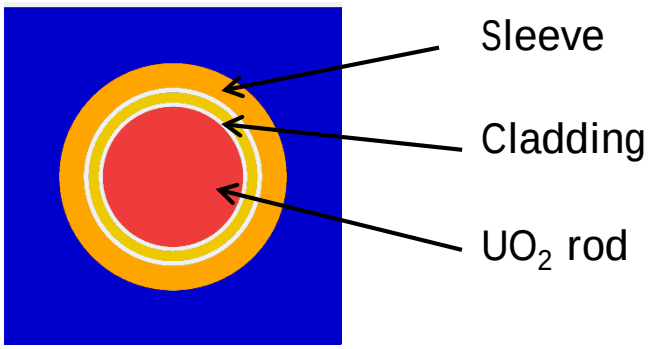
- Sleeves of Mo surrounding 7uPCX rods
  - Already tested in MIRTE 2.3 for Fe and Cu
- Two zones: with Mo sleeves and without
- Thickness of sleeves and pitch: variable



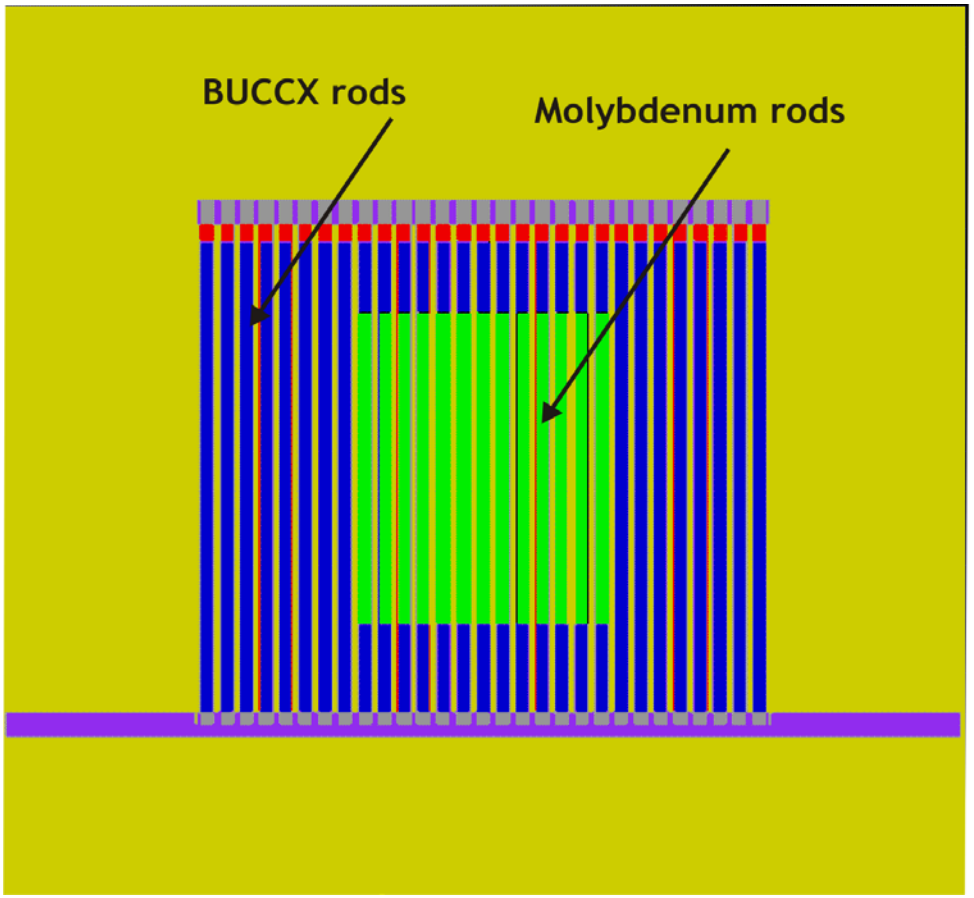
Design with 7uPCX rods and Mo sleeves

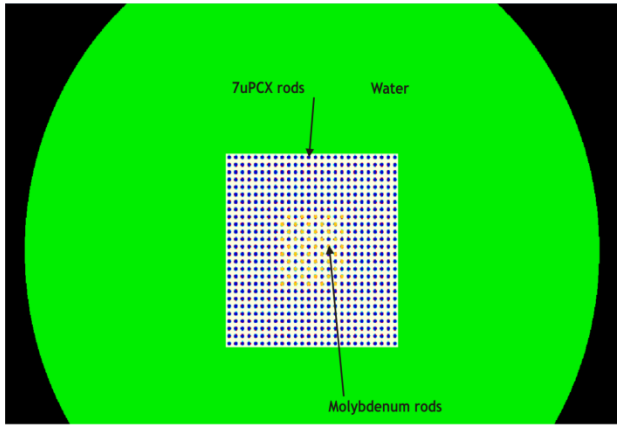


- Two zones:
  - Un-sleeved cross shaped 7uPCX rods
  - Sleeved rods outside the cross
- Thickness of sleeves and pitch: variable



Design with molybdenum rods

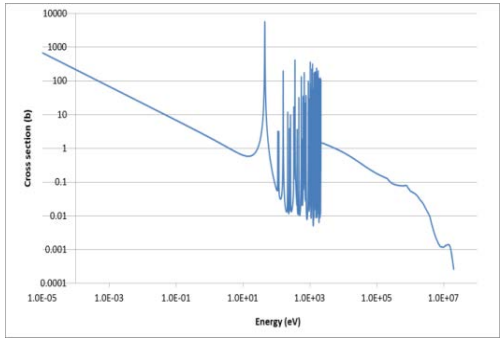


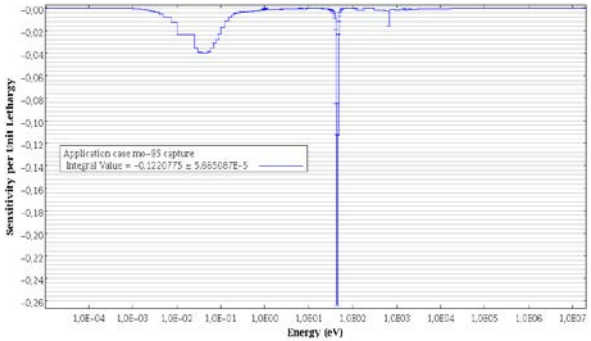


- Mo metallic rods inside lattice of UO_2 rods (BUCCX or 7uPCX)

Optimization of the design

- Need to optimize k_{eff} sensitivity to ^{95}Mo capture in thermal and epithermal energy ranges



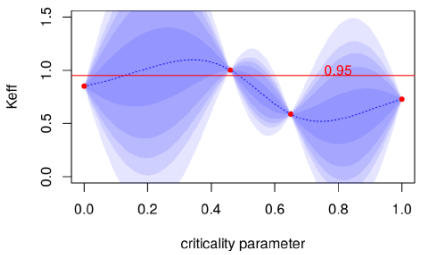


- Need to remain close to critical state

- Use of the SCALE6.1 package and associated ENDF/B-VII.0 library
  - Anticipate potential under-estimation of codes and nuclear data
    - Target k_{eff} = 1 + Additional margin

- Many parameters monitored at the same time
  - Use of advanced algorithms EGO and ECEGO via PROMETHEE workbench
    - Identify the “best” configuration in a reasonable amount of time

EGO and ECEGO algorithms



- Different steps
  - Parametrization of the SCALE 6.1 input decks for monitoring with PROMETHEE workbench
    - TSUNAMI-3D calculation for k_{eff} sensitivity to the capture of ^{95}Mo
  - Optimization on both k_{eff} and sensitivity to ^{95}Mo capture
  - Definition of a first set of calculation points
    - Step by step approach using kriging algorithms EGO and/or ECEGO

- Two types of algorithms
  - **EGO: optimization of k_{eff} sensitivity to ^{95}Mo capture without constraint**
  - ECEGO: optimization of k_{eff} sensitivity to ^{95}Mo capture with k_{eff} comprised between 0.98 and 1.02

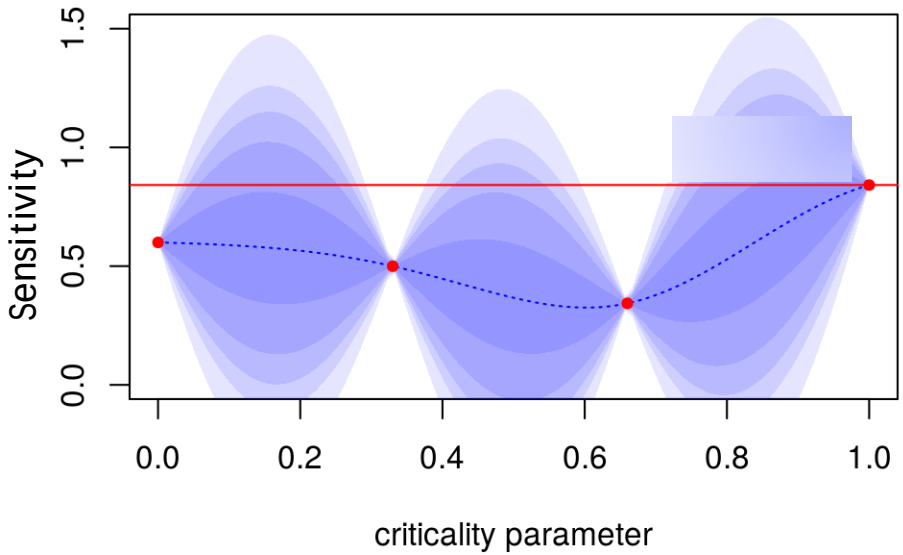
- Outputs
  - Response surfaces with iterations in the zones of interest
  - EGO: superimposition of response surfaces to determine the optimal configuration

“Optimization”

Surrogate function
Sensitivity(pitch, $R_{sleeves}$)

Random function

Interpolates calculated points



Gaussian predictor mean, sd:

$E[\text{Sensitivity}(\text{pitch}, \mathbf{R_{sleeves}})] = \text{mean}(\text{pitch}, R_{sleeves})$

$\text{Var}[\text{Sensitivity}(\text{pitch}, \mathbf{R_{sleeves}})] = \text{sd}(\text{pitch}, \mathbf{R_{sleeves}})^2$

“Optimization”

Surrogate function
Sensitivity(pitch, $R_{sleeves}$)

Random function

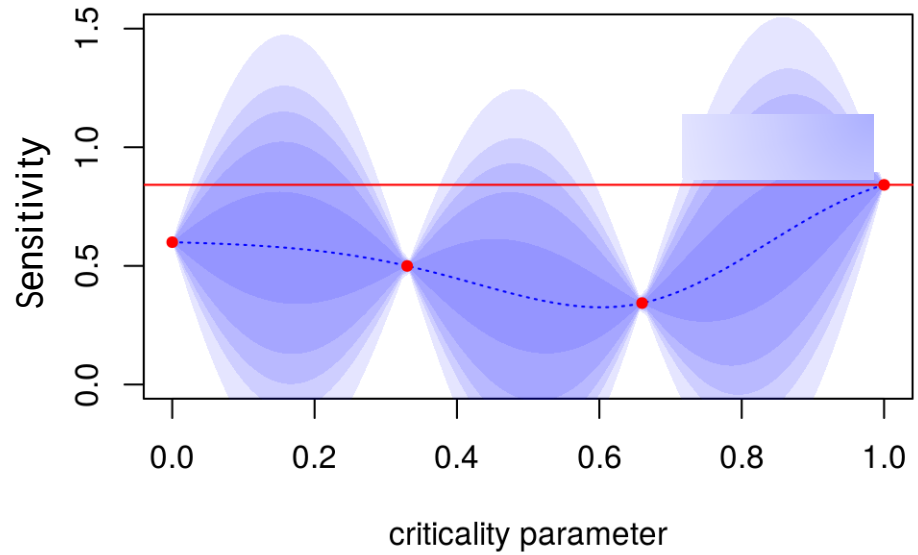
Interpolates calculated points

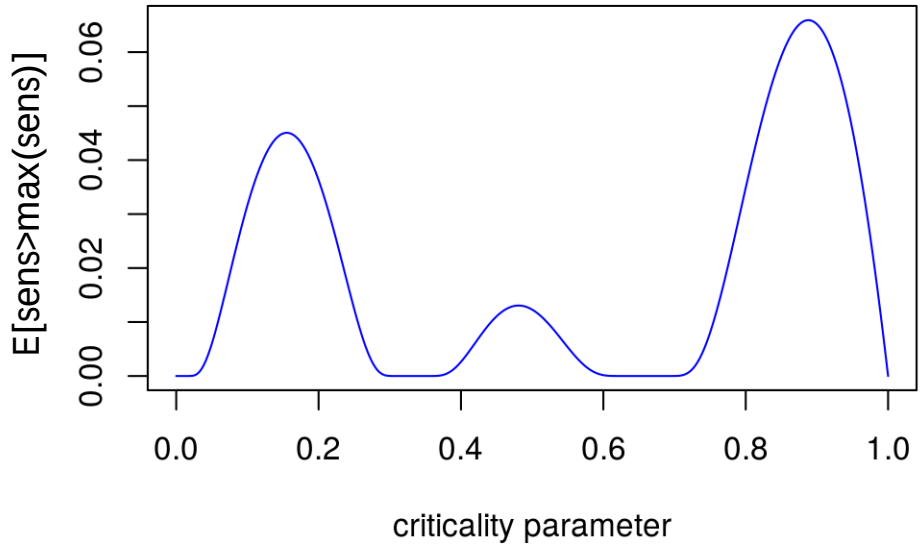
Gaussian predictor mean, sd:

E[Sens(pitch, $R_{sleeves}$)] = mean(pitch, $R_{sleeves}$)

Var[Sens(pitch, $R_{sleeves}$)] = sd(pitch, $R_{sleeves}$)^2

➔ Convenient to estimate:
E[Sens(pitch,water) > max{Sensitivity}]

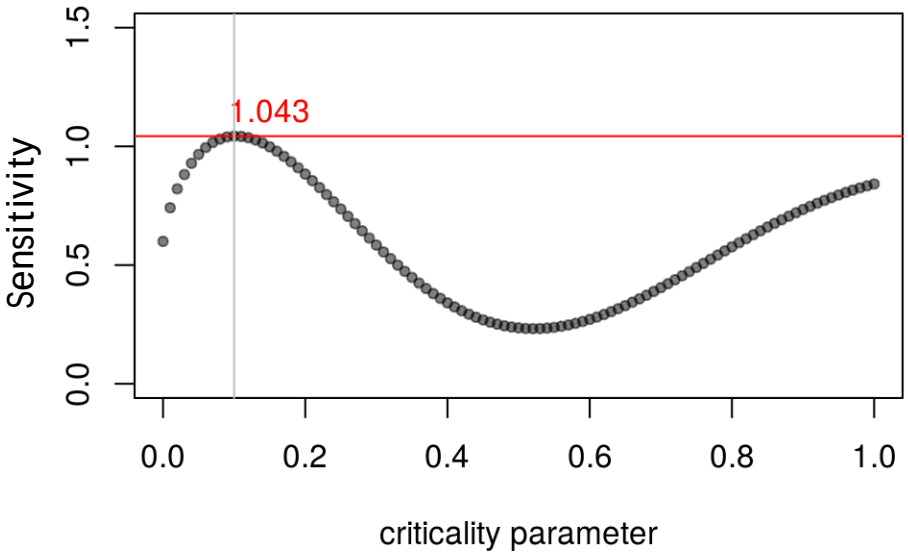




“Optimization”

“Valuable” point (pitch, $R_{sleeves}$)

Aim at reaching highest sensitivity to ^{95}Mo capture

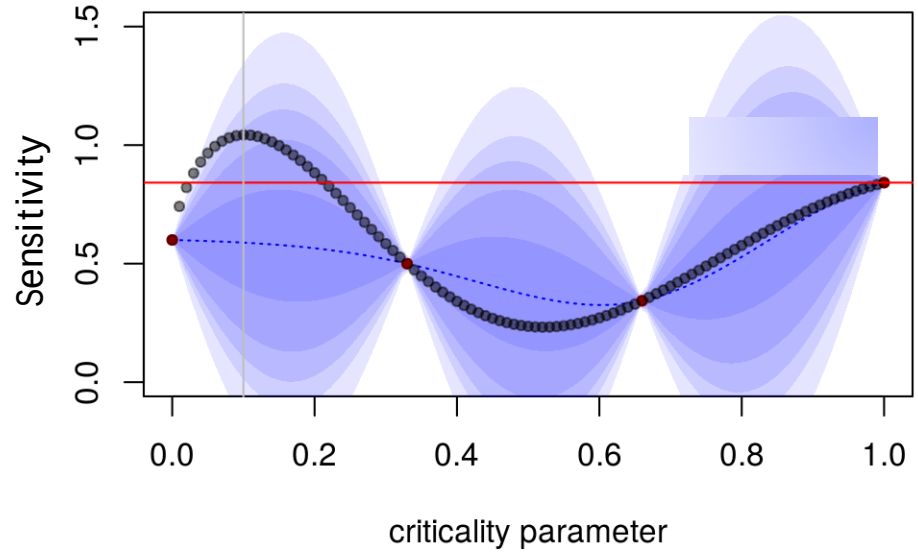


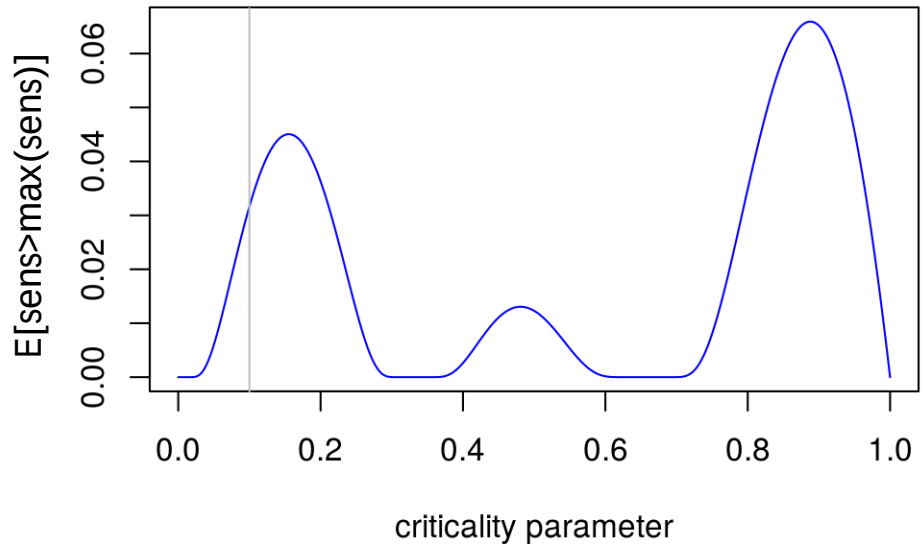
“Optimization”

“Valuable” point (pitch, $R_{sleeves}$)

Aim at reaching highest sensitivity to ^{95}Mo capture

Where to add next points/calculations?





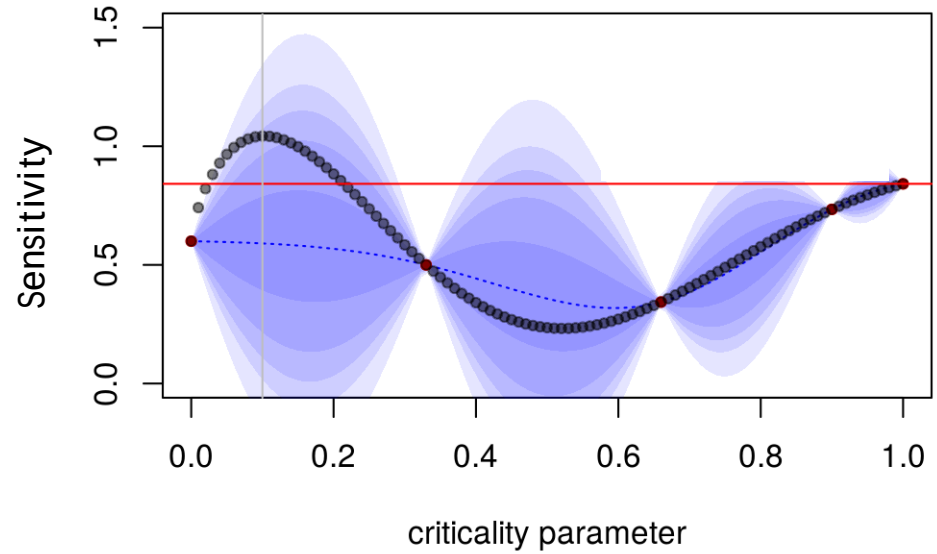
“Optimization”

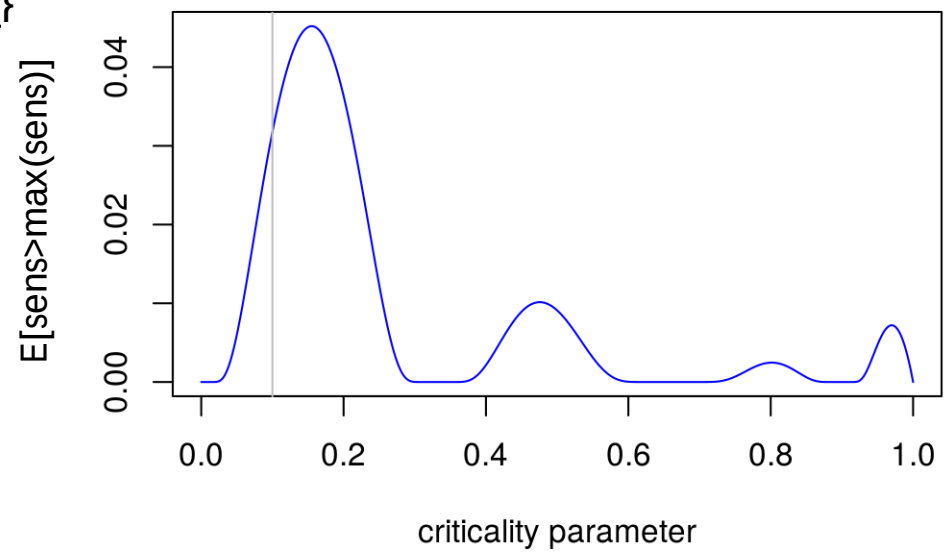
“Valuable” point (pitch, $R_{sleeves}$)

Aim at reaching highest sensitivity to ^{95}Mo capture

Where to add next points/calculations?

where is the highest E[Sens > max{Sens}]





“Optimization”

“Valuable” point (pitch, $R_{sleeves}$)

Aim at reaching highest sensitivity to ^{95}Mo capture

Where to add next points/calculations?

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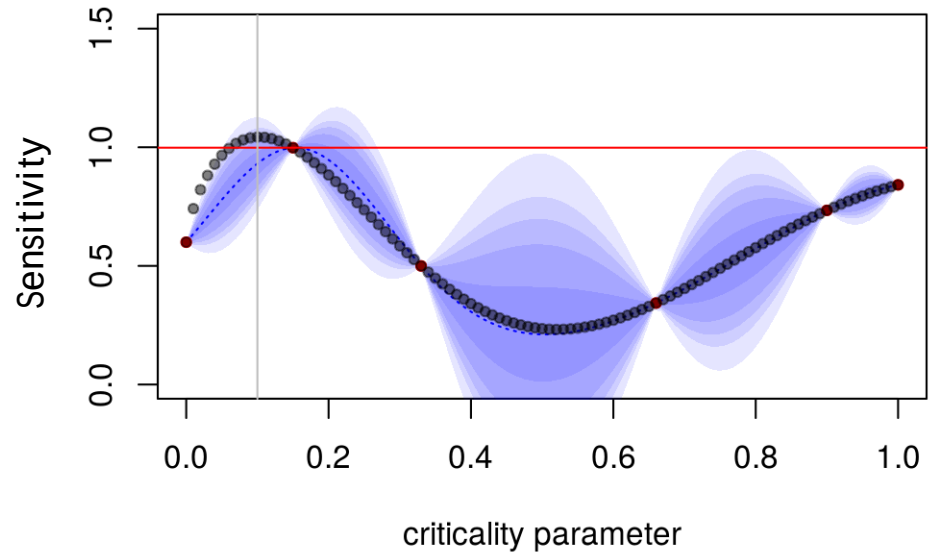
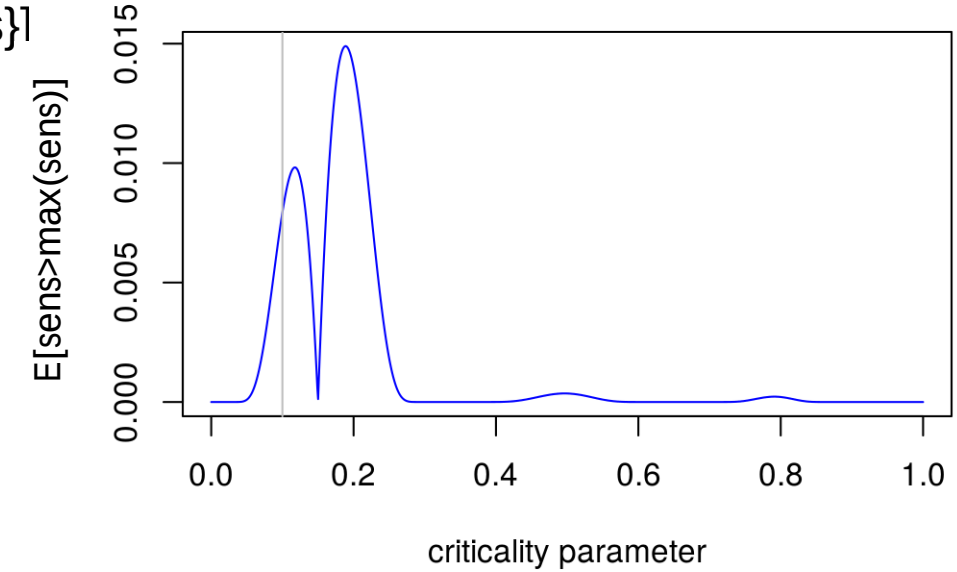




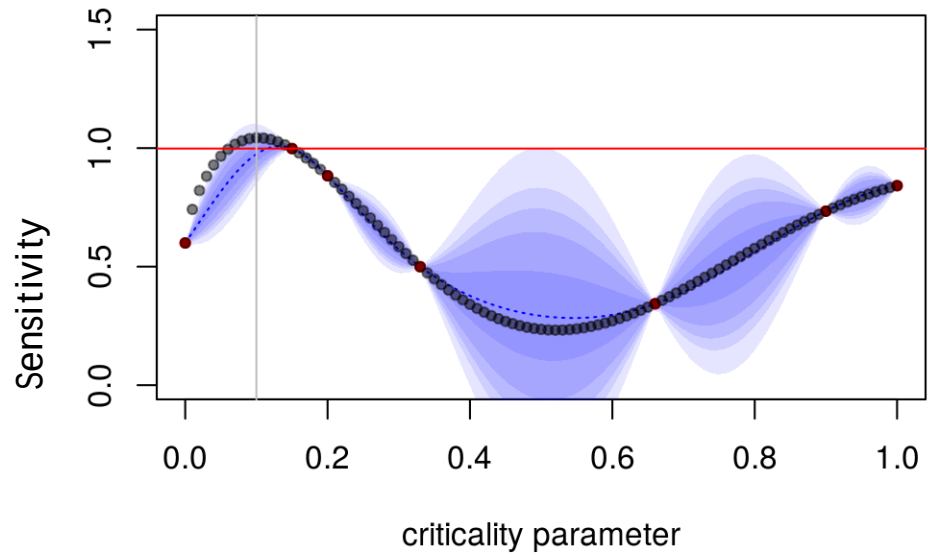
“Optimization”

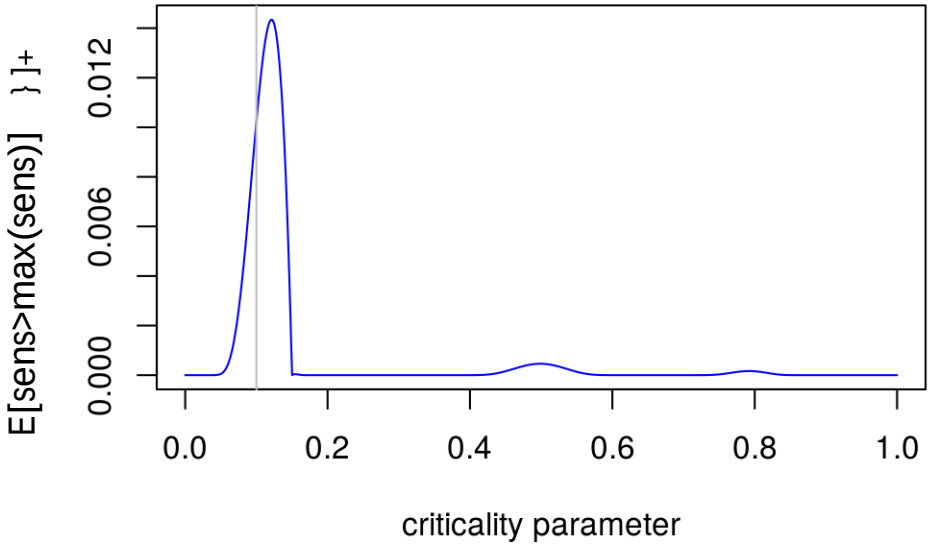
“Valuable” point (pitch, $R_{sleeves}$)

Aim at reaching highest sensitivity to ^{95}Mo capture

Where to add next points/calculations?

where is the highest E[Sens > max{Sens}]





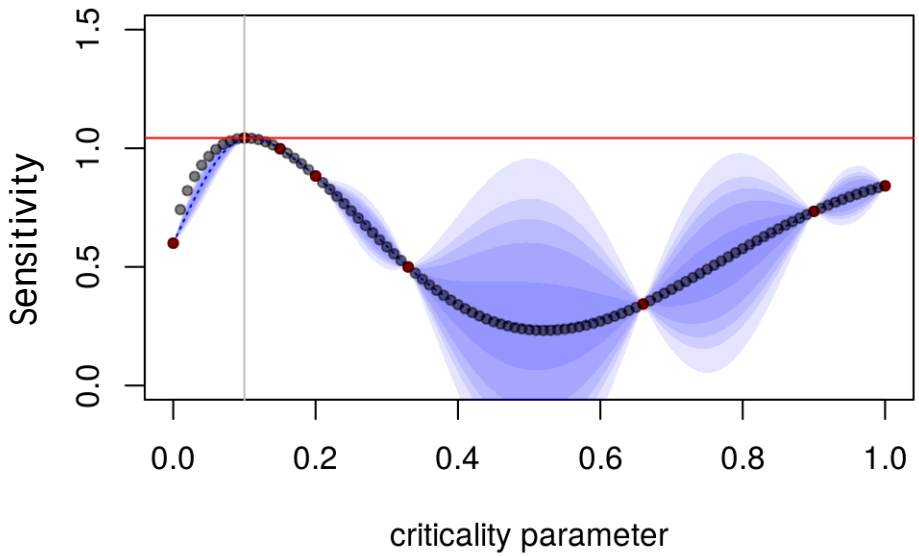
“Optimization”

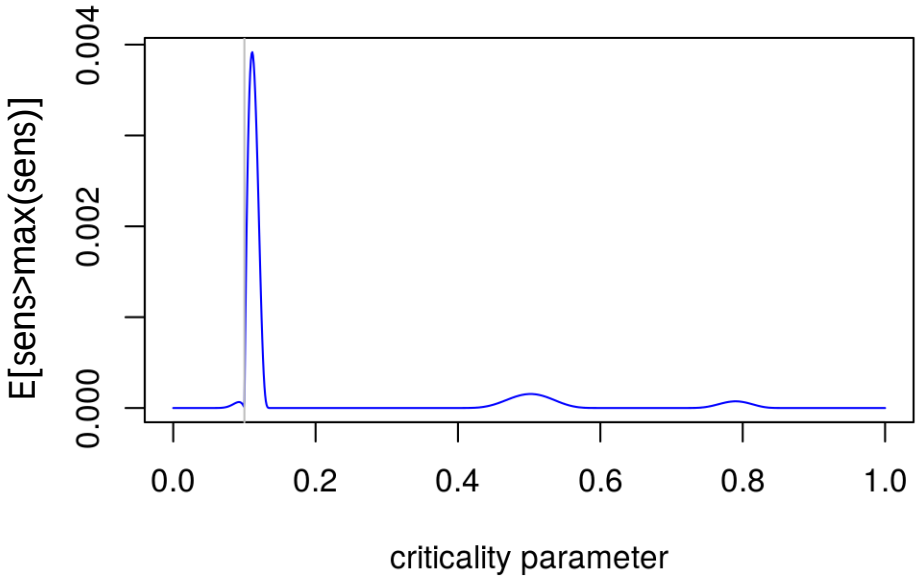
“Valuable” point (pitch, $R_{sleeves}$)

Aim at reaching highest sensitivity to ^{95}Mo capture

Where to add next points/calculations?

where is the highest E[sens > max{sens}]





“Optimization”

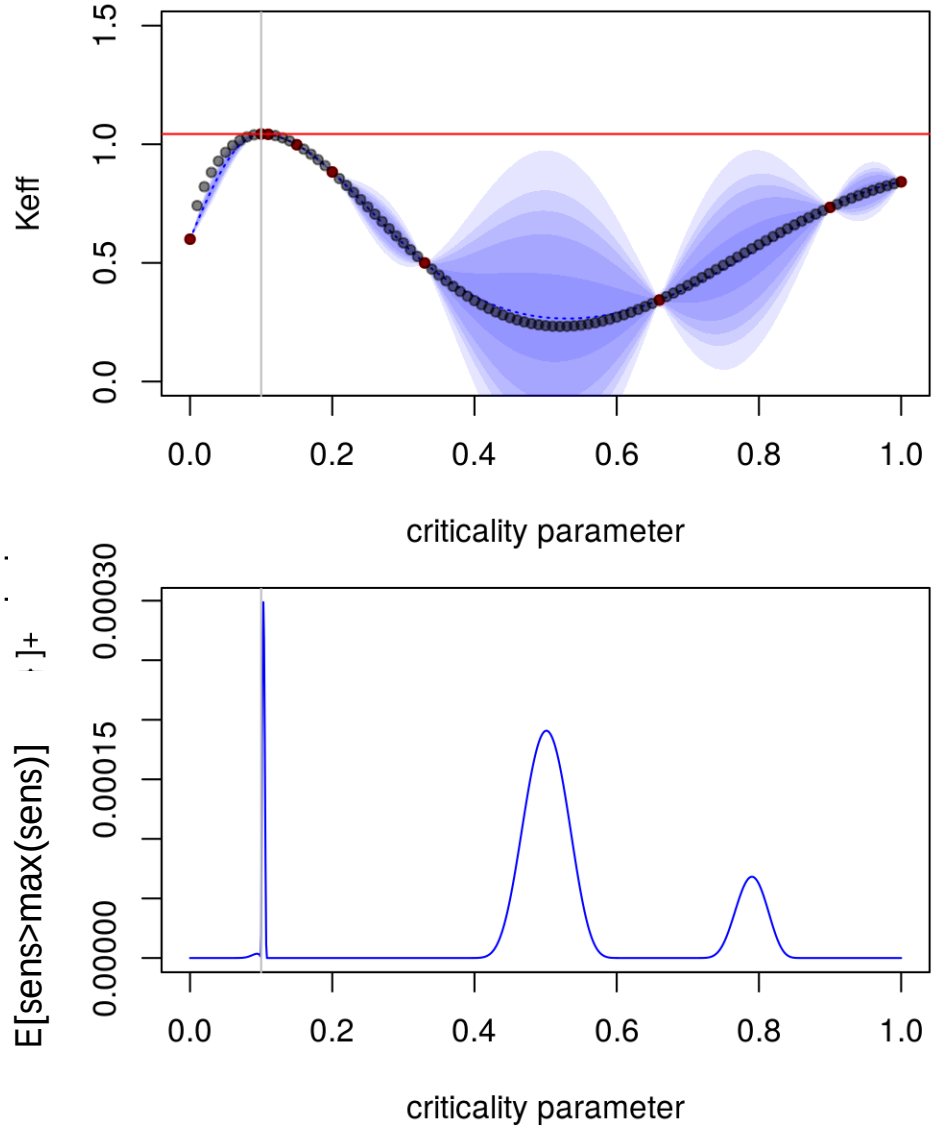
“Valuable” point (pitch, $R_{sleeves}$)

Aim at reaching highest Sensitivity to ^{95}Mo capture

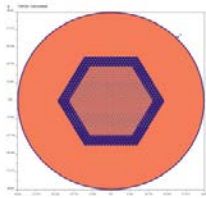
Where to add next points/calculations?

where is the highest E[Sens > max{Sens}]

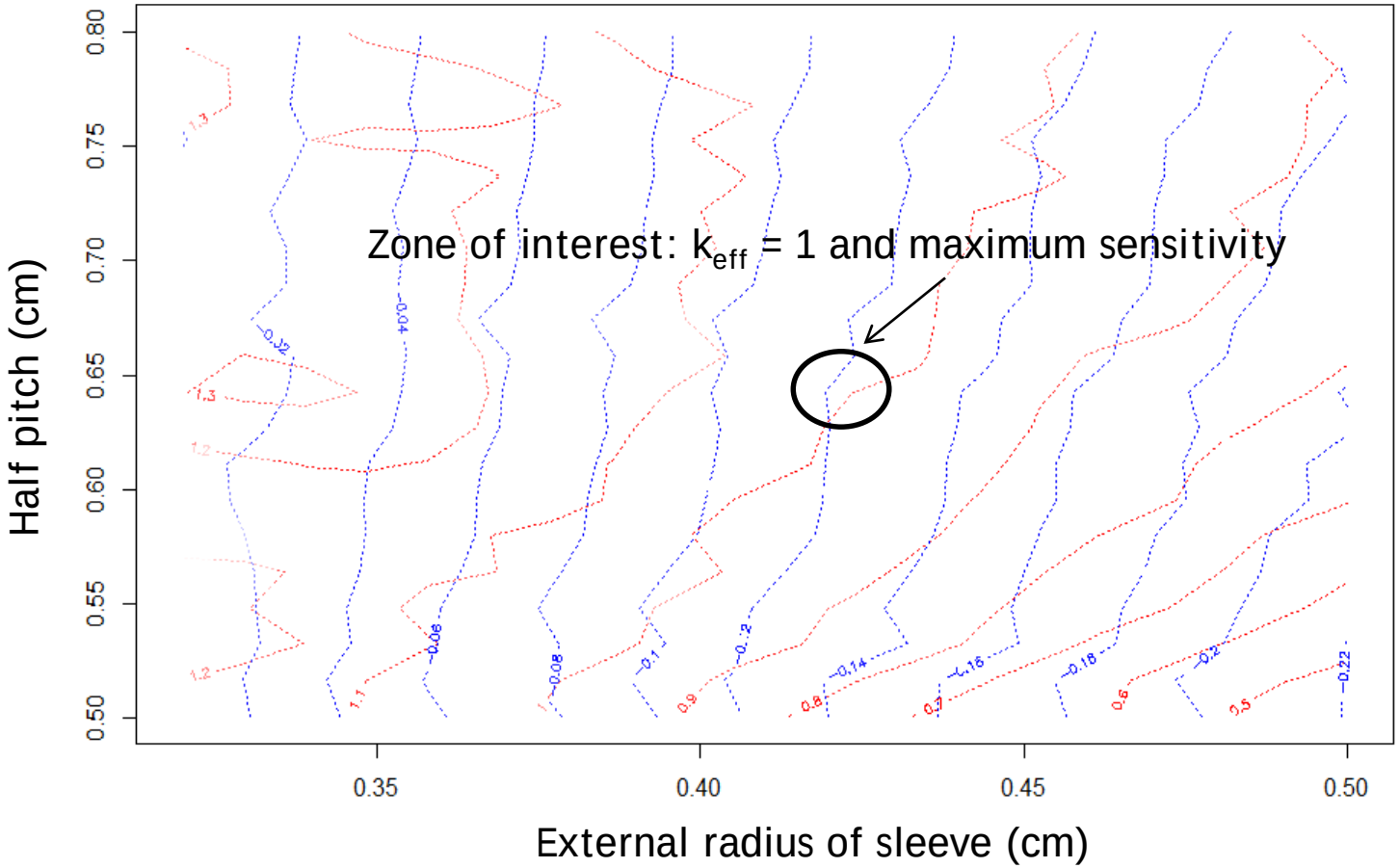
In the end,
we reached the highest sensitivity



EGO algorithm

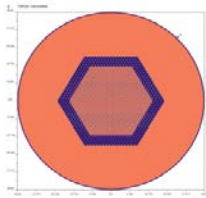


27 crowns Hexagonal lattice of 7uPCX rods surrounded by sleeves

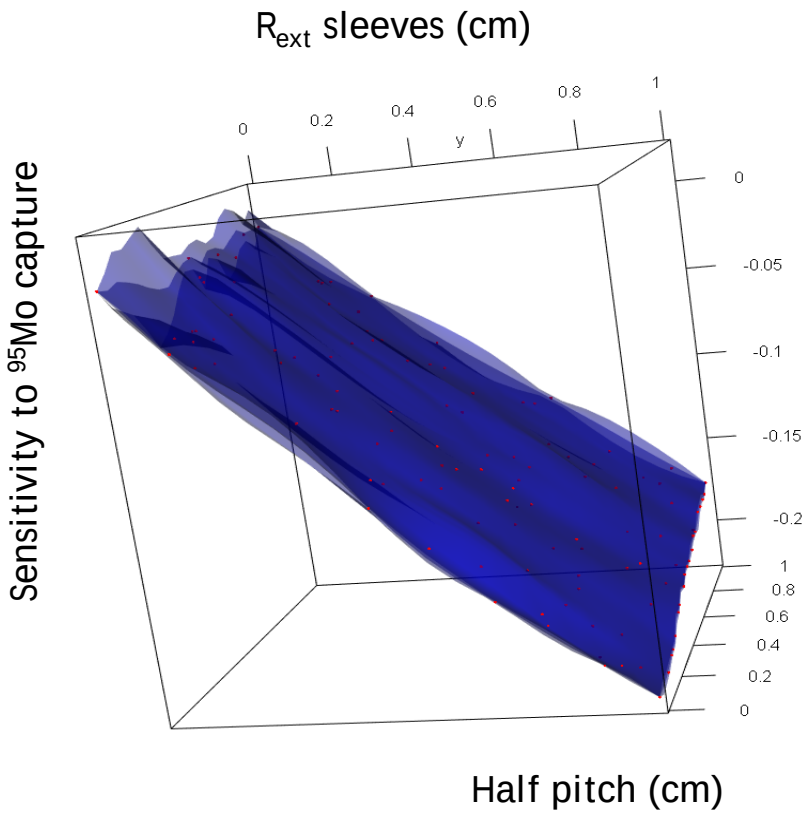


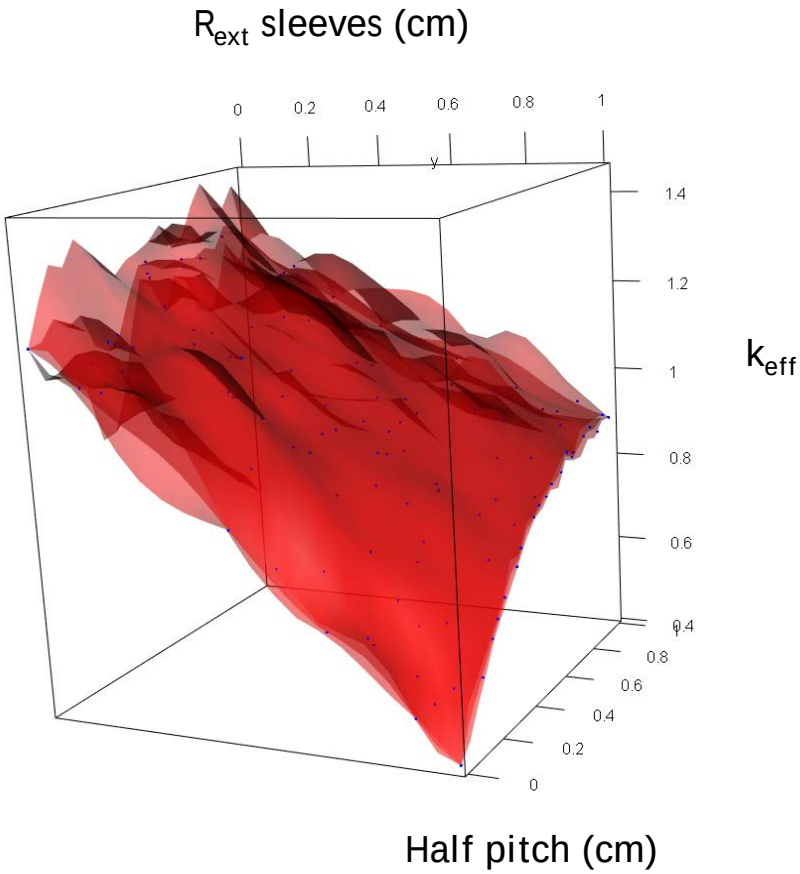
↳ Maximum sensitivity to ^{95}Mo capture = 0.2 %/%

ECEGO algorithm

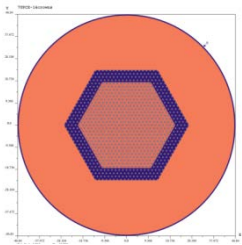


Hexagonal configuration with 27 crowns of 7uPCX rods and molybdenum sleeves (red and blue dots correspond to measurement points)

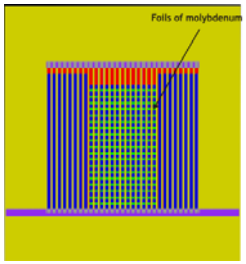




Tested configurations



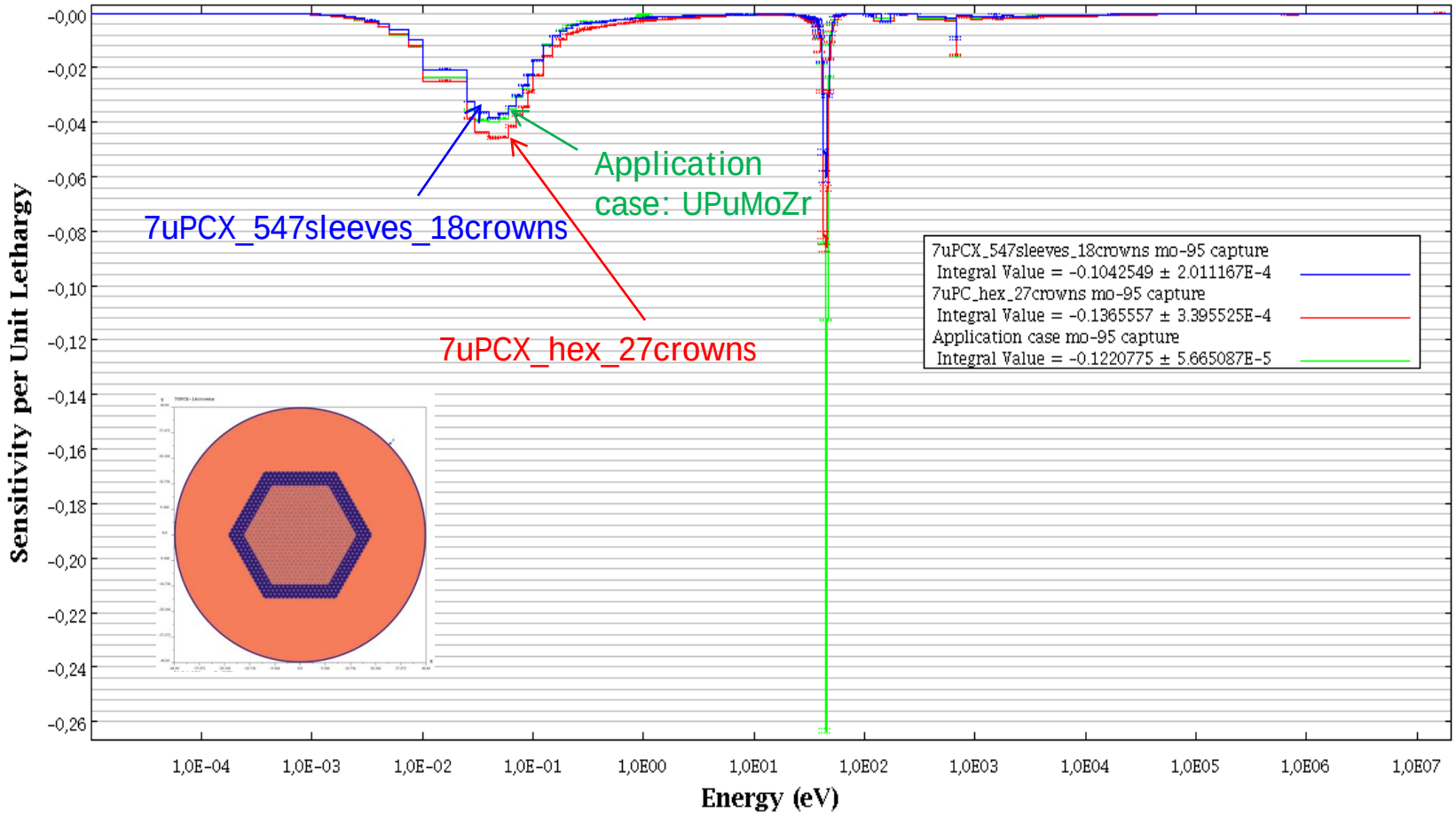
- Mo metallic rods inside lattice of BUCCX or 7uPCX rods: not promising
- Sleeves of Mo surrounding 7uPCX rods
  - 7uPCX: number of sleeves (up to 547), sleeves thickness variable
- Metallic foils incorporated in BUCCX rods
  - BUCCX: number of foils per rod (1 to 23), thickness of foils variable



↳ For each configurations: square or hexagonal pitch was studied and set variable

Configuration	Description	Thickness of foils/sleeves (cm)	Pitch (cm)	Integral sensitivity (%/%) ^{95}Mo capture
BUCCX_18 x 18_144	Square lattice of 324 BUCCX rods with internal "test" zone of 144 BUCCX rods with Mo foils	{0.01-0.578} **0.578**	{1.4-2.4} **2.02**	**-0.038**
7uPCX_547sleeves_ 18 crowns	Hexagonal lattice of 7uPCX rods without sleeves (18 crowns) with an internal "test" zone of 547 7uPCX rods with Mo sleeves	{0.02-0.182} **0.112**	{1-1.6} **1.566**	**-0.100**

Comparison with industrial case



↳ Sensitivity profiles close in shape and integral value to the application case, even if the sensitivity at the resonance peak still stays lower

Conclusions

- Use of algorithms allows
  - Reducing considerably the calculation time for determining the optimal case
  - Ensuring that the optimal case is not forgotten

- Configurations involving molybdenum were determined for realization at SNL on SPRF/CX
  - Configuration with Mo sleeves around 7uPCX rods leads to best sensitivities
  - Improvement of k_{eff} sensitivity to ^{95}Mo capture in thermal and epithermal energy ranges compared to other available experiments
  - Partial coverage of the resonance peak of the application case (UPuMoZr in reprocessing plants residues)
    - Determination of the bias due to nuclear data of ^{95}Mo

- Prospects
  - Apply the same methodology on ^{103}Rh to improve sensitivity of k_{eff} to ^{103}Rh capture of LCT-079

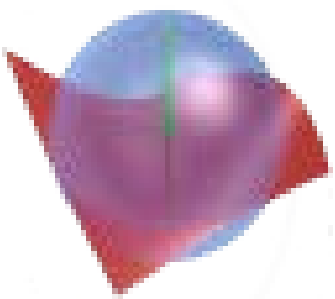
Thank You For Your Attention!

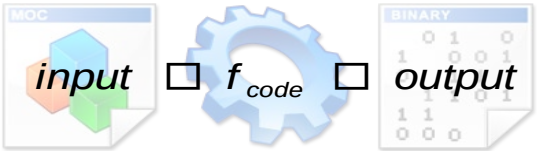
PROMETHEE Workbench

- Some feedback from criticality assessment engineering
  - Lot of time spent on computer dependent problems
    - Less time on safety and physics
  - Some issues seem too *expensive* to solve
    - Splitting problems (independency of variables), maybe oversimplifying safety analysis

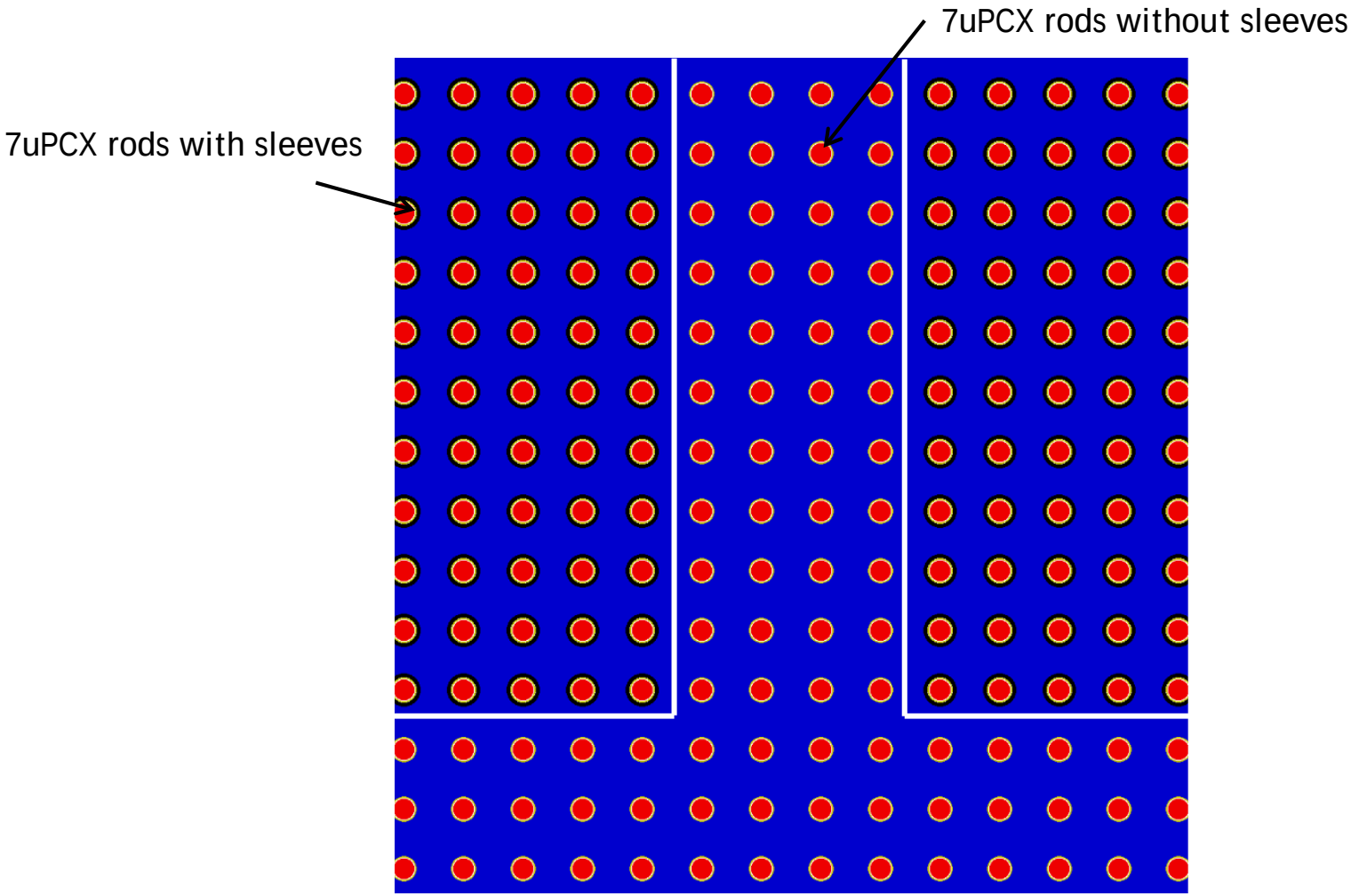
- PROMETHEE project
  - Improve usability for real world computing
    - Computing task to become **fast and easy**
    - Reliable **remote execution** on largest computing resource available
  - Extend reachable engineering issues
    - **Encapsulation** of code as input/output numerical function (MCNP, SCALE-KENO, MORET, APOLLO, TRIPOLI, …)
    - Provide robust **algorithms** toolbox for common use ([R] wrapping)
      - Monte Carlo sampling methods
      - **EGO and ECEGO:**

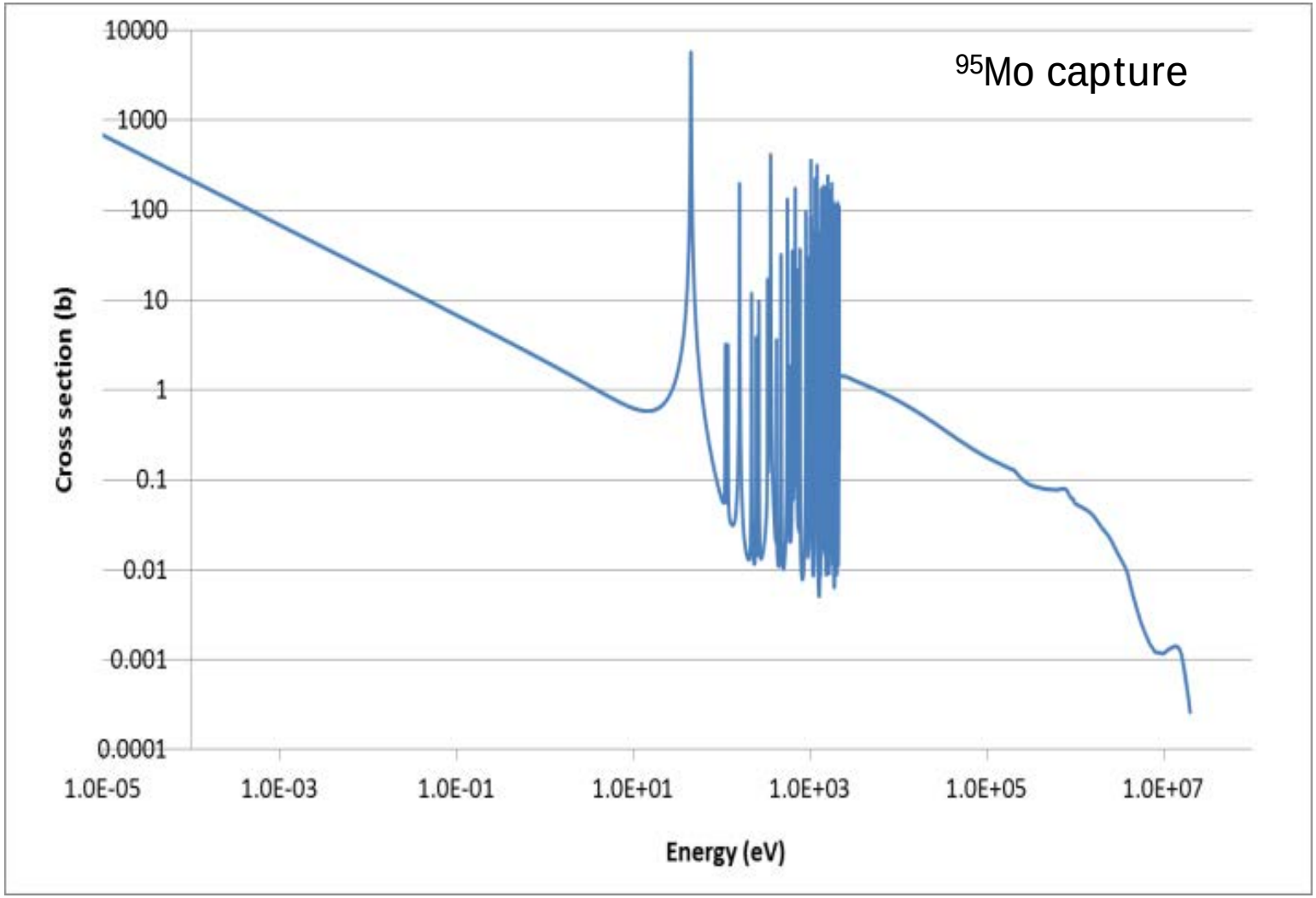
        Optimization w/wo constraint





Design with 7uPCX rods




95Mo capture
10000
1000
100
10
1
0.1
0.01
0.001
0.0001
Cross section (b)
1.0E-05
1.0E-03
1.0E-01
1.0E+01
1.0E+03
1.0E+05
1.0E+07
Energy (eV)