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# PROPOSAL OF POINT-WISE POWER RECONSTRUCTION FOR IRT-4M FUEL ASSEMBLIES IN COUPLED MONTE-CARLO CALCULATIONS

Pavel Jíška*, Jan Frýbort

*Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Department of Nuclear Reactors, V Holešovičkách 2, 180 00 Prague 8, Czech Republic*

* corresponding author: jiskapav@fjfi.cvut.cz

Abstract. Current efforts to develop high-fidelity multi-physics tools for research reactors with IRT-4M fuel leads to the involvement of Monte-Carlo transport and subchannel thermo-hydraulic codes in the process of safety assessment. Monte-Carlo based neutronic codes are often used as a reference tool and are suitable for a prediction of a detailed power distribution. This paper proposes a method of the point-wise power reconstruction based on a Radial Basis Function (RBF) interpolation for complicated irregular geometries and compares different detector functionalities of the Serpent2 code from the time efficiency point of view. Furthermore, a preliminary validation of the applied method for IRT-4M in a subchannel code SUBSALS mesh is presented. This code is currently under the development at the Research Centre Řež and the Czech Technical University in Prague and focuses on the thermohydraulic analysis of IRT type fuel assemblies.

Keywords: Power reconstruction, multi-physics coupling, IRT-4M, Serpent2, SUBSALS.

## 1. Introduction

The main motivation behind the development and the application of advanced calculation tools and methods is the ensurement of ability to simulate the processes in the reactor core with a lower degree of uncertainity than nowadays computing resources allow, and even beyond operational safety analyses. Most of the attention is predominantly given to power reactors. However, research reactors can also have difficulties to simulate specific phenomena.

Two Czech research reactors LVR-15 [1] and VR-1 [2] are operated with IRT-4M fuel assemblies. This type of fuel has an unusual irregular geometry as demostrated by Figures 1a or 1b. Its basic description is provided by Table 1.

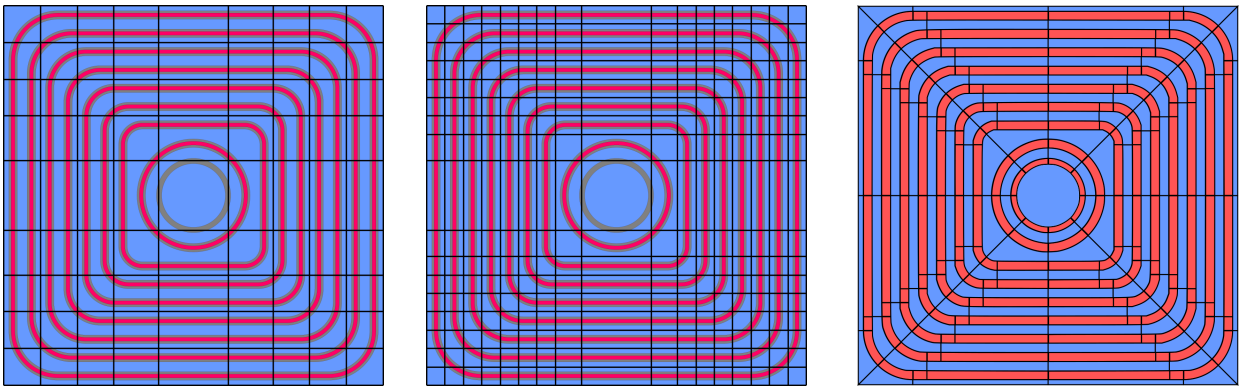
| **Designation** | **Value** |
|---|---|
| Fuel assembly type | IRT-4M standard |
| Number of fuel tubes in FA | 8 |
| Fuel meat material | $UO_2$ + Al |
| Enrichment | 19.7 % |
| Cladding material | SAV-1 alloy |
| Mass of $^{235}$U in FA | 300 g |
| Core pitch | 71.5 mm |
| Cladding thickness | 0.45 mm |
| Fuel meat thickness | 0.70 mm |
| Water gap between fuel tubes | 1.85 mm |
| Active height of fuel meat | 600 mm |
| Outer dimensions of tubes and corner radius: | |
| 1st tube | 69.6 mm; 9.3 mm |
| 2nd tube | 62.7 mm; 8.5 mm |
| 3rd tube | 55.8 mm; 7.7 mm |
| 4th tube | 48.9 mm; 6.9 mm |
| 5th tube | 42.0 mm; 6.1 mm |
| 6th tube | 35.1 mm; 5.3 mm |
| 7th tube | 28.2 mm; 4.5 mm |
| 8th tube (cylindrical) | 21.3 mm |

Table 1. Basic characteristics of standard IRT-4M fuel assembly [3].

Because of its unique concentric square annular fuel elements with rounded corners, the coolant flow is subjected to a relatively significant pressure driven crossflow. A detailed calculation of such thermal-hydraulic characteristics is beyond capabilities of standard dedicated one-dimensional system codes. A new subchannel code SUBSALS (SUBchannel Square Annular Layout Solver) is under the development at the Research Centre Řež and the Czech Technical University in Prague. The code is currently in the phase of concept verification. Nevertheless, its further utilisations are considered, for instance, its coupling with neutronic codes.

Monte-Carlo based neutronic codes are often used as a reference tool and are suitable for prediction of a detailed power distribution. For multi-physical coupling, it is essential to ensure the appropriate data transfer between individual codes in a required data structure. Different embedded funcionalities for power reconstruction (i.e. different detector types) are implemented in Monte-Carlo code Serpent2 [4]. However, some approaches appear to be more computationally challenging or difficult to implement in such a complex IRT-4M geometry.

Fuel assembly power mapping can be regarded as an interpolation problem of scattered data which is common in many fields. The radial basis function interpolation offers excellent tool for interpolating multidimensional scattered data whose value is dependant only on system coordinates. Thus, it is an



(A) . Mesh 9 × 9 (B) . Mesh 17 × 17 (C) . SUBSALS mesh

Figure 1. Cartesian mesh detectors 9 × 9 and 17 × 17, and SUBSALS thermal-hydraulic model for 8-tube IRT-4M fuel assembly.

appropriate approach for a power and temperature mapping in situations where values of scattered variables varies gently. In addition, the round-off error of a piecewise constant distribution could be minimized by a continuous function. However, it should be noted that the application of RBF interpolation is prone to uncertainty of sampled data, which may apply especially for Monte-Carlo tallies.

## 2. Theory

Within this work two different types of response detector meshes were considered for power reconstruction in the IRT-4M fuel assembly. Those meshes are denoted here as:

(1.) **mesh of cell detectors (MOCD)** is a general mesh made of individual cell detectors (see option `dc` in [5]) situated only in the fuelled regions in accordance with required SUBSALS layout (see Figure 1c),

(2.) **irregular Cartesian mesh detector (ICMD)** is a standard Serpent2 irregular Cartesian mesh (see option `dmesh` with `datamesh` type 6 in [5]).

MOCD enables to determine values of a variable in a general spatial mesh superimposed on the base area of an fuel assembly, whereas IRMD can be applicable only to an irregular Cartesian grid problem. Therefore MOCD is here considered as a reference mesh for point-wise *RBF-based power reconstruction* testing. The ICMD is here utilized as an auxiliary grid on which the mean values of an intensive variable (i.e. power density) are interpolated by RBF interpolation. Here should be noted, that the term *point-wise* power reconstruction is here used to distinquish from a frequently used term *pin-wise* or *plate-wise* power reconstruction since the process of evaluation is different and the final value is not connected with any fuel pins or plates, but rather with a general volume and its center of mass.

Basic descriptions of mesh and cell detectors are mentioned in this section. Further, basic information about RBF interpolation for the *pin-wise* power reconstruction in IRT-4M fuel assemblies are provided.

### 2.1. Mesh/cell detectors

Monte-Carlo mesh detectors are able to determine various integral quantities in user-defined detector bins. The fundamental idea is based on a division of space into partial regions and a selection of events of particular interest. The resultant spatial description of integral quantities has the character of a piecewise constant function.

For fission energy production $P$ is evaluated integral of type

$$P = \int_V \int_E \kappa\Sigma_f(\mathbf{r}, E)\, \phi(\mathbf{r}, E)\, d^3r\, dE, \qquad (1)$$

where $\kappa\Sigma_f(\mathbf{r}, E)$ is macroscopic total fission energy production cross section and $\phi(\mathbf{r}, E)$ is neutron flux density [6].

In order to achieve the highest possible level of statistical accuracy, it is reasonable to increase the size of cells in mesh detectors or to increase the number of neutron tallies. On the contrary, in an effort to characterize the distribution function as accurately as possible, it is necessary to minimize the rounding error of the mesh detector approximation. However, the common limit condition is the computational performance. For any simulation, it is necessary to find the balance between the level of the detail and the simulation time [7].

### 2.2. Radial basis function theory

Radial basis functions interpolation is one of the commonly used methods to interpolate multi-dimensional data and have gained popularity over the last few decades in a variety of areas such as a surface reconstruction, multivariate interpolation, approximation theory, neural networks, machine learning, etc. RBFs are typically used to approximate an unknown func-

tion $f : \mathbb{R}^n \to \mathbb{R}$ by the continuous function

$$s(\mathbf{x}) = \sum_{i=1}^{N} \lambda_i \, \varphi(||\mathbf{x} - \mathbf{x}_i||), \tag{2}$$

where $\{\mathbf{x}_i, i = 1, 2, ..., N\} \in \mathbb{R}^n$ are given scattered data coordinates, $\varphi : \langle 0, \infty) \to \mathbb{R}$ denotes a radial basis function, and $||\mathbf{x} - \mathbf{x_i}||$ is the Euclidean norm between coordinates $\mathbf{x}$ and $\mathbf{x_i}$ [8].

The approximating function, to be constructed over $N$ sampled coordinates, satisfies

$$s(\mathbf{x}_i) = f_i, \quad i = 1, 2, ..., N, \tag{3}$$

where values $f_i$ of unknown function $f$ are assumed to fulfill $f_i = f(\mathbf{x}_i)$. The Equation (2) could be rewritten in terms of linear system of equations

$$\mathbb{A}\lambda = \mathbf{f}, \tag{4}$$

or in matrix form

$$\begin{pmatrix} \varphi(r_{1,1}) & \dots & \varphi(r_{N,1}) \\ \vdots & \ddots & \vdots \\ \varphi(r_{1,N}) & \dots & \varphi(r_{N,N}) \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \vdots \\ \lambda_N \end{pmatrix} = \begin{pmatrix} f_1 \\ \vdots \\ f_N \end{pmatrix}, \tag{5}$$

where $r_{j,i} = ||\mathbf{x}_j - \mathbf{x}_i||$. From the definition of the Euclidean norm, it is clear that matrix $\mathbb{A}$ is symmetric with dimensions $N \times N$. To ensure a unique solution, the matrix $\mathbb{A}$ has to be non-singular. Specific form of the radial basis function $\varphi(r)$ may have a different prescription (e.g. gaussian, multiquadric, polyharmonic, etc.).

## 3. Power reconstruction

Currently, the Serpent2 program focuses predominantly on reactor systems with regular grids, similar to standard power reactors. Its coupling interface is not fully adapted to generally irregular geometries, as required in the SUBSALS code for IRT-4M representation. However, this minor deficiency can be easily circumvented using a specific type of *mesh of cell detectors* and an individual coupling wrapper.

In the proposed subchannel model, for the IRT-4M fuel assembly in SUBSALS program (see Figure 1c), three different types of heat sources occur:

- one-eighth annular section,
- large straight plate,
- small straight plate.

### 3.1. Models description

Serpent2 models includes simplified three-dimensional LVR-15 reactor core configuration with standard (8-tube) fresh fuel assemblies IRT-4M surrounded by beryllium blocks (see Figure 2). Depending on the level of detail of fuel meat division inside one preselected fuel assembly, two geometrically different models can be distinguished:

(1.) **simplified FA model**
where all fuel tube cells and water channels are considered as an unique material cell circumscribed by square prisms with rounded corners,

(2.) **detailed FA model**
which is almost identical to the *simplified FA model* with the only exception in the one core position (B6 or E6), where fuel meat materials are replaced by the identical material azimuthally divided into the SUBSALS computational mesh (i.e. 8 fuel meat cells replaced by 168 cells).

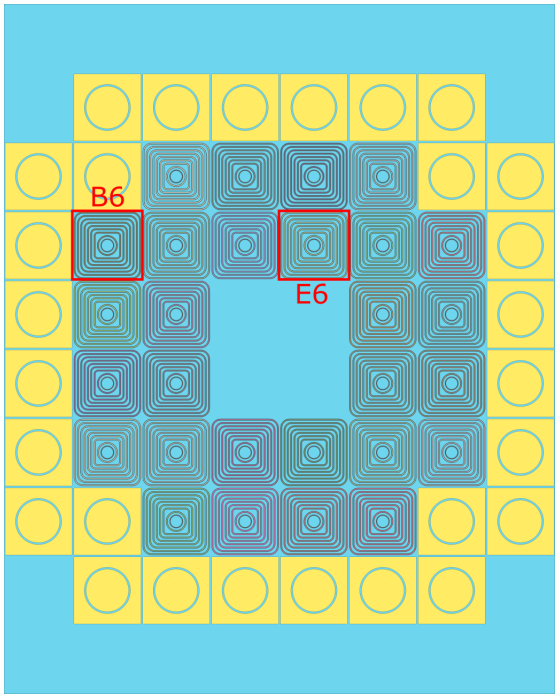


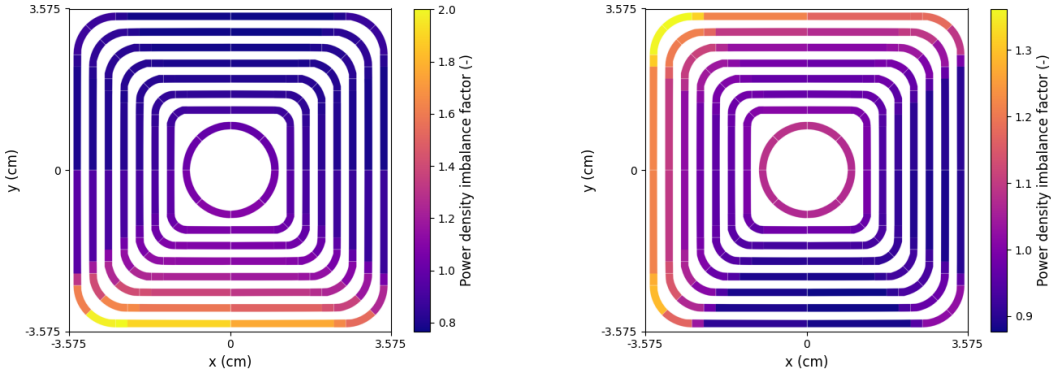

Figure 2. Serpent2 model with IRT-4M fuel assemblies surrounded by beryllium blocks (framed positions B6 and E6 of particular interest).

Depending on the implementation of response detector meshes (see MOCD and ICMD), three different approaches were considered for determining the *point-wise* power distribution in the SUBSALS layout. The nomenclature for each approach is stated below. These notations will be used throughout this work for a simplification:

(1.) **cell-based model**
where the *detailed FA model* is utilized and a *mesh of cell detectors* (MOCD) is directly included in the main universe as individual fuel meat cells,

(2.) **universe-based model**
where the *simplified FA model* is utilized and a *mesh of cell detectors* (MOCD) is included in a separate universe as mesh of individual detector cells overlapping the main universe,

(3.) **RBF-based model**
where the *simplified FA model* is utilized and an *irregular Cartesian mesh detector* (ICMD) is applied




(A) . Position E6 (B) . Position B6

Figure 3. Reference power density imbalance factors $k_q^{(i)}$ in the SUBSALS mesh.

for a subsequent two-dimensional RBF interpolation.[1]

### 3.2. Testing settings

All results were generated by running Serpent2 (version 2.1.32) in a criticality source simulation mode. The run parameters were set with 40 inactive cycles to populate the fission source, 400 active cycles to collect results, and 500 000 neutrons per cycle. All calculations were performed on one computer using 32 OpenMP threads with processor AMD EPYC 7351. The host operating system was an Ubuntu 20.04.4 LTS.

### 3.3. Implementation of RBF-based power reconstruction

It is necessary to mention at the outset that tested *RBF-based power reconstruction* method utilizing RBF interpolation is established on rough simplifying assumptions. The method is based on the known distribution function in the auxiliary grid (e.g. ICMD). The auxilliary mesh selection for IRT-4M fuel assembly is considerably complicated task and can have a significant effect on reconstruction outputs.

Source data for the *RBF-based power reconstruction* are total values of power in auxiliary Cartesian mesh (i.e. ICMD), or respectively mean power density if related to the relevant fuel meat volume. However, the question how to assign function values (i.e. power densities) to the spatial coordinate remains. Usually they are assigned to the center of mass of given fuel meat element (e.g. in *pin-wise* reconstruction). Nevertheless, the center of mass of ICMD cell may not coincide with the center of mass of the fuel meat cell. Unfortunately, this may result in the incorrect assignation of function values (especially when multiple fuel cells are in Cartesian mesh cell or when rounded corners are included) and thus resultant interpolant could be disorted. In this work, the mean values were always assigned to the center of mass of Cartesian mesh cell detector. The common aim was to create Cartesian mesh so that center of masses matches (at least in planar segments).

Another assumption is that resulting power distribution is obtained by quantifying the interpolation function at predefined coordinates and by volumetric multiplication of given fuel meat element. Predefined coordinates were chosen manually to correspond approximately to the center of mass of fuel meat element in SUBSALS layout. However, the assumption is fulfilled only if the course of the function is not convex or concave in the given interval.

Within this work, the polyharmonic radial basis function

$$\varphi(r) = r^3 \tag{6}$$

was selected for testing. The choice of RBF was based on the good practice and meaningful reconstruction outputs. The utilisation of other radial basis function is possible, but their impact on results was not evaluated here.

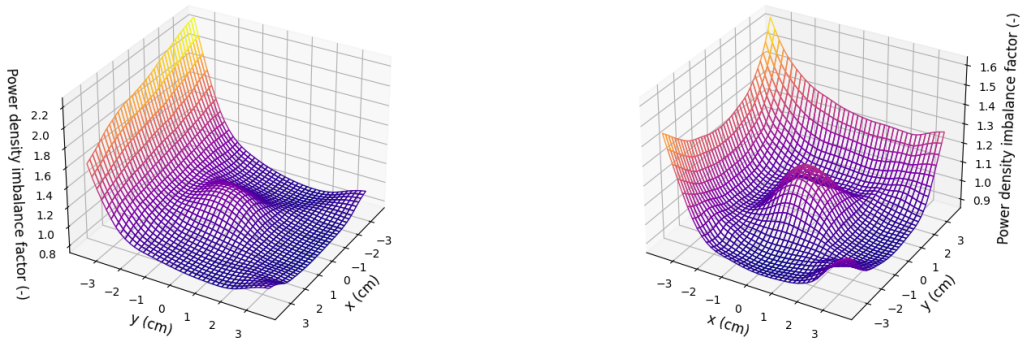
An auxiliary program for the *RBF-based power reconstruction* has been created. The program utilizes Python3 language and is based on NumPy and SciPy libraries (version 1.23.1, respectively 1.9.0). The program has an automatic procedure, which can evaluate IRT-4M fuel meat volumes almost in any ICMD cell to ensure proper volume division and also includes plotter in SUBSALS mesh (see Figure 1c) for result visualisation such as Figures 3.

### 3.4. Testing RBF-based power reconstruction

The point-wise *RBF based power reconstruction* was tested on two different auxiliary ICMD, specifically $9 \times 9$ and $17 \times 17$. Meshes were set as demonstrated on Figures 1a and 1b. The division of the detector in the vertical direction was not considered.

Performed point-wise *RBF based power reconstructions* were compared against the reference data obtained directly in SUBSALS layout (i.e. direct comparison with *universe-based model* results). It was

[1] Please note, that the manner of response detector mesh implementation is external for *universe-based* and *RBF-based models*, whereas internal for a *cell-based model*.




(A) . Position E6 (B) . Position B6

FIGURE 4. RBF interpolation of reference data.

ensured, by the calculation settings, that the statistical uncertainity for individual fuel meat elements was below 0.5 % and the case of Cartesian meshes for individual cells up to 1 % (especially for cells with lowest contain of fuel meat, i.e. cells (4,4) and (5,5) in mesh $17 \times 17$).

In the Figure 3, reference values of power density imbalance factors $k_q^{(i)}$ for fuel tubes cells in core positions E6 and B6 are depicted. Power density imbalance factors can be expressed by equation:

$$k_q^{(i)} = \frac{q_v^{(i)}}{\overline{q_v}}, \tag{7}$$

where $q_v^{(i)}$ is a power density in cell $i$ and $\overline{q_v}$ denotes a mean fuel assembly power density in given axial layer. In the Figure 4 are demonstrated RBF interpolations of reference data in positions E6 and B6.

When comparing point-wise *RBF-based power reconstructions* for both Cartesian meshes with reference data (see Figures 5 and 6), it is possible to quantify relative deviations. Those are summarized by the Table 2.

Overall, presented and roughly simplified *RBF based power reconstruction* gives reasonable results, because the maximal fission power density difference between neigbouring fuel meat elements could reach roughly 13 % for fuel assembly in the B6 possition and 23 % in the E6. The round-off error of irregular mesh reconstruction is higher than the error of point-wise *RBF based power reconstruction.*

| Position and ICMD | Max. deviation | RMSE |
|---|---|---|
| B6 mesh $9 \times 9$ | 3.29 % | 1.15 % |
| E6 mesh $9 \times 9$ | 4.29 % | 1.28 % |
| B6 mesh $17 \times 17$ | 2.33 % | 0.91 % |
| E6 mesh $17 \times 17$ | 3.51 % | 1.03 % |

TABLE 2. Max. relative differences of *RBF-based power reconstruction* from reference data.

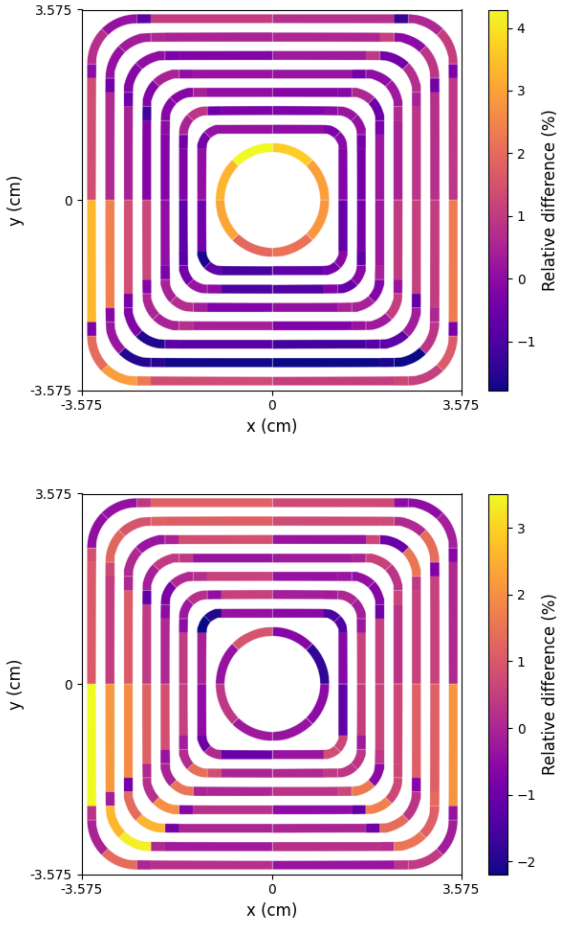



FIGURE 5. Relative differences between *RBF-based power reconstruction* and reference data for Cartesian meshes $9 \times 9$ (top) and $17 \times 17$ (bottom), both for fuel assembly in E6.

## 4. COMPUTATIONAL SPEED

The computational performance of the Monte-Carlo simulation depends predominantly on the complexity of created model. The total number of cells and their boundary surfaces play an important role in this case. Creating strongly heterogeneous discrete models (i.e. models whose properties are characterized by many

| Parameter | simplified FA w/o detectors | detailed FA w/o detectors | RBF-based model 9 × 9 | RBF-based model 17 × 17 | cell-based model | universe-based model |
|---|---|---|---|---|---|---|
| Total CPU time [min] | 2358.83 | 2694.85 | 2378.52 | 2522.38 | 5745.35 | 7721.40 |
| Total wall-clock running time [min] | 92.74 | 105.12 | 92.73 | 95.19 | 197.83 | 260.95 |
| Wall-clock time for transport simulation [min] | 92.00 | 104.50 | 92.00 | 94.52 | 197.18 | 260.33 |
| CPU usage fraction in transport simulation [–] | 25.70 | 26.10 | 25.90 | 26.85 | 29.23 | 29.78 |
| Allocated memory size [Mb] | 7586.46 | 7589.86 | 7586.46 | 7586.46 | 7590.06 | 7588.57 |
| Memory used for storing cross sections [Mb] | 2809.81 | 2809.81 | 2809.81 | 2809.81 | 2809.81 | 2809.81 |
| Memory used for storing material-wise data [Mb] | 1086.42 | 1086.42 | 1086.42 | 1086.42 | 1086.42 | 1086.42 |
| Total number of cells [–] | 3305 | 3465 | 3305 | 3305 | 3465 | 3473 |
| Total number of cells using unions [–] | 0 | 0 | 0 | 0 | 0 | 0 |

Table 3. Comparison of Serpent2 simulation characteristics for different cases.

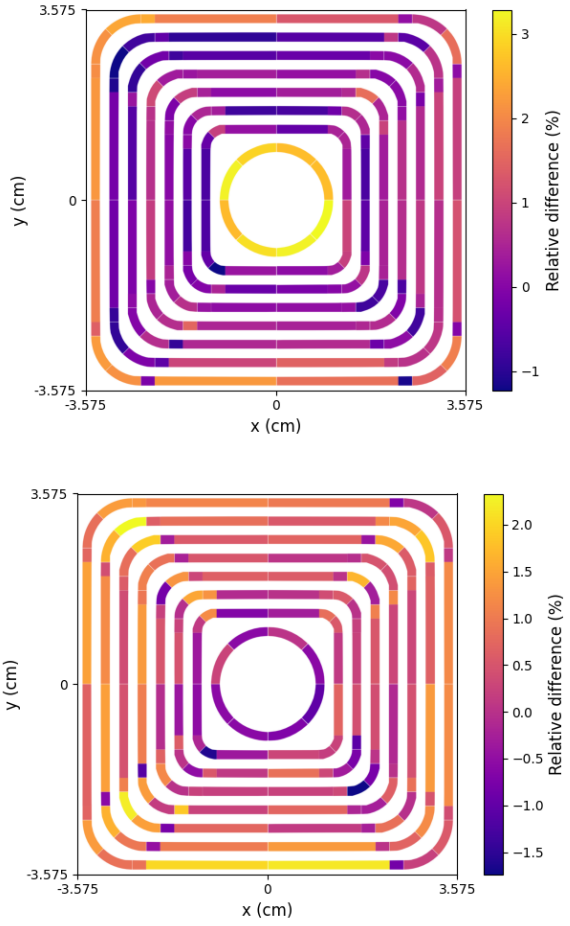



Figure 6. Relative differences between *RBF-based power reconstruction* and reference data for Cartesian meshes $9 \times 9$ (top) and $17 \times 17$ (bottom), both for fuel assembly in B6.

materials and a common, usually mean, value of state variable) can be not only computationally inefficient, but also user-unfavorable.

The comparison of main computational characteristics is provided in Table 3. As can be seen, the utilisation of a finer model division of fuel meat in the position B6 leads to an extension of computing time by approximately 14 % (from the dirrect comparison of *simplified FA* and *detailed FA model* without any detectors). If other fuel meat elements were divided, for instance in other fuel assemblies, the effect of the time increase will be even more significant. Consequently, performing full core calculations with cell detectors can be considerably time disadvantageous.

In terms of the *pin-wise* power distribution reconstruction, a significant increase of computational time was observed in the case of *cell-based* and *universe-based models*. From Table 3 is evident that the utilization of cell detectors has considerable impact on the transport simulation time. In direct comparison with *RBF-based models* (i.e. standard ICMD), this increase can be quantified for *cell-based model* by 144 % and for *universe-based model* even by 224 %. In both cases, an increase of fraction of time spent in OpenMP parallel loops was observed (by 15 % and 19 %, respectively).

## 5. Discussion

Modification of the cell detectors implementation in Monte-Carlo code Serpent2 may allow to detect local neutron-physical characteristics more efficiently, with lower computing time and a more user-friendly model definition (i.e. without any update of model, which also applies to models considering detailed burnup distributions). To focus on the cell of particular interest, which is not included in geometry, could be crucial in neutron-physical and thermal-hydraulic coupling. In that case, several iterations (or criticality source simulations) are performed until the set convergence criterion is met. Observed time increase will be multiplied, and even more if simulating full core coupled calculations. However, the author is not fully acquainted with the implementation of cell detectors in the Serpent2 code. This could be further discussed with code developers.

If the modification is not feasible, a simplificated method of *RBF-based power reconstruction* for IRT-4M fuel assembly was presented to shorten the computational time. For application of this method, the reduction of statistical uncertainty is necessary and ensurement of proper values to coordinates pairing. Further optimization of this method is possible as demostrated in the Section 3.4. Furthermore, this method could be applicable to the temperature characteristics of fuel and coolant materials in coupled

calculations. The pleasant benefit is that coupled Monte-Carlo models could not have to be geometrically complicated (not necessary to use a discrete material segmentation) and potentially save computinal time spent in a neutron transport simulation. The local temperatures of each fuel meat element, or coolant channel, could be also described by RBF interpolation (i.e. one function prescription) for given material region. This may result in a potential reduction of computing time in coupled calculations, because of less number of cells in transport calculation. However, this temperature field interpolation has not been computationally verified so far.

## 6. Conclusions

In this work a new method for power reconstruction for IRT-4M fuel assemblies was presented. The *RBF-based power reconstruction* method was tested to provide quantitative characterization of method error and the computational demands. Testing was performed on simplified LVR-15 reactor core for two selected fuel assembly positions B6 and E6 with different assembly-wise power distribution.

Demonstrated application gives reasonable results with errors lower than a round-off error of neighbouring fuel element cells. Although rough simplifications were used, the maximal observed deviation was approximately 4.3 %. Maximal power density imbalance RMSE for fuel assembly reaches less then 1.3 %. Maximal deviations decrease with finer division of mesh. Nevertheless, with finer mesh cells, larger local uncertainties may appear. Attention need to be paid, when choosing input data from a Cartesian data mesh.

As a part of this work was found, that cell detectors implemented in Monte-Carlo code Serpent2 (version 2.1.32) has a significant impact on computational time. When using *cell-based model* for direct power reconstruction (see Section 3.1), an increase in computing time around 144 % was observed. If *universe-based model* (see Section 3.1) was used, the time extension was approx. 227 %. This outcome is going to be further discussed with code developers. The new update of cell detectors of Serpent2 may allow to detect local neutron-physical characteristics more efficiently, with lower computing time and a more user-friendly model definition (i.e. without any update of model).

### List of symbols

$\mathbb{A}$ Matrix of evaluated kernels
$CPU$ Central Processing Unit
$E$ Energy [J]
$f_i$ Function value in $\mathbf{x}_i$
$ICMD$ Irregular Cartesian mesh detector
$\kappa$ Recoverable energy per fission [J]
$k_q^{(i)}$ Power density imbalance factor for node $i$ [–]
$\lambda_i$ Linear combination coefficient
$max$ Maximum
$MOCD$ Mesh of cell detectors
$P$ Total power [W]
$q_v^{(i)}$ Power density in node $i$ [$\mathrm{W\,m^{-3}}$]
$\overline{q_v}$ Mean fuel assembly power density [$\mathrm{W\,m^{-3}}$]
$\mathbf{r}$ Position vector
$||r||$ Euclidean norm
$RBF$ Radial Basis Function
$RMSE$ Root Mean Square Error
$\Sigma_f$ Fission macroscopic cross section [$\mathrm{m^{-1}}$]
$s(\mathbf{x})$ Aproximating Radial Basis Function interpolation
$\phi$ Neutron flux [$\mathrm{m^{-2}\,s^{-1}}$]
$\varphi$ Radial Basis Function kernel
$V$ Volume [$\mathrm{m^3}$]
$x$ Coordinates x-axis [cm]
$y$ Coordinates y-axis [cm]

### Acknowledgements

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