Decay Heat Curve Generation for High Temperature Reactors Using Exponentials, Support Vector Machines and Dynamic Mode Decomposition Within the RAVEN Framework

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INTRODUCTION

This paper is aimed to present a methodology based on the usage of the RAVEN code [1,2] for the construction of a multi-dimensional decay heat (DH) curve for High Temperature Reactors, via DH calculations performed by ORIGEN [3]. The main goal of this activity has been the identification of a model able to surrogate the phenomenology of the DH after shutdown, satisfying the following requirements:

- Reasonable prediction accuracy till 3 months after the shutdown
- Ability to capture the main deviation effects determined by field conditions (e.g. burn-up, fuel temperature, fissile enrichment, etc.)
- As easy as possible formalism in order to possibly allow the implementation of the curve into system codes (e.g. RELAP5-3D [4]) inputs exploiting, for example, control variable systems

Three surrogate models (also known as DH curves in the safety analysis nomenclature) has been identified:

- A Spline Exponential surrogate model
- A Support Vector Regression [5] model
- A Dynamic Mode Decomposition [6] model

In the following paragraphs, after a brief introduction of the tools that have been used, details regarding the Surrogate models and their performance are reported.

RAVEN

RAVEN is a probabilistic risk assessment, uncertainty quantification, parameter optimization and data analysis framework developed at INL since 2013.

RAVEN is designed to perform parametric and probabilistic analysis based on the response of complex system codes; it is capable of investigating the system response as well as the input space using Monte Carlo, Grid, or Latin Hyper Cube sampling schemes. Its main strength is focused toward system feature discovery, such as limit surfaces, separating regions of the input space leading to system failure, using dynamic supervised learning techniques. RAVEN includes the following major capabilities:

- Sampling of codes for uncertainty quantification and reliability analyses (dynamic probability risk assessment)
- Generation and use of reduced-order models (also known as surrogate models)
- Data post-processing (time dependent and steady state)
- Time dependent and steady state, statistical estimation and sensitivity analysis (mean, variance, sensitivity coefficients, etc.)
- Parameter Optimization (i.e. design optimization)
- Deep-learning.

The RAVEN statistical analysis framework can be employed for several types of applications:

- Uncertainty Quantification
- Sensitivity Analysis / Regression Analysis
- Probabilistic Risk and Reliability Analysis (PRA)
- Data Mining Analysis
- Model Optimization

RAVEN provides a set of basic and advanced capabilities that ranges from data generation, data processing and data visualization.

A subset of the RAVEN capabilities has been used for this activity: the Reduced Order Model (ROM) entity (also known as Surrogate models). A ROM is a mathematical model (e.g. a multi-dimensional polynomial regression model) consisting of a fast solution algorithm trained to predict a response of interest of a physical system. The "training" process is performed by sampling the response of a physical model with respect to variations of its input parameters (e.g. burnup, enrichment, etc.). The results (outcomes of the physical model) of the sampling are fed into the algorithm representing the ROM that tunes itself to replicate those results. RAVEN supports several different types of ROMs, among which the Spline Exponential, Support Vector Regression and Dynamic Mode Decomposition models, which are the subject of this work.

EMPLOYED SURROGATE MODELS

As previously mentioned, the following surrogate models have been investigated:

- Spline Exponential Model

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- Support Vector Regression
- Dynamic Mode Decomposition

In the following paragraphs a brief description of the above reported models is provided.

Spline Exponential Model

The Spline Exponential Model (SEM) is a newly developed surrogate model within the RAVEN framework. This surrogate is aimed to capture the behavior of a response of interest $\mathrm{F}(\boldsymbol{x},t)$ (e.g. DH power) using a blend of tensor spline regression and series of exponential terms ($G(\boldsymbol{x},t) \cong F(\boldsymbol{x},t)$):

$$G(\boldsymbol{x},t) = \sum_{i=1}^{N} P_i(\boldsymbol{x}) e^{-Q_i(\boldsymbol{x})} \quad (1)$$

where:

- N is the number of exponential terms requested by the user
- t is the independent monotonic variable (e.g. time)
- $\boldsymbol{x}$ is the vector of the other independent variables (burnup, enrichment, etc.)
- $P_i(\boldsymbol{x})$ and $Q_i(\boldsymbol{x})$ are spline polynomial functions of the parametric space $\boldsymbol{x}$.

The training process is performed in two distinct steps:

1. outcome (e.g. $DH_r(t)$) and the predicted one
2. once all the coefficients have been identified, tensor splines are constructed in order to predict the coefficients as function of $\boldsymbol{x}$.

Since the final formalism involves, in the prediction stage, basic mathematical functions such as exponentials and polynomials, this surrogate model is simple enough to be coded in a system code input exploiting, for example, control variable systems.

Support Vector Regression

Since a detailed explanation of the SVR is beyond the scope of this paper, just a simplistic description is here reported.

The Support Vector Regression (SVR) is an extension of the Support Vector Machine (SVM) surrogate models used in classification problems [5]. A SVR is aimed to identify the hyperplanes that maximize the margin among the "training" realizations of the response of interest. The vectors that characterize the hyperplanes are the support vectors. The main idea of SVM is to maximize the width ($\boldsymbol{w}$) of the margins, minimizing the error in predicting the outcomes. As for any model-based surrogate, the training process is characterized by an optimization search:

$$\min_{\boldsymbol{w}, b, \boldsymbol{\zeta}, \boldsymbol{\zeta}^*} \frac{1}{2} \boldsymbol{w}^T \boldsymbol{w} + C \sum_{i=1}^{n} (\zeta_i + \zeta_i^*)$$

$$\text{subject to} \begin{cases} y_i - \boldsymbol{w}^T \phi(x_i) - b \le \varepsilon + \zeta_i \\ \boldsymbol{w}^T \phi(x_i) + b - y_i \le \varepsilon + \zeta_i^* \\ \zeta_i, \zeta_i^* \ge 0, i = 1, \dots, n \end{cases} \quad (2)$$

Its dual is:

$$\min_{\boldsymbol{\alpha}, \boldsymbol{\alpha}^*} \frac{1}{2} (\boldsymbol{\alpha} - \boldsymbol{\alpha}^*)^T \boldsymbol{Q} (\boldsymbol{\alpha} - \boldsymbol{\alpha}^*) + \varepsilon \boldsymbol{g}^T (\boldsymbol{\alpha} - \boldsymbol{\alpha}^*) - \boldsymbol{y}^T (\boldsymbol{\alpha} - \boldsymbol{\alpha}^*)$$

$$\text{subject to} \begin{cases} \boldsymbol{g}^T (\boldsymbol{\alpha} - \boldsymbol{\alpha}^*) = 0 \\ 0 \le \alpha_i, \alpha_i^* \le C, i = 1, \dots, n \end{cases} \quad (3)$$

where:

- $\boldsymbol{g}$ is a unit vector
- C is the upper bound
- $\boldsymbol{Q}$ is a n by n positive semidefinite matrix containing the kernel mapping $K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$, that is aimed to implicitly map the training vectors into a higher dimensional space by the function ϕ
- $(\boldsymbol{\alpha} - \boldsymbol{\alpha}^*)$ is the vector of the dual coefficients.

The decision function is finally:

$$\sum_{i=1}^{n} (\alpha_i - \alpha_i^*) K(x_i, x) + \rho \quad (4)$$

Even if the formalism of the prediction model is a bit more complicated than the one for the SEM, it is still feasible to code this SM in a system code input (e.g. RELAP5-3D).

Dynamic Mode Decomposition

The Dynamic Mode Decomposition (DMD) is a novel methodology that demonstrated high accuracy in surrogating the dynamics of large non-linear systems, especially in the fluid dynamic field [6]. The DMD is a method that analyze data computing eigenvalues and eigenmodes of an approximate linear reduced order model.

Given a dynamic model $F(\boldsymbol{x},t)$ (e.g. $DH(\boldsymbol{x},t)$), discretized in N time steps, the data are organized in a sequence of snapshots:

$$\boldsymbol{F}_{\boldsymbol{1}}^{\boldsymbol{N}} = \{F(\boldsymbol{x}, ts_1), \dots, F(\boldsymbol{x}, ts_N)\} \quad (5)$$

where:

- $F(\boldsymbol{x}, ts_i)$ is the i-th snapshots of the system
- $\boldsymbol{F}_{\boldsymbol{1}}^{\boldsymbol{N}}$ is the MxN data matrix[2] containing all the snapshots

[2] The superscript and subscript of the matrix $\boldsymbol{F}$ indicates the index of the snapshots in the last and first column

All the snapshots are assumed to be related via a linear combination $F(\boldsymbol{x}, ts_{i+1}) = \boldsymbol{A}\,F(\boldsymbol{x}, ts_i)$:

$$\boldsymbol{F_2^N} = \boldsymbol{A}\boldsymbol{F_1^{N-1}} + \boldsymbol{r}\boldsymbol{e_{N-1}^T} \quad (6)$$

where:

- $\boldsymbol{r}$ is the vector of the residuals that take in account for what cannot be completely described by $\boldsymbol{A}$
- $\boldsymbol{e_{N-1}} = \{0, \ldots, 1\}$ is the $N-1$-th unit vector

The scope of the method is then to compute the eigenvalues and eigenvectors of $\boldsymbol{A}$ in order to reduce the dimensionality of the problem and capture its dynamics. In order to do so, an Single Value Decomposition (SVD) is performed:

$$\boldsymbol{F_1^{N-1}} = \boldsymbol{U\Sigma W^T} \quad (7)$$

$\boldsymbol{A}$ is chosen such as the snapshots in $\boldsymbol{F_2^N}$ **c**an be written as linear superposition of the columns in $\boldsymbol{U}$:

$$\boldsymbol{U^T A U} = \boldsymbol{U^T F_2^N W \Sigma^{-1}} \equiv \boldsymbol{\tilde{S}} \quad (8)$$

The eigenvalues of $\boldsymbol{\tilde{S}}$ are the eigenvalues of $\boldsymbol{A}$ and if $\boldsymbol{y}$ is an eigenvector of $\boldsymbol{\tilde{S}}$, then $\boldsymbol{Uy}$ is an eigenvector of $\boldsymbol{A}$ (since $\boldsymbol{A}$ and $\boldsymbol{\tilde{S}}$ are related via similarity transform).

Finally, the dynamic modes are:

$$\Phi_i = \boldsymbol{U}y_i \quad (9)$$

Unfortunately, the formalism of this methodology does not allow coding of the SM directly into a system code input file. The SM constructed by DMD needs to be coded directly in the software source or used for generation of lookup tables when needed.

TRAINING SET GENERATION

The construction of any surrogate model requires multiple realizations of the response of interest. In order to demonstrate the methodology and the surrogate construction the initial enrichment, burnup exposure and fuel temperature have been perturbed for a typical HTGR prismatic assembly, using ORIGEN for the decay heat calculation. The perturbation grid (48 ORIGEN realizations) is reported in TABLE I.

TABLE I. Input space perturbation discretization

Enrichment (wt.%)	Fuel Temperature (K)	Burnup (GWd/tHM)
3.4	600	16.5
5.9	900	18.8
7.2	1200	22.0
9.9		26.5

As it can be seen, the number of perturbation points is quite low to obtain a fully converged surrogate, but it is enough to present the methodology and to rank the surrogate modeling techniques in terms of ability to replicate the training results.

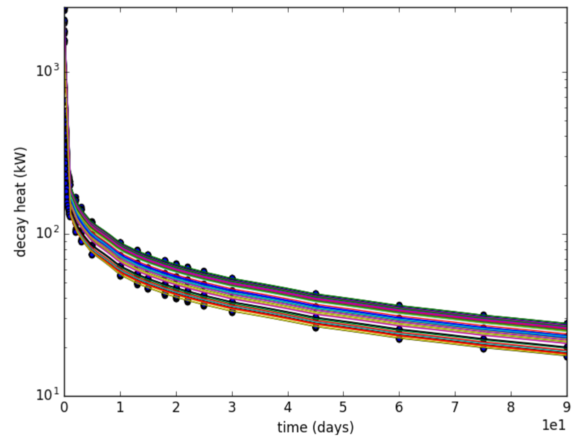

Figure 1 – 48 MC SVR predictions (line) vs. original data (scatter)

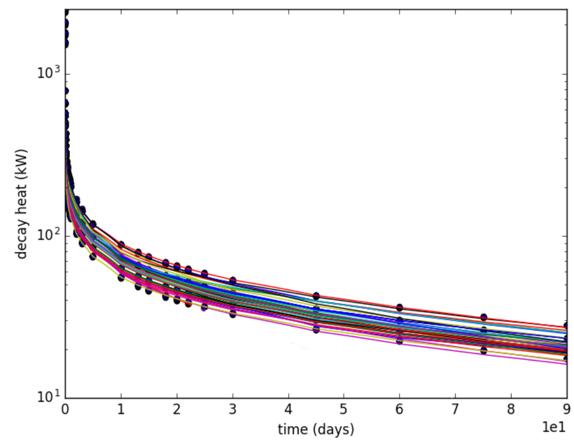

Figure 2 – 48 MC SEM predictions (line) vs. original data (scatter)

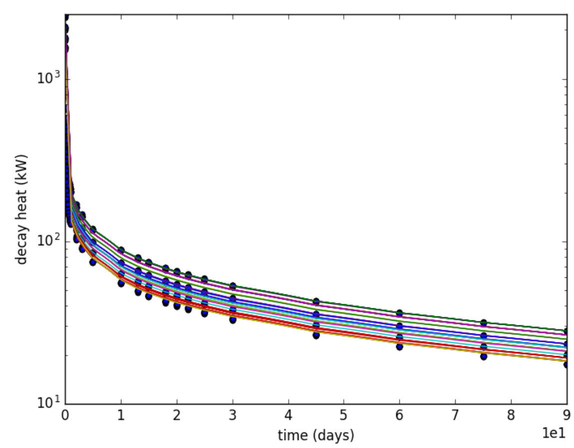

Figure 3 - 48 MC DMD prediction (line) vs. original data (scatter)

RESULTS

As already mentioned, 3 different surrogate modeling approaches have been considered, trying to find the best compromise between simplicity and accuracy. Even if RAVEN owns several complex capabilities to assess the accuracy of SMs [2], in this work, simple qualitative comparison approaches, based on two sampling strategies, have been employed: 1) a Monte-Carlo (MC) perturbation, aimed to testify the stability of the trained SMs within the training domain and 2) a Grid sampling (see TABLE I) meant to guarantee that prediction capabilities of the 3 SMs on the training points.

Figures 1,2,3 show the decay heat evolution, superimposed on the training data, predicted by the SVR, SEM and DMD surrogates in the MC sampling. It can be noticed that all three SMs are capable to predict the DH in the training domain, even if the SEM presents some oscillations. This is expected since two of the SM features (fuel temperature and enrichment) are much less relevant if compared with the burnup, leading to flat correlation regions that are difficult to be capture with a spline interpolant (in the feature space).

Figures 4,5,6 show the expected value (mean), 5% and 95% percentiles of the SVR, SEM and DMD. Although all SMs are able to predict the DH evolution with a relative error of ~0.01% (off the training points), it can be observed that the DMD outperforms the other two SMs, guaranteeing a perfect matching between the original and the predicted data.

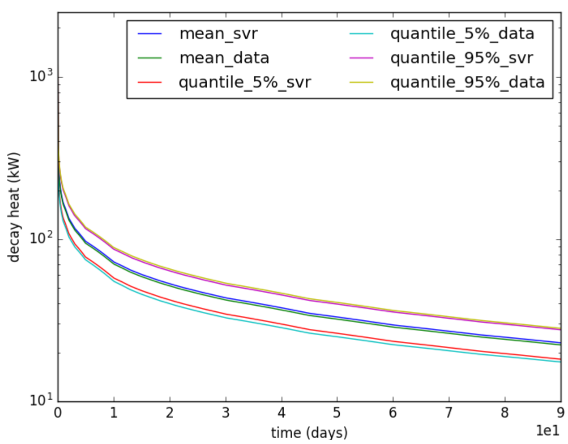

Figure 4 - Mean and Quantiles comparison SVR vs. Data

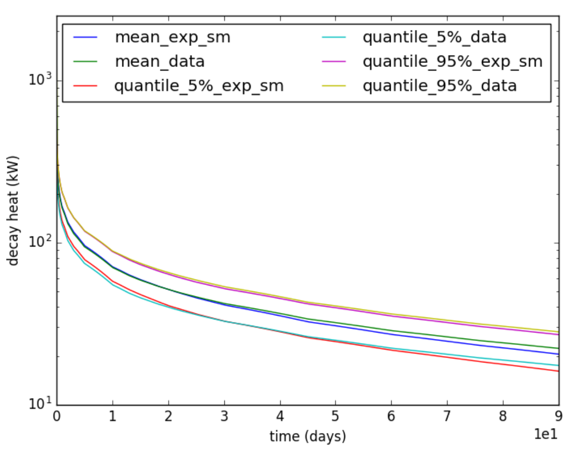

Figure 5 - Mean and Quantiles comparison SEM vs. Data

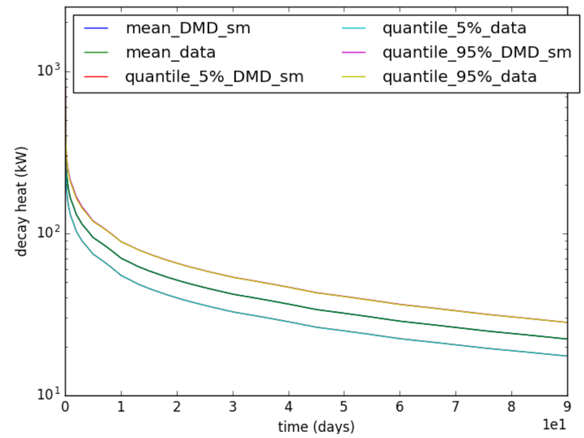

Figure 6 Mean and Quantiles comparison DMD vs. Data

CONCLUSIONS AND FUTURE WORK

In this paper, preliminary results of the construction of new DH models for HTR applications have been reported. The creation of SMs have been performed using ORIGEN and RAVEN codes. Three different models got investigated: 1) SEM, 2) SVR and 3) DMD. The 3 SMs have demonstrated a good potential in approximating and surrogating the DH phenomena.

In the near future, a more rigorous converge validation study needs to be performed, increasing the training points and exploiting the validation techniques in the RAVEN code. Finally, the best SM will be implemented in a system code (RELAP5-3D) for comparison against the ANS standard curves and the decay heat curves used by JAEA for the simulation of the HTTR.

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