INL/MIS-18-51628-Revision-0

Decay Heat Surrogate Modeling for High Temperature Reactors

Andrea Alfonsi, Gerhard Strydom, Hans D Gougar, Andrew Hummel, Jihaho Chen

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DECAY HEAT SURROGATE MODELING FOR HIGH TEMPERATURE REACTORS

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HTR-2018, 8-10 October, 2018, Warsaw, Poland

RAVEN

PHISICS

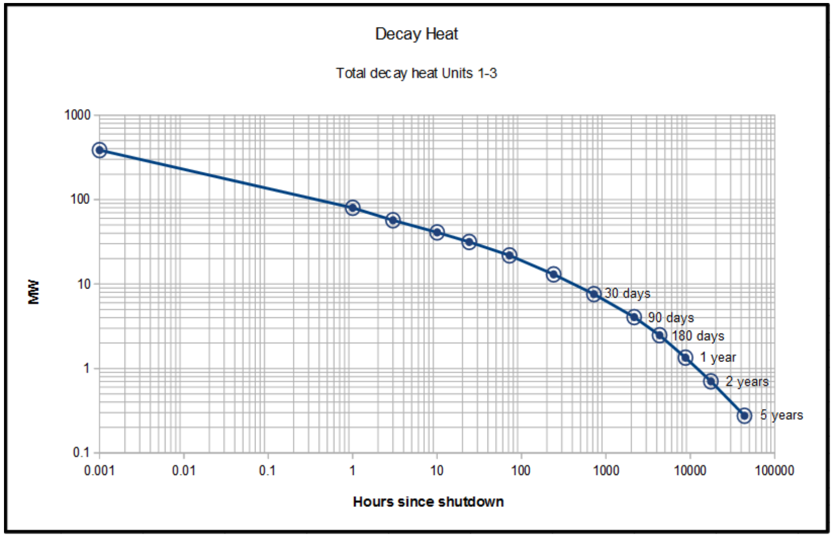
ART
ADVANCED REACTOR TECHNOLOGIES

Outline

- Goals and requirements
- Toolkit that has been used:
  - RAVEN
  - PHISICS
  - SCALE
- Identified surrogate models
  - Spline Exponentials
  - Dynamic Mode Decomposition
  - Support Vector Machines
- Surrogate model construction flow
- Preliminary results
- Future outlook

Goals and requirements

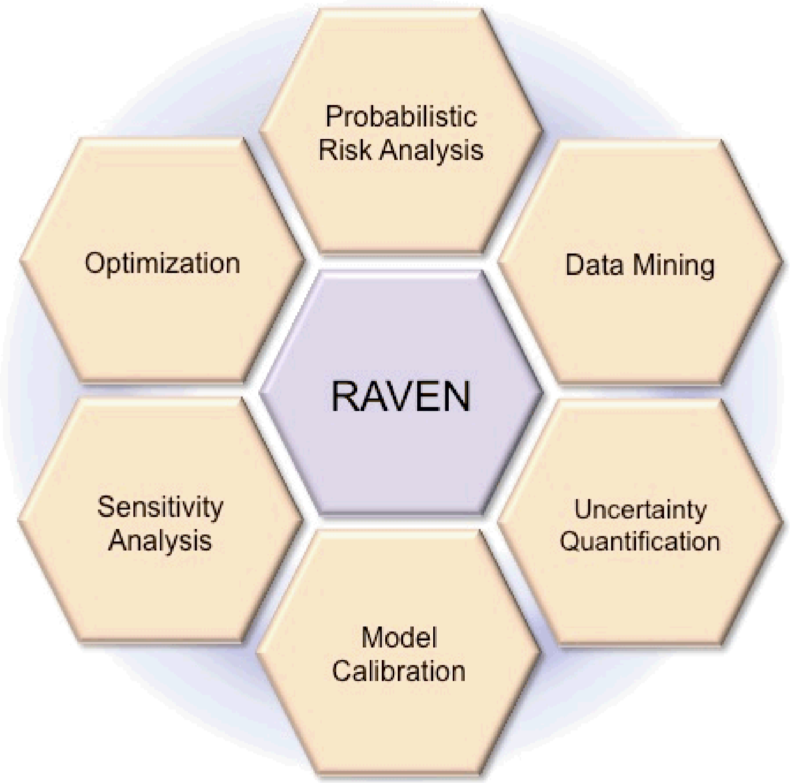
- Identification of a model, tight to HTR technology, able to surrogate the DH evolution after shutdown
- Requirements:
  - Reasonable prediction accuracy till 3 months after the shutdown
  - Ability to capture the main deviation effects determined by field conditions
  - As easy as possible formalism in order to possibly allow the implementation of the curve into system codes (e.g. RELAP5-3D)
  - Nodal and Core-wise prediction capabilities



ADVANCED REACTOR TECHNOLOGIES

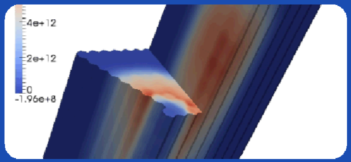
RAVEN overview

- Flexible and multi-purpose uncertainty quantification, regression analysis, probabilistic risk assessment, data analysis and model optimization framework.
- Depending on the tasks to be accomplished and on the probabilistic characterization of the problem, RAVEN perturbs the response of the system under consideration by altering its own parameters
- The data generated by the sampling process is analyzed using classical statistical and more advanced data mining approaches.
- RAVEN heavily relies on artificial intelligence algorithms to construct surrogate models of complex physical systems

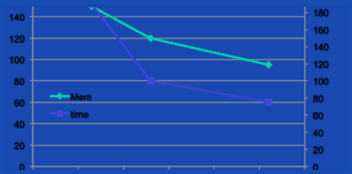


PHISICS overview

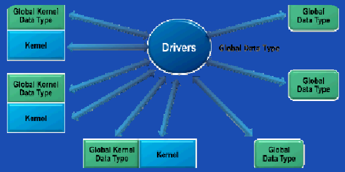
Parallel and **H**ighly **I**nnovative **S**imulation for the **I**NL **C**ode **S**ystem (PHISICS) principal purposes are:



Provide state of the art simulation capability to reactor designers, especially for advanced reactors such as Generation IV systems



Provide an optimal trade off between needed computational resources and accuracy



Simplify the independent development of modules by different teams and future maintenance

PHISICS Modules

INSTANT
Intelligent Nodal and Semi-structured Treatment for Advanced Neutron Transport

MIXER

MRTAU
Multi-Reactor Transmutation Analysis Utility

CRITICALITY

TIME INTEGRATOR

SPH XS Correction

Perturbation Theory

RELAP5-3D coupling

Fuel Management

PARALLEL (MPI) ENVIRONMENT

Identified surrogate models

- In order to try to fulfill the requirements, 3 surrogate models (SMs) have been identified:
  - Spline Exponential SM
  - Dynamic Mode Decomposition SM
  - Support Vector Machine Regressor

- Consider a set of *N* data points

output

$$\left(x_i, F(x_i)\right) \quad i = 1, \ldots, N$$

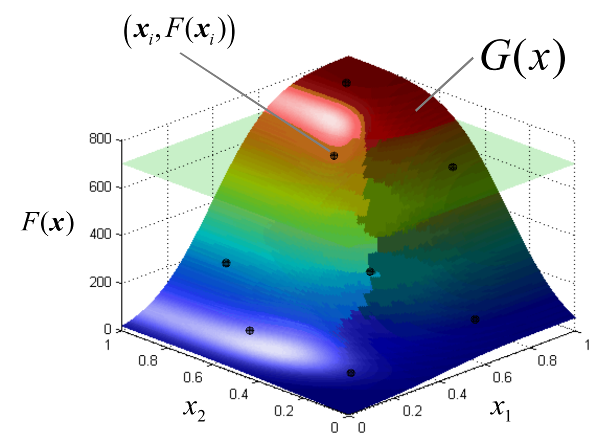
input

Simulation outcome (decay heat)

Initial and boundary conditions (e.g. burnup, enrichment)

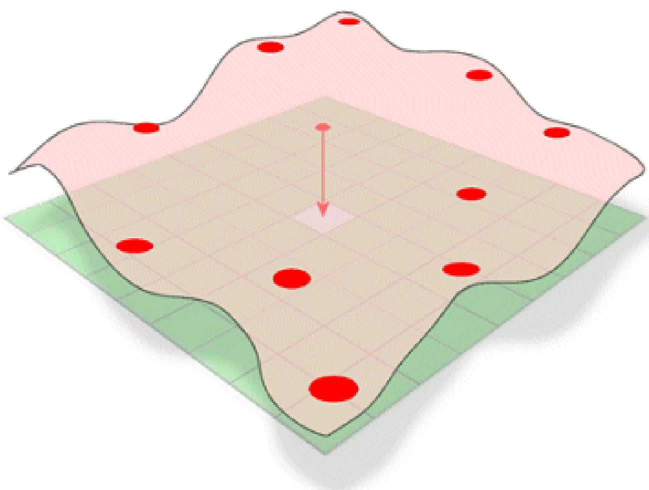
- Build a surrogate model
  - Reduced Order Model $G(x)$

$$G(x) : x_i \longrightarrow G(x_i) \cong \mathrm{F}(x_i)$$



Spline Exponential

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



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.)
- $P_i(\boldsymbol{x}, t)$ and $Q_i(\boldsymbol{x}, t)$ are spline polynomial functions of the parametric space $\boldsymbol{x}$.

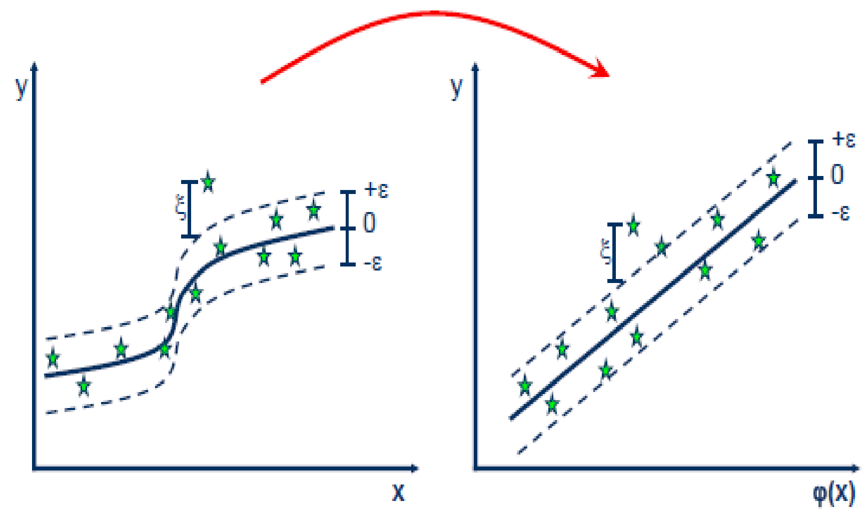
Support Vector Regression

$$\min_{\boldsymbol{\alpha},\boldsymbol{\alpha}^*} \left({}^1\!/_2 (\boldsymbol{\alpha}-\boldsymbol{\alpha}^*)^T \boldsymbol{Q}(\boldsymbol{\alpha}-\boldsymbol{\alpha}^*) + \varepsilon \boldsymbol{g}^T(\boldsymbol{\alpha}-\boldsymbol{\alpha}^*) - \boldsymbol{y}^T(\boldsymbol{\alpha}-\boldsymbol{\alpha}^*) \right)$$

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

where:

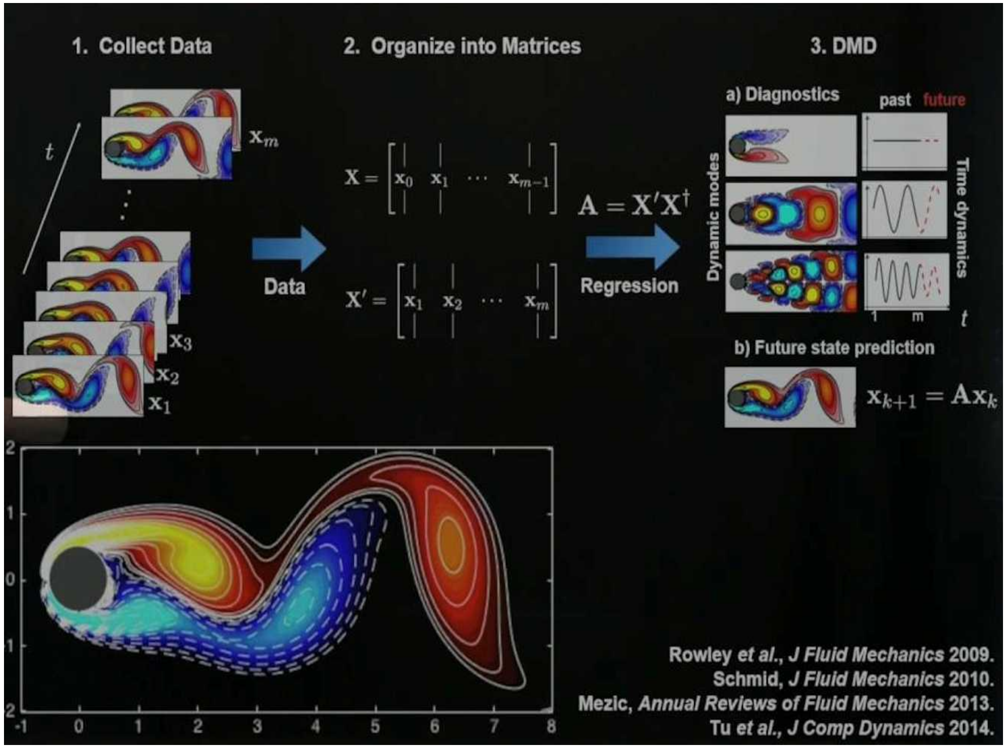
- $\boldsymbol{g}$ is a unit vector
- C is the upper bound
- $\boldsymbol{Q}$ is a n by n positive semidefinite matrix containing the kernel mapping $K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$
- $(\boldsymbol{\alpha}-\boldsymbol{\alpha}^*)$ is the vector of the dual coefficients.



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

Dynamic Mode Decomposition

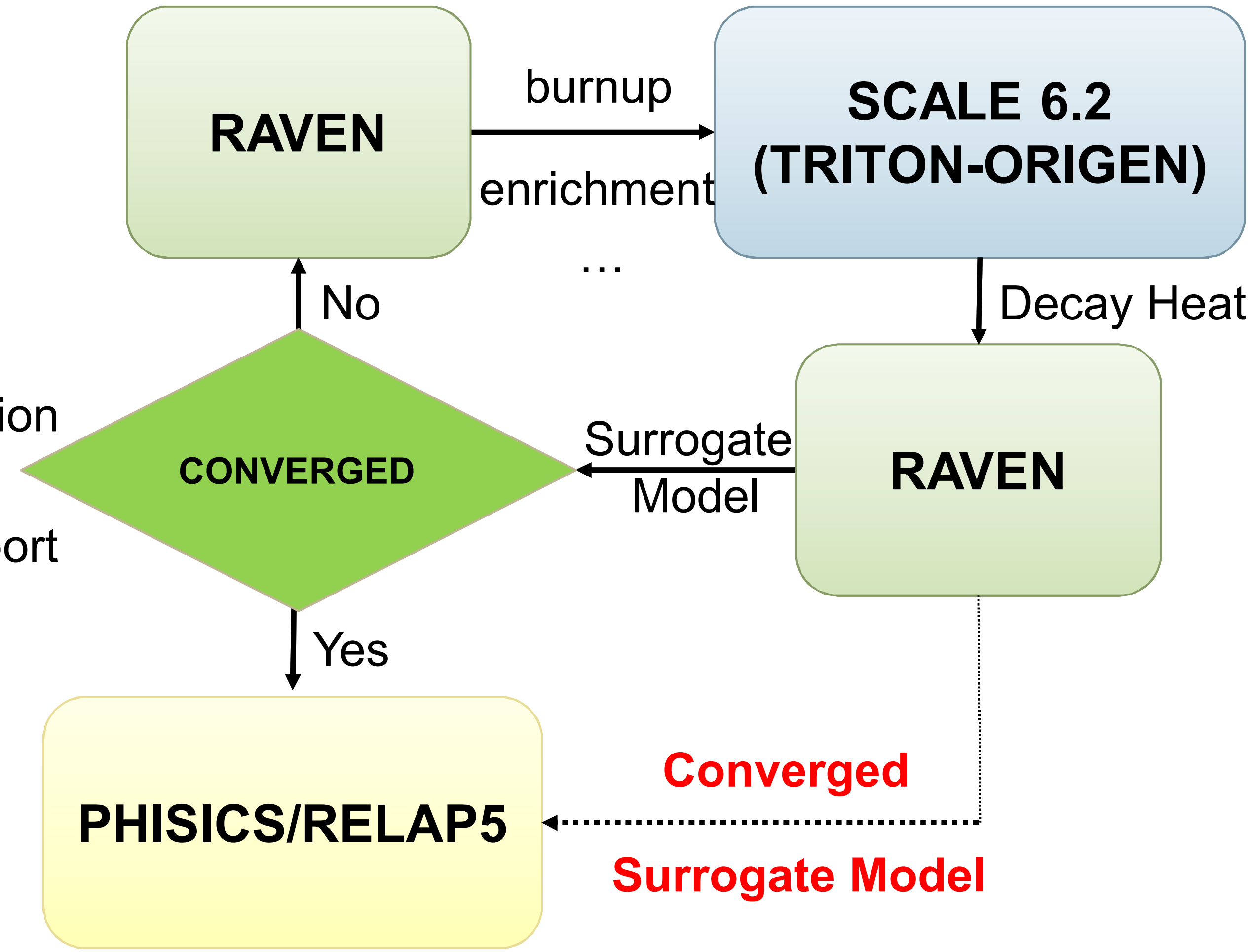
- Analyze data computing eigenvalues and eigenmodes of an approximate linear reduced order model
- Data are organized in a sequence of snapshots
- Snapshots are assumed to be related via a linear mapping
- Eigenvalue and Eigenvectors computation (SVD)



$$\Phi_i = \boldsymbol{U} y_i$$

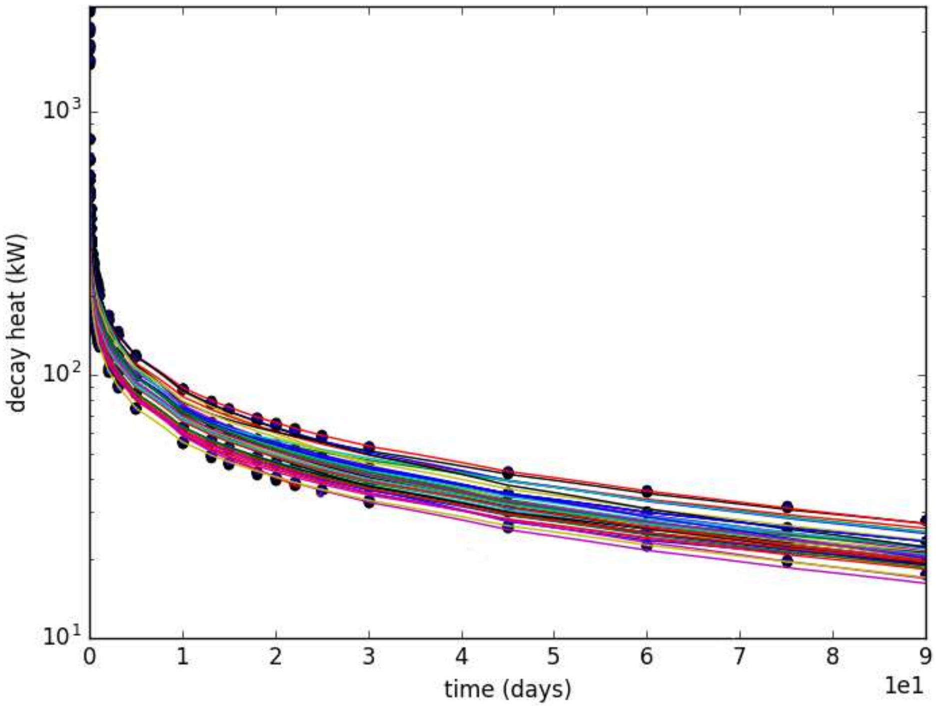
Calculation Flow Scheme

- **RAVEN:**
  - Sampling
  - Surrogate Model
- **SCALE 6.2:**
  - Lattice
  - Decay Heat Calculation
- **PHISICS/RELAP5:**
  - Surrogate Model import
  - Depletion/Transient calculations

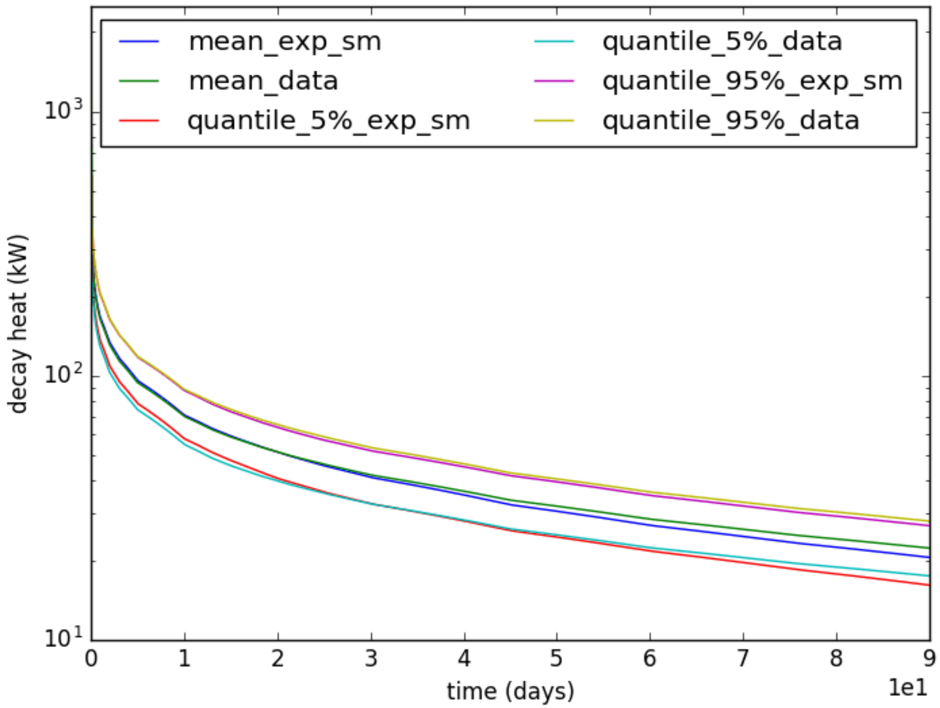


Comparison DH prediction (Spline Exponential) vs ORIGEN

Poly-Exponential prediction (line) vs. original data (scatter)

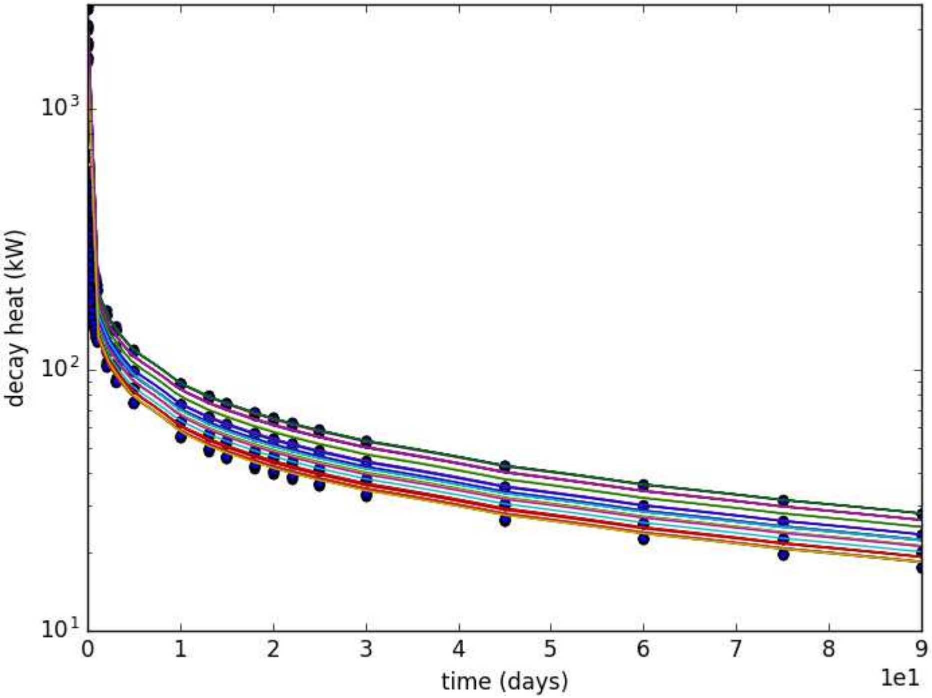


Maximum Relative Error 5E-2 p.u.

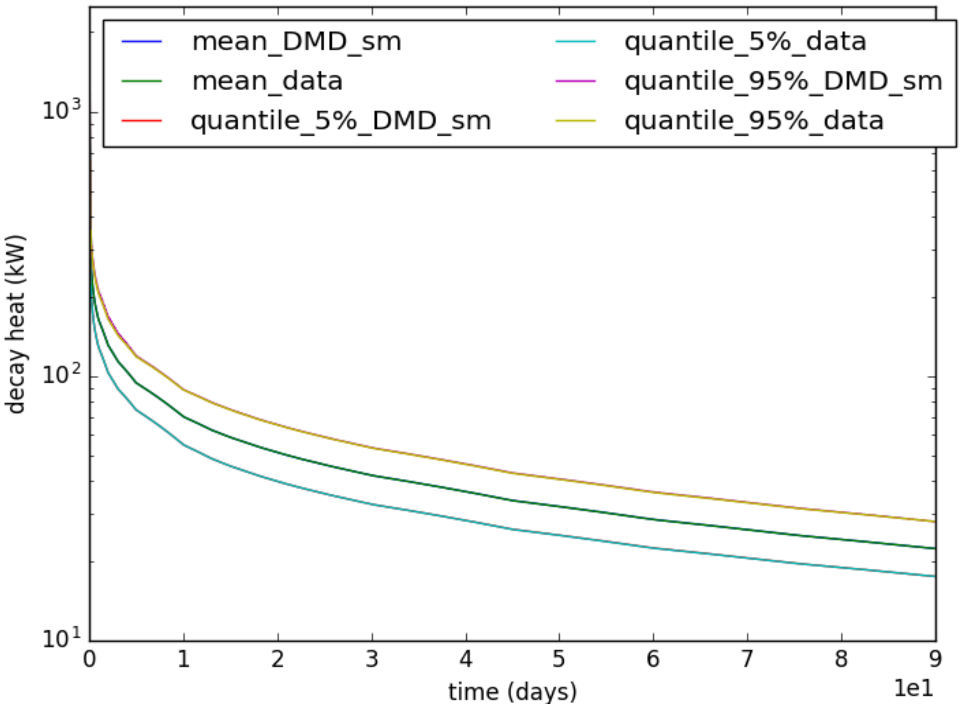


Comparison DH prediction (DMD) vs ORIGEN

DMD prediction (line)
vs.
original data (scatter)

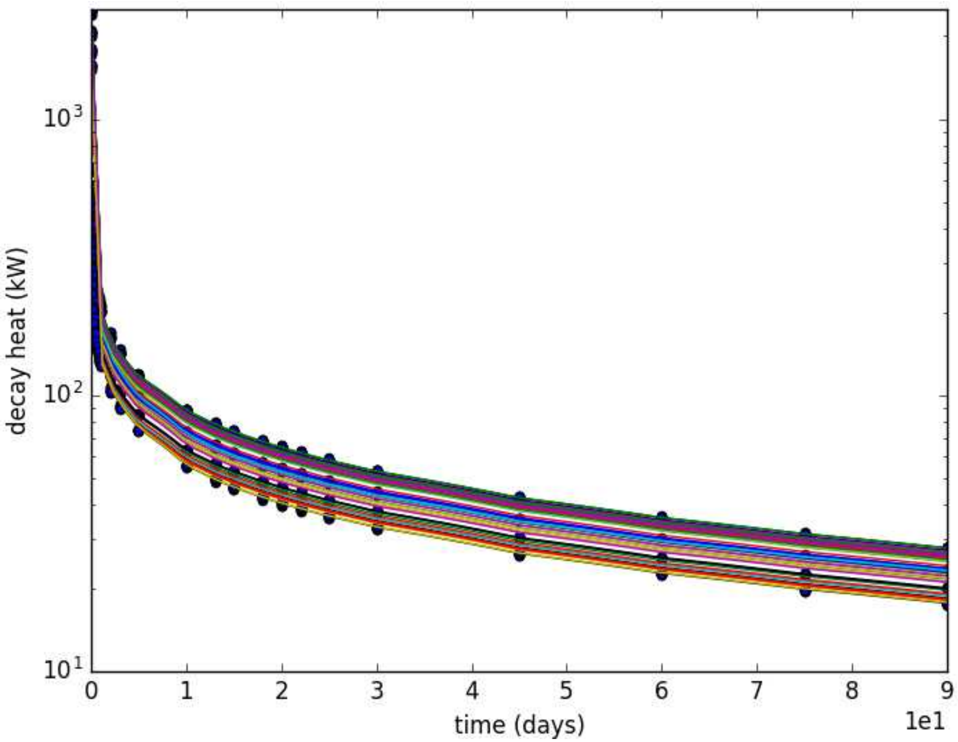


Maximum Relative Error 1E-12 p.u.

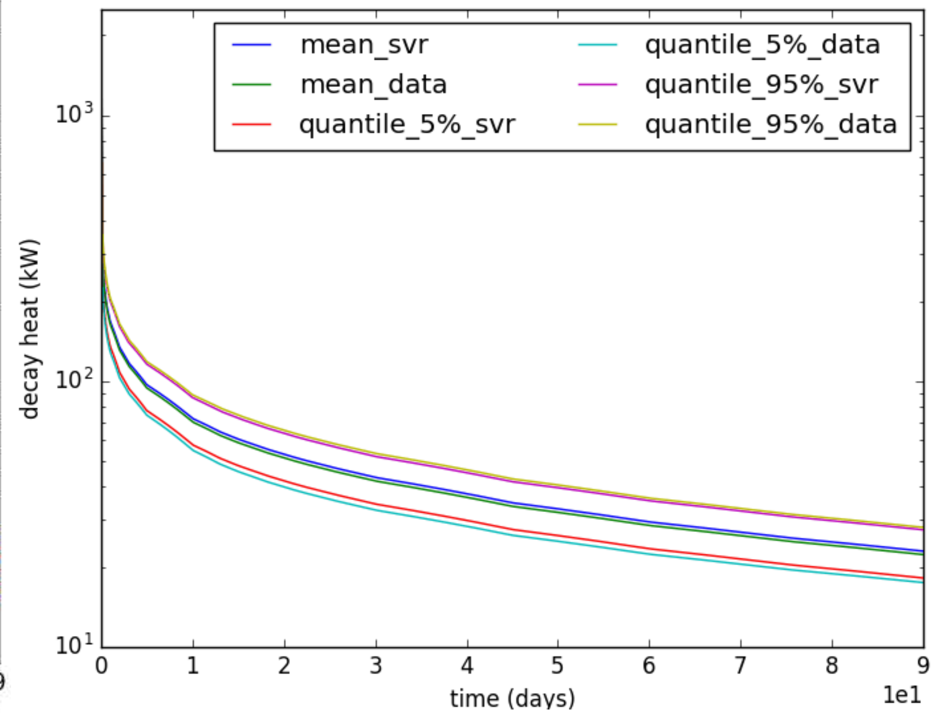


Comparison DH prediction (SVR) vs ORIGEN

SVR prediction (line)
vs.
original data (scatter)



Maximum Relative Error 1E-6 p.u.



Final Remarks and Future Work

- Status:
  - The calculation scheme for SM construction has been deployed (RAVEN-SCALE) and is envisioned to be applicable to any reactor design/concept
  - Implementation of DH SMs DMD, SVR and SplineExponential in PHISICS-RELAP5-3D is finalized
  - DH SM is highly customizable (e.g. different time scales, different field parameters, etc.)
  - SMs is able to predict operational and transient (e.g. after-scram) DH evaluation
  - Mechanics and Results have been tested on simple problems
- Short-term Future Work:
  - Comparison of DH SM predictions against ANS standard curves and MHGTR-350 benchmark decay data
- Mid-term Future Work:
  - Finalization of the construction of DH SM dependent on isotope inventory only:
    - Remove reactor-dependency
    - Cross-technology model

Grazie Mille
Dziękuję Ci
Thank you
Je vous remercie
Vielen Dank

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