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Error Propagation for Fuel Cycle Calculation

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Technical Workscope Identifier: FC-5.1b
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Time Frame: 3 years
Estimated Cost: $800,000

1 Proposed Scope/Context Description

The fuel cycle simulation tool can have a large scope of application, from the study of the behavior of some type of fuel or reactor inside an existing nuclear fleet to the prospective analysis of a complete nuclear transition. Beside the study of fleet evolution it can also been used to assess the possibility of material hijacking in the context of non-proliferation study or policy...
Each application field of the nuclear fuel cycle calculation requires a specific level of confidence, which are up to now very un-precisely assessed, if assessed. There is a real need of validation the those kind of calculation, which can hardly been reached. Indeed, the only existing way to validate any fuel cycle calculation/tool, is the benchmark with other similar tools, or other existing data... When the first is generally conclude with a list of why the different softwares end up with different results (without concluding on the precision of any), the second allow only the validation on existing concept and have no impact on calculation implying the use of new concept.
The aim of this project is to add error propagation capability to the CYCLUS fuel cycle simulator [1]. By their usage for predicting the evolution of a large industrial enterprise in an uncertain future, nuclear fuel cycle simulations are generally based on approximations and uncertain input data. Since validation is largely considered to be impractical, such simulations are seen as indications of future behavior rather than predictions of that behavior. Nevertheless, it would be valuable to be able to place some confidence bounds on those indications, both to assess the robustness of conclusions that derive from those indications and

to provide information about the sensitivity of those conclusions to the uncertain data and algorithms.
Having a broad distribution for each metric calculated in a fuel cycle simulation instead of unique values will allow a better comparison between different fuel cycle scenarios.
Moreover for some critical analysis such as retrospective non-proliferation analysis, it could be extremely valuable to add some degree of confidence on the simulation performed. This could allow at least to confirm or invalidate the possibility to use those calculation tools for such purpose.
This project will extend the Cyclus concept of resources to include error information and then develop a number of archetypes that can perform operations to propagate that error in a rigorous fashion. Ultimate calculation of fuel cycle performance metrics will also need to be updated in order to represent final results as distributions rather than single values.

2 Logical Path to Work Accomplishment

The goal of this project is to add optional extensions to Cyclus that will allow an assessment of the error as it propagates through a fuel cycle.

2.1 Add uncertainty to ressources

The first step of this work, is to update the principal CYCLUS metric : the material and associate the isotopic composition with a uncertainty. Because for this is the first introduction of uncertainty in CYCLUS (or fuel cycle calculation tool in general), we will consider the uncertainty on the material independent of any previous operation on this materials.

2.2 Archetypes uncertainty management

In a fuel cycle calculation, there are three different uncertainty/error sources :

- the material uncertainty, $\delta\vec{N}_{in}$, which is the input and the output of each archetypes,
- the "tolerance", τ_i, on the input parameter, which corresponds the possible variation range of any physics parameter, i,
- the error, ϵ_{mod}, introduce by the archetypes modeling/operation on the material.

The uncertainty on the output material is a function of all those uncertainties :

$$\delta\vec{N}_{out} = \mathcal{F}\{\ \delta\vec{N}_{in}\ ,\ \tau_0\ ,\ \dots\ ,\ \tau_n\ ,\ \epsilon_{mod}\ \} \tag{1}$$

The work we are proposing to do on this project, is to allows all archetypes of CYCLUS, to combine all those sources and computes the resulting uncertainties on the output materials. In the following parts, one will tried to detail the work which need to be done on the different archetypes, we are proposing to update.

2.2.1 Enrichment facility

The enrichment facility is probably the easiest facility to model, since the only error come from the tails and feed stream enrichments, the enrichment process could be linearly models. This can be easily analytically combine and propagate.

Is it true with any enrichment technic ?

do we want the exact error propagation formula ?

2.2.2 Separation

As the enrichment process, the separation should be very easy to model including uncertainty. Indeed, the only parameter which can introduce extra variance is the separation efficiency, τ_{eff}.

do we want the exact error propagation formula ?

2.2.3 Reactor

As all archetypes the reactor, are subject to physical parameter fluctuation.The different parameter one should consider are the discharge burnup, the effective power/capacity factor... Variation consideration on those parameters will affect the discharge time, which should be very difficult to include in the uncertainty calculation. Nevertheless, a brute force study (also sometimes called "Total Monte Carlo method") could allow the determine their impact, running many time the same simulation choosing randomly the parameter value at each cycle of the reactor, the distribution of the results will provides a precise measurement of the sensivity.

We are envisaging two kind of the reactor, which will be both capable to handle uncertainty. The first one will be built as an upgrade of the existing CYCAMORE reactor, making it error aware. The CYCAMORE reactor is a recipe base reactor, in addition of all the classical reactor parameter (batch number, cycle length, power, capacity factor,...) the user provides the input and output fuel recipes. The only requirement is to force user to provide the output recipe with the according sensitivity to input uncertainty. From this sensitivity, one will be able to compute directly the output uncertainty on the output composition from the input one.

The second version of reactor will be able to calculate the evolution of the fuel provided by the fuel fabrication (see §2.2.4). To do so, we propose investigating two ways, both using pre-trained models, allowing the prediction of key physics parameters needed to compute the evolution of a fuel during the irradiation. It has been proven that from pre-trained neural network models, one can predict the evolution of the one group cross section during the irradiation of the fuel from its initial isotopic composition, and is working for a various range of reactor, from LWR to SFR [**?**, **?**].

The first application using the neural network predictive models, is to train a model to

directly predict the composition evolution as the function of the burnup. This application might not work, since the usage of neural network has been proven to predict one group macroscopic cross section.
If the neural network model fail to directly predict precisely the isotopic composition evolution, one have to consider the second option, which imply to predict the 1 group cross section, then integrate the Bateman equation.

The main reason leading the try of direct prediction of the isotopic evolution, is the error/uncertainty propagation. As express prevsiously :

$$\delta \vec{N}_{out} = \mathcal{F}\{\ \delta \vec{N}_{in}\ ,\ \tau_0\ ,\ ...\ ,\ \tau_n\ ,\ \epsilon_{mod}\ \} \tag{2}$$

The determination and the propagation of all uncertainty source is, for this kind of reactor, a complicated matter. The error due to the computation of the depletion calculation are wild:

- the error of the neural network predictor, ϵ_i^{nn}, with $i \in [0..N]$, N the number of predicted parameter,
- the convolution of the uncertainty on the material composition with the neural network prediction.
- the calculation error on the data sets used to train the neural network, $\epsilon_{T.D.}$.

And then can be expressed as :

$$\epsilon_{mod} = \mathcal{G}\{\ \delta \vec{N}_{in}\ ,\ \epsilon_0^{nn}\ ,\ ...\ ,\ \epsilon_n^{nn}\ ,\ \epsilon_{T.D.}\ \} \tag{3}$$

Because, the predictive model are trained on sample populated using few thousand of depletion calculation, which are subject to computation error, $\epsilon_{T.D.}$. On one side, a depletion calculation take as input, the nuclear data. Those nuclear data are interpolated/extrapolated from many different experimental measurement using many different models. Therefore the nuclear data contain uncertainty... Those uncertainty are extremely difficult to propagate properly through a full depletion calculation because of the coupling between neutron transport and depletion calculation: the composition of the fuel impact the shape of the neutron spectrum, which impact the reaction rate on the nuclei... On the other side, the depletion calculation require different approximation to be completed. There is nearly impossible using Monte Carlo technique on a PWR full core calculation due to source convergence issue. It is also extremely complicate to follow precisely the different reactor parameter, such as boron concentration, rod control management, charge factor evolution, neutron leakage... The study and the propagation of the modeling uncertainty, such as the modeling simplification and the nuclear data uncertainty is way beyond the scope of this project...
This require a full dedicated research project (and probably more). Therefore, those error, $\epsilon_{T.D.}$, will not be considered on the first version of this work. This might need to be reconsidered when the depletion calculation error propagation capacity will have done important

progress.

The direct error induced by the use of predictive model, ϵ_i^{nn} on each parameter, i, need to be assessed. This could be performed with a mapping the error on the isotopic space populated with the training sample. This will allow to determine the error of the model on each point on the isotopic space populated. We might use then a other neural network, or other interpolation method to predict the error of the prediction as the function of the isotopic composition.
Once we have a working predictive model and a map of the error on the prediction, one need to build the covariance matrix which will allow to convolute the uncertainty on the input material, δN_{in}, with the prediction of the model.

If the direct prediction of the composition is not precise enough, one have to use solve Bateman equation using predicted one group cross section and then compute the error coming from a numerical resolution of the Bateman equation and propagate the error of the one group cross section. The Bateman equation resolution will be a step by step process. After having discretize the irradiation time (or burnup), one will use the model to predict the cross section at each time step (closer the time step are preciser the calculation will be) and then solve numerically the Bateman equation step after step, ending with the final isotopic composition of the fuel. Because the predictive model will be able to predict the one cross section as the function of time (or burnup), one should be able to propagate those error using sensitivity analysis. The time discretization as well as the other approximation require to solve the Bateman equation will also introduce computation error that need to be determined and added to the final uncertainty. This could be made with the comparison of depletion calculation made with those extra approximation with the reference one performed using the same modeling approximation as the training depletion all along the isotopic space.

2.2.4 Fabrication

The aim of the fuel fabrication is to mix different incoming material streams in order to build a fuel which validate the neutronics/physics requirement of the reactor. Depending of the reactor, the criterium could be various. We are considering in the first time including fabrication model for MOX fuel only, in LWR and SFR, used as burner and breeder for SFR. One will use algorithm building fuel allowing to build fuel reaching the targeted burnup according to either criticality criterium either conversion ratio criterium. Those algorithm will relies on the capabilities of some predictive model to predict the maximal achievable burnup depending on the the criticality or conversion ratio evolution according to burnup. The predictive model as the reactor model, will be based on the use of neural network formerly trained on the same set of training depletion calculation used for the reactor models. The capability of the neural network have been proven to predict the evolution of the criticality in PWR reactor using MOX fuel [**?**, **?**], as well as the the initial criticality of MOX fuel in SFR [**?**] and should be possible to extend it to conversion ratio evolution.

The error/uncertainty propagation for fuel fabrication should be pretty similar than for reactor. Indeed the uncertainty can be expressed as :

$$\delta \vec{N}_{out} = \mathcal{H}\{ \ \delta \vec{N}_{in} \ , \ \epsilon_{mod} \ \}. \tag{4}$$

In this case there is no tolerance, since the parameter are goal to achieve, not physicals characteristics. As well as previously the error of the model can be expressed as :

$$\epsilon_{mod} = \mathcal{K}\{ \ \delta \vec{N}_{in} \ , \ \epsilon_0^{nn} \ , \ \dots \ , \ \epsilon_n^{nn} \ , \ \epsilon_{T.D.} \ \}, \tag{5}$$

where ϵ_i^{nn} represent the error on the prediction of the parameter i by the neural network predictive model and $\epsilon_{T.D.}$ the error due to the error on the depletion calculation composing the training set, which will not be considered since we dont have any way to correctly estimate it.

As for the reactor model, the ϵ_i^{nn} component of the error can be determined through a mapping of the error along the isotopic space, and the impact of the material input uncertainty needed the be assessed by the calculation of the covariance matrix which need to be build.

2.3 Problems/Applications/Validations

During the realization of this work we would like to validate each step of the uncertainty propagation process. First, with a mid/early-term validation, after the enrichment facilities, the separation and the recipes reactor will be implemented, it will be possible to confirm the uncertainty is correctly propagated, using a brute force validation (with the "Total Monte Carlo" method). This validation will be continued with new archetypes will be implemented in CYCLUS...
An other gaol we want to achieve, is an sensitivity analysis, allowing to determine the impact of the different uncertainty/error/tolerance on the final calculation uncertainty. This should allow to define precisely where the future effort should be focus to reduce those uncertainty sources accordingly to the object of the calculation and also to validate (or un-validate) the use of fuel cycle simulation tool for some specialized study (such as non-proliferation study...)
With all the necessary components in place, a series of demonstration simulations will be conducted using fuel cycles of increasing complexity: once through, MOX LWR recycle, and fast reactor recycle. These scenarios will be constructed to highlight the role of error and uncertainty and identify metrics in which the presence uncertainty may impact fuel cycle analysis conclusions.

3 Relevance of Proposed Research

This proposal aims to provide an important feature needed in the fuel cycle simulator. Given the appropriate estimation of the error relative to any fuel cycle simulation, the simulator would be able to make decisions about fuel cycle transition like fuel reprocessing, or the launching of new technologies or types of reactors. Furthermore, the project will be one of the first of its kind to introducing error propagation in fuel cycle calculation, increasing the utility of the Cyclus kernel. Since the precision of fuel cycle tool have never been assessed, this work might the first step providing more confidence in the fuel cycle calculation. And even if this wok will be applied to the fuel cycle simulation tool CYCLUS, the concept should be a theoretically applicable on any agent based fuel cycle simulation tool.

Additionally, new archetypes will be contributed to the Cyclus ecosystem, including not only error propagation but also different fuel fabrication methods, cross-section prediction models and a Bateman equation solver. These features will permit future comparison between the different fuel fabrication models and improve the user experience and confidence in the interpretations of Cyclus simulations.

4 Milestone Task Listing

This research project consist in four major tasks that could be conducted in parallel. The first one will be very short (< 6 month), dedicated to update CYCLUS and allow it to handle uncertainty. The second one should be the longer task (12 - 24 months) where the models will be developed. The predictive model development can/should/will be started at the start of the project. The third will be started after the end of the TASK 1 and corresponds to CYCLUS archetypes update and included in a separated package. The development of some archetypes will depends on the progress on the TASK2. The last task is the validation and application one and will be started with the completion of the different TASK3-subtasks. The ideal progression is represented on the figure 1.

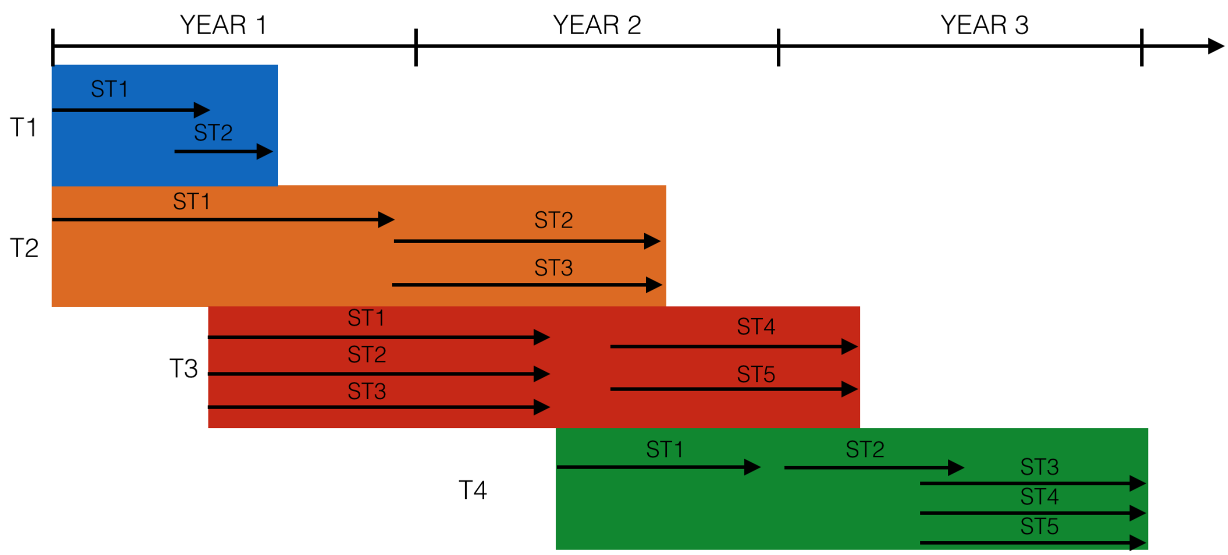

Figure 1: Preliminary schedule of the project, with the different Task (T#) (1 in blue, 2 orange, 3 red, 4 green) and the corresponding subtask (SB#).

TASK 1: CYCLUS update for uncertainty awareness

- subtask 1: update material to uncertainty,
- subtask 2: validate the backward compatibility,
- subtask 3: Add a default uncertainty behavior when using both uncertainty aware archetypes and standard one in the same time ?

TASK 2: Updating the CYCLUS Archetypes to uncertainty management

- subtask 1: enrichment facility,
- subtask 2: separation facility,

- subtask 3: recipe reactor,
- subtask 4: reactor archetypes, depletion calculation/prediction, uncertainty propagation,
- subtask 5: fuel fab archetypes, mixing calculation/prediction, uncertainty propagation.

TASK 3: Modeling development

- subtask 1: isotopic space definition, training sample realization
- subtask 2: reactor models development: parameter prediction, error analysis
- subtask 3: fuel fabrication model development: parameter prediction, error analysis

TASK 4: Validation & application

- subtask 1: validation of the overall process with simple calculation : enrichment + separation + recipe reactor
- subtask 2: validation of modeling capabilities (Fab + reactor)
- subtask 3: exemple calculation: PWR, transition from PWR to FBR
- subtask 4: full sensitivity analysis
- subtask 5: time dependent parameters sensitivity analysis (discharge burnup, capacity factor...)
- subtask X: comparison with other physic modeling capabilities such as Bright-Lite ?