The GPT saga at École Polytechnique

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Abstract

An important contribution of Prof. Daniel Rozon to research is related to the introduction and use of Generalized Perturbation Theory (GPT) in reactor physics. This approach was first reported in 1977, in the context of equilibrium refueling optimization for CANDU reactors. The combination of GPT and Mathematical Programming led to the OPTEX research project, still active thirty years later. Today, GPT is implemented in many important reactor physics codes still in development at École Polytechnique. It is available in DONJON for full-core analyses, mainly as a support for OPTEX. It is also available in DRAGON where it is currently used to evaluate the sensitivities of global or local system parameters to basic cross-section data or isotopic concentration that are required for uncertainty calculations.

1. Introduction

Generalized Perturbation Theory (GPT) is a fundamental approach in reactor physics and in nuclear data processing. One of the useful features of GPT is its ability to predict the combined effect of several perturbations on the characteristics of a system as a linear superposition of the effects of each of the perturbations. In addition to well-known classical perturbation method, dedicated to the prediction of the effective multiplication factor, a considerable use is being made of GPT, dealing with variations of any ratio of functionals, linear or bilinear, of the flux and/or flux adjoint. The initial introduction of GPT in reactor physics was proposed in two fundamental papers of G. C. Pomraning describing the perturbation of a source and eigenvalue equation, respectively.[1,2] It is worth noting that the perturbation of an eigenvalue equation leads to a *fixed source eigenvalue problem*, a type of problem with very specific and unusual characteristics. Another well-known contributor of GPT is reactor physics is W. M. Stacey in 1972.[3]

Back in 1976, Daniel Rozon was leading a team of graduate students and research associates for the development of optimization techniques related to the fuel management of CANDU reactors. At this time, the research team was puzzled by the failure to converge of the optimization process. A simple 1D prototype based on GPT was proposed as a possible fix to ensure convergence. The OPTEX approach was then developed as the application of GPT and Mathematical Programming to the equilibrium refuelling optimization in CANDU reactors. The OPTEX approach was first reported in 1977 [4] and has been developed and applied in the subsequent years to increasingly complicated situations.[5–8] An overview of OPTEX developments is the subject of a specific presentation at this meeting.[9]

More recently, a new research axis was initiated to develop tools for sensitivity and uncertainty methodology inside the DRAGON framework.[10–13] The goal of this research was to implement in DRAGON a tool to produce the sensitivities of a general system characteristics to constituent cross-section data and isotopic concentrations. These sensitivities can be coupled with covariance data to propagate through the code the uncertainties in the evaluated nuclear data.[14]

In Section 2 of this paper we will discuss the use of general perturbation theory for reactor optimization studies as applied in the OPTEX code. This will be followed in Section 3 by a description of how this technique has been applied to sensitivity and uncertainty calculations in DRAGON. Finally we will conclude.

2. GPT for optimization studies

System design in reactor physics involves a number of system characteristics that are function of control or decision variables. Exit irradiation and fuel enrichment in a reactor zone are example of such control variables. Zonal power factors, fuel cost per megawatt, adjuster reactivity weight and effective multiplication factor of the reactor are examples of system characteristics. The goal of an optimization procedure is to adjust the control variables in such a way as to optimized a single system characteristics while maintaining other system characteristics equal, above or below reference values.

In reactor physics studies, many system characteristics are of the form

$$R = \int_{\rho} d\rho F[\phi(\rho), \dot{X}(\rho)]$$

where ρ stands for the phase space variables, and F is an explicit function of the flux $\phi(\rho)$ and of I independent system variables:

$$\dot{X}(\rho) = \{X_1(\rho), \mathsf{K}, X_I(\rho)\}.$$

The system equation governing the neutron flux for a reactor in a critical system takes the form

$$[A(\rho) + \lambda(\rho) B(\rho)]\phi(\rho) = 0$$

where in diffusion theory $A(\rho)$ contains both the neutron diffusion and removal operator, $B(\rho)$ is the fission operator and $\lambda(\rho) = 1/K_{eff}(\rho)$ is the eigenvalue of the problem. The standard optimization process then consists in selecting the optimal value of R from tables $R_{\text{pert}}(\dot{X}(\rho) + \delta\dot{X}(\rho))$ obtained with multiple perturbations $\delta\dot{X}(\rho)$ in the system variables $\dot{X}(\rho)$.

Generally, the tabulation of $R_{\text{pert}}(\dot{X}(\rho) + \delta\dot{X}(\rho))$ implies that multiple solutions of the system equation covering the available space for $\dot{X}(\rho)$ must be generated. On way to simplify this evaluation is to use a GPT formulation where one assumes that $R_{\text{pert}}(\dot{X}(\rho) + \delta\dot{X}(\rho))$ can be approximated by first order functional Taylor series expansion around a reference value [15]

$$R_{\text{pert}}(\dot{X}(\rho) + \delta\dot{X}(\rho)) = R(\dot{X}(\rho)) + \delta R_{\delta X}^{\mathsf{r}}$$

where

$$\delta R_{\delta X}^{\mathsf{r}} = \sum_{i=1}^{I} \int_{\rho} d\rho \frac{\partial R}{\partial X_i(\rho)} \delta X_i(\rho) + O(\delta^2 X).$$

Here will present two basic approaches to determine the first order variation $\delta R_{\delta X}^{\mathsf{r}}$.

2.1 The explicit approach

In this approach, the flux variations introduced by the perturbations are treated explicitly. These perturbations are the result of a variation in the control variables $\dot{X}(\rho)$.

Let $\psi_i(\eta,\rho)$ be the variation in the neutron flux distribution at phase space position η resulting from the variation of the control variable X_i at ρ:

$$\psi_i(\eta,\rho) = \frac{\partial\phi(\eta)}{\partial X_i(\rho)}.$$

Using this equation, the expression for $\partial R_{\frac{\mathrm{r}}{\partial X}}$ becomes

$$\partial R_{\frac{\mathrm{r}}{\partial X}} = \sum_{i=1}^{I} \int_{\rho} d\rho \left[\frac{\partial F}{\partial X_i(\rho)} + \int_{\eta} d\eta \frac{\partial F}{\partial \phi(\eta)} \cdot \psi_i(\eta,\rho) \right] \delta X_i(\rho)$$

where the distribution $\psi_i(\eta,\rho)$ is the solution of a direct *fixed source eigenvalue equation* written as

$$\left[A(\eta) + \lambda(\eta) B(\eta)\right] \psi_i(\eta,\rho) = -\left[\frac{\partial A(\eta)}{\partial X_i(\rho)} + \lambda(\eta) \frac{\partial B(\eta)}{\partial X_i(\rho)} + \frac{\partial \lambda(\eta)}{\partial X_i(\rho)} B(\eta) \right] \phi(\eta).$$

In this equation, the flux distribution $\phi(\eta)$ and fundamental eigenvalue $\lambda(\eta)$ are the known solution of the eigenvalue equation corresponding to the reference–or non-perturbed– system. The operator on the LHS is singular and, for a solution to exist, the RHS must be orthogonal to the fundamental adjoint $\phi^*(\eta)$ of the reference system that satisfies

$$\left[A^*(\rho) + \lambda(\rho) B^*(\rho)\right] \phi^*(\rho) = 0$$

where the operators $A^*(\rho)$ and $B^*(\rho)$ are the adjoints of operators $A(\rho)$ and $B(\rho)$. A unique solution of the fixed source eigenvalue equation can be obtained by decontaminating $\psi_i(\eta,\rho)$ using the fundamental adjoint $\phi^*(\eta)$.

2.2 The implicit approach

In cases where *R* is a linear or bilinear ratio defined in term of the neutron flux $\phi(\eta)$, an alternative approach is possible. This approach, called the implicit approach, yields the same estimate for the variation in *R*, but requires the solution of a different number of fixed source eigenvalue equations. To avoid the necessity of solving fixed source eigenvalue equations for every control variable, the second term in the expression of $R_{\mathrm{pert}}(\dot{X}(\rho) + \delta\dot{X}(\rho))$ $(\partial R_{\frac{\mathrm{r}}{\partial X}})$ can be written in terms of an importance function

$$\delta R_{\frac{\mathrm{r}}{\delta X}} = \sum_{i=1}^{I} \int_{\rho} d\rho \left\{ \frac{\delta F}{\delta X_i(\rho)} - \int_{\eta} d\eta \Gamma_R(\eta) \left[\frac{\partial A(\eta)}{\partial X_i(\rho)} + \lambda(\eta) \frac{\partial B(\eta)}{\partial X_i(\rho)} + \frac{\partial \lambda(\eta)}{\partial X_i(\rho)} B(\eta) \right] \phi(\eta) \right\} \delta X_i(\rho).$$

Here, Γ_R, is the solution of an adjoint fixed source eigenvalue equation defined as

$$\left[A^*(\eta)+\lambda(\eta)B^*(\eta)\right]\Gamma_R(\eta)=\frac{\partial F}{\partial\phi(\eta)}$$

The importance function $\Gamma_R(\eta)$ can be interpreted as the contribution of an additional neutron at η to the value of the system characteristics *R*. It plays a role similar to that of the adjoint flux with regards to changes in the fundamental eigenvalue λ, but related specifically to *R* because of the source term $\partial F/\partial\phi(\eta)$.

In the context of the implicit approach, there is one fixed source eigenvalue equation to be solved for each system characteristics *R* to be controlled, regardless of the number of control variables.

The efficiency of the GPT approach as a substitute to repeated direct calculations will depend on the number of fixed source eigenvalue equations to be solved for a given problem. Therefore, the choice between an implicit or an explicit approach can be significant to the applicability of GPT to the optimization problem.

2.3 GPT in DONJON

The use of GPT in DONJON is reminiscent of the 1977 implementation in OPTEX1. The GPT-related modules are used to construct the RHS of the fixed source eigenvalues equations (both the generalized direct and adjoint system equations) and then solve them over the full-core. Two specific modules are implemented in DRONON:

`DELTA:` This module is used to compute the source of a fixed source eigenvalue equation corresponding to a set of unperturbed and perturbation system matrices.

`GPTFLU:` This module is used to compute the solution to a fixed source eigenvalue problem corresponding to a set of unperturbed system matrices and sources vectors. It uses the full core diffusion solver of TRIVAC.

The `DELTA:` module is mainly used for non-regression testing, since the code OPTEX, which call directly the `GPTFLU:` module of DONJON, contains dedicated modules for computing the source components required for optimization studies.

3. GPT for sensitivity and uncertainty calculations

Evaluation of the uncertainties in cell averaged and group condensed lattice cell properties is another domain of research where the use of GPT is of utmost importance. Assume that the uncertainties σ in a given set of lattice properties $\vec{x}$ (temperature, densities, microscopic cross sections or isotopic concentrations) are statistical in nature (due to the experimental measurement process). We will suppose that these uncertainties are normally distributed around $\bar{x}$, meaning that $\vec{x}$ can be sampled from a probability density function of the form

$$p(x_n)=\frac{1}{\sigma\sqrt{2\pi}}e^{-\left(\frac{x_n-\bar{x}_n}{\sqrt{2}\sigma}\right)^2}$$

where $\bar{x}_n$ is the reference value of parameter $x_n \in \vec{x}$ (N elements). The uncertainty in the functional R (a cell averaged and group condensed macroscopic cross section for example) that depends on $\vec{x}$, can be evaluated using

$$\sigma_R = \sqrt{\frac{1}{K-1}\sum_{i=1}^{K}\left(R(\vec{x}_i) - \bar{R}(\vec{x})\right)^2}$$

with $\vec{x}_i$ a set of values for $\vec{x}$ drawn (K times) from the normal distribution using a random number generator. This means that in order to evaluate σ_R, one must first solve K times the system equation governing the neutron flux using transport or diffusion theory. In order to obtain reasonable statistics for σ_R large values of K >1000 are generally required.[14]

As we will now see, the GPT approach can be used to accelerate substantially this calculation assuming R has the form

$$R = \frac{\int_\rho P\Sigma_y(\rho)\phi(\rho)}{\int_\rho P\phi(\rho)}$$

where Σ_y is the macroscopic cross section for reaction type y and P an operator that projects the complete phase space to a specific sub phase space (homogenized region and condensed group selected).

3.1 The statistical GPT approach

We can first use the GPT technique to accelerate the evaluation of $R(\vec{x}_i)$ using

$$\delta R_{\delta\vec{x}_i} = \int_\rho d\rho \left\{ \frac{P(\Sigma_y(\vec{x}_i) - \Sigma_y(\bar{x}))}{\int_\alpha P\phi(\alpha)} - \sum_k \Gamma_{R,k}(\rho)\, x_{i,k}\left[\frac{\partial A(\rho)}{\partial x_{i,k}} + \lambda(\rho)\frac{\partial B(\rho)}{\partial x_{i,k}}\right]\right\}\phi(\rho) \qquad (1)$$

$$R(\vec{x}_i) = \bar{R}(\vec{x}_i) + \delta R(\vec{x}_i)$$

where $\Gamma_{R,k}(\rho)$ is the generalized adjoint defined as the solution to the following transport equation

$$(A^* + \lambda B^*)\Gamma = Q$$

with S the adjoint source associated with the functional $R(\vec{x}_i)$. The procedure to obtain σ_R in this case follows:

1. Solve the transport for the flux using the reference values for $\vec{x}$
2. Solve a series of transport equations for the generalized adjoints, each element corresponding to a source Q_n given by (N)

$$Q_y^* = \frac{P(\Sigma_y - \overline{R}_y)}{\int_\rho P\phi(\rho)d\rho} \tag{2}$$

3. Select $\dot{x}_i$ statistically from the probability distribution function and evaluate $\delta R_{\delta x_i}$ using equation (1). Repeat K times until a sufficient large number of perturbations have been considered.
4. Perform a statistical analysis of $\delta R_{\delta x_i}$ and determine evaluate σ_R.

Typically this technique will be faster than solving K times the transport equation since the flux and adjoints can be computed before the analysis starts. However, N evaluations of equation (1) are still required as well as a final statistical analysis of the results.

3.2 The deterministic GPT approach

For the general case where σ_n is the variance of parameter $x_n \in \vec{x}$ and c_{nm} the covariance factor between x_n and x_m, then the variance σ_R in R can be computed using

$$\frac{\sigma_R}{R(\overline{x})} = \sqrt{\sum_n \left(\frac{\sigma_n S_R^n}{x_n}\right)^2 + \sum_n \sum_{m \neq n} c_{nm} \left(\frac{\sigma_n S_R^n}{x_n}\right)\left(\frac{\sigma_m S_R^m}{x_m}\right)} \tag{3}$$

with S_R^n, the sensitivity coefficient of functional R with respect to parameter x_n:

$$S_R^n = \frac{x_n}{R}\frac{\partial R}{\partial x_n}$$

The problem with this form is that S_R^n is very difficult to evaluate in the general case. However, using a first order GPT approach it can be approximated using

$$S_R^n = \frac{x_n}{R}\int_\rho d\rho \left[\frac{P}{\int_\alpha P\phi(\alpha)}\frac{\partial \Sigma_y(\rho)}{\partial x_n} - \Gamma(\rho)\left(\frac{\partial A}{\partial x_n} - \lambda\frac{\partial B}{\partial x_n}\right)\right]\phi(\rho) \tag{4}$$

The solution in this case is even simpler and consists of

1. Solve the transport for the flux using the reference values for $\dot{x}$
2. Solve a series of transport equation for the generalized adjoints, each element corresponding to a source Q_n given by in equation (2)
3. Evaluate the sensitivity coefficients using equation (4) and determine directly σ_R using equation (3).

The main advantage here is that there is no need for any statistical analysis including repetitive evaluations of perturbed functional. However the evaluation of N generalized adjoints is still required.

3.3 Example of application

The problem we have considered is a PWR pin cell fueled with 3.9 % enriched uranium oxide. [14] The fuel and the coolant are respectively at a temperature of 600 K and 500 K respectively. Our

transport calculations were performed in DRAGON using the collision probability method on a cell subdivided into 5 regions (3 for the fuel, one for the cladding and one for the coolant) and a 69 group library. The flux distributions resulting from these calculations were then used to generate cell averaged and 2 group cross sections. The upper energy limit of the thermal group (group 2) was set at 0.625 eV.

The effect of uncertainties in both the fuel and coolant temperatures on the two group cell averaged absorption cross sections. The uncertainty in the coolant temperature also affects its density (the fuel density is not strongly affected by the fuel temperature). Here, we assumed that the coolant density varies linearly with temperature and that there is a complete correlation between the coolant density and temperature and no correlation between fuel and coolant temperature. In Table 1 and 2 the results of a direct statistical analysis, a statistical GPT approach and a deterministic GPT approach (1000 simulations) are presented for the cell averaged fast and thermal absorption cross sections respectively when σ_T=5, 10 and 50 K.

Table 1 Uncertainties in the fast absorption cross section.

σ_T (K)	σ_{Σ^1} (%) Direct statistical	σ_{Σ^1} (%) GPT statistical	σ_{Σ^1} (%) GPT deterministic
5	0.11	0.11	0.11
10	0.22	0.22	0.22
50	1.17	1.15	1.10

Table 2 Uncertainties in the thermal absorption cross section.

σ_T (K)	σ_{Σ^2} (%) Direct statistical	σ_{Σ^2} (%) GPT statistical	σ_{Σ^2} (%) GPT deterministic
5	0.46	0.46	0.47
10	0.90	0.90	0.93
50	4.77	4.75	4.67

As one can see, the deterministic evaluations yield very good results for $\sigma_T \leq 10$ K, the results being consistent with the statistical method (both the direct and GPT approach). For the case where $\sigma_T = 50$ K, the uncertainties in the absorption cross sections are underestimated by up to 7 %. The gain in computing time for the statistical GPT approach is near 3 while for the deterministic GPT method it reaches 10.

4. Conclusion

We have presented an overview of methodology based on GPT and developed at École Polytechnique during the last thirty years. The origin of this development is a research project in fuel management of CANDU reactors, directed by Daniel Rozon. This technique is currently implemented in both our lattice cell DRAGON, where it is used for uncertainties propagation and perturbation calculations and in OPTEX for optimization studies.

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