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A Generalized Perturbation Theory Solver In Rattlesnake Based On PETSc With Application To TREAT Steady State Uncertainty Quantification

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Abstract - *Rattlesnake and MAMMOTH are the designated TREAT analysis tools currently being developed at the Idaho National Laboratory. Concurrent with development of the multi-physics, multi-scale capabilities, sensitivity analysis and uncertainty quantification (SA/UQ) capabilities are implemented for predicitive modeling of the TREAT reactor. For steady-state SA/UQ, that is essential for setting initial conditions for the transients, generalized perturbation theory (GPT) will be used. This work describes the implementation of a Krylov subspace based solver for the generalized adjoint equations that constitute a inhomogeneous, rank deficient problem. The standard approach is to use an outer iteration strategy with repeated removal of the fundamental mode contamination. The proposed new GPT algorithm directly solves the GPT equations without the need of an outer iteration procedure by constructing Krylov subspaces that are orthogonal to the operator's nullspace. Three test problems are solved and provide verification for the Rattlesnake's GPT capability. We conclude with a preliminary example evaluating the impact of the boron distribution in the TREAT reactor using perturbation theory.*

I. INTRODUCTION

Perturbation theory is an efficient tool for quantifying changes of output parameters to changes of input parameters if the number of output parameters is small. Perturbation theory for fixed source problems and eigenvalue problems is discussed in [1]. For eigenvalue problems, standard perturbation theory is confined to quantifying changes of the eigenvalue to changes of the input parameters. If the perturbation of other quantities is desired, a rank-deficient fixed source problem must be solved to obtain the generalized adjoint function [2]. The theory of obtaining changes of general quantities due to changes in input parameters for eigenvalue problems is referred to as generalized perturbation theory (GPT). Within this work, GPT is exclusively applied to the radiation transport problem without multiphysics feedback.

At the center of GPT is the solution of an inhomogeneous, rank-deficient problem. Traditionally, an outer iteration procedure is applied fixing the eigenvalue, and iterating on the fission source [2]. After a set number of outer iterations the fundamental mode contamination is removed. This method is for example implemented in the SCALE code NEWT for supporting the TSUNAMI module [3]. Within this work, we implement a new algorithm for the solution of the GPT equations into the radiation transport code Rattlesnake, [4], that directly solves for the generalized eigenfunction without the need of an outer iteration procedure. The basic idea is to utilize a modified Krylov subspace method such as GMRES, [5], implemented in PETSc, [6], to solve a singular linear problem by removing the null space from the Krylov space and the nullspace of the transpose from the right hand side. In the described case, Krylov methods will always provide the solution of the linear set of eqations [7].

Within this work, we first introduce the GPT equations and the implementation in Rattlesnake. Then we provide three analytical test problems illustrating the correct implementation in Rattlesnake: (1) discrete laplacian eigenvalue problem, (2) a one-dimensional, one-group neutron diffusion problem, (3) a two-dimensional, two-group neutron diffusion problem. Finally, we exercise the adjoint capability to compute the change of the eigenvalue due to changes of the boron contamination distribution in the steady state version of the Transient Test Reactor's (TREAT) transient 15 setup [8]. This work is the first step on the way to TREAT centered SA/UQ effort that is important due to the lack of detailed configuration information including boron contamination, control rod position, and steady-state conditions before a transient.

II. THE GENERALIZED ADJOINT PROBLEM

The radiation transport GPT equations comprise the rank-deficient adjoint eigenvalue operator on the left hand side and a source on the right hand side. Depending on the source, this equation has either no solution or infinitely many solutions. In this section, the generalized adjoint equations are introduced, solvability conditions are introduced, the solution procedure algorithm is discussed, and a normalization condition that yields a unique solution is introduced.

The adjoint eigenvalue problem in operator notation is given by:

$$L^*\phi^* = \frac{1}{k}P^*\phi^*, \tag{1}$$

where ϕ^* is the adjoint solution vector comprising all group fluxes (scalar or angular for diffusion or transport problems, respectively), L^* is the adjoint operator comprising all terms except the fission term but including boundary conditions, k is the multiplication factor, and P^* is the operator comprising the fission contributions. After discretization, the operators L^* and P^* become matrices. The fundamental mode solution is denoted by (k_0, ϕ_0^*). The corresponding forward problem is given by:

$$L\phi = \frac{1}{k}P\phi, \tag{2}$$

and the fundamental eigenpair is given by (k_0, ϕ_0) noting that the adjoint and forward multiplication factors are the same. The generalized adjoint equations are given by:

$$(L^* - \frac{1}{k_0}P^*)\Gamma^* = S^*, \tag{3}$$

where Γ^* is the generalized adjoint function and S^* is a so-far undetermined source. The generalized adjoint equations feature the following properties:

- $(L^* - \frac{1}{k_0}P^*)$ is rank deficient and the nullspace of dimension one is spanned by ϕ_0^*.
- The equation has infinitely many solutions if and only if

  $$(\phi_0, S^*) = 0, \tag{4}$$

  where $(\cdot, \cdot)$ is an inner product over the corresponding phase space (energy and space for diffusion, energy, space and angle for transport). PETSc ensures that this condition is always satisfied.
- The general solution consists of a homogeneous and a particular solution:

  $$\Gamma^* = c\phi_0^* + \Gamma_p^*, \tag{5}$$

  where c is an arbitrary constant.

In case Eq. (4) holds, a unique solution can be obtained by enforcing the normalization condition adopted from [2]:

$$(\phi_0, P^*\Gamma^*) = (P\phi_0, \Gamma^*) = 0. \tag{6}$$

We split the operator P into two pieces:

$$P = F^*F, \tag{7}$$

where $F^* = (\chi_1, \chi_2, ..., \chi_G)$ incorporates the fission spectrum and $F = (\nu\sigma_{f,1}, \nu\sigma_{f,2}, ..., \nu\sigma_{f,G})$ contains the fission neutron production cross sections. The pertinent fission sources can be constructed using these operators:

$$\begin{aligned} f_0^* &= F^*\phi_0^* \\ f_0 &= F\phi_0 \\ F_p^* &= F^*\Gamma_p^*. \end{aligned} \tag{8}$$

The normalization condition Eq. (6) becomes:

$$(P\phi_0, \Gamma^*) = (F\phi_0, F^*\Gamma^*) = (f_0, cf_0^* + f_p^*) = 0. \tag{9}$$

Solving for c yields:

$$c = -\frac{(f_0, f_p^*)}{(f_0, f_0^*)}. \tag{10}$$

The adjoint and forward eigenvalue problems Eq. (1) and (2) are solved as sub-apps using the MOOSE MultiApp system, [9]. The adjoint fundamental mode is supplied to PETSc for constructing a basis of the null space. The forward fundamental mode is used for ensuring that condition Eq. (4) is satisfied and for computing the fission source and constant c.

III. GENERALIZED PERTURBATION THEORY

A. Perturbation of the Eigenvalue

Perturbation of the eigenvalue follows the description in Ref. [1]. It is more convenient to work with the reactivity defined by:

$$\rho = \frac{k-1}{k}. \tag{11}$$

To first order, the change in reactivity to changes in the input parameters can be computed by [1]:

$$\delta\rho \approx \frac{(\phi^*, (1-\rho)\delta P\phi - \delta L\phi)}{(\phi^*, P\phi)}. \tag{12}$$

The significance of Eq. (12) is that it does not depend on the perturbed flux and hence the perturbed equations do not have to be solved.

B. Perturbation of Reaction Rate Ratios

For computing the changes of reaction rate ratios to changes in the input parameters using linear perturbation theory, the generalized adjoint problem Eq. (3) normalized according to Eq. (6) must be solved. We consider reaction rate ratios of the form

$$R = \frac{(\sigma_1, \phi_0)}{(\sigma_2, \phi_0)}. \tag{13}$$

The perturbation up to linear terms can be determined to be:

$$\begin{aligned} \delta R/R \approx &\frac{(\delta\sigma_1, \phi_0)}{(\sigma_1, \phi_0)} - \frac{(\delta\sigma_2, \phi_0)}{(\sigma_2, \phi_0)} \\ &+ (-\delta L\phi_0 + (1-\rho)\delta P\phi_0, \Gamma^*). \end{aligned} \tag{14}$$

where we have chosen S^* in Eq. (3) as

$$S^* = \frac{\sigma_1}{(\sigma_1, \phi_0)} - \frac{\sigma_2}{(\sigma_2, \phi_0)}. \tag{15}$$

IV. ANALYTICAL TEST PROBLEMS

In this section we demonstrate by using simple analytical test problems that Rattlesnake correctly solves the generalized adjoint equations. The first problem is a one-dimensional, discrete Laplacian eigenvalue problem, the second problem is a one-group, slab geometry neutron diffusion problem, and the third problem is a two-group, two-dimensional bare reactor problem.

1. Discrete Laplacian Problem

The setup of this test problem slightly adapts the description in Ref. [10]. The eigenvalue problem of the continuous Laplacian operator is given by:

$$\begin{aligned} -\frac{d^2u}{dx^2} &= \frac{1}{\lambda}u(x) \\ u(0) &= u(L) = 0, \end{aligned} \tag{16}$$

where u is the function we seek, λ is the eigenvalue, and the domain extends from $x = 0$ to $x = L$. For any given discretization, a discrete Laplacian operator can be constructed that for

TABLE I. Rattlesnake solution of Eq. (20) at interior nodes.

Node	x	Γ
1	1.25	1.002323
2	2.5	1.417499
3	3.75	1.002323
4	5	0
5	6.25	-1.002323
6	7.5	-1.417499
7	8.75	-1.002323

a continuous FEM implementation with linear Lagrange shape functions looks like:

$$\mathbf{D}\vec{u} = \frac{1}{\lambda}\mathbf{M}\vec{u}, \tag{17}$$

where **D** and **M** are the stiffness and mass matrices, respectively, and $\vec{u}$ are the values of u at the internal nodes. Let the discrete problem be defined on a mesh featuring n elements with a mesh spacing of $h = L/n$; this mesh has $n-1$ interior nodes. The m-th eigenpair is given by:

$$\begin{aligned} \frac{1}{\lambda_m} &= \frac{12}{h^2}\frac{\sin^2\omega_m}{1+2\cos^2\omega_m} \\ u_{m,j} &= \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x_j}{L}\right), \end{aligned} \tag{18}$$

where

$$\begin{aligned} \omega_m &= \frac{m\pi}{2n} \\ x_j &= jh. \end{aligned} \tag{19}$$

The fundamental mode is indicated by $m = 1$. A test problem is set up using $L = 10$ and $n = 8$ resulting in an eigenvalue of $\lambda_1 = 10.00292$.

To test Rattlesnake's ability to **exactly** [i.e. without discretization error] solve the rank deficient, inhomogeneous problem, a source term is added to Eq. (17):

$$\mathbf{D}\vec{\Gamma} - \frac{1}{\lambda_1}\mathbf{M}\vec{\Gamma} = \vec{S}^*, \tag{20}$$

where $\vec{S}^*$ is given by:

$$S_j^* = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x_j}{L}\right) + \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x_j}{L}\right) \tag{21}$$

It should be noted that the right hand side of Eq. (21) is not within the range of the left hand side operator of Eq. (20) and hence the problem tests the ability of PETSc to properly prepare the right hand side of the provided linear system before solving it. Rattlesnake is used to solve Eq. (20) and then the solution is extracted and subsituted back into Eq. (20). The computed solution that is listed in Table I satisfies Eq. (20).

2. One-group Slab Geometry Diffusion Problem

This test uses the slab-geometry, one-group neutron diffusion equation in a homogeneous medium as model equation. The one-group diffusion equation in its eigenvalue form is given by:

$$\begin{aligned} -D\frac{d^2\phi}{dx^2} + \sigma_a\phi &= \frac{1}{k}\nu\sigma_f\phi,\ 0 < x < a, \\ \phi(0) &= 0, \\ \phi(a) &= 0. \end{aligned} \tag{22}$$

where D is the diffusion coefficient, σ_a is the absorption cross section, and $\nu\sigma_f$ is the fission neutron production cross section. As Eq. (22) is self-adjoint $\phi = \phi^*$. The fundamental mode solution of Eq. (22) is:

$$\begin{aligned} \phi &= \alpha\sin\left(\frac{\pi x}{a}\right), \\ k &= \frac{\nu\sigma_f/\sigma_a}{1 + D/\sigma_a B_g^2}, \end{aligned} \tag{23}$$

where α is an arbitrary constant and the geometric buckling B_g is given by:

$$B_g = \frac{\pi}{a}. \tag{24}$$

We select the following parameter $D = 0.72\ cm$, $\sigma_a = 0.2\ cm^{-1}$, $k = 1.1$, $a = 100\ cm$, and compute $\nu\sigma_f = 0.220782$.

The inhomogeneous, rank-deficient GPT system is set up as:

$$\begin{aligned} \left[-D\frac{d^2}{dx^2} + \sigma_a - \frac{1}{k}\nu\sigma_f\right]^*\Gamma^* &= S^*(x),\ 0 < x < a, \\ \Gamma^*(0) &= 0, \\ \Gamma^*(a) &= 0. \end{aligned} \tag{25}$$

Using Eq. (23), we can simplify Eq. (25):

$$\begin{aligned} -D\left[\frac{d}{dx^2} + \left(\frac{\pi}{a}\right)^2\right]^*\Gamma^* &= S^*(x),\ 0 < x < a, \\ \Gamma^*(0) &= 0, \\ \Gamma^*(a) &= 0. \end{aligned} \tag{26}$$

We first determine a source that satisfies the condition $(\phi, S^*) = 0$ and the boundary conditions in Eq (26). A suitable choice is:

$$S^*(x) = \sin\left(\frac{2\pi x}{a}\right). \tag{27}$$

The solution Γ^* is the linear combination of the homogeneous solution ϕ and a particular solution Γ_p^* according to Eq. (5). where c is an arbitrary constant. The particular solution Γ_p^* is given by:

$$\Gamma_p^* = \frac{1}{3D}\left(\frac{a}{\pi}\right)^2\sin\left(\frac{2\pi x}{a}\right). \tag{28}$$

PETSc returns the particular solution without fundamental mode contamination, i.e. Γ_p^*. To check this, we set up the test problem in Rattlesnake and compute the L_2 norm of the difference between the exact and numerical solutions for mesh

element's thicknesses 10, 5, 2.5, 1.25, and 0.625 cm discretizing the diffusion equations with first order continuous finite elements. The results are compiled in Table II. In addition to the source $S^*(x)$ given in Eq. (27), we also use the source

$$S_2^*(x) = S^*(x) + \phi. \tag{29}$$

$S_2^*(x)$ does not satisfy the orthogonality condition and hence we again test if PETSc properly removes the fraction of the right hand side that is outside of the range of the left hand side operator. Therefore, the solution is expected to be identical up to numerical integration error to the one that uses $S^*(x)$ as right hand side. The results in Table II indicate that the error reduces with the theoretical predicted order two confirming that Rattlesnake correctly solves the rank deficient problem.

3. A Two-Dimensional, Two-group Bare Reactor Benchmark Problem

A. Analytical Solution

For the two-group, neutron diffusion problem an inner product is defined as:

$$\sum_{g=1}^{2}\left(f_g, p_g\right) = \sum_{g=1}^{2}\int_0^a dx \int_0^b dy\, f_g p_g. \tag{30}$$

The two-group diffusion equations for a homogeneous reactor extending from $0 < x < a$, $0 < y < b$ are given by:

$$\begin{aligned} -D_1\nabla^2\phi_1 + \sigma_{r,1}\phi_1 &= \frac{1}{k}\left(\nu\sigma_{f,1}\phi_1 + \nu\sigma_{f,2}\phi_2\right) \\ -D_2\nabla^2\phi_2 + \sigma_{r,2}\phi_2 &= \sigma_s^{1\to 2}\phi_1, \text{ on } V, \\ \phi_1 = \phi_2 &= 0 \text{ on } \partial V. \end{aligned} \tag{31}$$

Note that the subscript now indicates the group index and not the fundamental mode. The geometric buckling B^2 defined in [1] is slightly generalized to:

$$B_{n,m}^2 = \left(\frac{n\pi}{a}\right)^2 + \left(\frac{m\pi}{b}\right)^2, \tag{32}$$

where we note that $B_{1,1}^2 = B^2$. The multiplication factor can be computed as:

$$k = \frac{\nu\sigma_{f,1}}{\sigma_{r,1} + D_1B^2} + \frac{\sigma_s^{1\to 2}}{\sigma_{r,1} + D_1B^2}\frac{\nu\sigma_{f,2}}{\sigma_{r,2} + D_2B^2}. \tag{33}$$

The fundamental mode is given by:

$$\vec{\phi} = \alpha\begin{pmatrix}\Phi_1\\ \Phi_2\end{pmatrix}\sin\frac{\pi x}{a}\sin\frac{\pi y}{b}, \tag{34}$$

where α is an arbitrary real number representing the magnitude of the flux. The ratio Φ_1/Φ_2 is fixed and can be computed by determining the nullspace of the matrix:

$$\begin{bmatrix} D_1B^2 + \sigma_{r,1} - \frac{1}{k}\nu\sigma_{f,1} & -\frac{1}{k}\nu\sigma_{f,1} \\ -\sigma_s^{1\to 2} & D_2B^2 + \sigma_{r,2}\end{bmatrix}\begin{pmatrix}\Phi_1\\ \Phi_2\end{pmatrix} = 0 \tag{35}$$

Similarly, the adjoint fundamental mode is given by:

$$\vec{\phi}^* = \alpha^*\begin{pmatrix}\Phi_1^*\\ \Phi_2^*\end{pmatrix}\sin\frac{\pi x}{a}\sin\frac{\pi y}{b}. \tag{36}$$

We define the matrix $\mathbf{A}_{n,m}^*$ as:

$$\mathbf{A}_{n,m}^* = \begin{bmatrix} D_1B_{n,m}^2 + \sigma_{r,1} - \frac{1}{k}\nu\sigma_{f,1} & -\sigma_s^{1\to 2} \\ -\frac{1}{k}\nu\sigma_{f,1} & D_2B_{n,m}^2 + \sigma_{r,2}\end{bmatrix}. \tag{37}$$

The ratio Φ_1^*/Φ_2^* can be determined by obtaining the nullspace of the matrix $\mathbf{A}^* = \mathbf{A}_{1,1}$.

The response of interest is a ratio of reaction rates integrated over a subset of the domain. Let us denote the subset of the domain by V_s:

$$V_s : x_{min} < x < x_{max},\ y_{min} < y < y_{max}, \tag{38}$$

and the integal over region V_s by:

$$(f,g)_{V_s} = \int_{x_{min}}^{x_{max}} dx \int_{y_{min}}^{y_{max}} dy\, f\, g. \tag{39}$$

The response of interest is then given by:

$$R = \frac{(\sigma_{x,1}, \phi_1)_{V_s}}{(\sigma_{x,2}, \phi_2)_{V_s}}, \tag{40}$$

and the corresponding adjoint source is computed from Eq. (15):

$$\vec{S}^* = \begin{cases} \begin{pmatrix} \frac{\sigma_{x,1}}{(\sigma_{x,1},\phi_1)_{V_s}} \\ -\frac{\sigma_{x,2}}{(\sigma_{x,2},\phi_2)_{V_s}}\end{pmatrix} & \vec{r}\in V_s \\ \vec{0} & \text{otherwise}\end{cases} \tag{41}$$

The GPT problem written in matrix form is given by:

$$\mathbf{A}^*\vec{\Gamma}^* = \vec{S}^*. \tag{42}$$

The particular solution is sought as superposition of orthogonal functions on the domain V:

$$\vec{\Gamma}_p^* = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\begin{pmatrix}\Phi_{p,1}^{n,m,*}\\ \Phi_{p,2}^{n,m,*}\end{pmatrix}\sin\frac{n\pi x}{a}\sin\frac{m\pi y}{b}, \tag{43}$$

with the source similarly expanded:

$$S_g^* = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} S_g^{n,m,*}\sin\frac{n\pi x}{a}\sin\frac{m\pi y}{b}. \tag{44}$$

The expansion coefficients can be computed as:

$$\begin{aligned}\vec{S}^{n,m,*} = &\begin{pmatrix} \frac{\sigma_{x,1}}{(\sigma_{x,1},\phi_1)_{V_s}} \\ -\frac{\sigma_{x,2}}{(\sigma_{x,2},\phi_2)_{V_s}}\end{pmatrix} \\ &\times\frac{4}{n\,m}\left(\cos\frac{n\pi x_{max}}{a} - \cos\frac{n\pi x_{min}}{a}\right) \\ &\times\left(\cos\frac{m\pi y_{max}}{b} - \cos\frac{m\pi y_{min}}{b}\right).\end{aligned} \tag{45}$$

TABLE II. L2 error of the numerical and exact solution for the one-group diffusion test problem.

	L2 error			
Mesh size (cm)	$S^*(x)$	order	$S_2^*(x)$	order
10	2.36E+02		2.36E+02	
5	6.08E+01	1.96E+00	6.08E+01	1.96E+00
2.5	1.53E+01	1.99E+00	1.53E+01	1.99E+00
1.25	4.67E+00	1.71E+00	4.03E+00	1.92E+00
0.625	9.74E-01	2.26E+00	9.63E-01	2.06E+00

TABLE III. Two-dimensional, two-group test problem specifications.

Quantity	Value
a	300
b	300
$x_{min},\ x_{max} = y_{min},\ x_{yax}$	$\{133.\overline{3}, 166.\overline{6}\}$
σ_r	$\{0.027, 0.07\}$
$\nu\sigma_f$	$\{0.006, 0.1\}$
D	$\{1.51515, 0.4166667\}$
$\sigma_s^{1\to 2}$	0.017
σ_x	$\{0.002, 0.0417\}$
k	1.106897

Substituting Eq. (43) into Eq. (42) and collecting terms with identical n and m leads to:

$$\mathbf{A}_{n,m}\vec{\Gamma}_p^{n,m,*} = \vec{S}^{n,m,*}, \tag{46}$$

Using the pseudo-inverse, the expansion coefficients can be computed:

$$\vec{\Gamma}_p^{n,m,*} = \mathbf{A}_{n,m}^{\dagger}\vec{S}^{n,m,*}, \tag{47}$$

We require the generalized adjoint solution $\vec{\Gamma}^{*,T}$ to be normalized such that it satisfies:

$$\left(\vec{\Gamma}^{*,T}, \mathbf{P}\vec{\phi}\right) = 0. \tag{48}$$

Explicitly evaluating this condition yields:

$$\Gamma_1^{1,1,*}\left(\nu\sigma_{f,1}\Phi_1 + \nu\sigma_{f,2}\Phi_2\right) \times\left(\int_0^a dx \sin^2\frac{\pi x}{a}\right)\left(\int_0^b dy \sin^2\frac{\pi y}{b}\right) = 0, \tag{49}$$

which can only be satisfied if $\Gamma_1^{1,1,*} = 0$. The properly normalized generalized adjoint flux is therefore obtained by:

$$\vec{\Gamma}^* = \vec{\Gamma}_p^* - \frac{\Gamma_{p,1}^{1,1,*}}{\Phi_1^*}\vec{\phi}^*. \tag{50}$$

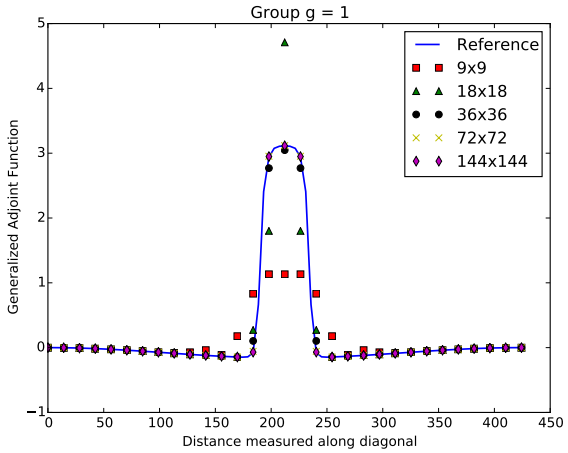

Fig. 1. Comparison of the numerical and reference solution for the two-dimensional, two-group, bare reactor test for group $g = 1$.

B. Numerical Results

We sample the numerical solution and the analytical solution along the diagonal ($x = y$) at distances of $\sqrt{2}\cdot 10$ cm (31 locations) and compare as the numerical model is refined. For the analytical solution, the series expansion is truncated at $N = M = 200$. The comparison of the reference solution with the numerical solution on meshes featuring 9×9, 18×18, 36×36, 72×72 and 144×144 rectangular elements is depicted in Fig. 1 and Fig. 2 for group 1 and group 2, respectively. The numerical solution uses first order continuous shape functions in space. The results show convergence of the numerical solution to the reference solution as the mesh is refined. The generalized adjoint function computed on the finest mesh is depicted in Fig. 3.

V. APPLICATION OF PERTURBATION THEORY TO TREAT

This summary contains preliminary results for TREAT perturbation analysis. We focus on the eigenvalue version of the transient 15 model described in Ref. [8] that is used to obtain the initial conditions for the subsequent transient analysis. This model features vacuum boundary conditions on all exterior sides. In particular, we use Rattlesnake's perturbation capability to compute the change in the eigenvalue

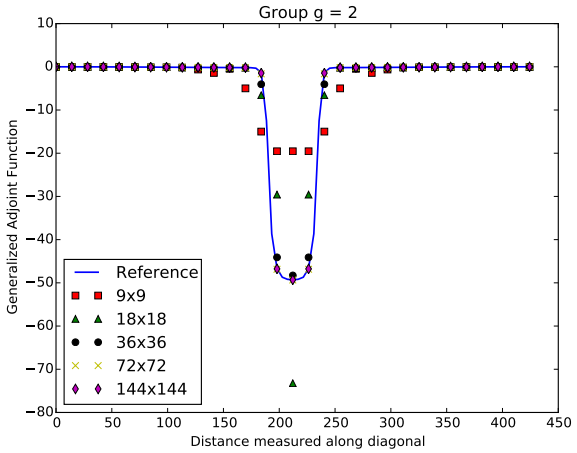

Fig. 2. Comparison of the numerical and reference solution for the two-dimensional, two-group, bare reactor test for group $g = 2$.

due to boron contamination in the fuel. During the baking process for the manufacture of TREAT fuel, borated steel dividers were used to reduce the chance of inadvertant criticality. However, due to direct contact with some of the fuel blocks, some boron migrated into the graphite. It is estimated to average either 5.6 or 7.9 weight parts per million (wppm) [11]. The transient 15 model already contains 7.9 wppm of boron distributed uniformly within the fuel and the computed eigenvalue is $k = 0.9917$. As the detailed spatial distribution is unknown, we analyze the following cases within this work: (1) uniform spatial distribution in the fuel using the lower estimate of 5.6 wppm of boron [essentially we compute the worth of 2.3 wppm of boron uniformly distributed within the core], (2) boron is distributed according to the following periodic function:

$$N(\vec{r}) = \alpha\left(1 - \left|sin\frac{x\pi}{L}\right|\right)\left(1 - \left|sin\frac{y\pi}{L}\right|\right), \qquad (51)$$

where α is chosen to conserve the total amount of boron in the core, and $L = 10.22$ cm is the size of a fuel assembly. The postulated distribution attempts to model the fact that boron migrated into the fuel assemblies from the outside so it is expected to vary on the assembly length scale. In fact, the true distribution is more complicated because not all outer surfaces were exposed to borated steel.

Thermal absorption cross sections of boron are obtained by assuming a Maxwellian flux spectrum, $1/v$ dependence of the cross section and a value of 755 b at $v = 2250$m/s [1]. We solve the transient 15 steady-state model in forward and adjoint mode using the continuous finite element diffusion solver in Rattlesnake and an 11 group energy structure described in [12].

Using Eq. (12), we find that the eigenvalue changes by about 1,700 pcm when decreasing the boron content unformly by 2.3 wppm. In Ref. [11] it is found that this change leads to a 1,200 pcm change of the eigenvalue for an infinite lattice of TREAT assemblies. Finally, the case where boron is distributed according to the periodic function Eq. (51) leads

TABLE IV. $\Delta k/k$ found for the various changes in boron distribution in the TREAT transient 15 core.

Case	$\Delta k/k$ [pcm]
Change by 2.3 wppm	1695
Periodic	42

to almost no change in the eigenvalue. While the spatial distribution of boron matters in principle, the length scale of realistic boron distributions [the typical distance over which changes are observed] is smaller or equal to the assembly pitch that is much smaller than the length scale over which the fluxes change. Hence the shape of the boron distribution does not play a significant role, but characterizing the total boron content is critical for accurate TREAT models.

VI. CONCLUSIONS AND FUTURE WORK

In this summary we introduce and verify Rattlesnake's capability for computing generalized adjoint functions. The generalized adjoint problem is solved using PETSc requiring no outer iteration procedure as typically performed. Three test problems: a discrete laplacian problem, a slab-geometry, one-group neutron diffusion problem, and a two-dimensional, two-group bare reactor are proposed and used to verify the implementation. The described GPT capability in Rattlesnake is the first step in a SA/UQ effort for TREAT modeling and simulation. Perturbation of the eigenvalue for the TREAT transient 15 core due to changes in the boron distribution are presented. Future work will focus on the TREAT M8CAL core and investigate more closely the effect of boron contamination, and control rod position on the eigenvalue and assembly powers. Future work will include SA/UQ on transient, multiphysics TREAT models.

VII. ACKNOWLEDGMENTS

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REFERENCES

1. J. J. DUDERSTADT and L. J. HAMILTON, *Nuclear Reactor Analysis*, John Wiley & Sons, Inc., New York (1976).
2. R. L. CHILDS, "Generalized Perturbation Theory Using Two-Dimensional, Discrete Ordinates Transport Theory," Research Report ORNL/CSD/TM-127, Oak Ridge National Laboratory (1980).
3. M. A. JESSEE, M. L. WILLIAMS, and M. D. DEHART, "Development of generalized perturbation theory capability within the SCALE code package," in "Proceedings of the International Conference on Mathematics, Computational Methods, and Reactor Physics (MC 09)," American Nuclear Society, Saratoga Spring, NY, USA (May, 2009).

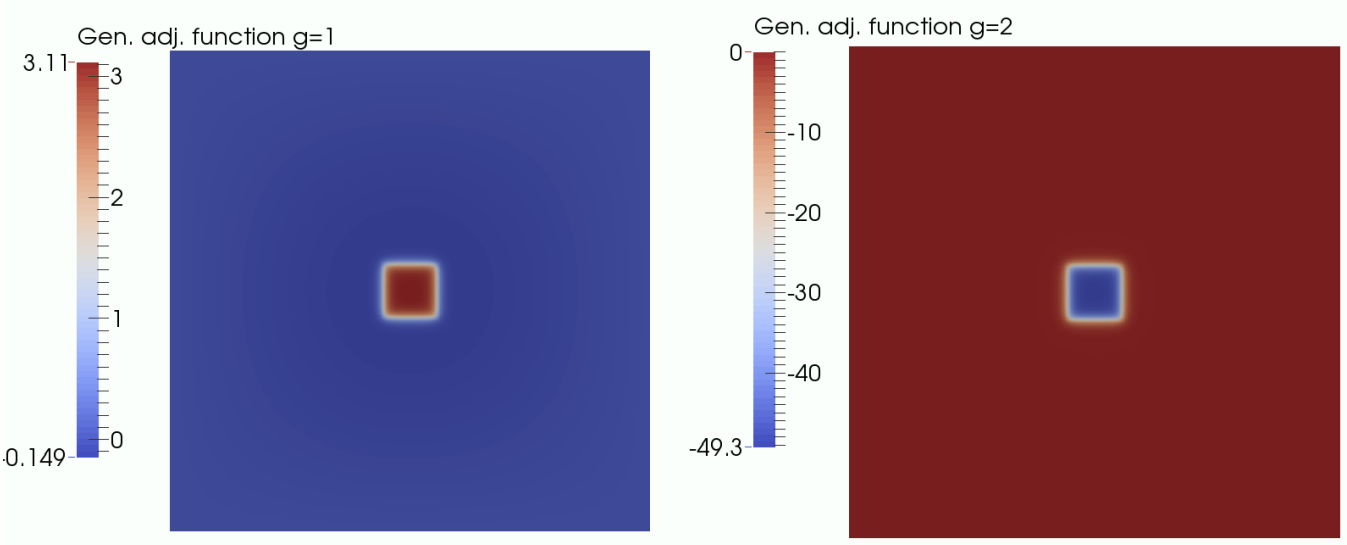

Fig. 3. Generalized adjoint fluxes computed with the $144x144$ mesh for $g = 1$ and $g = 2$.

4. Y. WANG, S. SCHUNERT, B. A. BAKER, F. G. GLEICHER, J. ORTENSI, M. D. DEHART, and R. C. MARTINEAU, *Rattlesnake User Manual*, INL (2016).
5. Y. SAAD and M. SCHULTZ, "GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems," *SIAM Journal on Scientific and Statistical Computing*, **7**, 856–869 (1986).
6. S. BALAY, S. ABHYANKAR, M. F. ADAMS, J. BROWN, P. BRUNE, K. BUSCHELMAN, L. DALCIN, V. EIJKHOUT, W. D. GROPP, D. KAUSHIK, M. G. KNEPLEY, L. C. MCINNES, K. RUPP, B. F. SMITH, S. ZAMPINI, H. ZHANG, and H. ZHANG, "PETSc Users Manual," Tech. Rep. ANL-95/11 - Revision 3.7, Argonne National Laboratory (2016).
7. I. IPSEN and C. MEYER, "Idea Behind Krylov Methods," Research Report CRSC-TR97-3, Center for Research in Scientific Computation, Department of Mathematics, North Carolina State University, Raleigh, NC (1997).
8. M. DEHART ET AL., "Research in Support of TREAT Kinetics Calculations using Rattlesnake/BISON Coupling within MAMMOTH," in "Physor 2016 -Unifying Theory and Experiments in the 21st Century," American Nuclear Society, Sun Valley, ID, USA (May 1-5, 2016).
9. D. GASTON and ET AL., "Physics-based multiscale coupling for full core nuclear reactor simulation," *Annals of Nuclear Energy*, **84**, *1*, 45–54 (2015).
10. B. SMITH, "Eigenvalues and Eigenvectors of the Discrete Laplacian," (2012).
11. J. D. BESS and M. D. DEHART, "Baseline Assessment of TREAT for Modeling and Analysis Needs," Research Report INL/EXT–15-35372, Idaho National Laboratory, Idaho Falls, ID (2015).
12. J. ORTENSI, Y. WANG, B. BAKER, S. SCHUNERT, F. GLEICHER, M. DEHART, A. LAURIER, and A. HEBERT, "Preparation of a Neutron Transport Data Set for Simulations of the Transient Test Reactor Facility," in "Proc. PHYSOR 2016 Unifying Theory and Experiments in the 21st Century," ANS, Sun Valley, Idaho (2016).