High Energy Density Physics 22 (2017) 12–16

Contents lists available at ScienceDirect

High Energy Density Physics

journal homepage: www.elsevier.com/locate/hedp

Adjoint-based sensitivity analysis for high-energy density radiative transfer using flux-limited diffusion

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ARTICLE INFO

Article History:
Received 6 June 2016
Revised 8 September 2016
Accepted 6 December 2016
Available online 7 December 2016

Keywords:
Flux limited diffusion
Radiative diffusion
Sensitivity analysis
Adjoint

ABSTRACT

Uncertainty quantification and sensitivity analyses are a vital component for predictive modeling in the sciences and engineering. The adjoint approach to sensitivity analysis requires solving a primary system of equations and a mathematically related set of adjoint equations. The information contained in the equations can be combined to produce sensitivity information in a computationally efficient manner. In this work, sensitivity analyses are performed on systems described by flux-limited radiative diffusion using the adjoint approach. The sensitivities computed are shown to agree with standard perturbation theory and require significantly less computational time. The adjoint approach saves the computational cost of one forward solve per sensitivity, making the method attractive when multiple sensitivities are of interest.

1. Introduction

The adjoint approach to performing sensitivity analyses is an efficient method for identifying parameters that have the greatest influence on a particular quantity of interest (QOI). The adjoint method requires formulation of a second problem, mathematically related to the forward system of equations, and uses the solution to obtain sensitivity information. This approach allows multiple sensitivities to be computed by solving the forward and adjointequations once, and evaluating inner products for each sensitivity. This is computationally efficient compared to the perturbation approach to finding sensitivities, which requires solving the forward problem twice per perturbed parameter. The sensitivity is then found by dividing the change in the QOI by the change in the perturbed parameter.

The main disadvantage of the adjoint approach is that can quickly become memory intensive [1,2]. The forward and adjoint solutions, along with parameter values, must be stored for all time, and at all spatial locations, in order to compute the sensitivities. For high fidelity, transient calculations the memory demand can rapidly exceed that available on standard computers. Typically, writing and reading to files is required, or a subset of information is stored and the solutions are recomputed from these checkpoints [3].

The methodology for deriving an adjoint system of coupled differential equations is well documented [4–6]. In this work, the adjoint equations are derived for a system of coupled partial differential equations describing radiative flux-limited diffusion. Approximations to complex expressions that result from the nonlinear flux-limited diffusion model are shown not to introduce significant error when computing sensitivities. The resulting system of adjoint equations are linear, thus it takes less computational time to perform a full sensitivity analysis using the adjoint approach than it takes to compute a single sensitivity using the perturbation method.

2. Adjoint-based sensitivity analysis

An adjoint-based sensitivity analysis is performed on a system described by flux-limited radiative diffusion with material temperature feedback. The evolution of the forward system is described by a set of coupled partial differential equations [7–9]:

$$\begin{aligned} &\frac{1}{c}\frac{\partial \phi}{\partial t} - \nabla\cdot D\nabla\phi = S - \kappa\rho(\phi - acT^4),\\ &\rho C_v\frac{\partial T}{\partial t} = \kappa\rho(\phi - acT^4), \end{aligned} \tag{1}$$

where $\phi = \phi(r, t)$ is the scalar intensity with units of GJ/cm^{2}ns, $T = T(r, t)$ is the temperature in keV, c is 29.98 cm/ns, a is 0.01372 GJ/cm^3-keV^4, S is an external volumetric source, κ is the opacity, ρ is the density, C_v is the specific heat, and D is the flux-limited diffusion coefficient. Note that the solutions, ϕ and T, depend implicitly on the material constants and the diffusion coefficient.

Flux-limited diffusion coefficients are designed to correct for non-physical results related to the speed of propagation of information. In the diffusion approximation, the current is given by the expression:

$$J = -D\nabla\phi. \tag{2}$$

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http://dx.doi.org/10.1016/j.hedp.2016.12.002
1574-1818/

The approximation is inaccurate where the gradient of the scalar intensity is large; flux-limited diffusion coefficients prevent the current from exceeding physical values in such regions. The Larsen coefficient is used in this work [10]:

$$D = \left((3\kappa\rho)^n + \left(\frac{1}{\phi} |\nabla\phi| \right)^n \right)^{-1/n}. \tag{3}$$

When the gradient of the scalar intensity is small, this reduces to the standard diffusion coefficient; when the gradient is large, the second term in the denominator dominates, thus preventing the current from exceeding the scalar intensity. Typically n is chosen to be two, but it can be adjusted such that the diffusion solution agrees more closely with transport calculations [11].

To derive the equations for the adjoint scalar intensity, $\phi^\dagger$, and the adjoint temperature, $T^\dagger$, we use the Lagrangian approach to form the sensitivity expression. First, the differential equations are combined to form the operator F:

$$F = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix} = \begin{pmatrix} \dot{\phi}/c - f(\phi, T) \\ \dot{T} - g(\phi, T) \end{pmatrix} = 0, \tag{4}$$

with

$$\begin{aligned} f(\phi, T) &= \nabla \cdot D\nabla\phi - \kappa\rho(\phi - acT^4) + S, \\ g(\phi, T) &= \frac{\kappa\rho}{\rho C_v}(\phi - acT^4). \end{aligned} \tag{5}$$

Following the work of Stripling [3] and Stripling, Anitescu, and Adams [12], to find the adjoint system for the coupled set of equations, a Lagrangian is formed:

$$\mathcal{L} = \int [\langle Q\rangle - \langle\lambda, F\rangle] dt, \tag{6}$$

where the angular brackets denote integrals over all space and $\langle Q\rangle$ is the quantity of interest. The integral over time is taken from t_0 to t_f. The operator F is defined to be zero, thus the sensitivities of $\langle Q\rangle$ and $\mathcal{L}$ are equivalent. To derive the expression for the sensitivity, the functional derivative of the Lagrangian is taken with respect to θ using the chain rule:

$$\frac{\partial\mathcal{L}}{\partial\theta} = \int \left[\langle Q\rangle_\theta + \langle Q\rangle_x x_\theta - \frac{\partial}{\partial\dot{x}}\langle\lambda, F\rangle\dot{x}_\theta - \frac{\partial}{\partial x}\langle\lambda, F\rangle x_\theta - \frac{\partial}{\partial\theta}\langle\lambda, F\rangle \right] dt. \tag{7}$$

In this equation, $x = (\phi\ T)^T$, the subscripts denote partial derivatives, $\dot{x}$ is the time derivative of x, and λ is an undetermined two component Lagrange multiplier. Using integration by parts, the integral can be rewritten as:

$$\begin{aligned} \frac{\partial\mathcal{L}}{\partial\theta} = &\left[-\frac{\partial}{\partial\dot{x}}\langle\lambda, F\rangle x_\theta \right]_{t_0}^{t_f} + \int \left[\langle Q_\theta\rangle - \frac{\partial}{\partial\theta}\langle\lambda, F\rangle \right] dt \\ &+ \int \left[\langle Q_x\rangle + \frac{d}{dt}\left(\frac{\partial}{\partial\dot{x}}\langle\lambda, F\rangle \right) - \frac{\partial}{\partial x}\langle\lambda, F\rangle \right] x_\theta\, dt, \end{aligned} \tag{8}$$

The only term in the above expression that cannot be computed directly is x_θ, the derivative of the solution vector with respect to θ. If this term was known, the adjoint approach would not be necessary as the sensitivity could be computed by direct differentiation of the QOI.

The adjoint equations are defined to be the conditions that are imposed on $\lambda \equiv (\phi^\dagger\ T^\dagger)^T$ such that the integrand of the final term is eliminated. Thus, the adjoint equations are given by the expression:

$$\left[-\frac{\partial}{\partial\dot{x}}\langle\lambda, F\rangle x_\theta \right]_{t_0} + \langle Q_x\rangle + \frac{d}{dt}\left(\frac{\partial}{\partial\dot{x}}\langle\lambda, F\rangle \right) - \frac{\partial}{\partial x}\langle\lambda, F\rangle = 0. \tag{9}$$

Note that the first term in (9) includes the sensitivity of the initial conditions to the parameter θ. This term can be included if known; in the work that follows it is simply assumed that the sensitivity of the initial conditions is not of interest and the term is taken to be zero; this assumption is not necessary in general. However, the value of x_θ at the final time is not known, and must be eliminated by imposing appropriate terminal conditions on the adjoint variables. The resulting system of adjoint equations evolve backward in time, with the terminal condition:

$$\lambda(t_f) = 0. \tag{10}$$

Physically, the terminal condition states that events occurring beyond the final time step do not influence the adjoint solution [3,13].

To summarize, the forward system of equations (Eq. (1)) are solved provided initial conditions and the adjoint system of equations (Eq. (9)) are solved by imposing terminal conditions (Eq. (16)). The forward and adjoint solutions can then be used to evaluate the sensitivity of the QOI with respect to any parameter, θ, by evaluating Eq. (11):

$$\frac{\partial\mathcal{L}}{\partial\theta} = \int \left[\langle Q_\theta\rangle - \frac{\partial}{\partial\theta}\langle\lambda, F\rangle \right] dt. \tag{11}$$

The QOI for the following examples is the time integrated absorption, $\mathcal{A}$, in particular regions, thus:

$$\langle Q\rangle = \int \rho\kappa\phi\ dV, \tag{12}$$

where the spatial integral is taken over the volume of interest. The expressions for F and $\langle Q\rangle$ are substituted into Eq. (9), and the system is split into its constituent components. The result is a set of coupled equations for the adjoint scalar intensity and the adjoint temperature:

$$\begin{aligned} &-\frac{1}{c}\frac{\partial\phi^\dagger}{\partial t} - \frac{\partial}{\partial\phi}\nabla\cdot(D\nabla\phi)\phi^\dagger + \kappa\rho\phi^\dagger = \kappa\rho + \frac{\kappa}{C_v}T^\dagger, \\ &-\frac{\partial T^\dagger}{\partial t} = -4ac\kappa\rho T^3\left(\frac{T^\dagger}{\rho C_v} - \phi^\dagger \right) + \left(\nabla\frac{\partial D}{\partial T}\nabla\phi - \frac{\partial(\kappa\rho)}{\partial T}(\phi - acT^4) \right)\phi^\dagger \\ &+ \frac{T^\dagger}{\rho C_v}(\phi - acT^4)\frac{\partial(\kappa\rho)}{\partial T} + \phi\frac{\partial(\kappa\rho)}{\partial T} \end{aligned} \tag{13}$$

The final expression for the sensitivity of the absorption, $\mathcal{A}$, with respect to an arbitrary parameter θ is given by:

$$\frac{\partial\mathcal{A}}{\partial\theta} = \left[\frac{\partial}{\partial\dot{x}}\langle\lambda, F\rangle x_\theta \right]_{t_0} + \int \left[\langle Q_\theta\rangle - \frac{\partial}{\partial\theta}\langle\lambda, F\rangle \right] dt. \tag{14}$$

2.1. Sensitivity examples

In this study the primary quantity of interest is the total absorption within particular volumes:

$$\mathcal{A} = \int\int \kappa\rho\phi\ dV\, dt,$$

where the integration over time is taken from t_0 to t_f and the spatial integration is taken over a region of interest. When computing sensitivities, a few complicated derivatives must be evaluated. For example, when computing the sensitivity of the absorption with respect to the opacity, the following derivative appears in the final term of Eq. (14):

$$\frac{\partial}{\partial\kappa}\left(-\nabla\cdot\left(\left\{ (3\kappa\rho)^n + \left(\frac{1}{\phi}|\nabla\phi| \right)^n \right\}^{-1/n} \nabla\phi \right) \right). \tag{15}$$

The flux-limited form of the diffusion coefficient complicates the spatial derivative. To avoid performing this derivative analytically, a second-order centered finite difference approximation is employed. For a particular direction in Cartesian geometry, the expression above is estimated by:

$$-\frac{\partial}{\partial\kappa}\left(\frac{\partial}{\partial r}D\frac{\partial\phi}{\partial r} \right)_i \approx -\frac{1}{\Delta r}\left(\left(\frac{\partial D}{\partial\kappa}\frac{\partial\phi}{\partial r} \right)_{i+1/2} - \left(\frac{\partial D}{\partial\kappa}\frac{\partial\phi}{\partial r} \right)_{i-1/2} \right), \tag{16}$$