Improved Differential Evolution Implementation for Solving Inverse Transport Problems

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INTRODUCTION

In the problem of inverse radiation transport, measurements of particle leakages from radioactive source/shield systems are used to infer unknown parameters within the system. Recently, inverse transport problems in spherical source/shield geometries were successfully solved using two stochastic optimization algorithms, differential evolution (DE) [1] and mesh-adaptive direct search (MADS) [2]. Since Ref. [2] was published, we have made improvements to our DE implementation that have further increased the method's efficacy for solving inverse transport problems. This paper reports on these improvements.

PROBLEM FORMULATION

Consider spherical multilayered source/shield systems where the material in each layer is homogeneous and the source is isotropic. An example of such a geometry is shown in Fig. 1. Suppose that some parameters, such as the locations between layers or the enrichment of the source, are unknown and we want to identify these unknown quantities by analyzing the passive (decay) radiation leakage. This problem can be solved by optimization-based inverse techniques that find the parameter values which minimize a cost difference between the measured quantities of interest for the system and the quantities of interest calculated using a set of postulated parameter values. The measurements considered in this paper are uncollided fluxes of discrete gamma-ray lines at points external to the source/shield system. Because scattering is neglected, the scalar flux at each line can be computed by a ray-trace technique [3]. We define the following cost functional to represent the difference between the measured and calculated values of the flux:

$$f(\mathbf{x}) = \sum_{g=1}^{G} \left(\frac{R_g - R_g(\mathbf{x})}{\sigma_g} \right)^2,$$

where R_g is the measured value of the flux for detector g, $R_g(\mathbf{x})$ is the value of the flux at detector g calculated using the postulated parameter set $\mathbf{x}$, σ_g is the uncertainty associated with the measurement at detector g, and G is the number of detectors. In this inverse problem, we seek to find a feasible global optimal solution $\mathbf{x}^* \in \mathbf{\Omega}$ such that $f(\mathbf{x}^*) \leq f(\mathbf{x})$ for all $\mathbf{x} \in \mathbf{\Omega}$, where $\mathbf{\Omega}$ is the feasible region.

In Ref. [2], the geometry shown in Fig. 1 was used as a test problem. The region between 0.00 cm and r_1 = 8.741 cm contained a high-enriched uranium source (94.73% ^{235}U and 5.27% ^{238}U) of density 18.74 g/cm^3. This was surrounded by a void between r_1 = 8.741 cm and r_2 = 12.40 cm. A layer of lead shielding was between r_2 = 12.40 cm and r_3 = 12.90 cm and a layer of aluminum shielding between r_3 = 12.90 cm and r_4 = 13.20 cm. External leakage measurements of the four strongest emission lines of uranium (144, 186, 766, and 1001 keV) were the quantities of interest for the system. It was noted in Ref. [2] that the MADS method was capable of solving an inverse transport problem in which r_1, r_2, and r_3 were unknown, but the DE method was not.

This conclusion led us to reevaluate our implementation of DE. We have made modifications and greatly improved the performance of DE.

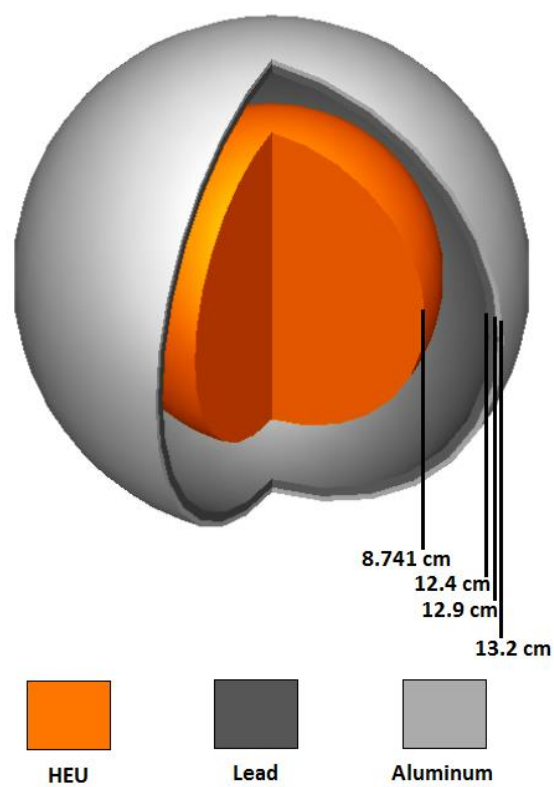

Fig. 1. Spherical Test Geometry 1.

IMPROVEMENTS TO THE DIFFERENTIAL EVOLUTION METHOD IMPLEMENTATION

The DE method is an evolutionary algorithm based on a generational approach in which a population of solutions is evolved. A new generation of "child" solutions is created using information contained in the current, or "parent," generation of solutions. Often, a maximum number of generations is specified for the method. In our initial implementation of DE, an unrealistically low number of maximum generations was specified, causing the method to stop running before it was complete. This led to the failure of the method that is noted in Ref. [2].

We have also made an improvement in the strategy by which DE handles constraint violations. In our initial implementation of DE, when an unknown interface violated a constraint, the violation was fixed by constraining the solution between the parameter values of the parent. As an example of how this hindered performance of the algorithm, consider the geometry in Fig. 1. Suppose that r_1 = 8.741 cm and r_2 = 12.40 cm are unknown, and suppose that r_3 = 12.90 cm and r_4 = 13.20 cm are known (and thus fixed). Further suppose that in the DE method a given parent has calculated values of r_1 = 2.00 cm and r_2 = 4.00 cm for the unknown radii. Now suppose the child of that parent has calculated values of r_1 = 13.00 cm and r_2 = 13.40 cm, thus violating a constraint because they are both greater than the (known) value of r_3 = 12.90 cm. In our previous implementation of DE, the method for fixing this constraint violation was to set r_1 equal to a random value between 0.00 cm and the r_2 value of the *parent*, or r_2 = 4.00 cm, thus overly constraining the child's value of r_1. We have taken a new approach in which two random values are generated between 0.00 cm and 12.90 cm, with the smaller value being set to r_1 and the larger to r_2. This improvement has led to enormous reductions in the time required to solve many problems.

NUMERICAL TEST PROBLEMS

The improved DE implementation was tested on two sets of numerical test problems. The first set is based on a geometry (Fig. 1) that was used in Ref. [2]. In this set, the first problem is taken directly from Ref. [2], where it was noted that DE failed, and the second and third problems are difficult inverse problems that our initial DE method also fails to solve. The second set is based on inverse transport problems from Ref [1]. Although the DE method was successful in Ref. [1], here we will show the enormous time reduction obtained with our improved method.

Since DE is stochastic in nature, starting from randomly generated initial solutions and employing random numbers to proceed through the generational process, ten 10 separate DE calculations will be considered for each test problem in order to establish average behavior.

Problem Set 1 Using Figure 1

These three test problems and their DE results are summarized in Table I.

Problem 1: Three Unknown Radii

Consider the case in which the first three radii in Fig. 1 are unknown. The previous DE implementation failed for this problem in Ref. [2]. With the improved DE implementation, all 10 calculations found the correct parameter values to within 0.001 cm with an average run time of 1.96 seconds.

This problem was run with the Levenberg-Marquardt method [4] with 30 random initial starting models (the initial population used in one run of the DE method). Only three of the 30 converged to within 0.01% for all four lines.

Problem 2: Four Unknown Radii

Now consider the case where all four radii in Fig. 1 are unknown. Here we constrain the radii to all be less than 40 cm. A calculation using our initial implementation of DE required 50.65 seconds to run and yielded an inaccurate solution of r_1 = 8.586 cm, r_2 = 11.89 cm, r_3 = 12.39 cm, and r_4 = 12.49 cm. All 10 calculations of our improved DE method found the correct radii to within 0.001 cm with an average run time of 6.66 seconds.

This problem was run with the Levenberg-Marquardt method [4] with 40 random initial starting models (the initial population used in one run of the DE method). Only three of the 40 converged to within 0.01% for all four lines.

Problem 3: Three Unknown Radii and Unknown Source Weight Fractions

In the third test problem, the first three radii and the weight fractions of the uranium source (94.73% ^{235}U and 5.27% ^{238}U – this results in a single unknown because weight fractions are constrained to sum to 1.0) are unknown. A calculation using our initial implementation of DE required 58.18 seconds to run and yielded inaccurate values of r_1 = 8.136 cm, r_2 = 12.24 cm, r_3 = 12.74 cm, and a ^{235}U weight fraction of 93.57%. All 10 calculations of our improved DE method found the correct radii to within 0.001 cm and the correct uranium weight fractions to within 0.01%, with an average run time of 5.02 seconds.

This problem was run with the Levenberg-Marquardt method [4] with 50 random initial starting models (the

initial population used in one run of the DE method). None of the 50 converged to within 0.01% for all four lines.

TABLE I. DE Results for Problem Set 1

Problem	Unknown Quantities	Percent of Successful DE Trials	Average Run Time (seconds)
1	r_1 = 8.741 cm r_2 = 12.40 cm r_3 = 12.90 cm	100%	1.96
2	r_1 = 8.741 cm r_2 = 12.40 cm r_3 = 12.90 cm r_4 = 13.20 cm	100%	6.66
3	r_1 = 8.741 cm r_2 = 12.40 cm r_3 = 12.90 cm ^{235}U = 94.73%	100%	5.02

Problem Set 2 Using Figure 2

The second set of problems is based on the geometry shown in Fig. 2. The HEU source has a radius of r_1 = 7.00 cm and is surrounded by a void layer with radius r_2 = 10.00 cm, followed by a layer of aluminum shielding with radius r_3 = 12.00 cm. The two test problems in this set are taken directly from Ref. [1].

These two test problems and their DE results are summarized in Table II.

Problem 4: Two Unknown Radii and Unknown Source Weight Fractions

In the fourth test problem, r_1 (7.00 cm), r_2 (10.00 cm), and the weight fractions of the uranium source (94.73% ^{235}U and 5.27% ^{238}U) are all unknown. This was case 1 of Ref [1], where our initial DE method (referred to as DEO in Ref. [1]) successfully solved this problem for every trial case, but required an average of 41.1 seconds to do so. Here, all 10 runs of the new DE method were also successful but required only an average of 2.47 seconds of run time.

This problem was run with the Levenberg-Marquardt method [4] with 40 random initial starting models (the initial population used in one run of the DE method). Only 23 of the 40 converged to within 0.01% for all four lines. This is much better performance than in problems 1, 2, and 3, but it is much worse than DE.

Problem 5: One Unknown Radius, Unknown Source Weight Fractions, and Unknown Source Density

Consider now a case in which r_1 (7.00 cm), the weight fractions of the uranium source (94.73% ^{235}U and 5.27% ^{238}U), and the density of the uranium source

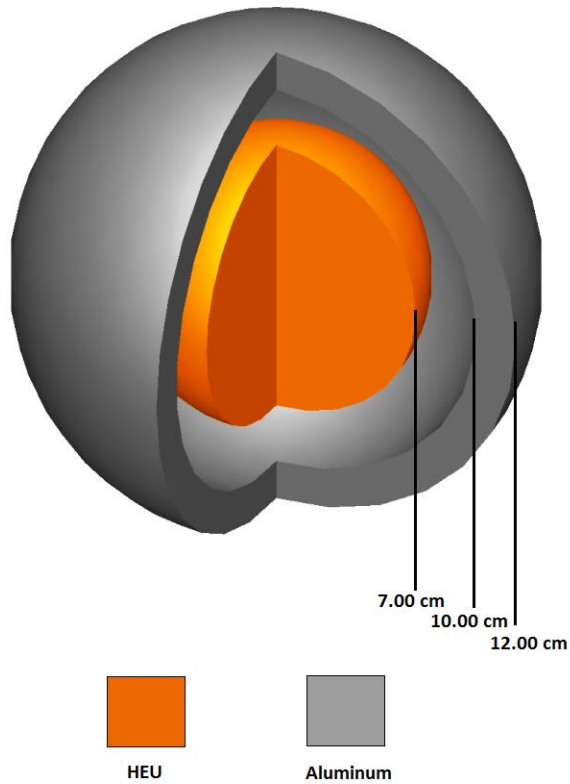

Fig. 2. Spherical Test Geometry 2.

(18.74 g/cm^3) are unknown. This was case 2 of Ref. [1], where all runs of the original DE method were successful, with an average run time of 34.20 seconds. Here, all 10 runs of the new DE method were also successful but with an average run time of just 2.40 seconds.

This problem was run with the Levenberg-Marquardt method [4] with 40 random initial starting models (the initial population used in one run of the DE method). Only 23 of the 40 converged to within 0.01% for all four lines.

TABLE II. DE Results for Problem Set 2

Problem	Unknown Quantities	Average Run Time for Initial DE Method (seconds)	Average Run Time for Improved DE Method (seconds)
4	r_1 = 7.00 cm r_2 = 10.00 cm ^{235}U = 94.73%	41.11	2.47
5	r_1 = 7.00 cm ^{235}U = 94.73% ρ(U) = 18.74 g/cm^3	34.20	2.40

SUMMARY AND CONCLUSIONS

Recently, the differential evolution method was applied to solve inverse transport problems. Since our initial results were published, we have made improvements to our implementation of this method that have resulted in significant improvements over our previous results. In this paper, we have shown that the DE method went from being unable to solve some inverse transport problems to solving those problems with average run times of less than 7 seconds. We have also applied DE to two problems in which our old implementation was successful. For these problems, the improved method runs 15–20 times faster than the original method.

We compared our DE implementation with our Marquardt implementation for these problems. This is not necessarily an equitable comparison because the methods are so different. For example, the Marquardt method is extremely sensitive to the initial model, but DE is not. Nevertheless, our recent implementation of DE very clearly outperforms Marquardt for these problems, in which the initial model is essentially random. Marquardt's performance would improve if the initial model were constrained.

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