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Samoa Updater: An Application of the Levenberg–Marquardt Method to Update DELFIC Predictions Using Field Measurements

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ABSTRACT

The US Department of Energy (DOE) Forensics Operations (DFO) is a member of the Ground Collections Task Force (GCTF), which is responsible for sample collection of radiological debris for attribution should a nuclear detonation ever occur in the United States. The DFO runs the Defense Land Fallout Interpretive Code (DELFIC) Fallout Planning Tool to predict the deposition of fallout from a nuclear detonation. This prediction is refined using the DELFIC Updater tool, which takes ground measurements and adjusts DELFIC inputs to minimize the difference between prediction and observation, yielding improved predictions of fallout in locations both measured and not yet measured.

Samoa, a framework for uncertainty analysis and optimization, is used to improve DELFIC predictive fallout modeling. This new capability using Samoa, dubbed "Samoa Updater," is compared with the current DELFIC Updater, a brute-force sampling approach. Samoa Updater uses the Levenberg–Marquardt (LM) method, a gradient-based nonlinear least squares approach that uses the functional shape of the input space to increase optimization speed. In simulated test cases Samoa Updater yields faster and more accurate solutions than the current Updater.

1. INTRODUCTION

Updater [1], a tool developed by DOE's Oak Ridge National Laboratory (ORNL) in 2015, uses measured data to improve fallout modeling predictions by DELFIC. Updater varies physical inputs for the simulations until the difference between calculated and measured dose rates is minimized. The DELFIC input deck with the physical inputs that produce this minimum can then be used to predict fallout in regions not yet measured. Although Updater's approach will almost always reduce this difference and improve the fallout model, the sampling technique is computationally expensive and has difficulty fine-tuning to find the inputs that minimize the difference. In this work, the LM method, implemented in ORNL's Samoa toolset, was used to improve the speed and accuracy of the minimization. This new approach is called Samoa Updater. Here, a comparison between Updater and Samoa Updater is documented.

This report is broken down as follows. Section 2 briefly reviews the Updater approach. Section 3 discusses the new Samoa Updater method, and Section 4 compares the performances of the two methods.

2. CURRENT METHOD: UPDATER

Updater begins with a DELFIC model that contains the best initial guess for the inputs (e.g., yield, height of burst, meteorological conditions) of the scenario of interest and a set of measured data. The initial DELFIC model predictions are compared with these measured data, and then the DELFIC input is adjusted for three physical inputs: yield, wind speed factor (WSF), and wind direction offset (WDO). These values are updated via brute force—no functional information (such as gradients) is used to determine the direction or size of the adjustments. The only information used to choose the updated values is whether results are trending better or worse. If the DELFIC models are producing results closer to the measured data, then larger adjustments are made to the inputs. If the results are diverging from the measured data, then smaller adjustments are made. This process of expanding and contracting adjustment sizes continues until the calculated dose rates match the measured dose rates within a prescribed tolerance or until a maximum number of iterations are performed. The Updater code operates in the following fashion:

1. Read in the measurement data, appending to any existing measurement data if desired.
2. Calculate DELFIC predictions to compare to the time/location-stamped measurement data.

Calculate the overall error between the measurements and predictions.

3. Vary the DELFIC inputs to create a new series of predictions and calculate new overall errors. From this series and from the previous best prediction, find the input that provides the lowest error.
4. Taking the best input at this point, repeat step 3 until the error no longer improves (convergence) or until a specified maximum number of iterations have occurred (to prevent excessively long calculations).
5. Produce a new input deck for DELFIC using the input values that minimize error.

This updating is not intended for predicting the varied inputs like yield and wind speed. Instead, updating is performed to help understand dose rates, mass chain activities, particle sizes, and other fallout characteristics in regions of the fallout field where measurement data have not yet been collected. This information can be useful for forensics or consequence management personnel who may have to work with incomplete information.

The search array is always centered around the best-known set of inputs. However, Updater does not always use an all-possible-subsets approach to creating an array of data points. To speed the solution, Updater attempts to recognize when a particular array (or one very similar to it) has already been tried. Because previous points (that were not selected as the best match) are known to be a less suitable solution, they do not have to be re-evaluated. Updater may also omit variations of a variable if that variable does not change across solutions. For example, if the best value for wind direction is always at 90° in this scenario, then Updater will occasionally skip variations of the wind direction to accelerate the convergence.

Despite the optimizations in place, Updater does not use particularly sophisticated search methods. At the time of Updater's inception, there was no readily available framework to provide a better search algorithm. Updater's approach made minimal assumptions about the shape and characteristics of the search space but could be susceptible to local minima or other artifacts that prevented convergence on the globally minimal solution. Hence the desire to create a new approach to the prediction update process.

3. A NEW APPROACH: SAMOA UPDATER

In this work, a new tool called Samoa Updater was developed to find better matches to the measured data in fewer evaluations than are required by Updater. The Samoa framework is a generalized optimization and uncertainty analysis tool developed at ORNL. It can solve optimization problems such as minimizing the difference between measured and calculated values by using a variety of methods, including gradient-based techniques, evolutionary algorithms, and Markov chain Monte Carlo approaches. Because of its potential to be much faster than the other methods, the gradient-based LM [2] optimization algorithm was chosen.

In the LM method, the problem is cast in a nonlinear least squares formulation, with the goal of minimizing a metric that expresses the difference between the logarithms of the measured and calculated dose rate values:

$$\chi^2 = \frac{1}{N}\sum_{i=1}^{N}\left(\ln(C_i) - \ln(M_i)\right)^2,$$

where N is the number of measurement points, M_i is the measured value at point i, and C_i is the calculated value at point i, determined by a DELFIC calculation given postulated values for yield, WSF, and WDO. A log difference is used to weight points by the relative difference between calculated and measured values and avoid the χ^2 value being determined by only the points with the largest measurements. The dose rates in a fallout field can vary by orders of magnitude; if the values were used directly, differences in the peak values would overwhelm differences in the rest of the field. Applying a logarithmic transform allows all measured data to provide meaningful contribution to the updating approach. The LM approach uses interpolation between the Gauss–Newton algorithm and the gradient descent technique, tending more toward the Gauss–Newton approach in regions where χ^2 is approximately quadratic and more toward gradient descent elsewhere. LM requires an initial guess for the three input values, and then it chooses updated input values by using information contained in the gradients of χ^2 with respect to the inputs. These gradients are approximated using a central differencing technique:

$$\frac{\partial \chi^2}{\partial x} \approx \frac{\chi^2(x+h) - \chi^2(x-h)}{2h},$$

where x is the value of yield, WSF, or WDO, and h is a small finite difference step size. Because χ^2 is calculated at two values, each iteration takes two DELFIC calculations for each unknown input. Thus, if all three inputs were evaluated simultaneously, then LM would require six DELFIC calculations per iteration.

Samoa Updater provides a constraint-handling mechanism so that results do not go beyond user-defined maximum and minimum values[1]. Constraints are handled via an active-set method. This approach works by turning off an input that violates a constraint and setting it to the maximum or minimum value. The χ^2 metric is then minimized as a function of the remaining inputs, and then the input that had been turned off is turned back on (i.e., the algorithm then proceeds to again minimize χ^2 as a function of all the inputs). For example, suppose yield and wind speed factor are being determined, and the user has specified that the maximum yield is 21.0 kt. Further suppose that LM calculates a yield of 25.0 kt. The yield is larger than the maximum and is therefore set to 21.0 kt. LM then proceeds to find the wind speed factor that minimizes χ^2 when yield is 21.0 kt. After this value is found, the yield is again turned on, and LM finds both the yield and wind speed factor that minimize χ^2.

4. COMPARISON OF SAMOA UPDATER AND DELFIC UPDATER RESULTS

Updater and Samoa Updater were compared using data collected from the 2023 GCTF Cranky Cockroach Prominent Hunt Exercise. The Prominent Hunt exercise is an interagency exercise in which a nuclear detonation scenario is modeled to simulate a real event. Ground truth contours for the Cranky Cockroach exercise are shown in Figure 1. The ground truth is the result of a burst with a yield of 3.0 kt, WSF of 1.0, and WDO of 0.0 given a set of ground truth meteorological conditions.

In a real event, knowledge about the event may be sparse and uncertain. Knowledge may be limited to estimates of yield, ground zero location, and the meteorological conditions from the nearest airport or a numerical weather prediction model. All these estimates may have high uncertainties, particularly during the first few hours after detonation when information may be conflicting and unresolved. This variability introduces large uncertainties in predictions of fallout deposition. As time progresses, reanalysis methods refine the estimated meteorological conditions for ground zero. Test cases were designed to illustrate this post-detonation refinement of inputs.

Two test cases were developed. To compare Updater and Samoa Updater directly, both tests used the same 500 measurement points. Test Case 1 was a simulation of a time soon after the burst when only a

[1] Such constraints are necessary because the data for updating may be from geographically constrained regions. The user may know that the yield and other inputs are in a given range based upon other external evidence, but the mathematical best fit to the given data may be from unrealistic combinations of DELFIC inputs. The ability to manually constrain the solution allows the user to control for this phenomenon.

single wind observation or numerical prediction was available. In this case, small errors in wind direction (<5°) are present at various altitudes. The initial yield, WSF, and WDO were 10.0 kt, 1.0, and 0.0, respectively. Note that the initial yield estimate is greater than the ground truth of 3.0 kt, simulating a situation where the present understanding of the yield is only approximate. The contours resulting from the initial guess are shown in Figure 2. These contours result in a far wider deposition field than that of the ground truth deposition.

For comparing Updater and Samoa Updater we consider how many DELFIC evaluations each method required to find a solution. One evaluation of DELFIC estimates the dose rate at all 500 ground measurement points.

For Test Case 1, Updater required 353 DELFIC evaluations to reach a χ^2 value of 0.3202, which corresponded to a yield of 9.65 kt, a WSF of 0.82, and a WDO of 4.10. Samoa Updater required 304 DELFIC evaluations but reached a lower χ^2 value of 0.1134. This value corresponded to a yield of 3.87 kt, WSF of 1.81, and WDO of -2.15. The contour lines calculated by the two methods are shown in Figure 3 (note that for comparison purposes the domain was limited to the ground-truth domain, thus truncating some of the calculated contours). Samoa Updater did a superior job of matching the contour lines of ground truth. This result is expected because it reached a smaller χ^2 metric, indicating a better match between calculated and measured values.

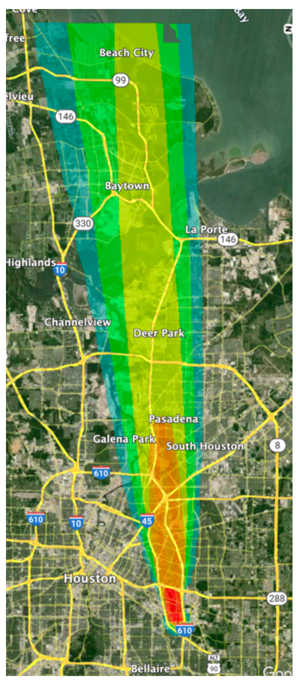

Figure 1. Ground truth deposition contours for Cranky Cockroach.

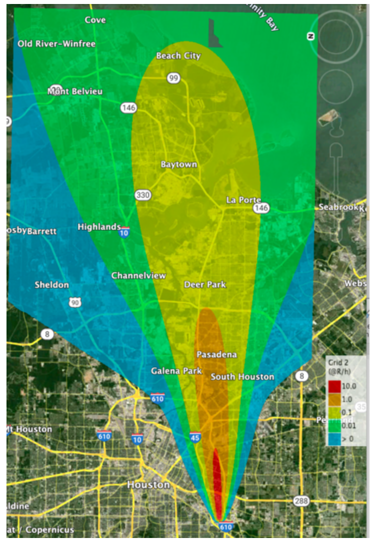

Figure 2. Deposition contours for Test Case 1. Contours corresponding to the initial guess (yield = 10.0 kt, WSF = 1.0, WDO = 0.0).

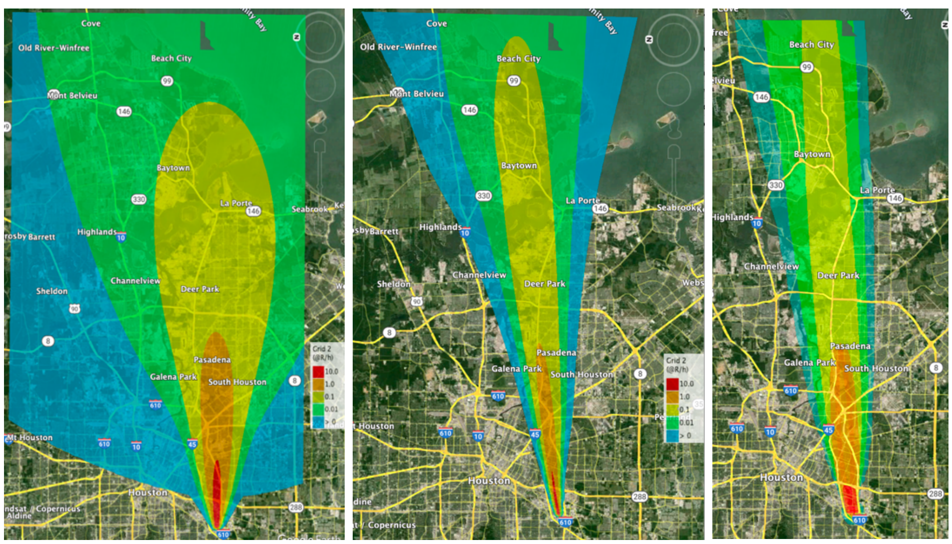

Figure 3. Deposition contours for Test Case 1. (left) Contours calculated by Updater, (center) contours calculated by Samoa Updater, and (right) ground truth contours.

Test Case 2 was a simulation at 24 hours after detonation, when additional weather data have been added to get the correct wind field, and a better estimation of the yield has become available. In this case, the estimated yield is 5.0 kt, with updated weather data. WSF and WDO remain 1.0, and 0.0, respectively. The contour values corresponding to these conditions are shown in Figure 4.

Updater required 213 DELFIC evaluations to reach a χ^2 value of 0.1610, corresponding to a yield of 4.54 kt, a WSF of 1.50, and a WDO of -0.30. Samoa Updater required 116 DELFIC evaluations to reach a χ^2 value of 0.0903, corresponding to a yield of 3.87 kt, a WSF of 1.66, and a WDO of -0.57. The contours corresponding to these values are shown in Figure 5. Again Samoa Updater found a much better match than Updater, this time using far fewer DELFIC evaluations.

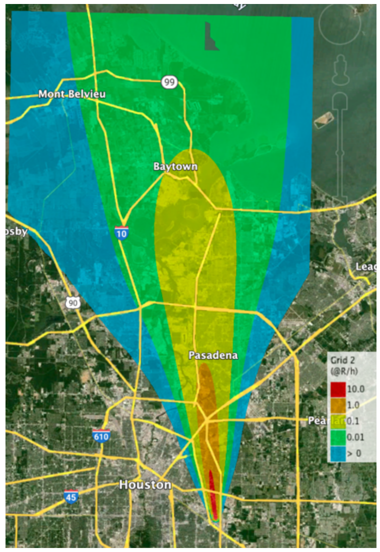

Figure 4. Deposition contours for Test Case 2. Contours corresponding to the initial conditions (yield = 5.0 kt, WFT = 1.0, WDO = 0.0).

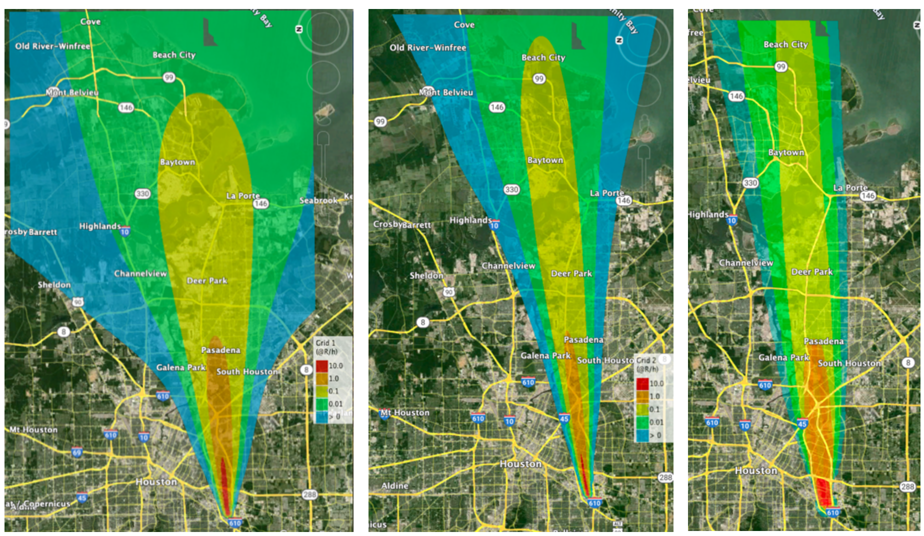

Figure 5. Deposition contours for Test Case 2. (left) Contours calculated by Updater, (center) contours calculated by Samoa Updater, and (right) the ground truth contours, which are the same as in Test Case 1.

The results of the two test cases are summarized in Table 1.

Table 1. Results of test cases

Test Case 1		
Initial guess	Updater result (353 evaluations) $\chi^2 = 0.3202$	Samoa Updater result (304 evaluations) $\chi^2 = 0.1134$
Yield: 10.0 kt WSF: 1.0 WDO: 0.0	Yield: 9.65 kt WSF: 0.82 WDO: 4.10	Yield: 3.87 kt WSF: 1.81 WDO: -2.15
Test Case 2		
Initial guess	Updater result (213 evaluations) $\chi^2 = 0.1610$	Samoa Updater result (116 evaluations) $\chi^2 = 0.0903$
Yield: 5.0 kt WSF: 1.0 WDO: 0.0	Yield: 4.54 kt WSF: 1.50 WDO: -0.30	Yield: 3.87 kt WSF: 1.66 WDO: -0.57

5. CONCLUSIONS

By using the LM approach and employing gradient information to guide the search, the new Samoa Updater method finds solutions for the predictive fallout modeling problem that led to better matches to the measured values and required fewer evaluations than the Updater method. In a test case modeling a situation soon after the burst so that wind information was inaccurate and the initial yield was over three times the ground truth yield, Samoa Updater calculated contour lines far closer to the ground truth lines than Updater. In a test case modeling a later time when more information was available, Samoa Updater again produced better contour lines and required 46% fewer DELFIC evaluations than Updater. When deployed, Samoa Updater will allow the GCTF to generate updated plume models more quickly and with higher confidence in the unmeasured regions compared with the current Updater method.

6. REFERENCES

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[2] Press, W. H., et al. 1994. “Statistical Description of Data.” In: *Numerical Recipes in FORTRAN: The Art of Scientific Computing*, 2nd ed. (reprinted with corrections). Cambridge, United Kingdom.