

Tools for Predicting Uncertainty and Confidence Intervals in Radiometric Data Products

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ABSTRACT

Spaced-based observations of atmospheric energetics, such as those provided by NASA's Clouds and the Earth's Radiant Energy System (CERES), produce data products intended to be shared with the larger scientific community and merged with other complementary data sets. Meaningful fusion of complementary data requires a well-founded common statistical basis for cited precision and accuracy. A high-level numerical model is available capable of predicting the dynamic opto-electrothermal behavior of CERES-like radiometric channels. The paper reports use of this model to explore the sensitivity of data products to variations in individual optical, thermal and electronic parameters. The optical/thermal radiative part of the model is based on the Monte-Carlo Ray-Trace (MCRT) method in which millions of rays are traced. Several hours of execution time on a large computer are required to simulate a single scan across the Earth's surface, thus making it impractical to run the simulation for every possible variation of each parameter. A key element of the research involves an effort to determine the minimum number of simulations required to produce statistically meaningful results.

SINOPSIS

Las observaciones provistas por el Sistema de Nube y Energía Radiante de la Tierra (Clouds and the Earth's Radiant Energy System, CERES) de la Administración Nacional de Aeronáutica y del Espacio (National Aeronautics and Space Administration, NASA) proporciona datos que tienen que ser completados y compartidos por la comunidad científica. Para obtener la precisión y

exactitud requerida en la fusión de los datos, es necesario contar con una base estadística bien fundamentada. Existe un modelo numérico de alto nivel para predecir el comportamiento opto-electrotérmico dinámico de los canales radiométricos de CERES. Este trabajo utiliza dicho modelo para investigar la variación en la sensibilidad de los parámetros ópticos, electrónicos y térmicos. La parte de radiación óptica-térmica del modelo es basada en el método de rastreo de rayos de Monte Carlo (Monte Carlo Ray Trace, MCRT), en el cual millones de rayos son rastreados por superficie. La simulación de una simple observación sobre la superficie terrestre tomaría varias horas de ejecución del programa en una computadora de gran capacidad de procesamiento de datos, lo que hace impráctico la simulación para todas las posibles variaciones de cada parámetro. El objetivo principal de esta investigación es el determinar el número mínimo de simulaciones requeridas para producir resultados estadísticamente significativos.

I- INTRODUCTION

This paper describes an effort to combine standard statistical methods with simulation using a high-level numerical model to predict uncertainty intervals in the data product of space-based observations of atmospheric energetics. The method proposed is initially applied to the numerical model for a thermopile linear-array thermal radiation detector intended for geostationary earth radiation budget applications. Since the optical/thermal radiative part of the model is based on the Monte-Carlo Ray-Trace (MCRT) method, the first part of the paper is focused on a probabilistic analysis of the MCRT method and the

underlying random number generator. Next, a study is described to determine the minimum number of simulations required to obtain results to a stated confidence interval. Finally, a study of auto-regression methods to perform level-one data retrieval from instruments such as those carried on NASA's Clouds and the Earth's Radiant Energy System (CERES) are reported. Auto-correlation or auto-regression coefficients may be retrieved during dynamic on-board calibration of spaceborne radiometers and then used to invert instrument count time series to obtain the corresponding radiance time series. This would allow radiances to be down-linked directly, thereby greatly reducing data management costs.

II- THERMOPILE LINEAR-ARRAY THERMAL RADIATION DETECTOR

A new detector concept, originally conceived for use on the Geostationary Earth Radiation Budget (GERB) experiment, has been proposed for earth radiation budget radiometry applications [1, 2, 3]. The detector consists of a linear array of single-junction-pair thermocouples mounted in one wall of a mirrored, wedge-shaped cavity, as shown in Figure 1. Each of the 256 pixels of the linear-array detector consists of the darkened active junction of

a two-junction thermopile. The incident collimated radiation enters the cavity through the 60- μm wide slit at the top and strikes the blackened active junction of the thermopile.

III- PROBABILISTIC CHARACTERIZATION OF THE MONTE-CARLO RAY TRACE METHOD

The Monte-Carlo ray-trace (MCRT) method has been used for decades in the development of thermal radiative models to predict the opto-electrothermal behavior of radiometric channels [4]. In this approach the radiation energy emitted from a given surface i is divided into a large number N_i of discrete and uniform energy bundles. The MCRT technique consists of tracing the history of these bundles from their emission to their absorption. Using the properties of the enclosure and the laws of probability, it is possible to determine the number of energy bundles N_{ij} emitted by surface i and absorbed by surface j . Then the distribution factors may be estimated as

$$D_{ij} \cong \frac{N_{ij}}{N_i} \quad (1)$$

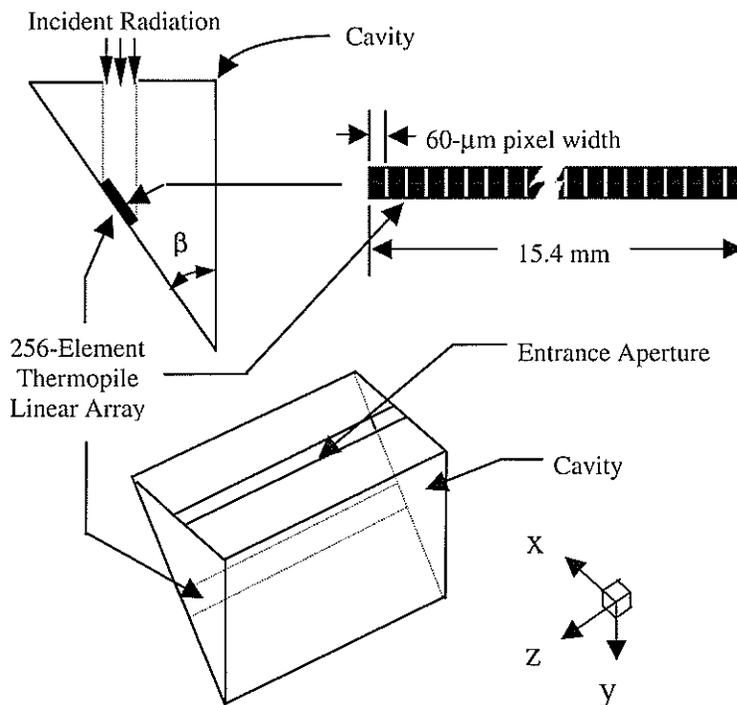


Figure 1: Thermopile linear-array thermal radiation detector

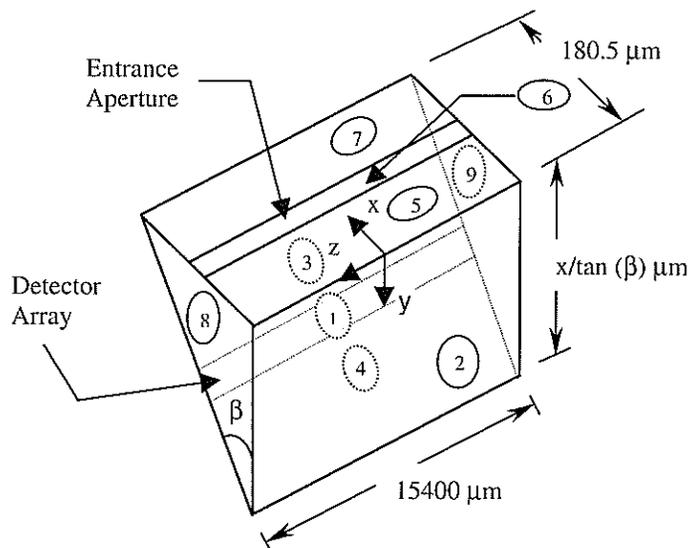


Figure 2: Division of the detector cavity in surfaces

and the contribution of radiation heat transfer to surface element j due to emission from surface element i at temperature T_i is

$$Q_{ij} = \epsilon_i A_i \sigma T_i^4 D_{ij} \quad (2)$$

In Equation 2, ϵ_i is the emissivity of surface element i and A_i is its surface area.

As an illustrative example the MCRT method is used here to compose an optical model of the detector and the cavity of an instrument originally conceived for geostationary earth radiation budget applications [1, 2, 3]. The cavity consists of nine plane surfaces, as shown in Figure 2. The numerical model has been implemented as a FORTRAN program that permits calculations of optical cross-talk among pixels as well as all the radiation distribution factors among surfaces [3]. The model simulates a collimated beam that enters through the aperture. The beam's energy is traced throughout the cavity until it is completely absorbed by the surfaces or escapes through the aperture.

The accuracy of any MCRT simulation depends on the quality of the random number generator used. Typically a pseudorandom number generator is used in which deterministic formulas produce sequences of numbers whose statistical properties approach those of true random number sequences. In the case at hand a double-precision FORTRAN version of a multiplicative linear congruent generator algorithm, RANMAR [5], has been adapted for use in the mathematical model of the linear-array detector shown in Figures 1 and 2. Although this random number generator has been used in other applications for many years, its

statistical properties have not been reported in the open literature.

This model is presented here as an illustrative example. The principles developed would be applicable to a wide range of MCRT-based radiometric channel models.

A- QUALITY OF RANMAR

1- Uniformity of distribution

The sequence of numbers generated should be uniformly distributed. Uniformity of distribution of a sequence of pseudorandom numbers was tested using the standard goodness-of-fit χ^2 -test from statistics. This test compares the observed and the expected frequencies of the pseudorandom numbers in the sequence. If the observed frequencies agree with corresponding expected frequencies, the value of χ^2 will be small, indicating a good fit. However, if the observed frequencies differ considerably from the expected frequencies, the value will be large, indicating a poor fit. In the current study a sequence of pseudorandom numbers of length of 1000 was sorted according to the range into which its individual members fell. The 1000 numbers were sorted into 20 bins and the count of numbers in each bin was obtained. Of course, the expected count for each bin is $1000/20 = 50$. The χ^2 statistic was computed using

$$\chi^2 = \sum_{i=1}^{20} \frac{(O_i - E_i)^2}{E_i} \quad (3)$$

where O_i is observed count in bin i and E_i is expected count in bin i .

Because a highly uniform distribution was expected, the value of χ^2 should correspond to the “very good fit” range when interpreting the value of χ^2 obtained. In the case at hand, with a degree of freedom of 19 (degree of freedom = number of observations – number of conditions imposed to the distribution), at a significance level of 0.05 a value of χ^2 less than 31.144 is expected. The value computed in the test is 13.04. Therefore it may be concluded that the distribution is uniform to a 5-percent significance level.

RANMAR was also compared with three other pseudorandom number generators available in the literature [6]: RAN0, RAN1, and RAN2. These produce χ^2 values of, respectively, 29.92, 28.48, and 18.08. While all three produce uniformly distributed random number sequences with a 5-percent significance level, RANMAR produces the most uniform sequences.

2- Randomness

The second property of interest is randomness of the sequence of random numbers. By randomness it is meant that a procedure cannot be devised to predict the next number in the sequence based on knowledge of the preceding numbers. In

other words, the correlation between each number in the sequence and the numbers that precede it should be low. Arguably the most general prediction of future values of an equally spaced time series based on past values is obtained using an auto-regression model [7]. For any uniformly spaced sequence x_1, x_2, x_3, \dots , it is possible to find an auto-regression model of order n such that

$$x_i = b_1 x_{i-1} + b_2 x_{i-2} + b_3 x_{i-3} + \dots + b_n x_{i-n} + \varepsilon_n \quad (4)$$

where ε_n is the unknown error in the model. If a given member of the sequence is correlated with immediately anterior members, i.e. if a deterministic relationship exists among members of the sequence, the error can usually be minimized to an acceptable value, on the order of a few percent, with judicious choice of order n and the length of the sequence used to define the n^{th} -order model. In the current study, a sequence of 15 random numbers was used to define a fifth-order auto-regression formula to predict the next (sixteenth) number in the sequence. Equation 4 with $n = 5$ was used to compute a “predicted” sequence of random numbers, and this sequence was then compared with the actual sequence of random numbers. The χ^2 statistic was then used to test the deviation of the predicted sequence of random numbers (observed, O_i) from the actual sequence (expected, E_i) using

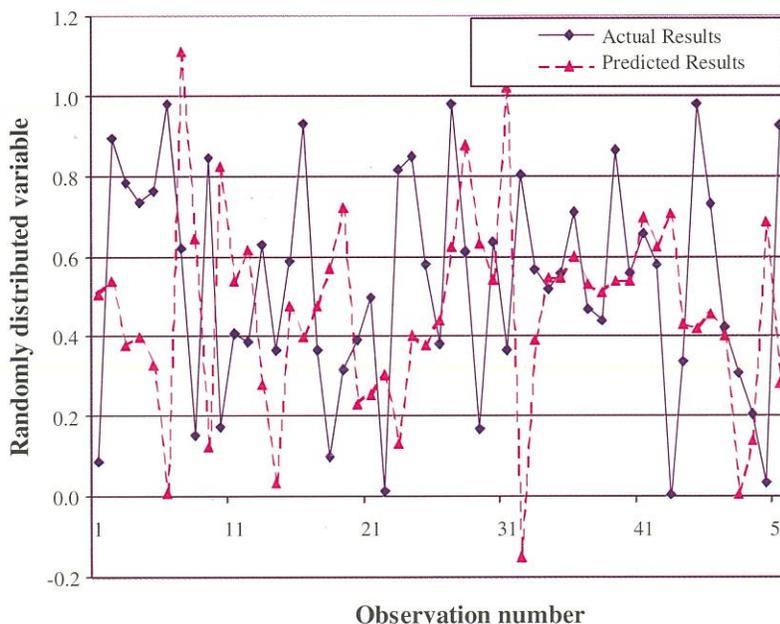


Figure 3: Actual random numbers generated by RANMAR and corresponding values predicted using an auto-regression model

Equation 3. A very large value of χ^2 (=494,243) was obtained, indicating a random relationship between the predicted and actual random number sequence. This may be taken as strong evidence that the original sequence is random.

In addition to the χ^2 test described above, deviation of the predicted sequence from the actual sequence was tested for normality using the Ryan-Joiner test [8]. In this test a very high correlation (R-value) is consistent with normality. Usually, for a confidence interval of 95 percent, the hypothesis of normality is accepted if the R-value exceeds than 0.9835. Figure 3 shows values of the actual random numbers obtained using RANMAR and the corresponding values predicted using the auto-regression model. If the pseudorandom number sequence is truly random, then the auto-regression model should fail to predict the next member of the sequence. Further, this failure should itself be random.

Figure 4 is a plot of the logarithm of the cumulative distribution function of the difference between actual and predicted members of the pseudorandom number sequence. If this difference is random, then the logarithm of the cumulative distribution function should be a linear function of the difference. Figure 4 demonstrates that, in the case at hand, a linear regression fits the data with an R-value of 0.9988. We conclude that the difference between the actual (pseudo) random number sequence and the corresponding sequence predicted using the auto-regression model is random. In summary, we have shown that the χ^2 statistic is very large, indicating very low correlation between the actual and predicted random number sequences,

and that the differences themselves are randomly distributed. These are the necessary and sufficient conditions to conclude that the original (pseudo) random number sequence is indeed random.

3- Number of rays necessary for statistically meaningful results

Several simulations of the behavior of the cavity were run in which the number of rays traced was studied as a parameter. In these experiments the radiative properties of the walls of the cavity are maintained at a constant value ($\alpha = \epsilon = 0.5$, $\rho^s/\rho = 0.9$). The entrance aperture (surface 6 in Figure 2) is modeled as a membrane that emits collimated radiation into the cavity toward the sloped wall where the detector is mounted. For each experiment the distribution factor D_{62} between the aperture and surface 2 is computed each time changing the seeds used to initiate of the random number sequence. An experiment consists of one run of the program for a given set of instrument parameters and specified seeds to initiate the random number sequence. For every combination of number of rays and number of experiments, the results were tested for normality using the Ryan-Joiner test in which a very high correlation (R-value) is consistent with normality. For a 95-percent confidence interval the hypothesis of normality is accepted if the R-value exceeds 0.9835. Table 1 gives the values of R for different combinations of number of rays traced and number of experiments. Table 1 shows that for a given number of rays traced (10,000), the distribution of the values of D_{62} obtained becomes more normal as

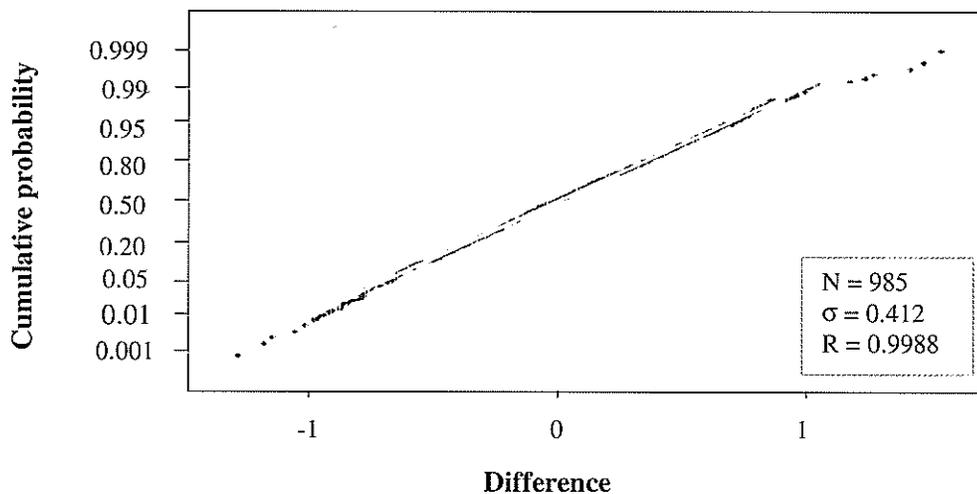


Figure 4: Test for normality of the difference between the actual and predicted sequences of random numbers

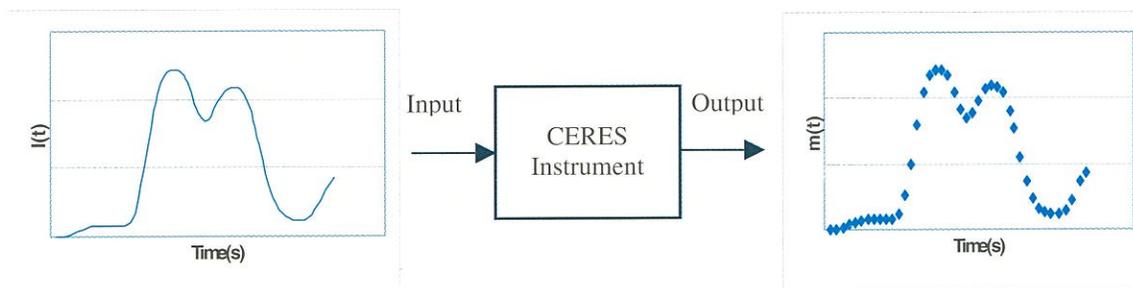


Figure 5: CERES instrument operation (actual instrument and model)

the number of experiments run increases. This is the expected result. We note further that even for this relatively low number of rays traced, the distribution of values of D_{62} is acceptably normal ($R > 0.9835$) even when only ten experiments are run. On the other hand the degree of normality is insensitive to the number of rays traced for a given number of experiments (100). Table 1 seems to suggest that it is more effective to repeat a simulation n times with a relatively low number of rays traced in each simulation, and then to use the mean value of the result obtained for the n simulations, than to run a single simulation with a large number of rays traced.

Table 2 gives several statistics pertaining to the estimation of D_{62} . The first three columns contain, respectively, the number of rays traced per experiment, the number of experiments run, and the product of these two quantities (i.e. the total number of rays traced in all of the experiments).

Column four contains the mean value of the distribution factor, $\langle D_{62} \rangle$, obtained for the number of experiments given in the first column, and column five contains the corresponding standard deviations. Finally, column six contains the range of values of D_{62} into which the actual value would be expected to fall with 95-percent confidence.

The 95-percent confidence interval was computed in three steps. First, the value of D_{62} was computed for a single experiment using the MCRT method with the indicated number of rays traced. Then the mean value of D_{62} , $\langle D_{62} \rangle$, and its standard deviation σ_{62} were computed for the indicated number of MCRT experiments. Finally, the 95-percent confidence interval was computed as

$$\langle D_{62} \rangle - D_{62} = \pm \frac{t s}{\sqrt{n}} \quad (5)$$

where $t = 1.960$ is the value of the Student's t statistic corresponding to a large number of degrees of freedom for a 95-percent confidence interval, s is

Table 1: Values of R in the Ryan-Joiner test for D_{62}

Number of Experiments	Number of Rays					
	10	100	1,000	10,000	100,000	1,000,000
10				0.9664		
100	0.9966	0.9980	0.9945	0.9908	0.9962	0.9969
1000				0.9995		

Table 2: Standard deviation and confidence intervals for D_{62}

Number of Rays	Number of Experiments	Rays per Experiment	$\langle D_{62} \rangle$	σ_{62}	95-% Confidence interval
10	100	1000	0.242	0.131947	0.242 ± 0.051723 ($\pm 21.37\%$)
100	100	10000	0.2558	0.042928	0.2558 ± 0.016828 ($\pm 6.58\%$)
1000	100	100000	0.26508	0.013106	0.26508 ± 0.005138 ($\pm 1.938\%$)
10000	10	100000	0.26476	0.002505	0.26476 ± 0.003105 ($\pm 1.172\%$)
10000	100	1000000	0.26391	0.004552	0.26391 ± 0.001784 ($\pm 0.676\%$)
100000	100	10000000	0.26397	0.001553	0.26397 ± 0.000609 ($\pm 0.23\%$)
10000	1000	10000000	0.26411	0.004547	0.26411 ± 0.000564 ($\pm 0.213\%$)
1000000	100	100000000	0.26407	0.000429	0.26407 ± 0.000168 ($\pm 0.036\%$)

the estimate of the standard deviation (σ_{62} in this case), and n is the number of experiments.

The results in Table 2 show that the 95-percent confidence interval narrows as the total number of rays traced (column 3) increases. When the product of number of rays traced and number of experiments run reaches one million, the uncertainty in the result obtained for the radiation distribution factor is less than one percent. It is also noted that, for sufficiently large numbers of total rays traced, slightly better performance is obtained when the number of experiments is increased while holding the total number of rays traced constant (second and third rows from the bottom). The opposite seems to be true for smaller numbers of total rays traced (fourth and fifth rows of the table).

Finally, it should be pointed out that when only one experiment is run with m rays traced, the 95-percent confidence interval is computed treating the radiation distribution factor as a proportion rather than as a mean. In this case,

$$\{D_{62}\} - D_{62} = \pm W_c \sqrt{\frac{\{D_{62}\}(1 - \{D_{62}\})}{m}} \quad (6)$$

where $\{D_{62}\}$ is the estimate of the actual value of the radiation distribution factor D_{62} and W_c plays the same role as the Student t statistic in Equation 5 and also has a value of 1.960. If only one experiment is run with a given number of rays traced, the 95-percent confidence interval obtained using Equation 6 is roughly the same as the 95-

percent confidence interval obtained using Equation 5 when multiple experiments are run with the same total number of rays traced (number of rays per experiment times number of experiments).

We conclude from Table 2 that no significant statistical advantage is obtained by running a large number of experiments with the same total number of rays traced as in a single experiment. However, other advantages may be obtained using a relatively large number of experiments with a relatively small number of rays traced per experiment. For example, the experiments could be distributed over a number of processors, thereby saving wall-clock time for the overall simulation. Other ideas are currently under study.

IV- MODEL-BASED USE OF AUTOCORRELATION ALGORITHMS FOR DYNAMIC RETRIEVAL OF SPACEBORNE RADIOMETRIC DATA

A- CERES INSTRUMENT

The CERES instrument consists of three scanning thermistor bolometer radiometers, an elevation axis drive system, an azimuth axis drive system and associated electronics. The shortwave channel measures the earth-reflected solar radiance in the 0.3-to-5 μm spectral region. The longwave channel measures the earth-emitted solar radiance in the 8-to-12 μm spectral region. The total channel is unfiltered and thus responds to both earth-reflected solar and earth-emitted radiance in

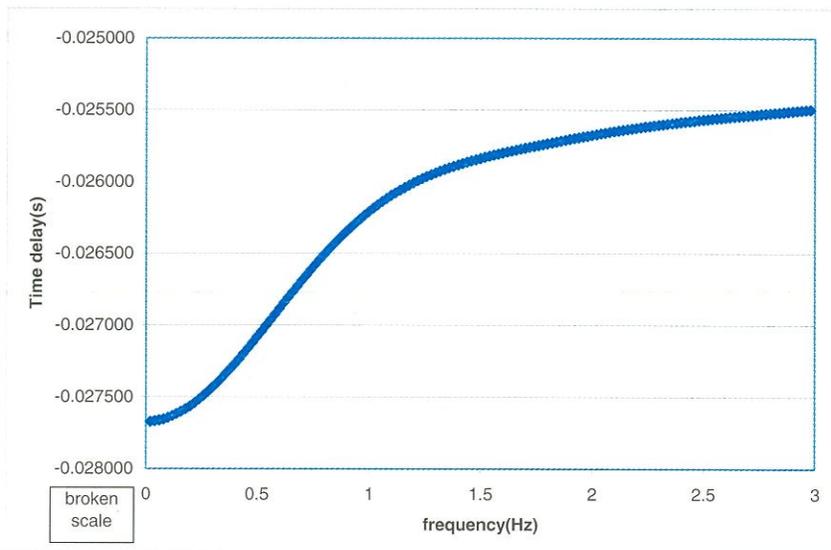


Figure 6: Model-predicted CERES total channel time delay versus frequency

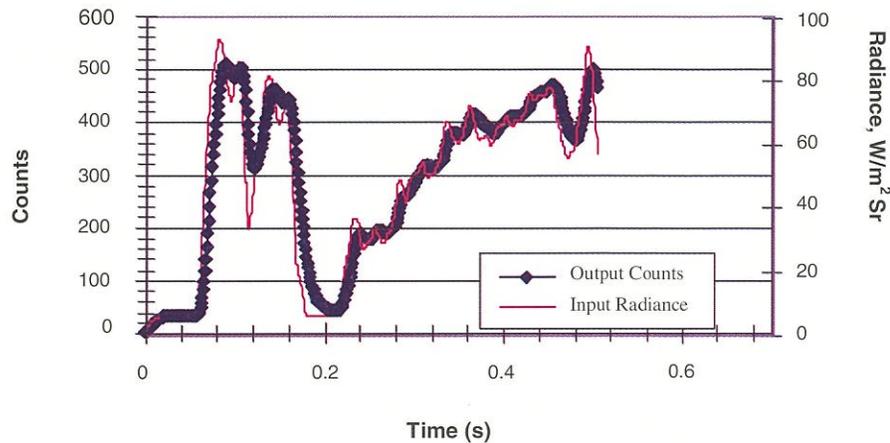


Figure 7: Input radiance and output count time series

the 0.3-to-100 μm spectral region. Each radiometric channel consists of a baffle, Cassegrain optics, and a thermistor bolometer detector module consisting of active and references sensors.

The CERES instrument scans the earth using biaxial and cross-track scan modes. For the cross-track mode, the azimuth axis is fixed and the sensor scans about the elevation plane perpendicular to the orbital direction. The biaxial scan mode is an operational mode in which the azimuth axis rotates at a constant rate of 6 deg/s in one direction for 30 s and then rotates in the opposite direction at 6 deg/s for 30 s. All zenith scan cycles last 6.6 s and includes an internal calibration and spaces views. The data sample rate is 100 Hz.

Conditioning of the electronic signals is a requirement of typical remote sensing instruments because of the need to amplify, filter and sample the signal. A low noise pre-amplifier is used to

amplify the signal. A Bessel low-pass filter downstream of the pre-amplifier avoids aliasing error and assures a relatively constant time shift between the input and output for all frequency components of interest.

B- HIGH-LEVEL DYNAMIC OPTO-ELECTROTHERMAL RADIOMETRIC MODEL

Haefflin et al. [3] and Priestley et al. [9, 10] completed the high-level dynamic opto-electrothermal model for the CERES radiometer in 1997. This radiometric model is used to study data retrieval methods. It was developed based on a combination of the Monte-Carlo ray-trace method (MCRT) and finite-difference and finite-element methods. The model is capable of simulating the end-to-end response of the CERES instrument to simulated earth scenes. On the basis of simulated

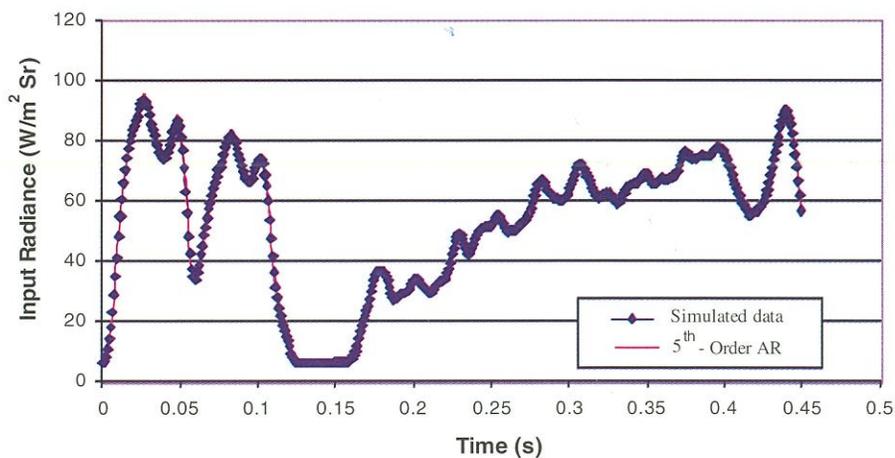


Figure 8: Input radiance recovered using Equation 7

input radiance $I(t)$, the model produces a sampled output discrete time series in proportional counts $m(i)$ at 0.01-s time intervals. The relationships among the input radiance signal, the instrument (both actual and simulated), and the output count time series are indicated schematically in Figure 5.

Priestley et al. [9, 10] combined the optical, thermal and electrical models developed by previous investigators to create a Practical Numerical Model (PNM) of the CERES protoflight total channel. Validation and certification of the model was accomplished by simulating the ground calibration process of the actual instrument. High-confidence prediction ability was demonstrated.

A simulated output count time series can be obtained based on a simulated radiance input time series $I'(t)$ incident to the Practical Numerical Model. The counts are proportional to the output voltage of the instrument. It is important that the simulated data obtained by the PNM represent accurately that of the real instrument. This was established by Priestley [9, 10].

A Bessel low-pass filter is used after the pre-amplifier to maintain time-delay independence of frequency. A random noise input was used to obtain the spectral response of the instrument model (and thus of the instrument itself) for all frequencies. The resulting data set consists of 25 blocks of 51,200 points, each sampled at 1-ms intervals. This corresponds to a resolution for 0.02 Hz. A Fourier transform and frequency response function approach was used to obtain the time delay as a function of frequency. Results are shown Figure 6. Based on this test, it may be concluded that the Bessel filter maintains the time delay essentially constant in narrow range between 25.5 and 27.5 ms.

C- PROPOSED METHOD TO PERFORM LEVEL-ONE DATA ANALYSIS

The first step in data analysis involves converting the instrument counts to radiance at the instrument entrance aperture (before filtering). This is currently done using a count-conversion scheme based on time shifting and multiplying the result by a calibration constant. An alternative approach is considered here.

The simulated output data obtained from the PNM depends on time; therefore, it is hypothesized that an auto-regression model can be used to predict the next value of this time series based on previous values in the sequence. An auto-regression model of order n has been described in Section 3.1 (Equation 4). The coefficients b_i , $i = 1, 2, \dots, n$, are calculated based on N observations. The Akaike information Criterion (AIC) [11] criterion is used to estimate the order n of the auto-regression..

The auto-regression model is studied using the order as a parameter to determine the most accurate model. Generally the matrix of coefficients of the system produced by auto-regression is not square. In this case the transpose and the inverse matrices are employed to solve the system [11]. Auto-regression representations of the input radiance and the output counts are given by

$$I_i = c_1 I_{i-1} + c_2 I_{i-2} + c_3 I_{i-3} + \dots + c_n I_{i-n} + \varepsilon_{n,i} \quad (7)$$

and

$$m_i = d_1 m_{i-1} + d_2 m_{i-2} + d_3 m_{i-3} + \dots + d_n m_{i-n} + \varepsilon_{n,m} \quad (8)$$

Villeneuve [12] has created a realistic cloudy earth scene simulation that was used as the input

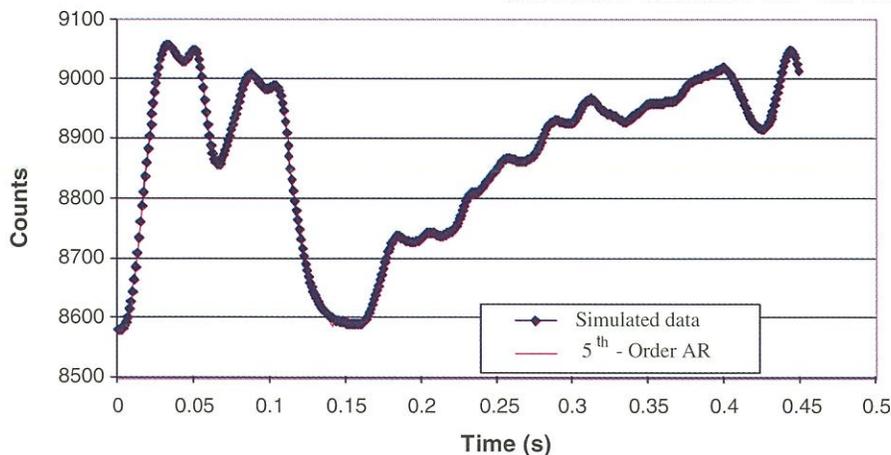


Figure 9: Output count recovered using Equation 9

radiance time series in the PNM to produce the simulated count time series data shown Figure 7.

Auto-regression models were created using the ten previous values in the time series, that is $N = 10$. The five coefficients b_i , $i = 1, 2, \dots, 5$, that result are then used to predict the next value based on the five previous observations. Results for the input radiance and corresponding output count time series are shown in Figures 8 and 9. From these results it is evident that the auto-regression model is capable of accurately predicting the evolution of these time series based on previous observations.

The next logical step would be to find the relationship between the coefficients c_i and d_i that permit the count time series to be used to predict the corresponding radiance time series. The result sought would be an auto-regression model of the form:

$$I_i = a_0 m_i + a_1 m_{i-1} + a_2 m_{i-2} + a_3 m_{i-3} + \dots + a_n m_{i-n} + \epsilon_n \quad (9)$$

where the coefficients a_i account for both the dynamic response of the instrument and the dynamic nature of the radiance field. Work in progress involves using the CERES Practical Numerical Model to determine the relationships among the various auto-regression coefficients that would allow the instrument dynamics to be separated from those of the radiance field.

V- CONCLUSIONS

An essential step in the process of predicting uncertainty and confidence intervals in radiometric models is establishment of the quality of the random number generator used in the underlying Monte-Carlo ray-trace method. This paper establishes that the random number generator used in the current model of the CERES Practical Numerical Model meets very high standards of randomness and uniformity of distribution. It is also established through study of another radiometric model that, to a 95-percent level of confidence, such MCRT-based models are capable of providing better than one-percent simulation accuracy when at least one million rays are traced per surface. Finally, model-based studies using the auto-regression method show promise of providing an alternative approach to level-one radiometric data analysis.

VI- ACKNOWLEDGMENTS

The authors are indebted to NASA's Langley Research Center for its partial support of this effort under Grant NAG-1-2128. A debt of gratitude is

also owed to Ondrej Lanik for his contributions to this effort.

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