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ACCURACY CONTROL IN MONTECARLO RADIATIVE CALCULATIONS

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SUMMARY

This paper presents the general accuracy law that rules the MonteCarlo, ray-tracing algorithms used commonly for the calculation of the radiative entities in the thermal analysis of spacecraft. These entities involve transfer of radiative energy either from a single source to a target (e.g., the configuration factors), or from several sources to a target (e.g., the absorbed heat fluxes). In fact, the former is just a particular case of the latter. The accuracy model is later applied to the calculation of some specific radiative entities. Furthermore, some issues related to the implementation of such a model in a software tool are discussed. Although only the relative error is considered through the discussion, similar results can be derived for the absolute error.

INTRODUCTION

Monte Carlo methods are often used in combination with ray-tracing algorithms to perform the radiative analysis of spacecraft (ref. [1]). Using this approach (MCRT from now on), the radiative couplings between the faces of a model, as well as the external heat loads applied on these faces, are calculated. Normally, these radiative values are passed to a thermal solver in order to produce the temperature predictions for the spacecraft model.

While MCRT-based tools present some interesting advantages with respect to other methods, they also show a major drawback, which is the often large computational effort required to produce the radiative values. The results of a MCRT simulation are taken as an estimation of the actual values of the radiative entities. Since these results are of random nature, the accuracy of the estimation depends on the number of rays fired in the simulation. In general, the thermal engineer performs a trade off between the accuracy of the results and the computational effort required to achieve them. This paper presents models which allow the automatic accuracy control of the results in an efficient way.

It is important to point out that the simulation inaccuracies only account for a part of the uncertainty in the results of the thermal analysis. Other sources of error are the validity of the modelling assumptions and the uncertainty of the data used in these models (ref. [2]). The "engineering judgement" shall be used to decide which level of accuracy in the simulation is sensibly required, especially when compared to the uncertainties in the other areas. Once the simulation's accuracy requirements have been established, their efficient achievement can be guaranteed by the techniques presented in this paper.

BASIC ACCURACY MODEL

MCRT methods are based on the repetition of a given random process, which reproduces the physical problem of interest (ref. [3]). For each trial, values of the random parameters that play a role in the process are uniformly sampled from their cumulative distribution functions, and a score T , representative of the physical phenomenon, is tallied. T is a random variable that follows an arbitrary distribution:

$$T \sim (E(T), V(T)) \quad (\text{EQ 1})$$

where $E(T)$ is the expectation of T and $V(T)$ the variance of T . The estimation r^* of the radiative parameter R is then calculated by averaging the scores over a large number of trials:

$$r^* = \frac{1}{N} \cdot \sum_{i=1}^N t_i \quad (\text{EQ 2})$$

where t_i is the score for the i -th trial and N is the total number of trials. In the MCRT simulations, each trial involves firing a ray from the source. Because of the random nature of the process, every simulation produces a different estimated value, and therefore the estimation R^* is a random variable itself. By the central limit theorem (ref. [4]), given N reasonably large, R^* is normally distributed, regardless of the actual shape of the distribution for the basic random variable T .

$$R^* \sim N(E(R^*), V(R^*)) \quad (\text{EQ 3})$$

where:

$$E(R^*) \equiv \mu_{R^*} = E(T) = R \quad (\text{EQ 4})$$

$$V(R^*) \equiv \sigma_{R^*}^2 = \frac{V(T)}{N} \quad (\text{EQ 5})$$

By definition, the relative error of an estimated value r^* is:

$$e \equiv \frac{r^* - R}{R} \quad (\text{EQ 6})$$

By applying the algebra of random variables, it is possible to show that the relative error of the estimated values is also normally distributed:

$$E - N(E(E), V(E)) \quad (\text{EQ 7})$$

with expectation and variance given by:

$$E(E) \equiv \mu_E = 0 \quad (\text{EQ 8})$$

$$V(E) \equiv \sigma_E^2 = \frac{V(R^*)}{R^2} = \frac{V(T)}{N \cdot R^2} \quad (\text{EQ 9})$$

Given the normal law followed by the simulation error, the probability α of having a relative error smaller than ε is:

$$\alpha \equiv \text{Prob}(e < \varepsilon) = \text{erf}\left(\frac{\varepsilon}{\sqrt{2 \cdot \sigma_E^2}}\right) \quad (\text{EQ 10})$$

and replacing (eq 9) into (eq 10) the fundamental accuracy model is derived:

$$N_\varepsilon = 2 \cdot \left(\frac{\text{erf}^{-1}(\alpha)}{\varepsilon}\right)^2 \cdot \frac{V(T)}{R^2} \quad (\text{EQ 11})$$

This expression is very important for our purposes, because it provides a relationship between the accuracy ε to be achieved and the computational effort (number of rays N_ε) required for it, in terms of the radiative value itself, the variance of the basic random process used in the MCRT simulation and the confidence level α . Furthermore, (eq 11) shows that the accuracy achieved is inversely proportional to the square root of the number of rays fired in the simulation (i. e., to halve the relative error the number of rays has to be multiplied by four).

For a given confidence level α , if N_ε rays are fired to ensure a level of accuracy of ε , the variance of the relative error depends only on ε :

$$V(E_\varepsilon) = \frac{1}{2} \cdot \left(\frac{\varepsilon}{\text{erf}^{-1}(\alpha)}\right)^2 \quad (\text{EQ 12})$$

That is, the variance of the relative error is directly proportional to the square of the level of accuracy specified. Once the accuracy requirements are fixed, the variance of the errors associated to the estimation of different values do not depend on the actual values or on the variance of the basic random processes. This is an interesting property which is used later in the paper to introduce an efficient way to calculate reciprocal couplings.

ACCURACY CONTROL FOR RADIATIVE PARAMETERS

Configuration Factors

The configuration (or view) factors represent the fraction of diffuse energy uniformly emitted by a radiative face and reaching directly (i. e., without suffering any intermediate reflection) a target face. The procedure followed in the MCRT approach to determine the configuration factors is based on the repetition of a process consisting of the following steps:

- calculate a random emission point on the emitting radiative face
- calculate a random emission direction
- calculate the intersection between the ray fired from the emission point and directed along the emission direction, and the target radiative face
- tally the ray if the intersection is not void

Finally, the estimated value f^* is calculated as the average of all the trials performed:

$$f^* = \frac{1}{N} \cdot \sum_{i=1}^N t_i \quad (\text{EQ 13})$$

Thus, this algorithm tallies the random variable T , which in this case represents the intersection between a randomly emitted ray and the target radiative face. T is a discrete random variable, which only can take two possible values: 0 if the intersection is void and 1 if the ray strikes the target radiative face. Since this is a rather simple process, the distribution function of the random variable T can be determined by only knowing the value of the configuration factor F , as shown in Figure 1.

The expectation and variance of T can be calculated by applying the expressions used for discrete random variables:

$$E(T) = \sum_{k=1}^s t_k \cdot P(t_k) \quad (\text{EQ 14})$$

$$V(T) = \sum_{k=1}^s (t_k - E(T))^2 \cdot P(t_k) \quad (\text{EQ 15})$$

where s is the number of discrete values which the random variable can take. Applying these expressions to T , with $s = 2$ corresponding to the only two possible values 0 and 1, we obtain:

$$E(T) = F \quad (\text{EQ 16})$$

$$V(T) = F \cdot (1 - F) \quad (\text{EQ 17})$$

where F is the actual value of the configuration factor.

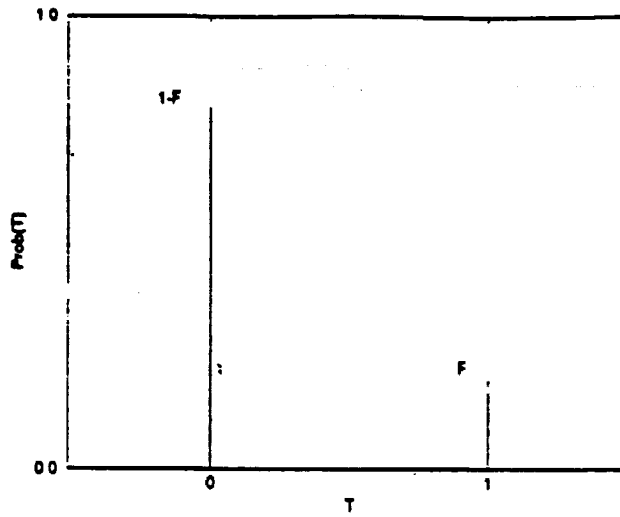


FIGURE 1. Probability distribution function for the random variable T, intersection ray/target face

Introducing these values into the general accuracy model given by (eq 11), the accuracy control law for the configuration factors can be derived:

$$N_{\epsilon} = 2 \cdot \left(\frac{\text{erf}^{-1}(\alpha)}{\epsilon} \right)^2 \cdot \frac{1-F}{F} \quad (\text{EQ 18})$$

From this expression it can be appreciated that, in agreement with the experience, bounding the accuracy for small configuration factors is much more computationally demanding than doing so for large values.

Due to the fact that the variance of the basic random process depends exclusively on the value of the configuration factor, once this value F is fixed it is possible to specify the number of rays to be fired in order to achieve the desired accuracy. Figure 2 shows the computational effort (i. e. number of rays fired from the radiative face) required to achieve three different accuracy levels (relative errors of 100%, 10% and 1%) for the whole range of configuration factor values.

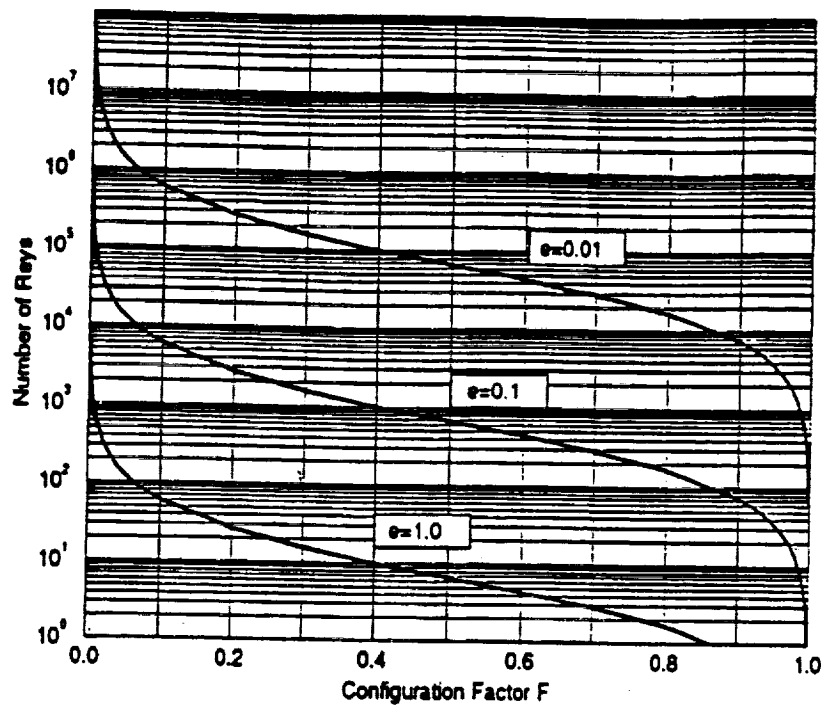


FIGURE 2. Computational effort vs configuration factor value for several levels of accuracy (confidence level of 99%)

Radiative exchange factors

The radiative exchange factors (REF) are defined as the fraction of diffuse energy uniformly emitted by a radiative face and being finally absorbed by a target face. Multi-reflection paths are included in this definition. These values can be derived from the configuration factors, following Gebhart's method (ref. [5]). Alternatively, the MCRT approach offers some advantages, taking into account the non-uniform nature of the radiative transfer exchange between radiative faces, as well as allowing the inclusion of specular behaviour. The procedure followed for each radiative face is in this case:

- calculate a random emission point on the emitting radiative face
- calculate a random emission direction
- propagate the ray fired from the emission point and directed along the emission direction through the model. For the propagation take into account the radiative behaviour of the surfaces
- tally the fraction of the original ray's energy which is finally absorbed by the target face (random variable T)

Following this algorithm, the estimation of the REF value G is calculated by the expression:

$$g^* = \frac{1}{N} \cdot \sum_{i=1}^N t_i \quad (\text{EQ 19})$$

The main difference with the configuration factors case is that it is not possible to know a priori the nature of the probability distribution function of the random variable T . Indeed, T can take different values depending on the path followed by the rays, and the number of possible paths grows significantly with the number of radiative faces in the model. Nevertheless, regardless of this fact the powerful central limit theorem is valid and (eq 11) still applies. Therefore, the accuracy control model for REF can be expressed as:

$$N_{\epsilon} = 2 \cdot \left(\frac{\text{erf}^{-1}(\alpha)}{\epsilon} \right)^2 \cdot \frac{V(T)}{G^2} \quad (\text{EQ 20})$$

Thus, in the REF case, the computational effort depends explicitly not only on the value of the REF but also on the variance of the basic random process.

Direct Solar Flux

The heat flux emitted by the Sun and being intercepted by a given target radiative face can be calculated as:

$$D = SC \cdot A^{\perp} \quad (\text{EQ 21})$$

where SC is the solar constant and A^{\perp} is the visible cross section area of the face.

The MCRT method can also be used to calculate an estimation of D . Once the solar constant and the solar aspect ratio are known, the problem is reduced to find the visible cross section area of the radiative face. Although for non-occluded planar faces this is a simple operation, a MCRT procedure can be followed whenever the faces are curved or shading effects exist:

- calculate a random emission point on the radiative face
- fire a ray from the emission point towards the sun
- find whether the emission point "sees" the Sun. A discrete random variable H , taking only two possible values (0 if the Sun is not visible and 1 if it is) shall be tallied for this purpose
- tally the $\cos \theta$ value (where θ is the angle between the Sun direction and the face's normal vector at the emission point), only if the emission point is not occluded by any other part of the model

An estimation of A^{\perp} is then calculated as:

$$a^{\perp} = \frac{1}{N} \cdot A \cdot \sum_{l=1}^N (\cos \Theta)_l \cdot h_l \quad (\text{EQ 22})$$

where A is the radiative node area, h_l is the value of the random variable H and $(\cos \Theta)_l$ is the value of the random variable $\cos \theta$. The subscript l refers to the l -th trial.

Applying the general accuracy model to this specific case, the following equation is obtained:

$$N_{\epsilon} = 2 \cdot \left(\frac{\text{erf}^{-1}(\alpha)}{\epsilon} \right)^2 \cdot (SC \cdot A)^2 \cdot \frac{V(\cos \Theta \cdot H)}{D^2} \quad (\text{EQ 23})$$

SOME IMPLEMENTATION ISSUES

Parameter pre-estimation

The application of the accuracy models to the estimation of radiative values presents the paradox of requiring as input the value whose calculation is the goal of the simulation. Furthermore, the variance of the basic random process used to calculate the estimation is not generally known a priori. These apparent drawbacks can be satisfactorily overcome by pre-estimating both the radiative value R and the variance of the basic process $V(T)$, so that the accuracy models can be applied. The pre-estimated values can be obtained after a first batch of M rays is fired in the simulation. Indeed:

$$R = \bar{i} = \sum_{i=1}^M \frac{t_i}{M} \quad (\text{EQ 24})$$

$$V(T) = S^2_T = \frac{1}{M-1} \cdot \sum_{i=1}^M (t_i - \bar{i})^2 \quad (\text{EQ 25})$$

The number of rays M to be fired in order to pre-estimate R and $V(T)$ shall be determined as a compromise between having reasonably accurate pre-estimations and not spending too much computational effort in this previous phase of the algorithm. In practice, it has been checked that even with sample sizes which are small when compared to N_{ϵ} , the accuracy control based on the accuracy model produces excellent results.

For instance, Figure 3 shows the histogram of the relative error associated to the estimation of a particular configuration factor, with a reference value of 0.01832. To produce the histogram, 1000 different simulations were performed, each of them using a pre-estimation sample size of 1000 rays. The accuracy model was then applied to ensure an accuracy of 3% with a level of confidence of 99%. The application of (eq 11) shows that these requirements are achieved by firing approximately 398000 rays in each simulation. The tails of the histogram, filled in black, show that only 10 out of the 1000 simulations performed had an error beyond the specified limits. This is in agreement with the confidence level used for this particular case.

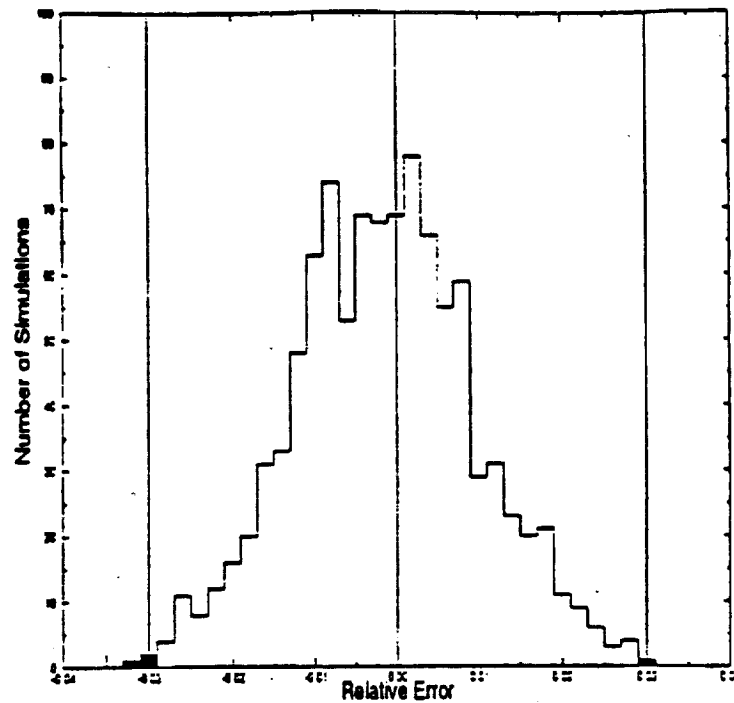


FIGURE 3. Histogram of the relative error associated to the estimation of a configuration factor with reference value 0.01832

A particular problem arising when introducing the pre-estimated values into (eq 11) is that this expression becomes singular for $\bar{i} = 0$. A null pre-estimated value can indicate either that:

- the actual radiative value is indeed null, in which case its actual variance will also be null, or that
- the actual radiative value is so small that the size of the sample it is not large enough to provide a non-null pre-estimated value.

In the first case, no additional rays need to be fired. In the second, a very large number of rays are likely to be needed. Practical considerations impose a limit to this number, which for very small couplings might become computationally prohibitive. Generally speaking, once this limit is imposed it will not be possible to guarantee the accuracy of the radiative values below a threshold value.

Enforcement of the reciprocity law

In general, and for efficiency reasons, the software tools that implement MCRT methods do not calculate the couplings individually. Indeed, the couplings from one face to all the other faces in the model are normally calculated in one pass. Due to this fact, the couplings' line sum adds up to 1. However, the reciprocity law between couplings is in principle not satisfied, because of the statistical inaccuracy associated to the estimations.

Often, the manipulation of couplings that satisfy the reciprocity law is preferred, especially because of the reduction in memory requirements. The enforcement of the reciprocity law brings about a

line sum which does not add up to 1. This imbalance is sometimes taken as a measure of the error in the estimation of the couplings. The enforcement of the couplings' reciprocity is normally performed after both couplings have been independently calculated. This is not very efficient, since computational time is wasted to guarantee the specified level of accuracy for both the direct and inverse couplings. Furthermore, a systematic error is introduced by the enforcement method.

On the other hand, the general error model shows that, given a reciprocal pair of faces, one of the associated couplings is privileged in the sense that identical accuracy levels can be achieved with a smaller number of rays. This fact suggests the idea of estimating the non-privileged coupling by simply applying the reciprocity law to the one calculated via MCRT from the privileged face. Of course, this operation shall ensure that both coupling's errors meet the specified accuracy requirements.

To apply this approach, the privileged face shall be identified. Therefore, the question to be answered is: given a reciprocal pair of couplings R_{ij} and R_{ji} such that:

$$R_{ij} = \Psi \cdot R_{ji} \quad (\text{EQ 26})$$

where Ψ is the reciprocity factor, and assuming that the accuracy requirements are respectively set to ϵ_{ij} and ϵ_{ji} , which face shall be used to fire rays from?

To identify the privileged face, let's assume that the MCRT simulation is performed by firing rays from face i. Therefore, the coupling R_{ij} is directly estimated via the simulation, while the coupling R_{ji} is estimated by enforcing the reciprocity law:

$$r'_{ij} = r^*_{ij} \quad (\text{EQ 27})$$

$$r'_{ji} = \frac{r^*_{ij}}{\Psi} \quad (\text{EQ 28})$$

The reciprocal values estimated in such a way follow normal distributions:

$$R'_{ij} - R^*_{ij} \quad (\text{EQ 29})$$

$$R'_{ji} - N(E(R'_{ji}), V(R'_{ji})) \quad (\text{EQ 30})$$

Furthermore, it can be shown that the variance of the relative error associated to the estimation of R_{ji} via (eq 28) is:

$$V(E'_{ji}) = V(E^*_{ij}) = \frac{V(T_{ij})}{N_{ij} \cdot R_{ij}^2} \quad (\text{EQ 31})$$

On the other hand, if the estimation of R_{ji} was calculated by the MCRT procedure, by firing from face j the number of rays needed to meet the accuracy target ϵ_{ji} , the variance of the relative error would be:

$$V(E_{\epsilon_j}) = \frac{1}{2} \cdot \left(\frac{\epsilon_{jj}}{\text{erf}^{-1}(\alpha)} \right)^2 \quad (\text{EQ 32})$$

Since the accuracy requirements must be also achieved by the enforced estimation R'_{jj} , the variance of its error must be equal to the variance of the error obtained in the MCRT procedure:

$$V(E'_{jj}) = V(E_{\epsilon_j}) \quad (\text{EQ 33})$$

From this equation, it can be proved that i is the privileged face if the following condition holds:

$$V(T_{ij}) \leq \Psi^2 \cdot V(T_{ji}) \quad (\text{EQ 34})$$

This expression relates the variance of the basic random processes used to estimate the couplings. If (eq 34) is applied to the configuration factors case, it can be seen that the privileged face is the one with larger associated coupling. In the REF case, the privileged face cannot be determined by simply looking at the relative size of the reciprocal couplings, and (eq 34) shall be used instead.

To clarify the interest of firing rays from the privileged face, let's present an example. For the model in Figure 4, reference values are available in the literature (ref. [6]). In particular, $F_{12} = 0.29176$. Assuming we are interested in the calculation of the view factors with an accuracy of 5%, the most efficient way to proceed is to fire rays from face 1, which is the privileged one. This can be seen by checking the condition given by (eq 34). If the accuracy law for view factors (eq 18) is applied, it can be seen that approximately 6500 rays are needed to guarantee the accuracy requirements for both reciprocal couplings. If the same accuracy level had to be achieved by firing rays from face 2, roughly 25000 rays would be needed.

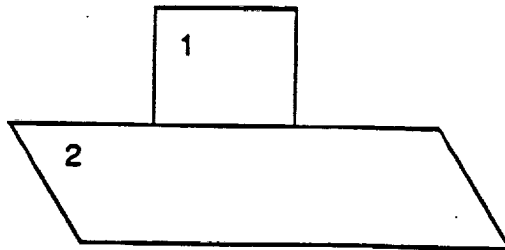


FIGURE 4. Model consisting of two perpendicular rectangular plates, with areas of 1 and 3 units respectively. The reciprocity factor between the configuration factors is in this case $\Psi = 3$.

ACCURACY CONTROL FOR ABSORBED HEAT FLUXES

The estimation of the absorbed heat flux on a radiative face differs of that of the simple radiative values presented above in that the absorbed value can be seen as the contribution of several source terms. Indeed, the heat flux striking the spacecraft follows different multi-reflection paths until it is finally absorbed by the face. Obviously, some multi-reflection paths will contribute more than others to the final absorbed flux. The purpose of this section is to apply the general accuracy model to this problem, taking into account the relevance of the mentioned radiative paths into the final value. The results that follow are applicable to either solar or planetary (infrared and albedo) absorbed heat fluxes.

A proper accuracy control for the absorbed heat flux is especially interesting when trying to quantify the absorbed heat flux on a spacecraft radiator. Because of the radiator's heat rejection requirements, the direct heat loads are generally small, and most of the absorbed flux reaches the radiator after several reflections.

As previously stated, the heat flux Φ absorbed by a given radiative face can be expressed as the addition of a number of contributing terms Φ_j :

$$\Phi = \sum_{j=1}^n \Phi_j \quad (\text{EQ 35})$$

where each Φ_j is the flux being absorbed by the target face, with origin in the reflection of direct heat flux in the source face j . The summation is therefore extended to the n faces in the model which have non-null direct heat flux.

The concept of source faces is clarified with the help of Figure 5. Assuming an idealised model consisting of 4 surfaces illuminated by the Sun, only faces 1 and 3 are source faces, as far as the calculation of the heat flux absorbed by face 4 is concerned. Face 2 does not see the Sun, and therefore it will not contribute with a source term in (eq 35).

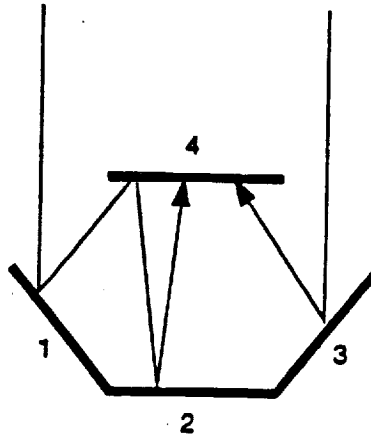


FIGURE 5. Source faces 1 and 3 contribute to the heat flux absorbed by face 4. In this case, face 2 only contributes through multi-reflections.

In the actual MCRT simulation, the Φ_j term is estimated by uniformly firing N_j rays from face j and averaging the random variable T_j , i. e. amount of the energy carried by the ray that is finally absorbed by the target face:

$$\phi_j^* = \frac{1}{N_j} \cdot \sum_{i=1}^{N_j} (t_j)_i \quad (\text{EQ 36})$$

The estimated value for the absorbed heat flux is therefore:

$$\phi^* = \sum_{j=1}^n \phi_j^* \quad (\text{EQ 37})$$

and follows a normal law:

$$\Phi^* \sim N(E(\Phi^*), V(\Phi^*)) \quad (\text{EQ 38})$$

The variance of the relative error associated to the estimation is:

$$V(E) = \frac{1}{\Phi^2} \cdot V(\Phi^*) = \frac{1}{\Phi^2} \cdot \sum_{j=1}^n \frac{V(T_j)}{N_j} \quad (\text{EQ 39})$$

This expression shows that the variance of the relative error, which is directly related to the accuracy achieved by the simulation, depends on several terms, one for each source face. The question here is, given a fixed amount N of rays to be fired:

$$N = \sum_{j=1}^n N_j \quad (\text{EQ 40})$$

how shall these N rays be distributed among the source faces so that (eq 39) is minimised? The solution to this problem can be found by applying standard techniques of non-linear programming. It can be shown that the optimal solution is given by:

$$N_j^o = \frac{\sqrt{V(T_j)}}{\sum_{k=1}^n \sqrt{V(T_k)}} \cdot N \quad (\text{EQ 41})$$

For this optimal distribution of the rays, the variance of the error becomes:

$$V(E) = \frac{1}{\Phi^2 \cdot N} \cdot \left(\sum_{j=1}^n \sqrt{V(T_j)} \right)^2 \quad (\text{EQ 42})$$

Replacing (eq 42) in the general error model, the accuracy control law for the estimation of the absorbed heat fluxes can be obtained:

$$N_\varepsilon = 2 \cdot \left(\frac{\text{erf}^{-1}(\alpha)}{\varepsilon} \right)^2 \cdot \frac{1}{\Phi^2} \cdot \left(\sum_{j=1}^n \sqrt{V(T_j)} \right)^2 \quad (\text{EQ 43})$$

This multi-source model is the most general expression of the accuracy law for MCRT calculations. In fact, the accuracy model previously obtained for the simple radiative entities is just a particular case of (eq 43), with $n = 1$. Indeed, one can regard the calculations of couplings as a mono-source phenomenon, being the unique source the radiative face emitting the radiation. Similarly, the Sun (or the planet) are the unique sources emitting radiation when the direct fluxes are calculated.

The considerations about the pre-estimation of the values are also relevant for the implementation of this accuracy model.

CONCLUSIONS

This paper has presented a model which can be used to control the accuracy of the radiative values estimated by using MCRT methods. The generality of the model allows its application to the radiative values relevant to the thermal analysis of spacecraft.

A prototyping activity has confirmed the validity of the assumptions used in the derivation of the accuracy models, as well as the feasibility of their implementation. The results obtained are in excellent agreement with the values predicted by the statistical models, even if pre-estimation of some parameters is required.

Full scale implementation of the error models is in progress, with the intention to enhance ESARAD, the radiative analysis software developed for the European Space Agency (ref. [7]). Significant improvements in terms of accuracy control, efficiency and performance are expected in relation to other radiative codes currently available in Europe.

NOMENCLATURE

The following conventions have been followed in naming the random variables:

- Star indicates estimation of a radiative entity. For example, F^* represents the random variable "estimation of the view factor F ".
- Upper case is reserved to denote the distribution of the random variable, while lower case denotes a sample value from this distribution. For example, f^* is the estimation of the view factor F , as provided by a single simulation run.

Furthermore, the notation:

$$R - N(E(R), V(R))$$

indicates that the random variable R follows a normal distribution with expectation $E(R)$ and variance $V(R)$.

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