where Im $\left(r_{X_1+\Delta X_1,X_2,\ldots,X_J}\right)$ is the imaginary part of the result, r [4]. The advantage of this complex-step method is that very small values of ΔX_1 can be used without affecting the accuracy of the approximation for the derivative. The iterations required in Eqs. (3.33) and (3.35) are not necessary. This is very important in simulation uncertainty determinations, in computational fluid dynamics (CFD) for example, where one solution may take many hours of computer time.

3-2 MONTE CARLO METHOD FOR PROPAGATION OF UNCERTAINTIES

An introduction to the Monte Carlo Method (MCM) was given in Section 2-5.4 for a measured variable. That discussion illustrated the random sampling from assumed distributions for each error source to estimate the distribution of the measured variable. With the computing power and speed now available, even in personal computers, it has become feasible to perform an uncertainty analysis directly by Monte Carlo simulation for a result that is a function of multiple variables. This method is not limited to simple expressions but can also be used for highly complicated experiment data reduction equations or for numerical solutions of advanced simulation equations. The Joint Committee for Guides in Metrology (JCGM) has recently published a supplement to the GUM [1] presenting the MCM for uncertainty analysis [5].

In this section, we will present the general approach for the MCM for uncertainty propagation and will then illustrate the technique with an example. The section concludes with a discussion of the general methodology for determining a specific percent coverage interval for the true result from the Monte Carlo distribution of results.

3-2.1 General Approach for MCM

Figure 3.4 presents a flowchart that shows the steps involved in performing an uncertainty analysis by the MCM. The figure shows the sampling technique for a function of two variables, but the methodology is general for DREs or simulations that are functions of multiple variables. In many cases, more than one result is desired in the test or simulation, that is, pressure drop and friction factor for a given Reynolds number, and that possibility is illustrated in the figure.

Figure 3.4 illustrates the MCM case that is analogous to the TSM case in which random standard uncertainties s_{X_i} are used in the propagation equation (3.12) to obtain s_r. The MCM case analogous to the TSM case in which s_r is directly calculated from multiple results using Eq. (3.13) is shown in Figure 3.5.

Using the approach shown in Figure 3.4 for MCM propagation as the basis for the discussion, first the assumed true value of each variable in the result is input. These would be the X_{best} values that we have for each variable. Then the estimates of the random standard uncertainty s and the elemental systematic standard uncertainties b_k for each variable are input. An appropriate probability distribution function is assumed for each error source. The random errors are usually assumed to come from a Gaussian distribution, but if s is from a very

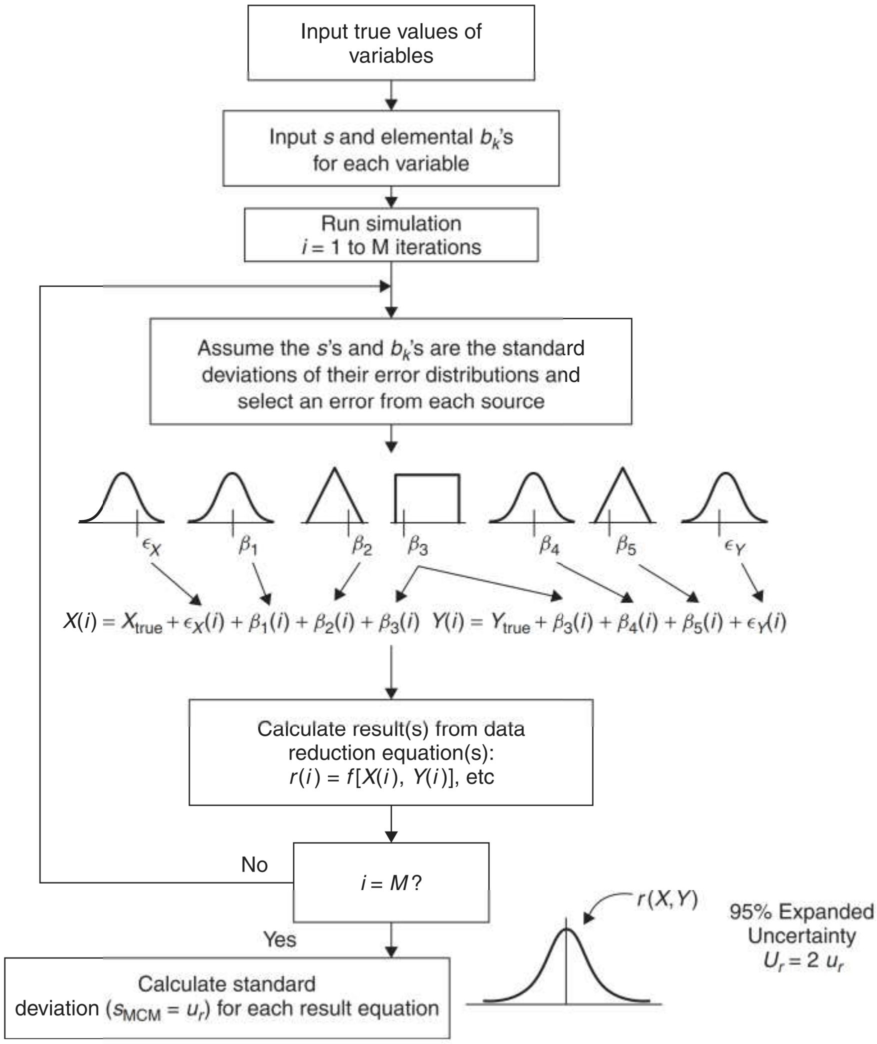

Figure 3.4 Schematic of MCM for uncertainty propagation when random standard uncertainties for individual variables are used.

small sample, the t distribution at the appropriate degrees of freedom ν_s could be more appropriate. The systematic error distributions are chosen based on the user's judgment, as discussed in Section 2-5.1. For the flowchart in Figure 3.4, we have assumed that the random standard uncertainties for X and Y come from Gaussian distributions and that each variable has three elemental systematic standard uncertainties, one Gaussian, one triangular, and one rectangular.

For each variable, random values for the random errors and each elemental systematic error are found using an appropriate random number generator (Gaussian,

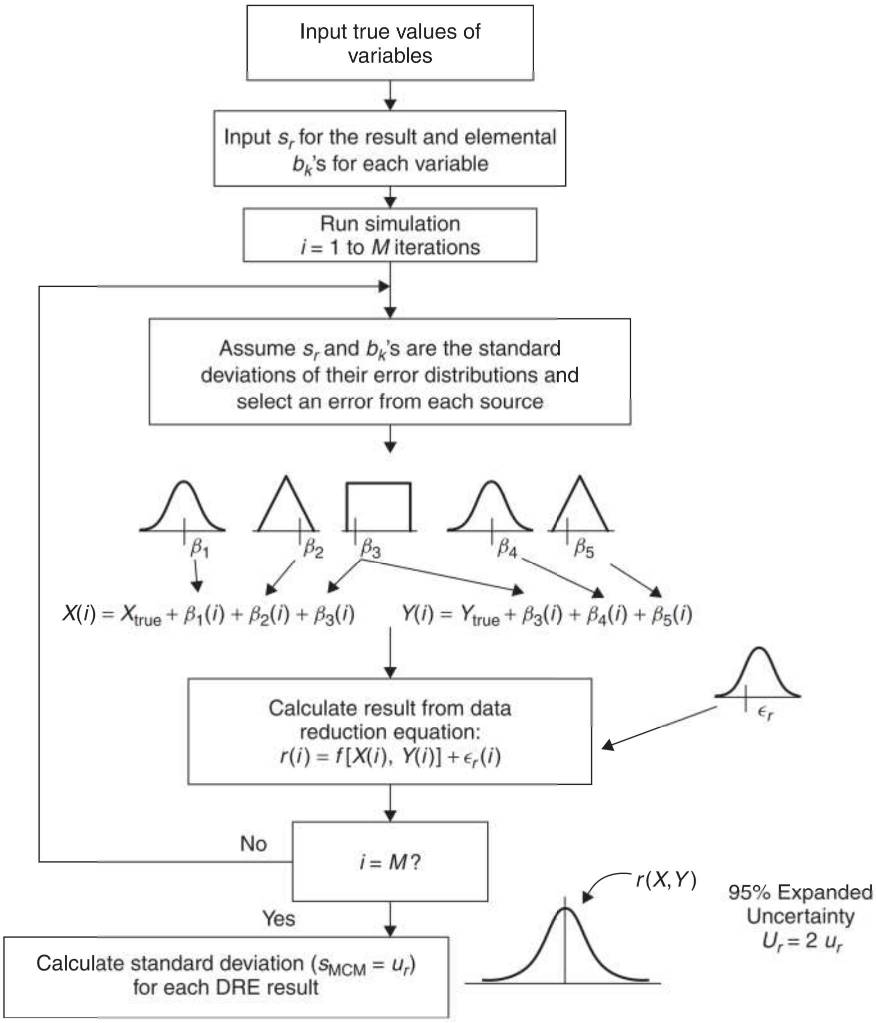

Figure 3.5 Schematic of MCM for uncertainty propagation when directly calculated random standard uncertainty for the result, s_r, is used.

rectangular, triangular, etc.). The individual error values are then summed and added to the true values of the variables to obtain "measured" values. Using these measured values, the result is calculated. This process corresponds to running the test or simulation once.

The sampling process is repeated M times to obtain a distribution for the possible result values. The primary goal of the MCM propagation technique is to estimate a converged value for the standard deviation, s_{MCM}, of this distribution. An appropriate value for M is determined by periodically calculating s_{MCM} during the MCM process and stopping the process when a converged value of s_{MCM} is obtained. Keep in mind that s_{MCM} is the estimate of the combined standard uncertainty of the result, u_r. We do not need to have a perfectly converged value of s_{MCM} to have a reasonable estimate of u_r. Once the s_{MCM} values are converged to within 1–5%, then the value of s_{MCM} is a good approximation of the combined standard uncertainty of the result. The level of convergence is a matter of judgment based on the cost of the sampling process (e.g., costly CFD simulations) and the application for u_r. Once a converged value of u_r is determined and assuming that the central limit theorem applies, the expanded uncertainty for the result at a 95% level of confidence is $U_r = 2u_r$.

The number of iterations required in the MCM to reach a reasonable estimate of the converged value of s_{MCM} can be reduced significantly by using special sampling techniques, such as Latin hypercube sampling. This technique is described in Ref. 6–10 and is very popular for determining the uncertainty in complex simulation results.

Note that in Figure 3.4 we used the same value of β_3 for X and Y during each iteration. Here we are assuming that X and Y have a common, correlated, systematic error that has the same value for both variables. As we discussed in Section 3-1.1, the effects of these correlated errors have to be taken into account in order to get the correct value for u_r. We see in Figure 3.4 that handling correlated systematic errors is very straightforward using the MCM.

In Section 3-1.1, we also pointed out that sometimes the random errors might be correlated because of effects that vary with time that affect the variables in the same manner. These effects are taken into account using the approach shown in Figure 3.5. In the next section, we give an example of using the MCM for uncertainty propagation.

3-2.2 Example of MCM Uncertainty Propagation

Considering the same example used in Section 3-1.4, the uncertainties of the three test results, friction factor f, Reynolds number Re, and relative roughness ϵ/d, can be found with the MCM method as shown in Figure 3.6. The nominal values for all of the variables are input to the MCM process. Standard uncertainties and associated error distributions are assumed for each variable. Error values are randomly chosen from the distributions and added to the nominal values to get the measurement values for each variable and then the values of the three results. The iteration process is continued until converged values of u_f, u_{Re}, and $u_{\epsilon/d}$ are obtained. In this example, we have taken one error source for each variable to simplify the presentation. Of course, the MCM process is straightforward for multiple error sources for each variable, as shown in the previous section.

In the TSM solution of this problem in Section 3-1.4, percent expanded uncertainties at a 95% level of confidence were used for each of the variables. If we assume that all distributions are Gaussian, then the standard uncertainty inputs for the MCM will be the previous percent uncertainties divided by 2. Therefore for 1% expanded uncertainties

$$u_{X_i} = \tfrac{1}{2}(0.01)X_i \tag{3.37}$$

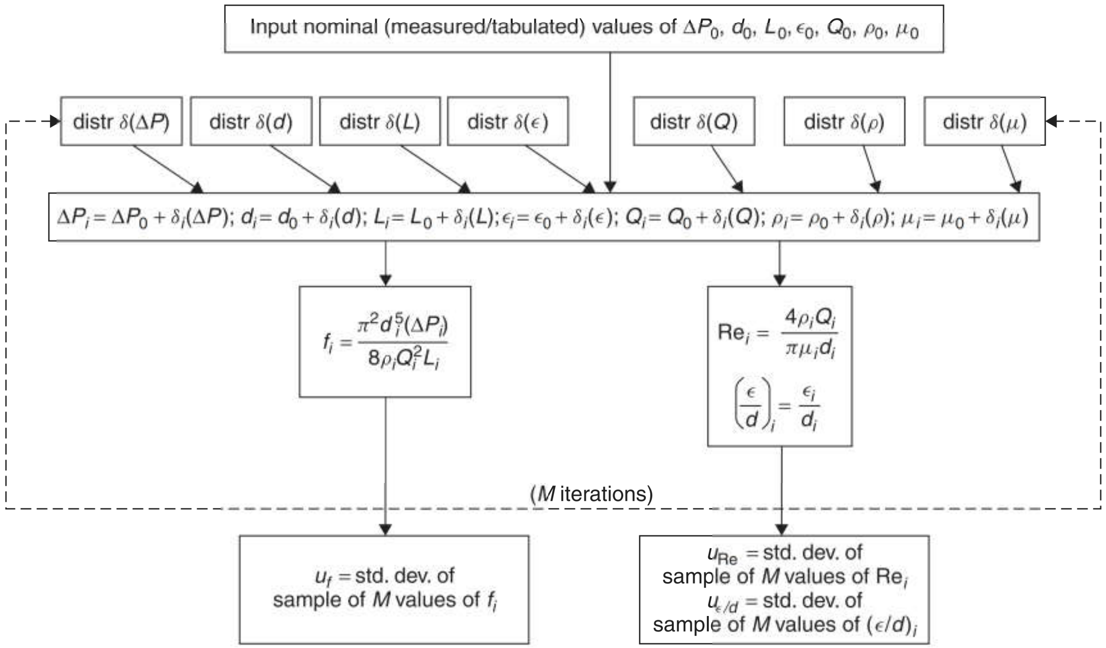

Figure 3.6 Schematic flowchart of MCM for fluid flow example problem.

Using the same nominal values for the variables as before, the MCM yields for the friction factor

$$(u_f)_{\mathrm{MCM}} = 0.00049 \tag{3.38}$$

or

$$\left(\frac{U_f}{f}\right)_{\mathrm{MCM}} = \left(\frac{2u_f}{f}\right)_{\mathrm{MCM}} = 5.7\% \tag{3.39}$$

which is the same value as that obtained using the TSM. The distribution of the results from the MCM is shown in Figure 3.7.

The convergence of the combined standard uncertainty u_f in this MCM example is shown in Figure 3.8. The value of s_f was calculated after 200 iterations and then again for every 200 additional iterations using the total number of iterations to that point. The plot of these s_f, or u_f, values is shown in Figure 3.8. The value of $(U_f/f)_{\mathrm{MCM}}$ in Eq. (3.39) was a fully converged value from a large number of iterations. We see that after only 200 iterations the value has converged to within about 3% and by 1000 iterations to within less than 1% of the fully converged value.

When the 95% expanded uncertainties for each variable are 5%, the MCM results for the friction factor yield

$$(u_f)_{\mathrm{MCM}} = 0.00244 \tag{3.40}$$

or

$$\left(\frac{U_f}{f}\right)_{\mathrm{MCM}} = \left(\frac{2u_f}{f}\right)_{\mathrm{MCM}} = 28.5\% \tag{3.41}$$

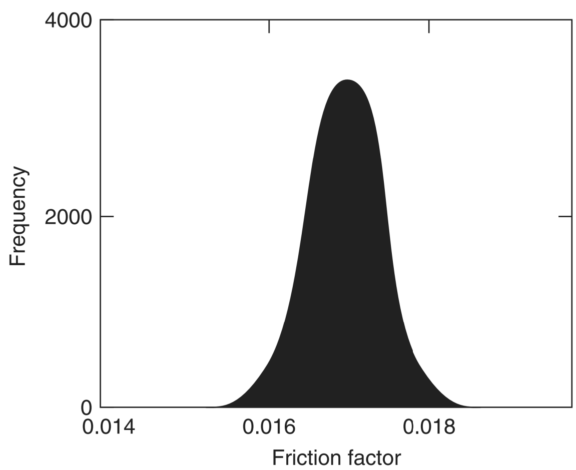

Figure 3.7 Distribution of MCM results for friction factor for 1% expanded uncertainty (95%) for each variable.

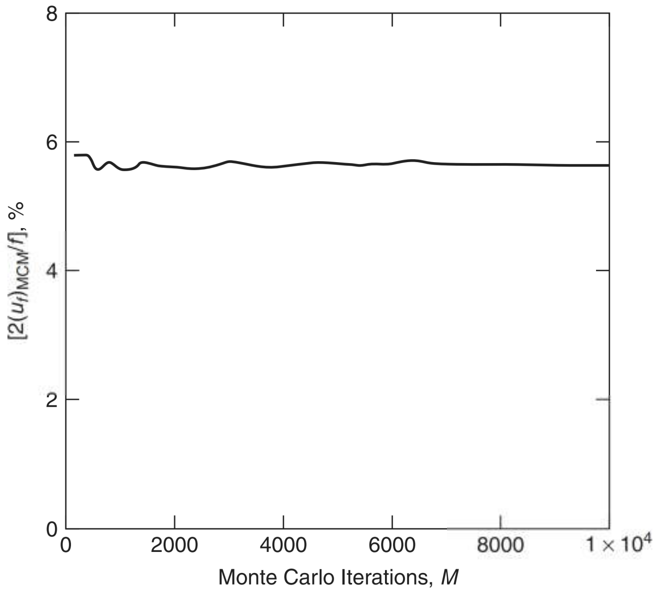

Figure 3.8 Convergence study for MCM value of u_f for 1% expanded uncertainty (95%) for each variable.

This value is compared to the value for $(U_f/f)_{\mathrm{TSM}}$ of 28.3%, which is essentially the same value. Looking at the distribution of the results for this case from the MCM given in Figure 3.9, we see that when the expanded uncertainties of the variables are 5% the distribution of MCM results is slightly skewed toward higher values of friction factor.

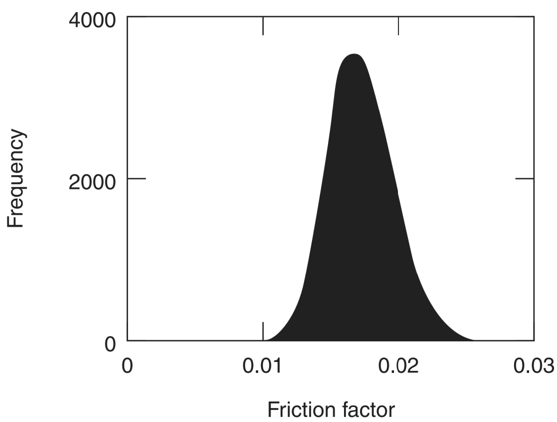

Figure 3.9 Distribution of MCM results for friction factor for 5% expanded uncertainties (95%) for each variable.

The difference between the MCM and TSM uncertainty results in this example is negligible, but if the distribution of MCM results is highly skewed, the plus and minus uncertainty limits will not be equal. The general methodology for determining a specific percent coverage interval for the true result from the MCM is presented next.

3-2.3 Coverage Intervals for MCM Simulations

If the uncertainties of the variables are relatively large and/or the DRE or simulation is highly nonlinear, the distribution of Monte Carlo results can be asymmetric, as shown in Figure 3.10. The result calculated using the nominal values of all the input variables will not coincide with the peak, or mode (the most probable value), of the distribution of the MCM results as shown. For these cases, calculating the standard deviation s_{MCM} and assuming that the central limit theorem applies to obtain the expanded uncertainty will not necessarily be appropriate depending on the degree of asymmetry.

The GUM supplement [5] presents methods for determining the coverage intervals for MCM simulations when the distributions are asymmetric. These coverage intervals are described below.

The coverage interval that provides "probabilistically symmetric coverage" is shown in Figure 3.11 for a 95% level of confidence. The interval contains $100p\%$ of the results of the MCM simulation, where in this case $p = 0.95$ for 95% coverage. The lower bound of the interval is the result value that corresponds to the upper end of the lowest 2.5% of the MCM results. The upper bound of the interval is the result that corresponds to the upper end of the range that contains 97.5% of the MCM results. The interval between these bounds contains 95% of the MCM results with a symmetric percentage of the MCM results (2.5% in this case) outside of the coverage interval on each end.

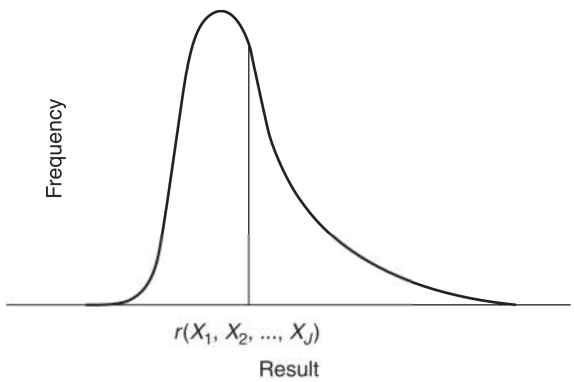

Figure 3.10 MCM results for large uncertainties in variables and/or nonlinear result equations.

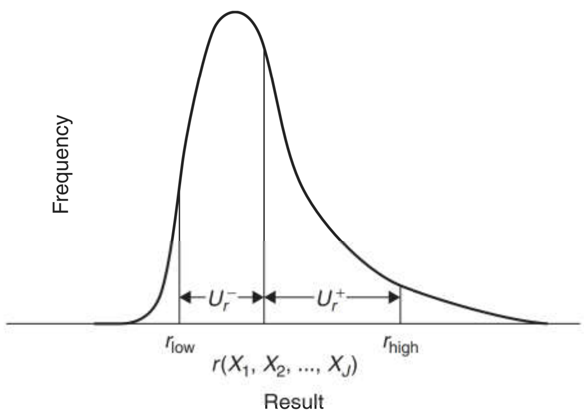

Figure 3.11 Probabilistically symmetric coverage interval for 95% level of confidence.

The procedure for determining the 95% probabilistically symmetric coverage interval and associated uncertainty limits is given below:

1. Sort the M Monte Carlo simulation results from lowest value to the highest value.
2. For a 95% coverage interval

$$r_{\text{low}} = \text{result number}(0.025M) \tag{3.42}$$

and

$$r_{\text{high}} = \text{result number}(0.975M) \tag{3.43}$$

If the numbers $0.025M$ and $0.975M$ are not integers, then add $\frac{1}{2}$ and take the integer part as the result number [5].

3. For 95% expanded uncertainty limits

$$U_r^- = r(X_1, X_2, \ldots, X_J) - r_{\text{low}} \tag{3.44}$$

and

$$U_r^+ = r_{\text{high}} - r(X_1, X_2, \ldots, X_J) \tag{3.45}$$

4. The interval that contains r_{true} at a 95% level of confidence is then

$$r - U_r^- \leq r_{\text{true}} \leq r + U_r^+ \tag{3.46}$$

The general procedure for determining the probabilistically symmetric coverage interval for any $100p\%$ level of confidence ($p = 0.99$ for 99% for instance) is step 1 above followed by

$$r_{\text{low}} = \text{result number}\{[\tfrac{1}{2}(1 - p)]M\} \tag{3.47}$$

and

$$r_{\text{high}} = \text{result number}\{[\tfrac{1}{2}(1+p)]M\} \tag{3.48}$$

Once again, if these numbers are not integers, then $\frac{1}{2}$ is added to each and the integer part is used as the result number. The expressions for the asymmetric uncertainty limits, U_r^- and U_r^+, and the $100p\%$ coverage interval for r_{true} are the same as in steps 3 and 4 above.

The GUM supplement [5] provides an alternative coverage interval called the "shortest coverage interval," which is described in Appendix D. If the distribution of MCM results is symmetric, the shortest coverage interval, the probabilistically symmetric coverage interval, and the interval given by $\pm(k_{100p\%})s_{\text{MCM}}$ will be the same for a $100p\%$ level of confidence.

3-2.4 Example of Determination of MCM Coverage Interval

Consider again the example in Sections 3-1.4 and 3-2.2. We saw in Section 3-2.2 that when the 95% expanded uncertainties for each variable were 5% the 95% expanded uncertainty for the friction factor was 28.5% using $2s_{\text{MCM}}/f$. The uncertainty value from the TSM was $(U_f/f)_{\text{TSM}} = 28.3\%$. We also observed that the distribution of friction factor results for this case was slightly skewed toward larger values, as shown in Figure 3.9.

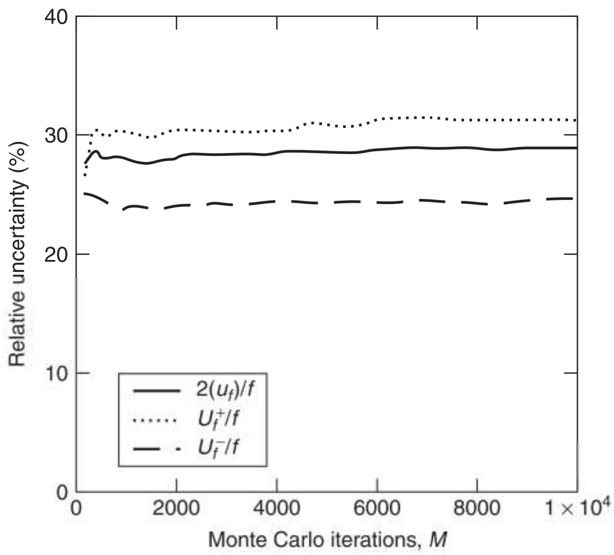

Figure 3.12 Convergence of coverage intervals for MCM example.

Using the probabilistically symmetric coverage interval method, $p = 0.95$, and the distribution of friction factor results in Figure 3.9, the plus and minus uncertainty limits were obtained as

$$U_f^+ = 31.5\% \tag{3.49}$$

and

$$U_f^- = 24.5\% \tag{3.50}$$

These values along with the value in Eq. (3.41) represent the converged uncertainty limits for a large number of iterations. The convergence of these limits is shown in Figure 3.12. We see that with about 2000 iterations the values for U_f^- and U_f^+ have converged to within about 5% and by 10,000 iterations to within about 2% of the fully converged values.

For this example, the TSM uncertainty interval, the $2(u_f)_{\mathrm{MCM}}/f$ interval, and the asymmetric uncertainty interval all provide about 95% coverage of the results from the MCM distribution given in Figure 3.9. However, for extreme cases where the Monte Carlo distribution is highly skewed, the asymmetric uncertainty limits will be more appropriate to provide a given level of confidence for the uncertainty estimate.

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