LA-UR-01-1487
*Approved for public release;
distribution is unlimited.*

Title:

Verification of Transport Codes by the Method of Manufactured Solutions: The ATTILA Experience

Author(s):

Shawn D. Pautz

Submitted to:

http://lib-www.lanl.gov/la-pubs/00796073.pdf

Verification of Transport Codes by the Method of Manufactured Solutions: The ATTILA Experience

Shawn D. Pautz
Transport Methods Group, CCS-4, MS-D409
Los Alamos National Laboratory
Los Alamos, NM 87545
pautz@lanl.gov

Keywords: verification, manufactured solutions, transport

ABSTRACT

We extend the Method of Manufactured Solutions (MMS) to the verification of transport codes. We derive analytic fixed sources required by the MMS procedure for several types of transport problems and apply the method to the Attila transport code. By means of this method we discover and correct several coding mistakes in Attila and ultimately verify its correct implementation for the problems studied. Our studies reveal that the MMS procedure is a useful tool for transport code development.

1 INTRODUCTION

A critical task in the development of scientific computer codes is the verification that a given code has been implemented correctly. Here we distinguish verification, which determines whether the intended (discretized) equations are solved correctly by a code, from validation, which determines whether these equations are an adequate model of physical reality for the code's domain of interest. Both verification and validation are required in order to have confidence in a code's capabilities.

There are numerous methods of verification. One commonly used one is the Method of Exact Solutions (MES) (Salari, 2000). With MES one attempts to derive exact solutions (benchmarks) to the relevant equations for particular problems and then compares these solutions to the code results for the same problems. Drawbacks of this method include the difficulty of obtaining exact solutions and the fact that the solutions that have been derived are very often for simplified problems that do not exercise the full functionality of a code. Thus with MES one may not be able to fully verify a code.

One alternative to MES is the Method of Manufactured Solutions (MMS) (Salari, 2000). With MMS one first defines a solution that will necessarily exercise desired parts of a code and then constructs a problem that yields that solution. Advantages of the MMS procedure include the ease with which analytic problems may be constructed and that in principle all parts of the code may be tested. In this work we will extend the MMS verification procedure to transport codes, in particular to the Attila discrete ordinates code (Wareing, 1996).

The rest of this paper is organized as follows. In Section 2 we will review the general MMS procedure. In Section 3 we will extend the MMS procedure for use with the transport equation, deriving several equations needed for verification tests. We will apply the MMS procedure to the Attila code to verify it for several types of problems in Section 4, and we will discuss our experience with the MMS method more generally in Section 5. Finally, in Section 6 we will present some conclusions.

2 REVIEW OF MMS PROCEDURE

Suppose that one wishes to verify a computer code that attempts to approximately solve an equation of the form

$$Du = f, \tag{1}$$

where D is an operator (such as the transport operator), f is a fixed source, and u is the solution. In the MES method of verification one carefully chooses a source f such that, often with great effort, one can derive the exact solution u. By executing the computer code with the selected source and increasingly fine grids one can determine whether the code results converge to the correct solution. As noted in the introduction, however, it can be very difficult to apply the MES procedure in a manner that exercises the full functionality of the code.

In the MMS procedure we approach Eq. (1) in the reverse manner. First we choose ("manufacture") a solution u with properties that will exercise desired parts of the computer code. For example, if u has a complex spatial variation we will be able to test the spatial discretizations in the code. We may also choose complicated expressions for coefficient functions in D such as material properties. We then simply evaluate Du to obtain the analytic expression for f. We follow the same procedure as in MES to test the code for convergence to the exact solution.

Salari and Knupp (2000) give guidelines for manufacturing solutions for the MMS procedure. Among other recommendations, the solution should be smooth enough that one can actually evaluate Du, the solution should be complicated enough that one can test the order of accuracy of the code, and the solution should be general enough that one can exercise all of the terms in the governing equations. One important note is that the manufactured problem need not be a physically realistic one. The code itself makes no distinction between "real" problems and artificial ones; it should solve the same set of equations in the same manner in either case.

One major strength of the MMS procedure is that it can identify any coding mistake that affects the order of accuracy of the numerical method (Salari, 2000). Since we know the exact solution we can determine the exact discretization error of any calculation; by executing the code on increasingly fine grids we can observe the asymptotic convergence rate of any variable we wish. If the solution is general enough we will exercise all parts of the code, and the existence of those coding mistakes that affect the order of accuracy will be obvious from the convergence studies. The above property, coupled with the ease of constructing many different problems with solutions, makes MMS a very powerful verification tool.

3 EXTENSION OF MMS TO TRANSPORT

The MMS verification procedure has been used in many application areas, but it has received little attention in the transport community. Some of the basic ideas of the method were applied to transport calculations in Lingus (1971), Martin (1975), and Martin and Duderstadt (1977), but their development of the method is more limited than the more recent and general treatment by Salari and Knupp (2000). We will attempt to update the previous transport verification work with the current understanding of the MMS method. In this section we derive general analytic sources and solutions for several types of transport problems that may be used with MMS verification of transport codes. We will use these analytic results in the next section to verify the Attila code.

3.1 Steady State, Monoenergetic

The steady state, monoenergetic form of the transport equation is

$$[\Omega \cdot \nabla + \sigma_t]\,\psi(\mathbf{r},\Omega) = \sum_{n,m} Y_{nm}(\Omega)\,\varphi_{nm}(\mathbf{r})\,\sigma_{sn} + q(\mathbf{r},\Omega)\,, \tag{2a}$$

$$\varphi_{nm}(\mathbf{r}) = \int_{4\pi} d\Omega' Y^*_{nm}(\Omega')\,\psi(\mathbf{r},\Omega')\,, \tag{2b}$$

where ψ is the angular flux, φ_{nm} are the angular flux moments, σ_{sn} is the nth Legendre moment of the scattering cross section, and the Y_{nm} are spherical harmonics functions. In order to apply the MMS procedure we need to specify an analytic form for the solution (in this case, ψ) and then determine the corresponding fixed source. Let us choose the following general form for ψ:

$$\psi(\mathbf{r},\Omega) \equiv f(\mathbf{r}) \sum_{n,m} \varphi_{nm} Y_{nm}(\Omega)\,. \tag{3}$$

Substitution of Eq. (3) into Eq. (2) yields the following analytic fixed source:

$$q(\mathbf{r},\Omega)=\sum_{n,m}\varphi_{nm}Y_{nm}(\Omega)\left[\Omega\cdot\nabla+(\sigma_t-\sigma_{sn})\right]f(\mathbf{r})\,. \tag{4}$$

Boundary conditions are obtained simply by evaluating Eq. (3) at the boundaries.

We note that many other forms for ψ would also be valid choices, yielding fixed sources different from that given above. However, the above choice is sufficient for several verification tests. For example, if we choose $f(\mathbf{r})=1$ and several non-zero flux moments we can verify whether a code handles angular terms correctly. Alternatively, if we let $f(\mathbf{r})$ have a non-trivial spatial variation we may verify the spatial discretizations of a code.

3.2 Steady State, Multigroup

The steady state, continuous energy form of the transport equation is

$$\begin{aligned}&\left[\Omega\cdot\nabla+\sigma_t(E)\right]\psi(\mathbf{r},\Omega,E)\\ =&\int dE'\sum_{n,m}Y_{nm}(\Omega)\,\varphi_{nm}(\mathbf{r},E')\,\sigma_{sn}(E\to E')+q(\mathbf{r},\Omega,E)\,.\end{aligned} \tag{5}$$

If we define the flux and cross sections to be

$$\psi(\mathbf{r},\Omega,E)\equiv f(E)\sum_{n,m}\varphi_{nm}Y_{nm}(\Omega)\,, \tag{6a}$$

$$\sigma_t(E)=\sigma_t g_t(E)\,,\qquad \sigma_{sn}(E\to E')=\sigma_{sn}g_s(E,E')\,, \tag{6b}$$

then the multigroup sources and cross sections are given by

$$q_g=\sum_{n,m}\varphi_{nm}Y_{nm}(\Omega)\left[\sigma_{t,g}f_g-\sum_{g'}\sigma_{sn,gg'}f_{g'}\right], \tag{7a}$$

$$\sigma_{t,g}\equiv\sigma_t\int_g dE\,g_t(E)\,\frac{f(E)}{f_g},\qquad \sigma_{sn,gg'}\equiv\sigma_{sn}\int_{g'}dE'\,g_{s,g}(E')\,\frac{f(E')}{f_{g'}}, \tag{7b}$$

$$g_{s,g}(E')\equiv\int_g dE\,g_s(E,E')\,,\qquad f_g\equiv\int_g dE\,f(E) \tag{7c}$$

Note that there are no discretization errors in the multigroup treatment if the spatial and energy dependence of the exact flux is separable (as above) and if the correct flux spectrum is used to generate the cross sections. Therefore in a properly implemented multigroup transport code we should observe no energy discretization errors with the above problem. On the other hand, if we use cross sections generated from a different analytic solution we should observe energy discretization errors. Although cross section sets may not be considered to be part of a transport code per se, the code should use them in a manner consistent with the multigroup treatment, and hence we should observe the proper convergence behavior as we refine the group structure.

3.3 Monoenergetic K-Eigenvalue

The monoenergetic, k-eigenvalue form of the transport equation is

$$[\Omega \cdot \nabla + \sigma_t]\, \psi(\mathbf{r}, \Omega) = \sum_{n,m} Y_{nm}(\Omega)\, \varphi_{nm}(\mathbf{r})\, \sigma_{sn} + \frac{\nu \sigma_f}{k} \varphi_{00}(\mathbf{r}) + q(\mathbf{r}, \Omega)\,. \tag{8}$$

As required by the MMS procedure we have included a fixed source in Eq. (8). This is markedly different from a normal k-eigenvalue calculation, in which we determine the eigenvalue and eigenmode of a homogeneous equation. In the above form we are attempting to determine the response of a system to a forcing term; the k-eigenvalue calculation is just a special case in which the forcing term is zero. It may be necessary to rewrite the transport code to properly normalize the discrete solution (otherwise there will be too many unknowns) and to include a fixed source, but otherwise we may test the implementation of the k-eigenvalue calculation by the MMS method.

If we choose Eq. (3) as the form for the analytic solution then the corresponding fixed source is

$$q(\mathbf{r}, \Omega) = \sum_{n,m} \varphi_{nm} Y_{nm}(\Omega)\, [\Omega \cdot \nabla + (\sigma_t - \sigma_{sn})]\, f(\mathbf{r}) - \frac{\nu \sigma_f}{k} \varphi_{00} f(\mathbf{r})\,, \tag{9}$$

where we recognize that we must also choose a value for k.

3.4 Gray Infrared

The gray infrared form of the transport equation is

$$[\Omega \cdot \nabla + \sigma_t]\, \psi(\mathbf{r}, \Omega) = \sum_{n,m} Y_{nm}(\Omega)\, \varphi_{nm}(\mathbf{r})\, \sigma_{sn} + \sigma_e \varphi_{00}(\mathbf{r}) + q(\mathbf{r}, \Omega)\,. \tag{10a}$$

$$T(\mathbf{r}) = \left[\frac{1}{4\sigma} \varphi_{00}(\mathbf{r}) \right]^{1/4}, \tag{10b}$$

where σ is the Stefan-Boltzmann constant. If we use Eq. (3) as the analytic solution then the required fixed source is

$$q(\mathbf{r}, \Omega) = \sum_{n,m} \varphi_{nm} Y_{nm}(\Omega)\, [\Omega \cdot \nabla + (\sigma_t - \sigma_{sn})]\, f(\mathbf{r}) - \sigma_e \varphi_{00} f(\mathbf{r})\,. \tag{11}$$

4 MMS VERIFICATION OF ATTILA

In the previous section we derived a set of analytic transport problems and solutions for use with the MMS verification method. In this section we report verification tests of the Attila code. Attila is a discrete ordinates transport code developed at

Los Alamos National Laboratory (Wareing, 1996). It uses linear discontinuous finite element differencing of the first-order form of the transport equation on tetrahedral elements; it can perform all of the calculations (as well as others) discussed in the previous section. It has functionality to accept sources that vary in space, energy, and/or angle, making it relatively easy to use the complicated sources needed by the MMS procedure.

To perform the spatial convergence studies we need a set of increasingly refined meshes. Although Attila can use irregularly structured tetrahedral meshes, in order to have a well-defined measure of "refinement" we will use a set of meshes that are highly regular. Each of the meshes will consist of a unit cube that has been subdivided into an $n \times n \times n$ array of cubes (with n being a power of 2); each of the cubes in the array is further subdivided into 24 tetrahedra. We will define h, the representative length scale of a mesh, as the length of any of the small cubes in the array, i.e. $h = 2^{1-n}$.

Although in theory one could define problems with enough complexity to test many different aspects of a code simultaneously, in practice this can result in unacceptably large transport calculations due to concurrent refinements in energy, angle, and space. We will instead use a larger set of less complicated problems, each of which is designed to explore only a portion of Attila's functionality. An added benefit of this approach is that it helps to isolate the effects of different sections of code. We will also divide our verification tests into two different types. In one type of verification test the problem will be simple enough that Attila should display no truncation errors at all if it is properly coded; in the second type of test we should observe convergent truncation errors in at least one of the problem dimensions.

4.1 Steady State, Monoenergetic Problems

4.1.1 Tests Without Truncation Error

We conduct several tests of steady state, monoenergetic problems in which we expect to observe no truncation errors. In the first series of tests we wish to verify Attila's handling of angular terms including anisotropic scattering. We use Eq. (3) for the desired solution with $f(\mathbf{r}) = 1$ and several non-zero angular flux moments and scattering cross section moments. When executed with appropriate quadratures Attila should obtain the exact solution, ignoring round-off errors. However, in our initial execution of these tests we did not obtain the correct solution, which we eventually traced to coding mistakes in the input routines. We also discovered divide-by-zero errors when $\sigma_{s0} = \sigma_{s1}$. After correcting these mistakes we reran these tests and obtained the exact results, as expected. These tests demonstrate the value of MMS with simple problems.

In a second series of tests we wish to verify Attila's handling of spatial terms. We choose fluxes that are isotropic and spatially linearly varying, i.e. for which $f(\mathbf{r}) = a + bx + cy + dz$. The linear discontinuous representation of internal and boundary

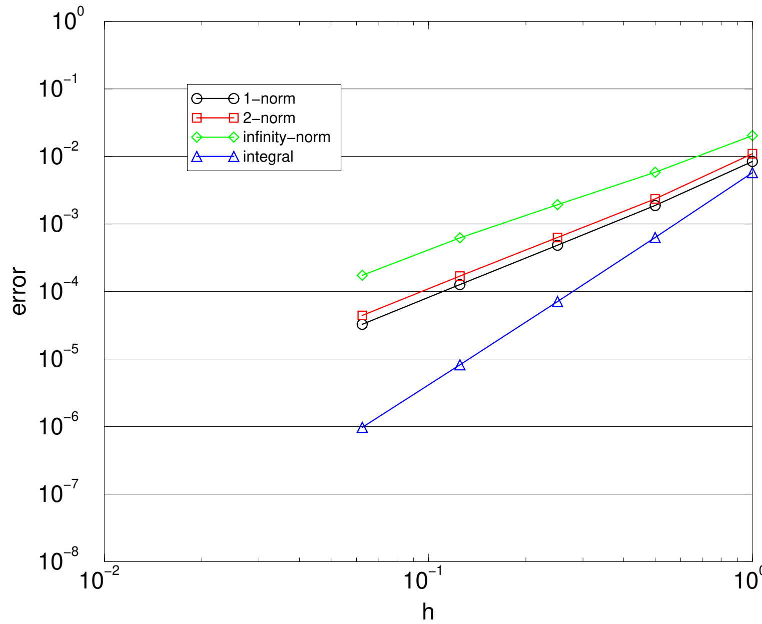

Figure 1: Attila errors for steady state, monoenergetic problem.

fluxes in Attila should exactly capture solutions of this form. We ran several problems of this form and obtained the exact solution in all cases, as expected.

4.1.2 Tests With Truncation Error

We have conducted several steady state, monoenergetic tests in which the spatial variation of the solution is sufficiently complicated that we expect to observe truncation errors in Attila results. We report one such test here. In this test we use $f(\mathbf{r}) = (1 + x^2)(1 + y^2)(1 + z^2)$. We executed Attila with the corresponding source given by Eq. (4) and with S_2 level-symmetric quadrature, $\sigma_t = 1$, and $\sigma_a = 0$. In Figure 1 we show the errors as calculated by different methods for several levels of spatial refinement. The norms in Figure 1 are applied to cell average fluxes, while the “integral” error compares the problem average discrete flux with the analytic value. We see that the error norms reveal second-order convergence and the integral error reveals third-order convergence. This is consistent with the discretization in Attila (Wareing, 1999, Wareing, 2000), so the MMS method has verified the spatial discretization in Attila for this general type of problem.

4.2 Steady State, Multigroup Problems

4.2.1 Tests Without Truncation Error

To verify the steady state multigroup capability of Attila for problems in which there should be no energy truncation error we use problems defined by Eqs. (6) and (7) with $\sigma_t = \sigma_{sn} = 1$ and the following cross section kernels:

$$g_t(E) = 1 + 100e^{-5E}, \quad 0 \le E \le 5, \tag{12a}$$

$$g_s(E, E') = \begin{cases} e^{-(E'-E)}, & E' \ge E \\ 0, & E' < E \end{cases}, \quad 0 \le E \le 5. \tag{12b}$$

We divide the energy range into energy groups of equal width. For our first test we use $f(E) = 1$, isotropic fluxes, S_2 quadrature, and one of the coarser spatial meshes. When we execute this problem with Attila with any amount of energy group refinement we obtain the exact results. In a second test we use $f(E) = Ee^{-E}$; it too is calculated exactly by Attila.

4.2.2 Tests With Truncation Error

To test the energy convergence of Attila we run a problem in which the fixed source and boundary conditions are those given by Eqs. (6) and (7) with $f(E) = Ee^{-E}$, but rather than using this flux spectrum to generate the cross section set we use $f(E) = 1$ as the weighting function. We expect the multigroup treatment in Attila to display truncation errors for this problem. We plot the errors in Attila results with S_2 quadrature and a coarse spatial mesh in Figure 2. All of the error measures show second-order convergence in energy, which is consistent with the multigroup treatment. Thus we have verified Attila's multigroup capabilities for downscattering problems; we have yet to verify the upscattering treatment.

4.3 Monoenergetic K-Eigenvalue Problems

4.3.1 Tests Without Truncation Error

For verification of monoenergetic k-eigenvalue calculations in Attila we examine several problems of the form suggested in Section 3.3 in which $f(\mathbf{r})$ is at most linearly varying. In all cases that we have run we have obtained the correct spatial flux shape and value for k.

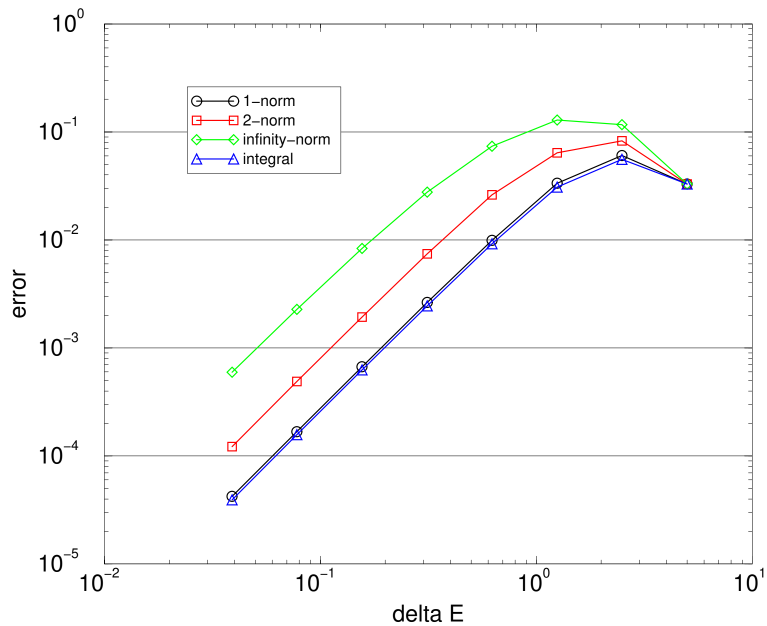

Figure 2: Attila errors for steady state, multigroup problem.

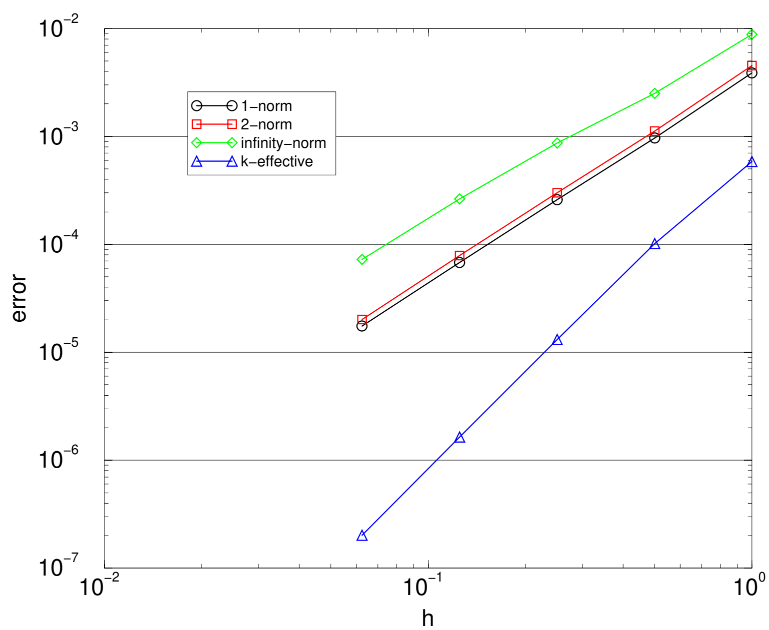

Figure 3: Attila errors for monoenergetic k-eigenvalue problem.

4.3.2 Tests With Truncation Error

We have run several verification tests in which $f(\mathbf{r})$ should produce spatial truncation errors with linear discontinuous differencing. We report results for the case in which $f(\mathbf{r}) = e^{(\lambda_x x + \lambda_y y + \lambda_z z)}$, with $\lambda_x = 1$, $\lambda_y = 1/2$, and $\lambda_z = -1$. For this case we use $\sigma_a = \nu\sigma_f = \sigma_t = 1$, S_2 quadrature, and an expected value of $k = 1/2$. The errors in Attila results are shown in Figure 3. In this plot the error norms are again defined with cell average fluxes, whereas the "k-effective" measure is the difference between the expected and calculated value of k. The norms display second-order convergence and the k-effective error displays third-order convergence, as expected.

4.4 Gray Infrared Problems

4.4.1 Tests Without Truncation Error

We conducted a series of infrared tests with solution forms given in Section 3.4 with $f(\mathbf{r})$ at most linearly varying. We expect to find no errors in Attila with such problems. However, in our initial executions of these tests we discovered errors that were eventually traced to the manner in which Attila handled certain boundary data. After correcting these mistakes we reran Attila and obtained the exact results.

4.4.2 Tests With Truncation Error

To test Attila's spatial error convergence with infrared problems we define a problem with the same exponential variation we used in the previous subsection. For this problem we use $\sigma_a = \sigma_t = 1$ and S_2 quadrature. The errors in the radiation flux and in the temperature are plotted in Figures 4 and 5, respectively. We again see second-order convergence for the error norms and third-order errors for integral (average) quantities, so we have provided verification of Attila for spatial discretizations with infrared problems.

In summary, we have used the MMS procedure to verify the Attila code for several problem types, both for problems in which Attila should have no truncation error and for problems in which the truncation error should be convergent. These tests have not been exhaustive; we have not exercised every code option or certain problem types such as electron transport. However, the tests we have performed have verified the correctness of a large subset of Attila's coding. We believe that this demonstrates the utility of MMS verification for transport applications.

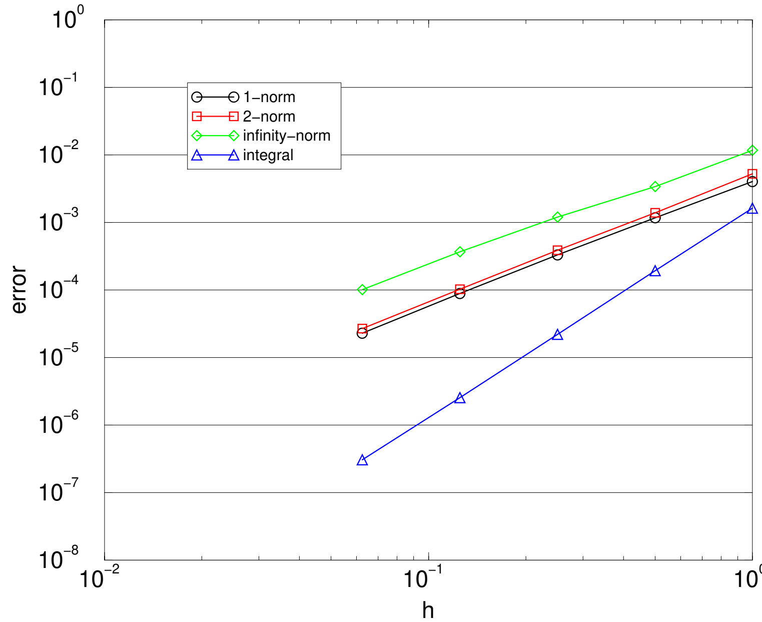

Figure 4: Attila flux errors for gray infrared problem.

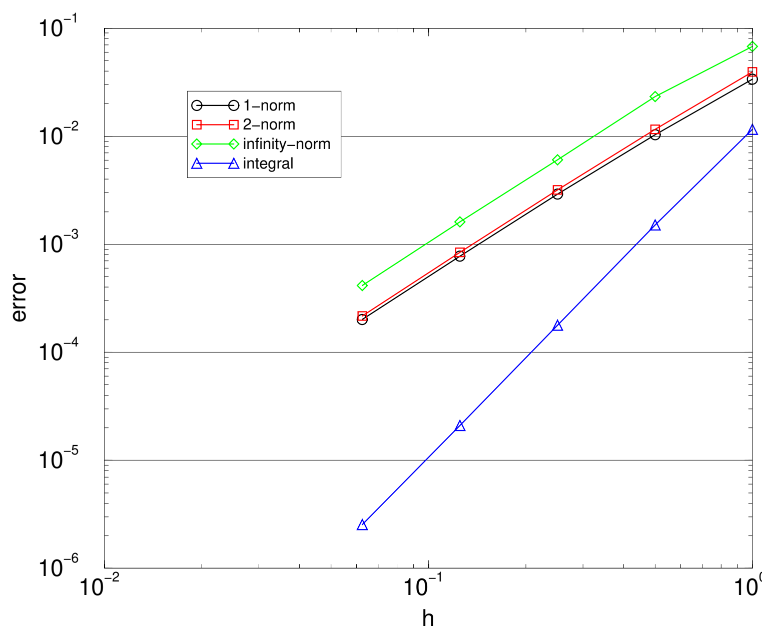

Figure 5: Attila temperature errors for gray infrared problem.

5 DISCUSSION

Our attempts to verify the Attila code by means of the MMS method were ultimately successful for the problem types that we examined. However, as we applied the method we discovered some subtle characteristics of MMS verification that we had to consider as we constructed test problems. We also discovered that MMS can be used as a tool for the analysis of numerical methods as well as for verifying code correctness.

In order to apply the MMS method a code must be able to accept general source and boundary conditions. These "general" conditions will necessarily be discrete, rather than analytic, values. It is important that the error introduced by mapping analytic functions to discrete values be asymptotically no larger than that introduced by the numerical method itself, or the true order-of-convergence of the code will be masked by the input errors. In our initial tests with Attila we had merely evaluated the analytic sources and boundary conditions at the required spatial locations, but this had the effect of changing the convergence order of the code. Only after applying the correct finite element weighting to the analytic functions did we observe the correct convergence order in the results.

Another property of the MMS method that we had not anticipated is its potential utility to characterize numerical methods. If, for example, one does not know the convergence order of a given method, the application of MMS can reveal it. In the case of Attila we had originally believed that all quantities had third-order spatial convergence, but our tests reveal that this is true only of integral quantities; our previous analyses had not included multiple spatial dimensions. Strictly speaking, one needs to conduct both mathematical analyses as well as MMS verification to determine whether observed convergence rates are the result of coding mistakes or are inherent to the numerical method being implemented.

6 CONCLUSIONS

The MMS method has previously been shown to be a useful code verification tool in a number of fields. In this paper we extended it to transport applications, in particular to the Attila discrete ordinates code. We have verified the Attila implementation for several problem types, thus increasing our confidence in the reliability of that code. We recommend that the utility of MMS verification be explored with other transport codes.

ACKNOWLEDGMENTS

This work was performed under the auspices of the U.S. Department of Energy by the University of California Los Alamos National Laboratory under contract No. W-

7405-Eng-36.

References

[1] Lingus, C. Analytical Test Cases for Neutron and Radiation Transport Codes. *Proc. 2nd Conf. Transport Theory*, CONF-710107, p.655, Los Alamos Scientific Laboratory, 1971.

[2] Martin, W.R., 1975. Convergence of the Finite Element Method in Neutron Transport. *Trans. Am. Nucl. Soc.*, **22**, 251.

[3] Martin, W.R., Duderstadt, J.J., 1977. Finite Element Solutions of the Neutron Transport Equation with Applications to Strong Heterogeneities. *Nucl. Sci. Eng.*, **62**, 371.

[4] Salari, K., Knupp, P. Code Verification by the Method of Manufactured Solutions, SAND2000-1444, Sandia National Laboratory, 2000.

[5] Wareing, T.A., McGhee, J.M., Morel, J.E., 1996. ATTILA: A Three-Dimensional, Unstructured Tetrahedral Mesh Discrete Ordinates Transport Code. *Trans. Am. Nucl. Soc.*, **75**, 146.

[6] Wareing, T.A., McGhee, J.M., Morel, J.E., Pautz, S.D., 1999. Discontinuous Finite Element S_N Methods on 3-D Unstructured Grids. *Proc. Int. Conf. Mathematics and Computations, Reactor Physics and Environmental Analysis in Nuclear Applications*, Madrid, Spain, September 27-30, 1999, Vol. 2, p. 1185.

[7] Wareing, T.A., McGhee, J.M., Morel, J.E., Pautz, S.D., 2000. Discontinuous Finite Element S_N Methods on 3-D Unstructured Grids, *Nucl. Sci. Eng.* **138**, 1.