

# An Analysis of Mass Matrix Lumping in NIMROD

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## 1 Introduction to Lumping

The  $(i, j)$ th element of a consistent mass matrix is given by

$$\mathbf{M}_{ij} = \int_V \alpha_i \alpha_j dV, \quad (1)$$

where  $\alpha_i$  and  $\alpha_j$  are the basis functions for finite element expansions. However, in early usage of the finite element formulation, a diagonal or “lumped” approximation was used because of the reduction in the number of calculations. We define the diagonal elements of an *ad hoc* lumped mass matrix of dimension  $n$  to be

$$\mathbf{M}_{L,ii} \equiv \sum_{j=1}^n \mathbf{M}_{ij} \quad (2)$$

There is often a physical basis for lumping. In structural dynamics problems, “lumping” simply means assuming all of the mass is at the nodes in the problem. In this context, this is a reasonable physical approximation. It should be noted that in general there is not a mathematical basis for *ad hoc* lumping of mass matrices, and hence no reason to expect *a priori* that the convergence rate of an algorithm will be maintained.

In NIMROD, the mass matrix arises as a result of the expansion into polynomial basis functions for a weak form of the problem [6]. Note that if the basis functions were orthogonal over the element, there would be no off-diagonal terms in the integral. One can make the rough interpretation that lumping is the approximation that the basis functions are actually orthogonal. This interpretation will return when we discuss optimal lumping in a later section.

As a quantitative example of how mass matrices arise, take the example of pressure. First we do the basis function expansion of pressure,  $p \rightarrow \sum_j p_j \alpha_j(\mathbf{x})$ . Then, use this in the weak form of the problem by multiplying by the test function and then integrating over volume. You will arrive at an equation

including a mass matrix.

$$\begin{aligned} \int dV \alpha_i(\mathbf{x}) \sum_j p_j \alpha_j(\mathbf{x}) &= \sum_j \left( \int \alpha_i(\mathbf{x}) \alpha_j(\mathbf{x}) dV \right) p_j \\ &= \sum_j \mathbf{M}_{ij} p_j \end{aligned} \tag{3}$$

Similar mass matrices occur for every field that arises in NIMROD.

Mass matrices are calculated with the `get_mass` procedure in `integrand.f` by performing numerical quadrature of equation (1). The code to lump mass matrices is found in subroutines near the end of `matrix_mod.f`. The *ad hoc* lumping procedure in NIMROD calls for the calculation of the consistent mass matrix as normal, but then followed by having each diagonal element become the sum of all elements in that element’s row, while setting the off-diagonal elements to zero.

The main advantage to lumping is obvious. Using only a diagonal mass matrix has the potential to save a lot of computational time by making the inversion of these matrices much simpler. Instead of having to do implicit matrix solves for each subcycle, one can simply divide by the diagonal element of the mass matrix (assuming there are no other implicit terms in the subcycle).

## 2 Testing Convergence Rates for Lumped and Consistent Mass Matrices

In this investigation, we hoped to discover the effects lumping has on the accuracy and convergence rate of NIMROD. We assume that the numerical solution is of the form

$$\Gamma_{num} = \Gamma_{true} + a(\Delta x)^C, \tag{4}$$

where  $\Gamma$  is a measured value in the code that converges (often a growth rate or period),  $a$  is the error coefficient,  $\Delta x$  is the mesh spacing, and  $C$  is the convergence rate. By solving the system of equations we get for the mesh spacings  $\Delta x$ ,  $r\Delta x$ , and  $r^2\Delta x$ , we find that the convergence rate is given by

$$C = \frac{1}{\ln r} \ln \left[ \frac{\Gamma_{r^2\Delta x} - \Gamma_{r\Delta x}}{\Gamma_{r\Delta x} - \Gamma_{\Delta x}} \right]. \tag{5}$$

Here,  $r$  is the ratio between mesh spacings for different otherwise identical runs of NIMROD. Generally,  $r \in \{\frac{4}{3}, \frac{3}{2}, \frac{5}{3}, 1.827, 2\}$  but  $r = 2$  is the most common case. Note that there is a bias towards calculating a higher convergence rate when coarse resolutions are used as part of this formula. This is because there are additional sources of error besides the leading Taylor series term that are significant at low  $\Delta x$ . Care must be taken to choose mesh spacings that are small enough to avoid this effect, but large enough so that the remaining errors can be distinguished.

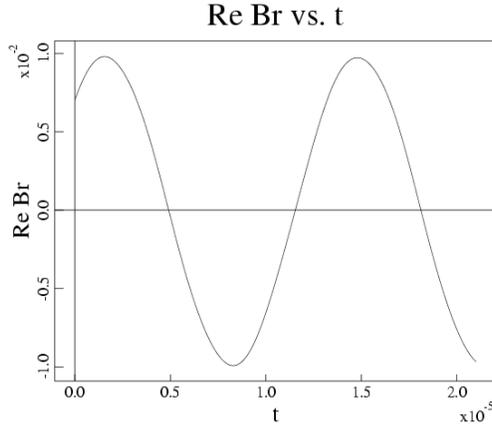


Figure 1: Shear Alfvén wave in a box. The measured quantities were the first, second, and third crossings of the y-axis [ $\text{Re}(B_r) = 0$ ] as well as the period.

An additional method is to plot  $\log \|\nabla \cdot \mathbf{B}\|$  against  $\log \Delta x$ . The slope as  $\Delta x \rightarrow 0$  is the negative of the convergence rate, assuming the dominant source of error is the lowest order remaining term in the Taylor series expansion. Here we define  $\Gamma \equiv \nabla \cdot \mathbf{B}$  so we then have  $\Gamma_{true} = 0$ . This is only done in the linear resistive tearing mode case.

For trials with consistent mass matrices, it is expected that the order of convergence for derivatives is identical to the order of the basis function polynomials. This is not always the case, and there are instances where the convergence rates vary significantly from what is expected from finite element analysis. This is puzzling, but even with these disparities, we can still make comparisons about the accuracy and convergence rate of NIMROD when either lumped or consistent mass matrices are used.

## 2.1 Shear Alfvén Wave Test

The first test regarding the effects of lumping used the input file `nimrod.inx`, which has a shear Alfvén wave traveling in a  $1 \text{ m}^2$  box. There was a rectangular grid, and  $\Delta x$  was constant and identical for both the  $x$  and  $y$  directions. In this case,  $\Gamma$  can be the first period of a wave, i.e. the location where the perturbed magnetic field reaches a minimum in magnitude. Graphically, this is where the wave crosses the  $x$ -axis.

The first set of trials involve having zero resistivity. From these, convergence rates for consistent mass matrices were obtained up until  $p = 3$  and for lumped mass matrices of  $p = 1$ , where  $p$  is defined to be the degree of the polynomial

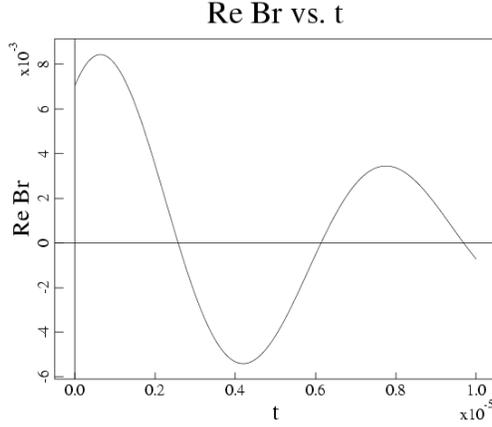


Figure 2: Shear Alfvén wave in a box with a significant electrical diffusivity. The measured quantities are qualitatively the same as in the case with zero resistivity.

basis functions. There were no results for cases with lumped mass matrices when  $p \geq 2$  because of the numerical problems described in the next paragraph. For  $p = 1$ , the convergence rates were near identical at 2 for both lumped and consistent mass matrices. However, lumped mass matrices gave significantly less accurate results. The results for  $p = 2$  with consistent mass matrices were not conclusive, but hinted at a convergence rate of 3. The  $p = 3$  consistent trials showed evidence of a convergence rate of 4. Both of these results are higher than the expected convergence rate for their respective polynomial basis function degrees.

The second set of trials included an electrical diffusivity of usually  $\eta/\mu_o = 1600 \text{ m}^2 \text{ s}^{-1}$  to prevent the numerical problems associated with lumping for  $p \geq 2$ . When the mass matrices were lumped in cases with zero electrical diffusivity, an explosive behavior occurred when the perturbed magnetic field was close to zero. The wave would suddenly divert from good behavior and increase inexplicably. Including a resistivity allowed the numerical solution to remain much more stable. Why this is the case is uncertain. This gives an instance where *ad hoc* lumping provides unacceptable errors.

The results for  $p = 1$  were verified by finding a convergence rate of 2 for both lumped and consistent mass matrices and poorer accuracy for the lumped trials. There were still problems with  $p = 2$ , disallowing reasonable solutions. For  $p = 3$  there was still fourth order convergence inferred for consistent mass matrices and second order convergence for lumped mass matrices.

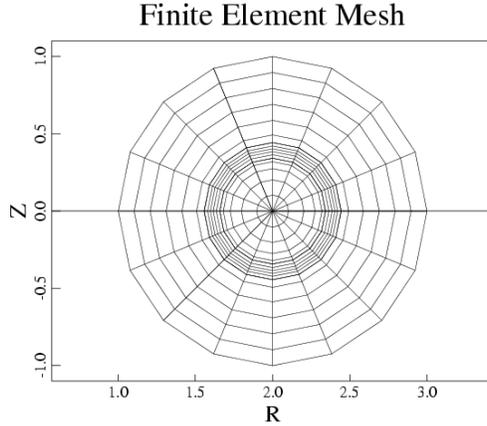


Figure 3: A 16x16 circular nonuniform mesh used for the linear resistive tearing mode test.

For  $p \geq 4$  it was very difficult to get convergence rates for trials with consistent mass matrices because of the extremely high accuracy achieved at low resolutions. However, the trials for lumped mass matrices were inaccurate enough that convergence rates were able to be obtained. There was significant evidence that the convergence rate remained close to 2 regardless of the degree of the polynomial for trials with lumped mass matrices. One danger with this conclusion is that the changes in solutions between runs were often  $10^{-3}$  times the solution, and high order convergence might not be recordable with solutions already this accurate. The fact that the results for lumped mass matrices were inaccurate enough to measure convergence rates shows that there is a definite disadvantage to the *ad hoc* lumped approximation, regardless of convergence rates.

## 2.2 Resistive Tearing Mode Test

In this section, we describe tests of a linear resistive tearing mode. Here, we define  $\Gamma$  as the growth rate of the tearing mode. These trials were done after the shear Alfvén trials, and are a more challenging computation for NIMROD. There is also the presence of a nonuniform circular mesh (see Fig. 3), allowing us to test convergence for a nonconstant  $\Delta x$ .

There was at first a general difficulty in using *ad hoc* lumped mass matrices with this test. Initially, the circular mesh trials with lumped mass matrices were not successful. This was traced back to a problem with the degenerate node at the center of the grid. In `rblock.f` there is a simplification in the Jacobian that

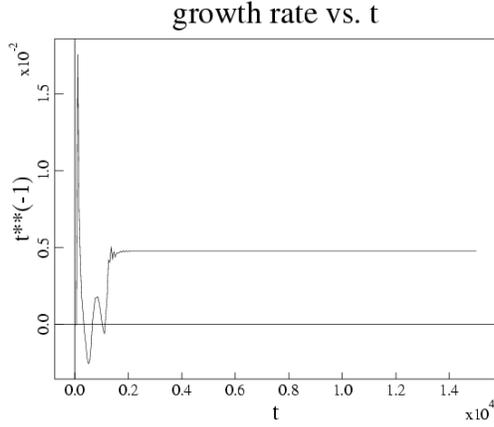


Figure 4: Typical result for growth rate vs. time. The recorded value was that of the converged flat line for higher  $t$ .

prevents the lumped mass for higher order elements from becoming singular. Cases with  $p \geq 2$  were not able to run while using this simplification. After commenting this simplification out, lumped cases were generally able to run smoothly.

With the initial input file, it was common that for low resolution lumped trials there would not be convergence of the growth rate. The simplest way to fix this problem was to increase the resistivity to make the eigenfunction smoother, but this tended to make the simulation less strenuous on NIMROD and hence convergence would be less well defined. Thus, a balance is needed to increase the resistivity enough to get enough working trials, but keeping it low enough so that we have a difficult enough simulation to measure a representative convergence rate. Generally, a range of resistivities was needed to ensure the results were realistic.

For  $p = 3$  it appears that  $C \approx 3$  for lumped mass matrices and  $C \approx 4$  for consistent mass matrices. The value for  $C$  with consistent mass matrices matches what was found from the shear Alfvén wave runs. However, the previous tests found that  $C \approx 2$  for lumped trials. Additional tests measuring the  $\kappa_{\nabla \cdot B}$  convergence rate further suggest that this is second order. Why this difference exists is uncertain.

The trials for  $p = 4$  showed that the lumped convergence rate was of order 2, drawing the same conclusion as before. The consistent mass matrix convergence rate was difficult to achieve so resistivities as low as  $2 \times 10^{-6} \Omega \cdot \text{m}$  were used, about a factor of 10-15 less than trials testing lumped mass matrices.

Test Type	Mass Matrix	Quantity	$p = 1$	$p = 2$	$p = 3$	$p = 4$
Wave Test	consistent	period	2	3	4	ND
Wave Test	lumped	period	2	NI	NI	NI
Damped Wave Test	consistent	period	2	NI	4	ND
Damped Wave Test	lumped	period	2	NI	2	2
Tearing Mode	consistent	growth rate	-	-	4	2-3
Tearing Mode	lumped	growth rate	-	-	3	2-3
Tearing Mode	consistent	$\ \nabla \cdot \mathbf{B}\ $	-	3	3	2-3
Tearing Mode	lumped	$\ \nabla \cdot \mathbf{B}\ $	-	3	2	3

Table 1: A summary of results comparing the convergence rates of NIMROD when using *ad hoc* lumped mass matrices and consistent mass matrices. These specific results should be considered approximate, but the general result that *ad hoc* lumped mass matrices provide much less accurate solutions has considerable evidence. NI indicates that numerical instabilities disallowed using this method, ND indicates the errors are not distinguishable, and a dash indicates no test was attempted.

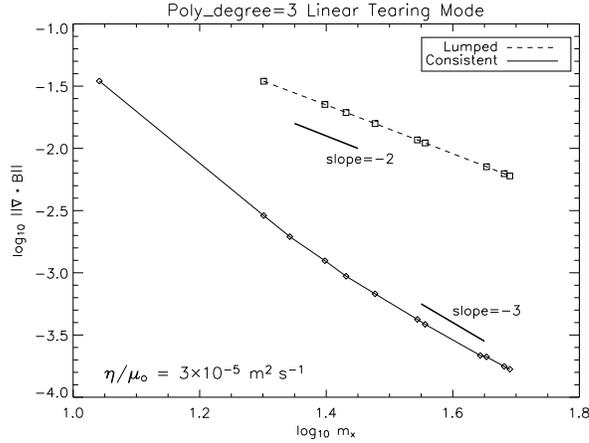


Figure 5:  $\|\nabla \cdot \mathbf{B}\|$  scalings for a linear resistive tearing mode. For  $p = 3$  the convergence rate is 3 for consistent mass matrices and 2 for *ad hoc* lumped mass matrices. The accuracy is also greatly reduced for the lumped case.

### 3 Summary of Accuracy and Convergence with *ad hoc* Lumped Mass Matrices

The results from the previous section are included in Table 1. The tests indicate that the *ad hoc* lumping scheme implemented in NIMROD as of October 2004 brings the convergence rate down to roughly second or third order convergence when using high order finite elements. An additional concern is that the accuracy for lumped trials has been shown to be much lower than for consistent trials. It is also typical for lumping to create numerical problems and add undesired and unphysical behavior to the code. In the shear Alfvén wave test, there was an explosive behavior associated with lumping in higher order elements. In the circular resistive tearing mode test, a combination of a low resistivity and lumping prevented convergence to a single well-defined growth rate in tests with low to moderate resolution. Both of these are significant departures from a stable numerical solution.

The recommendation of this paper is to not use the current implementation of lumping. However, this does not rule out other techniques, including optimal lumping [2]. As described in the next section, changing the polynomial basis functions allows a form of optimal lumping that in test cases maintains a high convergence rate without loss of accuracy.

### 4 Theory of Optimal Lumping

In Ref. [1], two additional lumping techniques are discussed. The first is HRZ lumping, a technique first advocated by Hinton, Rock, and Zienkiewicz [3]. With this method, only the diagonal elements of the mass matrix for each element are computed. Then each diagonal element is multiplied by the same constant so that the total mass of the element is correct. HRZ lumping is similar in principle to *ad hoc* lumping, and for many cases both will produce the same diagonal mass matrix. Thus, HRZ lumping is not expected to maintain a high order convergence rate any better than *ad hoc* lumping.

This brings us to the next technique described in Ref. [1]. Optimal lumping uses Lobatto quadrature to integrate the basis functions when determining the mass matrix [2]. The mathematics behind optimal lumping have been thoroughly investigated in Ref. [5]. An  $n$ -point Lobatto quadrature rule takes the form

$$\int_{-1}^{+1} f(x)dx \cong \sum_{i=1}^n w_i f(x_i) \quad (6)$$

with the weights being given by

$$w_i = \begin{cases} \frac{2}{n(n-1)} & \text{if } i \in \{1, n\} \\ \frac{2}{n(n-1)[P_{n-1}(x_i)]^2} & \text{if } i \notin \{1, n\} \end{cases} \quad (7)$$

Each nodal point  $x_i$  for  $i \notin \{1, n\}$  is the  $(i - 1)$ th zero of  $P'_{n-1}(x)$ , where  $P_k(x)$  is the Legendre polynomial of degree  $k$ . This is equivalent to  $x_i$  being the  $(i - 1)$ th maxima or minima of  $P_{n-1}(x)$ . An  $n$ -point Lobatto quadrature rule will exactly integrate a polynomial of degree  $2n - 1$ , and differs from normal Gaussian quadrature by including the endpoints in the integration scheme [7].

When using Lobatto quadrature for numerical integration, the nodes of the discrete sum lie at the zeros of the Legendre polynomials. This is particularly convenient when using a nodal expansion of the polynomial basis functions where the nodes lie at the same points because the integration scheme gives

$$\begin{aligned} \int_{-1}^1 \alpha_i(\mathbf{x})\alpha_j(\mathbf{x})dx &\cong \sum_{i=1}^n w_i\alpha_i(x_i)\alpha_j(x_i) \\ &= \begin{cases} 0 & \text{if } i \neq j \\ w_i & \text{if } i = j \end{cases} \end{aligned} \quad (8)$$

In essence, Lobatto quadrature naturally gives a diagonal mass matrix by not generating any nonzero off-diagonal elements.

I will give an example of optimal lumping with Lobatto quadrature for  $p = 3$  (cubic basis functions). This will require four quadrature points. Assume we are dealing with a one-dimensional element with  $x \in [-1, 1]$ . The nodes of integration will be at  $x_{1,4} = \pm 1$  and  $x_{2,3} = \pm 1/\sqrt{5}$  with weights  $w_{1,4} = 1/6$  and  $w_{2,3} = 5/6$  [4]. The basis functions are

$$\begin{aligned} \alpha_1(x) &= -\frac{5}{8}\left(x + \frac{1}{\sqrt{5}}\right)\left(x - \frac{1}{\sqrt{5}}\right)(x - 1) \\ \alpha_2(x) &= \frac{5\sqrt{5}}{8}(x + 1)\left(x - \frac{1}{\sqrt{5}}\right)(x - 1) \\ \alpha_3(x) &= -\frac{5\sqrt{5}}{8}(x + 1)\left(x + \frac{1}{\sqrt{5}}\right)(x - 1) \\ \alpha_4(x) &= \frac{5}{8}(x + 1)\left(x + \frac{1}{\sqrt{5}}\right)\left(x - \frac{1}{\sqrt{5}}\right) \end{aligned}$$

We then make the approximation

$$\int_{-1}^{+1} \alpha_i(x)\alpha_j(x)dx \cong \sum_{i=1}^4 w_i\alpha_i(x_i)\alpha_j(x_j) \quad (9)$$

When we do this summation, we find that  $\alpha_i(x_i)\alpha_j(x_i) = \delta_{ij}$ . Hence, there are no off-diagonal terms generated, and the numerically integrated mass matrix is

$$\mathbf{M} = \frac{1}{6} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (10)$$

You will note that the diagonal elements are in fact the weights of the 4-point Lobatto quadrature rule.

Optimal lumping has the nice property of being able to maintain a high order convergence rate. If  $p$  is the degree of the basis functions and  $m$  is the highest order derivative in the strain energy expression, then a quadrature rule with degree of precision  $2(p - m)$  will not reduce the convergence rate nor significantly reduce the accuracy [2]. The Lobatto quadrature is appropriate to do this, and has the additional property of having its weights be positive definite. Cook et. al. [1] warns that triangular and other types of elements may have some negative or zero values in an optimally lumped mass matrix. This is because it is not possible in general to specify a quadrature rule with fixed node locations and positive weights. The consequences of negative and zero masses is discussed in detail in [5].

## 5 Optimal Lumping with Gaussian Quadrature and Gauss-Legendre-Lobatto Nodes

The addition of Lobatto quadrature was attempted during this project, and it was noted there was a bug in the recursion relation for Legendre polynomials in the `legendre_poly` function in `polynomials.f`. The correct recursion relation for Legendre polynomials of degree  $\geq 2$  is given by [8]

$$P_n(x) = \frac{1}{n} [(2n - 1)xP_{n-1}(x) - (n - 1)P_{n-2}(x)]. \quad (11)$$

This function was called by `poly_nodes` to get the nodes for Gauss-Legendre-Lobatto (GLL) basis functions. The basis functions were still valid, but were not GLL polynomials.

Once this correction was made, we discovered that using GLL polynomials along with *ad hoc* lumping gave convergence at rates nearly identical to those when we used consistent mass matrices. In addition, the accuracy for these lumped mass matrices was very close to the accuracy when consistent mass matrices were used. Hence, it is not necessary to implement Lobatto quadrature in NIMROD to achieve optimal lumping (note that there are some possible restrictions given below). All that needs to be done for optimal lumping is to use GLL basis functions (to keep the node locations identical to the Lobatto nodes) along with normal *ad hoc* lumping.

The numerical results from a representative linear tearing mode case are shown in Fig. 6. Here we compare values for  $\|\nabla \cdot \mathbf{B}\|$  for the case of a consistent mass matrix with uniform nodes and a lumped mass matrix with GLL nodes. The lines essentially overlap. Lumping with this method did not reduce the accuracy or convergence rate of NIMROD. This result was tested for several different values of  $p$ , and they all show the same trend. It should be pointed out that for very coarse resolutions, consistent mass matrices give NIMROD a better chance of working than when using optimally lumped mass matrices. For example, in the case shown in Fig. 6, with  $m_x = 12$  the optimally lumped case did not converge to a single growth rate while the case using consistent mass matrices was successful.

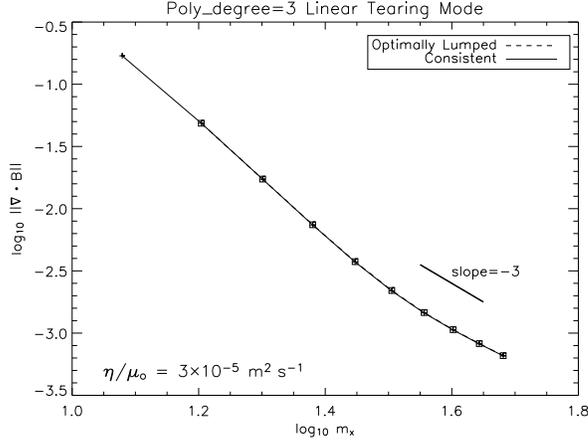


Figure 6: Results comparing  $\|\nabla \cdot \mathbf{B}\|$  when using consistent and optimally lumped mass matrices. Optimal lumping was brought about by using Gauss-Legendre-Lobatto nodes for the basis functions combined with the *ad hoc* lumping scheme previously in use. Consistent data points are marked by a plus and lumped data points are marked by a square. The setup for this case differs from Fig. 5 because of different values for the divergence cleaning coefficient.

To understand why the relationship between true lumping and the scheme used above, we can prove an equivalence between Lobatto and Gaussian quadrature rules as applied to mass matrices. The  $i$ th element of the lumped mass matrix for  $n$  basis functions is given by

$$\mathbf{M}_{L,ii} \equiv \sum_{j=1}^n \mathbf{M}_{ij} = \sum_{j=1}^n \left( \int_{-1}^{+1} \alpha_i(x) \alpha_j(x) dx \right) \quad (12)$$

where the summation is given over all basis functions. Each of the  $\alpha_i(x)$  and  $\alpha_j(x)$  are polynomials of degree  $n - 1$ . Note that by switching the summation and integration we can arrive at

$$\mathbf{M}_{L,ii} = \int_{-1}^{+1} \left( \alpha_i(x) \sum_{j=1}^n \alpha_j(x) \right) dx \quad (13)$$

Now define the polynomial

$$f(x) \equiv \sum_{j=1}^n \alpha_j(x) \quad (14)$$

At each of the  $n$  node locations  $x_i$  we have  $f(x_i) = 1$ . There is only one unique polynomial of degree  $n - 1$  that will interpolate these points, which tells us that

$f(x) \equiv 1$ . Hence we have

$$\mathbf{M}_{L,ii} = \int_{-1}^{+1} \alpha_i(x) dx \quad (15)$$

Given  $n$  nodal points, Gaussian quadrature will exactly integrate a polynomial of degree  $2n + 1$  and Lobatto quadrature will exactly integrate a polynomial of degree  $2n - 1$ . Since  $\alpha_i(x)$  is a polynomial of degree  $n - 1$  we have for all  $n$  that both Lobatto and Gaussian quadrature will integrate this function exactly.

Note that the only assumptions made about the nature of the basis functions are that they are polynomials of degree  $n - 1$  and that for each  $\alpha_i$  there will exist a point  $x_i$  such that  $\alpha_i(x_i) = 1$  and  $\alpha_i(x_j) = 0$  for all  $j \neq i$ . Lobatto and Gaussian quadrature will give identical lumped mass matrices as long as these assumptions are met. The difference between using Legendre and GLL nodes is that Lobatto quadrature naturally generates a diagonal mass matrix when used with GLL nodes, but not when used with Legendre nodes.

In NIMROD, the integrals are not over a single dimension. We need to multiply the integrand above by the Jacobian

$$J \equiv \frac{\partial R}{\partial x} \frac{\partial Z}{\partial y} + \frac{\partial R}{\partial y} \frac{\partial Z}{\partial x} \quad (16)$$

$R$  and  $Z$  are polynomials of  $x$  and  $y$ . Whether the equivalence between Gaussian and Lobatto quadrature for lumped masses holds depends on the Jacobian resulting from the mapping. If the sum of the degrees of the polynomials  $\alpha_i(x)$  and  $J$  is greater than  $2n - 1$  then Lobatto quadrature will no longer be exact. In the case where Gaussian quadrature is exact and Lobatto quadrature is not, it is not known whether Gaussian quadrature will continue to produce optimally lumped *ad hoc* mass matrices.

## 6 Summary and Conclusions

An analysis of mass matrix lumping in NIMROD was performed to determine whether lumping adversely effects the convergence rate and accuracy of the algorithm. Two lumping techniques were used, an *ad hoc* method, which simply sums the rows of the consistent mass matrix, and optimal lumping, which normally uses Lobatto quadrature and GLL node spacing to ensure that no off-diagonal mass matrix elements are generated. It was determined that *ad hoc* lumping significantly reduced both the accuracy and convergence rate in most test cases. After correcting an error in the recursion relation in the function `legendre_poly` in `polynomials.f` it was determined that optimal lumping does not require the implementation of Lobatto quadrature in the code. Using *ad hoc* lumping, Gauss-Legendre-Lobatto polynomials as basis functions, and Gaussian quadrature produces optimally lumped mass matrices. It remains to be seen whether using more complicated mappings will maintain this form of optimal lumping. The recommendation of this paper is to lump mass matrices

using the normal *ad hoc* scheme along with Gauss-Legendre-Lobatto polynomials.

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