D

Mass Matrix Diagonalization

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The construction of the consistent mass matrix (CMM) is fully defined by the choice of kinetic energy functional and shape functions. No significant procedural deviation is possible, other than possibly using reduced integration to obtain a singular matrix. On the other hand, the construction of a diagonally lumped mass matrix (DLMM) is not so clear cut, except for simple elements in which the lumping is uniquely defined by conservation and symmetry considerations. A consequence of this ambiguity is that various methods have been proposed in the literature, ranging from heuristic through algorithmic. A good discussion of mass diagonalization schemes starting from the CMM can be found in the textbook by Cook *et al.* [148]. Its use in explicit DTI is well covered in [74]. This Appendix gives a quick overview of proven methods, as well as a promising but as yet untried one.

§D.1. HRZ Lumping

This scheme is acronymed after the authors of [363]. It produces a DLMM given the CMM. Let m^e denote the total element mass. The procedure is as follows.

1. For each coordinate direction, select the DOFs that contribute to motion in that direction. From this set, separate translational DOF and rotational DOF subsets.
2. Add up the CMM diagonal entries pertaining to the translational DOF subset only. Call the sum S.
3. Apportion m^e to DLMM entries of both subsets on dividing the CMM diagonal entries by S.
4. Repeat for all coordinate directions.

The see HRZ in action, consider the three-node prismatic bar with CMM given by (17.2). Only one direction (x) is involved and all DOFs are translational. Excluding the factor $\rho A\ell/30$, which does not affect the results, the diagonal entries are 4, 4 and 16, which add up to $S = 24$. Apportion the total element mass $\rho A\ell$ to nodes with weights $4/S = 1/6$, $4/S = 1/6$ and $16/S = 2/3$. The result is the DLMM (17.3).

Next consider the 2-node Bernoulli-Euler plane beam element. Again only one direction (y) is involved but now there are translational and rotational freedoms. Excluding the factor $\rho A\ell/420$, the diagonal entries of the CMM (**?**), are 156, $4\ell^2$, 156 and $4\ell^2$. Add the translational DOF entries: $S = 156+156 = 312$. Apportion the element mass $\rho A\ell$ to the four DOFs with weights $156/312 = 1/2$, $4\ell^2/312 = \ell^2/78$, $156/312 = 1/2$ and $4\ell^2/312 = \ell^2/78$. The result is the DLMM (18.4) with $\alpha = 1/78$.

The procedure is heuristic but widely used on account of three advantages: easy to explain and implement, applicable to any element as long as a CMM is available, and retaining nonnegativity. The last attribute is particularly important: it means that the DLMM is physically admissible, precluding numerical instability headaches. As a general assessment, it gives reasonable results if the element has only translational freedoms. If there are rotational freedoms the results can be poor compared to customized templates.

Table D.1. One-Dimensional Lobatto Integration Rules

Points	*Abscissas* $\xi_i \in [-1, 1]$	*Weights* w_i
2	$-\xi_1 = 1 = \xi_2$	$w_1 = w_2 = 1$
3	$-\xi_1 = 1 = \xi_3,\ \xi_2 = 0$	$w_1 = w_3 = \frac{1}{3},\ w_2 = \frac{4}{3}$
4	$-\xi_1 = 1 = \xi_4,\ -\xi_2 = 1/\sqrt{5} = \xi_3$	$w_1 = w_4 = \frac{1}{6},\ w_2 = w_3 = \frac{5}{6}$

Common names: Trapezoidal rule and Simpson's rule for $p = 2, 3$, respectively.
In the $p = 4$ rule, interior points are not thirdpoints, since $1/\sqrt{5} \approx 0.447213596 \neq \frac{1}{3}$.
Lobatto rules with $5 \leq p \leq 10$, rarely important in FEM work, are tabulated in [2, Table 25.6].

Table D.2. One-Dimensional Newton-Cotes Integration Rules

Points	*Abscissas* $\xi_i \in [-1, 1]$	*Weights* w_i
2	Same as 2-point Lobatto; see Table D.1	
3	Same as 3-point Lobatto; see Table D.1	
4	$-\xi_1 = 1 = \xi_4,\ -\xi_2 = 1/3 = \xi_3$	$w_1 = w_4 = \frac{1}{4},\ w_2 = w_3 = \frac{3}{4}$
5	$-\xi_1 = 1 = \xi_5,\ -\xi_2 = 1/2 = \xi_4,\ \xi_3 = 0$	$w_1 = w_5 = \frac{7}{90},\ w_2 = w_3 = \frac{32}{90},\ w_3 = \frac{12}{90}$

Common names for $p = 4, 5$: Simpson's 3/8 rule and Boole's rule, respectively.
Additional NC formulas may be found in [2, Table 25.4]. For $p > 5$ they have negative weights.

§D.2. Lobatto Mass Lumping

A DLMM with n_F^e diagonal entries m_i is formally equivalent to a numerical integration formula with n_F^e points for the element kinetic energy:

$$T^e = \sum_{i=1}^{n_F^e} m_i T_i, \quad \text{where} \quad T_i = \tfrac{1}{2}\dot{u}_i^2 \tag{D.1}$$

Assume the element is one-dimensional (1D), possesses only translational DOF, and that its geometry is described by the natural coordinate ξ that varies from -1 through 1 at the end nodes. Then (D.1) can be placed in correspondence with the so-called *Lobatto quadrature* in numerical analysis. (Also called Radau quadrature by some authors, e.g. [130]; however the handbook [2, p. 888] says that Lobatto and Radau rules are slightly different.)

A Lobatto rule is a 1D Gaussian quadrature formula in which the endpoints of the interval $\xi \in [-1, 1]$ are sample points. If the formula has $p \geq 2$ abscissas, only $p - 2$ of those are free. Abscissas are symmetric about the origin $\xi = 0$ and all weights are positive. The general form is

$$\int_{-1}^{1} f(\xi)\, d\xi = w_1 f(-1) + w_p f(1) + \sum_{i=2}^{p-1} w_i f(\xi_i). \tag{D.2}$$

The rules for $p = 2, 3, 4$ are collected in Table D.1. Comparing (D.1) with (D.2) clearly indicates that if the nodes of a 1D element are placed at the Lobatto abscissas, the diagonal masses m_i are simply the weights w_i. This correspondence was first observed in [285], and further explored in [463,464]. For the type of elements noted, the equivalence works well for $p = 2, 3$. For $p = 4$ a minor difficulty arises: the interior Lobatto points are not at the thirdpoints, as can be seen in

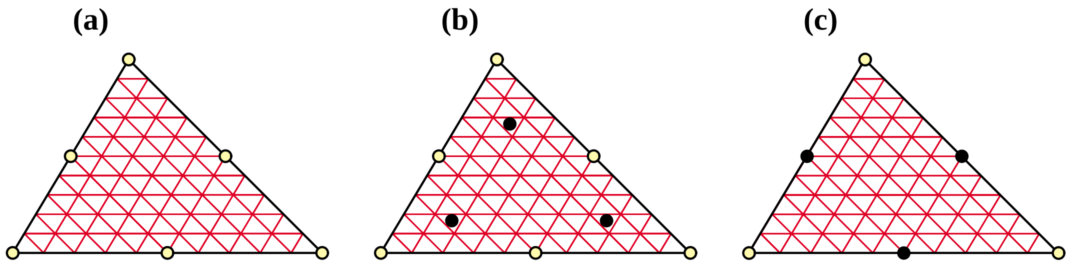

FIGURE D.1. A pair of degree-2, 3-point Gauss quadrature rules for the six-node plane stress triangle with constant metric: (a) node configuration; (b) the 3-interior point rule; (c) the 3-midpoint rule, which is a Lobatto rule for this node configuration. All weights are 1/3. Lines within triangle mark triangular natural coordinates (a.k.a. barycentric coordinates) of constant value, to illustrate constant metric.

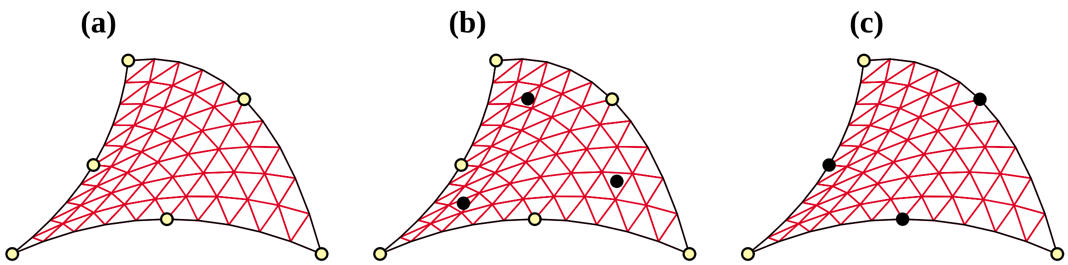

FIGURE D.2. As in Figure D.1, but triangle has now curved sides and variable metric.

Table D.1. If the element nodes are collocated there, one must switch to the "Simpson 3/8 rule", which is a Newton-Cotes formula listed in Table D.2. and adjust diagonal masses accordingly.

As a generalization to multiple dimensions, for conciseness we call *FEM Lobatto quadrature* one in which the DOF-endowed element nodes are sample points of an integration rule. (Sample points at other than nodal locations are precluded.) If so, the equivalence with (D.1) still holds. But one quickly runs into difficulties:

Negative Masses. If one insists in higher order accuracy, weights of 2D and 3D Lobatto rules are not necessarily positive, a feature noted in [203]. The subject is studied in detail in [285]. This shortcoming can be alleviated, however, by accepting lower accuracy, or sticking to product rules in suitable geometries. For example, applying a product 1D Lobatto rule over each side of a triangle or quadrilateral. Of course a more flexible alternative is provided by templates, because these allow the stiffness to be concurrently adjusted.

Rotational Freedoms. If the element has rotational DOF, Lobatto rules do not exist. Any attempt to extend (D.2) to node rotations inevitably leads to translation-rotation coupling.

Varying Properties. If the element is nonhomogeneous or has varying properties (for instance, a tapered bar element, or a plate of variable thickness) the construction of accurate Lobatto rules runs into additional difficulties, for the problem effectively becomes the construction of a quadrature formula with non-unity kernel.

As a general assessment, Lobatto mass lumping is useful when the diagonalization problem happens to fit a Gaussian quadrature rule with *element nodes as sample points* and *nonnegative weights*. Formulas of that type were developed for multidimensional domains of simple geometry during the 1950s and 60s. They are can be found in handbooks such as [706,707], along with many other rules.

As noted above, an obvious hindrance is the *emergence of negative weights* as the rule degree gets higher. This feature excludes those from contention except under extreme caution, whereas zero weights are less deadly. Rules useful for FEM work are compiled in [244], as well as Appendix I of [253], for seven element geometries.

The six-node plane stress triangle, shown in Figure D.1(a), illuminates obstacles typically encountered in multiple space dimensions. The total element mass is $m^e = \rho\, A\, h$, in which A denotes the plane area and h the plate thickness, assumed uniform. There are two 3-point Gauss quadrature rules of degree 2 for a constant metric triangle, shown in Figure D.1(b,c), which is extracted from [255]. The midpoint rule, illustrated in Figure D.1(c), is also a Lobatto rule for this element, but the 3-interior-point rule pictured in Figure D.1(b) is not.

Using the midpoint rule to build the DLMM results in three masses of $m^e/3$ collocated at the midpoints, while all corner masses vanish [203]. The HRZ scheme leads to the same result. This DLMM has rank 6 and rank deficiency 6. To attain full rank one must take some mass from the midpoints and move it to the corners: not a well defined process. An heuristic way out would be to apply the Simpson rule line lumping along the three edges. This results in $m^e/9$ at corners and $2m^e/9$ at midpoints but the degree drops to 1. To retain accuracy, a simultaneous change of the stiffness matrix could be tried within the template framework.

For a curved-side six-node triangle with variable metric, a case illustrated in Figure D.2, node and sample points remain at the same location in terms of natural coordinates, but local Jacobian determinants enter the formula.

§D.3. Nonconforming Velocity Shape Functions

This is a variational technique based on assuming velocity shape functions (VSF) that differ from the usual displacement shape functions (DSF). To produce a diagonal mass matrix, the VSF must satisfy additional "mass orthogonality" conditions that effectively decouples each VSF with respect to all others in the kinetic energy integral. This can be practically realized by making each VSF vanish at all points of a Gauss integration rule except one. Which rule? That appropriate to the correct integration of the kinetic energy over the element.

Rather than explaining the technique further, the interested reader may want to study the examples provided in Appendix V.

§D.4. Congruential Mass Transformation

A *congruential mass transformation*, or CMT, is a general framework than can be applied to transform a given *source* mass matrix into a *target* one. In particular all model reduction techniques mentioned in §H.3. Here it is specialized to the following case of importance in diagonalization:

(i) The source mass matrix $\mathbf{M}_S$ is nondiagonal and positive definite (PD); for example a CMM.

(ii) The target mass matrix $\mathbf{M}_T$ is diagonal and nonnegative (that is, zero diagonal entries are permitted)

Both matrices have order n_{DOF}. The congruential transformation that converts source to target is

$$\mathbf{M}_T = \mathbf{H}^T\, \mathbf{M}_S\, \mathbf{H}. \tag{D.3}$$

If $\mathbf{H}$ is nonsingular, the inverse mapping is $\mathbf{M}_S = \mathbf{G}^T \mathbf{M}_T \mathbf{G}$, in which $\mathbf{G} = \mathbf{H}^{-1}$. We will say that $\mathbf{M}_S$ and $\mathbf{M}_T$ are *congruentially linked* through $\mathbf{H}$. Even if $\mathbf{M}_S$ and $\mathbf{M}_T$ are both given and parameter-free, there are generally many $\mathbf{H}$ matrices that satisfy (D.3). In fact the number of solutions typically grows exponentially with n_{DOF}.

One particular form, however, is unique under conditions (i)-(ii). Perform the Cholesky factorization $\mathbf{M}_S = \mathbf{L}_S \mathbf{L}_S^T = \mathbf{L}_S \mathbf{U}_S$, where $\mathbf{L}_S$ is lower triangular and $\mathbf{U}_S = \mathbf{L}_S^T$ is upper triangular. If $\mathbf{M}_S$ is PD, this factorization is unique and both $\mathbf{L}_S$ and $\mathbf{U}_S$ are nonsingular [797]. Let $\mathbf{M}_T^{1/2}$ be the principal square root of $\mathbf{M}_T$, obtained by taking the positive square root of each diagonal entry. By inspection

$$\mathbf{H} = \mathbf{U}_S \mathbf{M}_T^{1/2}, \qquad \mathbf{H}^T = \mathbf{M}_T^{1/2} \mathbf{L}_S^{-1}. \tag{D.4}$$

This will be called the *Cholesky form* of $\mathbf{H}$, and identified by subscript 'CF' if necessary. Since the inverse of a nonsingular upper triangular matrix is also lower triangular, and scaling by the diagonal matrix $\mathbf{M}_T^{1/2}$ does not alter that configuration, $\mathbf{H}^T$ and $\mathbf{H}$ are lower and upper triangular, respectively.

As an example, the CMM and DLMM of the two-node prismatic bar given in (**?**) are linked by the Cholesky form

$$\mathbf{H}_{CF} = \frac{1}{\sqrt{2}} \begin{bmatrix} \sqrt{3} & -1 \\ 0 & 2 \end{bmatrix} = \begin{bmatrix} 1.22474 & -0.707107 \\ 0 & 1.41421 \end{bmatrix}. \tag{D.5}$$

For the CMM and DLMM of the three-node prismatic bar studied in **?**, the Cholesky form is

$$\mathbf{H}_{CF} = \begin{bmatrix} \sqrt{5}/2 & 1/(2\sqrt{3}) & -\sqrt{2/3} \\ 0 & 2/\sqrt{3} & -\sqrt{2/3} \\ 0 & 0 & \sqrt{3/2} \end{bmatrix} = \begin{bmatrix} 1.180303 & 0.288675 & -0.816497 \\ 0 & 1.154701 & -0.816497 \\ 0 & 0 & 1.224745 \end{bmatrix}. \tag{D.6}$$

The Cholesky form of (D.3) is unique and easy to obtain, but does not link naturally to the algebraic Riccati equation mentioned below. For that purpose finding a symmetric $\mathbf{H}$ is more convenient. Those will be identified by subscript 'Sy' if necessary. Symmetric forms are not unique; in fact typically one generally finds $2^{n_{DOF}}$ different solutions. It is rather easy, however, to extract a principal solution.

For the two-node prismatic bar, the transformation (D.3) from CMM to DLMM with symmetric $\mathbf{H}$ has $2^2 = 4$ solutions. The only one with positive eigenvalues is

$$\mathbf{H}_{Sy} = \tfrac{1}{2} \begin{bmatrix} 1+\sqrt{3} & 1-\sqrt{3} \\ 1-\sqrt{3} & 1+\sqrt{3} \end{bmatrix} = \begin{bmatrix} 1.366025 & -0.366025 \\ -0.366025 & 1.366025 \end{bmatrix}. \tag{D.7}$$

For the 3-node pristamic bar, one gets $2^3 = 8$ solutions. The only one with all eigenvalues positive is (only given numerically, as its analytical expression is complicated):

$$\mathbf{H}_{Sy} = \begin{bmatrix} 1.2051889 & 0.2051889 & -0.1472036 \\ 0.2051889 & 1.2051889 & -0.1472036 \\ -0.1472036 & -0.1472036 & 1.1518024 \end{bmatrix}. \tag{D.8}$$

The determination of $\mathbf{H}$ in (D.3) is related to the quadratic matrix equation $\mathbf{X}^T \mathbf{A} \mathbf{X} = \mathbf{B}$, where $\mathbf{M}_S \to \mathbf{A}$ and $\mathbf{M}_T \to \mathbf{B}$ are data and $\mathbf{H} \to \mathbf{X}$ the unknown. If $\mathbf{H} \to \mathbf{X}$ is symmetric so $\mathbf{X}^T = \mathbf{X}$, the equation $\mathbf{X}\,\mathbf{A}\mathbf{X} = \mathbf{B}$ is a specialization of the algebraic Riccati equation extensively studied in optimal control systems [7,433]. Hopefully this interdisciplinary resource could be eventually be applied to devise robust mass diagonalization schemes using a matrix function library [359]. But as of now, templates remain the most practical method to find optimal diagonalizations.