constrained boundary conditions

We explain the principle of using **Lagrange multipliers** to solve **linear systems** under **affine constraints** resulting from the imposition of kinematic boundary conditions. The stiffness matrix that is obtained is no longer positive definite. As a result, certain solution algorithms become unusable.

We therefore seek a technique that will permit us to continue to use the $\mathbf{LDL}^T$ factorization algorithm **without permutation and without elimination**. The proposed technique is called "double Lagrange" (and used in the `Castem2000` code). This technique is shown to be effective. We give some indications on the conditioning of the matrices obtained by this technique.

The problem of the search for the **eigenmodes of constrained systems** is then examined. We show that a possible solution is to add **dualized** boundary conditions dualized to the stiffness matrix and not to modify the mass matrix.

11.2.1. Introduction

We are interested in this document in the dualization of the boundary conditions (say kinematics). Two distinct linear algebra problems are examined:

- the solution of linear systems: sections 2, 3, 4, 5, 6,
- the search for the eigenmodes: section 7

11.2.2. Dualization of kinematic boundary conditions, Lagrange multipliers

In `Code_Aster` (as in other finite element codes), one is required to to solve many linear systems.

Such a system can often be regarded as the result of the minimization of a positive quadratic functional $\mathcal{J}(\mathbf{u})$ where $\mathbf{u}$ belongs to $\mathbb{R}^n$ where n is the number of nodal unknowns. The minimization problem is subject to a set of constraints of the form $C_i(\mathbf{u}) - \mathbf{d}_i = 0$ which arise from Dirichlet boundary conditions.

It is in this problem of minimization under affine constraints that we are interested here. In the rest of this document, we will take as an example the case (and the vocabulary) of linear static mechanics. We will speak of stiffness matrix, of displacement vector, but the proposed technique remains valid for problems involving heat transfer, whether linear or nonlinear.

The discrete minimization problem can be stated as:

$$\min_{\mathbf{u} \in V \subset \mathbb{R}^n} \mathcal{J}(\mathbf{u})$$

where:

- $\mathcal{J}(\mathbf{u})$ is a quadratic form (total potential energy) given by

  $$\mathcal{J}(\mathbf{u}) = \frac{1}{2}(\mathbf{A}\mathbf{u}, \mathbf{u}) - (\mathbf{b}, \mathbf{u})$$

  $\mathbf{A}$ is a symmetric, positive semidefinite, matrix such that $(\mathbf{A}\mathbf{u}, \mathbf{u}) \geq 0 \ \forall \ \mathbf{u}$, but not necessarily invertible ($\mathbf{A}\mathbf{u} = 0$ is possible for $\mathbf{u} \neq 0$)

- V is the space of kinematically acceptable displacements (it is an affine subspace of $\mathbb{R}^n$)

This discrete problem is solved numerically by setting the derivative of $\mathcal{J}(\mathbf{u})$ in V to zero. That leads to a linear system of equations that can be solved for $\mathbf{u}$. The problem is to find the derivative of $\mathcal{J}(\mathbf{u})$ in $V \in \mathbb{R}^n$.

In general, for practical reasons, the expression for $\mathcal{J}(\mathbf{u})$ is calculated in the basis of the nodal displacements (without taking account of the constraints): $\mathbf{u}$ then belongs to $\mathbb{R}^n$ where n is the total number of nodal unknowns.

- If V is a vector subspace of $\mathbb{R}^n$ generated by $(n - p)$ nodal displacements as basis, the derivative of $\mathcal{J}(\mathbf{u})$ in V is computed in a straightforward manner: it is enough to “forget” in the matrices $\mathbf{A}$ and $\mathbf{b}$ rows and columns that correspond to the p fixed displacements $(u_i = 0)$.
- If the constrained degrees of freedom are not zero but assigned a given value $(u_i = d_i)$, it is necessary to modify $\mathbf{b}$.
- Finally, if the constraints ared “mixed” (linear relations between unknown degrees of freedom) it is necessary to modify both $\mathbf{A}$ and $\mathbf{b}$.

The Lagrange multiplier method makes it possible to solve the problem without modifying matrices $\mathbf{A}$ and $\mathbf{b}$. The price that is paid for this convenience is an increase in the number of unknowns in the system to be solved.

Instead of solving the problem in space V of dimension $n - p$, one solves it in the space $\mathbb{R}^n + p$ with the additional unknown factors λ_i being called Lagrange multipliers.

11.2.2.1. Principle and justification

The formal definition of space V for the three cases listed above, can be expressed as two minimization problems.

Problem 1

$$\begin{aligned}
&\min_{\mathbf{u} \in V} \mathcal{J}(\mathbf{u}) \\
&\mathcal{J}(\mathbf{u}) = \frac{1}{2}(\mathbf{A}\mathbf{u}, \mathbf{u}) - (\mathbf{b}, \mathbf{u}) \\
&V = \{\mathbf{u} \in \mathbb{R}^n / C_i(\mathbf{u}) = d_i, \ \ \forall \ \ i = 1, p\}
\end{aligned}$$

Here, C_i are linear functions on $\mathbb{R}^n$ and d_i are constant data. We also assume that the p linear relations C_i are independent, i.e., the dimension of the space generated by C_i is p.

We can show (see Appendix 1) that this problem is equivalent to the following:

Problem 2

$$\begin{aligned} &\text{Find } \mathbf{u} \in \mathbf{V} \text{ where} \\ &\qquad \mathbf{V} = \{\mathbf{u} \in \mathbb{R}^n / C_i(\mathbf{u}) = d_i, \ \forall \ i = 1, p\} \\ &\text{such that } (\mathbf{A}\mathbf{u} - \mathbf{b})\mathbf{v} = 0 \ \forall \ \mathbf{v} \in \mathbf{V}_0 \text{ where} \\ &\qquad \mathbf{V}_0 = \{\mathbf{v} \in \mathbb{R}^n \text{ such that } C_i(\mathbf{u}) = 0, \ \forall \ i = 1, p\} \end{aligned}$$

Problem 2 can also be expressed as follows.

Problem 3

$$\begin{aligned} &\text{Find } \mathbf{u} \in \mathbf{V} \\ &\text{such that} \\ &\text{(a)} \qquad \mathbf{C}_i\mathbf{u} = \mathbf{d}_i \ \forall \ i \\ &\text{(b)} \qquad \mathbf{C}_i\mathbf{v} = 0 \ \forall \ \mathbf{v} \in \mathbf{V}_0 \\ &\text{(c)} \qquad (\mathbf{A}\mathbf{u} - \mathbf{b})\mathbf{v} = 0 \ \forall \ \mathbf{v} \in \mathbf{V}_0 \end{aligned} \tag{11.2.1}$$

equations (11.2.1) (b) and (c) show (while identifying $\mathbb{R}^n$ and its dual) that

- $\mathbf{C}_i$ is orthogonal to $\mathbf{V}_0$ for all i
- $(\mathbf{A}\mathbf{u} - \mathbf{b})$ is also orthogonal to $\mathbf{V}_0$

where $\mathbf{V}_0$ is the $n - p$ dimensional subspace of the vector space $\mathbb{R}^n$ which is orthogonal to the space spanned by the constraints $\{\mathbf{C}_i \ , i = 1, p\}$ because the p constraints are independent.

Since the decomposition of $\mathbb{R}^n$ into the sum of two orthogonal subspaces is unique, it follows that $(\mathbf{A}\mathbf{u} - \mathbf{b})$ belongs to the subspace generated by the constraints $\mathbf{C}_i$.

There thus exists a family of scalars λ_i called Lagrange multipliers such that

$$(\mathbf{A}\mathbf{u} - \mathbf{b}) + \sum_i \lambda_i \mathbf{C}_i = 0$$

This equality is true in $\mathbb{R}^n$.

Problem 3 can then be expressed as follows.

Problem 4

$$\begin{aligned} &\text{Find } \mathbf{u} \in \mathbb{R}^n \ , \ \ \lambda_i \in \mathbb{R}, \ , \ \ i = 1 \dots p \\ &\quad \text{s.t.} \ \forall \ \ i \in 1 \dots p \\ &\qquad \mathbf{C}_i\mathbf{u} = \mathbf{d}_i \\ &\qquad (\mathbf{A}\mathbf{u} - \mathbf{b}) + \sum_i \lambda_i \mathbf{C}_i = 0 \end{aligned}$$

We can also recover Problem 3 from Problem 4 as follows.

If there exist λ_i such that

$$(\mathbf{Au} - \mathbf{b}) + \sum_i \lambda_i \mathbf{C}_i = 0$$

then

$$(\mathbf{Au} - \mathbf{b})\mathbf{v} = -\left(\sum_i \lambda_i \mathbf{C}_i\right)\mathbf{v} = 0 \ \ \forall \mathbf{v} \in \mathbf{V}_0$$

Problem 4 is the one that we seek. It is referred to here as the problem with **dualized kinematic conditions**. In matrix form, this problem can be written as:

$$\begin{bmatrix} \mathbf{A} & \mathbf{C}^T \\ \mathbf{C} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{d} \end{bmatrix} \qquad (11.2.2)$$

or

$$\mathbf{KX} = \mathbf{F}$$

where

$$\mathbf{u} \in \mathbb{R}^n \ , \ \ \lambda \in \mathbb{R}^p \ , \ \ \mathbf{X} \in \mathbb{R}^{n+p}$$
$$\mathbf{A} \in \mathbb{R}^n \times \mathbb{R}^n \ , \ \ \mathbf{C} \in \mathbb{R}^p \times \mathbb{R}^n \ , \ \ \mathbf{K} \in \mathbb{R}^{n+p} \times \mathbb{R}^{n+p}$$

This problem can be interpreted as the extremum of the functional

$$\mathcal{L}(\mathbf{u}, \lambda) = \tfrac{1}{2}(\mathbf{Au}, \mathbf{u}) - (\mathbf{b}, \mathbf{u}) + \lambda(\mathbf{Cu} - \mathbf{d}) \qquad (11.2.3)$$

This functional is called the Lagrangian of the initial problem. The main advantage of this method is that it incorporates the constraints in the system of equations: $\mathbf{u}$ and λ are sought in $\mathbb{R}^n$ and $\mathbb{R}^p$ ($\mathbf{X}$ in $\mathbb{R}^{n+p}$.

The coefficients λ_i are called the Lagrange coefficients of the problem (sometimes just the "Lagrange").

11.2.3. Disadvantages of this dualization

From the expression of the Lagrangian (11.2.2), we can see that the matrix $\mathbf{K}$ is not positive definite any longer (unlike $\mathbf{A}$). In effect, if there exists a $\mathbf{u}_0$ for which $\mathbf{Cu}_0 \neq 0$ then there exists a λ_0 for which $\mathcal{L}(\mathbf{u}_0, \lambda_0) \ldots = \tfrac{1}{2}(\mathbf{Au_0}, \mathbf{u_0}) + \lambda_0 \mathbf{Cu}_0 < 0$.

The loss of positive definiteness of $\mathbf{K}$ implies that the the system $\mathbf{KX} = \mathbf{F}$ cannot be solved (in general) by classical gradient algorithms or by Cholesky factorization. The $\mathbf{LDL}^T$ factorization algorithms without permutation of rows and columns is not guaranteed either: it is the latter algorithm which one wants to be able to continue to use.

Necessary and sufficient conditions for $\mathbf{LDL}^T$ (without permutation)

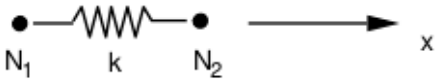
The block submatrix $\mathbf{K}_i$ of $\mathbf{K}$ is formed from the first i rows and columns of $\mathbf{K}$ (i.e., if $\mathbf{K}$ is of order n then $\mathbf{K}_n = \mathbf{K}$ and if $n = 1$ then $\mathbf{K}_1 = [k_{11}]$).

There will be no zero pivot in the $\mathbf{LDL}^T$ algorithm if and only if $\mathbf{K}_i$ is invertible for all $i \in [1, n]$.

Let us call this requirement `cond1` .

Let us illustrate the problem with the following example.

Example 1:



A spring of stiffness k connects 2 nodes N1 and N2. This problem involves 2 unknowns ($n = 2$): u_1, u_2 and 2 nodal forces: f_1, f_2. The stiffness matrix is

$$\mathbf{A} = \begin{bmatrix} k & -k \\ -k & k \end{bmatrix}$$

Consider a constraint ($p = 1$) that ties the unknowns at the two nodes,

$$\alpha u_1 + \beta u_2 = \gamma$$

The dualized problem is written as $\mathbf{KX} = \mathbf{F}$ where

$$\mathbf{K} = \begin{bmatrix} k & -k & \alpha \\ -k & k & \beta \\ \alpha & \beta & 0 \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} u_1 \\ u_2 \\ \lambda \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} f_1 \\ f_2 \\ \gamma \end{bmatrix}$$

The matrix $\mathbf{K}$ is written according to the ordering of the unknowns. For example, if the order of the components of $\mathbf{X}$ is

- $\mathbf{X} = (u_1, u_2, \lambda)$, then

$$\mathbf{K} = \begin{bmatrix} k & -k & \alpha \\ -k & k & \beta \\ \alpha & \beta & 0 \end{bmatrix}$$

and

$$\mathbf{K}_2 = \begin{bmatrix} k & -k \\ -k & k \end{bmatrix}$$

which is not invertible (determinant is 0). Therefore, cond1 is not satisfied.

- $\mathbf{X} = (\lambda, u_1, u_2)$, then

$$\mathbf{K} = \begin{bmatrix} 0 & \alpha & \beta \\ \alpha & k & -k \\ \beta & -k & k \end{bmatrix}$$

and

$$\mathbf{K}_1 = [0]$$

which is not invertible. Therefore, cond1 is not satisfied.

- $\mathbf{X} = (u_1, \lambda, u_2)$, then

$$\mathbf{K} = \begin{bmatrix} k & \alpha & -k \\ \alpha & 0 & \beta \\ -k & \beta & k \end{bmatrix}$$

In this case

$$\det \mathbf{K}_1 = k, \quad \det \mathbf{K}_2 = \alpha^2, \quad \det \mathbf{K}_3 = -k(\alpha + \beta)^2$$

- k is the spring stiffness, hence strictly positive
- $\mathbf{K}_3$ is invertible only if $\alpha + \beta \neq 0$. The case $\alpha + \beta = 0$ corresponds to a "bad" physical condition, rigid-body motion ($u_1 - u_2 = \text{constant}$) without energy.

  So the problem has a singular solution. It is necessary that the constraint conditions generate a space of acceptable displacements which do not contain any rigid body motion.

  Using the notation of [1] one can write:

$$\ker \mathbf{A} \cap \mathbf{V}_0 = \{0\}$$

  In the rest of the document we will assume that this condition is checked (or at least whether the constraint leads to rigid body motion). When this condition is checked and the constraints $\mathbf{C}_i$ are linearly independent, one will say that the problem is physically well-posed.
- $\mathbf{K}_2$ is invertible only if $\alpha \neq 0$ and the condition cond1 is met only if this is true..

  If constraint $\alpha u_1 + \beta u_2 = \gamma$ is reduced to:

  - $u_1 = \delta$, i.e., $(\alpha, \beta) = (1, 0)$, then cond1 is satisfied
  - $u_2 = \delta$, i.e., $(\alpha, \beta) = (0, 1)$, then cond1 is not satisfied

  From the symmetry of the problem, it can be seen that for the LDL algorithm to be usable for the case where $(\alpha, \beta) = (0, 1)$, it is necessary that the permutation $\mathbf{X} = (u_2, \lambda, u_1)$ be used (the first and last columns have to be interchanged).

From this very simple example, one can draw some general conclusions (all negative):

- if the Lagrange multipliers λ_i are all added to the matrix after the unknowns $\mathbf{u}_i$, if $\mathbf{A}$ is singular, the condition cond1 will not be satisfied for $\mathbf{K}_i = \mathbf{A}$

- in a constraint $\mathbf{Cu} = \mathbf{d}$, not all the n unknown values of $\mathbf{u}$ are typically used and only a subset are constrained. If the associated Lagrange multiplier (λ) is placed before a degree of freedom that the constraint is applied to, then condition cond1 will not be satisfied.

  For example, if the j th row/column is associated with λ, then the matrix $\mathbf{K}_j$ has the form

$$\mathbf{K}_j = \begin{bmatrix} \mathbf{K}_{j-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

  and is therefore singular.

- for the case of a physical structure which, by bad luck, is supported by its physical last degree of freedom, i.e., such that if one does not prescribe this dof the matrix is singular, but if one prescribes it, the matrix becomes invertible. The use of a multiplier λ for this constraint is impossible. Indeed, if one orders λ such that it comes before the last degree of physical freedom, there will be a null pivot on the row of λ , and if one numbers it after (thus making it the last degree of freedom), the matrix $\mathbf{K}_{n-1}$ will not be invertible since the constraint has not yet been taken yet into account. One will see in section The "double Lagrange" technique that the "double Lagrange" technique makes it possible to solve this problem.

To conclude this section we make the following remark: If $\mathbf{K}$ is invertible, one knows that there exists a permutation of the unknowns that makes it possible to factorize $\mathbf{K}$ using $\mathbf{LDL}^T$. This ordering can be that resulting from the algorithm with permutation allowed (based on the maximum pivot, for example). But this ordering relates to only the rows of the matrix; there is thus a loss of symmetry of $\mathbf{K}$. Consider the following example.

Example

$$\mathbf{A} = [0]\ ,\quad \mathbf{C} = [1]\ ,\quad \mathbf{K} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \mathbf{X} = \begin{bmatrix} \mathbf{u} \\ \lambda \end{bmatrix}$$

mathbf{K} is invertible, but there does not exist any common permutation of the lines and columns of mathbf{K} allowing a resolution by $\mathbf{LDL}^T$.

These observations show that the Lagrange dualization proposed in this section does not make it possible to use $\mathbf{LDL}^T$ without permutation.

11.2.4. The "double Lagrange" technique

This method is based on the approach used in the `CASTEM 2000` code (developed by Th. CHARAS and P. VERPEAUX).

From (11.2.2) it can seen that the matrix form of the dual problem has zero terms on the diagonal that correspond to the Lagrange degrees of freedom. This property is also observed in the Lagrangian problem (11.2.3) because there are no quadratic terms in λ.

The null diagonal terms prevent certain permutations of rows and columns: one can only place a Lagrange multiplier before the physical degrees of freedom it constrains.

The “double Lagrange” idea is to break up each Lagrange multiplier into 2 equal parts, λ^1 and λ^2. The constraint equation $\mathbf{Cu} = \mathbf{d}$ is then replaced by:

$$\mathbf{Cu} - \alpha(\lambda^1 - \lambda^2) = \mathbf{d} \quad \text{and} \quad \mathbf{Cu} + \alpha(\lambda^1 - \lambda^2) = \mathbf{d}$$

where α is a non-zero constant.

To see the equivalence of the old problem and the new one, observe that:

Problem 1 : Simple Lagrange

$$\text{Find} \begin{cases} \mathbf{u} \in \mathbb{R}^n \\ \lambda \in \mathbb{R}^p \end{cases}$$
$$\text{such that} (S) : \begin{cases} \mathbf{Au} + \mathbf{C}^T\lambda = \mathbf{b} \\ \mathbf{Cu} = \mathbf{d} \end{cases}$$

We can split the multiplier and write

$$(S) : \begin{cases} \lambda^1 = \lambda^2 \\ \lambda = \lambda^1 + \lambda^2 \\ \mathbf{Au} + \mathbf{C}^T\lambda = \mathbf{b} \\ \mathbf{Cu} = \mathbf{d} \end{cases}$$
$$\leftrightarrow$$
$$(S) : \begin{cases} \mathbf{Au} + \mathbf{C}^T\lambda^1 + \mathbf{C}^T\lambda^2 = \mathbf{b} \\ \mathbf{Cu} - \alpha\lambda^1 + \alpha\lambda^2 = \mathbf{d} \\ \mathbf{Cu} + \alpha\lambda^1 - \alpha\lambda^2 = \mathbf{d} \end{cases}$$

From the above we can write the problem in alternative form as,

Problem 2 : Double Lagrange

$$\text{Find} \begin{cases} \mathbf{u} \in \mathbb{R}^n \\ \lambda^1, \lambda^2 \in \mathbb{R}^p \times \mathbb{R}^p \end{cases}$$
$$\text{such that} (S) : \begin{cases} \mathbf{Au} + \mathbf{C}^T\lambda^1 + \mathbf{C}^T\lambda^2 = \mathbf{b} \\ \mathbf{Cu} - \alpha\lambda^1 + \alpha\lambda^2 = \mathbf{d} \\ \mathbf{Cu} + \alpha\lambda^1 - \alpha\lambda^2 = \mathbf{d} \end{cases}$$

In matrix form:

$$\begin{bmatrix} \mathbf{A} & \mathbf{C}^T & \mathbf{C}^T \\ \mathbf{C} & -\alpha\mathbf{I} & \alpha\mathbf{I} \\ \mathbf{C} & \alpha\mathbf{I} & -\alpha\mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \lambda^1 \\ \lambda^2 \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{d} \\ \mathbf{d} \end{bmatrix}$$
or
$$\mathbf{K}^\star\mathbf{X}^\star = \mathbf{F}^\star$$

The associated Lagrangian is

$$\mathcal{L}(\mathbf{u}, \lambda^1, \lambda^2) = \tfrac{1}{2}(\mathbf{Au}, \mathbf{u}) - (\mathbf{b}, \mathbf{u}) + (\lambda^1, \mathbf{Cu} - \mathbf{d}) + (\lambda^2, \mathbf{Cu} - \mathbf{d}) - \frac{\alpha}{2}(\lambda^1 - \lambda^2, \lambda^1 - \lambda^2)$$

One can show (see Appendix 2) that if one observes certain rules of ordering of the unknowns, and by choosing the constant $\alpha > 0$, the matrix $\mathbf{K}^\star$ satisfies the condition cond1.

This rule can briefly be expressed as follows. Suppose a constraint relation $\mathbf{Cu} - \mathbf{d} = 0$ corresponds to the 2 Lagrange multipliers λ^1 and λ^2. This relation utilizes a certain number of physical degrees of freedom.

Rule R0

For each constraint relation, it is necessary to place λ^1 before the first degree of freedom that is constrained and λ^2 after the last degree of freedom constrained.

To decrease the memory needed to store matrix $\mathbf{K}$, it is necessary to minimize the bandwidth. `Code_Aster` achieves this by "framing" the relations "with the closest" constraints: λ^1 is placed right before the first constrained degree of freedom, and λ^2 is placed just after the last constrained last dof.

Illustration

Consider a problem with 4 physical degrees of freedom: u_1, u_2, u_3, u_4. This system is subjected to 2 constraints:

$$\begin{cases} a_{11}u_1 + a_{13}u_3 = b_1 \\ a_{22}u_2 + a_{24}u_4 = b_2 \end{cases}$$

Let the Lagrange multiples associated with the first condition be λ_1^1, λ_1^2 and those associated with the second condition be λ_2^1, λ_2^2.

If we assume that the degrees of freedom are ordered: u_1, u_2, u_3, u_4, the global ordering of the degrees of freedom determined by `Aster` is then:

$$\lambda_1^1, u_1, \lambda_2^1, u_2, u_3, \lambda_1^2, u_4, \lambda_2^2$$

That is,

- λ_1^1, λ_1^2 frame the "closer" constrained degrees of freedom (u_1 and u_3)
- λ_2^1, λ_2^2 frame the "closer" constrained degrees of freedom (u_2 and u_4)

The "double Lagrange" technique, in conjunction with Rule R0, thus allows the solution of any linear system that is physically well-posed with the $\mathbf{LDL}^T$ algorithm without permutation.

Note

This demonstration supposes, nevertheless, that matrix $\mathbf{A}$ is symmetric and positive semi-definite (not necessarily positive definite).

Note that a symmetric and positive matrix is necessary for LDLT (or LU) decompositions without permutation. Two counterexamples are given below:

- Symmetric but non-positive:

$$\mathbf{A} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

- Positive but non-symmetric :

$$\mathbf{A} = \begin{bmatrix} 0 & 1 \\ -1 & 1 \end{bmatrix}$$

11.2.5. Additional advantage

In this section we show that the "double Lagrange" technique can make it possible to economically solve a series of problems which differ only by their kinematic boundary conditions (for example, in a variable zone of contact).

Warning

This possibility is not currently exploited in the code.

Suppose we have a system with constraints: $\mathbf{KX} = \mathbf{X}$. Let us write this system while emphasizing a particular constraint, $\mathbf{Cu} - \mathbf{d} = 0$. Note that this calculation remains valid even when there are several constraints. To simplify matters, let us choose $\alpha = 1$.

In that case, we have

- λ^1 is the first Lagrange degree of freedom associated with the constraint
- λ^2 is the second Lagrange degree of freedom associated with the constraint

- $\mathbf{U} = \mathbf{X} - \{\lambda^1, \lambda^2\}$
- $\tilde{\mathbf{K}}$ is the matrix $\mathbf{K}$ projected on $\mathbf{U}$
- $\tilde{\mathbf{b}}$ is the vector $\mathbf{F}$ projected on $\mathbf{U}$

The system can then be written with these variables as

$$\begin{bmatrix} \tilde{\mathbf{K}} & \mathbf{C}^T & \mathbf{C}^T \\ \mathbf{C} & -1 & 1 \\ \mathbf{C} & 1 & -11 \end{bmatrix} \begin{bmatrix} \mathbf{U} \\ \lambda^1 \\ \lambda^2 \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{d} \\ \mathbf{d} \end{bmatrix}$$

Let us now change the coefficients (λ^2) from -1 to 3. The new system is:

$$(S) : \left\{ \tilde{\mathbf{K}}\mathbf{U} + \mathbf{C}^T(\lambda^1 + \lambda^2) = \mathbf{b} \mathbf{C}\mathbf{U} - \lambda^1 + 3\lambda^2 = \mathbf{d} \mathbf{C}\mathbf{U} + \lambda^1 - 3\lambda^2 = \mathbf{d} \right.$$

Combining the last two equations gives, $\lambda^1 + \lambda^2 = 0$. Hence, the first equation becomes uncoupled from the Lagrange multipliers:

$$\tilde{\mathbf{K}}\mathbf{U} = \mathbf{b} \tag{11.2.4}$$

and can be solved for $\mathbf{U}$, which can then be used to compute λ^1, λ^2.

Notice that the solution of (11.2.4) corresponds to the initial problem without the constraint $\mathbf{C}\mathbf{u} - \mathbf{d} = 0$. Therefore, values of λ^1, λ^2 no longer have the same physical meaning. In other words, the system (S) has the same solution $\mathbf{U}$ as the system $\tilde{\mathbf{K}}\mathbf{U} = \mathbf{b}$, the two additional unknown factors λ^1, λ^2 do not disturb the solution in $\mathbf{U}$. The global system can appear to be of larger size (+2) to what is necessary, but the modern computers can reduce that problem.

Indeed, let us imagine now that we know in advance that certain kinematic relations are likely to be released. Let us order the Lagrange multiplier (λ^2) associated with these relations to the end of the system. We can then partially triangularize the system once and for all before stopping at these dof. The triangularized part of the matrix is the most important: it contains all the physical degrees of freedom and all the λ^1 factors. When a concrete problem arises, i.e., when one knows the list of the active linear relations, it is enough to update the last rows of the matrix ($-\alpha$ if the relation is active, 3α if it is not). One can then finish the triangularization and solve the problem economically.

11.2.6. Note on the conditioning of the system

When one examines the matrix ($\mathbf{K}^\star$) that will be decomposed (see The “double Lagrange” technique), it can be observed that the orders of magnitude of the various submatrices, $\mathbf{A}$, $\mathbf{C}$, $\alpha\mathbf{I}$, can be very different. It is known that in general this situation is not favorable numerically (due to limited precision of computers).

It should be noted that the constraint equations $\mathbf{C}\mathbf{u} - \mathbf{d} = 0$ can be multiplied by an arbitrary constant (β) without changing the problem. Moreover, we saw that the matrices $\alpha\mathbf{I}$ were also arbitrary $(\alpha > 0)$. We thus have two parameters that can “regulate” the

conditioning of the matrix.

We will not make a general demonstration but we have to be satisfied by the examination of the simplest case, which is a spring, a dof, and a connection.

If k is the stiffness of the spring, the matrix $\mathbf{K}^\star$ is written as:

$$\mathbf{K}^\star = \begin{bmatrix} k & \beta & \beta \\ \beta & -\alpha & \alpha \\ \beta & \alpha & -\alpha \end{bmatrix}$$

The conditioning of this matrix is related to the dispersion of its eigenvalues m_i.

Let us calculate the roots of the characteristic polynomial of $\mathbf{K}^\star$:

$$\begin{aligned} P(\mu) &= (\mu + 2\alpha)(-\mu^2 + k\mu + 2\beta^2) = 0 \\ \mu_1 &= -2\alpha \quad &< 0 \\ \mu_2 &= \frac{k + \sqrt{k^2 + 8\beta^2}}{2} \quad &> 0 \\ \mu_3 &= \frac{k - \sqrt{k^2 + 8\beta^2}}{2} \quad &< 0 \end{aligned}$$

where k is the eigenvalue of the unconstrained system. This eigenvalue is the order of magnitude of μ_1, μ_2, μ_3. Note that $\mu_1, \mu_3 < 0$ and $\mu_2 > 0$.

One seeks to obtain eigenvalues of the same order of magnitude:

$$\begin{aligned} &|\mu_1| \approx |\mu_2| \approx |\mu_3| \\ &\implies |\mu_2 \mu_3| \approx |\mu_1|^2 \quad \implies \quad 2\beta^2 = 4\alpha^2 \end{aligned} \tag{11.2.5}$$

If $\beta << k$ then $\mu_3 \approx 0$ and $\mu_2 \approx k$, which is not desirable. If $\beta >> k$ then $|\mu_3| \approx |\mu_2| \approx \sqrt{2}\beta \approx |\mu_1|$.

Then the three eigenvalues are, in absolute value, approximately of the order of β which is a large arbitrary constant that multiplies k . This solution is not that which one will retain because the value of k is in the general case (with a large number of degrees of freedom) of an order of magnitude comparable to the other eigenvalues of the system.

One will choose rather, $\beta = \alpha = k$, win which case

$$\mu_1 \approx -2k\ , \quad \mu_2 \approx 2k\ , \quad \mu_3 \approx -k$$

Practically, in `Code_Aster` , we choose a single value of α for the whole system. This value is the average of the extreme values of the diagonal terms associated with the physical degrees of freedom:

$$(\min(A_{ii}) + \max(A_{ii}))/2.$$

Moreover, we use $\beta = \alpha$.

11.2.7. Eigenmodes and Lagrange parameters

11.2.7.1. Introduction

This section wants to answer the following two questions:

> Q1: What is the reduced system of eigenvalues (and vectors) to be solved when a mechanical model is subjected to linear homogeneous kinematic constraints?
>
> Q2: What is the dualized model (with Lagrange multipliers) that is equivalent to the reduced system?

11.2.7.2. The mechanical problem

Let us start with a mechanical system that has already been discretized with finite elements.

The nodal unknowns are $\mathbf{U} = \{u_i \ , \ \ i = 1 \dots n\}$.

Nodal displacements are not all independent: there exist $p < n$ homogeneous linear relations between these displacements: $B_j(\mathbf{U}) = 0 \ \ , \ j = 1 \dots p$.

However, these linear relations are independent, i.e., the pth row of the matrix $\mathbf{B}$ contains the coefficient of the pth relation.

The matrix $\mathbf{K}$ is the stiffness matrix and $\mathbf{M}$ is the mass matrix, both without constraints included.

11.2.7.3. Reduced system

Suppose the constraint equations are written in the form

$$\mathbf{B}\mathbf{U} = 0 \tag{11.2.6}$$

where $\mathbf{B}$ is a $p \times n$ matrix, and $\mathbf{U}$ is the vector of nodal unknowns, a $n \times 1$ matrix. Then,

$$\mathbf{B}\dot{\mathbf{U}} = 0 \tag{11.2.7}$$

is also valid for time rates of the unknowns.

Moreover, if $\mathbf{B}$ has p rows, there there exists a **square** submatrix of $\mathbf{B}$ that has p rows. Let us call this submatrix $\mathbf{B}_1$.

Let us next partition the unknowns into $\mathbf{U}_1$ and $\mathbf{U}_2$ such that

$$\mathbf{B}\mathbf{U} = 0 \leftrightarrow [\mathbf{B}_1 \quad \mathbf{B}_2] \begin{bmatrix} \mathbf{U}_1 \\ \mathbf{B}_2 \end{bmatrix} = 0$$

where $\mathbf{U}_1 \in \mathbb{R}^p, \mathbf{U}_2 \in \mathbb{R}^{n-p}, \mathbf{B}_1 \in \mathbb{R}^p \times \mathbb{R}^p, \mathbf{B}_2 \in \mathbb{R}^p \times \mathbb{R}^{n-p}$. The constraint relations can then be written as

$$\mathbf{B}_1\mathbf{U}_1 + \mathbf{B}_2\mathbf{U}_2 = 0$$

Since $\mathbf{B}_1$ is invertible, this makes it possible to write

$$\mathbf{U}_1 = \mathbf{B}_1^{-1}\mathbf{B}_2\mathbf{U}_2 \tag{11.2.8}$$

Reduced stiffness matrix

The elastic energy of the unforced discrete structure is

$$W_{\text{def}} = \frac{1}{2}\mathbf{U}^T\mathbf{K}\mathbf{U}$$

If one partitions the matrix $\mathbf{K}$ in the same manner as $\mathbf{U}$, we get

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_1 & \mathbf{K}_{12} \\ \mathbf{K}_{12}^T & \mathbf{K}_2 \end{bmatrix}$$

Then,

$$2W_{\text{def}} = \mathbf{U}_1^T\mathbf{K}_1\mathbf{U}_1 + \mathbf{U}_2^T\mathbf{K}_2\mathbf{U}_2 + \mathbf{U}_2^T\mathbf{K}_{12}\mathbf{U}_1 + \mathbf{U}_1^T\mathbf{K}_{12}^T\mathbf{U}_2$$

Let us introduce the linear constraints (11.2.8):

$$\begin{aligned} 2W_{\text{def}} &= \mathbf{U}_2^T\mathbf{B}_2^T\mathbf{B}_1^{-T}\mathbf{K}_1\mathbf{B}_1^{-1}\mathbf{B}_2\mathbf{U}_2 + \mathbf{U}_2^T\mathbf{K}_2\mathbf{U}_2 - \\ &\quad \mathbf{U}_2^T\mathbf{K}_{12}\mathbf{B}_1^{-1}\mathbf{B}_2\mathbf{U}_2 - \mathbf{U}_2^T\mathbf{B}_2^T\mathbf{b}_1^{-T}\mathbf{K}_{12}^T\mathbf{U}_2 \\ &= \mathbf{U}_2^T\widetilde{\mathbf{K}}_2\mathbf{U}_2 \end{aligned}$$

with

$$\widetilde{\mathbf{K}}_2 = \mathbf{K}_2 + \mathbf{B}_2^T\mathbf{B}_1^{-T}\mathbf{K}_1\mathbf{B}_1^{-1}\mathbf{B}_2 - \mathbf{K}_{12}\mathbf{B}_1^{-1}\mathbf{B}_2 - \mathbf{B}_2^T\mathbf{B}_1^{-T}\mathbf{K}_{12}^T \tag{11.2.9}$$

The deformation energy of the reduced structure can therefore be expressed in the form of a bilinear form in $\mathbf{U}_2$. The nodal unknowns $\mathbf{U}_1$ have been **eliminated** and the nodal unknowns $\mathbf{U}_2$ are **no longer forced**.

Reduced mass matrix

Let us adopt the same partition for the mass matrix $\mathbf{M}$. We can write (11.2.7) as

$$\mathbf{B}_1\dot{\mathbf{U}}_1 + \mathbf{B}_2\dot{\mathbf{U}}_2 = 0$$

The process used for the stiffness matrix leads to

$$2W_{\text{mass}} = \dot{\mathbf{U}}_2^T\widetilde{\mathbf{M}}_2\dot{\mathbf{U}}_2$$

where

$$\widetilde{\mathbf{M}}_2 = \mathbf{M}_2 + \mathbf{B}_2^T\mathbf{B}_1^{-T}\mathbf{M}_1\mathbf{B}_1^{-1}\mathbf{B}_2 - \mathbf{M}_{12}\mathbf{B}_1^{-1}\mathbf{B}_2 - \mathbf{B}_2^T\mathbf{B}_1^{-T}\mathbf{M}_{12}^T \tag{11.2.10}$$

Conclusion

The system that has to be solved to find the $(n-p)$ eigenmodes of the forced structure is:

$$(\widetilde{\mathbf{K}}_2 - \omega_i^2\widetilde{\mathbf{M}}_2)\mathbf{X}_i = 0$$

where $\mathbf{X}_i \in \mathbb{R}^{n-p}$, $\omega^2 \in \mathbb{R}$, and $\widetilde{\mathbf{K}}_2$, $\widetilde{\mathbf{M}}_2$ are defined in (11.2.9) and (11.2.10).

Application to the constrained degrees of freedom

In this case

$$\mathbf{B}_1 = \mathbf{I} \quad \text{and} \quad \mathbf{B}_2 = 0$$

from which: $\widetilde{\mathbf{K}}_2 = \mathbf{K}_2$ and $\widetilde{\mathbf{M}}_2 = \mathbf{M}_2$, i.e., it is enough to ignore the constrained rows and columns of the two matrices.

11.2.7.4. Dual system

We saw in Section 11.2.4 that the double Lagrange method led to the matrix

$$\mathbf{A}^\star = \begin{bmatrix} \mathbf{A} & \beta\mathbf{B}^T & \beta\mathbf{B}^T \\ \beta\mathbf{B}^T & -\alpha\mathbf{I} & \alpha\mathbf{I} \\ \beta\mathbf{B}^T & \alpha\mathbf{I} & -\alpha\mathbf{I} \end{bmatrix}$$

where $\mathbf{B}$ is the matrix of kinematic constraints ($\mathbf{BU} = 0$), $\alpha \in \mathbb{R}^+$ is arbitrary and $\alpha \neq 0$, and $\beta \in \mathbb{R}$ is arbitrary and $\beta \neq 0$.

Let us apply the Lagrange dualization of boundary conditions to the matrices $\mathbf{K}$ and $\mathbf{M}$ by partitioning the degrees of freedom into $\mathbf{X}_,\mathbf{X}_2$ as in Section 11.2.7.3. The eigenvalue problem then becomes:

$$(S) \quad \left(\begin{bmatrix} \mathbf{K}_1 & \mathbf{K}_{12} & \beta_k\mathbf{B}_1^T & \beta_k\mathbf{B}_1^T \\ \mathbf{K}_{12} & \mathbf{K}_2 & \beta_k\mathbf{B}_2^T & \beta_k\mathbf{B}_2^T \\ \beta_k\mathbf{B}_1 & \beta_k\mathbf{B}_2 & -\alpha_k\mathbf{I} & \alpha_k\mathbf{I} \\ \beta_k\mathbf{B}_1 & \beta_k\mathbf{B}_2 & \alpha_k\mathbf{I} & -\alpha_k\mathbf{I} \end{bmatrix} - \omega^2 \begin{bmatrix} \mathbf{M}_1 & \mathbf{M}_{12} & \beta_m\mathbf{B}_1^T & \beta_m\mathbf{B}_1^T \\ \mathbf{M}_{12} & \mathbf{M}_2 & \beta_m\mathbf{B}_2^T & \beta_m\mathbf{B}_2^T \\ \beta_m\mathbf{B}_1 & \beta_m\mathbf{B}_2 & -\alpha_m\mathbf{I} & \alpha_m\mathbf{I} \\ \beta_m\mathbf{B}_1 & \beta_m\mathbf{B}_2 & \alpha_m\mathbf{I} & -\alpha_m\mathbf{I} \end{bmatrix} \right) \mathbf{X} = 0$$

For a self-excitation ω and an eigenvector $\mathbf{X}$, we can write

$$\bar{\mathbf{K}}_1\mathbf{X}_1 + \bar{\mathbf{K}}_{12}\mathbf{X}_2 + \beta\mathbf{B}_1^T(\lambda_1 + \lambda_2) = 0 \tag{11.2.11}$$

$$\bar{\mathbf{K}}_{12}\mathbf{X}_1 + \bar{\mathbf{K}}_2\mathbf{X}_2 + \beta\mathbf{B}_2^T(\lambda_1 + \lambda_2) = 0 \tag{11.2.12}$$

$$\beta(\mathbf{B}_1\mathbf{X}_1 + \mathbf{B}_2\mathbf{X}_2) - \alpha(\lambda_1 - \lambda_2) = 0 \tag{11.2.13}$$

$$\beta(\mathbf{B}_1\mathbf{X}_1 + \mathbf{B}_2\mathbf{X}_2) + \alpha(\lambda_1 - \lambda_2) = 0 \tag{11.2.14}$$

The system (S) is of order $(n + 2p)$ if n is the number of physical dofs and p is the number of kinematic constraint relations.

The characteristic polynomial in ω^2 is a-priori of degree $n + 2p$, and its higher order terms have the form

$$\prod_{i=1}^{n}(-m_i)(\alpha_m)^{2p}$$

where m_i is the i-th diagonal term of $\mathbf{M}$.

- One thus sees that if $\alpha_m \neq 0$, the higher order terms are non-zero and the dualized system has more eigenvalues ($n+2p$) than the reduced system ($n-p$). Therefore the two systems appear not to be equivalent (see Example below).

- If we choose $\alpha_n = \beta_n = 0$, then from (11.2.13) and (11.2.14), we have

$$\lambda_1 = \lambda_2 \ , \quad \mathbf{X}_1 = -\mathbf{B}_1^{-1}\mathbf{B}_2\mathbf{X}_2$$

From (11.2.11), we have

$$\lambda_1 = \lambda_2 = -\frac{1}{2\beta}(-\bar{\mathbf{K}}_1\mathbf{B}_1^{-1}\mathbf{B}_2 + \bar{\mathbf{K}}_{12})\mathbf{X}_2$$

and from (11.2.12), we have

$$-\bar{\mathbf{K}}_{12}\mathbf{B}_1^{-1}\mathbf{B}_2\mathbf{X}_2 + \bar{\mathbf{K}}_2)\mathbf{X}_2 - \mathbf{B}_2^T\mathbf{B}_1^{-T}(-\bar{\mathbf{K}}_1\mathbf{B}_1^{-1}\mathbf{B}_2 + \bar{\mathbf{K}}_{12})\mathbf{X}_2 = 0$$

Therefore,

$$(\widetilde{\mathbf{K}}_2 - \omega^2\widetilde{\mathbf{M}}_2)\mathbf{X}_2 = 0$$

where

$$\begin{aligned}
\widetilde{\mathbf{K}}_2 &= -\bar{\mathbf{K}}_{12}\mathbf{B}_1^{-1}\mathbf{B}_2 + \bar{\mathbf{K}}_2 + \mathbf{B}_2^T\mathbf{B}_1^{-T}\bar{\mathbf{K}}_1\mathbf{B}_1^{-1}\mathbf{B}_2 - \mathbf{B}_2^T\mathbf{B}_1^{-T}\bar{\mathbf{K}}_{12} \\
\widetilde{\mathbf{M}}_2 &= -\bar{\mathbf{M}}_{12}\mathbf{B}_1^{-1}\mathbf{B}_2 + \bar{\mathbf{M}}_2 + \mathbf{B}_2^T\mathbf{B}_1^{-T}\bar{\mathbf{M}}_1\mathbf{B}_1^{-1}\mathbf{B}_2 - \mathbf{B}_2^T\mathbf{B}_1^{-T}\bar{\mathbf{M}}_{12}
\end{aligned}$$

Note that these definitions are identical to those in (11.2.9) and (11.2.10).

If is thus seen that any eigenvector $\mathbf{X}$ of the dualized system is also an eigenvector of the reduced system (with the same harmonic forcing) if one projects it on the space $\mathbf{U}_2$.

Reciprocally, any eigenvector $\mathbf{X}_2$ of the reduced problem can be extended into one for the dualized system using $\mathbf{X}^T = [\mathbf{X}_1^T, \mathbf{X}_2^T, \lambda_1^T, \lambda_2^T]$. with

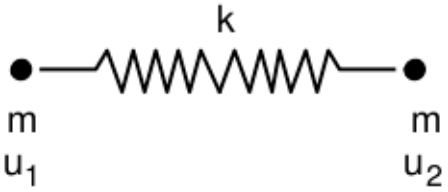
$$\begin{aligned}
\mathbf{X}_1 &= -\mathbf{B}_1^{-1}\mathbf{B}_2\mathbf{X}_2 \\
\lambda_1 &= \frac{1}{2\beta}\mathbf{B}_1^{-T}(-\bar{\mathbf{K}}_1\mathbf{B}_1^{-1}\mathbf{B}_2 + \bar{\mathbf{K}}_{12})\mathbf{X}_2 \\
\lambda_2 &= \frac{1}{2\beta}\mathbf{B}_1^{-T}(-\bar{\mathbf{K}}_1\mathbf{B}_1^{-1}\mathbf{B}_2 + \bar{\mathbf{K}}_{12})\mathbf{X}_2
\end{aligned}$$

The two systems are therefore equivalent; they have the same eigenmodes and eigenvalues, The dualized system does not have more eigenvalues than the reduced system.

Note

The dualized system is equivalent to the reduced system as soon as one chooses $\alpha_m = \beta_m = 0$. This is equivalent to observing that the dualized stiffness matrix is modified but the mass matrix is not. This approach has been used in the `Aster` implementation.

Example 2:



Consider the spring-mass system with stiffness and mass matrices

$$\mathbf{K} = \begin{bmatrix} k & -k \\ -k & k \end{bmatrix}, \quad \mathbf{M} = \begin{bmatrix} m & 0 \\ 0 & m \end{bmatrix}$$

Let us add the constraint $\alpha u_1 + \beta u_2 = 0$ with $\alpha \neq 0$, i.e., $\gamma = \beta/\alpha$.

The reduced system is then:

$$\begin{aligned} &\mathbf{K}_1 = k\,, \quad \mathbf{K}_2 = k\,, \quad \mathbf{K}_{12} = -k\,, \\ &\mathbf{M}_1 = m\,, \quad \mathbf{M}_2 = m\,, \quad \mathbf{M}_{12} = 0\,, \\ &\mathbf{B}_1 = \alpha\,, \quad \mathbf{B}_2 = \beta \end{aligned}$$

Therefore,

$$\widetilde{\mathbf{K}}_2 = k(1+\gamma)^2\,, \quad \widetilde{\mathbf{M}}_2 = m(1+\gamma)^2$$

which leads to

\[\omega^2 = \frac{k}{m} \frac{(1+\gamma)^2}{1+\gamma^2) ~,~~ \mathbf{X}_2 = 1\]

Some special cases are:

- If $\gamma = 0, \omega^2 = k/m.$
- If $\gamma = 1, \omega^2 = 2k/m.$
- If $\gamma \to \infty 1, \omega^2 \to 2k/m.$

Let us choose $\alpha = \beta = 1$ to simplify writing the dualized system:

$$\left(\begin{bmatrix} k & -k & \beta_k & \beta_k \\ -k & k & \beta_k & \beta_k \\ \beta_k & \beta_k & -\alpha_k & \alpha_k \\ \beta_k & \beta_k & \alpha_k & -\alpha_k \end{bmatrix} - \omega^2 \begin{bmatrix} m & 0 & \beta_m & \beta_m \\ 0 & m & \beta_m & \beta_m \\ \beta_m & \beta_m & -\alpha_m & \alpha_m \\ \beta_m & \beta_m & \alpha_m & -\alpha_m \end{bmatrix} \right) \begin{bmatrix} x_1 \\ x_2 \\ \lambda_1 \\ \lambda_2 \end{bmatrix} = 0$$

The eigenvalues of this system are

$$\omega^2 = \left\{ \frac{\beta_k}{\beta_m}, \frac{\beta_k}{\beta_m}, \frac{\beta_k}{\beta_m}, \frac{2k}{m} \right\}$$

Therefore, we find one real eigenvalue and three spurious ones because α_m and β_m are non-zero.

If one chooses $\alpha_m = \beta_m = 0$, then the only solution is $\omega^2 = 2k/m$ with eigenvectors $\mathbf{X} = (-1, 1)$, which is the desired solution.

11.2.7.5. Conclusions

- If $\mathbf{K}$ and $\mathbf{M}$ are the stiffness and mass matrices of a non-constrained system
- and if the linear constraints can be written as

$$[\mathbf{B}_1 \quad \mathbf{B}_2] \begin{bmatrix} \mathbf{U}_1 \\ \mathbf{U}_2 \end{bmatrix} = 0$$

  with $\mathbf{B}_1$ invertible

- then the eigenmodes of the forced structure are those of the reduced system

$$(\widetilde{\mathbf{K}}_2 - \omega^2 \widetilde{\mathbf{M}}_2)\mathbf{X}_2 = 0$$

  where

$$\begin{aligned} \widetilde{\mathbf{K}}_2 &= -\bar{\mathbf{K}}_{12}\mathbf{B}_1^{-1}\mathbf{B}_2 + \bar{\mathbf{K}}_2 + \mathbf{B}_2^T\mathbf{B}_1^{-T}\bar{\mathbf{K}}_1\mathbf{B}_1^{-1}\mathbf{B}_2 - \mathbf{B}_2^T\mathbf{B}_1^{-T}\bar{\mathbf{K}}_{12} \\ \widetilde{\mathbf{M}}_2 &= -\bar{\mathbf{M}}_{12}\mathbf{B}_1^{-1}\mathbf{B}_2 + \bar{\mathbf{M}}_2 + \mathbf{B}_2^T\mathbf{B}_1^{-T}\bar{\mathbf{M}}_1\mathbf{B}_1^{-1}\mathbf{B}_2 - \mathbf{B}_2^T\mathbf{B}_1^{-T}\bar{\mathbf{M}}_{12} \end{aligned}$$

- and the dualized system (double Lagrange) is written

$$(\widehat{\mathbf{K}} - \omega^2 \widehat{\mathbf{M}})\widehat{\mathbf{X}} = 0$$

  with

$$\begin{aligned} \widehat{\mathbf{X}}^T &= [\mathbf{X}_1 \quad \mathbf{X}_{12} \quad \lambda_1 \quad \lambda_2] \\ \widehat{\mathbf{K}} &= \begin{bmatrix} \mathbf{K}_1 & \mathbf{K}_{12} & \mathbf{B}_1^T & \mathbf{B}_1^T \\ \mathbf{K}_{12}^T & \mathbf{K}_2 & \mathbf{B}_2^T & \mathbf{B}_2^T \\ \mathbf{B}_1 & \mathbf{B}_2 & -\mathbf{I} & \mathbf{I} \\ \mathbf{B}_1 & \mathbf{B}_2 & \mathbf{I} & -\mathbf{I} \end{bmatrix} \\ \widehat{\mathbf{M}} &= \begin{bmatrix} \mathbf{M}_1 & \mathbf{M}_{12} & 0 & 0 \\ \mathbf{M}_{12}^T & \mathbf{M}_2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \end{aligned}$$

  and has the same solutions as the reduced system.

11.2.8. Appendix 1

In this appendix, we show that the problem of constrained minimization of the functional $\mathcal{J}(\mathbf{u})$ is equivalent to an algebraic problem.

The minimization problem can be stated as:

$$\min_{\mathbf{u}\in\mathbf{V}} \mathcal{J}(\mathbf{u}) \quad \text{where} \quad \mathcal{J}(\mathbf{u}) = \frac{1}{2}(\mathbf{A}\mathbf{u}, \mathbf{u}) - (\mathbf{b}, \mathbf{u}) \tag{11.2.15}$$

where the subspace $\mathbf{V} \subset \mathbb{R}^n$ is spans the set of n unknowns $\mathbf{u}$ minus the p affine constraints

$\mathbf{C}_i\mathbf{u} - \mathbf{d}_i = 0\ ,\ \ i = 1 \ldots p$. Both $\mathbf{A}$ and $\mathbf{b}$ are defined on $\mathbb{R}^n$, and $\mathbf{A}$ is positive and symmetric.

The algebraic problem can be stated as:

$$\text{Find } \mathbf{u} \in \mathbf{V} \quad \text{such that} \quad (\mathbf{Au}, \mathbf{v}_0) - (\mathbf{b}, \mathbf{v}_0) = 0 \quad \forall \mathbf{v}_0 \in \mathbf{V}_0 \tag{11.2.16}$$

Here, the space $\mathbf{V}$ is the same as that in (11.2.15), i.e.,

$$\mathbf{V} = \{\mathbf{u} \in \mathbb{R}^n \quad \text{such that} \quad \mathbf{C}_i\mathbf{u} - \mathbf{d}_i = 0, i = 1 \ldots p\}$$

The space $\mathbf{V}_0$ is a variation of $\mathbf{V}$:

$$\mathbf{V}_0 = \{\mathbf{v}_0 \in \mathbb{R}^n \quad \text{such that} \quad \mathbf{C}_i\mathbf{v}_0 = 0, i = 1 \ldots p\}$$

We wish to show that problems (11.2.15) and (11.2.16) are equivalent.

To start, observe that (11.2.16) can be expressed as:

$$\text{Find } \mathbf{u} \in \mathbf{V} \quad \text{such that} \quad (\mathbf{Au}, \mathbf{v} - \mathbf{u}) - (\mathbf{b}, \mathbf{v} - \mathbf{u}) = 0 \quad \forall \mathbf{v} \in \mathbf{V} \tag{11.2.17}$$

because of the bijection between $\{\mathbf{v} - \mathbf{u}, (\mathbf{u}, \mathbf{v}) \in \mathbf{V}\}$ and $\mathbf{V}_0$.

To show that (11.2.17) is equivalent to (11.2.15), we note that for all $\mathbf{v} \in \mathbf{V}$,

$$\begin{aligned}
\mathcal{J}(\mathbf{v}) - \mathcal{J}(\mathbf{u}) &= \frac{1}{2}(\mathbf{Av}, \mathbf{v}) - (\mathbf{b}, \mathbf{v}) - \frac{1}{2}(\mathbf{Au}, \mathbf{u}) - (\mathbf{b}, \mathbf{u}) \\
&= \frac{1}{2}(\mathbf{Av}, \mathbf{v}) - (\mathbf{Au}, \mathbf{v} - \mathbf{u}) - \frac{1}{2}(\mathbf{Au}, \mathbf{u}) \\
&= \frac{1}{2}(\mathbf{Av}, \mathbf{v}) - (\mathbf{Au}, \mathbf{v}) + \frac{1}{2}(\mathbf{Au}, \mathbf{u}) \\
&= \frac{1}{2}\mathbf{A}(\mathbf{u} - \mathbf{v}, \mathbf{u} - \mathbf{v}) \geq 0
\end{aligned}$$

The directional directive of $\mathcal{J}(\mathbf{u})$ in the direction $\mathbf{v}_0$ is

$$\begin{aligned}
\mathcal{J}^{'}(\mathbf{u}) \cdot \mathbf{v}_0 &= \lim_{\varepsilon \to 0} \frac{\mathcal{J}(\mathbf{u} + \varepsilon\mathbf{v}_0) - \mathcal{J}(\mathbf{u})}{\varepsilon} \\
&= \lim_{\varepsilon \to 0}(\mathbf{Au}, \mathbf{v}_0) + \frac{\varepsilon}{2}(\mathbf{Av}_0, \mathbf{v}_0) - (\mathbf{b}, \mathbf{v}_0) \\
&= (\mathbf{Au} - \mathbf{b})\mathbf{v}_0
\end{aligned}$$

Now, if we take $\mathbf{v} \in \mathbf{V}$ and let $\mathbf{v}_0 = \mathbf{v} - \mathbf{u},\ \ \mathbf{v}_0 \in \mathbf{V}_0$, we have, for all $\varepsilon > 0$,

$$\frac{\mathcal{J}(\mathbf{u} + \varepsilon\mathbf{v}_0) - \mathcal{J}(\mathbf{u})}{\varepsilon} \geq 0 \quad \Longrightarrow \quad \mathcal{J}^{'}(\mathbf{u}) \cdot \mathbf{v}_0 \geq 0$$

This is only possible if the derivative is zero. Therefore,

$$\mathcal{J}^{'}(\mathbf{u}) \cdot (\mathbf{v} - \mathbf{u}) = (\mathbf{Au} - \mathbf{b})(\mathbf{v} - \mathbf{u}) = 0 \quad \forall \mathbf{v} \in \mathbf{V}$$

which is equivalent to (11.2.17).

11.2.9. Appendix 2

In this appendix, we will see that the block submatrix matrix $\mathbf{K}_i$ can be made invertible by appropriate ordering of the rows and columns (cond1).

Definitions

Recall that

- $\mathbf{A}$ is the $n \times n$ unconstrained stiffness matrix (symmetric and positive)
- $\mathbf{C}$ is the $n \times p$ ($p < n$) constraint matrix : $\mathbf{C}\mathbf{u} - \mathbf{d} = 0$.
- $\mathbf{u}$ is the $n \times 1$ vector of the physical degrees of freedom
- λ^1 is the $p \times 1$ vector of the first Lagrange multiplier degrees of freedom
- λ^2 is the $p \times 1$ vector of the second Lagrange multiplier degrees of freedom

The combined vector of degrees of freedom is

$$\mathbf{x} = (\mathbf{u}, \lambda^1, \lambda^2) \quad \in \mathbb{R}^n \times \mathbb{R}^p \times \mathbb{R}^p$$

We use the notation:

- $\mathbf{U}$ for the global vector of physical degrees of freedom
- $\mathbf{\Lambda}^1$ for the global vector of the first set of Lagrange multipliers
- $\mathbf{\Lambda}^2$ for the global vector of the second set of Lagrange multipliers

The combined stiffness $\mathbf{K}$ is a symmetric, $(n + 2p) \times (n + 2p)$, matrix given by

$$\mathbf{K} = \begin{bmatrix} \mathbf{A} & \mathbf{C}^T & \mathbf{C}^T \\ \mathbf{C} & -\alpha\mathbf{I} & \alpha\mathbf{I} \\ \mathbf{C} & \alpha\mathbf{I} & -\alpha\mathbf{I} \end{bmatrix} \quad \alpha \in \mathbb{R}^+$$

This organization of matrix $\mathbf{K}$ corresponds to the following ordering of the unknowns: $\mathbf{x} = (\mathbf{u}, \lambda^1, \lambda^2)$. However, if we wish to obtain a $\mathbf{LDL}^T$ factorization of this matrix (without permutation of the row/columns), we cannot write the matrix in this order.

In the following, we will take $\alpha = 1$ to simplify the discussion.

The rule that is used in `Aster` to determine the correct order of the rows and columns is called **Rule R0** (discussed earlier):

Rule R0

The two Lagrange multiplier degrees of freedom associated with the constraint equation $\mathbf{C}_i - \mathbf{U} - \mathbf{d}_i = 0$ frame the physical dofs constrained by this equation.

We seek to show that every sub-matrix $\mathbf{K}_i$ of $\mathbf{K}$ is invertible. Recall that a submatrix divides the original matrix into two parts and corresponds to a division of the degrees of freedom:

those before (and including) row i and those after row i.

Notation

In the following discussion, we will use the following notation:

- $\widetilde{\mathbf{U}}$ is the subset of $\mathbf{U}$ that corresponds to dof of rows $\leq i$.
- $\widehat{\mathbf{U}}$ is the subset of $\mathbf{U}$ that corresponds to dof of rows $> i$.
- L_1 the set of pairs $(\lambda_1^1, \lambda_1^2)$ such that for the associated constrained dofs we have $\text{range}(\lambda_1^1) < \text{range}(\lambda_1^2) \leq i$.
- $L_1^1 = \{\lambda_1^1\}, L_1^2 = \{\lambda_1^2\}$
- L_2 the set of pairs $(\lambda_2^1, \lambda_2^2)$ such that for the associated constrained dofs we have $\text{range}(\lambda_2^1) \leq i < \text{range}(\lambda_2^2)$.
- $L_2^1 = \{\lambda_2^1\},\ L_2^2 = \{\lambda_1^2\}$
- L_3 the set of pairs $(\lambda_3^1, \lambda_3^2)$ such that for the associated constrained dofs we have $i < \text{range}(\lambda_3^1) < \text{range}(\lambda_3^2)$.
- $L_3^1 = \{\lambda_3^1\}, L_3^2 = \{\lambda_3^2\}$

The combined set is

$$L = \cup_{i=1,3;\, j=1,2} L_i^j$$

The constraint matrix $\mathbf{C}$ can be divided (along rows) into three blocks $(\mathbf{C}_1, \mathbf{C}_2, \mathbf{C}_3)$ that correspond to the sets (L_1, L_2, L_3). Each row block matrix $\mathbf{C}_i$ can be divided into two column blocks $(\widetilde{\mathbf{C}}_i, \widehat{\mathbf{C}}_i)$ that correspond to the dof blocks $\widetilde{\mathbf{U}}$ and $\widehat{\mathbf{U}}$. That is,

$$\mathbf{C} = \begin{bmatrix} \mathbf{C}_1 \\ \mathbf{C}_2 \\ \mathbf{C}_3 \end{bmatrix} = \begin{bmatrix} \widetilde{\mathbf{C}}_1 & \widehat{\mathbf{C}}_1 \\ \widetilde{\mathbf{C}}_2 & \widehat{\mathbf{C}}_2 \\ \widetilde{\mathbf{C}}_3 & \widehat{\mathbf{C}}_3 \end{bmatrix}$$

Similarly, the matrix $\mathbf{A}$ can be divided into blocks:

$$\mathbf{A} = \begin{bmatrix} \widetilde{\mathbf{A}} & \bar{\mathbf{A}} \\ \bar{\mathbf{A}}^T & \widehat{\mathbf{A}} \end{bmatrix}$$

Now consider the constrained stiffness sub-matrix ($\mathbf{K}_i$) organized as follows:

$$\mathbf{K}_i = \begin{bmatrix} -\mathbf{I} & \mathbf{I} & 0 & \widetilde{\mathbf{C}}_1 \\ \mathbf{I} & -\mathbf{I} & 0 & \widetilde{\mathbf{C}}_1 \\ 0 & 0 & -\mathbf{I} & \widetilde{\mathbf{C}}_2 \\ \widetilde{\mathbf{C}}_1^T & \widetilde{\mathbf{C}}_1^T & \widetilde{\mathbf{C}}_2^T & \widetilde{\mathbf{A}} \end{bmatrix}$$

This matrix corresponds to the vector

$$\mathbf{X}_i = \begin{bmatrix} \lambda_1^1 \\ \lambda_1^2 \\ \lambda_2^1 \\ \widetilde{\mathbf{U}} \end{bmatrix}$$

We have to show that the matrix $\mathbf{K}_i$ is invertible, i.e.,

$$\mathbf{K}_i \mathbf{X}_i = 0 \quad \Longrightarrow \quad \mathbf{X}_i = 0$$

This problem is equivalent to:

Problem 1

$$(S) = \begin{cases} -\lambda_1^1 + \lambda_1^2 + \widetilde{\mathbf{C}}_1 \widetilde{\mathbf{U}} = 0 \\ \lambda_1^1 - \lambda_1^2 + \widetilde{\mathbf{C}}_1 \widetilde{\mathbf{U}} = 0 \\ -\lambda_1^2 + \widetilde{\mathbf{C}}_2 \widetilde{\mathbf{U}} = 0 \\ \widetilde{\mathbf{C}}_1^T (\lambda_1^1 + \lambda_1^2) + \widetilde{\mathbf{C}}_2^T \lambda_2^1 + \widetilde{\mathbf{A}} \widetilde{\mathbf{U}} = 0 \end{cases}$$

which implies that

$$\widetilde{\mathbf{U}} = 0\,, \quad \lambda_1^1 = \lambda_1^2 = 0\,, \quad \lambda_2^1 = 0$$

General case:

Suppose that $\widetilde{\mathbf{U}} \neq \emptyset, L_1 \neq \emptyset, L_2 \neq \emptyset$. Then

$$\lambda_1^1 = \lambda_1^2 \tag{11.2.18}$$

$$\widetilde{\mathbf{C}}_1 \widetilde{\mathbf{U}} = 0 \tag{11.2.19}$$

$$\lambda_2^1 = \widetilde{\mathbf{C}}_2 \widetilde{\mathbf{U}} \tag{11.2.20}$$

$$2\widetilde{\mathbf{C}}_1^T \lambda_1^1 + (\widetilde{\mathbf{C}}_2^T \widetilde{\mathbf{C}}_2 + \widetilde{\mathbf{A}}) \widetilde{\mathbf{U}} = 0 \tag{11.2.21}$$

From (11.2.21) we observe that

$$2\widetilde{\mathbf{U}}^T \widetilde{\mathbf{C}}_1^T \lambda_1^1 + \widetilde{\mathbf{U}}^T (\widetilde{\mathbf{C}}_2^T \widetilde{\mathbf{C}}_2 + \widetilde{\mathbf{A}}) \widetilde{\mathbf{U}} = 0$$

Using (11.2.19), we have $\widetilde{\mathbf{U}}^T \widetilde{\mathbf{C}}_1^T = 0$, and we obtain

$$\widetilde{\mathbf{U}}^T \widetilde{\mathbf{C}}_2^T \widetilde{\mathbf{C}}_2 \widetilde{\mathbf{U}} + \widetilde{\mathbf{U}}^T \widetilde{\mathbf{A}} \widetilde{\mathbf{U}} = 0$$

Since $\widetilde{\mathbf{A}}$ is a submatrix of a symmetric, positive, matrix, it is also symmetric and positive. Also, $\widetilde{\mathbf{C}}_2^T \widetilde{\mathbf{C}}_2$ is a symmetric positive matrix. Therefore, their sum will be zero only if bot the terms are zero, i.e.,

$$\widetilde{\mathbf{U}}^T \widetilde{\mathbf{C}}_2^T \widetilde{\mathbf{C}}_2 \widetilde{\mathbf{U}} = 0 \quad \text{and} \quad \widetilde{\mathbf{U}}^T \widetilde{\mathbf{A}} \widetilde{\mathbf{U}} = 0$$

The first equation implies that

$$\widetilde{\mathbf{C}}_2\widetilde{\mathbf{U}} = 0 \quad \Longrightarrow \quad \lambda_2^1 = 0 \tag{11.2.22}$$

From the second equation we want to show that

$$\widetilde{\mathbf{U}}^T\widetilde{\mathbf{A}}\widetilde{\mathbf{U}} = 0 \quad \Longrightarrow \quad \widetilde{\mathbf{U}} = 0 \tag{11.2.23}$$

We also have to show that $\lambda_1^1 = 0$.

- $\widetilde{\mathbf{U}} = 0$:

  In the decomposition of $\mathbf{U} = (\widetilde{\mathbf{U}}, \widehat{\mathbf{U}})$ let us set $\widehat{\mathbf{U}} = 0$. Then

  $$\mathbf{U}^T\mathbf{A}\mathbf{U} = 0 \quad \Longrightarrow \quad \widetilde{\mathbf{U}}^T\widetilde{\mathbf{A}}\widetilde{\mathbf{U}} = 0$$

  Therefore, in this case, $\mathbf{U} \in \ker(\mathbf{A})$ and

  $$\mathbf{C}\mathbf{U} = \begin{bmatrix}\mathbf{C}_1\mathbf{U}\\ \mathbf{C}_2\mathbf{U}\\ \mathbf{C}_3\mathbf{U}\end{bmatrix} = \begin{bmatrix}\widetilde{\mathbf{C}}_1\widetilde{\mathbf{U}}\\ \widetilde{\mathbf{C}}_2\widetilde{\mathbf{U}}\\ \widetilde{\mathbf{C}}_3\widetilde{\mathbf{U}}\end{bmatrix} = \begin{bmatrix}0\\0\\0\end{bmatrix}$$

  Also note that if $\widetilde{\mathbf{C}}_3 \neq 0$, then there would exist dofs of $\widetilde{\mathbf{U}}$ that are constrained by equations that have not yet been taken into account (rows $> i$) which is contrary to Rule R0.

  Therefore the vector $\mathbf{U}$ is in the null-space of both $\mathbf{A}$ and $\mathbf{C}$. We have to show that $\mathbf{U} = 0$. Consider the "single" Lagrange multiplier problem

  $$(S_2) : \begin{cases}\mathbf{A}\mathbf{U} + \mathbf{C}^T\lambda = \mathbf{B}\\ \mathbf{C}\mathbf{U} = \mathbf{d}\end{cases}$$

  Let us assume a solution $\mathbf{U}_0 \neq 0$ such that $\mathbf{A}\mathbf{U}_0 = 0$ and $\mathbf{C}\mathbf{U}_0 = 0$. If $\mathbf{U}_1$ is a solution of (S_2), then $\mathbf{U}_1 + \mu\mathbf{U}_0$ is also a solution, i.e., the solution is not unique. This is not possible because we have assumed that our problem is well-posed. Therefore, we must have $\mathbf{U} = 0$, i.e., $\widetilde{\mathbf{U}} = 0$.

- $\lambda_1^1 = 0$:

  Equation :eq: `appendix2_4` gives

  $$\widetilde{\mathbf{C}}_1^T\lambda_1^1 = 0 \tag{11.2.24}$$

  Using Rule R0 (and using the same argument that was used to show that $\widetilde{\mathbf{C}}_3 = 0$, we can show that $\widehat{\mathbf{C}}_1 = 0$.

  Equation (11.2.23) gives

  $$\mathbf{C}_1^T\lambda_1^1 = \begin{bmatrix}\widetilde{\mathbf{C}}_1^T\lambda_1^1\\ \widehat{\mathbf{C}}_1^T\lambda_1^1\end{bmatrix} = \begin{bmatrix}0\\0\end{bmatrix} = 0 \tag{11.2.25}$$

  If $\lambda_1^1 \neq 0$ but $\mathbf{C}_1^T\lambda_1^1 = 0$, there exists a linear combination of the rows of $\mathbf{C}_1$

which is zero, i.e., they are not independent. This contradicts the assumption that the constraints are linearly independent, which is required for physical well-posedness.

Therefore, $\lambda_1^1 = 0$.

Typical case

When one (or more) of the sets $\tilde{\mathbf{u}}$, L_1, L_2 is empty, the system (S) is simplified. One can check that the reasoning used in the general case makes it possible to show similar results.

Footnotes

[1] P.G. Ciarlet, “The finite element method for elliptic problems”, Studies in Applied Mathematics, North Holland, 1978