

Resolution of the modal problem quadratic (QEP)

Summary

The study of the dynamic stability of a deadened and/or revolving structure leads to the resolution of a modal problem higher than the traditional standard modal problems (SEP) or generalized (GEP).

To apprehend them, **Code_Aster propose a string of methods via operators** `CALC_MODES` : powers opposite and method of Müller, Lanczos, IRA and QZ. They have each one their perimeter of use, their advantages/disadvantages and their history of development.

In the first part of the document we summarize the problems of resolution of a quadratic problem and its variation in the general architecture of a modal calculation *Code_Aster* . Then we detail the digital, data-processing and functional aspects of each approach available in the code. The various results, algorithms or parameters approached in this document are often based on the modal methods of orders lower (SEP and GEP) described in the document [R5.01.01]. The reading of this last is thus pre-necessary advised.

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1 Introduction

A majority of study concerning **dynamic behavior of deadened and/or revolving structures** is realized by carrying out one **transitory analysis on modal basis**. To exhume these modes of vibrations, a string of algorithms have been developed for about sixty years. In order to cope with the continual increase in the size of the problems and with the degradation of conditionings of the discretized operators, only most effective and most robust, in practice, were built-in the modal operator of *Code_Aster*, `CALC_MODES`.

The optimal perimeters of use of the various methods available can be dissociated. When it is about to **determine some eigenvalues** (typically a half-dozen) or to **refine some estimates**, the option `'NEAR'` or `'ADJUSTS'` of `CALC_MODES` is completely indicated. That gathers heuristic algorithms and those of type powers (cf §3).

On the other hand, for **to capture a significant part of the spectrum**, one has resorts to one of the options `'CENTER'`, `'PLUS_PETITE'` or `'ALL'` of `CALC_MODES`. This last federates the methods known as of "subspace" (Lanczos, IRAM §4) which project the operator of work in order to obtain an approximated modal problem of more reduced size (treated then by a global method of the type QR).

This operator also allows to exhume in a robust way all the spectrum of the modal problem. With this intention, one uses a global method of reference (method **QZ** cf §4) who calculates all the modes exhaustively. It is thus to hold for certain uses: problem of small (< 1000 degrees of freedom) or benchmark of algorithms.

The two families of methods can be complementary besides, because the methods put in work with the option `'NEAR'` or `'ADJUSTS'` are very powerful to optimize clean modes already almost converged. In one or two iterations, they can thus improve the beforehand estimated clean vectors *via* one of the options `'CENTER'`, `'PLUS_PETITE'` or `'ALL'`. Projection on modal basis will be only better.

In the first part of the document we summarize the problems of resolution of a quadratic problem and its variation in the general architecture of a modal calculation *Code_Aster*. Then we detail the digital, data-processing and functional aspects of each approach available in the code. One tries to give, for each method, his principal properties and his limitations by connecting these considerations, which can sometimes appear a little "ethereal", to a precise parameter setting of the operators *Aster*.

The various results, algorithms or parameters approached in this document are often based on the modal methods of order lower (SEP and GEP) described in the document [Boi09]. The reading of this last is thus pre-necessary advised!

OPTION / Perimeter of application	Algorithm	Keyword	Advantages	Disadvantages Remarks
<code>'NEAR'</code> <code>'ADJUSTS'</code>				
1 ^{ère} phase (heuristics)				Only symmetrical reality
Calculation of some modes	Müller-Traub	<code>'ADJUSTS'</code>		Cost calculation
Improvement of some estimates	Initialization by the user	<code>'NEAR'</code>	Resumption of eigenvalues estimated by another process. Cost calculation of this phase quasi-no one	Pas de captures multiplicity
2 ^{ième} phase (method of the powers itself)				Only symmetrical reality
Basic method	Powers	<code>OPTION_INV</code>	Very good	Not very robust

OPTION / Perimeter of application	Algorithm	Keyword	Advantages	Disadvantages Remarks
	opposite (Jennings)	= 'DIRECT'	construction of clean vectors	
'CENTER' 'PLUS_PETITE' 'ALL'				
	Lanczos	METHODE= 'TRI_DIAG'		Only symmetrical reality
	IRAM (Sorensen)	METHODE= 'SORENSEN'	Increased robustness. Better complexities calculation and memory. Quality control of the modes.	Method by default. Range in nonsymmetrical and/or with With complex.
Calculation of all the spectrum then filtering of a part	QZ	METHODE= 'QZ'	Robustness. Method of reference.	Very expensive in CPU and memory. To reserve for the small case (<10 ³ degrees of freedom). Range in nonsymmetrical and/or with With complex.

Table 1-1. Summary of the modal methods to treat the QEP of Code_Aster.

Foot-note:

- *The effective establishment and the maintenance of the modal solveurs in Code_Aster are the fruit of a team work: D.Séligmann, B.Quinnez, G.Devesa, O.Boiteau, O.Nicolas, E.Boyère, I.Nistor...*
- *One tried constantly to bind different the items approached and to limit to the strict minimum the recourse to long mathematical demonstrations. In any event, the many references which enamel the text must make it possible to search the accurate information.*
- *The object of this document is not to detail all the aspects approached, of the complete works having already fulfilled this mission. One will find many references in the note [Boi09]. One will quote however the excellent synthesis on the QEP made by F.Tisseur and K.Meerbergen [TM01]. Our document exploits some of its illustrative elements and, in particular, some examples.*

2 Context

2.1 Problems

We consider the quadratic modal problem (QEP)

$$\text{To find } (\lambda, \mathbf{u}) \text{ such as } (\lambda^2 \mathbf{B} + \lambda \mathbf{C} + \mathbf{A}) \mathbf{u} = \mathbf{0}, \mathbf{u} \neq \mathbf{0} \quad (2.1-1)$$

where \mathbf{A} , \mathbf{B} and \mathbf{C} square matrices of size have n , with real or complex, symmetrical coefficients or not. This kind of problem corresponds, in mechanics, in particular with **the study of the free vibrations of a structure deadened and/or revolving**. For this structure, one searches the eigenvalues λ_i (and their associated own vectors \mathbf{u}_i) S closer, in the complex plan, of a given value of reference (the "shift" σ) to know if an exiting force can create a resonance. In this standard case,

- The matrix \mathbf{A} is the matrix of rigidity, noted \mathbf{K} , symmetrical real (possibly increased symmetrical matrix complexes, noted \mathbf{E}_{hyst} , if the structure presents a damping hysteretic): $\mathbf{A} = \mathbf{K} + \mathbf{E}_{hyst}$. Thus \mathbf{A} is symmetrical real or complex.
- The matrix \mathbf{B} is the matrix of mass or noted inertia \mathbf{M} (symmetrical real).
- The matrix \mathbf{C} gather, it, the possible gyroscopic effects and those of viscous damping *via* combination:

$$\mathbf{C} := \mathbf{E}_{visq} + \xi \mathbf{G} \quad (2.1-2)$$

with \mathbf{E}_{visq} , matrix (symmetrical real) of damping induced by dissipative forces, \mathbf{G} matrix of gyroscopy (antisymmetric real) and ξ a real parameter representative the number of revolutions. Thus \mathbf{C} is potentially nonsymmetrical real.

This kind of problems are activated by the keyword `TYPE_RESU= 'DYNAMIQUE'`. In the case general of the QEP (2.1-1) and by exploiting only their property of symmetry and arithmetic of the matrices, one can break up the perimeter of the modal operators `Code_Aster` as follows.

\mathbf{A} / \mathbf{C}	Real symmetrical	Real nonsymmetrical	Complex
Real symmetrical	Case more running SIMULT/INV without restriction on the methods; Real modes or complexes $(\lambda, \bar{\lambda})$.	SIMULT with 'SORENSEN' / 'QZ'; Real or complex modes $(\lambda, \bar{\lambda})$.	Case untreated
Real nonsymmetrical	SIMULT with 'SORENSEN' / 'QZ'; Real modes or complexes $(\lambda, \bar{\lambda})$.	SIMULT with 'SORENSEN' / 'QZ' Real or complex modes $(\lambda, \bar{\lambda})$.	Case untreated
Complex symmetrical	SIMULT with 'SORENSEN' / 'QZ' Real modes, unspecified complexes or $(\lambda, \bar{\lambda})$.	Case untreated	Case untreated
Other complexes (square, nonsymmetrical...)	Case untreated	Case untreated	Case untreated

Table 2.1-1. Perimeter of use of the operator Aster `CALC_MODES` according to the methods of analysis, according to properties matrices \mathbf{A} and \mathbf{C} QEP (2.1-1). \mathbf{B} is real unspecified.

In absence of damping hysteretic, it **Standard QEP** to solve thus consists of **symmetrical real matrices**. These eigenvalues, either real, or complex are combined per pair $(\lambda, \bar{\lambda})$. The clean vectors are then potentially with complex components.

In the presence of damping hysteretic, the QEP becomes complex and loses the preceding property¹. These modes then are real, complex by pair or odd.

Note:

- *Contrary to the GEP [Boi09] treated by Code_Aster, the keyword `TYPE_RESU= 'FLAMBEMENT'` is not licit within the framework of the QEP.*
- *By means of computer, the perimeter of the option ['CENTER', 'PLUS_PETITE', 'ALL'] was extended to the nonsymmetrical real matrices **A**, **B** et **C** QEP. It is not yet the case for the option ['NEAR', 'ADJUSTS'] who limits himself, for the moment, with symmetrical real matrices. These last cannot thus take into account gyroscopic effects.*
- *The modeling of damping [Lev96] in Code_Aster can break up into two classes: viscous damping proportional (known as of Rayleigh $\mathbf{E}_{visq} := \alpha \mathbf{K} + \beta \mathbf{M}$) or damping hysteretic ($\mathbf{E}_{hist} := (I + i \eta) \mathbf{K}$). Each one is declined at the total level of the structure or by means of localised depreciation (groups of meshes, discrete elements ad hoc). The latter allowing to better represent the heterogeneity of the structure compared to damping. Remain however the delicate question of the identification of the coefficients (α, β, η) and their influences on the result.*

2.2 Properties of the clean modes

Preceding table 2.2-1 does not take account of typical cases (pure gyroscopy, on-deadened structure...). For memory, one will state of them some which one often finds in the literature. But it is necessary well to keep in memory that the context of modelings *Code_Aster* (quasi-systematic use of Lagranges double) and the sorting of personal programs modes in the modal operators do not take account of these specificities. **Currently in QEP, one retains only the coupled modes $(\lambda, \bar{\lambda})$ and one preserves that at positive imaginary part.** According to the cases, the presence of eigenvalues of other natures (real or complex not combined) is announced by one `ALARM` or on a purely informative basis.

One thus has (by taking again the elements and the notations of §3.3 of [Boi09] and paper [TM01]), distribution of the following properties. Those are sometimes cumulative. Figures 2.2-1 and 2.2-2 illustrate, on canonical cases, certain cases.

	Properties of the matrices	Properties of the eigenvalues	Properties of the clean vectors	Example of links with modelings <i>Code_Aster</i>
1	B not singular	$2n$ eigenvalues λ finished	-	Structure not blocked or blocked by elimination
2	B singular	$2n$ eigenvalues λ finished or infinite	-	Structure blocked by dualisation
3	A , B and C real	Real or by pair $(\lambda, \bar{\lambda})$	If u clean vector on the right of λ , then $\bar{\mathbf{u}}$ is that of $\bar{\lambda}$	"Classical" QEP (not of damping hysteretic)
4	A , B and C square	Real or by pair $(\lambda, \bar{\lambda})$	If u clean vector on the right of λ , then it is also clean vector on the left of $\bar{\lambda}$	QEP without gyroscopy and with viscous damping
5	A , B et C square, B > 0 and A , C ≥ 0	$\text{Re}(\lambda) \leq 0$	-	Structure free or blocked by elimination, with one damping (dissipative) of Rayleigh and without gyroscopy

¹ To recover it, are needed that the matrices are, for example, complexes square.

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	Properties of the matrices	Properties of the eigenvalues	Properties of the clean vectors	Example of links with modelings Code_Aster
6	A, B and C symmetrical B, C > 0 and A ≥ 0 + Condition of on-damping ²	Negative real spectrum broken up into two packages of size <i>n</i>	<i>n</i> clean vectors linearly independent are associated with <i>n</i> greater (or smaller) eigenvalues	Structure free or blocked by elimination, with a damping <i>ad hoc</i> and without gyroscopy
7	A and B square, C = - C [*] (anti-square) B > 0	Imaginary pure or by pair (λ, -λ̄)	If u clean vector on the right of λ, then it is also clean vector on the left of -λ̄	Structure free or blocked by elimination, with gyroscopy
8	A et B symmetrical real > 0, C = - C ^T (antisymmetric)	Imaginary pure	-	-

Table 2.2-1. Properties of the modes of a standard QEP (of size *n*) according to those of its matrices. Possible links with Code_Aster modelings.

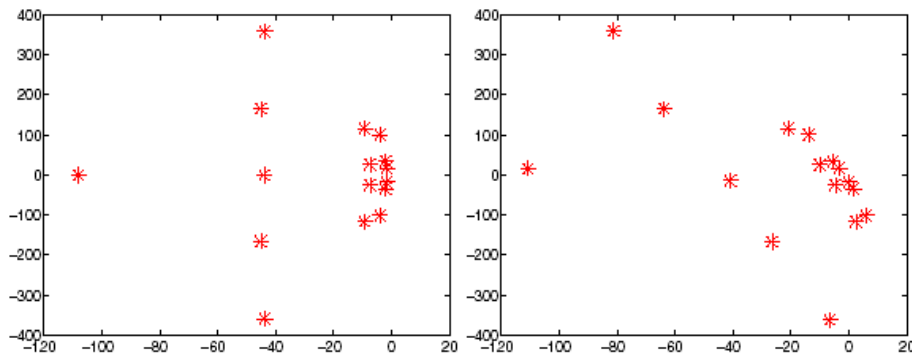


Figure 2.2-1. Examples of the spectrum of a QEP (*n* = 8) of a simplified model of nuclear enclosure [TM01]. Figure of left, one is in the case n°3 table 2.2-1. That of right-hand side, one adds with **K** damping hysteretic thus appear odd modes (case general n°1).

2 Condition of on-damping:
$$\gamma(\mathbf{A}, \mathbf{B}, \mathbf{C}) := \min_{\|\mathbf{x}\|_2=1} \left[(\mathbf{x}^* \mathbf{C} \mathbf{x})^2 - 4(\mathbf{x}^* \mathbf{M} \mathbf{x})(\mathbf{x}^* \mathbf{K} \mathbf{x}) \right] > 0 .$$

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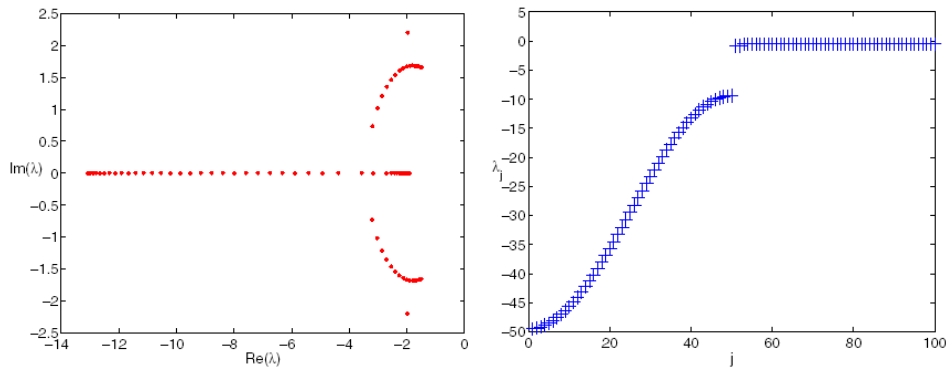


Figure 2.2-2. Examples of the spectrum of a QEP ($n=50$) of a system mass-springs deadened [TM01]. Figure of left, one is in the case $n^{\circ}5$ table 2.2-1. That of right-hand side, one adds the constraint of on-damping and the spectrum becomes real negative in two packages (case $n^{\circ}6$).

2.3 Specificities of the QEP and elements of theory

One **major algebraic specificity** between the QEP and the other classes of modal problems of level lower (GEP and SEP) is **the existence of twice more clean modes ($2n$) that size of the discretized problem**. The clean vectors cannot be linearly independent any more, in addition, the eigenvalues can finished or infinite and all “this small world” generally lives in the complex plan³. It is necessary then **to define the heuristic robust ones to filter the eigenvalues desired by the user** and to distinguish the real ones, of the odd complexes, complexes of those coupled...

Another complication inherent in the QEP is of order algorithmic. **There does not exist decomposition of Schur (resp. Schur generalized) as for the SEP (resp. GEP)** on which will be able to rest the algorithm of resolution. For example, for the SEP $\mathbf{A}\mathbf{u}=\lambda\mathbf{u}$, this decomposition ensures us the existence of a unit matrix (thus conditioned well and easily invertible) \mathbf{U} , allowing the rewriting of the matrix of work \mathbf{A} in a form easier to handle⁴: the higher triangular matrix \mathbf{T} .

$$\mathbf{U}\mathbf{A}\mathbf{U}^*=\mathbf{T} \quad (2.3-1)$$

The QEP thus constitute a very particular and important class⁵ nonlinear problems. Their resolution is less routine than for the other classes of modal problems. In particular, few methods make it possible to solve the problem directly, it is often necessary to forward by a GEP (via a linearization *ad hoc*) then a SEP (spectral transformation) what induces a loss of spectral information and digital instabilities (propagation of rounding errors).

In the theoretical literature, rather than in the QEP (2.1-1), one is interested in **matric polynomial** (quadratic in λ)

$$\mathbf{Q}(\lambda):=(\lambda^2\mathbf{B}+\lambda\mathbf{C}+\mathbf{A}) \quad (2.3-2)$$

One it call too λ -matrice **or stamps dynamic** and his noted spectrum is sought $spectre(\mathbf{Q}):=\{\lambda\in\mathbb{C}/det\mathbf{Q}(\lambda)=0\}$. When this determinant is null whatever λ , λ -matrice is known as singular. In the contrary case, it is known as regular (one places oneself in general within this framework!).

3 It is already the case for certain classes of GEP: nonsymmetrical or with complex matrix.

4 The eigenvalues of the problem are found on the principal diagonal of \mathbf{T} and one can deduce easily from the vectors of Schur (the vectors columns from \mathbf{Q}), their associated own vectors.

5 Fact in particular of these increasing applications in industry: analysis vibratory, vibro-acoustic, mechanics of the fluids with turbulence, electronics (VLSI)...

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The polynomial characteristic of the problem is thus written in the form $\det \mathbf{Q}(\lambda) = \det(\mathbf{B})\lambda^{2n} +$ terms of a lower nature in λ . Thus, as soon as $\mathbf{B} = \mathbf{M}$ is singular, this polynomial admits $r < 2n$ finite roots to which it is necessary to add $2n - r$ infinite. In addition, these distinct eigenvalues can divide the same clean vectors. It is the "dual situation" of the multiple eigenvalues of the SEP where the same eigenvalue is attached to several clean vectors. Thus, for the canonical QEP

$$\mathbf{A} = \mathbf{I}_3, \mathbf{B} = \begin{bmatrix} 0 & 6 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 1 \end{bmatrix} \text{ et } \mathbf{C} = \begin{bmatrix} 1 & -6 & 0 \\ 2 & -7 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (2.3-3)$$

there is the following spectrum

$$\begin{array}{cccccc} i & 1 & 2 & 3 & 4 & 5 & 6 \\ \lambda_i & 1/3 & 1/2 & 1 & i & -i & \infty \\ \mathbf{u}_i & \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} & \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} & \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} & \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} & \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} & \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \end{array} \quad (2.3-4)$$

Singularity of \mathbf{B} comes from the infinite eigenvalue. One notes also the division of clean vectors by the first two eigenvalues and the 4^{ème}/5^{ème}.

To more easily apprehend the infinite eigenvalues of $\mathbf{Q}(\lambda)$, one associates them with the worthless eigenvalues **opposite polynomial**

$$\text{rev } \mathbf{Q}(\lambda) := \lambda^2 \mathbf{Q}\left(\frac{1}{\lambda}\right) = (\mathbf{B} + \lambda \mathbf{C} + \lambda^2 \mathbf{A}) \quad (2.3-5)$$

These **eigenvalues finished of $\text{rev } \mathbf{Q}(\lambda)$ are easier to calculate** and the same spectral characteristics divide (multiplicities geometrical and algebraic, clean space...) that initial infinite values.

For further information on these theoretical aspects one will be able to consult, for example, the works of P.Lancaster [GLR82] [LT85] and the thesis of D.S.Mackey [Mac06] (and its many bibliographical references).

2.4 Strategy of linearization

2.4.1 Introduction

The standard approach to solve a modal problem is to transform it to reveal canonical matrices revealing the required modes. For example, decomposition of Schur for the SEP or that generalized for the GEP. Unfortunately, this practice cannot spread with the modal problems of a higher nature. Two solutions are offered then:

- **To solve the nonlinear problem directly** (root of polynomial, factorization of λ -matrice, methods of the Newton type...).
- **To linearize in a GEP**, then to treat this last *via* adapted methods [Boi09].

first strategy is declined in the options ['NEAR' , 'ADJUSTS'] (method of Müller-Traub) to capture a first estimate of the eigenvalues. One **plume then with the following strategy**, because to refine the estimates and to accelerate convergence, one calls on a method of the type powers opposite (alternative of Jennings) on the linearized QEP. Certain authors propose complete direct approaches. They are often based on alternatives of Newton. But their convergence is slow (a mode at the same time) and not always assured (cf Kublanovskaya 1970, G.Peters & J.H.Wilkinson 1979 and A.Ruhe 1973).

strategy of linearization is thus often privileged. It doubles the size of the modal problem to treat, changes its nature (with the risk to lose spectral information⁶) and introduced digital instabilities (sensitivities to the

6 One finds the solution exact of a "GEP approximate" but this one does not correspond inevitably to the exact solution of a "approximate QEP" because solveurs GEP do not respect the particular structure of the problem linearized (cf [TM01] §5).

rounding errors⁷ and with the digital parameters⁸). But she has the immense advantage of re-using all “digital artillery” already deployed for the GEP⁹.

One can thus capture simultaneously all the spectrum (cf method QZ usable with the options ['CENTER' , 'PLUS_PETITE' , 'ALL']) or only left it centered on a zone interest (cf IRAM or Lanczos) while resorting to the suitable spectral transformation.

2.4.2 Principle

Now that the context was brushed, to consolidate itself with the terminology employed in the literature, one from now on will simplify the notations by considering the QEP associated with λ -matrice $\mathbf{Q}(\lambda) := (\lambda^2 \mathbf{M} + \lambda \mathbf{C} + \mathbf{K})$. This matrix is also called “dynamic matrix” in the jargon of the dynamician of the structures (and in the data-processing documents/sources of *Code_Aster*). It is during that described in the note dedicated to the GEP: $\mathbf{Q}(\lambda) := (\mathbf{K} - \lambda \mathbf{M})$.

Definition 1

From a theoretical point of view, to linearize $\mathbf{Q}(\lambda)$ come down to find another λ -matrice (complex square of size $2n$) type $\mathbf{A} - \lambda \mathbf{B}$ such as there exist two different λ -matrices ($\mathbf{E}(\lambda)$ and $\mathbf{F}(\lambda)$) with determinant constant not no one, checking the relation

$$\begin{bmatrix} \mathbf{Q}(\lambda) & \mathbf{0}_n \\ \mathbf{0}_n & \mathbf{I}_n \end{bmatrix} = \mathbf{E}(\lambda) (\mathbf{A} - \lambda \mathbf{B}) \mathbf{F}(\lambda) \quad (2.4-1)$$

Matrices \mathbf{A} and \mathbf{B} the matrices are called “companion” of the linearization of the QEP.

Clearly, spectra of the initial QEP ($\mathbf{Q}(\lambda)$) and that of its linearization ($\mathbf{A} - \lambda \mathbf{B}$) coincide. However **this decomposition is not single** and it is necessary to choose, if possible, that which:

- **Preserve the properties** initial matrices (arithmetic, symmetry...),
- Present it **less sensitivity to the rounding errors** (“backward stable”: balanced, well conditioned, invertible matrices...),
- Handle **canonical matrices** (identity, triangular...),
- Adapt to one **broad perimeter of QEP** (viscous damping, gyroscopy, on-damping...).

A more intuitive manner to apprehend the techniques of linearization, consists in introducing a change of variable of the type $\mathbf{v} = \lambda \mathbf{u}$ ¹⁰ in (2.1-1) and to rearrange it in matrix form:

$$\left(\begin{bmatrix} \mathbf{0}_n & \mathbf{I}_n \\ -\mathbf{K} & -\mathbf{C} \end{bmatrix} - \lambda \begin{bmatrix} \mathbf{I}_n & \mathbf{0}_n \\ \mathbf{0}_n & \mathbf{M} \end{bmatrix} \right) \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} = \mathbf{0}_{2n} \quad (2.4-2)$$

This “very classical” linearization returns within the framework of definition 1 if they are used λ -matrices :

$$\mathbf{E}(\lambda) := \begin{bmatrix} -(\mathbf{C} + \lambda \mathbf{M}) & -\mathbf{I}_n \\ \mathbf{I}_n & \mathbf{0}_n \end{bmatrix}, \mathbf{F}(\lambda) := \begin{bmatrix} \mathbf{I}_n & \mathbf{0}_n \\ \lambda \mathbf{I}_n & \mathbf{I}_n \end{bmatrix} \quad (2.4-3)$$

In fact, the linearization of a QEP marries it **tally general of that of the matrix polynomials**. While posing

$\mathbf{Q}(\lambda) := \sum_{i=1}^k \lambda_i \mathbf{X}_i$ (here $k=2$, $\mathbf{X}_i = \mathbf{M}$ etc), one is always ensured to find two linearizations, known as

“companions”, of the form $\mathbf{A}_1 - \lambda \mathbf{B}_1$ and $\mathbf{A}_2 - \lambda \mathbf{B}_2$ with

7 The application of solver modal of GEP to a linearized QEP is not “backward stable”. I.e. this technique has a propensity to transmit/amplify the rounding errors.

8 The results can be sensitive to the various parameters of the modal solveurs used *in fine*, but more especially, with those of the two preprocessings: linearization and spectral transformation.

9 One made in the same way for transition GEP/SEP ([Boi09] §3.7).

10 How for the solutions of differential equations of the second order of the lower school!

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$$\mathbf{B}_1 = \mathbf{B}_2 := \begin{bmatrix} -\mathbf{X}_k & \mathbf{0}_{(k-1)n} \\ \mathbf{0}_{(k-1)n} & -\mathbf{I}_{(k-1)n} \end{bmatrix},$$

$$\mathbf{A}_1 := \begin{bmatrix} \mathbf{X}_{k-1} & \mathbf{X}_{k-2} & \dots & \mathbf{X}_0 \\ \mathbf{I}_n & \mathbf{0}_n & \dots & \mathbf{0}_n \\ \dots & \dots & \dots & \dots \\ \mathbf{0}_n & \dots & -\mathbf{I}_n & \mathbf{0}_n \end{bmatrix}, \quad \mathbf{A}_2 := \begin{bmatrix} \mathbf{X}_{k-1} & -\mathbf{I}_n & \dots & \mathbf{0}_n \\ \mathbf{X}_{k-2} & \mathbf{0}_n & \dots & \dots \\ \dots & \dots & \dots & -\mathbf{I}_n \\ \mathbf{X}_0 & \mathbf{0}_n & \dots & \mathbf{0}_n \end{bmatrix} \quad (2.4-4)$$

In practice, one prefers to them linearizations more adapted to the treated case (cf following paragraph).

2.4.3 Some examples

In the literature, it is often question of the following linearizations (with N a square regular matrix complexes of size n):

$$(L_1) \left(\begin{bmatrix} \mathbf{0}_n & \mathbf{N} \\ -\mathbf{K} & -\mathbf{C} \end{bmatrix} - \lambda \begin{bmatrix} \mathbf{N} & \mathbf{0}_n \\ \mathbf{0}_n & \mathbf{M} \end{bmatrix} \right) \begin{bmatrix} \mathbf{u} \\ \lambda \mathbf{u} \end{bmatrix} = \mathbf{0}_{2n} \quad (2.4-5)$$

$$(L_2) \left(\begin{bmatrix} -\mathbf{K} & \mathbf{0}_n \\ \mathbf{0}_n & \mathbf{N} \end{bmatrix} - \lambda \begin{bmatrix} \mathbf{C} & \mathbf{M} \\ \mathbf{N} & \mathbf{0}_n \end{bmatrix} \right) \begin{bmatrix} \mathbf{u} \\ \lambda \mathbf{u} \end{bmatrix} = \mathbf{0}_{2n} \quad (2.4-6)$$

The choice depends on the potential singularity of the matrices \mathbf{K} and \mathbf{M} . One wishes to be able to reverse the diagonal terms, therefore if \mathbf{K} is singular (resp. \mathbf{M}), one uses (L_1) (resp. (L_2)). To balance the terms of the matrices and to facilitate handling, one often takes $\mathbf{N} = \alpha \mathbf{I}_n$ with α real factor of balancing (cf [Boi09] appendix 1) built on the standard basis matrix of the other terms $\alpha = \alpha(\|\mathbf{K}\|, \|\mathbf{M}\|, \|\mathbf{C}\|)$. To work with a symmetrical GEP (even definite or semi-definite positive), one can also initialize the auxiliary matrix \mathbf{N} à $\alpha \mathbf{K}$ ou $\beta \mathbf{M}$ ($\alpha, \beta \in \mathbb{R}$).

To solve them more effectively **QEP with gyroscopic effects**, one advises in the literature hanging “the Hamiltonians¹¹” preceding linearizations. “Companions are the matrices”

$$(L_3) \left(\begin{bmatrix} \mathbf{K} & \mathbf{0}_n \\ \mathbf{C} & \mathbf{N} \end{bmatrix} - \lambda \begin{bmatrix} \mathbf{0}_n & \mathbf{K} \\ -\mathbf{M} & \mathbf{0}_n \end{bmatrix} \right) \begin{bmatrix} \mathbf{u} \\ \lambda \mathbf{u} \end{bmatrix} = \mathbf{0}_{2n} \quad (2.4-7)$$

$$(L_4) \left(\begin{bmatrix} \mathbf{0}_n & -\mathbf{K} \\ \mathbf{M} & \mathbf{N} \end{bmatrix} - \lambda \begin{bmatrix} \mathbf{M} & \mathbf{C} \\ \mathbf{0}_n & \mathbf{M} \end{bmatrix} \right) \begin{bmatrix} \mathbf{u} \\ \lambda \mathbf{u} \end{bmatrix} = \mathbf{0}_{2n} \quad (2.4-8)$$

Here the objective is not to respect a property of symmetry rather but those “Hamiltonian¹²” problem. If \mathbf{K} is singular (resp. \mathbf{M}), one uses (L_4) (resp. (L_3)).

11 A square matrix of order $2n$, \mathbf{A} , is known as Hamiltonian (resp. anti Hamiltonienne) if it checks the relation

$$(\mathbf{A}\mathbf{J})^T = \mathbf{A}\mathbf{J} \quad (\text{resp. } (\mathbf{A}\mathbf{J})^T = -\mathbf{A}\mathbf{J} \text{ with } \mathbf{J} \text{ the antisymmetric matrix unit } \mathbf{J} := \begin{bmatrix} \mathbf{0}_n & \mathbf{I}_n \\ -\mathbf{I}_n & \mathbf{0}_n \end{bmatrix}.$$

12 I.e. the solutions are symmetrical compared to the axes reality and imaginary: $(\lambda, \bar{\lambda}, -\lambda, -\bar{\lambda})$.

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In the case of one QEP says “T-palindromique” [Mac06] ($\mathbf{K} = \mathbf{M}^T$ et $\mathbf{C} = \mathbf{C}^T$) the linearization is preferred

$$(L_5) \left(\underbrace{\begin{bmatrix} \mathbf{K} & \mathbf{K} \\ \mathbf{C} - \mathbf{M} & \mathbf{K} \end{bmatrix}}_{\mathbf{A}} - \lambda \underbrace{\begin{bmatrix} -\mathbf{M} & \mathbf{K} - \mathbf{C} \\ -\mathbf{M} & -\mathbf{M} \end{bmatrix}}_{\mathbf{B}} \right) \begin{bmatrix} \mathbf{u} \\ \lambda \mathbf{u} \end{bmatrix} = \mathbf{0}_{2n} \quad (2.4-9)$$

2.4.4 Strategies retained in Code_Aster

One thus has a very large variety of choice to adapt the linearization of the QEP to each situation. For the moment, Code_Aster do not propose to the user of parameter allowing to modulate only the linearization. This one is fixed for a given modal solver:

- **With OPTION among ['NEAR' , 'ADJUSTS'] (2nd phase)** passage QEP/GEP is carried out via the matrices companions of (L₁), while posing $\mathbf{N} = \mathbf{I}_n$. The linearized system is not symmetrical but it is not pre-necessary for to apply a method of the type powers opposite.

$$(L_1) \left(\underbrace{\begin{bmatrix} \mathbf{0}_n & \mathbf{I}_n \\ -\mathbf{K} & -\mathbf{C} \end{bmatrix}}_{\mathbf{A}} - \lambda \underbrace{\begin{bmatrix} \mathbf{I}_n & \mathbf{0}_n \\ \mathbf{0}_n & \mathbf{M} \end{bmatrix}}_{\mathbf{B}} \right) \begin{bmatrix} \mathbf{u} \\ \lambda \mathbf{u} \end{bmatrix} = \mathbf{0}_{2n} \quad (2.4-10)$$

- **With OPTION among ['CENTER' , 'PLUS_PETITE'] and METHODE=' TRI_DIAG' or 'SORENSEN'**, passage QEP/GEP is carried out via the matrices companions of (L₂) while posing $\mathbf{N} = \mathbf{M}$. If the matrices of rigidity, mass and damping are symmetrical real, one falls down in the perimeter of the standard GEP (symmetrical realities). The methods of Lanczos and Sorensen are then accessible. If \mathbf{K} becomes complex or if one of them is nonsymmetrical, only IRAM remains in race (with QZ cf item according to)!

$$(L_2) \left(\underbrace{\begin{bmatrix} -\mathbf{K} & \mathbf{0}_n \\ \mathbf{0}_n & \mathbf{M} \end{bmatrix}}_{\mathbf{A}} - \lambda \underbrace{\begin{bmatrix} \mathbf{C} & \mathbf{M} \\ \mathbf{M} & \mathbf{0}_n \end{bmatrix}}_{\mathbf{B}} \right) \begin{bmatrix} \mathbf{u} \\ \lambda \mathbf{u} \end{bmatrix} = \mathbf{0}_{2n} \quad (2.4-11)$$

However, when \mathbf{M} is not invertible (fact for example of Lagranges of blocking), the inversion of the diagonal term of \mathbf{A} is not assured any more. To mitigate this problem, one introduces a “regularization” of the matrix \mathbf{M} , noted \mathbf{M}_R , in the diagonal term. This one has the property to cancel, by multiplication, all the components of the core of $\mathbf{M} : \mathbf{M}_R \mathbf{u} = \mathbf{0}$ si $\mathbf{u} \in \text{Ker}(\mathbf{M})$. Thus, one can define \mathbf{M}_R^{-1} who checks the property formally $\mathbf{M}_R^{-1} \mathbf{M} \approx \mathbf{M} \mathbf{M}_R^{-1} \approx \mathbf{I}_n$ on the components “except core of \mathbf{M} ” handled vectors. Because of particular structure of the dualized matrix \mathbf{M} (cf [Boi09] §3.2), this handling amounts proscribing the components related on Lagranges and the blocked degrees of freedom (them $\mathbf{v}_i^{2,3}$ demonstration of the property n°4 [Boi09]). What does not obstruct of anything the process since one is interested only in the physical modes and not in these artifacts of modelings¹³.

$$(L_2)'' \left(\underbrace{\begin{bmatrix} -\mathbf{K} & \mathbf{0}_n \\ \mathbf{0}_n & \mathbf{M}_R \end{bmatrix}}_{\mathbf{A}} - \lambda \underbrace{\begin{bmatrix} \mathbf{C} & \mathbf{M} \\ \mathbf{M} & \mathbf{0}_n \end{bmatrix}}_{\mathbf{B}} \right) \begin{bmatrix} \mathbf{u} \\ \lambda \mathbf{u} \end{bmatrix} = \mathbf{0}_{2n} \quad (2.4-12)$$

- **With OPTION among ['CENTER' , 'PLUS_PETITE' , 'ALL'] and METHODE=' QZ'**, one preferred to avoid these complications. The objective being of to privilege the digital robustness to treat

13 An identical process is often used to solve the GEP. It consists in initializing the algorithm of resolution by a vector of the image unit of \mathbf{M} (thus filtering the elements of the cores). Instead of the random vector \mathbf{u}_i , one takes $\mathbf{M} \mathbf{u}_i$.

the small ones case ($< 10^3$ degrees of freedom). The scenario (L_2) was empirically retained while posing $\mathbf{N} = \alpha \mathbf{I}_n$, with $\alpha := \frac{I}{3n} (\|\mathbf{K}\| + \|\mathbf{M}\| + \|\mathbf{C}\|)$

$$(L_2)^* \left(\underbrace{\begin{bmatrix} -\mathbf{K} & \mathbf{0}_n \\ \mathbf{0}_n & \alpha \mathbf{I}_n \end{bmatrix}}_{\mathbf{A}} - \lambda \underbrace{\begin{bmatrix} \mathbf{C} & \mathbf{M} \\ \alpha \mathbf{I}_n & \mathbf{0}_n \end{bmatrix}}_{\mathbf{B}} \right) \begin{bmatrix} \mathbf{u} \\ \lambda \mathbf{u} \end{bmatrix} = \mathbf{0}_{2n} \quad (2.4-13)$$

2.5 Establishment in Code_Aster

The course of a quadratic modal calculation is, by construction, very near to that of a generalized problem. One will thus be attached to the functional diagram of resolution of the GEP describes in [Boi09] (cf. § 3.8). Its stages break up as follows:

2.5.1 Preprocessings (linearization, calculation of the shift)

Determination of **form linearized and of the associated spectral transformation** according to the adopted method (power, Lanczos, IRAM and QZ) and the option of research 'ADJUSTS' / 'NEAR' or 'PLUS_PETITE' / 'CENTER'.

It should be noted that the clean modes being in the complex plan, the test of Sturm currently established is inoperative. Thus heuristics associated with OPTION 'NEAR' and 'ADJUSTS' is not based on the modal positions, and the option 'BAND' is proscribed. In the same way for the post-checking based on the test of Sturm [Boi12].

For **method of subspace** (OPTION among ['CENTER', 'PLUS_PETITE'] and METHODE= 'TRI_DIAG' or 'SORENSEN'), once the linearized problem (L_2)' updated, one applies a spectral transformation of standard "shift-and-invert" (cf [Boi09] §3.6/§5). That will make it possible to complete the transformation into a SEP¹⁴ (S_1), to direct the research of the spectrum in a zone of interest for the user and to better separate the eigenvalues.

$$(S_1) \underbrace{(\mathbf{A} - \sigma \mathbf{B})^{-1} \mathbf{B}}_{\mathbf{A}_\sigma} \begin{bmatrix} \mathbf{u} \\ \lambda \mathbf{u} \end{bmatrix} = \underbrace{\frac{I}{\lambda - \sigma}}_{\mu} \begin{bmatrix} \mathbf{u} \\ \lambda \mathbf{u} \end{bmatrix} \quad (2.5-1)$$

method of the powers opposite bracket it a spectral transformation particular to the linearized problem (L_1)'

As for **method QZ** (OPTION among ['CENTER', 'PLUS_PETITE', 'ALL'] and METHODE= 'QZ'), this spectral transformation is superfluous. The algorithm directly deals with the linearized problem (L_2)^{*} and calculates all its modes. According to the wishes of the user (OPTION, CALC_FREQ=_F (NMAX_FREQ...)), it filters then the results.

Note:

- As for the techniques of linearization, no parameter user makes it possible yet to change spectral transformation. Into quadratic, it would be interesting to use transformations more adapted to the complex plan than traditional "the shift-and-invert". For example, a transformation of the Cayley type to make converge simultaneously couples of combined eigenvalues ($\lambda, \bar{\lambda}$)

$$\underbrace{(\mathbf{A} - \sigma \mathbf{B}) \mathbf{B}^{-1} (\mathbf{A} - \bar{\sigma} \mathbf{B}) \mathbf{B}^{-1}}_{\mathbf{A}_\sigma} \mathbf{w} = \underbrace{\frac{I}{(\lambda - \sigma)(\bar{\lambda} - \sigma)}}_{\mu} \mathbf{W} \quad (2.5-2)$$

14 To which apply the classical modal solvers.

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- This strategy of Cayley spreads to treat the gyroscopy (cf V.Mehrman and D.Watkins 2001) and to make converge simultaneously the quadruplets $(\lambda, \bar{\lambda}, -\lambda, -\bar{\lambda})$
- Certain authors also propose to invert the phase of linearization and that of spectral transformation [Mee07].

2.5.2 Factorization of dynamic matrices

As one already underlined, these factorizations of dynamic matrices of the type $\mathbf{Q}(\lambda)$ are not used to implement a test of Sturm. This last being illicit for the QEP. However they remain an ingredient very present and very expensive¹⁵ for:

- To estimate the function cost of the heuristic part (method of Müller-Traub) with `OPTION=' AJUSTE'`.
- When one must handle a matrix of work comprising of the opposite. To be more effective, one seeks a formulation then utilizing only $\mathbf{Q}(\lambda)^{-1}$ (`OPTION` among [`'NEAR'`, `'ADJUSTS'`] + `SOLVEUR_MODAL=_F` (`OPTION_INV+` `'DIRECT'`), or `OPTION` among [`'CENTER'`, `'PLUS_PETITE'`] + `SOLVEUR_MODAL=_F` (`METHODE='TRI_DIAG'` / `'SORENSEN'`)).

Comprehensive approach (`OPTION` among [`'CENTER'`, `'PLUS_PETITE'`, `'ALL'`] + `SOLVEUR_MODAL=_F` (`METHODE='QZ'`)) is not concerned with this preliminary factorization of the dynamic matrix.

2.5.3 Modal calculation

Modal calculation itself is carried out: one solves standard problem SEP, one returns with the intermediate GEP, then with the initial QEP. Each one of these conversions, one filter and transcribes the results of preceding calculation. Concerning **eigenvalues** (cf. §2.1/2.2) only they are retained λ with positive imaginary part of the coupled modes $(\lambda, \bar{\lambda})$.

```
your problem is strongly deadened.  
value (S) clean (S) real (S) : 2  
value (S) clean (S) complex (S) with combined: 107  
value (S) clean (S) complex (S) without combined: 0
```

Example 1. Impressions in the file message of alarms recapitulating the number of modes not selected (here 2 realities). Extract of the CAS-test sdll123a.

For **clean vectors**, two possibilities remain open:

- To take them directly n first components of \mathbf{w} (part known as “high”),
- To choose them n last (part known as “low”) possibly divided by the same scalar.

In *Code_Aster*, it is the second option which was retained. This choice is not always pain-killer¹⁶ in particular with respect to the quality of the modes and their sensitivities to the rounding errors.

With `OPTION` among [`'NEAR'`, `'ADJUSTS'`], only one method is available, an alternative of the method of the iterations opposite due to Jennings (`OPTION_INV='DIRECT'`). It refines the eigenvalues detected beforehand by the method of Müller-Traub (`'AJUSTE'`) or estimates provided by the user (`'NEAR'`). As regards `OPTION` among [`'CENTER'`, `'PLUS_PETITE'`, `'ALL'`], one can use three distinct methods: method of Lanczos (`'TRI_DIAG'`), that of Sorensen (`'SORENSEN'`) and QZ (`'QZ'`). Only the two last are available with real or complex matrices nonsymmetrical symmetrical (for **K** only).

Remarks

- Each one of these methods has internal tests of stops. Not counting the methods of projection employ auxiliary modal methods: **QR/QL** for Lanczos and **IRAM**. They require also tests of stops. The user often has access to these parameters, although it is warmly recommended, at least initially, to preserve their values by default.

¹⁵ Calculation complexity in $O(bn^2)$ with b the bandwidth and n size of the problem has.

¹⁶ The alternative of method QZ suggested by F.Tisseur [TM01] is based on the values of “the opposite error” of each mode, to choose the high or low part clean vectors.

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- Contrary to the GEP, one does not force **M** - orthonormalisation of the clean vectors. It does not have any direction in QEP. Moreover, by applying the result of proposal 2 of [Boi09] to the linearized problem, it is clear that the clean vectors are **A** and **B** - orthogonal. But because of complexity of the linear reductions used, that does not lead (except typical case) to clean vectors **K**, **M** or **C** - orthogonal!

2.5.4 Postprocessings of checking

This last part gathers the only postprocessing which checks the good progress of calculation (in the absence of test of Sturm adapted to the complex case). One calculates **the relative error on the standard**¹⁷ **residue initial QEP**

$$\mathbf{u} \leftarrow \frac{\mathbf{u}}{\|\mathbf{u}\|_{\infty}}$$

Si $|\lambda| > \text{SEUIL_FREQ}$ alors

$$\frac{\|\lambda^2 \mathbf{M}\mathbf{u} + \lambda \mathbf{C}\mathbf{u} + \mathbf{K}\mathbf{u}\|_2}{\|\mathbf{K}\mathbf{u}\|_2} ? < \text{SEUIL},$$

Sinon

$$\|\lambda^2 \mathbf{M}\mathbf{u} + \lambda \mathbf{C}\mathbf{u} + \mathbf{K}\mathbf{u}\|_2 ? < \text{SEUIL},$$

Fin si.

Algorithm 1. Test of the standard of the residue.

This sequence is parameterized by the keyword `THRESHOLD` and `SEUIL_FREQ`, belonging respectively to the keyword factors `VERI_MODE` and `CALC_FREQ`. In addition, this post - treatment is activated by initialization with 'YES'(value by default) of `STOP_ERREUR` in the keyword factor `VERI_MODE`. When this rule is activated and non-observance, calculation stops, if not the error is just announced by an alarm. One could of course only too much recommend not to disable this parameter preferential treatment!

2.5.5 Posting in the file message

In the file message are mentioned the relative information with the modes selected. For example, in the case of a QEP, one specifies the modal solver used and lists its eigenvalues λ_i reserves by order ascending of imaginary part $\frac{\text{Im}(\lambda_i)}{2\pi}$ (column `FREQUENCY`). Then his damping is specified $\xi_i = \frac{-\text{Re}(\lambda_i)}{\lambda_i}$ and its standard of error (cf algorithm n°1).

```

-----
MODAL CALCULATION: GLOBAL METHOD OF THE TYPE QR
ALGORITHM QZ_EQUI

NUMBER    FREQUENCY (HZ)    DAMPING    ERROR NORMALIZES
1         1.23915E+02      1.55604E-08  9.93686E-02
2         1.24546E+02     -3.76772E-10  1.81854E-01
3         4.97033E+02     -5.88927E-10  1.41043E-03
4         4.99575E+02      1.41315E-12  2.14401E-03
5         1.11531E+03      4.75075E-12  1.17669E-04
.....
    
```

¹⁷ Square standard and only on the components of the physical degrees of freedom.

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Example 2. Impressions in the file message of the eigenvalues S retained at the time of QEP. Extract of the CAS-test sdll123a.

Now that context of the QEP in *Code_Aster* was brushed, we will be interested more particularly in the methods of type power and their establishment in 'CLOSE' OPTION and 'ADJUSTS'.

3 Method of the powers opposite (OPTION among ['NEAR' , 'ADJUSTS'])

3.1 Introduction

As for the treatment of the GEP, in QEP this operator functions in two parts:

- **localization of the eigenvalues.** One determines an approximation of each eigenvalue contained in an interval given by **the algorithm of Müller-Traub**[Mul56] [DB08] or one takes an estimate provided by the user.
- **Improvement of these estimates** and the calculation of their own vectors associated by a method **iterations opposite** (alternative of Jennings [Jen77]).

The search for a value approached for each eigenvalue considered is selected with the keyword `OPTION :`

- If `OPTION=' AJUSTE '`, in each interval of frequencies defined by the keyword `CALC_FREQ=_F (FREQ)`, an approximate value of each eigenvalue contained in this interval is calculated by using the method of Müller-Traub (cf §3.2).
- Either only they are retained `NMAX_FREQ` (under the keyword factor `CALC_FREQ`) the lowest frequencies contained in the maximum interval specified by the user, is one calculates all the values of this interval (if `NMAX_FREQ=0`).
- If `OPTION=' PROCHE '`, frequencies given by the keyword `CALC_FREQ=_F (FREQ)`, are regarded as the approximate values of the sought eigenvalues.

Note:

- *Of course, as one already specified, these options are to be used rather to determine or refine some eigenvalues. For a wider research it is necessary to use options ['CENTER' , 'PLUS_PETITE' , 'ALL'].*
- *With the option 'NEAR' one cannot calculate multiple modes.*
- *It is an expensive algorithm because he calls much on factorizations of a dynamic matrix of work $Q(\lambda)$.*

3.2 Method of Müller-Traub

As in QEP, the astute test of Sturm cannot apply any more, the heuristics of localization of the eigenvalues must be based on another strategy. One “folds back oneself” then on **classic searches of the zeros of the associated characteristic polynomial** with the QEP $p(\lambda) = \det Q(\lambda)$ in the complex plan.

As one then does not lay out any more a relation of order, it is not possible to apply the dichotomy put in work for the GEP. A generalization at three points of the method of the secant makes it possible however to be left there. It is the method suggested by D.E.Muller [Mul56] [DB08] in 1956. It is an iterative method using as curve of interpolation a parabola with horizontal axis. Whereas the method of the secant is based on a linear interpolation between the two reiterated last $\{(\lambda_{k-1}, p(\lambda_{k-1})), (\lambda_k, p(\lambda_k))\}$, the method known as of “Müller-Traub” seeks to build the interpolated quadratic one passing by the three last

$$\{(\lambda_{k-2}, p(\lambda_{k-2})), (\lambda_{k-1}, p(\lambda_{k-1})), (\lambda_k, p(\lambda_k))\}.$$

By writing that the interpolated quadratic one of Lagrange of the characteristic polynomial

$$p(\lambda) \approx a_0 \lambda^2 + a_1 \lambda + a_2 \tag{3.2-1}$$

must pass by the last three quoted points, one builds a system of three equations to three unknown factors. From his analytical resolution, one deduces the root nearest of the reiterated last

$$\rho_{k+1} = \frac{-2p(\lambda_k)\delta_k}{g_k \pm \sqrt{g_k^2 - 4p(\lambda_k)\delta_k \rho_k [p(\lambda_{k-2})\rho_k - p(\lambda_{k-1})\delta_k + p(\lambda_k)]}}$$

avec

$$g_k := p(\lambda_{k-2})\rho_k^2 - p(\lambda_{k-1})\delta_k^2 + p(\lambda_k)(\rho_k + \delta_k)$$

$$\rho_k := \frac{\lambda_k - \lambda_{k-1}}{\lambda_{k-1} - \lambda_{k-2}}$$
(3.2-2)

Of ρ_k , one deduces the new one easily then reiterated λ_{k+1} . The sign of the denominator is selected so as to minimize $|\rho_{k+1}|$ thus one privileges the “conservative” choice of the zero nearest to reiterated preceding λ_k . It is considered that the method converged, when the following relative criterion was reached (front $k+1 < \text{NMAX_ITER_AJUSTE}$ iterations)

$$\frac{|\lambda_{k+1} - \lambda_k|}{|\lambda_k|} < \varepsilon_{\text{PREC_AJUSTE}}$$
(3.2-3)

This method is relatively easy to implement but it lends itself badly in the searches of zeros of real functions with real roots, because it plunges the interpolation in the complex plan and this even on the basis of actual values. **Its interest is related to the class of this method called “by curves of interpolation”, namely:**

- The safety of the method of bisection, since research is carried out in a ball of approximated $(\lambda_k)_k$ being reduced gradually,
- Only the calculation of the function is necessary (not calculation of derived such as for example in the method of Newton-Raphson).
- Convergence is connected with a quadratic convergence (Q~1.89).

In practice, the evaluation is done not directly on the determinant of the polynomial $p(\lambda) := \det \mathbf{Q}(\lambda)$ characteristic but on its “déflaté” to take account of already exhumed spectral information (if not one reconverge always towards the same mode). In addition, after having calculated k eigenvalues $(\lambda_i)_{i=1}^k$, one déflate also by keeping account of their combined¹⁸ not to recompute them

$$p(\lambda) := \frac{\det \mathbf{Q}(\lambda)}{\prod_{i=1}^k (\lambda - \lambda_i)(\lambda - \bar{\lambda}_i)}$$
(3.2-4)

The evaluation of the denominator is commonplace. That of the numerator, $\det \mathbf{Q}(\lambda)$, is carried out while factorizing¹⁹ in form LDL^T the dynamic matrix $\mathbf{Q}(\lambda)$ and by carrying out the product of the diagonal terms of the diagonal matrix \mathbf{D} .

This factorization of dynamic matrix is very expensive with one calculation complexity in $O(bn^2)$ where b is the bandwidth and n size of the problem. It is the part rebukes it in capacity for treatment and place memory of the algorithm. It is to be reproduced $p(i+2)$ time with p the number of desired modes and i the average iteration count to convergence. **The algorithm is thus rather to reserve for the QEP small (<10⁴ degrees of freedom) or with the benchmarks of methods.**

Note:

- Müller [Mul56] proposes a particular and effective procedure to initialize the process if the function to be interpolated $p(\lambda)$ is a polynomial of order n whose coefficients are known. The case which interests us does not return unfortunately in this class of problem. The initialization of the algorithm requires 2 preliminary evaluations thus of p .

18 It is as for this reason as the perimeter of use of CALC_MODES with OPTION among ['NEAR', 'ADJUSTS'], is limited to the standard QEP (symmetrical reality). One expects to find only eigenvalues combined per pair.

19 One expects to be able to factorize without encumbers (without resorting to the swivelling) and to handle one factorized symmetrical. It is another reason which limits the perimeter of CALC_MODES with OPTION among ['NEAR', 'ADJUSTS'], with the real symmetrical QEP.

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- This method does not calculate a modal position, it thus manages badly the multiplicities. Contrary to the dichotomy put in work for the GEP. The concept of threshold in on this side which two digital values are supposed to be multiple is related to the parameter $\epsilon_{\text{PREC_AJUSTE}}$
- One does not retain in the formula (3.2-2) only the complex with positive imaginary part.

3.3 Method of the powers opposite (alternative of Jennings)

The second part consists in refining the estimates of the eigenvalues calculated by the method of Müller-Traub and calculating their associated own vectors. With this intention, **one linearizes the QEP according to the strategy**

(L₁) (cf §2.4) and one applies a particular spectral transformation due to Jennings [Jen77] (1977). Its objective is to reveal, like reverse of matrix, only that of the dynamic matrix $\mathbf{Q}(\lambda)^{-1}$. The algorithm set up in the code cuts out as follows:

- Initialization of the eigenvalue starting from the estimate of the first phase: λ_0 .
- Construction of the dynamic matrix $\mathbf{Q}(\lambda_0)$ and of its factorization.
- Initialization of the iterative process by the vectors: \mathbf{x}_0 aléatoire, $\mathbf{y}_0 = \lambda_0 \mathbf{x}_0$.
- For $k=0, \text{NMAX_ITER}-1$ to make
 - To standardize $\mathbf{x}_k \leftarrow \frac{\mathbf{x}_k}{(\bar{\mathbf{x}}_k)^T \mathbf{M} \mathbf{x}_k}, \mathbf{y}_k \leftarrow \frac{\mathbf{y}_k}{(\bar{\mathbf{y}}_k)^T \mathbf{M} \mathbf{y}_k}$
 - To solve $\mathbf{Q}(\lambda_0) \mathbf{x}_{k+1} = \mathbf{C} \mathbf{x}_k + \lambda_0 \mathbf{M} \mathbf{x}_{k-1} + \mathbf{M} \mathbf{y}_{k-1}$
 - To calculate $\mathbf{y}_{k+1} = -\lambda_0 \mathbf{x}_{k+1} + \mathbf{x}_k$
 - To evaluate $\lambda_k = \frac{(\bar{\mathbf{x}}_k)^T \mathbf{C} \mathbf{x}_k + \sqrt{((\bar{\mathbf{x}}_k)^T \mathbf{C} \mathbf{x}_k)^2 - 4((\bar{\mathbf{x}}_k)^T \mathbf{M} \mathbf{x}_k)((\bar{\mathbf{x}}_k)^T \mathbf{K} \mathbf{x}_k)}}{2((\bar{\mathbf{x}}_k)^T \mathbf{M} \mathbf{x}_k)}$ (3.3-1)
 - If $\frac{|\lambda_{k+1} - \lambda_k|}{|\lambda_k|} < \text{PREC}$ and $\max(|\text{Re}(\lambda_k - \lambda_0)|, |\text{Im}(\lambda_k - \lambda_0)|) < \text{PREC}$ then (3.3-2)
 - The clean mode solution is $(\lambda_k, \mathbf{x}_k)$, exit.

Algorithm 2. Method of the powers opposite (alternative of Jennings).

The criterion of stop PREC and the maximum number of authorized iterations NMAX_ITER are arguments of the keyword factor CALC_MODE .

Note:

- The criterion of stop is based on the extension of the quotient of Rayleigh (cf [Boi09] §4.3) with the QEP. Knowing a clean vector \mathbf{x}_k a good estimate of its eigenvalue λ_k is provided by the formula (3.3-1). The algorithm is stopped as soon as relative variations (in complex) and absolute (on the parts real and imaginary separately), compared to estimated initial, are lower than a certain value. Thus jointly, one refines estimated initial of the eigenvalue and one determines his associated own vector.
- In spite of the linearization of the initial problem, the "astute" formulation of Jennings handles only entities of size n . Actually, algorithm 2 can be schematized in the vectorial form
- $$\begin{bmatrix} \mathbf{Q}(\lambda_0) & \mathbf{0}_n \\ -\lambda_0 \mathbf{I}_n & \mathbf{I}_n \end{bmatrix} \begin{bmatrix} \mathbf{x}_{k+1} \\ \mathbf{y}_{k+1} \end{bmatrix} = \begin{bmatrix} -\mathbf{C} - \lambda_0 \mathbf{M} & -\mathbf{M} \\ -\mathbf{I}_n & \mathbf{0}_n \end{bmatrix} \begin{bmatrix} \mathbf{x}_k \\ \mathbf{y}_k \end{bmatrix} \quad (3.3-3)$$

3.4 Perimeter of use

QEP with symmetrical real matrices.

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The user can only specify `TYPE_RESU=' DYNAMIQUE'` like membership of its calculation classifies (not of buckling). One then informs possibly the vector `FREQ` (and not `CHAR_CRIT`).

3.5 Posting in the file message

In the file message, the results are displayed in the form of table

```

-----
THE NUMBER OF DDL
TOTAL IS:                               56
LAGRANGE IS:                             32
THE NUMBER OF ACTIVE DDL IS:             8
-----
MODAL CALCULATION:  METHOD OF ITERATION OPPOSITE
                     MULLER                OPPOSITE
NUMBER FREQUENCY (HZ) DAMPING NB_ITER PRECISION NB_ITER PRECISION ERROR NORMALIZES
1      5.52915E+00      1.52090E-02  5      9.49522E-07  1      4.47353E-17  2.17748E-15
2      1.08959E+01      2.87575E-02  3      1.17993E-05  1      3.24203E-17  4.83597E-15
3      1.59270E+01      3.95645E-02  5      2.53170E-05  1      8.86844E-18  7.12414E-16
...
-----
CHECKING A POSTERIORI OF THE MODES
-----

```

Example 3. Trace of `CALC_MODES (QEP)` in the file message. Extract of the CAS-test `sldd27b`.

For each eigenvalue (represented in the form $\text{FREQUENCY} = \frac{\text{Im}(\lambda_i)}{2\pi}$ and $\text{DAMPING} = \frac{-\text{Re}(\lambda_i)}{|\lambda_i|}$ cf §2.5), the iteration count and the precision obtained are traced²⁰ of the two phases of the modal operator. With the option 'NEAR', the columns concerning the method of Müller do not appear obviously. The last column, `ERROR NORMALIZES`, the standard of error of the determined residue following begins again the algorithm n°1 (§2.5).

3.6 Summary of the parameter setting

Let us recapitulate the parameter setting of the operator now `CALC_MODES` with `OPTION` among ['NEAR', 'ADJUSTS'].

Operand	Keyword	Value by default	References
	<code>TYPE_RESU=' DYNAMIQUE'</code>	'DYNAMIC'	§2.1
	<code>OPTION = 'AJUSTE'</code>	'ADJUSTS'	§3.1
	'NEAR'		§3.1
CALC_FREQ	FREQ (if NEAR)		§3.1
	NMAX_FREQ	0	§3.1
<i>SOLVEUR_MODAL</i>	<code>NMAX_ITER_AJUSTE</code>	15	§3.2
	<code>PREC_AJUSTE</code>	1.E-04	§3.2
	<code>OPTION_INV=' DIRECT'</code>	'DIRECT'	§3.3
	'RAYLEIGH' (even treatment)		§3.3
	<code>PREC_INV</code>	1.E-05	§3.3
	<code>NMAX_ITER_INV</code>	30	§3.3
<code>VERI_MODE</code>	<code>STOP_ERREUR=' OUI'</code>	'YES'	[Boi12] §3.2

²⁰ Precision of the method of Müller within the meaning of the formula (3.2-3), that of the method of Jennings takes again the formula (3.3-2).

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Operand	Keyword	Value by default	References
	'NOT'		
	THRESHOLD	1.E-02	[Boi12] §3.2

Table 3.6-1. Summary of the parameter setting of `CALC_MODES` with `OPTION` among ['NEAR' , 'ADJUSTS'] (QEP).

Note:

- One finds all the “tripaille” of parameters related to postprocessings of checking (`SEUIL_FREQ`, `VERI_MODE`).
- At the time of the first passages, it is strongly advised to modify only the principal parameters noted in fat. The others relate to more the mysteries of the algorithm and they were initialized empirically with values standards.

4 Method of subspace (METHODE= ' TRI_DIAG' / 'SORENSEN')

4.1 QEP with the SEP

4.1.1 Passage QEP /GEP: linearization

As one explained to §2.4, the passage of the QEP with the GEP is carried out *via* following linearization

$$(L_2)'' \left(\underbrace{\begin{bmatrix} -\mathbf{K} & \mathbf{0}_n \\ \mathbf{0}_n & \mathbf{M}_R \end{bmatrix}}_{\mathbf{A}} - \lambda \underbrace{\begin{bmatrix} -\mathbf{C} & \mathbf{M} \\ \mathbf{M} & \mathbf{0}_n \end{bmatrix}}_{\mathbf{B}} \right) \begin{bmatrix} \mathbf{u} \\ \lambda \mathbf{u} \end{bmatrix} = \mathbf{0}_{2n} \quad (4.1-1)$$

The GEP obtained is structurally symmetrical reality and inherits the properties of the matrices \mathbf{K} , \mathbf{M} and \mathbf{C} . As soon as one of them is nonsymmetrical or complex (possible only with \mathbf{K}), the GEP becomes nonsymmetrical or complex. The symmetrical aspect or not of the GEP is not in fact not blocking because **each method will get busy to find the couple “operator of scalar produced work” which enables him to function**. Moreover, only Lanczos needs a symmetrical couple. Method IRAM can it function very well in nonsymmetrical and with often more robustness²¹.

4.1.2 Passage GEP /SEP: spectral transformation

Then a spectral transformation (cf [Boi09] §3.7/§5) allows to complete the phase of preprocessing of the QEP by transforming the GEP $(L_2)''$ the preceding one in a SEP. When complex modes are handled, two cases are possible:

- To work completely in **arithmetic complex**,
- To generally remain **into arithmetic real** by isolating the contributions real and imaginary from the classical spectral transformation.

First strategy classically use the spectral transformation known as of “shift-and-invert” and metamorphose $(L_2)''$ in

$$(S_1) \quad \underbrace{(\mathbf{A} - \sigma \mathbf{B})^{-1}}_{\mathbf{A}_\sigma} \mathbf{B} \mathbf{w} = \mu \mathbf{w} \quad (4.1-2)$$

avec $\mu := \frac{I}{\lambda - \sigma}$, $\mathbf{w} := \begin{bmatrix} \mathbf{u} \\ \lambda \mathbf{u} \end{bmatrix}$

It is put in work by activating the complex approach of IRAM ('SORENSEN'+APPROCHE=' COMPLEXE'). It is the only alternative when a matrix is handled \mathbf{K} complex²². It is usable with \mathbf{K} , \mathbf{M} and \mathbf{C} symmetrical or not.

Second strategy rest on the spectral transformation with “double shifts summons” introduced in 1987 by B.N.Parlett & Y.Saad [PS87], which results in handling two types of SEP

$$(S_2) \quad \operatorname{Re} \left(\underbrace{(\mathbf{A} - \sigma \mathbf{B})^{-1}}_{\mathbf{A}_\sigma^+} \mathbf{B} \right) \mathbf{w} = \mu^+ \mathbf{w} \quad (4.1-3)$$

avec $\mu^+ := \frac{I}{2} \left(\frac{I}{\lambda - \sigma} + \frac{I}{\lambda - \bar{\sigma}} \right)$, $\mathbf{w} := \begin{bmatrix} \mathbf{u} \\ \lambda \mathbf{u} \end{bmatrix}$

21 At the price however of a surplus of calculations and storages.

22 As soon as \mathbf{K} is complex symmetrical and that one chose IRAM, some is the approach chosen in the command file, it is the approach 'COMPLEX' which is taken by default.

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$$(S_3) \quad \text{Im} \left(\underbrace{(\mathbf{A} - \sigma \mathbf{B})^{-1}}_{\mathbf{A}_\sigma^-} \mathbf{B} \right) \mathbf{w} = \mu^- \mathbf{w} \quad (4.1-4)$$

avec $\mu^- := \frac{I}{2i} \left(\frac{I}{\lambda - \sigma} + \frac{I}{\lambda - \bar{\sigma}} \right)$, $\mathbf{w} := \begin{bmatrix} \mathbf{u} \\ \lambda \mathbf{u} \end{bmatrix}$

These two alternatives are put in work with Lanczos and IRAM via values, respectively, 'REALITY' and 'IMAG' keyword APPROACH . With Lanczos, the perimeter of use is limited to the classical QEP (symmetrical realities), while IRAM is less restricted and allows also the nonsymmetrical one.

Note:

- The origin of the denomination "doubles shifts summons" spectral transformation above appears more clearly if one reformulates the operators as follows

$$\mathbf{A}_\sigma^+ := \frac{I}{2} [(\mathbf{A} - \sigma \mathbf{B})^{-1} + (\mathbf{A} - \bar{\sigma} \mathbf{B})^{-1}] \mathbf{B} \quad (4.1-5)$$

$$\mathbf{A}_\sigma^- := \frac{I}{2i} [(\mathbf{A} - \sigma \mathbf{B})^{-1} - (\mathbf{A} - \bar{\sigma} \mathbf{B})^{-1}] \mathbf{B}$$

- Besides the terminology "nap" in opposition to the "double shifts produced" is initially proposed by J.C.Francis and is used, in writing pad, by method QZ and the "implicit" restartings of IRAM (cf [Boi09] Appendix 1):

$$\mathbf{A}_\sigma := [(\mathbf{A} - \sigma \mathbf{B}) + (\mathbf{A} - \bar{\sigma} \mathbf{B})]^{-1} \mathbf{B} \quad (4.1-6)$$

This one has the major drawback to produce matrices of work very filled (thus more expensive to handle and store) compared to the strategy of Parlett & Saad.

Once determined the operator of work, it remains to choose its associated scalar product. For IRAM, one can be satisfied with a couple "scalar produced operator" nonsymmetrical (cf [Boi09] §6), but for Lanczos, this one must obligatorily be symmetrical (cf [Boi09] §7). Several choices of (pseudonym) matric product-scalars allow this symmetry:

$$\begin{aligned} (\mathbf{w}, \mathbf{z})_{\mathbf{B}} &:= \mathbf{z}^T \mathbf{B} \mathbf{w} \\ (\mathbf{w}, \mathbf{z})_+ &:= \mathbf{z}^T \text{Re} [(\mathbf{A} - \sigma \mathbf{B})^{-1}]^{-1} \mathbf{w} \\ (\mathbf{w}, \mathbf{z})_- &:= \mathbf{z}^T \text{Im} [(\mathbf{A} - \sigma \mathbf{B})^{-1}]^{-1} \mathbf{w} \end{aligned} \quad (4.1-7)$$

The first functions with the two formulations (S₂) and (S₃), while the second (resp. the third) only makes symmetrical \mathbf{A}_σ^+ (resp. \mathbf{A}_σ^-). In the effective establishment in Code_AsteR, these are the two last which are retained for the approaches real and imaginary of Lanczos.

Note:

- These scalar products are the "natural" extensions of (pseudonym) produced scalar matric used by the alternative of Newmann-Pipano in GEP:

$$(\mathbf{w}, \mathbf{z}) := \mathbf{z}^T (\mathbf{A} - \sigma \mathbf{B}) \mathbf{w} \quad (4.1-8)$$

4.2 Establishment in Code_Aster

4.2.1 Choice of the spectral shift

In GEP it there are four ways of choosing this shift (cf [Boi09]§5.4). In QEP, the option 'BAND'being proscribed because of L' absence of test of adapted Sturm, this figure is tiny room to three:

- $\sigma = 0$, one seeks the smallest eigenvalues of the starting problem. This corresponds to OPTION=' PLUS_PETITE ' under the keyword factor CALC_FREQ.
- $\sigma = \sigma_0$ avec $\sigma_0 = (2 \pi f_0)^2$, one seeks the frequencies close to the frequency $\text{FREQ} = f_0$ (OPTION=' CENTRE ').

- $\sigma = \sigma_0$ avec $\sigma_0 = (2\pi f_0)^2$ et $\sigma_1 = \eta(2\pi f_0)^2/2$ one seeks the frequencies close to the frequency $FREQ = f_0$ (OPTION='CENTRE') and of reduced damping $AMOR_REDUIT = \eta$ (OPTION='CENTRE').

The number of frequencies to be calculated is given in general by the user using `NMAX_FREQ` under the keyword factor `CALC_FREQ`.

4.2.2 Calculation of the operator and the scalar product of work

One recapitulates in the table according to the whole of the couples (operator of work, scalar product) possible, according to the options chosen by the user.

APPROCHE/METHODE	'TRI_DIAG'	'SORENSEN' (by default)
'COMPLEXE'	Inalienable	(A_σ, L^2)
'REAL' (by default)	$(A_\sigma^+, ()_+)$	(A_σ^+, L^2)
'IMAG'	$(A_\sigma^-, ()_-)$	(A_σ^-, L^2)

Table 4.2-1. Together couples (operator of work, scalar product) possible according to the options chosen by the user.

calculation of the operators of work A_σ^\pm can bring back itself to simple products matrix-vector and an inversion of the dynamic matrix $Q(\lambda)$ (factorized beforehand) via the formulation (astute) following

$$(A - \sigma B)^{-1} B = \begin{bmatrix} \mathbf{0}_n & \mathbf{0}_n \\ \mathbf{M}_R^{-1} \mathbf{M} & \mathbf{0}_n \end{bmatrix} - \begin{bmatrix} Q(\sigma)^{-1} & \mathbf{0}_n \\ \mathbf{0}_n & \sigma \mathbf{M}_R^{-1} \mathbf{M} Q(\sigma)^{-1} \end{bmatrix} \begin{bmatrix} C + \sigma M & M \\ C + \sigma M & M \end{bmatrix} \quad (4.2-1)$$

In addition, this formulation has the "good taste" to allow treatments into pure arithmetic real and to preserve the hollow structure of the matrices. One can thus build the following procedure:

- Preparation in C^{23} (only once, in phase of initialization of the algorithm, cf. § 2.5):
To form $Q(\sigma) := (\sigma^2 M + \sigma C + K)$
To factorize $Q(\sigma)$ in form LDL^T .
 - Calculation of $A_{\sigma^\pm} \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix}$ (several times by iteration of Lanczos or IRAM):
 \mathbf{w}
To form in R $\mathbf{u}_1 := C\mathbf{u}, \mathbf{u}_2 := M\mathbf{u}, \mathbf{u}_3 := M\mathbf{v}$,
To calculate in C $\mathbf{u}_4 := Q(\sigma)^{-1} + \sigma \mathbf{u}_2 + \mathbf{u}_3$
 - According to the choice of the approach
- $$A_\sigma^+ \mathbf{w} = \begin{bmatrix} -\text{Re}(\mathbf{u}_4) \\ \mathbf{M}_R^{-1} \mathbf{M} (\mathbf{u} - \text{Re}(\sigma \mathbf{u}_4)) \end{bmatrix}$$
- $$A_\sigma^- \mathbf{w} = \begin{bmatrix} -\text{Im}(\mathbf{u}_4) \\ -\mathbf{M}_R^{-1} \mathbf{M} (\mathbf{u} - \text{Im}(\sigma \mathbf{u}_4)) \end{bmatrix}$$

Algorithm 3. Procedure to calculate the operators of work A_σ^\pm .

23 Because the shift (like K with IRAM) can be complex.

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In complex approach, calculation is done directly *via* the formula (4.1-2) into arithmetic complex. Concerning the matrix scalar products, their handling in *Code_Aster* are based on the following formulations:

$$\begin{aligned} (\mathbf{w}, \mathbf{z})_+ &:= \mathbf{z}^T \left[(\mathbf{A} - \text{Re}(\sigma) \mathbf{B}) + \text{Im}^2(\sigma) \mathbf{B} (\mathbf{A} - \text{Re}(\sigma) \mathbf{B})^{-1} \mathbf{B} \right] \mathbf{w} \\ (\mathbf{w}, \mathbf{z})_- &:= \mathbf{z}^T \left[\frac{1}{\text{Im}(\sigma)} (\mathbf{A} - \text{Re}(\sigma) \mathbf{B}) \mathbf{B}^{-1} (\mathbf{A} - \text{Re}(\sigma) \mathbf{B}) + \text{Im}^2(\sigma) \mathbf{B} \right] \mathbf{w} \end{aligned} \quad (4.2-2)$$

Note:

- The calculation of the matrix scalar products can be carried out only into arithmetic real. For the first scalar product one needs an additional dynamic matrix $\mathbf{Q}(\text{Re}(\sigma))$ and of its factorized (from where a overcost calculation and memory).

4.3 Perimeter of use

QEP with real symmetrical matrices for Lanczos, **possibly nonsymmetrical** (and \mathbf{K} can be symmetrical complex) for IRAM.

The user can only specify `TYPE_RESU=' DYNAMIQUE'` like membership of its calculation classifies (not of buckling). One then informs possibly the vector `FREQ` (and not `CHAR_CRIT`).

4.4 Posting in the file message

In the file message, the results are displayed in the form of table

```

-----
THE NUMBER OF DDL
TOTAL IS:                130
LAGRANGE IS:            16
THE NUMBER OF ACTIVE DDL IS: 106
-----
MODAL CALCULATION:  METHOD OF SIMULTANEOUS ITERATION
                    METHOD OF SORENSEN
NUMBER   FREQUENCY (HZ)   DAMPING   ERROR NORMALIZES
  1      1.24163E+02     -1.89229E-02  1.16550E-09
  2      1.24164E+02      1.89229E-02  1.04882E-09
  ...
  6      1.07321E+03      1.63495E-01  1.36092E-13
NORMALIZES AVERAGE ERROR: 0.36947E-09

```

Example 4. Trace of `CALC_MODES` with `OPTION` among ['CENTER', 'PLUS_PETITE'] and `METHODE='SORENSEN'` (QEP) in the file message. Extract of the CAS-test `sdll123b`.

For each eigenvalue (represented in the form $\text{FREQUENCY} = \frac{\text{Im}(\lambda_i)}{2\pi}$ and $\text{DAMPING} = \frac{-\text{Re}(\lambda_i)}{|\lambda_i|}$ cf §2.5), one traces the standard of error of the determined residue following the algorithm n°1 (§2.5).

4.5 Summary of the parameter setting

Let us recapitulate the parameter setting of the operator now `CALC_MODES` with `OPTION` among ['CENTER', 'PLUS_PETITE'] for the methods of Lanczos and Sorensen.

Operand	Keyword	Value by default	References
	<code>TYPE_RESU= ' DYNAMIQUE'</code>	'DYNAMIC'	§2.1
	<code>OPTION = 'PLUS_PETITE'</code>	'PLUS_PETITE'	§4.2

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Operand	Keyword	Value by default	References
	'CENTER'		§4.2
CALC_FREQ	FREQ (if 'CENTRE')		§4.2
	AMOR_REDUIT (if 'CENTRE')		§4.2
	NMAX_FREQ	10	§4.2
SOLVEUR_MODAL	METHOD= 'TRI_DIAG'	'SORENSEN'	[Boi09] §6
	'SORENSEN'		[Boi09] §7
	APPROACH= 'REAL'	'REAL'	§4.1
	'IMAG'		§4.1
	'COMPLEXE' (if 'SORENSEN')		§4.1
	DIM_SOUS_ESPACE COEF_DIM_ESPACE	Calculated	[Boi09] §6/7
	...		
	Usual parameter setting of 'TRI_DIAG' / 'SORENSEN'		[Boi09] §6/7

Table 4.5-1. Summary of the parameter setting of **CALC_MODES** with **OPTION** among ['CENTER', 'PLUS_PETITE'] and **METHODE=** 'TRI_DIAG' or 'SORENSEN' (QEP).

Note:

- At the time as of first passages, it is strongly advised to modify only the principal parameters noted in fat. The others relate to more the mysteries of the algorithm and they were initialized empirically with values standards.
- In particular, to improve quality of a mode, the fundamental parameter is the dimension of the subspace of projection of the SEP, **DIM_SOUS_ESPACE**.

5 Global method QZ (METHODE=' QZ ')

5.1 QEP with the GEP

Contrary to the methods seen previously, method QZ is able to manage a GEP directly. One thus has **that only one transformation to be applied to the initial QEP, it is the linearization** . That empirically retained and detailed with § 2.4 is

$$(L_2)^* \left(\underbrace{\begin{bmatrix} -\mathbf{K} & \mathbf{0}_n \\ \mathbf{0}_n & \alpha \mathbf{I}_n \end{bmatrix}}_{\mathbf{A}} - \lambda \underbrace{\begin{bmatrix} \mathbf{C} & \mathbf{M} \\ \alpha \mathbf{I}_n & \mathbf{0}_n \end{bmatrix}}_{\mathbf{B}} \right) \begin{bmatrix} \mathbf{u} \\ \lambda \mathbf{u} \end{bmatrix} = \mathbf{0}_{2n} \quad (5.1-1)$$

The GEP obtained is not structurally symmetrical (or square) but it is not prejudicial with calculation because the drivers of adapted LAPACK work only in nonsymmetrical. **For more robustness and to simplify the structuring of the code**, and solved the GEP is formulated $(L_2)^*$ in **complex plan**. As for the GEP with complex modes one uses standard routines LAPACK (ZGGEV) or expert (ZGGEVX) according to the parameter TYPE_QZ=' QZ_SIMPLE' / 'QZ_EQUI'.

To resulting from modal calculation, QZ returns to Code_Aster the calculated modes and the latter will be checked, filtered and ordered according to the same recommendations as for the complex modes of the GEP (cf [Boi09] §9.4).

5.2 Perimeter of use

QEP with symmetrical matrices or not (and \mathbf{K} can be symmetrical complex).

The user can only specify TYPE_RESU=' DYNAMIQUE' like membership of its calculation classifies (not of buckling). One then informs possibly the vector FREQ (and not CHAR_CRIT).

5.3 Impressions in the file message

An extract with accompanying notes of the CAS-test sd11113a is taken again with the §2.5.

5.4 Summary of the parameter setting

Let us recapitulate the parameter setting of the operator now CALC_MODES with OPTION among ['CENTER', 'PLUS_PETITE', 'ALL'] for method QZ.

Operand	Keyword	Value by default	References
	TYPE_RESU=' DYNAMIQUE'	'DYNAMIC'	§2.1
	OPTION = 'PLUS_PETITE'	'PLUS_PETITE'	[Boi09] §9.4
	'CENTRE'		[Boi09] §9.4
	'ALL'		
CALC_FREQ	FREQ (if CENTER)		[Boi09] §9.4
	AMOR_REDUIT (if CENTER)		[Boi09] §9.4
	NMAX_FREQ	10	[Boi09] §9.4
	APPROCHE=...	Without object	
<i>SOLVEUR_MODAL</i>	METHOD = 'QZ'	'SORENSEN'	[Boi09] §9
	...		
	Usual parameter setting of 'QZ'		[Boi09] §9

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Table 5.4-1. Summary of the parameter setting of `CALC_MODES` with `OPTION` among [`"CENTRE"`, `"PLUS_PETITE"`, `"ALL"`] with `METHODE= 'QZ'` (QEP) .

Note:

- At the time of the first passages, it is strongly advised to modify only the principal parameters noted in fat. The others relate to more the details of the algorithm and they were initialized empirically with values standards.

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6.3 Resources Internet

- [Arp] Web site of ARPACK: <http://www.caam.rice.edu/software/ARPACK/>.

7 Description of the versions of the document

Version Aster	Author (S) Organization (S)	Description of the modifications
3	D.SELIGMANN- R&D/MMN	Initial text
...	...	
5	O.BOITEAU EDF-R&D/MMN	
V8.4	O.BOITEAU EDF-R&D/SINETICS O.NICOLAS EDF-R&D/AMA	
9.4	O.BOITEAU EDF-R&D/SINETICS	Recasting of the document, and extension of the perimeter of the solver QZ with nonsymmetrical
v10.4	O.BOITEAU EDF-R&D/SINETICS	large work of fitness (formula, figure, legend, notice, character white, cast iron...). Update concerning the parameters (in particular NPREC, COEF_DIM_ESPACE, ALL), the linear aspects solvers and parallelism.
V11.2	O.BOITEAU EDF-R&D/SINETICS	Work of fitness, correction of formulas in agreement with Docs. R 5.01.01/04.
V11.2.13	O.BOITEAU EDF-R&D/SINETICS	Still some fitness + taken into account EL16710.

8 Appendix 1. Interpretation of the complex eigenvalues

In the case of one **symmetrical damping and in internal absence of damping**, relations of orthogonalities and owing to the fact that the clean elements appear per combined pairs, one has the following relations:

$$\frac{\Phi_i^{*T} \mathbf{C} \Phi_i}{\Phi_i^{*T} \mathbf{M} \Phi_i} = \frac{c_i}{m_i} = 2 \operatorname{Re}(\lambda_i)$$

$$\frac{\Phi_i^{*T} \mathbf{K} \Phi_i}{\Phi_i^{*T} \mathbf{M} \Phi_i} = \frac{k_i}{m_i} = |\lambda_i|^2$$

If one notes $\lambda_i = \alpha_i \pm i \beta_i$, one can then define

$$\omega_i = |\lambda_i| = \sqrt{\alpha_i^2 + \beta_i^2} = \frac{\beta_i}{\xi_i}$$

$$\xi_i = \operatorname{Re} \frac{(\lambda_i)}{\omega_i} = \frac{\alpha_i}{\sqrt{\alpha_i^2 + \beta_i^2}} \omega_i$$

One can write the eigenvalue complexes in the following form

$$\lambda_i = -\xi_i \omega_i \pm i \omega_i \sqrt{1 - \xi_i^2}$$

This formulation induces its **physical interpretation** following:

- The real term represents the dissipative character of the system.
- The imaginary part represents the oscillatory part of the solution.
- ω_i is the pulsation of $i^{\text{ème}}$ mode.
- ξ_i is the damping of $i^{\text{ème}}$ mode,
- $\omega_{d_i} = \omega_i \sqrt{1 - \xi_i^2}$ is the reduced damping of $i^{\text{ème}}$ mode.

As for **the physical interpretation of the clean vectors**:

- The physical significance of the existence of a clean vector complexes, lies in the fact that if the structure vibrates on a clean mode, its various degrees of freedom do not vibrate with the same phase the ones compared to the others.
- The modal bellies and nodes do not correspond of the stationary points, but move during the movement.

Note:

- *One finds the classical formulation of the deadened systems with 1 degree of freedom.*
- *k_i, m_i and c_i are real. They are many intrinsic quantities with a mode (modal quantities) thus dependent on its standardisation.*
- *We point out that the modes of the GEP (just like complex modes of the GEP) do not diagonalise the matrices \mathbf{M} , \mathbf{K} et \mathbf{C} .*
- *If the real part of the eigenvalue is negative, then the clean mode is a deadened periodic movement of pulsation ω . If on the contrary, it is positive, then the clean mode is a periodic movement of amplitude increasing and thus unstable.*