

# Towards a robust a priori choice of Padé approximants for fast frequency sweeps of finite element problems

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## Résumé :

*Dans cette contribution, une approche se fondant sur l'utilisation d'approximants de Padé est étudiée afin de permettre une résolution efficace de problèmes dépendants d'une variable, tels que les balayages en fréquence. Une amélioration est ici proposée, concernant le développement de chaque composante du vecteur solution sous forme d'approximant, sur la base du calcul a priori des poles de la réponse. Ceci permet une décomposition a priori en sous-intervalles de convergence pour une reconstruction robuste de la solution sur l'intégralité du domaine de variation du paramètre d'intérêt (e.g. fréquence). Un exemple de problème d'acoustique est traité afin d'illustrer le potentiel de cette approche.*

## Abstract :

*In this work, a solution strategy based on the use of Padé approximants is investigated for efficient solution of parametric finite element problems such as, for example, frequency sweep analyses. An improvement to the Padé-based expansion of the solution vector components is proposed, suggesting the advantageous a priori estimate of the poles of the solution. This allows for the intervals of approximation to be chosen a priori in connection with the Padé approximants to be used. The choice of these approximants is supported by the Montessus de Ballore theorem, proving the convergence of a series of approximants with fixed denominator degrees. An acoustic case study is presented in order to illustrate the potential of the approach proposed by the authors.*

**Mots clés : Approximants de Padé; modèles réduits; balayage en fréquence; éléments finis.**

## 1 Introduction

The use of Padé approximants in order to improve the performance of Finite Element (FE) solution procedures, e.g. for frequency sweeps in structural-acoustic applications, has been given substantial attention in the last decade. These expansion methods have shown to be very efficient for a wide range of problems such as for the control theory [1, 2], acoustics or structural dynamics problems [3, 4, 5], or coupled problems [6, 7, 8, 9, 10].

In the work initiated with the present paper, the authors build upon previous contributions related to both a modal approach for coupled structural-acoustic problems with dissipative media [11, 12], and its combination with the component-wise solution approximation by Padé approximants [6]. The main idea is to introduce an early step in the Padé approximation procedure where poles of the response would be calculated. This step has a twofold objective: *i*) with an accurate estimate of the poles of the response, a solid foundation is provided for the Padé approximants to be calculated, thus ensuring a good convergence of these approximants, and *ii*) with the poles known early in the procedure, the choice of approximants in combination with their subdomains of convergence may be done a priori, thus ensuring an efficient reconstruction of the response over the entire domain of interest.

In the first part, the main steps of the component-wise Padé approximation procedure, as previously used by the authors [6], are recalled. In the following section, the addition of a priori knowledge of the poles of the response –an original step to best of the authors' knowledge– is detailed. It is then tested in the last part on an academic acoustic problem allowing for a detailed discussion of the potential of the proposed method. Further steps, currently under investigation by the authors, are presented in the conclusion.

## 2 Univariate solution expansion using Padé approximants

### 2.1 Numerical calculation of the Padé coefficients

The starting point of the component-wise Padé univariate sweep, as described in [6], is given by a linear system of equations in the following form,

$$\mathbf{Z}(x)\mathbf{U}(x) = \mathbf{F}(x), \quad (1)$$

where  $x$  is the independent variable of the problem, e.g. the angular frequency  $\omega$  for the problems of interest in this contribution. In an FE problem,  $\mathbf{Z}(x)$ ,  $\mathbf{U}(x)$ , and  $\mathbf{F}(x)$  represent the system matrix of the discretized problem, the solution vector and the vector of externally applied loads, respectively.

A component-wise solution expansion of the solution vector may be sought as Padé

approximants in the form

$$u(x_0 + \Delta x) \approx \frac{P_L(\Delta x)}{Q_M(\Delta x)}, \quad (2)$$

where the solution vector  $\mathbf{U}(x_0)$ , of which  $u(x_0)$  is a component, is assumed to be known after solving the system in Eq. (1).  $P_L(\Delta x)$  and  $Q_M(\Delta x)$  are two truncated power series in the variable  $\Delta x = (x - x_0)$ , to the orders  $L$  and  $M$  respectively, and given by

$$P_L(\Delta x) = \sum_{k=0}^L p_k(\Delta x)^k, \quad (3a)$$

$$Q_M(\Delta x) = \sum_{k=0}^M q_k(\Delta x)^k. \quad (3b)$$

In previous works, it was shown that the coefficients of these power series may be determined from the coefficients of the Taylor series expansion [13]

$$A_{L+M}(\Delta x) = \sum_{k=0}^{L+M} a_k(\Delta x)^k, \quad (4)$$

where

$$a_k = \frac{u^{(k)}(x_0)}{k!}, \text{ with } u^{(0)}(x_0) = u(x_0) = a_0. \quad (5)$$

These coefficients  $p_k$  and  $q_k$  are indeed solutions of the system of linear equations resulting from equating the Padé approximant in Eq. (2) to the Taylor series expansion Eq. (4), such that

$$P_L(\Delta x) - A_{L+M}(\Delta x)Q_M(\Delta x) = 0, \quad (6)$$

where the identification of the coefficients of equal order in  $\Delta x$  enables the formation of a set of  $(L+M+1)$  equations, after normalizing the zero-order denominator coefficient, i.e.  $q_0 = 1$ . In a first step, this leads to the following system of linear equations with the denominator coefficients  $q_k$  as unknowns,

$$\begin{bmatrix} a_L & \cdots & a_{L-M+1} \\ \vdots & & \vdots \\ a_{L+M-1} & \cdots & a_L \end{bmatrix} \begin{bmatrix} q_1 \\ \vdots \\ q_M \end{bmatrix} = - \begin{bmatrix} a_{L+1} \\ \vdots \\ a_{L+M} \end{bmatrix} \text{ with } a_i := 0 \text{ if } i < 0. \quad (7)$$

The numerator coefficients may subsequently be determined in a second step by simple algebraic operations,

$$p_k = \sum_{i=0}^M q_i a_{(k-i)}, \quad (8)$$

with

$$\begin{cases} k = 0 \cdots L \\ a_j := 0 \text{ if } j < 0 \end{cases}.$$

The calculation of these Padé coefficients however depends on the ability to efficiently calculate the  $L + M$  successive partial derivatives of the solution vector, at the reference point  $x = x_0$ , as implied by Eq. (5). This may be achieved via a recursive scheme, using a Leibniz formula resulting from the differentiation of Eq. (1) with respect to  $x$ , at order  $k$ , in  $x_0$ ,

$$\sum_{j=0}^k \binom{k}{j} \mathbf{Z}^{(k-j)}(x_0) \mathbf{U}^{(j)}(x_0) = \mathbf{F}^{(k)}(x_0), \text{ for } k = 1, \dots, (L + M), \quad (9)$$

where the zero-order derivatives correspond to the non differentiated functions, and the binomial coefficients are given by

$$\binom{k}{j} = \frac{k!}{j!(k-j)!}. \quad (10)$$

The recursive expression for  $\mathbf{U}^{(k)}(x_0)$  follows from extracting the highest-order term from the summation in Eq. (9),

$$\mathbf{Z}(x_0) \mathbf{U}^{(k)}(x_0) = \mathbf{F}^{(k)}(x_0) - \sum_{j=0}^{(k-1)} \binom{k}{j} \mathbf{Z}^{(k-j)}(x_0) \mathbf{U}^{(j)}(x_0), \text{ for } k = 1, \dots, (L+M), \quad (11)$$

This implies that the successive derivatives of  $\mathbf{U}$  with respect to  $x$ , required for the determination of the Padé approximations, can be efficiently calculated as the solution of a full-sized system of equations, with multiple right-hand sides.

## 2.2 Comments on the procedure

In agreement with the theoretical background recalled in the previous section, a corresponding efficient approach to calculate the Padé-expansion around a solution vector  $\mathbf{U}(x_0)$  (only one reference point at  $x_0$  is considered in the present discussion) essentially consists of 5 steps:

1. Factorize the system matrix  $\mathbf{Z}$  of Eq. 1 at  $x_0$ , and calculate the solution  $\mathbf{U}(x_0)$  (coefficient  $a_0$ ).
2. Solve for the  $L + M$  successive derivatives of  $\mathbf{U}$  with respect to  $x$  using an iterative multiple right-hand-side procedure, Eq. (11) (coefficients  $a_1 \dots a_{L+M}$ ).
3. For each component of interest in the solution vector, solve for the denominator coefficients via a small linear system of equations Eq. (7) (coefficients  $q_1 \dots q_M$ ,  $q_0 = 1$ ).
4. For each component of interest in the solution vector, evaluate the numerator coefficients via simple algebraic operations as presented in Eq. (8) (coefficients  $p_0 \dots p_L$ ).

5. For each component of interest in the solution vector, evaluate the solution expansion around  $x_0$  by evaluating Eq. (2).

Note that while the first two steps have to be performed at a global scale, involving the full size of the original problem, the last three steps may be limited to the degrees of freedom of interest for the solution. A few remarks may be made in relation with the five main steps detailed above:

- Step 2 involves a multiple right-hand-side problem with as many recursions as the number of numerator and denominator coefficients. In practice, there is a limit in the number of recursions that can be performed: the propagation of the small numerical error made at each recursion eventually affects the accuracy of the successive partial derivatives.
- More importantly, the system matrix involved in the solutions of Eq. (7) has the form of a Toeplitz matrix, which, although benefiting from very efficient algorithms, may become rapidly ill-conditioned with its increasing dimension. This implies that the solution of Eq. (7) may become sensitive to small errors of the right-hand-side, which consists of the Taylor coefficients, dependant on the accuracy of the successive partial derivatives.
- In addition to the previous points, the right-hand-side of Eq. (7), as well as the components of the system matrix, consist of the Taylor coefficients of highest order, i.e. those most costly to calculate (latest stages of the recursive procedure in step 2) and those with the most accumulated approximation error.

Even though the procedure presented in this section has proved to be very efficient for a wide variety of examples [4, 6, 7], it appears that some of its steps may be improved in light of the points aforementioned. The following section discusses one such possibility, which additionally opens for the possibility of an a priori choice of Padé approximants and their associated range of convergence.

## 3 A priori choice of Padé approximants and convergence

### 3.1 Convergence of Padé approximants

The convergence of Padé approximants is a broad topic which has been given much attention by specialists for decades [13]. In the present work, a key result from the so-called Montessus de Ballore theorem, on the convergence of a series of Padé approximants [14], is highlighted. This theorem guarantees, assuming a meromorphic function within a disk (which is typically the case for the FE solutions of interest in this work), the uniform convergence, except at poles of this function, of a sequence of Padé approximants of increasing numerator degree, fixed denominator degree, and whose poles correspond to simple poles of the approximated function within the considered disk. Thus, this result implies that, given a set of simple poles of the function to

be approximated, which define a disk of anticipated convergence, uniform convergence will be observed on this disk, except at the poles location, for a denominator degree corresponding to the number of poles, and an increasing numerator degree.

It is on the basis of this result that the following section suggests an improved approach in order to determine a priori, both the Padé approximants and their anticipated domain of convergence, thus enabling the systematic approximation of FE solutions involving parameter sweeps in a wide range.

### 3.2 An improved procedure with a priori control of the convergence

Following the observation made in the previous section, the poles of the Padé approximants play a key role in order to ensure a reliable reconstruction of the solution. Additionally, the poles of these Padé approximants should correspond to the zeros of the characteristic equation of the FE system matrix. Thus, starting with a step at a global scale (full-sized system of equations) by determining the zeros of this characteristic equation within subsets of the range of parametric sweep, would allow to address the comments made in Section 2.2:

- Replace the vector-component-wise step of solving for the denominator coefficients with Eq. (7).
- Ensure to have the same poles from one component to the other of the approximated solution vector, and thus, in light of the convergence properties recalled in the previous section, to enforce the same domain of convergence for all components.
- Reduce the number of Taylor coefficients required to be recursively calculated with Eq. (11), or reallocate them in order to have numerator polynomials of higher degrees, thus ensuring a more accurate approximation over the domain of convergence of the approximants.
- Use the information provided by the location of these poles in order to decompose the range of the parametric sweep into subdomains corresponding to one reference point of solution expansion and its associated convergence interval.

For the sake of validation in the scope of this contribution, the system matrix  $\mathbf{Z}(x)$  in Eq. (1) is here supposed to be a quadratic function of  $x$  with real-valued eigenvalues, solution of a polynomial characteristic equation. The application to more general cases is an important extension for the validation of such an approach which will be presented in further contributions by the authors. Thus, Step 3 in Section 2.2 would be replaced by a step at the global scale, including the calculation of the roots  $\{\hat{x}_{01}, \dots, \hat{x}_{0M}\}$  closest to  $x_0$ , solution of the characteristic equation

$$\det(\mathbf{Z}(x)) = 0. \quad (12)$$

The steps of Section 2.2, for the Padé-based approximation of the solution around  $x_0$  may therefore be updated to the following 6-step procedure aiming at the same domain of convergence (i.e. the same number of poles):

1. Solve for a set of roots  $\{\hat{x}_1, \dots, \hat{x}_n\}$ ,  $n > M$ , solution of the characteristic equation Eq. (12), including the subset of the  $M$  closest roots to  $x_0$  denoted  $\{\hat{x}_{01}, \dots, \hat{x}_{0M}\}$ .
2. Factorize the system matrix  $\mathbf{Z}$  of Eq. 1 at  $x_0$ , and calculate the solution  $\mathbf{U}(x_0)$  (coefficient  $a_0$ ).
3. Solve for the  $L'$  successive derivatives of  $\mathbf{U}$  with respect to  $x$  using an iterative multiple right-hand-side procedure corresponding to Eq. (11) (coefficients  $a_1 \dots a_{L'}$ ).
4. Once for all the components of interest in the solution vector, and assuming simple roots at this stage, identify the  $M$  coefficients  $q_1, \dots, q_M$  such that

$$\frac{(-1)^M}{\hat{x}_{01}\hat{x}_{02}\dots\hat{x}_{0M}}(x - \hat{x}_{01})(x - \hat{x}_{02})\dots(x - \hat{x}_{0M}) = 1 + q_1x + q_2x^2 + \dots + q_Mx^M. \quad (13)$$

(coefficients  $q_1 \dots q_M$ ,  $q_0 = 1$ ).

5. For each component of interest in the solution vector, evaluate the numerator coefficients via simple algebraic operations as presented in Eq. (8) (coefficients  $p_0 \dots p_{L'}$ ).
6. For each component of interest in the solution vector, evaluate the solution expansion around  $x_0$  by evaluating Eq. (2).

The first step becomes an important stage when considering a parametric sweep encompassing a large number of poles, as well as higher-multiplicity poles. An initial step where a sufficiently large number of poles may be determined –potentially all the poles in the range of interest– allows for an a priori decomposition in subintervals of Padé-based reconstructions. These intervals are typically defined by a fixed number of poles, or by pushing poles with a higher order multiplicity to their bounds. In contrast with the original procedure in Section 2.2, this latter point prevents the procedure from being potentially hampered by the appearance of a higher-multiplicity pole within an interval of reconstruction, which would concentrate the approximation at a singularity where no convergence can be expected in the sense of the Montessus de Ballore theorem. It may be argued that the pole-based bounds from one interval to the other can be chosen as distinct poles. Then, if we consider three consecutive intervals centered on the interval associated with  $x_0$ ,

$$\dots [\dots, \hat{x}_{01-1}] [\hat{x}_{01}, \hat{x}_{0M}] [\hat{x}_{0M+1}, \dots] \dots \quad (14)$$

This suggestion is supported by the empirical evidence available for engineering applications [4, 6, 7] showing the slow divergence of Padé approximants outside of the convergence bounds, especially for smooth responses. The analysis of the reconstruction of solutions around multiple intervals is however left for a discussion beyond the scope of this contribution where the attention is turned towards the validation of this procedure on a single interval of reconstruction.

Another point to be highlighted from the upgraded procedure presented above concerns the fact that the numerator polynomial degree  $L'$  may be increased ( $L' \geq L$ ) thanks to the reduced number of successive derivatives that need to be calculated in Step 3. In light of the Montessus de Ballore theorem on the convergence of a series of Padé approximants and the limitations associated with the number of successive derivatives of the global solution vector that may be iteratively calculated, this may imply the possibility to increase the range of convergence of each interval in the reconstruction procedure. As a consequence, the number of required intervals required to cover the entire parametric sweep may be subsequently reduced.

Finally, the reference point at  $x_0$  may be placed in the close vicinity ( $x_0$  should not coincide with a pole so as not to jeopardize the calculation of the successive derivatives of the solution vector) of the interval mid-point

$$x_0 = \frac{\hat{x}_{01} + \hat{x}_{0M}}{2}. \quad (15)$$

Note that if the poles are complex-valued, e.g. in the case of a frequency sweep for a damped dynamics problem, the mid-point may be calculated from the real part of the poles.

## 4 Numerical experiment and validation

In this section, some points of comparison between the original procedure in Section 2.2 and the updated one are analysed on a simple validation case consisting of a conservative acoustic problem. A rigid acoustic cavity of dimensions  $0.1 \times 0.15 \times 0.25 \text{ m}^3$  is excited at the corner  $(0, 0, 0)$  with a time-harmonic acoustic point source for consideration in the range  $f = [500, 2250]$  Hz. The acoustic pressure fluctuation at the arbitrary position  $(0.06\text{m}, 0.11\text{m}, 0.16\text{m})$  is used in order to compare the frequency sweeps obtained by using a Padé approximant on one interval with the reference solution. There are 11 eigenfrequencies of the acoustic cavity within the range of interest, see Table 1.

Table 1: Eigenfrequencies of the acoustic cavity in the range  $f = [500, 2250]$  Hz.

Mode order $(l, m, n)$	(0, 0, 1)	(0, 1, 0)	(0, 1, 1)	(0, 0, 2)	(1, 0, 0)	(0, 1, 2)
Eigenfrequency (Hz)	686	1143	1333	1372	1715	1786
Mode order $(l, m, n)$	(1, 0, 1)	(0, 0, 3)	(1, 1, 0)	(1, 1, 1)	(1, 0, 2)	
Eigenfrequency (Hz)	1847	2058	2060	2172	2196	



First, anticipating a limitation in the Padé approximants orders mostly due to the loss in precision associated with the recursive multiple-right-hand-side solution step, a convergence test is made for a fixed denominator degree of 7 (at most seven poles in the solution can be captured). The two procedures are compared, for one Padé approximant with increasing orders of its numerator, which should imply a uniform convergence on an interval encompassing the 7 closest poles to the reference frequency. The reference frequency is first chosen at 1500 Hz, thus limiting the convergence to an interval including the eigenfrequencies  $\{1143 \text{ Hz} \cdots 2058 \text{ Hz}\}$ . Fig. 1 compares the convergence for these two procedures with Padé approximants of numerator expansion orders 6, 9 and 11. The main conceptual difference between the two procedures can be clearly seen in Figs. 1a and 1b as the original procedure relies on the scalar-component data in order to determine the pole of the Padé approximant when the updated approach relies on the eigenfrequencies of the full-size problem. Consequently, the latter approach enforces the position of the poles no matter which step of convergence is reached thanks to the polynomial order of the numerator. Thus, as soon as expansion order  $L = 6$  for the numerator, the 7 expected poles are visible on the approximated solution of the updated procedure in Fig. 1b. In contrast, it appears that two poles are missing for the original procedure (at 1847 Hz and 2058 Hz). A typical behaviour is for the poles to be shifted away in such circumstances, in the higher frequency region in this case. Upon convergence with increasing numerator order, one of the missing poles is shifted down to the domain of interest, as can be seen in Figs 1c and 1e. It is however shifted from the eigenfrequencies of the cavity, and one pole remains uncaptured by the approximation. The updated procedure, however, manages to capture the dynamic content of the response in the entire interval, all 7 eigenfrequencies as well as the sound pressure level in between being accurately approximated after an expansion of the numerator to polynomial order 11.

The convergence limit of the original procedure is further illustrated in Figs 2, where 9 poles are considered, with a reference frequency of 1425 Hz, thus limiting the a priori convergence to an interval including the eigenfrequencies  $\{686 \text{ Hz} \cdots 2060 \text{ Hz}\}$ . Note that this interval includes two very close eigenfrequencies (2058 Hz and 2060 Hz) at one bound of the domain, a challenge for the approximation. Upon reaching limitations due to a combination of the high order of recursive derivatives in Eq. (11) and the ill-conditioned nature of the problem in Eq. (7), the Padé-approximation based upon the original procedure fails to capture the eigenfrequency at 686 Hz, and collapses in the region 1715 – 1847 Hz and above (see Figs 2a and 2c). Indeed, estimating the location of the 9 poles captured by the approximant ( $L = 12; M = 9$ ) in Fig. 2c gives two complex conjugate poles together with  $\{1143\text{Hz}, 1210\text{Hz}, 1333\text{Hz}, 1374\text{Hz}, 1717\text{Hz}, 1809\text{Hz}, 2431\text{Hz}\}$ . Note that only 4 eigenfrequencies are accurately captured as poles of the approximant. In contrast, the updated procedure allows to have a good representation over the entire domain anticipated, even giving a fair approximation of the response at the challenging upper bound, where two eigenfrequencies almost coincide (see Fig. 2d).

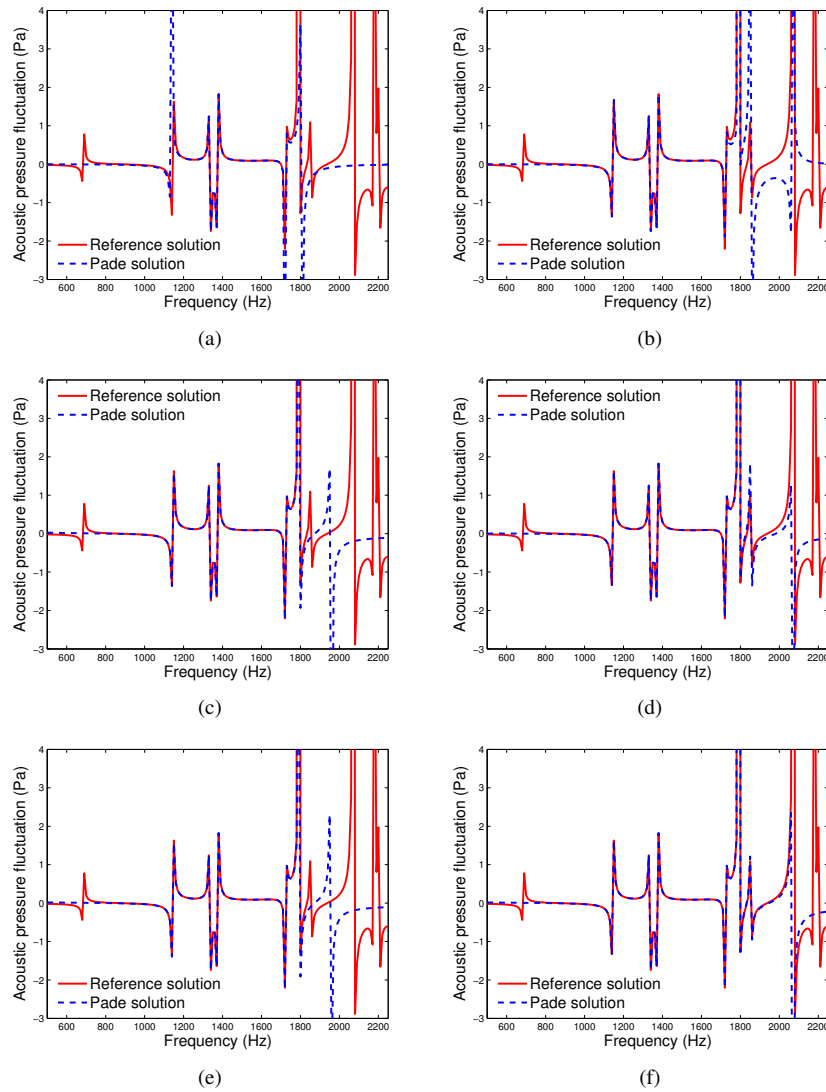


Figure 1: Convergence of the Padé-approximated solution with 7 poles ( $M = 7$ ), reference point at 1500 Hz: original procedure (Left) and updated procedure (Right); (a)–(b)  $L = 6$ , (c)–(d)  $L = 9$ , (e)–(f)  $L = 11$ .

## 5 Conclusions

In this contribution, a procedure for the scalar-component Padé approximation approach is proposed as an alternative to the method where the Padé coefficients are derived exclusively from the polynomial coefficients of the power series expansion of the solution.

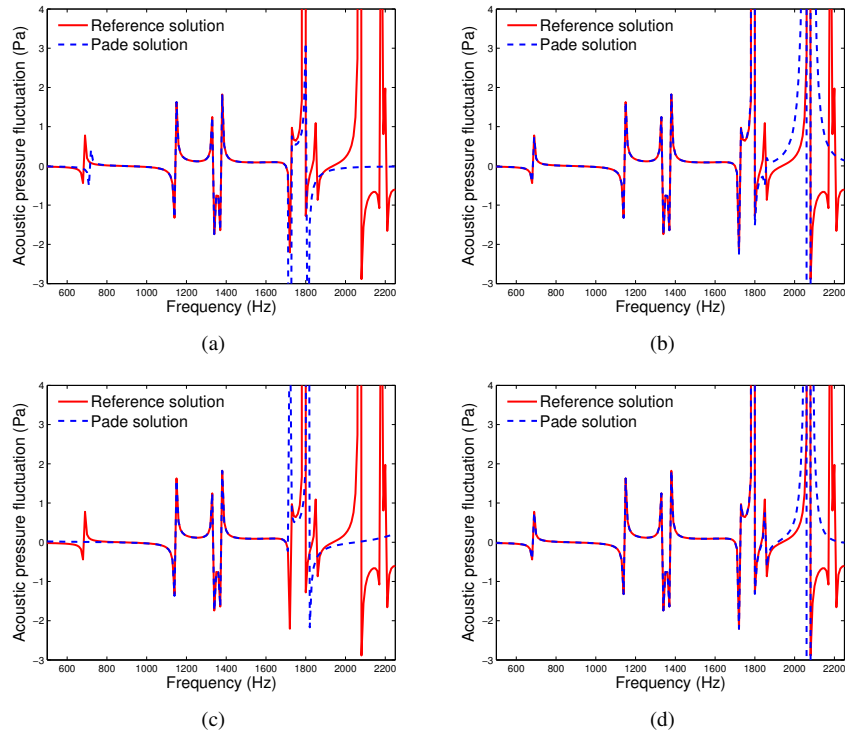


Figure 2: Convergence limits of the Padé-approximated solution with 9 poles ( $M = 9$ ), reference point at 1425 Hz: original procedure (Left) and updated procedure (Right); (a)–(b)  $L = 10$ , (c)–(d)  $L = 12$ .

This enhancement suggests that the denominator coefficients, i.e. the poles of the Padé approximant, may be advantageously determined from the full system of equations. Subsequently, the numerator coefficients may be determined, for each scalar component of the solution vector, from the polynomial coefficients of its power series expansion.

Several points of interest may be highlighted for the potential of this alternative approach: *i*) by calculating the denominator coefficients from the full system of equations, the polynomial coefficients of the power series expansion are used exclusively for the calculation of the numerator coefficients of the approximant, thus allowing to increase the order of expansion of this Padé approximant; *ii*) the calculation of the poles of the solution from the full system of equation may ensure that the accurate poles are enforced for the Padé approximant in the neighbourhood of the expansion point considered, which opens for the possibility to rely fully on the convergence theorem by Montessus de Ballore; *iii*) consequently, the bounds of the intervals of convergence may be determined a priori, which allows for an optimal decomposition of the parametric range of interest into several intervals of convergence.

After the illustration on a conservative acoustic problem in this contribution, current work aims at extending the method to fully coupled dissipative problems and integrating it in a multi-point solution reconstruction.

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