Improvement of crack-tip stress series with Padé approximants

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Abstract The most favored description of bi-dimensional crack-tip stress fields relies on Williams expansion. In this framework, each stress component is defined as a series which has a certain convergence behavior. Generally, the series is truncated after its first term since it is the most influential one at the vicinity of the crack-tip because of its well-known singularity. However, for some applications, the need for higher order terms arises and the study of truncation influence becomes important. The investigations performed by the authors for a specific fracture configuration have shown the existence of a convergence disk and of rather low convergence rates far from the crack-tip. In this communication, we propose to transform truncated stress series into Padé Approximants (PA) in order to improve both convergence domains and convergence rates. These approximants are rational functions whose coefficients are defined so as to fit the prescribed truncated series. The PA may be obtained following two different procedures. In practical tests, PA stemming from crack-tip stress series exhibit wider convergence domains and higher convergence rates.

Keywords Crack-tip, Williams series, Padé approximant

1. Introduction

The stress field at the vicinity of a crack-tip in a plane medium may be described using the so-called Williams series [1, 2]. Each term of the series is the product of three factors. Two of them concern respectively the angular and radial dependencies of the field. Their general expressions are known analytically and are the same for all fracture configurations [3, 4]. All the specific information related to the actual problem (geometry and loading conditions) is held by the third factor. Hence, to each fracture problem corresponds a specific infinite set of multi-order stress intensity factors.

Concerning the determination of these sets, research has been mainly focused on their first element (the Stress Intensity Factor "Ki" associated to the stress singularity) and on their second one (the T-stress "T" associated to a constant stress state). In [5], closed form asymptotic expansions for the problem of a finite straight crack in an infinite plane medium submitted to uniform remote loads have been proposed. Expressions are provided for the multi-order stress intensity factors in either mode I or mode II problems using both power series (Williams series) and Laurent series. Thanks to these expressions, the convergence behavior of crack-tip stress expansions may be studied. The existence of the expected radii of convergence is observed. Rates of convergence are quantified.

With the description of the crack-tip stress field by series arises the problem of truncation influence. The accuracy of the series representation improves as the number of terms increases. However, the convergence is rather slow and the summation procedure is numerically limited to a few hundreds terms. The aim of this work is then to improve the accuracy of the stress description based on the a-priori knowledge of a given number of terms in the series. A method based on Padé approximants (PA) is proposed [16-20]. These approximants are rational functions whose coefficients are defined so as to fit the prescribed truncated series.

The communication starts with the description of the procedure leading to closed-form crack-tip stress solutions, the presentation of techniques related to Padé approximation follows and the efficiency of the method is assessed for a practical fracture configuration.

2. Crack-tip stress series

The representation of crack-tip stress field at the vicinity of a crack-tip is generally performed with the so-called Williams crack-tip stress expansion [1, 2]:

$$\sigma_{ij}\left(r,\theta\right)=\sum_{m=1}^{2}\sum_{k=-\infty}^{\infty}a_k^m f_k^{m,ij}\left(\theta\right)r^{k/2-1} \tag{1}$$

This polar description establishes the separate nature of radial and angular dependencies. These dependencies also appear to be universal in the sense that they are the same for all fracture configurations. The particularity of each problem appears through an infinite set of specific coefficients – the first one of those being the Stress Intensity Factor (SIF). While SIF have been determined for numerous configurations, the evaluation of higher order coefficients has been less prolific (see [5] for a list of works on the subject). On the analytical point of view, just a few papers (for instance [6, 7]) have dealt with the subject. The authors have recently determined general closed form expressions for the following fracture configuration:

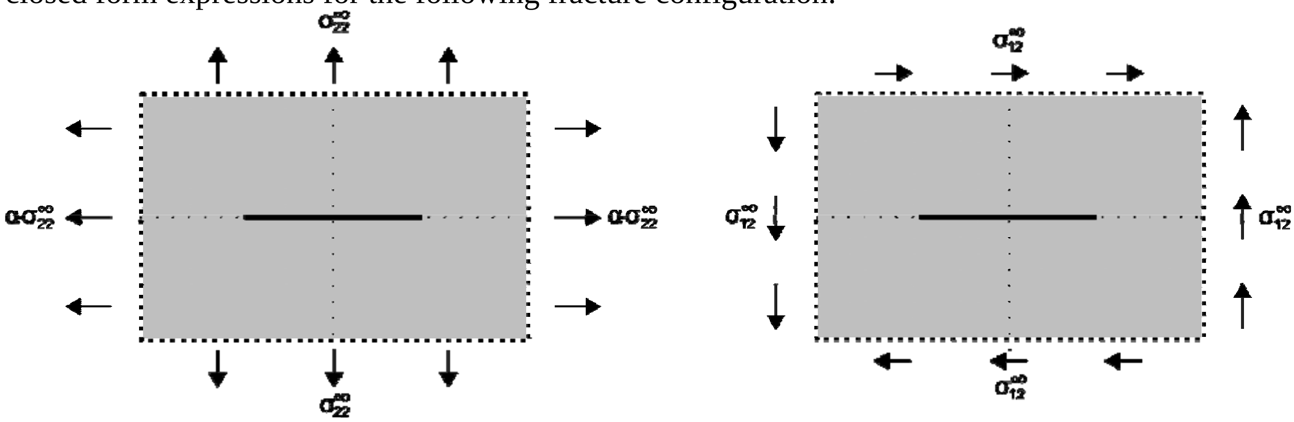

Figure 1. Fracture configuration: (left) mode-I, (right) mode-II

The procedure leading to coefficients exact definitions is described in the next subsections.

2.1. Complex solutions

Complex analysis provides a convenient way to deal with bi-dimensional elasticity. Positions are defined with a single complex number and Lamé-Navier equations may be expressed by simple “complex” operators. The formalism has largely beneficiated from the seminal works of Kolosov, Muskhelishvili and coworkers [8, 9]. A popular presentation of the method is due to Westergaard [10] who expressed the stress state in term of a complex potential (“Westergaard stress function”). Westergaard’s initial work has then been improved, for instance by Sih [11]. Stress functions have been found for several fracture configurations [12, 13]. The last improvement in the domain has been provided by Sanford [14, 15]. With his “generalized Westergaard approach”, he has shown that the solution should involve two complex potentials.

For mode-I, the stress state may be expressed with the potentials Z_1 and Y_1 according to:

$$\sigma_{11}^{1}=\operatorname{Re}Z_1-x_2\left(\operatorname{Im}Z_1'+\operatorname{Im}Y_1'\right)+2\operatorname{Re}Y_1 \tag{2}$$

$$\sigma_{22}^{1}=\operatorname{Re}Z_1+x_2\left(\operatorname{Im}Z_1'+\operatorname{Im}Y_1'\right) \tag{3}$$

$$\sigma_{12}^{1}=-\operatorname{Im}Y_1-x_2\left(\operatorname{Re}Z_1'+\operatorname{Re}Y_1'\right) \tag{4}$$

And for Mode-II with the potentials Z_2 and Y_2:

$$\sigma_{11}^{2}=\operatorname{Im}Y_2+x_2\left(\operatorname{Re}Y_2'+\operatorname{Re}Z_2'\right)+2\operatorname{Im}Z_2 \tag{5}$$

$$\sigma_{22}^{2} = \operatorname{Im} Y_2 - x_2 \left(\operatorname{Re} Y_2' + \operatorname{Re} Z_2' \right) \tag{6}$$

$$\sigma_{12}^{2} = -x_2 \left(\operatorname{Im} Y_2' + \operatorname{Im} Z_2' \right) + \operatorname{Re} Z_2 \tag{7}$$

The need for two complex potentials in the Westergaard approach appears coherent with the two complex potentials involved in the Kolosov-Muskhelishvili formalism.

For the fracture configuration depicted in (Fig. 1), mode-I complex potentials have the following expressions:

$$Z_1(z) = \sigma_{22}^{\infty} \frac{z}{\sqrt{z^2 - a^2}}, \quad Y_1(z) = \sigma_{22}^{\infty} \frac{(\alpha - 1)}{2} \tag{8}$$

While for mode-II:

$$Z_2(z) = \sigma_{12}^{\infty} \frac{z}{\sqrt{z^2 - a^2}}, \quad Y_2(z) = 0 \tag{9}$$

2.2. Identification of Williams series coefficients

In order to describe the stress-field in a planar cracked domain at the vicinity of the crack-tip, it is possible to use either Williams series (Eq. 1) or Sanford generalized Westergaard approach (Eq. 2-7). The stress state being unique, the two approaches must be equivalent. In [5], a procedure is described in order to transform the complex solution into the series one. Basically, complex potentials are expanded as closed-form convergent power series, these expression lead to complex stress series through (Eq. 2-7), and then, using the coordinates inter-relation $z = a + re^{i\theta}$, polar series may be retrieved.

For the configuration depicted in (Fig. 1), mode-I coefficients are then:

$$a_{2n+1}^{1} = \frac{(-1)^{n+1}(2n)!}{2^{3n+\frac{1}{2}}(n!)^2(2n-1)} \frac{\sigma_{22}^{\infty}}{a^{n-\frac{1}{2}}}, \quad n \geq 0 \tag{10}$$

$$a_2^1 = \frac{\sigma_{22}^{\infty}(\alpha - 1)}{4} \tag{11}$$

$$a_k^1 = 0, \quad otherwise \tag{12}$$

And for mode-II :

$$a_{2n+1}^{2} = \frac{(-1)^{n}(2n)!}{2^{3n+\frac{1}{2}}(n!)^2(2n-1)} \frac{\sigma_{12}^{\infty}}{a^{n-\frac{1}{2}}}, \quad n \geq 0 \tag{13}$$

$$a_k^2 = 0, \quad otherwise \tag{14}$$

If one considers the stress state along the radius associated with a given angle, it may be described by two polynomial series of r :

$$\sigma_{ij}^{m}(r,\theta) = \frac{1}{\sqrt{r}} \sum_{k=0}^{\infty} a_{2k+1}^{m,ij} f_{2k+1}^{m,ij}(\theta) r^k + \sum_{k=1}^{\infty} a_{2k}^{m,ij} f_{2k}^{m,ij}(\theta) r^{k-1} \tag{15}$$

3. Padé Approximants

3.1. Generalities

When series are used so as to describe physical quantities, the question of the accuracy of such a representation for practical purposes appears. Series are often truncated and in general the more terms there are, the better is the accuracy. However, sometimes it is neither possible nor accurate to include higher order terms of the expansion. In addition, the series has a radius of convergence beyond which the series diverges no matter how many terms are considered. Ideally, starting from a given truncated series, it would be interesting to devise a method that could both improve convergence rates and converge beyond the series radius of convergence. Padé approximants are known to provide such improvements [16-20]. The applicability of PA to crack-tip stress fields seems possible since (Eq. 15) holds polynomial series of the kind:

$$f\left(r,\theta\right) = \sum_{k=0}^{\infty} c_k\left(\theta\right) r^k \tag{16}$$

For the definition of PA in the general case, a function is supposed to a have a convergent polynomial expansion at the point $z = a$ where the coefficients $c_k \in$ £ are explicitly known:

$$f\left(z\right) = \sum_{k=0}^{\infty} c_k \cdot \left(z-a\right)^k \tag{17}$$

Associated with this function, the $\left[m,n\right]$ Padé approximant is the rational function:

$$f_{m,n}\left(z\right) = \frac{P_{m,n}\left(z\right)}{Q_{m,n}\left(z\right)} \tag{18}$$

Where the numerator and denominators are polynomials satisfying:

$$\begin{aligned} &\deg\left(P_{m,n}\left(z\right)\right) \le m, \quad \deg\left(Q_{m,n}\left(z\right)\right) \le n, \\ &f_{m,n}\left(z\right) Q_{m,n}\left(z\right) - P_{m,n}\left(z\right) = O\left(z-a\right)^{m+n+1}, \\ &Q_{m,n}\left(0\right) \ne 0. \end{aligned} \tag{19}$$

In order to enforce the uniqueness of the approximant, the first term of the denominator is set to one:

$$Q_{m,n}\left(0\right) = 1 \tag{20}$$

The numerator and denominator have then the expressions:

$$P_{m,n}\left(z\right) = \sum_{k=0}^{m} p_k \left(z-a\right)^k \tag{21}$$

$$Q_{m,n}\left(z\right) = 1 + \sum_{k=1}^{n} q_k \left(z-a\right)^k \tag{22}$$

The PA has $m+n+1$ unknown coefficients which requires the knowledge of the same amount of successive coefficients c_k in the initial series. The fact that coefficients p_k, q_k are not forced to be different from zero may lead to polynomials with maximum exponents lesser than the chosen ones $\left(m,n\right)$. In addition, the denominator being polynomial, it may exhibit spurious zeros that create non-physical singularities in addition to the expected ones.

3.2. Algebraic determination of Padé approximants coefficients

If the coefficients in the initial series are explicitly known, the coefficients in the $\left[m,n\right]$ Padé approximant may be determined with an algebraic process. We here suppose that $m \ge n$ without loss of generality. The enforcement of conditions (Eq. 19, 20) provides two linear systems. The first one enables to deduce $q_1,...,q_n$ from $c_{m-n+1},...,c_{m+n}$:

$$\begin{bmatrix} c_m & c_{m-1} & \cdots & c_{m-n+1} \\ c_{m+1} & c_m & \cdots & c_{m-n+2} \\ \vdots & \vdots & & \vdots \\ c_{m+n-1} & c_{m+n-2} & \cdots & c_m \end{bmatrix} \cdot \begin{bmatrix} q_1 \\ q_2 \\ \vdots \\ q_n \end{bmatrix} = - \begin{bmatrix} c_{m+1} \\ c_{m+2} \\ \vdots \\ c_{m+n} \end{bmatrix} \tag{23}$$

And the second one to determine $p_1,...,p_m$ from $q_1,...,q_n$ and $c_{m-n},...,c_m$

$$\begin{bmatrix} p_0 \\ p_1 \\ \vdots \\ p_m \end{bmatrix} = \begin{bmatrix} c_0 & 0 & \cdots & 0 \\ c_1 & c_0 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ c_m & c_{m-1} & \cdots & c_{m-n} \end{bmatrix} \cdot \begin{bmatrix} q_1 \\ q_2 \\ \vdots \\ q_n \end{bmatrix} \tag{24}$$

This algebraic computation of the PA may be performed either numerically or analytically. For the later, the use of a symbolic computation software like *Maple*, *Mathematica* or *Maxima* seems convenient. As an example, let's consider the following function:

$$f(x) = \frac{x}{\sqrt{x^2 - 1}} \tag{25}$$

A truncated series expansion at $x = 1$ can be derived analytically:

$$s_f(x,n)_{x=1} = \sum_{k=0}^{n} \left[\frac{1}{\sqrt{x-1}} \frac{1}{k!} \frac{d^k}{dx^k} \left(\frac{x}{\sqrt{x+1}} \right)_{x=1} \right] \cdot (x-1)^k \tag{26}$$

Its radius of convergence is equal to 2 and convergence rates are rather low near the border of the convergence domain. Based on the knowledge of 5 coefficients in (Eq. 26), the closed-form expression of the $[2,2]$ PA can be determined, here with the help of symbolic computations:

$$f_{2,2}(x) = \frac{1}{\sqrt{x-1}} \frac{\frac{1}{\sqrt{2}} + \frac{167}{136\sqrt{2}}(x-1) + \frac{249}{1088\sqrt{2}}(x-1)^2}{1 + \frac{65}{136}(x-1) + \frac{29}{1088}(x-1)^2} \tag{27}$$

For $x = 2.9$, the truncated series $s_f(x,4)_{x=1}$ (5 coefficients) provides a result with 6.117E-2 of relative error while the associated PA $f_{2,2}(x)$ has a lower error of 7.554E-4.

3.3. Numerical evaluation of Padé approximants values with the epsilon algorithm

If the practical purpose of the PA is to compute the value of the stress field for some points of interest, the calculation of coefficients p_k, q_k is just an intermediate step and not a goal in itself. It comes out that Wynn's epsilon algorithm [21, 22] is able to calculate directly the value of the PA from successive intermediate sums of the given truncated series. It the intermediate sum with $n+1$ terms of the series expansion of f is:

$$S_n = s_f(z,n) \tag{28}$$

Then the following algorithm produces the numerical evaluation of the associated PA:

$$\begin{aligned} &\varepsilon_{-1}^{j}=0, \quad j=0,1...,n \\ &\varepsilon_{0}^{j}=S_{j}, \quad j=0,1,...,n \\ &\varepsilon_{k}^{j}=\varepsilon_{k-2}^{j+1}+\left(\varepsilon_{k-1}^{j+1}-\varepsilon_{k-1}^{j}\right)^{-1}, \quad k=1,...,n \quad and \quad j=0,...,n-k \end{aligned} \tag{29}$$

This algorithm may be presented more conveniently using columns:

$$\begin{array}{lllll} 0 & \varepsilon_{0}^{0}=S_{0} & \varepsilon_{1}^{0} & \mathrm{K} & \varepsilon_{n}^{0} \\ \varepsilon_{-1}^{1}=0 & \varepsilon_{0}^{1}=S_{1} & \mathrm{M} & \mathrm{N} & \\ \mathrm{M} & \mathrm{M} & \varepsilon_{1}^{n-1} & & \\ \varepsilon_{-1}^{n}=0 & \varepsilon_{0}^{n}=S_{n} & & & \end{array} \tag{30}$$

As is appears in (Eq. 29), the evaluation of a new epsilon requires the inversion of a combination of previous epsilons. If the value of the last epsilon were to be expressed in terms of the initial partial sums, the observed expression would have the structure of a continued fraction. On the theoretical point of view, PA, the epsilon algorithm and continued fractions are deeply interrelated [18].

As an example, let's consider again the function (Eq. 25). The series representation of the function only converges within a disk of radius 2 centered at x=1. Employing the epsilon algorithm, is it possible to use the partial sums of successive truncated series in order to evaluate accurately the function for some points outside the convergence disk. For instance, even though the point x=4 lies outside the disk, a relative error of less than 10^{-6} can be achieved through the epsilon algorithm with 11 partial sums.

4. Tests

In order to assess the convergence improvement provided by PA, we consider the mode-I configuration depicted in (Fig. 1). For this problem, an exact complex solution is available with the injection of the complex potentials (Eq. 8) into Sanford's generalized Westergaard equations (Eq. 2-4). A closed-form series representation is available as well. Combining Williams general definition (Eq. 1) with the specific expressions of coefficients a_k^1 provided in (Eq. 10-12), an exact series like (Eq. 15) is defined.

From the exact series, three truncated series with respectively 5, 7 and 9 terms are considered. If the angle is fixed to zero, these truncated series may be transformed into PA using the algebraic procedure described in (Subsection 3.2). The series with 5 terms lead to the PA:

$$[2,2]_{\sigma_{22}^{1}(r,0)}=\frac{\sigma_{22}^{\infty}\sqrt{a}}{\sqrt{r}}\cdot\frac{\dfrac{1}{\sqrt{2}}+\dfrac{167}{136\sqrt{2}}\dfrac{r}{a}+\dfrac{249}{1088\sqrt{2}}\left(\dfrac{r}{a}\right)^{2}}{1+\dfrac{65}{136}\dfrac{r}{a}+\dfrac{29}{1088}\left(\dfrac{r}{a}\right)^{2}} \tag{31}$$

The series with 7 terms provide:

$$[3,3]_{\sigma_{22}^{1}(r,0)}=\frac{\sigma_{22}^{\infty}\sqrt{a}}{\sqrt{r}}\cdot\frac{\dfrac{1}{\sqrt{2}}+\dfrac{1171}{792\sqrt{2}}\dfrac{r}{a}+\dfrac{1649}{3168\sqrt{2}}\left(\dfrac{r}{a}\right)^{2}+\dfrac{709}{16896\sqrt{2}}\left(\dfrac{r}{a}\right)^{3}}{1+\dfrac{577}{792}\dfrac{r}{a}+\dfrac{413}{3168}\left(\dfrac{r}{a}\right)^{2}+\dfrac{169}{50688}\left(\dfrac{r}{a}\right)^{3}} \tag{32}$$

And the PA for the truncated series with 9 terms is:

$$[4,4]_{\sigma_{22}^{1}(r,0)} = \frac{\sigma_{22}^{\infty}\sqrt{a}}{\sqrt{r}} \cdot \frac{\frac{1}{\sqrt{2}} + \frac{7979}{4616\sqrt{2}}\frac{r}{a} + \frac{32295}{36928\sqrt{2}}\left(\frac{r}{a}\right)^2 + \frac{22585}{147712\sqrt{2}}\left(\frac{r}{a}\right)^3 + \frac{16337}{2363392\sqrt{2}}\left(\frac{r}{a}\right)^4}{1 + \frac{4517}{4616}\frac{r}{a} + \frac{19}{64}\left(\frac{r}{a}\right)^2 + \frac{4203}{147712}\left(\frac{r}{a}\right)^3 + \frac{985}{2363392}\left(\frac{r}{a}\right)^4} \quad (33)$$

In any case, the epsilon algorithm (Subsection 3.3) is able to provide the required value for the different PA at any point.

4.1. Qualitative comparison

The series expansion is performed at the crack-tip z=a. The radius of convergence is therefore equal to 2a. The series is not able to converge beyond this limit. In (Fig. 2), the exact complex solution, the truncated series representation with 9 terms, and the PA with 9 coefficients are compared. As expected, the series representation has only a good correspondence with the reference near the crack-tip and diverges beyond the radius of convergence. PA exhibits an excellent correspondence with the complex solution inside the whole convergence disk. The behavior outside the disk is also close to the reference. A spurious singular points appears at z=-2a. PA solution seems thus to have better convergence rates and a larger convergence domain.

4.2. Quantitative comparison

The approximate representations with truncated series and PA (Eq. 31-33) are now compared in (Fig. 3). Within the convergence disk, the more terms hold the series, the better is the solution. Beyond the convergence radius series diverge. PA approximations have far better convergence rates inside most of the convergence disk. PA are also able to provide accurate results far beyond the series convergence limit.

5. Conclusion

In this communication, Padé approximants have been used in order to improve the convergence behavior of crack-tip stress series. Starting from closed-form truncated series, it is possible to either determine exactly the coefficients in the PA or to estimate directly its value at any point. With the same amount of "information" (ie coefficients), the PA associated to a given truncated series provides better convergence rates inside the series convergence disk and is also able to converge outside the disk.

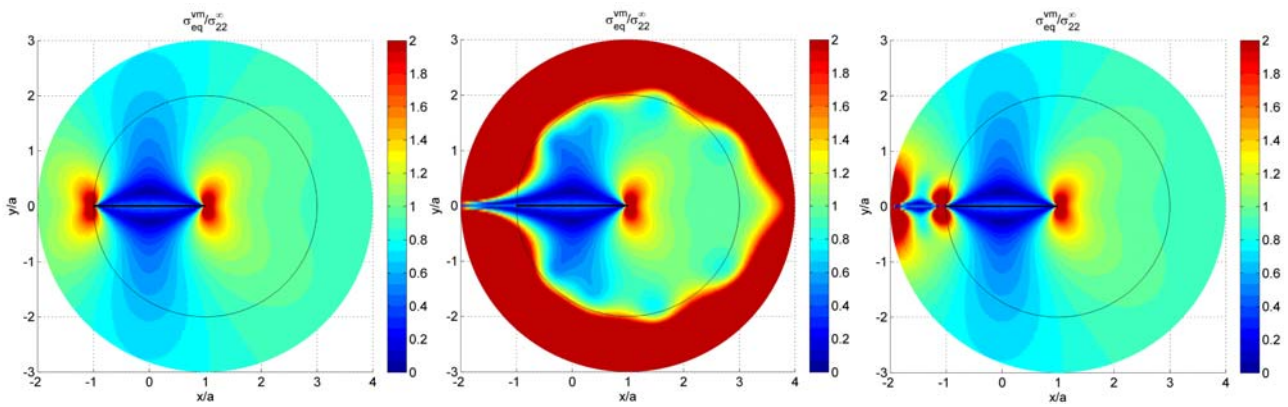

Figure 2. Stress state representation for: (left) Westergaard exact solution, (center) truncated series with 9 terms, (right) Padé approximant [4,4] with 9 coefficients.

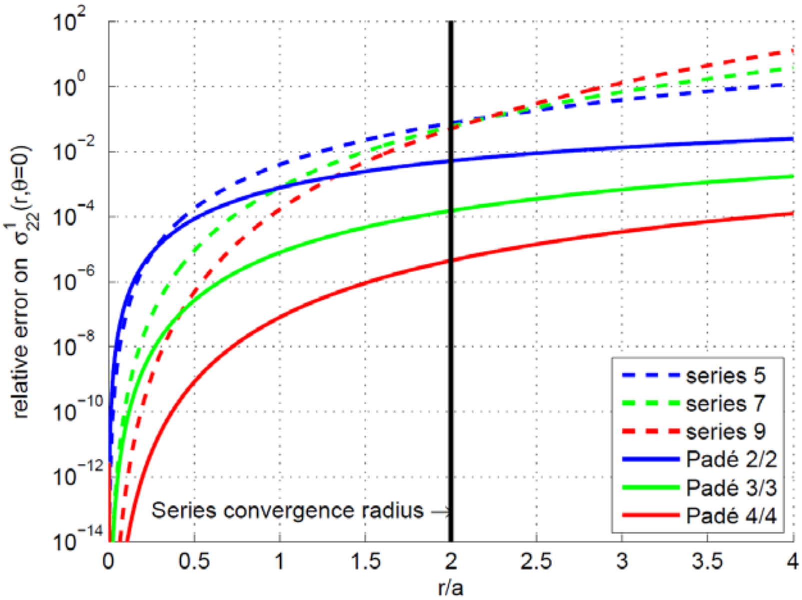

Figure 3. Relative error on $\sigma_{22}^{1}\left(r,\theta=0\right)$ for series representations with 5,7 and 9 terms and their associated Padé approximants $[2,2]$, $[3,3]$ and $[4,4]$.

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