Computer Assisted Mechanics and Engineering Sciences, 3: 121–132, 1996.

Two-point Padé approximants to Stieltjes series representation of bulk moduli of regular composites

Stanisław Tokarzewski and Józef Joachim Telega
Institute of Fundamental Technological Research, Polish Academy of Sciences
ul. Świętokrzyska 21, 00-049 Warsaw, Poland

(Received July 17, 1995)

The aim of this contribution is to present two-point Padé approximants method for the determination of upper and lower estimates on the effective transport coefficients of two-phase composite materials. The obtained formulae improve the corresponding one-point Padé approximants bounds [1,2,4,14,23]. As an example, a set of narrowing bounds for the overall conductivity of a square array of cylinders has been evaluated.

1. Introduction

The mathematical properties of one-point Padé approximants to the effective moduli λ_e of two-phase composites consisting of components of moduli λ_1, λ_2, were extensively investigated in recent years [4,14,16,23]. The most important result valid in the real domain reads: the sequence of diagonal and subdiagonal one-point Padé approximants to power expansion of $\lambda_e(x)$ at $x = 0$, $x = (\lambda_1/\lambda_2) - 1$, form the upper and lower bounds uniformly converging to $\lambda_e(x)$. Moreover, these bounds are the best with respect to the given number of power series coefficients [1,Th.15.2].

On the contrary, the mathematical properties of two-point Padé approximants to $\lambda_e(x)$ generated by two power expansions of $\lambda_e(x)$, namely at $x = 0$ and $x = \infty$, have not been examined as deeply as the one-point Padé ones. The results reported in mathematical literature [8–11] are concerned mostly with two-point Padé approximants to an equal number of coefficients of power expansions of Stieltjes function at zero and infinity ("balanced" situation). Some special type of two-point Padé approximants to Stieltjes function (2PTA) is studied in [6].

The convergence of sequences of two-point Padé approximants generated by non-equal number of coefficients of power expansions of Stieltjes function at zero and infinity has been investigated in [17,20]. General inequalities in real domain for unbalanced two-point Padé approximants to Stieltjes functions have been derived in [22].

Main aim of this paper is to present two-point Padé approximants method of determination, from the coefficients of a power series expansion of $\lambda_e(x)$, of the upper and lower bounds on $\lambda_e(x)$, for two-phase composite materials.

This paper is organized as follows: in Section 2 we introduce basic definitions, notations and assumptions dealing with Padé approximants to $\lambda_e(x)$. General two-point Padé approximants bounds on $\lambda_e(x)$ are presented in Section 3. Auxiliary algorithms for the determination of coefficients of a special continued fraction representation of two-point Padé approximants are demonstrated in Section 4. In Section 5 we present the exact recurrence formulae for finding two-point Padé approximants from the terms of power series expansions of $\lambda_e(x)$ around zero and infinity. In Sections 6 the correctness of the proposed algorithms is tested. A nontrivial example of practical calculation of two-point Padé approximants bounds on $\lambda_e(x)$ is provided in Section 7. In Section 8 we summarize and discuss the results achieved.

2. Basic assumptions, definitions and notations

From the physical point of view, our study is concerned with the effective conductivity Λ_e of a composite consisting of two isotropic components of conductivities λ_1, λ_2 and volume fractions φ and $1-\varphi$, respectively. The bulk effective conductivity is defined by the linear relationship $\langle \mathbf{J} \rangle = \Lambda_e \langle \nabla T \rangle$ between the volume-averaged temperature gradient $\langle \nabla T \rangle$ and the volume-averaged heat flux $\langle \mathbf{J} \rangle$. The average value $\langle \, . \, \rangle$ is evaluated over a representative volume or a basic cell. In general, Λ_e is a second-order symmetric tensor depending on the microstructure of a composite. Our study, however, will be focused upon one of the principal values of Λ_e denoted by λ_e. The remaining principal values can be studied similarly.

Analytical properties of the bulk dielectric coefficient $\lambda_e(\lambda_1, \lambda_2)$ were examined by Bergman in [4]. He proved that $\lambda_e(\lambda_1,\lambda_2)/\lambda_1 = \lambda_e(1, \lambda_2/\lambda_1)$ is a Stieltjes function of λ_2/λ_1, analytical everywhere except for the negative part of the real axis. Consequently, the effective conductivity $\lambda_e(x)$ has the following general Stieltjes-integral representation:

$$\frac{\lambda_e(x)}{\lambda_1} - 1 = R(x, C) = xF(x, C), \qquad F(x,C) = \int_0^\infty \frac{\mathrm{d}\Gamma(u, C)}{1+xu}, \tag{1}$$

defined for $0 < x < \infty$, where the spectrum $\Gamma(u, C)$:

$$\Gamma(u, C) = CH(u) + \gamma(u), \qquad H(u) = \begin{cases} 0 & \text{for } \ u \le 0 \\ 1 & \text{for } \ u > 0 \end{cases} \tag{2}$$

is a real-valued, bounded and non-decreasing function defined for $0 \le u < \infty$, while C and $H(u)$ denote a non-negative constant and Heaviside function, respectively.

Consider now the formal power expansion of the Stieltjes function $R(x, C)$ at $x = 0$,

$$R(x, C) \simeq \sum_{n=1}^{\infty} (C\delta_{n1} + c_n)\, x^n, \qquad \delta_{n1} = \begin{cases} 1 & \text{if } \ n = 1, \\ 0 & \text{if } \ n > 1. \end{cases} \tag{3}$$

The expansion coefficients c_n in (3) are given by

$$c_n = (-1)^{n+1} \int_0^\infty u^{n-1} \mathrm{d}\gamma(u) \quad n = 1, 2, \ldots . \tag{4}$$

Similarly at $x = \infty$ we have

$$R(x, C) \simeq Cx + \sum_{n=0}^{\infty} C_n x^{-n}, \tag{5}$$

where

$$C_n = (-1)^n \int_0^\infty u^{-n-1} \mathrm{d}\gamma(u), \quad n = 0, 1, \ldots . \tag{6}$$

The coefficients c_n and C_n are assumed to be finite, *cf.* [1–3]. Two-point Padé approximants to Stieltjes function $R(x, C)$ defined by (1) and (2) via the formal power series (3) and (5) with $C > 0$, have the following general form

$$[M+1/M]_k = \frac{a_{1,k}x + a_{2,k}x^2 + \ldots + a_{M+1,k}x^{M+1}}{1 + b_{1,k}x + b_{2,k}x^2 + \ldots + b_{M,k}x^M}. \tag{7}$$

Let us examine the power expansion of rational function (7) at $x = 0$

$$[M+1/M]_k = \sum_{n=1}^{\infty} c_{n,k} x^n \tag{8}$$

and at $x = \infty$

$$[M+1/M]_k = \sum_{n=-1}^{\infty} C_{n,k} x^{-n} . \tag{9}$$

By definition, the rational function (7) is a two-point Padé approximant to power series (3) and (5) with $C > 0$, if

$$c_{n,k} = C\delta_{1,n} + c_n \quad \text{for} \quad n = 1, 2, \ldots, 2M+1-k \tag{10}$$

and

$$C_{-1,k} = C, \quad C_{n,k} = C_n \quad \text{for} \quad n = 0, 1, \ldots, k-2. \tag{11}$$

According to the above notation, $[M+1/M]_0$ stands for the one-point Padé approximant.

Let us pass to the Stieltjes function $R(x, C)$ for $C = 0$. Then the two-point Padé approximants to power series (3) and (5) take the form

$$[M/M]_k = \frac{a'_{1,k}x + a'_{2,k}x^2 + \ldots + a'_{M,k}x^M}{1 + b'_{1,k}x + b'_{2,k}x^2 + \ldots + b'_{M,k}x^M}. \tag{12}$$

The rational function (12) is the two-point Padé approximant to the Stieltjes function $R(x, C)$, still for $C = 0$, with power expansions (3) and (5), if

$$c_{n,k} = c_n \quad \text{for} \quad n = 1, 2, \ldots, 2M-k \tag{13}$$

and

$$C_{n,k} = C_n \quad \text{for} \quad n = 0, 1, 2, \ldots, k-1, \tag{14}$$

cf. also (10) and (11). It is worth noting that on account of (7)–(11) and (12)–(14), one readily gets:

$$\text{if } C \to 0^+ \quad \text{then} \quad a_{M+1,k}x^{M+1} \to 0 \quad \text{and} \quad [M+1/M]_{k+1} \to [M/M]_k . \tag{15}$$

Thus by using (9)–(14) we obtain

$$[M+1/M]_{k+1} = Cx + [M/M]_k \quad \text{for} \quad k = 0, 1, \ldots . \tag{16}$$

Formula (16) determines the general relation between the two-point Padé approximants $[M+1/M]_{k+1}$ and $[M/M]_k$ constructed for the Stieltjes functions $R(x, C)$ with $C > 0$ and $R(x, C)$ for $C = 0$, respectively. Two-point Padé approximants (7) and (12) can also be expressed in the form of S-continued fractions [1]

$$[M+J/M]_k = \frac{g_1 x}{1} \, {}_{+} \cdots {}_{+} \, \frac{g_p x}{1} \, {}_{+} \cdots {}_{+} \, \frac{g_{p+1} x}{1} \, {}_{+} \cdots {}_{+} \, \frac{g_{2M+J} x}{1}, \quad J = 0, 1 \tag{17}$$

or alternatively

$$[M+J/M]_k = \frac{g_1 x}{s} \, {}_{+} \, \frac{g_2 x}{1} \, {}_{+} \, \frac{g_3 x}{s} \, {}_{+} \, \frac{g_4 x}{1} \, {}_{+} \cdots {}_{+} \, \frac{g_{p+1} x}{\alpha} \, {}_{+} \cdots {}_{+} \, \frac{g_{2M+J} x}{\alpha}, \quad \alpha = 0 \text{ or } 1 , \tag{18}$$

where $s = 1/x$, and $p = 2M + J - k$ ($j = 0, 1$). The coefficients $g_1, \ldots, g_p$ appearing in continued fractions (17) and (18) are uniquely determined by p coefficients c_n ($n = 1, 2, \ldots, p$) of a Stieltjes series (3). To determine the remaining coefficients $q_{p+1}, \ldots, q_{2M+J}$ ($J = 0, 1$), the values of k coefficients C_n of a series (5) are additionally needed. However, well known continued fractions (17)–(18) [1,2,3] are inconvenient for an investigation of two-point Padé approximants bounds on $\lambda_e(x)$. Below we will propose a special two-point continued fraction representation for $[M+J/M]_k$ ($J = 0, 1$), different from that given by (17)–(18).

3. Two-point Padé approximants bounds

The mathematical framework for the application of two-point Padé approximants for the investigation of overall properties of two-phase composites is provided by the present authors in [22], see also [17–20]. In particular, the following theorem indispensable for further development was proved in [22]:

Theorem 3.1. Two-point Padé approximants to Stieltjes power expansions (3) and (5) satisfy the following inequalities

$$(-1)^k[M/M]_k \quad < (-1)^k[M+1/M+1]_k \quad < (-1)^k R(x,C), \qquad \text{if} \quad C=0\,, \tag{19}$$

$$(-1)^{k-1}[M+1/M]_k < (-1)^{k-1}[M+2/M+1]_k < (-1)^{k-1}R(x,C), \quad \text{if} \quad C>0\,, \tag{20}$$

where $R(x,C)$ with $C=0$, $R(x,C)$ with $C>0$, defined by (1) and (2), stand for the limit as M goes to infinity of $[M/M]_k$, $[M+1/M]_k$, respectively, and x is real and positive.

These inequalities have the consequence that the $[M/M]_k$, $[M+1/M]_k$ bounds are obtainable using only the given number of coefficients, and that the use of additional coefficients (higher M) improves the bounds. Note that for $k=0$, the relations (19) and (20) take a form of well-known inequalities for one-point Padé approximants [1, Th.15.2].

An interrelation between two-point Padé approximants and continued fractions is furnished by:

Lemma 3.1. Two-point Padé approximants $[M/M]_k$ $(2M \leq k)$ and $[M+1/M]_k$ $(2M+1 \leq k)$ can be uniquely represented by the following two-point continued fractions:

(i) if k is odd, then

$$[M/M]_k = \frac{g_1 x}{1} + \cdots + \frac{g_p x}{(1+x)G_0} + \frac{G_1}{1} + \frac{G_2 s}{1} + \cdots + \frac{G_{k-1} s}{1}\,; \tag{21}$$

(ii) If k is even then

$$[M/M]_k = \frac{g_1 x}{1} + \cdots + \frac{g_p x}{1} + \frac{G_1}{1} + \frac{G_2 s}{1} + \cdots + \frac{G_k s}{1}\,; \tag{22}$$

(iii) If $k = 0, 1, 2, \ldots$, then

$$[M+1/M]_{k+1} = Cx + [M/M]_k\,. \tag{23}$$

Here the coefficients g_j and G_j

$$g_j > 0 \qquad (j = 1, 2, \ldots, p), \qquad G_j > 0 \qquad (j = 0, 1, \ldots, k) \tag{24}$$

are positive, whilst $s = 1/x$.

The recurrence formula for computing $[M/M]_k$ is given by:

$$\begin{aligned}
& s = 1/x\,,\; Q^{(k-1)} = \begin{cases} 0\,, & \text{if } k \text{ odd},\\ g_{k-1}s\,, & \text{if } k \text{ even},\end{cases}\\
& Q^{(k-2-n)} = g_{k-2-n}s/(1+Q^{(k-1-n)})\,, \qquad n = 0, 1, \ldots, k-3,\\
& Q^{(p+1)} = \begin{cases} Q^{(1)} + G_0 x\,, & \text{if } k \text{ odd},\\ Q^{(1)}/s\,, & \text{if } k \text{ even},\end{cases}\\
& Q^{(p-n)} = g_{p-n}x/(1+Q^{(p+1-n)})\,, \qquad n = 0, 1, \ldots, p-1,\quad [M/M]_k = Q^{(1)}\,,
\end{aligned} \tag{25}$$

where p, k and x are the input data for (25). It is convenient to rewrite the continued fractions (21) and (22) in terms of $s = 1/x$:

(i) if k is odd, then

$$[M/M]_k = \frac{g_1}{s} \,\frac{g_2}{+\,1} + \cdots + \frac{g_p}{s+G_0} + \frac{G_1 s}{1} + \frac{G_2 s}{1} + \cdots + \frac{G_{k-1} s}{1}\,; \tag{26}$$

(ii) If k is even, then

$$[M/M]_k = \frac{g_1}{s} \,\frac{g_2}{+\,1} + \cdots + \frac{g_{p-1}}{s} + \frac{g_p}{1} + \frac{G_1}{1} + \frac{G_2 s}{1} + \cdots + \frac{G_k s}{1}\,. \tag{27}$$

More details on relations (19)–(27) the reader will find in our paper [22]. Expressions (19)–(24) and (26)–(27) are indispensable for deriving an exact recurrence formulae for the determination of coefficients g_j $(j = 1, 2, \ldots, p)$ and G_j $(j = 0, 1, \ldots, k)$ appearing in (21)–(22).

4. Auxiliary recurrence formulae

Before the construction of an exact algorithm for the determination of coefficients g_j $(j = 1, 2, \ldots, p)$ and G_j $(j = 0, 1, \ldots, k)$ of continued fractions (21)–(22), some auxiliary recurrence formulae for infinite power expansions of Stieltjes functions will be proposed.

Let us introduce the two Stieltjes series: $R_{p+1}(x)$ $(p = 1, 3, \ldots)$ and $R_{p+1}(x)$ $(p = 0, 2, \ldots)$ defined by:

$$R(s) = \begin{cases} \dfrac{g_1}{s} \,\dfrac{g_2}{+\,1} + \cdots + \dfrac{g_p}{s + R_{p+1}(s)}\,, & \text{if} \quad p = 1, 3, \ldots, \\[2ex] \dfrac{g_1}{s} \,\dfrac{g_2}{+\,1} + \cdots + \dfrac{g_{p-1}}{s} + \dfrac{g_p}{1 + R_{p+1} s}\,, & \text{if} \quad p = 0, 2, \ldots, \end{cases} \tag{28}$$

where

$$R(s) = \sum_{j=0}^{\infty} C_j^{(1)} s^j, \qquad s = 1/x \tag{29}$$

is a power series (5) with $C = 0$, while $R_{(p+1)}(s)$ takes the form

$$R_{p+1}(s) = \begin{cases} \displaystyle\sum_{j=0}^{\infty} C_j^{(p+1)} s^j\,, & \text{if} \quad p = 1, 3, \ldots, \\[2ex] \displaystyle\sum_{j=0}^{\infty} C_j^{(p+1)} s^j\,, & \text{if} \quad p = 0, 2, \ldots. \end{cases} \tag{30}$$

From (28) one can easily derive the following recurrence formulae interrelating the coefficients $C_j^{(1)}$ with $C_j^{(2)}$:

$$C_0^{(2)} = g_1 / C_0^{(1)}\,, \tag{31}$$

$$C_j^{(2)} = -\frac{\sum_{k=0}^{j-1} C_{j-k}^{(1)} \left(C_k^{(2)} + \delta_{1k} \right)}{C_0^{(1)}} - \delta_{1j}\,, \qquad j = 1, 2, \ldots \tag{32}$$

and $C_j^{(2)}$ with $C_j^{(3)}$

$$C_0^{(3)} = g_2 / C_0^{(2)}\,, \tag{33}$$

$$C_j^{(3)} = -\frac{\sum_{k=0}^{j-1} C_{j-k}^{(2)} \left(C_k^{(3)} + \delta_{0k} \right)}{C_0^{(2)}} - \delta_{0j}\,, \qquad j = 1, 2, \ldots \tag{34}$$

Here we have introduced $\delta_s(p) = 1$ ($\delta_s(p) = 0$), if $s = p$ (if $s \neq p$). By starting from the $C_j^{(3)}$ given by (34) we obtain $C_j^{(4)}$ via (31)–(32), and then $C_j^{(5)}$ via (33)–(34), *etc.*

Motivated by a special continued fraction representation of $[M/M]_k$ given by (26)–(27), we can reformulate (28) in a slightly different form

$$R(s) = \begin{cases} \dfrac{g_1}{s} \, \dfrac{g_2}{+\,1} + \cdots + \dfrac{g_p}{s + G_0 + sR_{p+2}(s)}\,, & \text{if} \quad p = 1,3,\ldots, \\[2ex] \dfrac{g_1}{s} \, \dfrac{g_2}{+\,1} + \cdots + \dfrac{g_{p-1}}{s} \, \dfrac{g_p}{+\,1 + R_{p+1}s}\,, & \text{if} \quad p \quad \text{is even.} \end{cases} \tag{35}$$

Note that according to $(35)_1$ and $(30)_1$:

$$G_0 = C_0^{(p+1)}\,, \quad \text{if} \quad p = 1,3,\ldots; \tag{36}$$

while on account of (5) with $C = 0$ and due to $(30)_{1,2}$ we have:

$$R(x) \quad = \sum_{j=1}^{\infty} C_j^{(1)} x^j\,, \qquad \text{if} \quad p = 1,2,\ldots\,, \tag{37}$$

$$R_{p+2}(s) \;= \sum_{j=1}^{\infty} C_j^{(p+1)} s^j\,, \quad \text{if} \quad p = 1,3,\ldots\,, \tag{38}$$

$$sR_{p+1}(s) = \sum_{j=1}^{\infty} C_{j-1}^{(p+1)} s^j\,, \quad \text{if} \quad p = 0,2,\ldots\,. \tag{39}$$

Now we can construct S-continued fractions $[M/M]$ to Stieltjes functions (4.10), (4.11), (4.12) from:

(i) p terms of a Stieltjes series (37)

$$R(x) = \frac{g_1 x}{1} \, \frac{g_2 x}{+\,1} + \cdots + \frac{g_p x}{s + xR_{p+1}(s)}\,, \qquad s = 1/x\,; \tag{40}$$

(ii) $(k-1)$ terms of Stieltjes expansion (38)

$$R_{p+2}(s) = \frac{G_1 s}{1} \, \frac{G_2 s}{+\,1} + \cdots + \frac{G_{k-1} s}{1 + sf(s)}\,, \quad \text{if} \quad k = 1,3,\ldots; \tag{41}$$

(iii) k terms of the power series (39)

$$sR_{p+1}(s) = \frac{G_1 s}{1} \, \frac{G_2 s}{+\,1} + \cdots + \frac{G_k s}{1 + sf_{k+1}(s)}\,, \quad \text{if} \quad k \quad \text{is even.} \tag{42}$$

The problem of finding two-point Padé approximants $[M/M]_k$ to power series $R(x) = \sum_{j=1}^{\infty} c_j x^j$, $R(x) = \sum_{j=0}^{\infty} C_j s^j$, $s = 1/x$ has been reduced, via (31)–(34) and (40)–(42), to the determination of the S-continued fractions from power series (37), (38) and (39) respectively. Hence the following recurrence formula

$$\begin{cases} m = 1,2,\ldots\,, \quad D_m = d_1^{(m)}\,, \\[2ex] d_0^{(m+1)} = 1\,, \quad d_j^{(m+1)} = -\dfrac{\displaystyle\sum_{k=1}^{j} d_k^{(m)} d_{j-k}^{(m+1)}}{d_1^{(m)}}\,, \quad j = 1,2,\ldots\,, \end{cases} \tag{43}$$

for finding D_n from $\sum_{j=1}^{\infty} d_j^{(1)} x^j$, proposed in [22], can be applied directly to (37), (38) and (39). Here D_n represents g_n, G_n, while $d_j^{(1)}$ the coefficients $c_j^{(1)}$, $C_j^{(p+1)}$ ($p = 1,3,\ldots$), $C_{j-1}^{(p+1)}$ ($p = 0,2,\ldots$) respectively.

5. Exact recurrence formulae

Now we are in position to demonstrate the exact algorithm for the determination of the parameters g_n, G_n of a continued fraction $[M/M]_k$, given by (21) and (22). We start from p coefficients of a power series (3) with $C = 0$ and k coefficients of a power expansion (5) also with $C = 0$, where $p + k = 2M$. In the first step we compute the coefficients g_n $(n = 1, 2, \ldots, p)$ of a S-continued fraction to a Stieltjes expansion (3). On the basis of (43) we have

$$\left\{\begin{array}{l} m = 1,2,\ldots,p\ , \quad g_m = c_1^{(m)}\ , \\ \left\{\begin{array}{l} n = 1,2,\ldots,p-m\ , \\ c_0^{(1+m)} = 1\ , \quad c_n^{(1+m)} = -\dfrac{1}{c_1^{(m)}}\left(\displaystyle\sum_{j=0}^{n-1} c_j^{(1+m)} c_{n+1-j}^{(m)}\right), \end{array}\right. \end{array}\right. \tag{44}$$

where $c_m^{(1)}$ $(m = 1, 2, \ldots, p)$ given by (3) are the input data for (44).

The auxiliary formulae (31)–(35) with g_n $(n = 1, 2, \ldots, p)$ determined by $(44)_1$ take, for the data $C_m^{(m)} = C_m$ $(m = 0, 1, 2, \ldots, k-1)$ given by (5), the following exact form:

$$\left\{\begin{array}{l} m = \left\{\begin{array}{ll} 0,2,\ldots,(p-1)\ , & \text{if } p \text{ odd} \\ 0,2,\ldots,(p-2)\ , & \text{if } p \text{ even} \end{array}\right. , \quad C_0^{(n+2)} = g_{n+1}/C_0^{(n+1)}\ , \\ \left\{\begin{array}{l} n = 1,2,\ldots,k-1\ , \\ C_j^{(n+2)} = -\dfrac{\displaystyle\sum_{m=0}^{j-1} C_{j-m}^{(n+1)}\left(C_m^{(n+2)} + \delta_{1m}\right)}{C_0^{(n+1)}} - \delta_{1j}\ , \end{array}\right. \\ C_0^{(n+3)} = g_{n+2}/C_0^{(n+2)}\ , \\ \left\{\begin{array}{l} n = 1,2,\ldots,k-1\ , \\ C_j^{(n+3)} = -\dfrac{\displaystyle\sum_{m=0}^{j-1} C_{j-m}^{(n+2)}\left(C_m^{(n+3)} + \delta_{0m}\right)}{C_0^{(n+2)}} - \delta_{0j}\ , \end{array}\right. \end{array}\right. \tag{45}$$

If p is odd then $(45)_4$, if p is even then $(45)_7$ determines the coefficients $C_j^{(p+1)}$ $(j = 0, 1, \ldots, k-1)$ for recurrence relations (46) and (47) below:

(i) if p odd, then

$$C'_j = C_j^{(p+1)}\ , \quad j = 0,1,\ldots,k-1\ , \quad G_0 = C_0^{\prime(1)}\ ,$$

$$\left\{\begin{array}{l} m = 1,2,\ldots,k-1\ , \quad G_m = C_1^{\prime(m)}\ , \\ \left\{\begin{array}{l} n = 1,2,\ldots,k-1-m\ , \\ C_0^{\prime(1+m)} = 1\ , \quad C_n^{\prime(1+m)} = -\dfrac{\displaystyle\sum_{j=0}^{n-1} C_j^{\prime(1+m)} C_{n+1-j}^{\prime(m)}}{C_1^{\prime(m)}}\ . \end{array}\right. \end{array}\right. \tag{46}$$

(ii) If k is even, then

$$C'_{j+1} = C_j^{(p+1)} \;,\; j = 0, 1, \ldots, k-1 \;,$$

$$\begin{cases} m = 1, 2, \ldots, k-1 \;,\; G_m = C_1'^{(m)} \;, \\ \begin{cases} n = 1, 2, \ldots, k-1-m \;, \\ C_0'^{(1+m)} = 1 \;,\quad C_n'^{(1+m)} = -\dfrac{\sum_{j=0}^{n-1} C_j'^{(1+m)} C_{n+1-j}'^{(m)}}{C_1'^{(m)}} \;. \end{cases} \end{cases} \tag{47}$$

By starting from p terms of the power series expansion (3) and k terms of the series (5), where $p + k = 2M$, the recurrence relations (44)–(47) allow us to determine uniquely the coefficients g_n and G_n for continued fractions (21) or (22).

6. Numerical test

For testing the basic formulae given by (44)–(47), the following two Stieltjes series expanded at $x = 0$,

$$R(x) = +\frac{1}{\ln 1000} \sum_{n=1}^{\infty} \frac{1}{n}(1 - 1000^n)(-x)^n \;, \tag{48}$$

and at $x = \infty$

$$R(x) = 1 + \frac{1}{\ln 1000} \sum_{n=1}^{\infty} \frac{1}{n}(1 - 0.001^n)(-x)^n \;, \tag{49}$$

corresponding to the Stieltjes function

$$R(x) = x \int_1^{1000} \frac{du}{1 + xu} = \frac{1}{\ln 1000} \cdot \ln \frac{1 + 1000x}{1 + x} \tag{50}$$

have been used as the input data. Numerical results are shown in Figs. 1,2,3 and in Tables 1,2. Figs. 1,2 and 3 present the sequences of two-point Padé approximants forming, for odd k, upper and for even k – lower bounds on the Stieltjes function given by (50). The monotone sequences of $[M/M]_4$ and $[M/M]_5$ ($M = 7, 8, 9, 10$) converging to function (50) are evaluated and gathered in Table 1. Table 2 presents the positive continued fractions coefficients g_n and G_n for Padé approximant $[3/3]_k$ to the Stieltjes function (6.3). All numerical calculations performed by us confirm the theoretical predictions of Theorems 3.1.

7. Bounds on the effective modulus of micro-inhomogeneous media

As an example, the effective conductivity of microheterogeneous material consisting of equally-sized cylinders arranged in a square array has been examined. For such a composite the bulk conductivity $\lambda_e(x)$ is defined by the linear relationship between the volume-averaged temperature gradient $\langle \nabla T \rangle$ and heat flux $\langle \mathbf{J} \rangle$

$$\langle \mathbf{J} \rangle = \lambda_e(x) \langle \nabla T \rangle \;. \tag{51}$$

The averaging $\langle \,.\, \rangle$ is performed over the unit square cell. The temperature appearing in (51) satisfies the conductivity equation of the form

$$\nabla \cdot (1 + x\theta) \nabla T = 0, \tag{52}$$

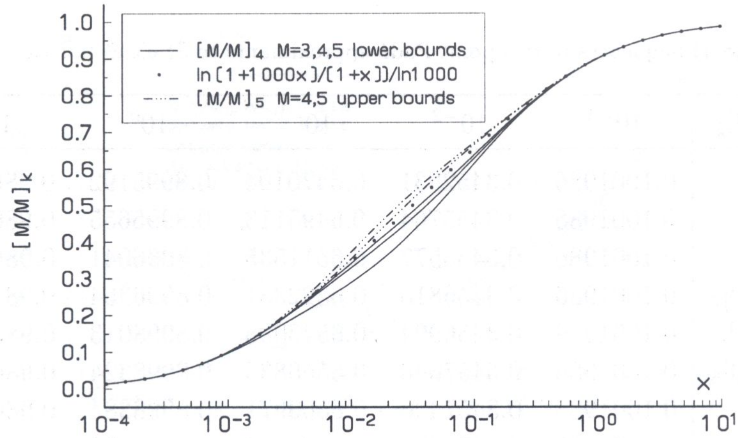

Fig. 1. Monotone sequences of two-point Padé approximants uniformly converging to Stieltjes function (6.3) for $k = 4$ and $k = 5$

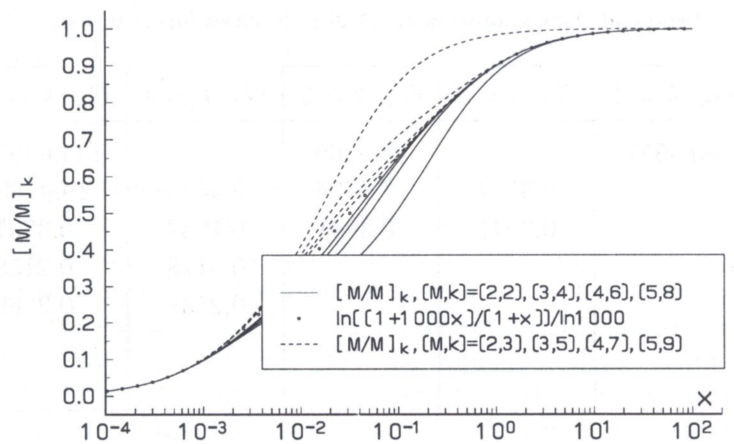

Fig. 2. Monotone sequences of two-point Padé approximants uniformly converging to Stieltjes function (6.3) for $2M - k = 1$ and $2M - k = 2$

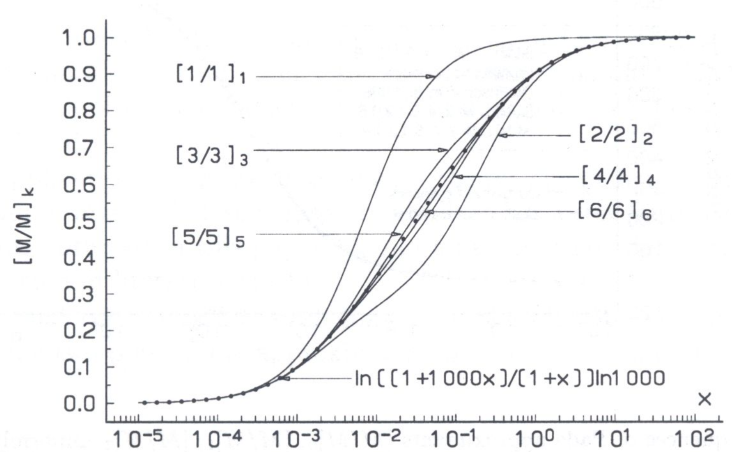

Fig. 3. Monotone sequences of two-point Padé approximants uniformly converging to Stieltjes function (6.3) for $k = M$

Table 1. Sequences of two-point Padé approximants to Stieltjes function (6.3)

$[M/M]_k$	10^{-3}	10^{-2}	10^{-1}	10^{0}	10^{1}
$[7/7]_4$	0.1001986	0.3452931	0.6470104	0.8995192	0.9862167
$[8/8]_4$	0.1001986	0.3455764	0.6495113	0.8995655	0.9862168
$[9/9]_4$	0.1001986	0.3456577	0.6511535	0.8996041	0.9862168
$[10/10]_4$	0.1001986	0.3456810	0.6522331	0.8996364	0.9862168
ex. val.	0.1001986	0.3456904	0.6543095	0.8998013	0.9862169
$[10/10]_5$	0.1001986	0.3457046	0.6556835	0.8998324	0.9862169
$[9/9]_5$	0.1001986	0.3457400	0.6563971	0.8998384	0.9862169
$[8/8]_5$	0.1001986	0.3458638	0.6574800	0.8998456	0.9862169
$[7/7]_5$	0.1001986	0.3462965	0.6591207	0.8998543	0.9862169

Table 2. Positive coefficients g_n, G_n of continued fraction (3.3) (k=1,3,5) and (3.4) (k=0,2,4,6) representing two-point Padé approximants [3/3] to Stieltjes function (6.3)

n	g_n	$G_n,\ k=1$	$G_n,\ k=2$	$G_n,\ k=3$	$G_n,\ k=4$	$G_n,\ k=5$	$G_n,\ k=6$
0		50.3657		67.5269		144.6200	
1	144.620		3.9512	12.0774	2.4608	19.9150	1.0000
2	500.500		0.2241	0.3441	0.1937	0.3737	0.1446
3	166.167				0.3178	0.2158	0.3559
4	334.332				0.2538	0.2889	0.2337
5	199.003						0.2668
6	301.496						0.2494

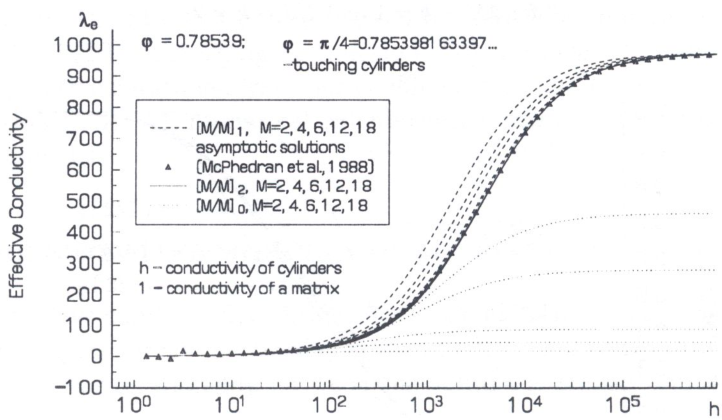

Fig. 4. Monotone sequences of Padé approximants $[M/M]_0$, $[M/M]_1$, $[M/M]_2$ uniformly converging to the effective conductivity λ_e ($h = \lambda_2/\lambda_1$) of the square array of cylinders for volume fraction $\varphi = 0.78539$. The curves $[M/M]_2$, $M = 2, 4, 6, 12, 18$ are indistinguishable (solid line). The bounds $[18/18]_2$ and $[18/18]_1$ are very restrictive

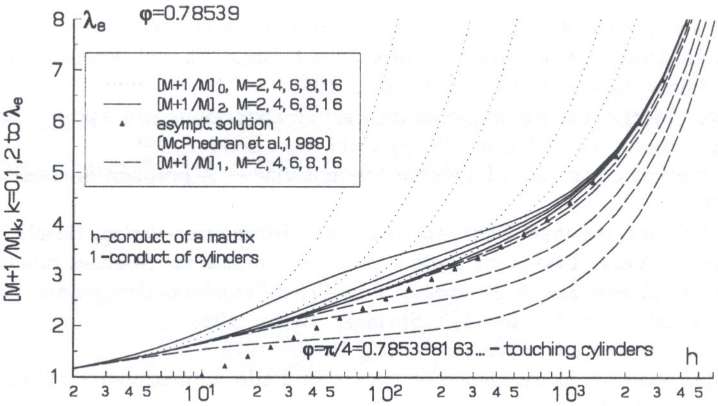

Fig. 5. Monotone sequences of Padé approximants $[M+1/M]_0$, $[M+1/M]_1$ $[M/M]_2$ uniformly converging to the effective conductivity $\lambda_e(h=\lambda_2/\lambda_1)$ of the square array of cylinders for volume fraction $\varphi = 0.78539$.

where θ is the characteristic function for cylinders. The continuity condition for the normal component of the heat current $\mathbf{J} = (1 + x\theta_2)\nabla T$ at the surfaces of the cylinders is expressed by

$$\mathbf{m} \cdot \mathbf{J}_- = \mathbf{m} \cdot \mathbf{J}_+ \, . \tag{53}$$

Here $\mathbf{m}$ is the unit vector normal to the surface of a cylinder, while $\mathbf{J}_-$ and $\mathbf{J}_+$ denote the heat currents on the inside and on the outside of the cylinder surface.

As the input data for calculation of two-point Padé approximants, the coefficients of the expansion of $\lambda_e(x)$ in powers of x have been obtained by solving the system of equations (51)–(53). The low order coefficients of the expansion of $\lambda_e(x)$ in powers of $s = 1/x$ are reported in [15]. Starting from these two series, we calculate via (44)–(47) the sequences of two-point Padé approximants $[M/M]_k$ and $[M+1/M]_k$ $(k = 0, 1, 2)$ uniformly converging to the effective conductivity $\lambda_e(x)$. The numerical results are shown in Figs. 4,5. For comparison, the asymptotic solution reported in [15] is also depicted.

8. Summary and discussion

By using the two-point continued fraction representation given by (21) or (22) the general algorithm (44)–(47) for the determination of two-point Padé approximants bounds $[M/M]_k$ on the effective transport coefficients $\lambda_e(x)$ of two-component composite materials have been proposed and tested for correctness (Figs. 1,2,3).

As an example of application to a physical problems, the set of narrowing bounds on the effective conductivity for a square array of closely spaced cylinders has been found (Figs. 4 and 5). The two-point Padé bounds obtained in this paper are more narrow than the corresponding one-point Padé estimations reported in literature [13,14].

It is worth noting that our study has been limited to the real domain only. In the future we would like to extend the two-point Padé approximants method to the complex domain as well.

Acknowledgment

This work was supported by the State Committee for Scientific Research (Poland) through the Grant No 3P40401306.

REFERENCES

[1] G.A. Baker. *Essentials of Padé Approximants.* Acad. Press, London, 1975.

[2] G.A. Baker, P. Graves–Morris. Padé Approximants. Part I: Basic Theory. *Encyclopedia of Mathematics and its Applications*, **13**, Addison–Wesley Publ. Co., London, 1981.

[3] G.A. Baker, P. Graves–Morris. Padé Approximants, Part II: Extensions and Applications. *Encyclopedia of Mathematics and its Applications*, **14**, Addison–Wesley Publ. Co., London, 1981.

[4] D.J. Bergman. The dielectric constant of a composite material — A problem in classical physics, *Phys. Report.*, **C 43**: 377–407, 1978.

[5] A. Bultheel. *Laurent Series and their Padé Approximants.* Birkhäuser-Verlag, Basel, 1987.

[6] L. Casasús, P. González–Vera. Two-point Padé type approximants for Stieltjes functions. In: C. Brezinski, A. Draux, A.P. Magnus, P. Moroni and A. Ronveaux, eds. *Proc. Polinômes Ortogonaux et Applications, Bar-le-Duc 1984, Lecture Notes in Math.*, **1171**: 408–418, Springer, Berlin, 1985.

[7] J. Gilewicz. *Approximants de Padé.* Springer–Verlag, Berlin, 1978.

[8] P. Gonzalez–Vera, O. Njåstad. Convergence of two-point Padé approximants to series of Stieltjes. J. Comp. Appl. Math., **32**: 97–105, 1990.

[9] W.B. Gragg. Truncation error bounds for T-fractions. In: E.W. Cheney, ed. *Approximation Theory III*, 455–460, Academic Press, New York, 1980.

[10] W.B. Jones, O. Njåstad, W.J. Thron. Two-point Padé expansions for a family of analytic functions. *J. Comp. Appl. Math.*, **9**: 105–123, 1983.

[11] W.B. Jones, W.J. Thron. A posteriori bound for truncation error of continued fraction. *SIAM J. Num. Anal.*, **8:** 693–705, 1970.

[12] W.B. Jones, W.J. Thron. Continued Fraction Analytic Theory and its Applications. *Encyclopedia of Mathematics and its Applications*, **11**, Addison–Wesley Publ. Co., London, 1980.

[13] S. May, S. Tokarzewski, A. Zachara, B. Cichocki. Continued fraction representation for the effective thermal conductivity coefficient of a periodic two component composite. *Int. J. of Heat and Mass Transf.*, **37**: 2165–2173, 1994.

[14] R.C. McPhedran, G.W. Milton. Bounds and exact theories for the transport properties of inhomogeneous media. *Appl. Phys. A*, 207–220, 1981.

[15] R.C. McPhedran, L. Poladian, G.W. Milton. Asymptotic studies of closely spaced highly conducting cylinders. *Proc. R. Soc. London A*, **415**: 185–196, 1988.

[16] S. Tokarzewski. Inequalities for the effective transport coefficients. *Arch. Mech.*, **46**: 611–623, 1994.

[17] S. Tokarzewski. Two-point Padé approximants for the expansions of Stieltjes functions in real domain. *J. Comp. Appl. Math.*, 1995 (in press).

[18] S. Tokarzewski, J. Bławzdziewicz, I.V. Andrianov. *Two-point Padé approximants for Stieltjes series*, IFTR Reports, 30/1993.

[19] S. Tokarzewski, J. Bławzdziewicz, I.V. Andrianov. Effective conductivity of densely packed highly conducting cylinders. *Appl. Phys.*, **A 59**: 601–604, 1994.

[20] S. Tokarzewski, J. Bławzdziewicz, I.V. Andrianov. Two-point Padé approximants for formal Stieltjes series. *Num. Algorithms*, **8**: 313–328, 1994.

[21] S. Tokarzewski, J.J. Telega. *S-continued fraction representation for effective transport coefficients of two-phase media*, IFTR Reports, 16/95.

[22] S. Tokarzewski, J.J. Telega. Inequalities for two-point Padé approximants to the expansions of Stieltjes functions in real domain (submitted).

[23] S. Tokarzewski, J.J. Telega. S-continued fraction bounds for real effective moduli of two-phase composite materials (submitted).

[24] H.S. Wall. *Analytic Theory of Continued Fractions.* New York, Van Nostrand, 1948.