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ESTIMATION OF EFFECTIVE TRANSPORT COEFFICIENTS FROM PARAMETRIC POWER SERIES

Motivation

Governing equations defining effective transport coefficients

Formulation of the approximation problem

Construction of C-Continued Fractions

Applications

Governing equations

$$f_1^{(jk)}(z) = \frac{q_{jk} - \delta_{jk}}{z} = \frac{1}{|Y|}\int_Y \Theta_2(y)\, \frac{\partial T^{(j)}(y)}{\partial y_k}\, dy, \quad z = \frac{\lambda_2}{\lambda_1} - 1$$

$$-\frac{\partial}{\partial y_j}\left(\left(1 + \Theta_2(y) z\right) \frac{\partial T^{(i)}(y)}{\partial y_j} \right) = 0 \qquad \left(y_i - T^{(i)}\right) \ \ Y - periodic$$

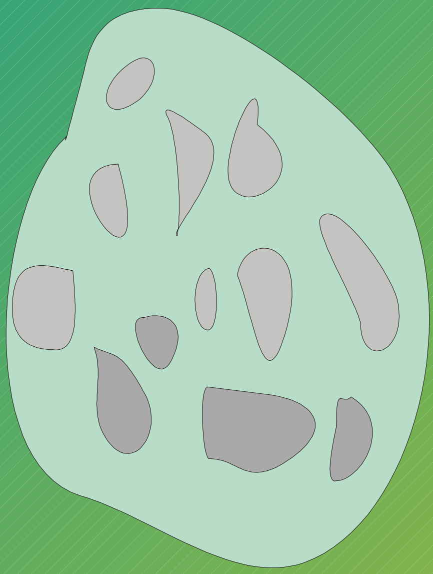
↓ Solution

$$f_1(z) = \frac{q(z) - 1}{z} = \sum_n \frac{A_n}{1 + zU_n} < \infty, \quad -1 < z =< \infty$$

$$0 \le U_n \le 1, \ \sum_n \frac{A_n}{1 - U_n} \le 1$$

↓ Stieltjes function

$$f_1(z) = \frac{q(z) - 1}{z} = \int_0^1 \frac{d\gamma(u)}{1 + zu}, \ d\gamma \ge 0$$



Two-phase material

Problem Formulation

By starting from the following power expansions of a Stieltjes function with complex coefficients

$$f_1(z) = f_1(z)_{z_j}^{p_j}, \quad z_j \in C, \quad j = 1,2,\dots,N,$$

$$f_1(z)_{z_j}^{p_j} = \sum_{i=0}^{p_j-1} c_{ij}(z-z_j)^i + O((z-z_j)^{p_j}), \quad j = 1,2,\dots,N, \quad f_1(-1) = 1$$

Power expansions

$$c_{ij} = c_i(z_j) = \frac{f_1^{(j)}(z_j)}{j!}, \quad f_1^{(i)}(z_j) = \left.\frac{d^j f_1(z)}{d^j(z)}\right|_{z=z_j}, \quad j = 0,1,\dots$$

$$z_{2(j-1)} = \alpha_{2(j-1)} + i\beta_{2(j-1)}, \quad z_{2j} = \bar{z}_{2(j-1)} = \alpha_{2(j-1)} - i\beta_{2(j-1)}$$

$$c_{kj} = \bar{c}_{k(j-1)}$$

Input data are complex conjugated

we find the best estimations of the effective transport coefficients valid in a complex domain

Basic equations

Padé inclusion regions

$$\left(\sum_{n=1}^{P/2}\frac{\Lambda_n(\alpha,\beta)}{1+zU_n(\alpha,\beta)}+\frac{\alpha}{1+\beta z}\right)_{z_1,z_2,\dots,z_N,-1}^{p_1,p_2,\dots,p_N,-1}=f_1(z)_{z_1,z_2,\dots,z_N,-1}^{p_1,p_2,\dots,p_N,-1}$$

$$0\le U_n(\alpha,\beta)\le 1,\quad \Lambda_n(\alpha,\beta)>0$$

Multipoint continued fraction expansion method

$$f_1(z)=\cfrac{f_1(x_1)}{1+\cfrac{(z-x_1)f_2(x_2)}{1+\cfrac{(z-x_2)f_3(x_2)}{1+\cfrac{(z-x_2)f_4(x_3)}{\ddots\,\cfrac{}{1+w_P(z-x_N)\cfrac{\alpha' z}{1+\beta' z}}}}}},\quad 0\le\alpha'\le 1,\quad \beta'=1-\alpha'$$

Method of solution

We start from the following linear fractional transformations

$$zf_1(z) = z_1 f_1(z_1) + \frac{f_1(z_1)(z-z_1)}{1+z\Theta_2 f_2(z)}, \qquad zf_2(z) = z_2 f_2(z_2) + \frac{f_2(z_2)(z-z_2)}{1+z\Theta_3 f_3(z)}, \; \dots,$$

$$zf_j(z) = z_j f_j(z_j) + \frac{f_j(z_j)(z-z_j)}{1+z\Theta_{j+1} f_{j+1}(z)}, \dots \qquad zf_N(z) = z_N f_N(z_N) + \frac{z_N f_N(z_N)(z-z_N)}{1+z\Theta_{N+1} f_{N+1}(z)},$$

where the coefficients Θ_k are chosen in such a way that

$$f_j(-1) = 1, \quad j - 1, 2, \dots, N+1.$$

It follows

$$zf_1(z) = z_1 f_1(z_1) + \cfrac{f_1(z_1)(z-z_1)}{1+z_2\Theta_2 f_2(z_2) + \cfrac{\Theta_2 f_2(z_2)(z-z_2)}{1+z_3\Theta_3 f_3(z_3) + \cfrac{\Theta_3 f_3(z_3)(z-z_3)}{1+z_4\Theta_4 f_4(z_4) + \cfrac{\Theta_4 f_4(z_4)(z-z_4)}{\ddots \cfrac{}{1+\Theta_{N+1} z \cfrac{\alpha' z}{1+\beta' z}}}}}}$$

Main property of C-continued fraction to effective transport coefficient

If $f_1(z)$ *is a Stieltjes function given by*

$$f_1(z) = \int_0^1 \frac{d\gamma_1(u)}{1+zu},\ d\gamma_1 \geq 0,\ f_1(-1) \leq 1$$

then $f_{N+1}(z)$ *appearing in*

$$zf_1(z) = \mathop{V}_{k=1}^{N}\left(z_k f_k(z_k) + \frac{z_k f_k(z_k)(z-z_k)}{1+\Theta_k} \times \right) zf_{N+1}(z)$$

is also a Stieltjes function

$$f_{N+1}(z) = \int_0^1 \frac{d\gamma_{N+1}(u)}{1+zu},\ d\gamma_{N+1} \geq 0,\ f_{N+1}(-1) \leq 1,$$

provided that

$$f_j(-1) = 1,\ z_{2j} = \bar{z}_{2(j-1)},\ \ j = 1,2,\ldots,N+1$$

Proof

$$zf_1(z) = z_1 f_1(z_1) + \cfrac{f_1(z_1)(z - z_1)}{1 + z_2\Theta_2 f_2(z_2) + \cfrac{\Theta_2 f_2(z_2)(z - z_2)}{1 + z\Theta_3 f_3(z)}}, \; z_2 = \bar{z}_1, \; f_1(-1) = f_2(-1) = f_3(-1) = 1$$

Without loss of generality we assume that

$$f_1(z) = \sum_{j=1}^{K-1} \frac{C_{1j}}{1 + zU_{1j}}, \;\; C_{1j} \geq 0, \, 0 \leq U_{1j} \leq 1$$

Then it follows that

$$f_3(z) = \sum_{j=1}^{K-2} \frac{C_{2j}}{1 + zU_{2j}}, \;\; C_{2j} \geq 0,$$

$$U_{1j} \leq U_{2j} \leq U_{1j}$$

Example

$$f_1(z) = \frac{0.09195402299}{1+0.5000000000z} + \frac{0.2758620690}{1+0.3333333333z} + \frac{0.3218390805}{1+0.2000000000z}$$

$$f_3(z) = \frac{0.2185277373}{1+0.4785356557z} + \frac{0.4199383519}{1+0.2771329970z}$$

Comments to proof

I. From the following relations

$$f_3(z) = \frac{B(z) + z_1 B(z) B(z_1) - B(z_1) - z_1 (B(z_1))^2}{-zB(z) + z_1 B(z) f_1(z_1) - z_1 B(z_1) - z_1 (B(z_1))^2},$$

$$B = \frac{f_1(z) + z_1 f_1(z) f_1(z_1) - f_1(z_1) - z_1 (f_1(z_1))^2}{-zf_1(z) + z_1 f_1(z) f_1(z_1) - z_1 f_1(z_1) - z_1 (f_1(z_1))^2},$$

It follows at once

$$\textit{if} \;\; f_1(z) = [m/m], [m-1/m] \;\; \textit{then} \;\; f_3(z) = [m-1/m-1], [m-2/m-1]$$

II. By solving the equations

$$f_3(z) = \infty \quad \textit{and} \quad f_3(z) = 0$$

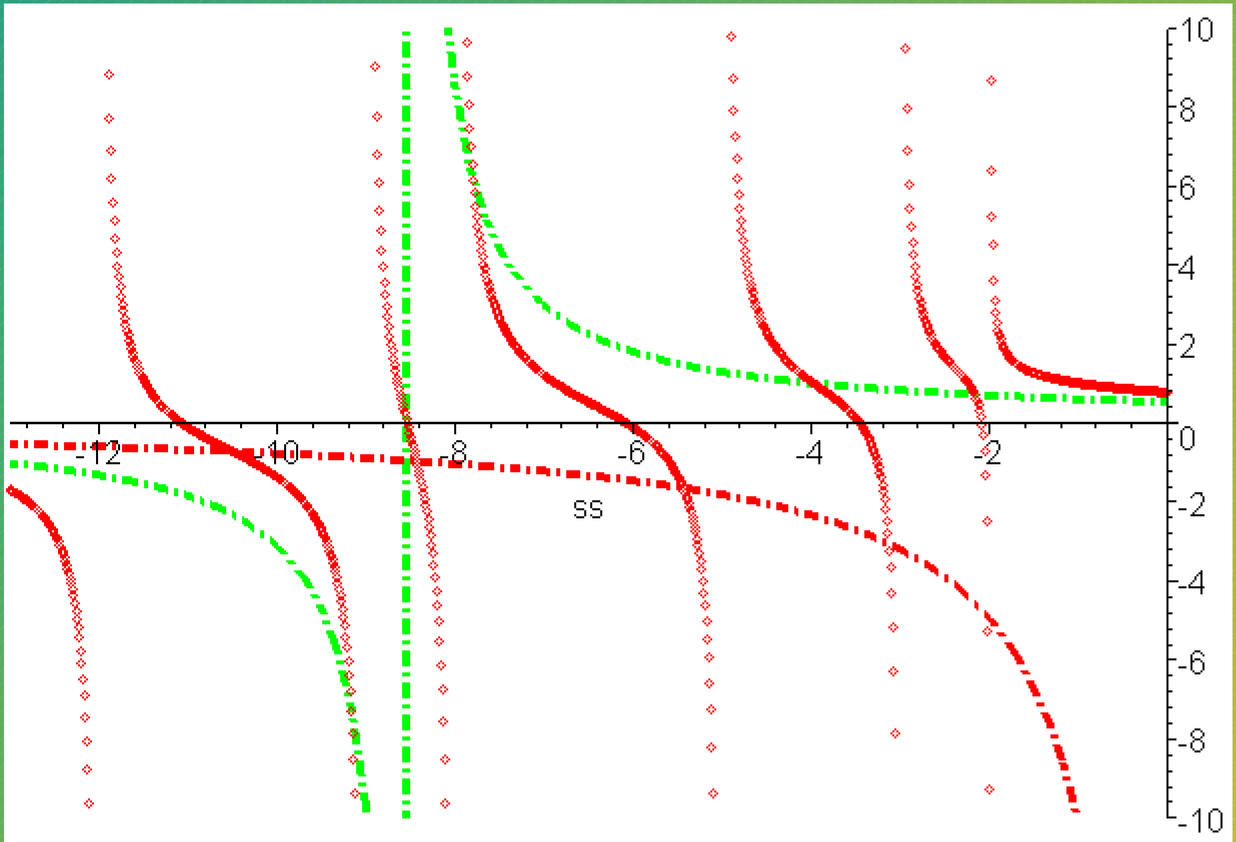
we arrive to the equalities

$$f_1(z) = \frac{-(ad - bc)}{b} + \frac{d(a^2 + b^2)}{zb}, \quad f_1(z) = \frac{(d^2 + c^2)}{-ad + zb + bc}$$

where

$$z_1 = a + ib, \quad z_2 = a - ib, \quad f_1(z_1) = c - id, \;\; f_1(z_2) = c + id, \;\; bd \geq 0$$

Final conclusion

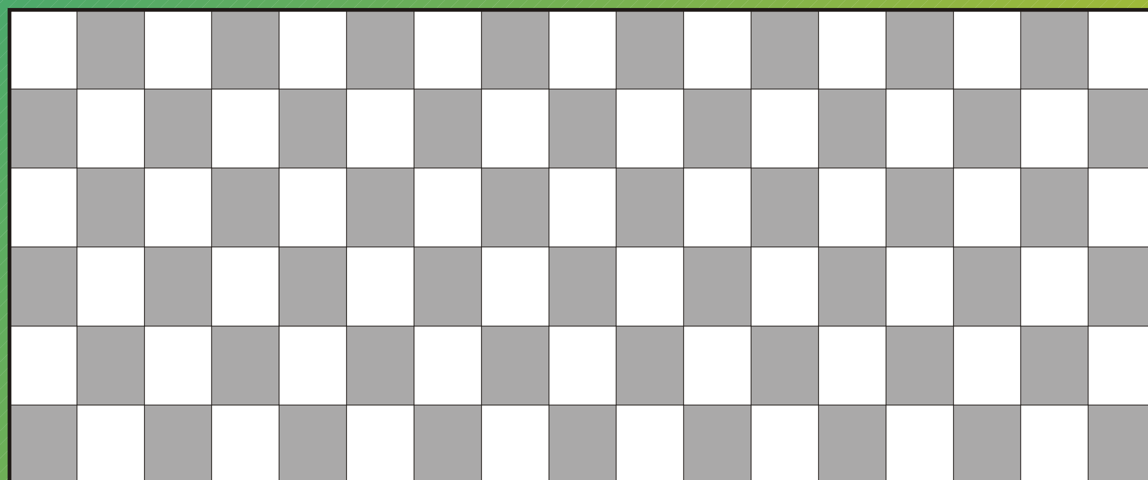


Roots of $f_3(z)$ lie between poles of $f_3(z)$. They are real and negative

Applications

$$f_1(z) = \frac{\sqrt{z+1}-1}{z}, \quad z = 1 - \frac{i}{\omega},$$

$$\omega_1 = \frac{1}{1000}, \quad \omega_3 = \frac{1}{50}, \quad \omega_5 = \frac{1}{10}, \quad \omega_7 = 10$$



Chekerboard

Local estimation

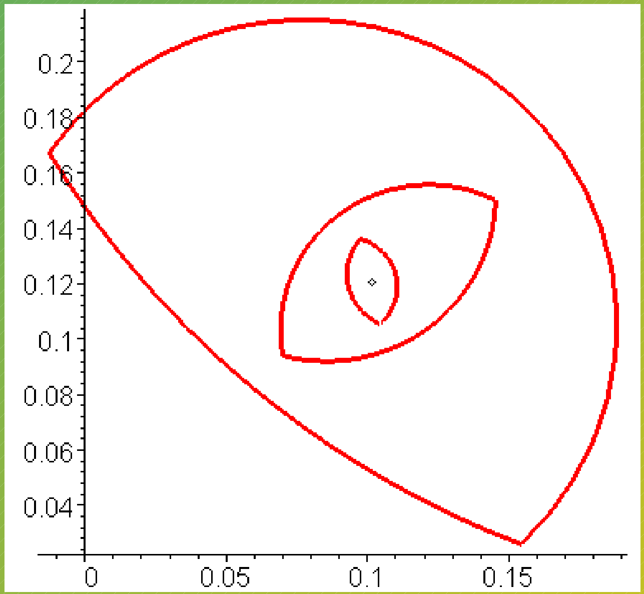
Complex input data

$$z_1=5+i3,\ \ z_3=7+i5,\ \ z_5=9+i8$$

$$f_1(z_1)=0.2761-i0.0467,\ \ f_1(z_3)=0.2419-i0.0518,\ \ f_1(z_5)=0.2129-i0.0576$$

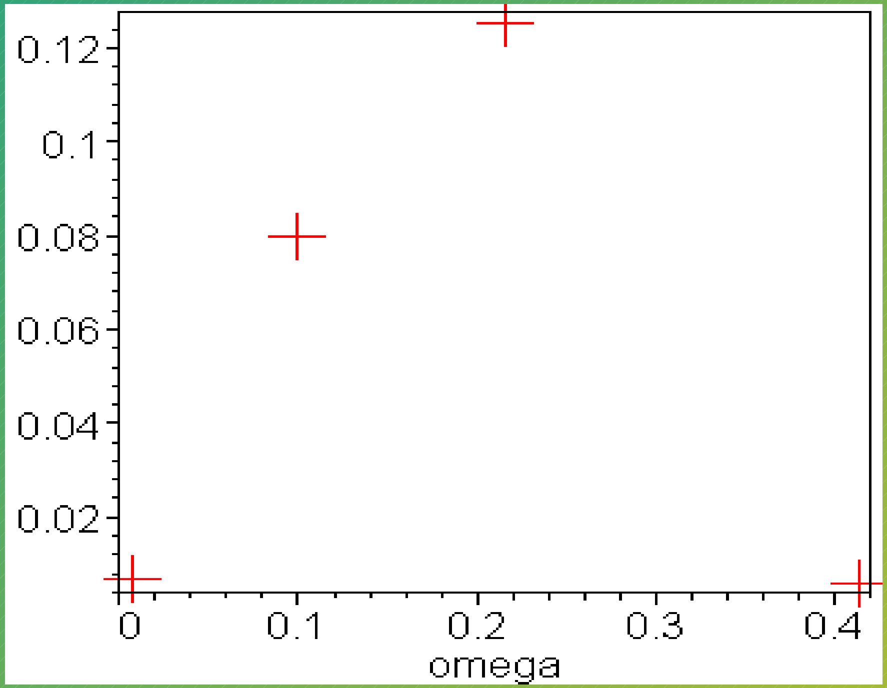
$$z_0=-15-i\,30$$

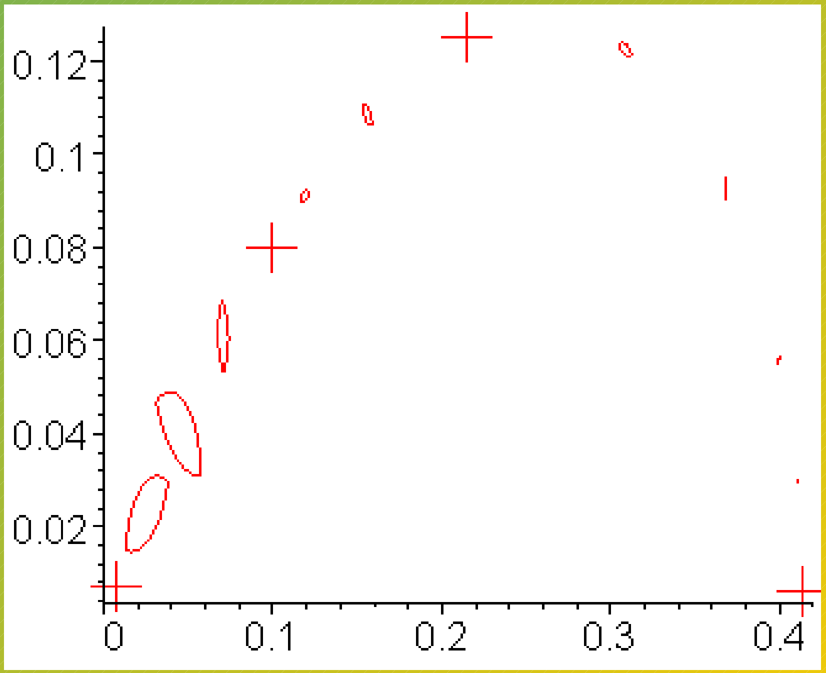
Complex bounds



Estimation from experimental data

	$f_1(z(\omega))$
ω_1	0.0070710578 - i 0.0069710678
ω_3	0.0996209331 - i 0.0800271716
ω_5	0.2150064827 - i 0.1254612822
ω_7	0.4140490983 - i 0.0060606072





Estimation of volume fraction

	$f_1(z(\omega))$
ω_1	0.0070710578 - i 0.0069710678
ω_3	0.0996209331 - i 0.0800271716
ω_5	0.2150064827 - i 0.1254612822
ω_7	0.4140490983 - i 0.0060606072

Lower bound	Exact value	Upper bound
0.1394492440	0.5000000000	0.9860550757
0.1758834168	0.5000000000	0.8241165830
0.3742922409	0.5000000000	0.6257077586
0.4962668372	0.5000000000	0.5037331625

Conclusions

1. **The C-Multipoint Continued Fraction Method incorporate into the estimates of the effective transport coefficients of composite matrials the truncated power series expanded at arbitrary number of complex points.**
2. **The CMCFM are especially suited for implementation as a fast, accurate, numerical algorithms, since they are simply recursive and do not involve the solutions of a large number of a coupled equations**
3. **The complex bounds derived by CMCFM are the best over the input data represented by the several truncated power series with complex coefficients**
4. **The CMCFM are especially suited for experimental investigations**