Over-deterministic method: The influence of rounding numbers on the accuracy of the values of Williams' expansion terms

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ABSTRACT. A study on the accuracy of the values of Williams' expansion terms influenced by rounding numbers is presented. The results are presented taking into account a three-point bend single edge notched beam. Crack tip stress tensor components are expressed using the linear elastic fracture mechanics (LEFM) theory in this work, more precisely via its multi-parameter formulation, i.e. by Williams' power series (WPS). Determination of the coefficients of the terms of this series is performed using the least squares-based regression technique known as the over-deterministic method (ODM), for which displacements data obtained numerically in software ANSYS are taken as inputs. The values of Williams' expansion terms based on the displacement data obtained are calculated by using various levels of rounding numbers and the results are compared and discussed.

KEYWORDS. Over-deterministic method; Rounding numbers; Williams' expansion; Fracture mechanics; Stress field.

INTRODUCTION

Sometimes it is necessary to describe the crack-tip stress field by means of more than only one singular term (the well-known stress intensity factor, see e.g. [1-4] or two-parameter fracture mechanics, see e.g. [5-10]) of Williams' expansion (WE). It has been shown that so-called multi-parameter fracture mechanics can be helpful when the fracture process occurs in the more extensive surroundings of the crack tip, see for material like concrete [11-19]. Then, a particular number of the WE terms needs to be taken into account for a more complex fracture analysis. In this paper, the focus is devoted to investigations into the accuracy of the higher-order terms of the WE when various types of rounding

numbers are considered. There exist various kinds of software that enable to calculate higher-order terms of the WE, see [20-22]. For each of them a specific accuracy of the numbers used is defined, which can play a key role when the WE terms are calculated.

The analysis presented deals with various numbers of the decimal places that are considered in the calculations of the WE terms and brings practical recommendations how the analysis should be performed in order to obtain accurate results.

THEORETICAL BACKGROUND

Fracture mechanics: Williams' expansion

As it has been mentioned, the paper is based on the idea that the near crack-tip stress field tensor components are approximated via Williams' expansion [23] that was originally derived for a homogeneous elastic isotropic cracked body subjected to arbitrary remote loading and is expressed via the infinite power series for loading mode I as follows:

$$\sigma_{ij} = \sum_{n=1}^{\infty} \frac{n}{2} r^{\frac{n}{2}-1} A_n f_{\sigma_{ij}}(\theta, n), \quad \text{where} \quad i,j \in \{x,y\}. \tag{1}$$

The meaning of the symbols used in Eq. 1 can be described in the following way: (r, θ) are polar coordinates centred at the crack tip; $f_{\sigma_{ij}}$ are known functions corresponding to the stress distribution; the symbols A_n correspond to the unknown coefficients of Williams' expansion terms (this is to emphasize that their values depend on the specimen geometry, relative crack length α and loading conditions).

Over-deterministic method

When the effect of rounding numbers is investigated, the over-deterministic method is assumed to be used for determination of various numbers of the WE terms [24]. This method is based on the least-squares technique and was used as one of the methods that do not require any special crack elements or implementation of other difficult fracture mechanics concepts. The method uses the displacement field estimated around the crack tip via the finite element method and together with the polar coordinates of the nodes, where the displacements are investigated, a system of linear equations is solved according to the definition:

$$u_i = \sum_{n=0}^{\infty} r^{n/2} A_n f_i^u(\theta, n, E, \nu), \quad \text{where} \quad i \in \{x,y\}. \tag{2}$$

When the k number of nodes is investigated, then $2k$ of displacements (u and v) can be used and $2k$ of equations can be formed in the following way [24]:

$$
\begin{bmatrix}
u_1 \\ u_2 \\ \vdots \\ u_k \\ v_1 \\ v_2 \\ \vdots \\ v_k
\end{bmatrix}
=
\begin{bmatrix}
f_{r0}^u(r_1,\theta_1) & f_{r1}^u(r_1,\theta_1) & \cdots & f_{rN}^u(r_1,\theta_1) \\
f_{r0}^u(r_2,\theta_2) & f_{r1}^u(r_2,\theta_2) & \cdots & f_{rN}^u(r_2,\theta_2) \\
\vdots & \vdots & \vdots & \vdots \\
f_{r0}^u(r_k,\theta_k) & f_{r1}^u(r_k,\theta_k) & \cdots & f_{rN}^u(r_k,\theta_k) \\
f_{r0}^v(r_1,\theta_1) & f_{r1}^v(r_1,\theta_1) & \cdots & f_{rN}^v(r_1,\theta_1) \\
f_{r0}^v(r_2,\theta_2) & f_{r1}^v(r_2,\theta_2) & \cdots & f_{rN}^v(r_2,\theta_2) \\
\vdots & \vdots & \vdots & \vdots \\
f_{r0}^v(r_k,\theta_k) & f_{r1}^v(r_k,\theta_k) & \cdots & f_{rN}^v(r_k,\theta_k)
\end{bmatrix}
\begin{bmatrix}
A_0 \\ A_1 \\ \vdots \\ A_N
\end{bmatrix}
\tag{3}
$$

The solution of the system of the equation can be written as:

$$[X] = \left([C]^{\mathrm{T}}[C]\right)^{-1}[C]^{\mathrm{T}}[U] \tag{4}$$

It is always necessary to prescribe the number of the terms of the WE terms, *N*, that shall be calculated. This is also one of the parameters that is varied in the analysis presented.

Data structure used in common software

Nowadays, most personal computers used for calculation of mathematical tasks are constructed by 32 or 64 bit data architecture, see [25, 26], i.e. 4 or 8 Bytes are used for one number. For representation of numbers, mathematical software can use a structure with or without a floating point. Counting with numbers without a floating point is not usable for very low and very high numbers, especially with some decimal numbers. For counting with decimal numbers, it is necessary to use a data structure with a floating point; it gives maximally 15 decimal numbers plus an exponent in 64 bit data architecture or only 6 decimal numbers in 32 bit data architecture. For this reason, all the common software (e.g. Maple [20], Matlab [21], Mathematica [22],) uses the data structure with a floating point or a special data structure to extend the count of decimal numbers. One of the methods how to increase the count of decimal numbers is to convert the original number to a string of characters and then to carry out calculating with strings in specially programmed procedures.

NUMERICAL EXAMPLE OF 3PB

For the analysis a very simple model of a three-point-bending specimen was used, see Fig. 1. The detailed geometry can be found in [27, 28] ($c = 0.2$ mm, $D = 1$ mm, $P = 1$ N). Because of the symmetry, only one half of the specimen could be modelled in order to obtain a set of displacement data at the distance of 0.1 mm from the crack tip.
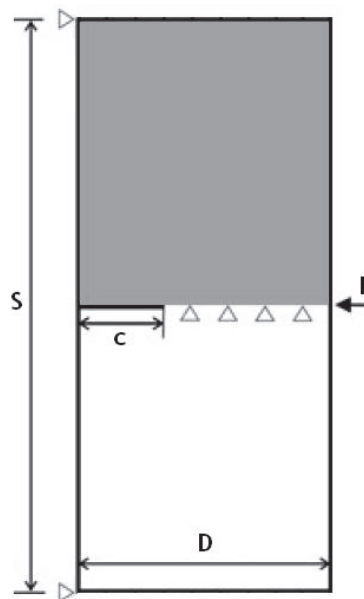

Figure 1: Schema of the three-point-bending specimen used for the analysis presented.

The data of the displacement vector obtained from the ANSYS finite element software [29] can be found in Tab. 1. The values introduced in the referred table were used as inputs for Eq. 3 and 4 respectively.

RESULTS AND DISCUSSION

The main goal was to validate the ODM concept in order to obtain a reliable procedure for further analysis of the stress field near the crack tip in civil engineering materials. Therefore, a basic cracked specimen configuration (3PB) has been investigated and higher-order terms coefficients estimated. Data comparison can be found in Tab. 2. Note that only the first five terms are mostly available in literature [27, 28, 30]. It can be seen in Tab. 2 that the coefficients calculated by means of the ODM correspond very well with the data published in literature.

Nr.	Node Nr.	Radius [mm]	Theta [deg]	u [mm]	v [mm]
1	2	0.1	0	-27.077	0.0000
2	13	0.1	9	-27.066	0.0639
3	14	0.1	18	-27.034	0.1325
4	15	0.1	27	-26.984	0.2100
5	16	0.1	36	-26.919	0.3000
6	17	0.1	45	-26.843	0.4072
7	18	0.1	54	-26.765	0.5292
8	19	0.1	63	-26.688	0.6691
9	20	0.1	72	-26.618	0.8250
10	21	0.1	81	-26.564	0.9945
11	12	0.1	90	-26.529	1.1737
12	97	0.1	99	-26.517	1.3584
13	98	0.1	108	-26.534	1.5431
14	99	0.1	117	-26.581	1.7226
15	100	0.1	126	-26.659	1.8915
16	101	0.1	135	-26.768	2.0460
17	102	0.1	144	-26.906	2.1766
18	103	0.1	153	-27.069	2.2843
19	104	0.1	162	-27.253	2.3634
20	105	0.1	171	-27.449	2.4105
21	87	0.1	180	-27.651	2.4236

Table 1: The displacements and polar coordinates of the selected nodes around the crack tip obtained from the ANSYS finite element software.

3PB	[27]	[28]	Data calculated
A_1	1.8530	1.8538	1.8538
A_2	-0.3533	-0.3527	-0.3527
A_3	-0.7149	-0.7202	-0.7202
A_4	-0.0896	-0.1019	-0.1019
A_5	-1.3717	-1.3565	-1.3565

Table 2: Higher-order terms coefficients determined by means of the ODM in comparison to data published in literature for 3PB, see [27, 28].

On the basis of PHP software [31] the special software tool was programmed considering various levels of rounding numbers in order to analyze how many decimal numbers are needed to obtain precise values of WE terms. The software was based on the idea of representation of numbers by means of strings. The values of the WE terms were calculated step by step assuming two changing parameters: the level of rounding numbers and the number of calculated WE terms.
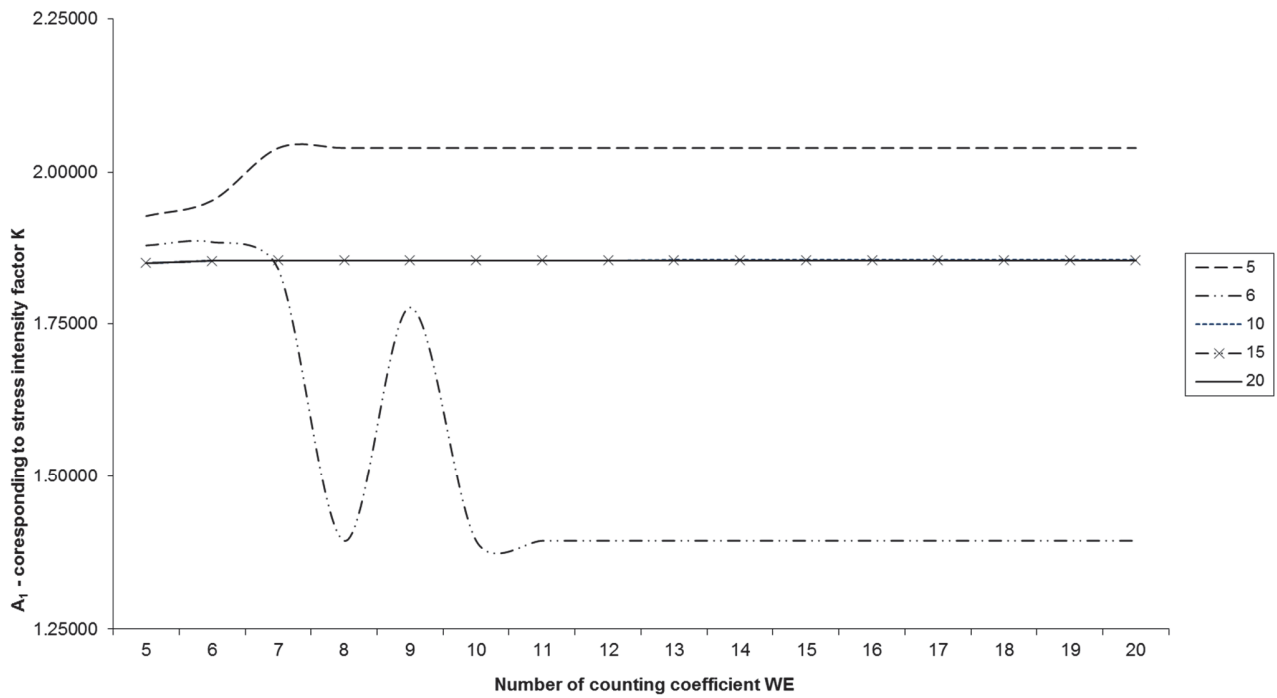
Figure 2: Dependence of A_1 corresponding to the stress intensity factor on the number of the WE terms considered for various numbers of the decimal places taken into account during the analysis.
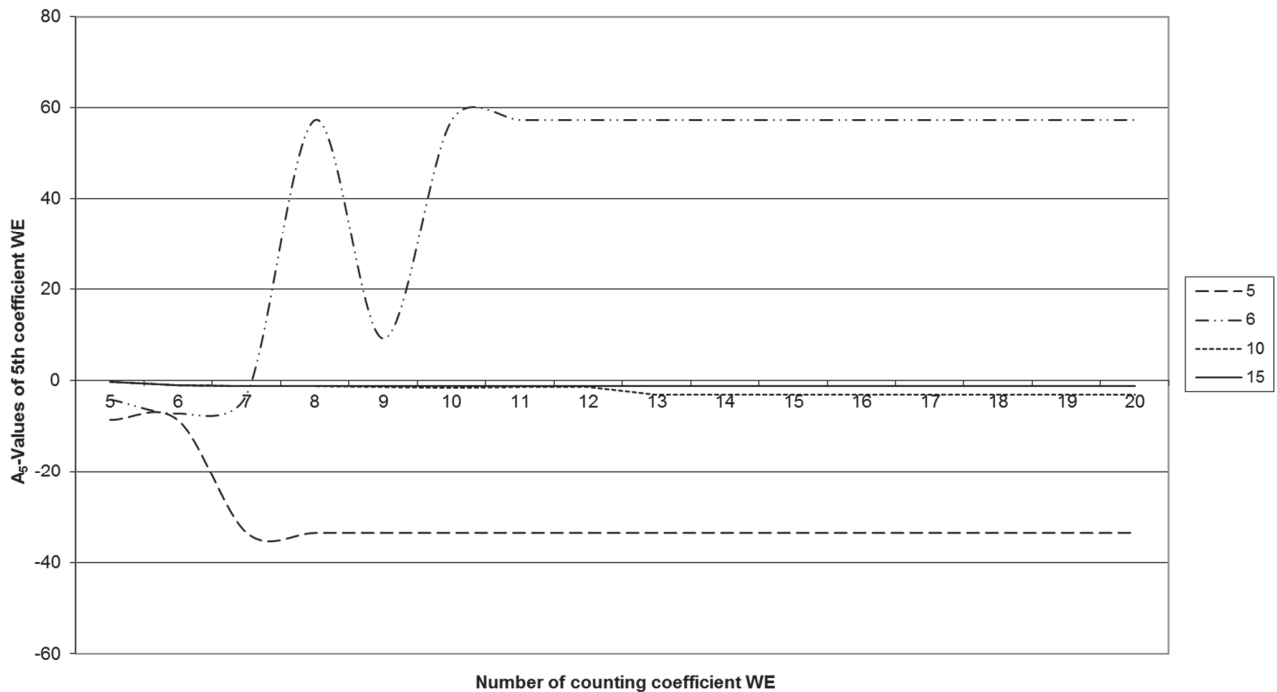

Figure 3: Dependence of the 5th WE term on the number of the WE terms considered for various numbers of the decimal places taken into account during the analysis.

Several phenomena can be observed from the investigation. For example the first coefficient A_1 (corresponding to the stress intensity factor K) differs significantly when 5, 6 or 10 decimal numbers are taken into account and these values are nearly independent of the number of the WE terms calculated (the minimum counted values were 5, the maximum 20), see Fig. 2.

Similar dependences can also be observed for other values of the WE terms of higher-orders. It holds that the level of rounding numbers is more important when the analysis for a higher index of the WE terms coefficients is performed. For example, A_5 (the 5th coefficient of WE) does not seem to be precise enough until 15 decimal numbers are considered within the counting numbers (see Fig. 3); and A_{10} (the 10th coefficient) needs rounding by 20 decimal numbers, see Fig. 4.
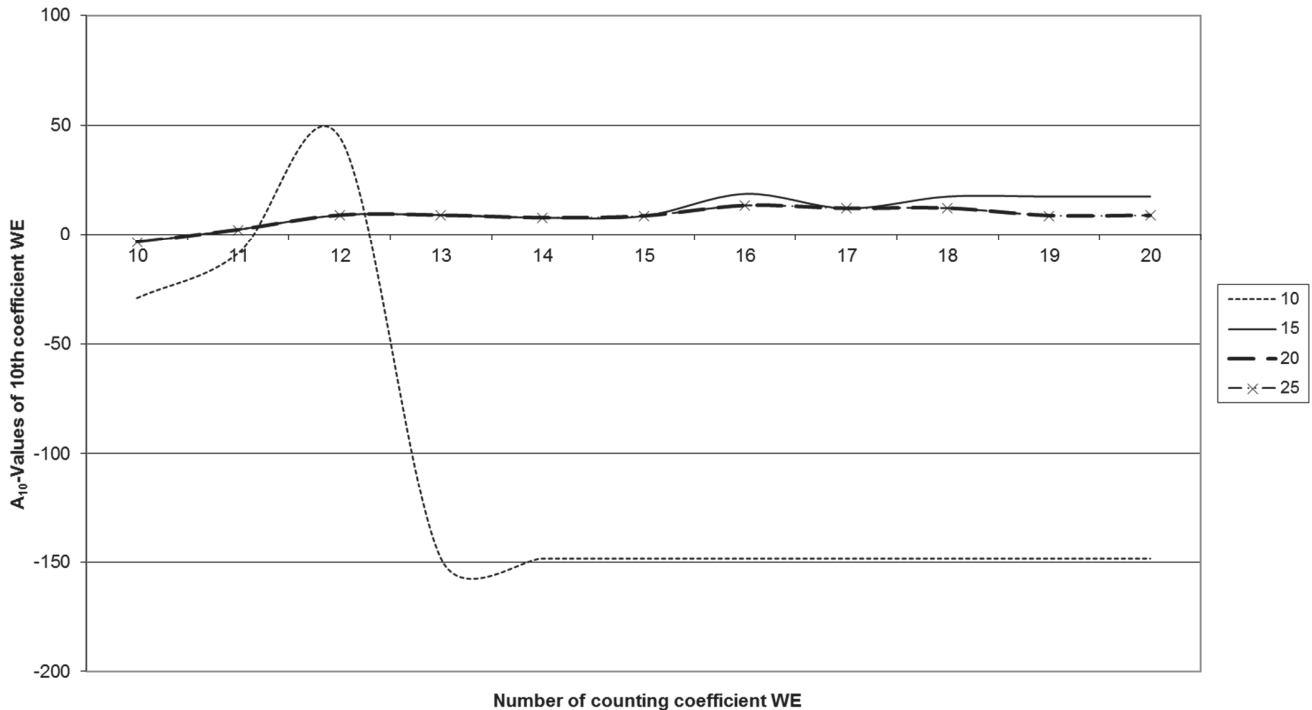

Figure 4: Dependence of the 10th WE term on the number of the WE terms considered for various numbers of the decimal places taken into account during the analysis.

A similar trend is also expected for the coefficients of the WE terms of higher orders: the higher index of the WE term, the higher number of decimal places needed. Simultaneously it holds that more WE terms need to be considered during the analysis when the coefficient of the WE term of some higher-order is required.

CONCLUSIONS

S pecial computing software tool based on the concept of representation of numbers by means of strings was developed which enables to calculate with numbers with up to 100 or 200 decimal places. The software was used in order to perform an extended analysis dealing with the influence of rounding numbers on the accuracy of the WE terms coefficients determined via the over-deterministic method. The results show that it is enough to use numbers with up to 20 decimal characters to obtain good results for 10 initial coefficients of Williams' expansion.
A final conclusion/recommendation based on the research presented can be stated: the higher number of the coefficients of WE terms is requested, the higher number of decimal places used within rounding numbers is needed.

ACKNOWLEDGEMENT

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