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Stepsize Control for Cubic Spline Interpolation

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Abstract Numerical algorithms which include a stepsize are affected by a global error, which consists of both a truncation error and a round-off error. In these algorithms as the stepsize decreases, the truncation error also decreases, but the round-off error may increase. The problem is now to find the stepsize which minimizes the global error. In this paper, by using the CESTAC method and the CADNA library a procedure is proposed to control the stepsize for determining interpolating cubic spline functions. Some numerical experiments are given to show the effectiveness of the proposed procedure.

Keywords Cubic spline · stepsize · CESTAC method · DSA · CADNA library.

Mathematics Subject Classification (2000) 65D07 · 65G50.

1 Introduction

Finite precision computations may affect the stability of algorithms and the accuracy of computed solutions. In fact, the numerical result provided by an algorithm is affected by a global error, which consists of both a truncation error and a round-off error. Computation of the solution of many problems in scientific computing involves a stepsize h. As h decreases, the truncation error also decreases, but the round-off error in the method may increase. Here, the problem is to find the optimal stepsize h_{opt} which minimizes the global error. In general, it is difficult to estimate the optimal stepsize in an algorithm.

In [4], Chesneaux and Jézéquel showed that by using the CESTAC (Contrôle et Estimation Stochastique des Arrondis de Calcul) method [20,19] and the CADNA (Control of Accuracy and Debugging for Numerical Application) library [2,3,17], one can estimate the optimal stepsize for the numerical computation of integrals using the trapezoidal and Simpson's rules. Then, Abbasbandy and Araghi [1] developed this method to general closed Newton-Cotes integration rules. The development of the method to multiple integrals can be found in [12]. In [14], Salkuyeh et al. proposed a procedure with stepsize control for solving n one-dimensional initial value problems. In this paper, a procedure is presented to control the stepsize for the cubic spline interpolations with equally spaced knots.

This paper is organized as follows. In section 2, some new results on the cubic splines are given. Section 3 is devoted to main results for definition of the procedure. A brief review of the CESTAC

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method, the DSA and the CADNA library is given in Section 4. In section 5, some numerical experiments are given. Section 6 is devoted to some concluding remarks.

2 Some results on the cubic splines

Let f be a real-valued function defined on $[a, b]$ and $\mathbf{T}_n = \{a = x_0 < x_1 < x_2 < \ldots < x_{n-1} < x_n = b\}$ be a partition of $[a, b]$ with equally spaced knots and stepsize h. Let S_n be the *clamped* interpolating cubic spline function on the partition $\mathbf{T}_n$ satisfying $S_n(x_i) = f(x_i) = f_i$, $i = 0, 1, \ldots, n$, and

$$S'_n(x_0) = f'(x_0), \quad S'_n(x_n) = f'(x_n). \tag{1}$$

It can be seen that (see [15, 9])

$$S_n(x) = \alpha_j + \beta_j(x - x_j) + \gamma_j(x - x_j)^2 + \delta_j(x - x_j)^3, \quad x \in [x_j, x_{j+1}], \tag{2}$$

where

$$\alpha_j = f_j, \quad \beta_j = \frac{f_{j+1} - f_j}{h} + \frac{2M_j + M_{j+1}}{6}h, \quad \gamma_j = \frac{M_j}{2}, \quad \delta_j = \frac{M_{j+1} - M_j}{6h},$$

in which M_j's satisfy

$$\begin{pmatrix} 2 & 1 & & & 0 \\ 1 & 4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 4 & 1 \\ 0 & & & 1 & 2 \end{pmatrix} \begin{pmatrix} M_0 \\ M_1 \\ M_2 \\ \vdots \\ M_n \end{pmatrix} = \begin{pmatrix} d_0 \\ d_1 \\ d_2 \\ \vdots \\ d_n \end{pmatrix}, \tag{3}$$

such that

$$d_j = \frac{6}{h^2}(f_{j+1} - 2f_j + f_{j-1}), \quad j = 1, 2, \ldots, n-1,$$
$$d_0 = \frac{6}{h}(\frac{f_1 - f_0}{h} - f'(x_0)), \quad d_n = \frac{6}{h}(f'(x_n) - \frac{f_n - f_{n-1}}{h}).$$

It is well-known that, if $f \in C^2[a, b]$, then $S''_n(x)$ tends to $f''(x)$ as h tends to zero for all $x \in [a, b]$, and

$$E_n := \int_a^b (f''(x) - S''_n(x))^2 dx = \int_a^b f''(x)^2 dx - \int_a^b S''_n(x)^2 dx \geq 0, \tag{4}$$

where equality holds if and only if $f = S_n$ (see [8, 13, 15]). Therefore, the evaluation of E_n would be very useful, because it may help us to state a stopping criterion for choosing suitable n. Hence, we are going to investigate how this difference depends on the stepsize h. We begin with the following theorem.

Theorem 1 *Let S_n be the clamped cubic spline interpolating f. Then*

$$\int_a^b S''_n(x)^2 dx = \frac{h}{3}(M_0^2 + 2\sum_{j=1}^{n-1} M_j^2 + M_n^2 + \sum_{j=0}^{n-1} M_j M_{j+1}).$$

Proof From (2), one can see that

$$S''_n(x) = M_j \frac{x_{j+1} - x}{h} + M_{j+1} \frac{x - x_j}{h}, \quad \forall x \in [x_j, x_{j+1}].$$

By this relation it is easy to see that

$$\int_{x_j}^{x_{j+1}} S''_n(x)^2 dx = \frac{h}{3}(M_j^2 + M_j M_{j+1} + M_{j+1}^2).$$

Therefore

$$\int_a^b S_n''(x)^2 dx = \sum_{i=0}^{n-1} \int_{x_j}^{x_{j+1}} S_n''(x)^2 dx = \frac{h}{3}(M_0^2 + 2\sum_{j=1}^{n-1} M_j^2 + M_n^2 + \sum_{j=0}^{n-1} M_j M_{j+1}).$$

This completes the proof. □

Theorem 2 *Let f be a sufficiently smooth function and S_n be the clamped cubic spline interpolating f. Then*

$$\int_a^b f''(x)^2 dx = \int_a^b S_n''(x)^2 dx + \frac{b-a}{720}(f^{(4)}(c))^2 h^4 + \mathcal{O}(h^6), \tag{5}$$

for some c in $[a, b]$.

Proof It is easy to see that (see [15, page 140])

$$\int_a^b (f''(x) - S_n''(x))^2 dx = \int_a^b (f(x) - S_n(x)) f^{(4)}(x) dx. \tag{6}$$

For the sake of simplicity, let $g(x) = (f(x) - S(x))f^{(4)}(x)$. By the Euler-Maclaurin formula [15, page 156] we have

$$\begin{aligned}\int_{x_i}^{x_{i+1}} g(x)dx = &\frac{h}{2}(g(x_i) + g(x_{i+1})) - \frac{h^2}{12}(g'(x_{i+1}) - g'(x_i)) + \frac{h^4}{720}(g^{(3)}(x_{i+1}^-) - g^{(3)}(x_i^+)) \\ &-\frac{h^6}{30240}(g^{(5)}(x_{i+1}^-) - g^{(5)}(x_i^+)) + \mathcal{O}(h^8).\end{aligned} \tag{7}$$

Obviously, $g(x_i) = g(x_{i+1}) = 0$. We now recall that (see [16, page 121] and [9, page 487])

$$f'(x_j) = S_n'(x_j) + \frac{1}{180}h^4 f^{(5)}(x_j) + \mathcal{O}(h^6), \quad j = i, i+1, \tag{8}$$

$$f''(x_j) = S_n''(x_j) + \frac{1}{12}h^2 f^{(4)}(x_j) + \mathcal{O}(h^4), \quad j = i, i+1, \tag{9}$$

$$f^{(3)}(x_i) = S_n^{(3)}(x_i^+) - \frac{h}{2}f^{(4)}(x_i) - \frac{h^2}{12}f^{(5)}(x_i) + \mathcal{O}(h^4), \tag{10}$$

$$f^{(3)}(x_{i+1}) = S_n^{(3)}(x_{i+1}^-) + \frac{h}{2}f^{(4)}(x_{i+1}) - \frac{h^2}{12}f^{(5)}(x_{i+1}) + \mathcal{O}(h^4). \tag{11}$$

Differentiating g and using Eq. (8) we get

$$g'(x_{i+1}) - g'(x_i) = \frac{1}{180}(f^{(5)}(x_{i+1})f^{(4)}(x_{i+1}) - f^{(5)}(x_i)f^{(4)}(x_i))h^4 + \mathcal{O}(h^6). \tag{12}$$

On the other hand, by three times differentiating of g and using Eqs. (8), (9) and (10), we obtain

$$\begin{aligned}g^{(3)}(x_i^+) &= (f^{(3)} - S_n^{(3)})(x_i^+)f^{(4)}(x_i) + 3(f'' - S_n'')(x_i^+)f^{(5)}(x_i) \\ &\quad +3(f' - S_n')(x_i^+)f^{(6)}(x_i) + (f - S_n)(x_i^+)f^{(7)}(x_i) \\ &= -\frac{h}{2}(f^{(4)}(x_i))^2 + \frac{h^2}{6}f^{(5)}(x_i)f^{(4)}(x_i) + \mathcal{O}(h^4).\end{aligned} \tag{13}$$

In the same manner, from Eqs. (8), (9) and (11), we deduce

$$g^{(3)}(x_{i+1}^-) = \frac{h}{2}(f^{(4)}(x_{i+1}))^2 + \frac{h^2}{6}f^{(5)}(x_{i+1})f^{(4)}(x_{i+1}) + \mathcal{O}(h^4). \tag{14}$$

Therefore, from Eqs. (13) and (14), we see that

$$\begin{aligned} g^{(3)}(x_{i+1}^-) - g^{(3)}(x_i^+) &= \frac{h}{2}((f^{(4)}(x_i))^2 + (f^{(4)}(x_{i+1}))^2) \\ &\quad + \frac{h^2}{6}(f^{(5)}(x_{i+1})f^{(4)}(x_{i+1}) - f^{(5)}(x_i)f^{(4)}(x_i)) + \mathcal{O}(h^4) \\ &= h(f^{(4)}(\xi_i))^2 + \frac{h^2}{6}(f^{(5)}(x_{i+1})f^{(4)}(x_{i+1}) - f^{(5)}(x_i)f^{(4)}(x_i)) + \mathcal{O}(h^4), \end{aligned}$$

for some $\xi_i \in [x_i, x_{i+1}]$. It is mentioned that the latter equality has been obtained by the intermediate value theorem. Substituting (12) and (15) in Eq.(11), yields

$$\begin{aligned} \int_{x_i}^{x_{i+1}} g(x)dx &= \frac{1}{720}(f^{(4)}(\xi_i))^2 h^5 - \frac{1}{4320}(f^{(5)}(x_{i+1})f^{(4)}(x_{i+1}) - f^{(5)}(x_i)f^{(4)}(x_i))h^6 \\ &\quad - \frac{h^6}{30240}(g^{(5)}(x_{i+1}^-) - g^{(5)}(x_i^+)) + \mathcal{O}(h^8). \\ &= \frac{1}{720}(f^{(4)}(\xi_i))^2 h^5 - \frac{1}{4320}(f^{(5)}(x_{i+1})f^{(4)}(x_{i+1}) - f^{(5)}(x_i)f^{(4)}(x_i))h^6 \\ &\quad - \frac{h^7}{30240} g^{(6)}(\eta_i) + \mathcal{O}(h^8), \end{aligned}$$

for some $\eta_i \in (x_i, x_{i+1})$. Here, it is noted that the latter equality is obtained by the mean value theorem. This together with (6) results in

$$\begin{aligned} \int_a^b (f''(x) - S_n''(x))^2 dx &= \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} (f(x) - S_n(x)) f^{(4)}(x) dx \\ &= \frac{1}{720} h^5 \sum_{i=0}^{n-1} (f^{(4)}(\xi_i))^2 - \frac{1}{4320}(f^{(5)}(b)f^{(4)}(b) - f^{(5)}(a)f^{(4)}(a))h^6 + \mathcal{O}(h^6) \\ &= \frac{b-a}{720}(f^{(4)}(c))^2 h^4 + \mathcal{O}(h^6), \end{aligned}$$

for some c in $[a, b]$ and the proof is completed. □

This theorem shows that $\int_a^b S_n''(x)^2 dx$ approximates $\int_a^b f''(x)^2 dx$ and the approximation error is of order 4. In the next section, we present a theorem which helps us to propose a procedure to control the stepsize for determining interpolating cubic spline functions.

3 Definition of the procedure

We first recall the following definition [4,10].

Definition 1 *Let r and s be two real numbers. The number of exact significant digits that are common to r and s can be defined in $(-\infty, +\infty)$ by*

1. *for $r \neq s$,*

$$C_{r,s} = \log_{10} \left| \frac{r+s}{2(r-s)} \right| .$$

2. $C_{r,r} = +\infty$.

Theorem 3 *(Jézéquel [10]). Let $I(h)$ be an approximation of order p of an exact value, i.e., $I - I(h) = Ch^p + \mathcal{O}(h^q)$ with $1 \leq p < q$ and $C \in \mathbb{R}$. If I_m is an approximation computed with the stepsize $h_0/2^m$, then*

$$C_{I_m,I_{m+1}} = C_{I_m,I} + \log_{10}(\frac{2^p}{2^p-1}) + \mathcal{O}(2^{m(p-q)}).$$

Theorem 4 *Let f be a sufficiently smooth function and S_m be the clamped cubic spline interpolating f with stepsize $(b-a)/2^m$. Moreover, let*

$$I = \int_a^b f''(x)^2 dx, \quad \text{and} \quad I_m = \int_a^b S''_m(x)^2 dx.$$

Then

$$C_{I_m,I_{m+1}} = C_{I_m,I} + \log_{10}(\frac{16}{15}) + \mathcal{O}(\frac{1}{4^m}). \tag{15}$$

Proof Let

$$I(h) = \int_a^b S''_n(x)^2 dx, \quad h = \frac{b-a}{n}.$$

In this case, by Theorem 2 we have

$$I - I(h) = Ch^4 + \mathcal{O}(h^6),$$

where

$$C = \frac{b-a}{720}(f^{(4)}(c))^2.$$

Now, letting $p = 4$, $q = 6$ and $h_0 = b - a$, from Theorem 3 the desired relation is obtained. □

This theorem shows that, if the convergence zone is reached, i.e., if the term $\mathcal{O}(\frac{1}{4^m})$ becomes negligible, then the significant digits common to two successive approximations I_m and I_{m+1} are also in common with I, up to one. Note that the term $\log_{10}(\frac{16}{15})$ corresponds at most to one bit.

These theoretical results have been obtained by taking into account only the truncation error on two successive approximations I_m and I_{m+1}. However computed results are also affected by round-off error propagation. Next, we describe how round-off errors can be estimated with a probabilistic approach in order to determine the exact significant digits of any computed result.

4 The CESTAC method, the DSA and the CADNA library

The Discrete Stochastic Arithmetic (DSA) [18] is a probabilistic approach for analyzing the round-off error propagation which is based on the synchronous implementation of the CESTAC method and the stochastic order relations. In the CESTAC method the floating-point arithmetic is replaced by a random arithmetic [5,7,18,20]. In fact, a computer program is run N times in parallel and in this way a new arithmetic called stochastic arithmetic is defined (for more details see [6]). The main idea is to use a random rounding to produce several samples of each result of any arithmetic operation and the number of common digits in these samples estimates the number of exactly significant digits in the floating-point result. From this point of view, Vignes [21] introduced the concept of computational zero which is denoted by @.0. A computational zero is a computed result which has no significant digit or which is the mathematical zero.

The CADNA software [2,3,17] is a library which implements automatically the DSA in any code written in Fortran. Using the CADNA library, each standard FP types have their corresponding stochastic types. Every intrinsic function and operator are overloaded for those types. When a stochastic variable is printed, only its significant digits are displayed to point out its accuracy. If a number has no significant digit (i.e., a computational zero), the symbol @.0 is displayed.

In the next section, we describe how the use of the CADNA library allows us to control the stepsize for the clamped interpolating cubic spline functions.

Table 1 Results for Example 1.

m	I_m	$\lvert I_m - I_{m-1}\rvert$
1	0.579606611372059E+000	-
2	0.409304598638124E+001	0.351343937500918E+001
3	0.282440641108701E+002	0.241510181244889E+002
4	0.137716622289053E+003	0.10947255817818E+003
5	0.283455313649822E+003	0.14573869136076E+003
6	0.291902821075508E+003	0.8447507425686E+001
7	0.29435093277108E+003	0.244811169558E+001
8	0.294515585171556E+003	0.16465240046E+000
9	0.294523788228367E+003	0.8203056810E-002
10	0.29452427212104E+003	0.48389267E-003
11	0.29452430193457E+003	0.2981353E-004
12	0.2945243037936E+003	0.18590E-005
13	0.2945243039109E+003	0.117E-006
14	0.2945243039189E+003	0.79E-008
15	0.294524303919E+003	@.0

5 Numerical examples

According to the previous section and Theorem 4, by using the CESTAC method and the CADNA library, we propose to use $|I_m - I_{m-1}| = @.0$ as a stopping criterion. The use of this stopping criterion allows us to estimate the optimal stepsize as soon as the difference between I_m and I_{m-1} is equal to the computational zero. In this case, by the theoretical results presented in Section 3, the common significant digits between I_m and I_{m-1} are also the common significant digits between I_m and I, up to one digit. By the proposed method, the best approximation of I provided by the computer is chosen. In this case, S_m is the best approximation of f provided by the computer. It is necessary to mention that in all the presented examples I_m's have been computed by Theorem 1.

Let us now present the examples and the results which we obtained by the Fortran code of the clamped interpolating cubic spline functions combined with the CADNA library, version BETA [17]. All the numerical experiments were computed in double precision. The `data_st` function of the CADNA library has been used to take into account the assignment error of some data of the examples which are not integer numbers and cannot be exactly coded on computer.

Example 1 Consider the Runge's function $f(x) = \frac{1}{1+25x^2}$ on $[-3, 3]$. Numerical results are given in Table 1. As we observe $|I_{15} - I_{14}| = @.0$. Therefore the optimal stepsize is estimated as $h = 6/2^{15} = 1.8310546875E - 004$. To show the effectiveness of the proposed method the values of $S_{15}(x)$ and $f(x)$ for midpoint of ten subintervals (denoted by $\bar{x}_j$) of $[-3, 3]$, for the obtained optimal stepsize, are given in Table 2. In column 1 of this table the index of the subinterval is given. Here we mention that the values of f are computed by a MATLAB code with 20 digits of accuracy and are presented by 15 digits with rounding. As we see, all of the digits of $S_{15}(\bar{x}_j)$, up to one, coincide with that of the $f(\bar{x}_j)$ for all j.

Example 2 In this example, we consider $f(x) = 3 + x + 5\sin x$ on $[0, 2]$. Numerical results are given in Table 3. Here, we have $|I_{10} - I_9| = @.0$. Therefore the optimal stepsize is estimated as $h = 2/2^{10} = 1.953125E - 003$. Similar to Example 1, the values of $S_{10}(x)$ and $f(x)$ for midpoint of ten subintervals of $[0, 2]$ for the obtained optimal stepsize are given in Table 4. Other assumptions are as before. As we see, all of the digits of $S_{10}(\bar{x}_j)$, up to one, coincide with that of the $f(\bar{x}_j)$.

Example 3 This example is devoted to the function $f(x) = \tan x$ on the interval $[0, 1]$. Numerical results are given in Table 5. In this example $|I_{11} - I_{10}| = @.0$. Therefore the optimal stepsize is

Table 2 Comparison between exact and numerical results for Example 1 at some points.

j	$\bar{x}_j = (x_j + x_{j+1})/2$	$f(\bar{x}_j)$	$S_{15}(\bar{x}_j)$
3000	-0.245059204101562E+001	0.661659957285500E-002	0.661659957285499E-002
6000	-0.190127563476562E+001	0.109443644783414E-001	0.109443644783414E-001
9000	-0.135195922851562E+001	0.214156407155478E-001	0.214156407155477E-001
12000	-0.802642822265625E+000	0.584594046817734E-001	0.584594046817734E-001
15000	-0.253326416015625E+000	0.383971961870989E+000	0.38397196187098E+000
18000	0.295989990234375E+000	0.313454875827633E+000	0.31345487582763E+000
21000	0.845306396484375E+000	0.530122273912718E-001	0.530122273912718E-001
24000	0.139462280273437E+001	0.201514100181291E-001	0.201514100181292E-001
27000	0.194393920898437E+001	0.104742212900443E-001	0.104742212900443E-001
30000	0.249325561523437E+001	0.639353121651417E-002	0.639353121651419E-002

Table 3 Results for Example 2.

m	I_m	$\lvert I_m - I_{m-1}\rvert$
1	0.296820840065746E+002	-
2	0.297273264567318E+002	0.452424501571E-001
3	0.29729852565359E+002	0.25261086277E-002
4	0.29730005487198E+002	0.152921838E-003
5	0.29730014965180E+002	0.9477982E-005
6	0.29730015556288E+002	0.591108E-006
7	0.29730015593213E+002	0.3692E-007
8	0.2973001559552E+002	0.230E-008
9	0.2973001559566E+002	0.1E-009
10	0.297300155956E+002	@.0

Table 4 Comparison between exact and numerical results for Example 2 at some points.

j	$\bar{x}_j = (x_j + x_{j+1})/2$	$f(\bar{x}_j)$	$S_{15}(\bar{x}_j)$
100	0.196289062500000E+000	0.417144408942271E+001	0.417144408942267E+001
200	0.391601562500000E+000	0.529994769532040E+001	0.52999476953203E+001
300	0.586914062500000E+000	0.635588479683488E+001	0.63558847968347E+001
400	0.782226562500000E+000	0.730652940267767E+001	0.73065294026775E+001
500	0.977539062500000E+000	0.812315935934277E+001	0.81231593593426E+001
600	0.117285156250000E+001	0.878214853571748E+001	0.87821485357173E+001
700	0.136816406250000E+001	0.926586522705502E+001	0.92658652270548E+001
800	0.156347656250000E+001	0.956334261572473E+001	0.95633426157245E+001
900	0.175878906250000E+001	0.967069579389256E+001	0.96706957938924E+001
1000	0.195410156250000E+001	0.959126949048556E+001	0.95912694904853E+001

estimated as $h = 1/2^{11} = 4.8828125E - 004$. The values of $S_{11}(x)$ and $f(x)$ for some points are given in Table 6. Other assumptions are similar to previous examples. As we see, all of the digits of $S_{11}(\bar{x}_j)$, up to one, coincide with that of $f(\bar{x}_j)$.

6 Conclusion

In this paper, a theorem has been stated to provide a stopping criterion to control the stepsize in the clamped interpolating cubic spline functions. We observed that the use of the CESTAC method and the CADNA library allows us to estimate the optimal stepsize. Numerical examples show that the proposed method is effective. It is easy to show that the results of this paper hold for other type of splines.

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Table 5 Results for Example 3.

m	I_m	$\lvert I_m - I_{m-1}\rvert$
1	0.11994926417854E+002	-
2	0.12322769199102E+002	0.3278427812480E+000
3	0.123633246653066E+002	0.405554662041E-001
4	0.12366443162187E+002	0.3118496880E-002
5	0.12366642535419E+002	0.199373231E-003
6	0.1236665491785E+002	0.1238243E-004
7	0.1236665568877E+002	0.770923E-006
8	0.1236665573689E+002	0.48120E-007
9	0.1236665573990E+002	0.300E-008
10	0.1236665574008E+002	0.18E-009
11	0.123666557400E+002	@.0

Table 6 Comparison between exact and numerical results for Example 3 at some points.

j	$\bar{x}_j = (x_j + x_{j+1})/2$	$f(\bar{x}_j)$	$S_{15}(\bar{x}_j)$
100	0.49072265625000E-001	0.491116937030549E-001	0.49111693703054E-001
300	0.14672851562500E+000	0.147790648659708E+000	0.14779064865970E+000
500	0.24438476562500E+000	0.249369077505914E+000	0.24936907750591E+000
700	0.34204101562500E+000	0.356034947855218E+000	0.3560349478552E+000
900	0.43969726562500E+000	0.470410749269861E+000	0.4704107492698E+000
1100	0.53735351562500E+000	0.595837904393136E+000	0.5958379043931E+000
1300	0.63500976562500E+000	0.736815922323845E+000	0.7368159223238E+000
1500	0.73266601562500E+000	0.899730190248084E+000	0.8997301902481E+000
1700	0.83032226562500E+000	0.109414073165260E+001	0.1094140731652E+001
1900	0.92797851562500E+000	0.133523311340313E+001	0.1335233113403E+001

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