SHARP APPROXIMANTS FOR THE ERROR FUNCTION VIA COSINE HYPERBOLIC POLYNOMIALS EXPANSION

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The aim of this paper is to provide new refinements for the error function using cosine hyperbolic, respectively mixed cosine polynomials expansion for even functions. These approximants are designed to be very accurate in large neighborhoods of the origin. Then we use them in unidimensional heat flow theory.

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1. Introduction and Motivation

The error function er$f$ is a special function. It is frequently used in probability theory and statistical computations, mathematical physics, mathematical models in biology.

The error function is related to the function expression for a Gaussian distribution and has the form

$$\mathrm{er}f\,(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2)dt.$$

The error function may be looked up in the tables given in standard texts on statistics, but it is convenient for computation to have it in analytical function form. Reviews of approximations of the error function have been given by Karlsson and Bjerle [9] or Abramowitz and Stegun [1].

In the study of the error function two fundamental aspects are approached. The first aspect refers to the establishment of some bounds for the error function. The second aspect is to approximate the error function with different analytical functions.

Finding sharp bounds for the error function have attracted the attention of many researches in the recent past. We refer to [1] - [15] and closely related references therein.

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Pólya [12] proved that the inequality

$$\operatorname{erf}(x) < \sqrt{1 - \exp\left(-\frac{4x^2}{\pi}\right)}$$

holds for all $x > 0$.

Neuman's inequalities assert that

$$\frac{2x}{\sqrt{\pi}} \cdot \exp\left(-\frac{x^2}{3}\right) \leq \operatorname{erf}(x) \leq \frac{2x}{\sqrt{\pi}} \cdot \frac{\exp(-x^2) + 2}{3}$$

hold for all $x > 0$.

In order to approximate the error function with different analytical functions, Hastings [6] suggested some expressions, of which the simplest are

$$\operatorname{erf}(x) \simeq 1 - \left(a_1 t + a_2 t^2 + a_3 t^3\right) \exp(-x^2), 0 \leq x$$

where

$$t = \frac{1}{1 + a_4 x},\ a_1 = 0.3480242,\ a_2 = -0.0958798,\ a_3 = 0.7478556,\ a_4 = 0.47047$$

and

$$\operatorname{erf}(x) \simeq 1 - \left(1 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4\right)^{-4},$$

where

$$a_1 = 0.278393,\ a_2 = 0.230389,\ a_3 = 0.000972,\ a_4 = 0.078108.$$

The absolute error $\varepsilon(x)$ is shown to be less 2×10^{-5} and 5×10^{-4}, respectively.

Norton [11] obtained the following approximation

$$\operatorname{erf}(x) \simeq \begin{cases} 1 - \exp\left(-\dfrac{2x^2 + 1.2\left(x\sqrt{2}\right)^{0.8}}{2}\right);\ 0 \leq x \leq 2.7 \\ -1 + \sqrt{\dfrac{2}{\pi}} \exp\left(-x^2\right);\ x > 2.7 \end{cases}$$

with absolute error $|\varepsilon(x)| < 8.07 \times 10^{-3}$, for all $x \geq 0$.

In this work we deepen the study of the error function started in a previous article [3].

The first idea is that the function $\exp\left(-x^2\right)$ is even, so it can be expanded as hyperbolic cosine polynomials

$$\exp\left(-x^2\right) = 1 - a - b + a\cosh x + b\cosh 2x + ...,$$

and

$$\exp\left(-x^2\right) = 1 - a - b - c + a\cosh x + b\cosh 2x + c\cosh 3x + ...$$

The second idea is to expand the function $\exp\left(-x^2\right)$ as *mixed* cosine polynomials

$$\exp\left(-x^2\right) = a + b\cos x + c\cosh x + d\cos 2x + e\cosh 2x + f\cos 3x + g\cosh 3x + ...$$

In the following we present our algorithm for the first expansion. We introduce the function $F_1(x)$ by

$$F_1(x) = 1 - a - b + a\cosh x + b\cosh 2x.$$

The power series expansion of $\exp\left(-x^2\right) - F_1(x)$ near 0 is

$$x^2\left(-\frac{a}{2} - 2b - 1\right) + x^4\left(-\frac{a}{24} - \frac{2b}{3} + \frac{1}{2}\right) + \mathcal{O}\left(x^6\right).$$

In order to increase the speed of the function $F_1(x)$ approximating $\exp\left(-x^2\right)$, we vanish the first coefficients as follows:

$$\begin{cases} -\frac{a}{2} - 2b - 1 = 0 \\ -\frac{a}{24} - \frac{2b}{3} + \frac{1}{2} = 0 \end{cases}$$

and we obtain $a = -\frac{20}{3}$ and $b = \frac{7}{6}$.

Therefore we have

$$\exp\left(-x^2\right) - \frac{13}{2} + \frac{20}{3}\cosh x - \frac{7}{6}\cosh 2x = -\frac{47}{180}x^6 + \frac{347}{10080}x^8 - \frac{97}{11200}x^{10} + \mathcal{O}\left(x^{12}\right).$$

Using the same algorithm, we find

$$\begin{aligned}\exp\left(-x^2\right) - \frac{211}{18} + \frac{29}{2}\cosh x - \frac{43}{10}\cosh 2x + \frac{47}{90}\cosh 3x = \frac{67}{672}x^8 - \\ -\frac{79}{75600}x^{10} + \frac{77101}{39916800}x^{12} + \mathcal{O}\left(x^{14}\right)\end{aligned}$$

and

$$\begin{aligned}\exp\left(-x^2\right) + \frac{14335}{36} - \frac{22461}{100}\cos x - \frac{4139}{20}\cosh x + \frac{783}{40}\cos 2x + \\ + \frac{37187}{2600}\cosh 2x - \frac{55}{52}\cos 3x - \frac{409}{900}\cosh 3x = -\frac{46469}{279417600}x^{14} + \\ + \frac{9500951}{435891456000}x^{16} - \frac{362727023}{133382785536000}x^{18} + \mathcal{O}\left(x^{20}\right).\end{aligned}$$

2. Main Results

In this section we will prove our approximations of the error function using cosine hyperbolic polynomials expansion for the function $\exp\left(-x^2\right)$.

Theorem 2.1. *The double inequality*

$$\begin{aligned}\frac{211}{18}x - \frac{29}{2}\sinh x + \frac{43}{20}\sinh 2x - \frac{47}{270}\sinh 3x < \frac{\sqrt{\pi}}{2}\mathrm{er}f(x) < \\ < \frac{13}{2}x - \frac{20}{3}\sinh x + \frac{7}{12}\sinh 2x\end{aligned} \tag{1}$$

hold for all $x > 0$.

Proof. For the right-hand side of inequality (1), we consider the function

$$f_1 : (0,\infty) \to \mathbb{R}, f_1(x) = \frac{\sqrt{\pi}}{2}\mathrm{er}f(x) - \frac{13}{2}x + \frac{20}{3}\sinh x - \frac{7}{12}\sinh 2x.$$

The function f_1 has the derivative

$$f_1'(x) = \exp(-x^2) - \frac{13}{2} + \frac{20}{3}\cosh x - \frac{7}{6}\cosh 2x.$$

We have to prove that $f_1'(x) < 0$ for all $x > 0$ or, equivalently,

$$\exp(-x^2) < \frac{13}{2} - \frac{20}{3}\cosh x + \frac{7}{6}\cosh 2x, \text{ for all } x > 0.$$

Since

$$\frac{13}{2} - \frac{20}{3}\cosh x + \frac{7}{6}\cosh 2x = \frac{7\cosh^2 x - 20\cosh x + 16}{3} > 0$$

for all $x > 0$, we can log the above inequality and it remains to be shown that

$$-x^2 < \log\left(\frac{13}{2} - \frac{20}{3}\cosh x + \frac{7}{6}\cosh 2x\right),$$

for all $x \in (0,\infty)$.

The function

$$f_2 : (0,\infty) \to \mathbb{R}, f_2(x) = -x^2 - \log\left(\frac{13}{2} - \frac{20}{3}\cosh x + \frac{7}{6}\cosh 2x\right)$$

has the derivatives

$$f_2'(x) = \frac{40\sinh x - 14\sinh 2x}{-40\cosh x + 7\cosh 2x + 39} - 2x$$

and

$$f_2^{(2)}(x) = \frac{-16\sinh^4\left(\frac{x}{2}\right)\left(98\cosh^2 x - 504\cosh x + 688\right)}{\left(-40\cosh x + 7\cosh 2x + 39\right)^2}.$$

We notice that $f_2^{(2)} < 0$ for all $x > 0$, hence f_2' is strictly decreasing on $(0,\infty)$. As $f_2'(x) = 0$, it follows that $f_2' < 0$ on $(0,\infty)$. Then f_2 is strictly decreasing on $(0,\infty)$. Since $f_2(0) = 0$, finally we find $f_2 < 0$ on $(0,\infty)$.

For the proof of left-hand side of inequality (1), we introduce the function

$$f_3 : (0,\infty) \to \mathbb{R}, f_3(x) = \frac{\sqrt{\pi}}{2}\mathrm{er}f(x) - \frac{211}{18}x + \frac{29}{2}\sinh x - \frac{43}{20}\sinh 2x + \frac{47}{270}\sinh 3x.$$

The derivative of the function f_3 is

$$f_3'(x) = \exp(-x^2) - \frac{211}{18} + \frac{29}{2}\cosh x - \frac{43}{10}\cosh 2x + \frac{47}{90}\cosh 3x.$$

We have to prove that $f_3'(x) > 0$ on $(0,\infty)$ or, equivalently,

$$\exp(-x^2) > \frac{211}{18}x - \frac{29}{2}\cosh x + \frac{43}{10}\cosh 2x - \frac{47}{90}\cosh 3x.$$

Since the only positive root of the function

$$f_4(x) = \frac{211}{18}x - \frac{29}{2}\cosh x + \frac{43}{10}\cosh 2x - \frac{47}{90}\cosh 3x$$

is $x \approx 1.13381$ and $f_4(x) > 0$ only on $(0, 1.13381)$, it remains to prove that $f_3' > 0$ only for $x \in (0, 1.13381)$.

We find

$$f_3^{(2)}(x) = -2x\exp(-x^2) + \frac{29}{2}\sinh x - \frac{43}{5}\sinh 2x + \frac{47}{30}\sinh 3x,$$
$$f_3^{(3)}(x) = \left(4x^2 - 2\right)\exp(-x^2) + \frac{29}{2}\cosh x - \frac{86}{5}\cosh 2x + \frac{47}{10}\cosh 3x,$$
$$f_3^{(4)}(x) = \left(-8x^3 + 12x\right)\exp(-x^2) + \frac{29}{2}\sinh x - \frac{172}{5}\sinh 2x + \frac{141}{10}\sinh 3x,$$

$$\begin{aligned} f_3^{(5)}(x) &= \frac{1}{10}\exp(-x^2)(160x^4 - 480x^2 + 145\exp(x^2)\cosh x - \\ &\quad -688\exp(x^2)\cosh 2x + 423\exp(x^2)\cosh 3x + 120), \end{aligned}$$

$$\begin{aligned} f_3^{(6)}(x) &= \frac{1}{10}\exp(-x^2)(-320x^5 + 1600x^3 + 145\exp(x^2)\sinh x - \\ &\quad -1376\exp(x^2)\sinh 2x + 1269\exp(x^2)\sinh 3x - 1200x) \end{aligned}$$

and

$$\begin{aligned} f_3^{(7)}(x) &= \frac{1}{10}\exp(-x^2)\left(640x^6 - 4800x^4 + 7200x^2 + 145\exp(x^2)\cosh x - \right. \\ &\quad \left. -2752\exp(x^2)\cosh 2x + 3807\exp(x^2)\cosh 3x - 1200\right) \\ &= \frac{1}{10}\exp(-x^2)\left[160x^2\left(4x^4 - 30x^2 + 45\right) + 145\left(\exp(x^2)\cosh x - 1\right) + \right. \\ &\quad \left. +2752\exp(x^2)\left(\cosh 3x - \cosh 2x\right) + 1055\left(\exp(x^2)\cosh 3x - 1\right)\right] \end{aligned}$$

Since the equation

$$4x^4 - 30x^2 + 45 = 0$$

has the roots

$$x_1 = \frac{1}{2}\sqrt{15 - 3\sqrt{5}} \approx 1.4397739 \text{ and } x_2 = \frac{1}{2}\sqrt{15 + 3\sqrt{5}} \approx 2.329603$$

and

$$4x^4 - 30x^2 + 45 > 0$$

for $x \in (0, x_1) = (0, 1.4397739) \supset (0.1.13381)$ we obtain $f_3^{(7)} > 0$ on $(0, 1.13381)$. Hence $f_3^{(6)}$ is strictly increasing on $(0, 1.13381)$. As $f_3^{(6)}(0) = 0$, it follows that $f_3^{(6)} > 0$ on $(0, 1.13381)$. Continuing the algorithm, finally we find $f_3' > 0$ on $(0, 1.13381)$.

The proof of Theorem 2.1 is complete. □

In the following we will prove that our bounds for the error function are more precise than Neuman's inequalities on large neighbourhoods of the origin.

Proposition 2.1. *(i) The inequality*

$$\frac{13}{2}x - \frac{20}{3}\sinh x + \frac{7}{12}\sinh 2x \leq \frac{x}{3}\left(\exp(-x^2) + 2\right)$$

holds for every $x \in [0, 1.08201]$.

(ii) The inequality

$$\frac{211}{18}x - \frac{29}{2}\sinh x + \frac{43}{20}\sinh 2x - \frac{47}{270}\sinh 3x \geq x\exp\left(-\frac{x^2}{3}\right)$$

holds for every $x \in [0, 1.22449]$.

Proof. (i) We introduce the function $g : [0, \infty) \to \mathbb{R}$,

$$g(x) = \frac{13}{2}x - \frac{20}{3}\sinh x + \frac{7}{12}\sinh 2x - \frac{x}{3}\left(\exp\left(-x^2\right) + 2\right).$$

In order to find all positive critical points, first we calculate $g'(x)$:

$$g'(x) = \frac{1}{3}\exp(-x^2)\left(2x^2 - 1\right) + \frac{1}{6}\left(-40\cosh x + 7\cosh 2x + 35\right).$$

The positive roots of the derivative g' are $x = 0$ and $x \approx 0.908029$.

Evaluate $g(x)$ at the critical points:

$$g(0) = 0, g(0.908029) = -0.010647 \text{ and } \lim_{x\to\infty} g(x) = \infty.$$

The equation $g(x) = 0$ has the positive roots: $x = 0$ and $x \approx 1.08201$.

Summarizing the results, we obtain that $g(x) \le 0$ for all $x \in [0, 1.08201]$.

(ii) We consider the function $h : [0, \infty) \to \mathbb{R}$,

$$h(x) = \frac{211}{18}x - \frac{29}{2}\sinh x + \frac{43}{20}\sinh 2x - \frac{47}{270}\sinh 3x - x\exp(-\frac{x^2}{3}).$$

The first derivative of h is

$$h'(x) = \exp(-\frac{x^2}{3})\left(\frac{2}{3}x^2 - 1\right) - \frac{29}{2}\cosh x + \frac{43}{10}\cosh 2x - \frac{47}{90}\cosh 3x + \frac{211}{18}.$$

The positive roots of the first derivative h' are $x = 0$ and $x \approx 1.049665$.

Evaluate $h(x)$ at the critical points:

$$h(0) = 0, h(1.049665) = 0.019944 \text{ and } \lim_{x\to\infty} h(x) = -\infty.$$

The equation $h(x) = 0$ has the positive roots: $x = 0$ and $x \approx 1.22449$.

Finally, we find that $h(x) \ge 0$ for all $x \in [0, 1.22449]$.

This completes the proof. □

We also improve the Pólya's inequality as follows.

Proposition 2.2. *The inequality*

$$\frac{2}{\sqrt{\pi}}\left(\frac{13}{2}x - \frac{20}{3}\sinh x + \frac{7}{12}\sinh 2x\right) \le \sqrt{1 - \exp\left(-\frac{4x^2}{\pi}\right)}$$

holds for every $x \in [0, 0.707118]$.

Proof. We define the function $p : (0, \infty) \to \mathbb{R}$,

$$p(x) = \exp\left(-\frac{4x^2}{\pi}\right) - 1 + \frac{4}{\pi}\left(\frac{13}{2}x - \frac{20}{3}\sinh x + \frac{7}{12}\sinh 2x\right)^2.$$

The first derivative of function $p(x)$ is

$$p'(x) = -\frac{8x}{\pi}\exp\left(-\frac{4x^2}{\pi}\right) - \frac{(-39 + 40\cosh x - 7\cosh 2x)(78x - 80\sinh x + 7\sinh 2x)}{9\pi}$$

and has the positive roots: $x_1 = 0$ and $x \approx 0.583826$.

Since $p'(0.5) \approx -0.00610245$ and $p'(1) \approx 0.484477$, it follows that $p' \leq 0$ on $[0, 0.583826]$ and $p' > 0$ on $(0.583826, \infty)$. Then p is strictly decreasing on $[0, 0.583826]$ and p is strictly increasing on $(0.583826, \infty)$.

Evaluate $p(x)$ at critical points:

$$p(0) = 0, p(0.583826) \approx -0.00168491 \text{ and } \lim_{x\to\infty} p(x) = \infty.$$

The positive roots of the function p are: $x_1 = 0$ and $x_2 \approx 0.707118$.

Summarizing the results, we find that $p(x) \leq 0$ for all $x \in [0, 0.707118]$ and $p(x) > 0$ for all $x \in (0.707118, \infty)$.

This completes the proof. $\square$

3. Approximation to six decimals of precision for er$f(x)$ on a large neighbourhood of the origin

In the following we derive approximation to six decimals of precision for the function er$f(x)$ on a large neighbourhood of the origin. Using the *mixed* cosine series of the function $\exp\left(-x^2\right)$, we find

$$\begin{gathered}\frac{\sqrt{\pi}}{2}\mathrm{er}f(x) + \frac{14335}{36}x - \frac{22461}{100}\sin x - \frac{4139}{20}\sinh x + \\ +\frac{783}{80}\sin 2x + \frac{37187}{5200}\sinh 2x - \frac{55}{156}\sin 3x - \frac{409}{2700}\sinh 3x = \\ -\frac{46469}{4191264000}x^{15} + \frac{9500951}{7410154752000}x^{17} - \frac{362727023}{2534272925184000}x^{19} + \mathcal{O}\left(x^{21}\right).\end{gathered}$$

Therefore, we consider the function $\varepsilon : (0, \infty) \to \mathbb{R}$,

$$\begin{aligned}\varepsilon(x) \quad = \quad & \mathrm{er}f(x) + \frac{2}{\sqrt{\pi}}\left(\frac{14335}{36}x - \frac{22461}{100}\sin x - \frac{4139}{20}\sinh x + \frac{783}{80}\sin 2x + \right. \\ & \left. +\frac{37187}{5200}\sinh 2x - \frac{55}{156}\sin 3x - \frac{409}{2700}\sinh 3x\right).\end{aligned}$$

The derivative of $\varepsilon(x)$ is

$$\begin{aligned}\varepsilon'(x) \quad = \quad & \frac{2}{\sqrt{\pi}}\exp(-x^2) + \frac{2}{\sqrt{\pi}}\left(-\frac{22461}{100}\cos x + \frac{783}{40}\cos 2x - \frac{55}{52}\cos 3x - \right. \\ & \left. -\frac{4139}{20}\cosh x + \frac{37187}{2600}\cosh 2x - \frac{409}{900}\cosh 3x + \frac{14335}{36}\right).\end{aligned}$$

The roots of the function $\varepsilon'(x)$ on the interval $[0, \infty)$ are $x = 0$ and $x \approx 0.5189134$. Then we partition the domain $[0, \infty)$ into intervals with endpoints at the critical points: $[0, 0.5189134]$ and $[0.5189134, \infty)$. Since $\varepsilon'(0.5) > 0$ and $\varepsilon'(1) < 0$, it follows that $\varepsilon' > 0$ on $[0, 0.5189134]$ and $\varepsilon' < 0$ on $[0.5189134, \infty)$. Then the function $\varepsilon(x)$ is strictly increasing on $[0, 0.5189134]$ and is strictly decreasing on $[0.5189134, \infty)$.

Summarizing the results, we obtain that the function $\varepsilon(x)$ has the maximum value $\max \varepsilon(x) \approx 4 \times 10^{-9}$ at $x \approx 0.5189134$.

We also have $\varepsilon(0.992) \approx -9.91852 \times 10^{-6}$, $\varepsilon(1.155) \approx -9.40334 \times 10^{-5}$, $\varepsilon(1.355) \approx -9.8332 \times 10^{-4}$.

Therefore we find the following approximation to six, five and respectively four decimals of precision for the error function $\mathrm{er}f(x)$ on large neighbourhoods of the origin: $(0, 0.992)$, $(0.1.155)$ and respectively $(0, 1.355)$: $\mathrm{er}f(x) \approx \theta(x)$, where

$$\begin{aligned}\theta(x) =& \frac{2}{\sqrt{\pi}}\left(-\frac{14335}{36}x + \frac{22461}{100}\sin x + \frac{4139}{20}\sinh x - \frac{783}{80}\sin 2x - \right. \\ & \left. -\frac{37187}{5200}\sinh 2x + \frac{55}{156}\sin 3x + \frac{409}{2700}\sinh 3x\right)\end{aligned} \tag{2}$$

with the absolute error $|\varepsilon(x)| = |\mathrm{er}f(x) - \theta(x)| \leq 9.91852 \times 10^{-6}$ on the interval $(0, 0.992)$, $|\varepsilon(x)| \leq 9.40334 \times 10^{-5}$ on the interval $(0, 1.155)$ and respectively $|\varepsilon(x)| \leq 9.8322 \times 10^{-4}$ on the interval $(0, 1.355)$.

4. **Application**

As an example to apply the error function, one case is considered for the unidimensional heat flow equation.

Consider the case of the nonstationary flux in an agriculture field due to the sun. Suppose that the initial distribution of temperature on the field is given by $T(x, 0) = T_f$, and the superficial temperature T_s is constant [5].

Consider the origin be on the surface of the field such that the positive end for x axis points inward the field. We can express T as a function of x and time t, $T(x, t)$.

From heat flow theory, it is known that $T(x, t)$ should satisfy the heat conduction equation:

$$a^2 \frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t},$$

where $a^2 = k$, known as thermal diffusivity.

The initial conditions are $T(0, t) = T_s$ and $T(x, 0) = T_f$.

Using the substitution $V(u) = T(x, t)$, where $u = u(x, t) = \frac{x}{2a\sqrt{t}}$, the heat conduction equation can be expressed as an ordinary single variable second - order differential equations:

$$\frac{d^2 V}{du^2} = -2u \frac{dV(u)}{du},$$

which has the solution

$$V(u) = C_1 \int_0^u \exp\left(-\rho^2\right) d\rho + C_2,$$

C_1 and C_2 being integration constants.

Therefore, the temperature distribution $T(x, t)$ can be express in terms of the error function by

$$T(x, t) = C_1 + C_2 \mathrm{er}f\left(\frac{x}{2a\sqrt{t}}\right).$$

Applying the initial conditions, finally we find

$$T\left(x,t\right)=\left(T_f-T_s\right)\mathrm{er}f\left(\frac{x}{2a\sqrt{t}}\right)+T_s.$$

Expressing $T\left(x,t\right)$ in terms of our approximation for the error function, we obtain the following approximate solution

$$T\left(x,t\right)\approx\left(T_f-T_s\right)\theta\left(\frac{x}{2a\sqrt{t}}\right)+T_s,$$

where $\frac{x}{2a\sqrt{t}}<1.355$.

The distance x is in meters, the temperature is in Kelvin, and time is measured in seconds. The field temperature is $T_f=285°K$, surface temperature is $T_s=300°K$, and the thermal conductivity value is $k=a^2=0.003m^2/s$.

5. **Conclusions**

In our work we expand the function $\exp\left(-x^2\right)$ as hyperbolic cosine polynomials and respectively as *mixed* cosine polynomials in order to obtain sharp approximations for the error function. Using the cosine hyperbolic polynomials expansion, we find the double inequality (1). Our new bounds for the error function improve Neuman's inequalities on large neighborhoods of the origin. Using the *mixed* cosine polynomials, we provide the approximation (2) for the error function. Our approximation has simple expression with acceptable deviation for engineering calculations. The approximate error function is used as a solution for the unidimensional heat flow equation.

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