Analysis of a Finite Difference Scheme for STC

Daniel Topa ERT Corp Albuquerque, NM

April 6, 2020

Abstract

A new finite difference scheme for the STC model is quickly analyzed to clarify the relationship between the discrete centered-difference derivative nx1 and a reformulation nx2. Sufficient details are provided to make the report useful as an independent check.

1 Finite Difference Scheme

1.1 Inputs

A finite difference scheme was recorded in the attached spreadsheet finite-difference. Unfortunately, the attachment excludes the algebraic relations between the columns. However, a Mathematica notebook was composed to recreate the algebra, and the attached file log-01.nb explicitly details the relationship between relevant parameters. The spreadsheet features explicit entries for a, b, Δ , and, x_0 to allow for numerical experimentation.

1.2 Mesh

The mesh presented is an equipartition of the domain $x \in [0, 600]$ with an interval size of $\Delta = 15$. The domain is composed of the set of points

$$x = \{x_k\}_{k=0}^{40} = \{k\Delta\}_{k=0}^{40}, \qquad k = 0, 1, 2, \dots 40.$$
 (1)

1.3 Functions of interest

The quantity nx1 represents a centered difference formulation of the derivative G'(x) while the quantity nx2 is intended as a new formulation which suppresses large spikes in velocity. The foundation function is of Gaussian form:

$$G(x) = ae^{-bx^2}, (2)$$

with the parameters given as $a = 10^{14}$ and b = 1/5000. For clarity, the Gaussian quantity nx1 is called G(x).

The goal of the analysis is to explore the relationship between the two putatively equivalent terms

$$\frac{G(x+\Delta) - G(x-\Delta)}{(x+\Delta) - (x-\Delta)} \quad \text{and} \quad G(x+\Delta) \left(\frac{\ln G(x+\Delta) - \ln G(x-\Delta)}{(x+\Delta) - (x-\Delta)}\right)$$

which we will see has a leading order equivalence.

Start by observing that the denominators evaluate to the same constant

$$(x + \Delta) - (x - \Delta) = 2\Delta,$$

and then define the functions $\eta(x)$, the classic discrete derivative, and $\eta(x)$, the reformulation:

$$\xi(x) = \frac{G(x+\Delta) - G(x-\Delta)}{2\Delta},$$

$$\eta(x) = \frac{G(x+\Delta)}{2\Delta} \left(\ln G(x+\Delta) - \ln G(x-\Delta) \right).$$
(3)

2 Analysis

The analysis entails computing series expansions for the two forms and comparing terms.

2.1 The Function $\xi(x)$

Using the identity

$$(x \pm \Delta)^2 = x^2 \mp 2\Delta x + \Delta^2,\tag{4}$$

the first function becomes

$$\xi(x) = \frac{G(x+\Delta) - G(x-\Delta)}{2\Delta}$$

$$= \frac{a}{\Delta} e^{-b(x^2 + \Delta^2)} \left(e^{-2b\Delta x} - e^{2b\Delta x} \right).$$
(5)

Simplification produces a form amenable to series expansion, a constant, an exponential function and the hyperbolic sine:

$$\xi(x) = \left(-\frac{2a}{\Delta}e^{-b\Delta^2}\right)e^{-bx^2}\sinh(2\Delta x) \tag{6}$$

2.2 The Function $\eta(x)$

The reformulation of the derivative uses the difference of the logarithmic terms:

$$\ln G(x + \Delta) - \ln G(x - \Delta) = \left(a - b(x + \Delta)^2\right) - \left(a - b(x - \Delta)^2\right)$$

$$= -b\left((x + \Delta)^2 - (x - \Delta)^2\right)$$

$$= -4b\Delta x$$
(7)

Use this identity in (3) and reduce the function to a constant multiplying an exponential function:

$$\eta(x) = -4b\Delta x \frac{G(x+\Delta)}{2\Delta}
= -2abxe^{-b(x^2+\Delta^2-2\Delta x)}
= \left(-2abxe^{-b\Delta^2}\right)e^{-b(x^2-2\Delta x)}$$
(8)

2.3 Series expansions

The equivalence of the two functions is determined by a term-by-term comparison of their respective expansions. Fortunately, we only need to recall a single series expansion, and it is

$$e^x = 1 + x + \frac{1}{2!}x^2 + \frac{1}{3!}x^3 + \dots = 1 + \sum_{k=1}^{\infty} \frac{x^k}{k!}.$$
 (9)

Two needed identities follow from this formulation. The first is the Gaussian function:

$$e^{-bx^2} = 1 - bx^2 + \frac{1}{2!}b^2x^4 - \frac{1}{3!}b^3x^6 + \dots = 1 + \sum_{k=1}^{\infty} (-1)^k \frac{b^k x^{2k}}{k!},$$
 (10)

the second, the hyperbolic sine function

$$\frac{1}{2} \left(e^x - e^{-x} \right) = \frac{1}{2} \left(1 + x + \frac{1}{2!} x^2 + \frac{1}{3!} x^3 + \dots \right) - \frac{1}{2} \left(1 - x + \frac{1}{2!} x^2 - \frac{1}{3!} x^3 + \dots \right) \\
= x + \frac{x^3}{3!} + \frac{x^5}{5!} + \dots \\
= \sum_{k=1}^{\infty} \frac{x^{2k-1}}{(2k-1)!}.$$
(11)

2.4 Comparing $\xi(x)$ to $\eta(x)$

To reduce algebraic clutter for both functions, define the constant

$$\alpha = abe^{-b\Delta^2}. (12)$$

2.4.1 Leading order terms for $\xi(x)$

Continue with the form of $\xi(x)$ given in (6). The two expansions to be multiplied are (10) and (11):

$$\xi(x) = -\frac{\alpha}{b\Delta} e^{-bx^2} \sinh(2b\Delta x)$$

$$= -\left(\frac{\alpha}{b\Delta}\right) \left(1 - bx^2 + \frac{1}{2!}b^2x^4 + \mathcal{O}\left(x^6\right)\right) \left(2b\Delta x + \frac{8b^3\Delta^3}{3!}x^3 + \frac{32b^5\Delta^5}{5!}x^5 + \mathcal{O}\left(x^7\right)\right)$$

$$= -\left(\frac{\alpha}{b\Delta}\right) \left(2b\Delta x - 2b^2\Delta x^3 + \frac{4b^3\Delta^3}{3}x^3 + \mathcal{O}\left(x^4\right)\right)$$
(13)

which reduces to:

$$\xi(x) = -2\alpha x + 2\alpha b \left(1 - \frac{2}{3}b\Delta^2\right)x^3 + \mathcal{O}\left(x^4\right)$$
(14)

2.4.2 Leading order terms for $\eta(x)$

Restate (8) using the parameter α and decompose the function into a product of basic expansions ((9) and (10)):

$$\eta(x) = -2\alpha x e^{-b(x^2 - 2\Delta x)}
= -2\alpha x \left(e^{-bx^2}\right) \left(e^{2b\Delta x}\right)
= -2\alpha x \left(1 - bx^2 + \frac{1}{2!}b^2x^4 + \mathcal{O}\left(x^6\right)\right) \left(1 + 2b\Delta x + 2b^2\Delta^2x^2 + \frac{4}{3}b^3\Delta^3x^3 + \mathcal{O}\left(x^4\right)\right)
= -2\alpha x \left(1 + 2b\Delta x - bx^2 + 2b^2\Delta^2x^2 - 2\Delta b^2x^3 + \frac{4}{3}b^3\Delta^3x^3\right) + \mathcal{O}\left(x^4\right).$$
(15)

The leading order terms are

$$\eta(x) = -2\alpha x + 4\alpha b\Delta x^2 + 2\alpha b\Delta \left(1 - 2b\Delta^2\right) x^3 + \mathcal{O}\left(x^4\right)$$
(16)

3 Results

Equations (14) and (16) establish a leading order equivalence between the functions $\xi(x)$ and $\eta(x)$. The issue is when will the errors dominate. The leading terms in the error are

$$\xi(x) - \eta(x) = -4\alpha b\Delta x^2 + \frac{8}{3}\alpha b^2 \Delta^2 x^3 + \mathcal{O}(x^4). \tag{17}$$

This functions is plotted in figure 1

The constant term

$$\alpha = abe^{-b\Delta^2} \approx 1.91199 \times 10^{10},$$
 (18)

and the factor b controls the growth of the error term as the terms can be thought of as $\frac{\Delta x^2}{5000}$. But the error will grow quickly if the maximum value of x increases or b decreases.

4 PDF Attachments

а	1.00E+14	X	n	nx	nx1	nx1 rel err	In n	nx2	nx2 rel err
b	0.0002	0	1.0000 E+14	0.0000 E+00			32.24		
Delta	15	15	9.5600 E+13	-5.7360 E+11	-5.4910 E+11	-4.27%	32.19	-5.7360 E+11	-1.7025 E-15
x0	0	30	8.3527 E+13	-1.0023 E+12	-9.6340 E+11	-3.88%	32.06	-1.0023 E+12	-1.7050 E-15
		45	6.6698 E+13	-1.2006 E+12	-1.1617 E+12	-3.23%	31.83	-1.2006 E+12	4.8805 E-15
		60	4.8675 E+13	-1.1682 E+12	-1.1411 E+12	-2.32%	31.52	-1.1682 E+12	-1.6719 E-15
		75	3.2465 E+13	-9.7396 E+11	-9.6285 E+11	-1.14%	31.11	-9.7396 E+11	-1.6293 E-15
		90	1.9790 E+13	-7.1244 E+11	-7.1467 E+11	0.31%	30.62	-7.1244 E+11	1.5421 E-15
		105	1.1025 E+13	-4.6305 E+11	-4.7255 E+11	2.05%	30.03	-4.6305 E+11	1.1863 E-15
		120	5.6135 E+12	-2.6945 E+11	-2.8043 E+11	4.08%	29.36	-2.6945 E+11	-1.8122 E-15
		135	2.6121 E+12	-1.4106 E+11	-1.5009 E+11	6.40%	28.59	-1.4106 E+11	-1.5145 E-15
		150	1.1109 E+12	-6.6654 E+10	-7.2679 E+10	9.04%	27.74	-6.6654 E+10	4.5785 E-16
		165	4.3178 E+11	-2.8498 E+10	-3.1917 E+10	12.00%	26.79	-2.8498 E+10	2.6772 E-16
		180	1.5338 E+11	-1.1043 E+10	-1.2733 E+10	15.30%	25.76	-1.1043 E+10	0.0000 E+00
		195	4.9796 E+10	-3.8841 E+09	-4.6202 E+09	18.95%	24.63	-3.8841 E+09	-1.2277 E-16
		210	1.4775 E+10	-1.2411 E+09	-1.5263 E+09	22.98%	23.42	-1.2411 E+09	-1.9210 E-16
		225	4.0065 E+09	-3.6059 E+08	-4.5940 E+08	27.40%	22.11	-3.6059 E+08	9.9179 E-16
		240	9.9295 E+08	-9.5323 E+07	-1.2605 E+08	32.24%	20.72	-9.5323 E+07	9.3793 E-16
		255	2.2491 E+08	-2.2940 E+07	-3.1546 E+07	37.51%	19.23	-2.2940 E+07	-4.8717 E-16
		270	4.6557 E+07	-5.0282 E+06	-7.2032 E+06	43.26%	17.66	-5.0282 E+06	0.0000 E+00
		285	8.8082 E+06	-1.0041 E+06	-1.5011 E+06	49.50%	15.99	-1.0041 E+06	-1.1594 E-16
		300	1.5230 E+06	-1.8276 E+05	-2.8558 E+05	56.26%	14.24	-1.8276 E+05	1.5925 E-16
		315	2.4067 E+05	-3.0325 E+04	-4.9608 E+04	63.59%	12.39	-3.0325 E+04	2.3994 E-16
		330	3.4759 E+04	-4.5882 E+03	-7.8695 E+03	71.52%	10.46	-4.5882 E+03	-7.9290 E-16
		345	4.5880 E+03	-6.3314 E+02	-1.1402 E+03	80.08%	8.43	-6.3314 E+02	1.7956 E-16
		360	5.5346 E+02	-7.9698 E+01	-1.5090 E+02	89.34%	6.32	-7.9698 E+01	-1.7831 E-16
		375	6.1019 E+01	-9.1529 E+00	-1.8244 E+01	99.32%	4.11	-9.1529 E+00	-1.9408 E-16
		390	6.1484 E+00	-9.5915 E-01	-2.0151 E+00	110.09%	1.82	-9.5915 E-01	-1.1575 E-16
		405	5.6620 E-01	-9.1724 E-02	-2.0336 E-01	121.71%	-0.57	-9.1724 E-02	-3.0260 E-16
		420	4.7653 E-02	-8.0057 E-03	-1.8751 E-02	134.22%	-3.04	-8.0057 E-03	-2.1669 E-16
		435	3.6654 E-03	-6.3779 E-04	-1.5798 E-03	147.71%	-5.61	-6.3779 E-04	-3.3999 E-16
		450	2.5768 E-04	-4.6382 E-05	-1.2163 E-04	162.24%	-8.26	-4.6382 E-05	1.1688 E-15
		465	1.6555 E-05	-3.0793 E-06	-8.5568 E-06	177.88%	-11.01	-3.0793 E-06	8.2523 E-16
		480	9.7210 E-07	-1.8664 E-07	-5.5010 E-07	194.73%	-13.84	-1.8664 E-07	-7.0910 E-16
		495	5.2167 E-08	-1.0329 E-08	-3.2318 E-08	212.88%	-16.77	-1.0329 E-08	-6.4066 E-16
		510	2.5586 E-09	-5.2195 E-10	-1.7351 E-09	232.42%	-19.78	-5.2195 E-10	-3.9620 E-16
		525	1.1469 E-10	-2.4084 E-11	-8.5130 E-11	253.46%	-22.89	-2.4084 E-11	-5.3664 E-16
		540	4.6984 E-12	-1.0148 E-12	-3.8171 E-12	276.12%	-26.08	-1.0148 E-12	5.9698 E-16
		555	1.7591 E-13	-3.9052 E-14	-1.5641 E-13	300.52%	-29.37	-3.9052 E-14	4.8481 E-16
		570	6.0193 E-15	-1.3724 E-15	-5.8574 E-15	326.80%	-32.74	-1.3724 E-15	2.8740 E-16
		585	1.8824 E-16	-4.4048 E-17	-2.0046 E-16	355.10%	-36.21	-4.4048 E-17	-5.5966 E-16
		600	5.3802 E-18	-1.2912 E-18			-39.76		



setup

overhead

tag

```
Im[383]:= home = "ert/stc/algorithms/";
   Get["utility modules.m", Path → dirPack];
   stamp1;
   maximum memory: 0.210887 GB
   seed file: /Users/dantopa/Mathematica_files/nb/seed 19_12.nb
   user: dantopa, CPU: Xiuhcoatl, MM v. 12.0.0 for Mac OS X x86
   date: Mar 30, 2020, time: 16:16:46
   nb: /Users/dantopa/Mathematica_files/nb/ert/stc/algorithms/log-01.nb

modules, functions, settings, ...
```

2 spreadsheet

```
In[411]:= (* column B *)
                               n = 10^{14} Exp \left[ -\frac{x^2}{5000} \right];
                                % // N
\text{Out}[412] = \left\{1.\times10^{14},\,9.55997\times10^{13},\,8.3527\times10^{13},\,6.66977\times10^{13},\,4.86752\times10^{13},\,3.24652\times10^{13},\,6.66977\times10^{13},\,4.86752\times10^{13},\,3.24652\times10^{13},\,6.66977\times10^{13},\,4.86752\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^{13},\,6.66977\times10^
                                       1.97899 \times 10^{13}, 1.10251 \times 10^{13}, 5.61348 \times 10^{12}, 2.61214 \times 10^{12}, 1.1109 \times 10^{12},
                                       4.31784 \times 10^{11}, 1.53381 \times 10^{11}, 4.97955 \times 10^{10}, 1.47748 \times 10^{10}, 4.00653 \times 10^{9},
                                       9.9295 \times 10^{8}, 2.24906 \times 10^{8}, 4.65572 \times 10^{7}, 8.80818 \times 10^{6}, 1.523 \times 10^{6}, 240672., 34758.9,
                                       4587.96, 553.461, 61.0194, 6.1484, 0.5662, 0.047653, 0.00366543, 0.000257676,
                                       0.0000165552, 9.72099 \times 10^{-7}, 5.21674 \times 10^{-8}, 2.55859 \times 10^{-9}, 1.14688 \times 10^{-10},
                                      4.69835 \times 10^{-12}, 1.75909 \times 10^{-13}, 6.01928 \times 10^{-15}, 1.88241 \times 10^{-16}, 5.38019 \times 10^{-18}
   In[409]:= (* column c *)
                              nx = \frac{-2 \times n}{5000};
Out[410]= \{0., -5.73598 \times 10^{11}, -1.00232 \times 10^{12}, -1.20056 \times 10^{12}, -1.16821 
                                      -9.73957 \times 10^{11}, -7.12435 \times 10^{11}, -4.63052 \times 10^{11}, -2.69447 \times 10^{11}, -1.41056 \times 10^{11},
                                       -6.6654 \times 10^{10}, -2.84977 \times 10^{10}, -1.10434 \times 10^{10}, -3.88405 \times 10^{9}, -1.24109 \times 10^{9},
                                       -3.60588 \times 10^{8}, -9.53232 \times 10^{7}, -2.29404 \times 10^{7}, -5.02817 \times 10^{6}, -1.00413 \times 10^{6},
                                       -182760., -30324.7, -4588.18, -633.139, -79.6984, -9.15291, -0.95915,
                                       -0.0917243, -0.00800571, -0.000637785, -0.0000463816, -3.07927 \times 10^{-6},
                                       -1.86643 \times 10^{-7}, -1.03291 \times 10^{-8}, -5.21953 \times 10^{-10}, -2.40844 \times 10^{-11}, -1.01484 \times 10^{-12},
                                       -3.90518 \times 10^{-14}, -1.3724 \times 10^{-15}, -4.40484 \times 10^{-17}, -1.29124 \times 10^{-18}}
   In[407]:= (* column d *)
                                nx1 = Table
                                                     n[[k+1]] - n[[k-1]]
                                                    x[[k+1]] - x[[k-1]]
                                                   , {k, 2, Length[x] - 1}];
Out[408]= \{-5.49099 \times 10^{11}, -9.63402 \times 10^{11}, -1.16173 \times 10^{12}, -1.14108 \times 10
                                      -9.62845 \times 10^{11}, -7.14673 \times 10^{11}, -4.72546 \times 10^{11}, -2.8043 \times 10^{11}, -1.50086 \times 10^{11},
                                      -7.26786 \times 10^{10}, -3.19173 \times 10^{10}, -1.27329 \times 10^{10}, -4.62021 \times 10^{9}, -1.5263 \times 10^{9},
                                       -4.59396 \times 10^{8}, -1.26054 \times 10^{8}, -3.15464 \times 10^{7}, -7.20325 \times 10^{6}, -1.50114 \times 10^{6},
                                       -285 584., -49 608., -7869.48, -1140.18, -150.898, -18.2438, -2.01511,
                                       -0.203358, -0.0187511, -0.00157985, -0.000121629, -8.55679 \times 10^{-6},
                                       -5.50102 \times 10^{-7}, -3.2318 \times 10^{-8}, -1.73509 \times 10^{-9}, -8.51298 \times 10^{-11},
                                       -3.81706 \times 10^{-12}, -1.56411 \times 10^{-13}, -5.85736 \times 10^{-15}, -2.00463 \times 10^{-16}}
```

```
In[437]:= (* column e *)
                               relerror1 = Table
                                                  nx1[[k]] - nx[[k+1]]
                                                                            nx[[k+1]]
                                                 , {k, Length[nx1]}];
                              % // N
Out[438] = \{-0.0427114, -0.0388318, -0.0323447, -0.0232187, -0.0114093, 0.00314109, 0.0205036, -0.0114093, 0.00314109, 0.0205036, -0.0114093, 0.00314109, 0.0205036, -0.0114093, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.0031409, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.00314109, 0.003140
                                    0.0407632, 0.0640192, 0.090386, 0.119993, 0.152988, 0.189533, 0.22981, 0.274021,
                                    0.322386, 0.37515, 0.432577, 0.494961, 0.562617, 0.635893, 0.715164, 0.80084,
                                    0.893365, 0.99322, 1.10093, 1.21706, 1.34222, 1.47708, 1.62236, 1.77883,
                                    1.94735, 2.12882, 2.32423, 2.53464, 2.76122, 3.00522, 3.26798, 3.55098}
                                (* column f *)
                              ln = Log[n];
                              % // N
Out[421] = \{32.2362, 32.1912, 32.0562, 31.8312, 31.5162, 31.1112, 30.6162, 30.0312, 29.3562, 31.8312, 31.5162, 31.1112, 30.6162, 30.0312, 29.3562, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.5162, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312, 31.8312
                                     28.5912, 27.7362, 26.7912, 25.7562, 24.6312, 23.4162, 22.1112, 20.7162, 19.2312,
                                    17.6562, 15.9912, 14.2362, 12.3912, 10.4562, 8.43119, 6.31619, 4.11119, 1.81619,
                                    -0.568809, -3.04381, -5.60881, -8.26381, -11.0088, -13.8438, -16.7688,
                                    -19.7838, -22.8888, -26.0838, -29.3688, -32.7438, -36.2088, -39.7638
  In[428]:= (* column g *)
                              nx2 = Table
                                               n[[k+1]] \ \frac{ln[[k]] - ln[[k+2]]}{x[[k]] - x[[k+2]]}
                                                , {k, Length[nx1]}];
                              % // N
Out[429]= \{-5.73598 \times 10^{11}, -1.00232 \times 10^{12}, -1.20056 \times 10^{12}, -1.16821 \times 10
                                    -9.73957 \times 10^{11}, -7.12435 \times 10^{11}, -4.63052 \times 10^{11}, -2.69447 \times 10^{11}, -1.41056 \times 10^{11},
                                    -6.6654 \times 10^{10}, -2.84977 \times 10^{10}, -1.10434 \times 10^{10}, -3.88405 \times 10^{9}, -1.24109 \times 10^{9},
                                    -3.60588 \times 10^{8}, -9.53232 \times 10^{7}, -2.29404 \times 10^{7}, -5.02817 \times 10^{6}, -1.00413 \times 10^{6},
                                    -182760., -30324.7, -4588.18, -633.139, -79.6984, -9.15291, -0.95915,
                                    -0.0917243, -0.00800571, -0.000637785, -0.0000463816, -3.07927 \times 10^{-6},
                                    -1.86643 \times 10^{-7}, -1.03291 \times 10^{-8}, -5.21953 \times 10^{-10}, -2.40844 \times 10^{-11},
                                    -1.01484 \times 10^{-12}, -3.90518 \times 10^{-14}, -1.3724 \times 10^{-15}, -4.40484 \times 10^{-17}}
```

```
 \begin{array}{l} \text{relerror2 = Table} \Big[ \\ & \underbrace{ \begin{array}{l} nx2[[k]] - nx[[k+1]] \\ nx[[k+1]] \\ \end{array} \\ & \underbrace{ \begin{array}{l} nx[[k+1]] \\ nx[[k+1]] \\ \end{array} \\ \end{array} \Big] \\ \text{s. } // \text{ N} \\ \\ \text{Out[443]= } \Big\{ -1.4897 \times 10^{-15}, -1.58323 \times 10^{-15}, 4.88054 \times 10^{-15}, -1.6719 \times 10^{-15}, -1.50401 \times 10^{-15}, \\ 1.88477 \times 10^{-15}, 1.31811 \times 10^{-15}, -1.58564 \times 10^{-15}, -1.51446 \times 10^{-15}, 3.43388 \times 10^{-16}, \\ 2.67719 \times 10^{-16}, 1.72713 \times 10^{-16}, 0., -1.92105 \times 10^{-16}, -1.65299 \times 10^{-16}, 9.37935 \times 10^{-16}, \\ 6.49561 \times 10^{-16}, 0., 0., -4.77739 \times 10^{-16}, 3.59903 \times 10^{-16}, 1.98226 \times 10^{-16}, \\ 1.79561 \times 10^{-16}, 0., -1.94076 \times 10^{-16}, 0., 0., -2.16686 \times 10^{-16}, -1.69995 \times 10^{-16}, \\ 0., -2.75076 \times 10^{-16}, 7.09102 \times 10^{-16}, 4.80493 \times 10^{-16}, -3.96195 \times 10^{-16}, \\ -4.02481 \times 10^{-16}, -3.97989 \times 10^{-16}, 4.84809 \times 10^{-16}, -4.31104 \times 10^{-16}, -5.59655 \times 10^{-16} \Big\} \end{array}
```

3 plots

```
In[436]:= ListLogPlot[{x, n}<sup>T</sup>,

PlotStyle \rightarrow Black,

PlotLabel \rightarrow "Gaussian function n(x)",

FrameLabel \rightarrow {"x", "n"},

Frame \rightarrow True]

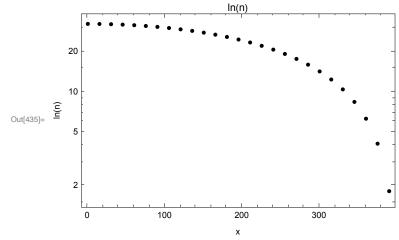
Gaussian function n(x)

10^{15}
10^{5}

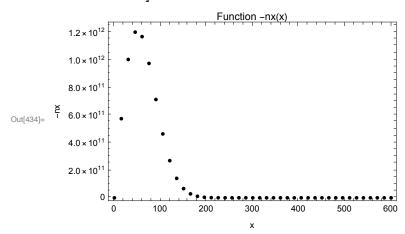
Out[436]=

Out[436]=
```

```
In[435]:= ListLogPlot[{x, ln}<sup>T</sup>,
        PlotStyle → Black,
        PlotLabel \rightarrow "ln(n)",
        FrameLabel \rightarrow {"x", "ln(n)"},
        Frame → True]
```



ln[434]:= ListPlot[{x, Abs[nx]}^T, PlotStyle → Black, PlotLabel \rightarrow "Function -nx(x)", FrameLabel $\rightarrow \{"x", "-nx"\},\$ PlotRange → All, Frame → True]



```
ln[432] = x = Drop[Drop[x, -1], 1];
         ListPlot[\{x, Abs[nx1]\}^{\mathsf{T}},
           PlotStyle \rightarrow Blue, PlotLabel \rightarrow "Function -nx1(x)",
           FrameLabel \rightarrow \{"x", "-nx1"\},
           PlotRange → All,
           Frame → True]
                                              Function -nx1(x)
             1.2 \times 10^{12}
             1.0 \times 10^{12}
             8.0 \times 10^{11}
         ₹ 6.0 × 10<sup>11</sup>
Out[433]=
             4.0 \times 10^{11}
             2.0\times10^{11}
                      0
                                 100
                                                      300
                                                                 400
                                                                            500
ln[431]:= ListPlot[{x, Abs[nx2]}^{T},
           PlotStyle → Blue,
           PlotLabel \rightarrow "Function -nx2(x)",
           FrameLabel → {"x", "-nx2"},
           PlotRange → All,
           Frame → True]
                                               Function -nx2(x)
             1.2 \times 10^{12}
             1.0 \times 10^{12}
             8.0 \times 10^{11}
         X
F 6.0 × 10<sup>11</sup>
Out[431]=
             4.0 \times 10^{11}
             2.0 \times 10^{11}
                    0
                      0
                                100
                                                      300
                                                                 400
                                                                            500
```

```
ln[447] = ListPlot[{x, Abs[relerror2 // N]}^T,
           PlotStyle → Blue,
           PlotLabel → "Function |relerror2|",
           FrameLabel → {"x", "|relerror2|"},
           PlotRange → All,
           Frame → True]
                                           Function |relerror2|
             5. × 10<sup>-15</sup>
             4. \times 10^{-15}
Out[447]= \frac{\overline{Q}}{\frac{b}{2}} 3. × 10<sup>-15</sup>
             1. \times 10^{-15}
                               100
                                         200
                                                             400
                                                                        500
                                                   300
```

relerror2

end

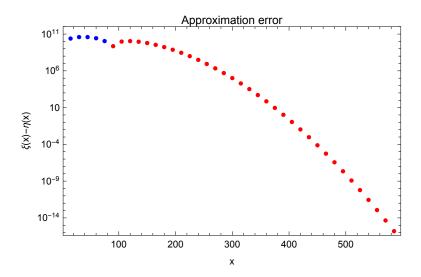


Figure 1: The error term in (17). Positive values are plotted in blue; the absolute value of the negative terms is plotted in red.