Four Methods of Numerical Double Integration: Sequential Simpson's Rule, Multitasking Simpson's Rule, Sequential Monte Carlo and Multitasking Monte Carlo Methods © Wednesday April 16 – 18, 2025, by James Pate Williams, Jr.

We use four two-dimensional functions to test our integration methods (Wolfram, 2025):

$$\int_0^\infty\int_0^\infty e^{-x^2-y^2}dxdy=\int_0^\infty\int_0^{\pi/2} e^{-r^2}rdrd\vartheta=-\frac{\pi r}{2}e^{-r^2}\Big]_{r=0}^{r=\infty}=\frac{\pi}{4}\approx 0.78539816$$

$$(4\pi)^2\int_0^\infty\left[\int_0^{r_1}\frac{1}{r_1}e^{-2\zeta_1 r_1-2\zeta_2 r_2}r_2^2dr_2+\int_{r_1}^\infty\frac{1}{r_2}e^{-2\zeta_1 r_1-2\zeta_2 r_2}r_2^2dr_2\right]r_1^2dr_1=\frac{5Z}{8}\forall\zeta_1=\zeta_2=Z$$

The second integral in P. A. M. Dirac's Bra-Ket notation (Dirac, 1958 Reprinted 1978) is:

$$\left\langle 1s(\zeta_1)1s(\zeta_2)\middle|\frac{1}{r_{12}}\middle|1s(\zeta_1)1s(\zeta_2)\right\rangle=1.25\ for\ Z=2$$

The second integral computation is in (Schiff, Chapter 8 Approximation Methods for Bound States Electron Interaction Energy, 1968)

The other two test functions are:

$$\left\langle 1s(\zeta_1)2s(\zeta_2)\middle|\frac{1}{r_{12}}\middle|1s(\zeta_1)2s(\zeta_2)\right\rangle$$

$$\left\langle 2s(\zeta_1)2s(\zeta_2)\middle|\frac{1}{r_{12}}\middle|2s(\zeta_1)2s(\zeta_2)\right\rangle$$

Where (Schiff, Chapter 4 Discete Eigenvalues: Bound States Hydrogen-Atom Wave Functions, 1968):

$$|1s(\zeta_1)\rangle=2\pi{\zeta_1}^{3/2}e^{-\zeta_1 r_1}$$

$$|2s(\zeta_1)\rangle=2\pi\left(\frac{\zeta_1}{2}\right)^{3/2}(2-\zeta_1 r_1)e^{-\zeta_1 r_1/2}$$

The first integrals using sequential Simpson's Rule and sequential Monte Carlo Method are:

```
Sequential Simpson's Rule 2D
b, d = 25
m, n = 1000
exp(-r * r) = +8.0252315412E-001
Percent Error % = 2.1804
Runtime in milliseconds = 151
```

```
Sequential Simpson's Rule 2D
b, d = 25
m, n = 2000
exp(-r * r) = +7.9398783493E-001
Percent Error % = 1.0937
Runtime in milliseconds = 603
Sequential Simpson's Rule 2D
b, d = 25
m, n = 3000
exp(-r * r) = +7.9113053930E-001
Percent Error % = 0.7299
Runtime in milliseconds = 1399
Sequential Simpson's Rule 2D
b, d = 25
m, n = 4000
exp(-r * r) = +7.8969965262E-001
Percent Error % = 0.5477
Runtime in milliseconds = 2404

Sequential Monte Carlo 2D
b, d = 25
m, n = 1000
exp(-r * r) = +8.2501213124E-001
Percent Error % = 5.0438
Runtime in milliseconds = 58
Sequential Monte Carlo 2D
b, d = 25
m, n = 2000
exp(-r * r) = +7.9512049650E-001
Percent Error % = 1.2379
Runtime in milliseconds = 228
Sequential Monte Carlo 2D
b, d = 25
m, n = 3000
exp(-r * r) = +7.8944065697E-001
Percent Error % = 0.5147
Runtime in milliseconds = 543
Sequential Monte Carlo 2D
b, d = 25
m, n = 4000
exp(-r * r) = +7.8335087500E-001
Percent Error % = 0.2607
Runtime in milliseconds = 953
```

The first integrals using the multitasking algorithms are:

```
Multitasking Simpson's Rule 2D
b, d = 25
m, n = 1000
exp(-r * r) = +8.2248862437E-001
Percent Error % = 4.7225
Runtime in milliseconds = 108
Multitasking Simpson's Rule 2D
b, d = 25
m, n = 2000
exp(-r * r) = +8.0390347056E-001
Percent Error % = 2.3562
Runtime in milliseconds = 351
Multitasking Simpson's Rule 2D
b, d = 25
m, n = 3000
exp(-r * r) = +7.9772581839E-001
Percent Error % = 1.5696
Runtime in milliseconds = 712
Multitasking Simpson's Rule 2D
b, d = 25
m, n = 4000
exp(-r * r) = +7.9464040016E-001
Percent Error % = 1.1768
Runtime in milliseconds = 1288

Multitasking Monte Carlo 2D
b, d = 25
m, n = 1000
exp(-r * r) = +8.1275362550E-001
Percent Error % = 3.4830
Runtime in milliseconds = 16
Multitasking Monte Carlo 2D
b, d = 25
m, n = 2000
exp(-r * r) = +7.8577820075E-001
Percent Error % = 0.0484
Runtime in milliseconds = 60
Multitasking Monte Carlo 2D
b, d = 25
m, n = 3000
exp(-r * r) = +7.9115851400E-001
Percent Error % = 0.7334
Runtime in milliseconds = 172
```

```
Multitasking Monte Carlo 2D
b, d = 25
m, n = 4000
exp(-r * r) = +7.8714426395E-001
Percent Error % = 0.2223
Runtime in milliseconds = 290
```

The second integrals are as illustrated next:

```
Sequential Simpson's Rule 2D
b, d = 25
m, n = 1000
<1s1s|r12|1s1s> = +1.2504518185E+000
Percent Error % = 0.0361
Runtime in milliseconds = 175
Sequential Simpson's Rule 2D
b, d = 25
m, n = 2000
<1s1s|r12|1s1s> = +1.2500811003E+000
Percent Error % = 0.0065
Runtime in milliseconds = 698
Sequential Simpson's Rule 2D
b, d = 25
m, n = 3000
<1s1s|r12|1s1s> = +1.2500316019E+000
Percent Error % = 0.0025
Runtime in milliseconds = 1571
Sequential Simpson's Rule 2D
b, d = 25
m, n = 4000
<1s1s|r12|1s1s> = +1.2500165548E+000
Percent Error % = 0.0013
Runtime in milliseconds = 2767
```

```
Sequential Monte Carlo 2D
b, d = 25
m, n = 1000
<1s1s|r12|1s1s> = +1.3274021639E+000
Percent Error % = 6.1922
Runtime in milliseconds = 62
Sequential Monte Carlo 2D
b, d = 25
m, n = 2000
<1s1s|r12|1s1s> = +1.2672928192E+000
Percent Error % = 1.3834
Runtime in milliseconds = 246
```

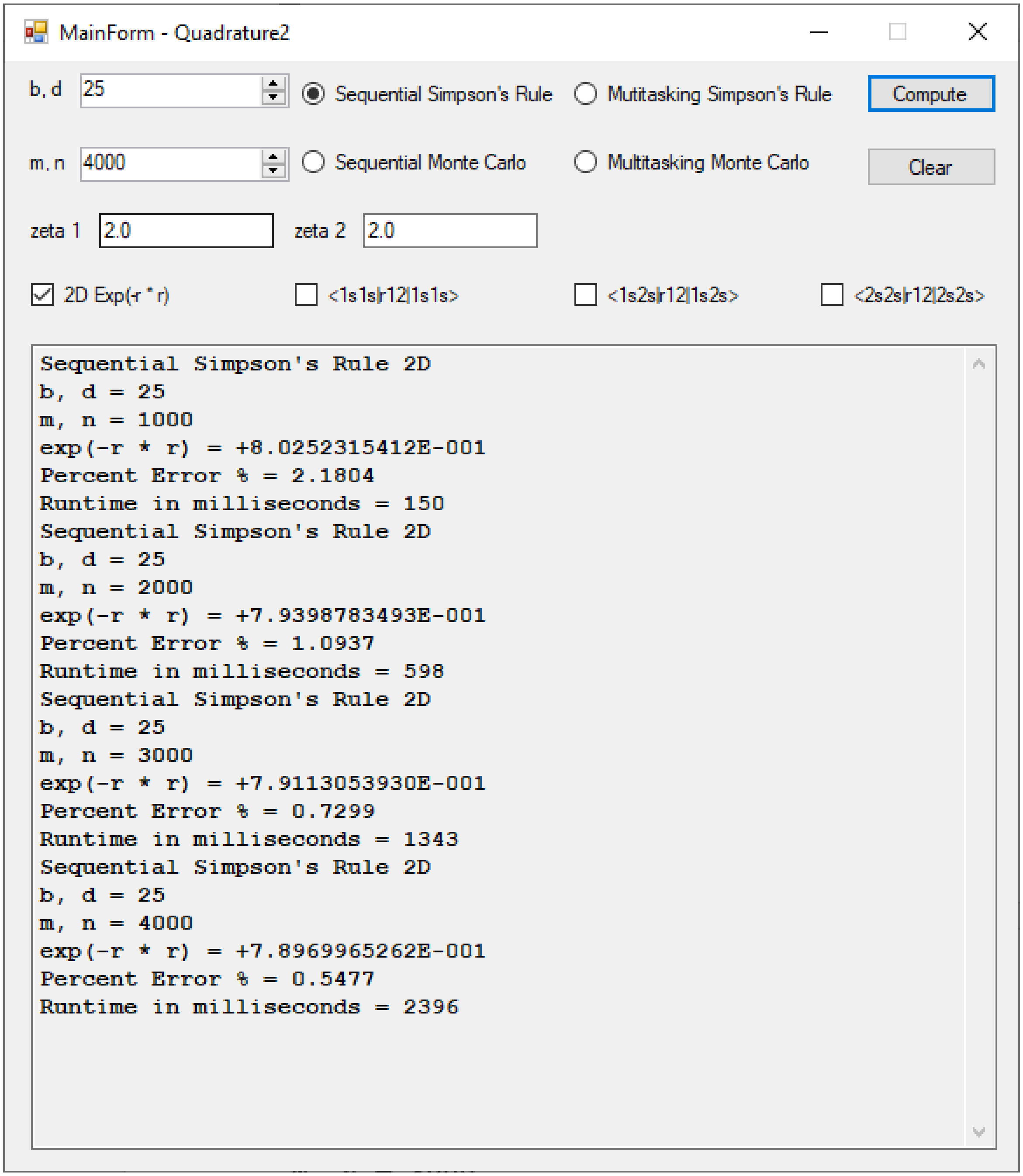
```
Sequential Monte Carlo 2D
b, d = 25
m, n = 3000
<1s1s|r12|1s1s> = +1.2480384345E+000
Percent Error % = 0.1569
Runtime in milliseconds = 553
Sequential Monte Carlo 2D
b, d = 25
m, n = 4000
<1s1s|r12|1s1s> = +1.2407146168E+000
Percent Error % = 0.7428
Runtime in milliseconds = 979

Sequential Simpson's Rule 2D
b, d = 25
m, n = 1000
<1s2s|r12|1s2s> = +1.3363752252E-001
Runtime in milliseconds = 185
Sequential Simpson's Rule 2D
b, d = 25
m, n = 2000
<1s2s|r12|1s2s> = +1.3361550637E-001
Runtime in milliseconds = 745
Sequential Simpson's Rule 2D
b, d = 25
m, n = 3000
<1s2s|r12|1s2s> = +1.3361295831E-001
Runtime in milliseconds = 1661
Sequential Simpson's Rule 2D
b, d = 25
m, n = 4000
<1s2s|r12|1s2s> = +1.3361224802E-001
Runtime in milliseconds = 2975

Sequential Monte Carlo 2D
b, d = 25
m, n = 1000
<1s2s|r12|1s2s> = +1.3614671566E-001
Runtime in milliseconds = 79
Sequential Monte Carlo 2D
b, d = 25
m, n = 2000
<1s2s|r12|1s2s> = +1.3395677562E-001
```

```
Runtime in milliseconds = 261
Sequential Monte Carlo 2D
b, d = 25
m, n = 3000
<1s2s|r12|1s2s> = +1.3318468738E-001
Runtime in milliseconds = 585
Sequential Monte Carlo 2D
b, d = 25
m, n = 4000
<1s2s|r12|1s2s> = +1.3296865354E-001
Runtime in milliseconds = 1066

Multitasking Simpson's Rule 2D
b, d = 25
m, n = 1000
<1s2s|r12|1s2s> = +1.3367656085E-001
Runtime in milliseconds = 96
Multitasking Simpson's Rule 2D
b, d = 25
m, n = 2000
<1s2s|r12|1s2s> = +1.3362014591E-001
Runtime in milliseconds = 379
Multitasking Simpson's Rule 2D
b, d = 25
m, n = 3000
<1s2s|r12|1s2s> = +1.3361430926E-001
Runtime in milliseconds = 928
Multitasking Simpson's Rule 2D
b, d = 25
m, n = 4000
<1s2s|r12|1s2s> = +1.3361281279E-001
Runtime in milliseconds = 1566

Multitasking Monte Carlo 2D
b, d = 25
m, n = 1000
<1s2s|r12|1s2s> = +1.3579830290E-001
Runtime in milliseconds = 17
Multitasking Monte Carlo 2D
b, d = 25
m, n = 2000
<1s2s|r12|1s2s> = +1.3396986474E-001
Runtime in milliseconds = 97
```

```
Multitasking Monte Carlo 2D
b, d = 25
m, n = 3000
<1s2s|r12|1s2s> = +1.3420144209E-001
Runtime in milliseconds = 202
Multitasking Monte Carlo 2D
b, d = 25
m, n = 4000
<1s2s|r12|1s2s> = +1.3364533843E-001
Runtime in milliseconds = 344

Sequential Simpson's Rule 2D
b, d = 25
m, n = 1000
<2s2s|r12|2s2s> = +3.8298144678E-001
Runtime in milliseconds = 375
Sequential Simpson's Rule 2D
b, d = 25
m, n = 2000
<2s2s|r12|2s2s> = +3.8296903139E-001
Runtime in milliseconds = 1576
Sequential Simpson's Rule 2D
b, d = 25
m, n = 3000
<2s2s|r12|2s2s> = +3.8296749379E-001
Runtime in milliseconds = 3364
Sequential Simpson's Rule 2D
b, d = 25
m, n = 4000
<2s2s|r12|2s2s> = +3.8296704621E-001
Runtime in milliseconds = 6039

Sequential Monte Carlo 2D
b, d = 25
m, n = 1000
<2s2s|r12|2s2s> = +3.8894699444E-001
Runtime in milliseconds = 133
Sequential Monte Carlo 2D
b, d = 25
m, n = 2000
<2s2s|r12|2s2s> = +3.8311914621E-001
Runtime in milliseconds = 530
```

```
Sequential Monte Carlo 2D
b, d = 25
m, n = 3000
<2s2s|r12|2s2s> = +3.8246631143E-001
Runtime in milliseconds = 1258
Sequential Monte Carlo 2D
b, d = 25
m, n = 4000
<2s2s|r12|2s2s> = +3.8252753278E-001
Runtime in milliseconds = 2147

Multitasking Simpson's Rule 2D
b, d = 25
m, n = 1000
<2s2s|r12|2s2s> = +3.8300095396E-001
Runtime in milliseconds = 191
Multitasking Simpson's Rule 2D
b, d = 25
m, n = 2000
<2s2s|r12|2s2s> = +3.8297135080E-001
Runtime in milliseconds = 764
Multitasking Simpson's Rule 2D
b, d = 25
m, n = 3000
<2s2s|r12|2s2s> = +3.8296816922E-001
Runtime in milliseconds = 1946
Multitasking Simpson's Rule 2D
b, d = 25
m, n = 4000
<2s2s|r12|2s2s> = +3.8296732858E-001
Runtime in milliseconds = 3287

Multitasking Monte Carlo 2D
b, d = 25
m, n = 1000
<2s2s|r12|2s2s> = +3.8294345091E-001
Runtime in milliseconds = 43
Multitasking Monte Carlo 2D
b, d = 25
m, n = 2000
<2s2s|r12|2s2s> = +3.8311197445E-001
Runtime in milliseconds = 177
```

```
Multitasking Monte Carlo 2D
b, d = 25
m, n = 3000
<2s2s|r12|2s2s> = +3.8258663720E-001
Runtime in milliseconds = 407
Multitasking Monte Carlo 2D
b, d = 25
m, n = 4000
<2s2s|r12|2s2s> = +3.8275796450E-001
Runtime in milliseconds = 736
```



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