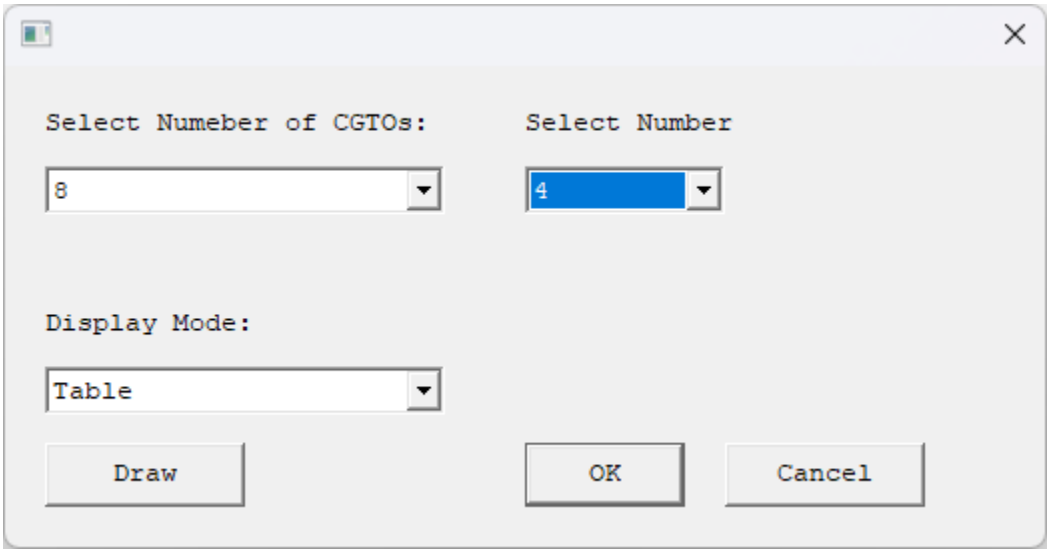
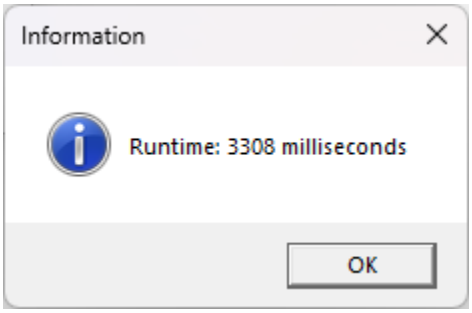
Blog Entry © Monday, August 18, 2025, by James Pate Williams, Jr. Curve Fitting Contracted Gaussian Type 1s Orbitals (CGTO-1s) to a Slater Type 1s Orbital

I translated a 2015 C# application which did the curve fitting mentioned above in this blog entry's title to a Win32 Desktop C++ Release x64 Configuration. I had some minor help from Microsoft Copilot. See Figure 3.2 page 157 of the following online textbook:

modern-quantum-chemistry.pdf



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Evolutionary Elitist Hill Climber Fit
Coefficient Exponent
+1.2449805200       0.1621838038
+0.5200133274       1.9312197241
+0.0104762932       0.0005272591
+0.3812456648       0.5888630848

Hill Climber Norm =  0.0228093466

Dr. H. T. Lau's Least Squares Fit
Coefficient Exponent
+0.2295772202       0.8463109183
+0.5344139072       0.3132735131
+0.9139620226       0.5245481629
+0.4572048093       0.4434528938
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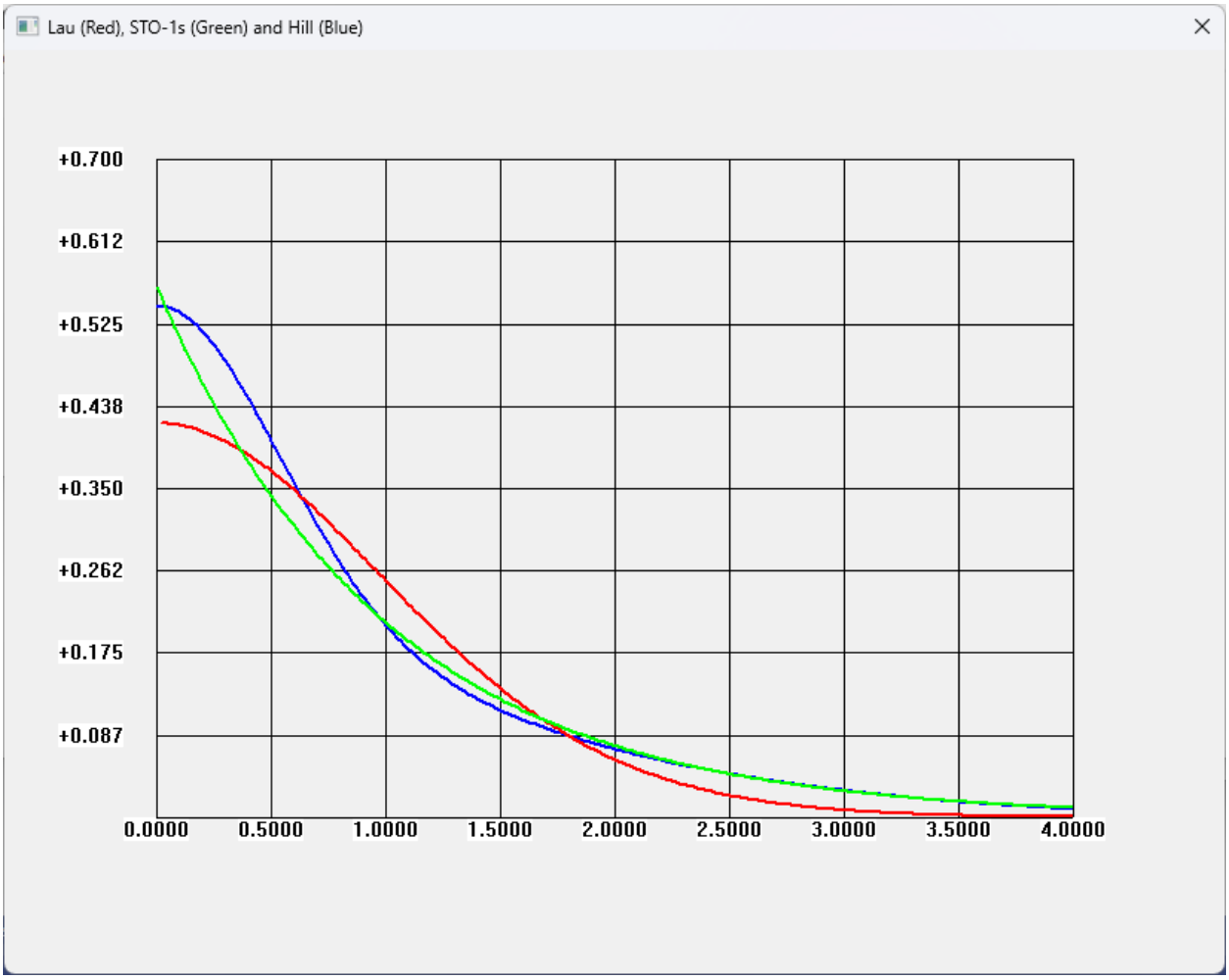
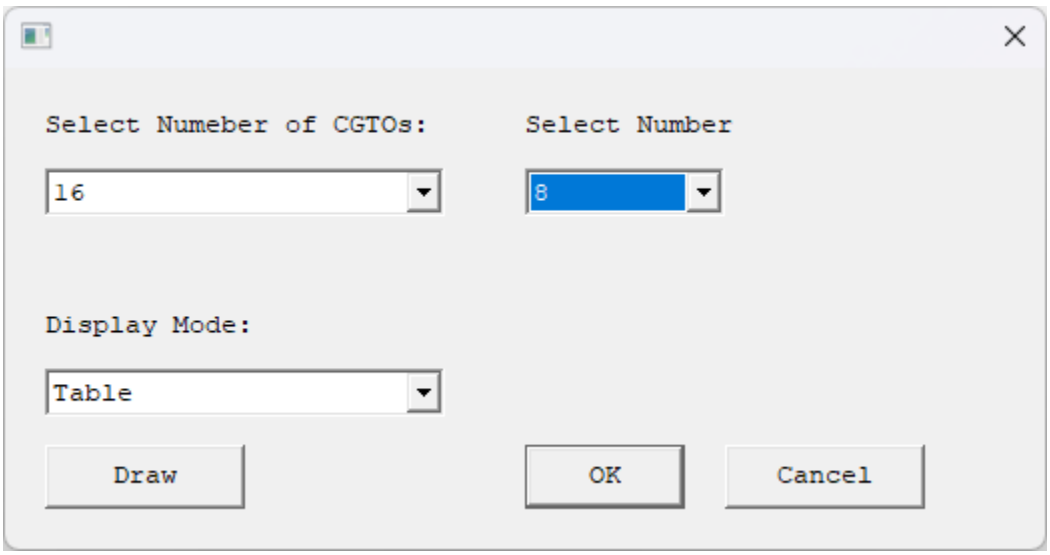
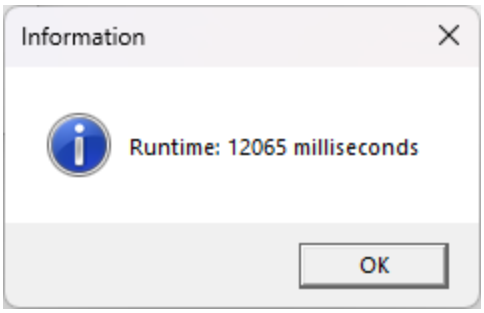
Least Squares Norm = 0.0331865471





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Evolutionary Elitist Hill Climber Fit
Coefficient    Exponent
+0.9947592608   0.5912435286
+1.3645520402   0.8151883511
-1.0179059206   0.2379528184
+0.3661390027   2.8303170873
+1.2981437635   0.2382969665
+0.2344211158   0.5777238289
-2.0655453139   0.9591967528
+0.2249298593   0.3246033113

Hill Climber Norm =  0.0159540765

Dr. H. T. Lau's Least Squares Fit
Coefficient    Exponent
+0.8650202455   0.4572048093
+0.8291469109   0.4306985702
+0.8296033647   0.9391277950
+0.2730499774   0.7783892355
+0.0592431971   0.7159705110
+0.6705280414   0.8027575035
+0.5930655168   0.0928008103
+0.6716540918   0.5181525484

Least Squares Norm =  0.0338618182
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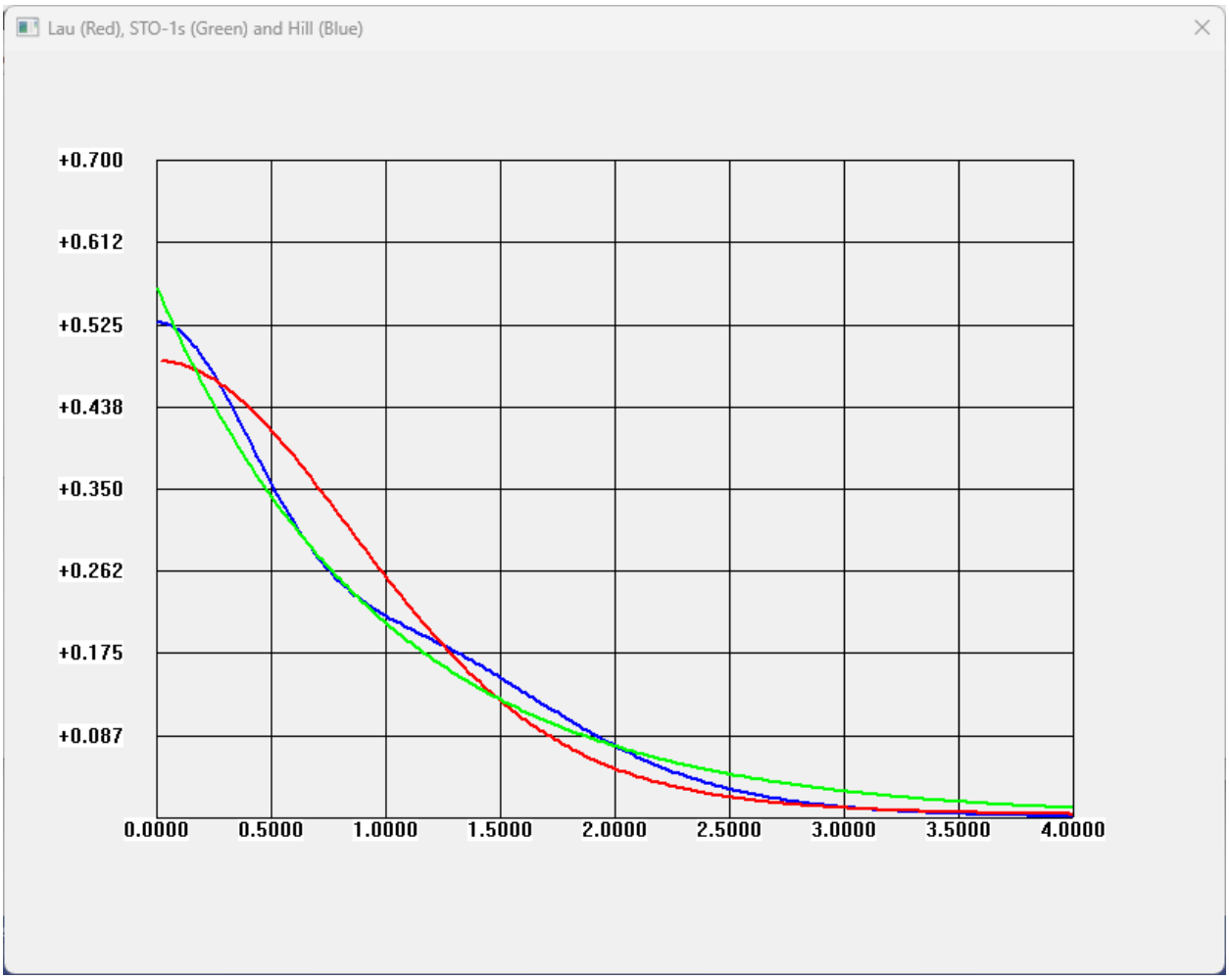
Lau (Red), STO-1s (Green) and Hill (Blue)
+0.700
+0.612
+0.525
+0.438
+0.350
+0.262
+0.175
+0.087
0.0000
0.5000
1.0000
1.5000
2.0000
2.5000
3.0000
3.5000
4.0000