### **Global Variables**

```
In[1]:= prec = 100;
      Nmax = 100;
      x = 20.0;
      xmax = 20.0;
      xmin = -20.0;
      xsize = 100;
      dx = (xmax - xmin) / (xsize - 1);
      Xvector = N[Range[xmin, xmax, dx], prec];
                 L. lintervalo de valores
      Nvector = Range[0, Nmax, 1];
                 intervalo de valores
      Wavefuntion_Wolfram_Mathematica_1
In[10]:= WavefunctionMathematica1[n_, x_, prec_] :=
        Module[{nPrec, xPrec, norm, H, wavefunction},
        módulo de código
         SetPrecision[n, prec];
         define precisão
         SetPrecision[x, prec];
         define precisão
         norm = (2^{(-0.5 * n)}) * (Gamma[n+1]^{(-0.5)}) * (Pi^{(-0.25)});
                                   função gama de Euler
         H = HermiteH[n, x];
             polinômios de Hermite
         wavefunction = SetPrecision[norm * Exp[-0.5 * x^2] * H, prec];
                         define precisão
                                             exponencial
         wavefunction];
      Wavefuntion Wolfram Mathematica 2
In[11]:= WavefunctionMathematica2[n_, x_, prec_] :=
        Module[{wavefunction, xsize, i}, SetPrecision[x, prec];
        módulo de código
                                           define precisão
         wavefunction = Table[SetPrecision[0, prec], {n + 1}, {Length[x]}];
                         tabela define precisão
                                                                  comprimento
         wavefunction[1] = SetPrecision[Pi^(-1/4) Exp[-(x^2)/2], prec];
                            define precisão número pi
                                                       exponencial
         wavefunction[2] = SetPrecision[(2 x wavefunction[1]) / Sqrt[2], prec];
                            define precisão
                                                                   raiz quadrada
         For [i = 3, i \le n + 1, i++, wavefunction[i]] = 2 \times (wavefunction[i - 1]] / Sqrt[2(i - 1)]) -
                                                                                 raiz quadrada
         para cada
              Sqrt[(i-2) / (i-1)] \times wavefunction[[i-2]];];
              raiz quadrada
         wavefunction[n + 1]];
```

## Wavefuntion\_Wolfram\_Mathematica\_3

```
In[12]:= WavefunctionMathematica3[n_, x_, prec_] :=
       Module[{wavefunction, i}, SetPrecision[x, prec];
       módulo de código
                                 define precisão
         wavefunction = Table[SetPrecision[0, prec], {n + 1}, {Length[x]}];
                       tabela define precisão
                                                             comprimento
         wavefunction[1] = SetPrecision[Pi^{(-1/4)} Exp[-(x^2)/2], prec];
                          For [i = 1, i \le n, i++,
        para cada
          wavefunction[i + 1] =
           SetPrecision[2 x (wavefunction[i] / Sqrt[2 (i)]) -
           define precisão
                                             raiz quadrada
             Sqrt[(i-1) / i] x wavefunction[i-1], prec]];
             raiz quadrada
         wavefunction];
```

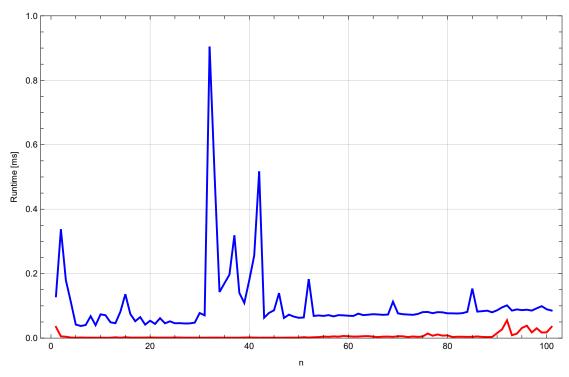
### **Tests**

★ Single-Mode and Onedimensional speed test

```
In[25]:= (*To use timeit.repeat in the Python is a option too*)
      FastWaveSMODList = Normal[ExternalEvaluate["Python",
                         normal execução externa
           "import fast_wave.wavefunction_numba as wn;import timeit;N_max = 100;x =
             20.0; [(timeit.timeit(lambda : wn.psi_n_single_fock_single_position(n,
             x) , number=10000) /10000) *1000 for n in range(N_max+1)];"]];
     WavefunctionWolframSMODList = {};
      For [i = 1, i \le (Nmax + 1), i++, AppendTo[WavefunctionWolframSMODList,]
         RepeatedTiming[WavefunctionMathematica1[i - 1, x, prec]] [1] * 1000];]
         cronometra repetidamente
      ListLinePlot[
     gráfico de linha de uma lista de valores
       {WavefunctionWolframSMODList, FastWaveSMODList},
       PlotStyle → {Blue, Red},
       estilo do gráfico azul vermelho
       Frame → True,
      quadro verdadeiro
       FrameLabel → {"n", "Runtime [ms]"},
      Legenda do quadro
       PlotLabel →
      etiqueta de gráfico
        Row[{Style["Wavefunction_Wolfram1 vs Wavefunction_Fast-Wave(sfmp)", Bold, 13],
        linha estilo
           "\n", Style["x: 20.0, to each value of n \n", 12]}],
                estilo
       GridLines → Automatic,
       grade de linhas automático
       PlotLegends →
      Legenda do gráfico
        Placed[{" avg[Wavefunction Wolfram1] = " <> ToString[SetPrecision[Mean[
        situado
                                                        converte··· define precisão média
               \label{lem:wavefunctionWolframSMODList], 20], TraditionalForm] <> " ms;", \\
                                                     _forma tradicional
          " avg[Fast-Wave(sfmp)] = " <> ToString[
                                           Lonverte em cadeia de caracteres
             SetPrecision[Mean[FastWaveSMODList], 20], TraditionalForm] <> " ms"}, Below],
             define precisão média
                                                          forma tradicional
                                                                                         abaixo
       ImageSize → Large ,
       tamanho da ··· grande
       PlotRange → {{Automatic, Automatic}, {0, 1.0}}
      intervalo do gráf··· automático automático
      Functionality Test Passed: True
```

## Wavefunction\_Wolfram1 vs Wavefunction\_Fast-Wave(sfmp)

x: 20.0, to each value of n



- avg[Wavefunction\_Wolfram1] = 0.10514299280147740290 ms;
- avg[Fast-Wave(sfmp)] = 0.0061750070297038476066 ms

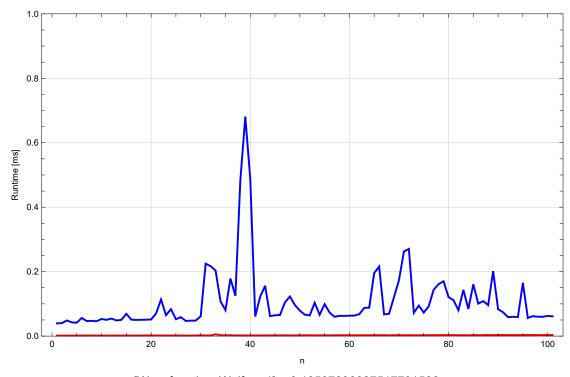
### ★ Single-Mode and Onedimensional speed test (less\_fast)

```
In[29]:= FastWaveSMODList =
                                                        "import fast_wave.wavefunction_numba
        Normal[ExternalEvaluate["Python",
        normal execução externa
             as wn;import timeit; N_max = 100; x = 20.0; [(timeit.timeit(lambda
             : wn.psi_n_single_fock_single_position(n, x, more_fast=False)
             , number=10000) /10000) *1000 for n in range(N_max+1)];"]];
     WavefunctionWolframSMODList = {};
      For [i = 1, i \le (Nmax + 1), i++, AppendTo[WavefunctionWolframSMODList,]
     para cada
         RepeatedTiming[WavefunctionMathematica1[i - 1, x, prec]] [1] * 1000];]
         cronometra repetidamente
      ListLinePlot[
     gráfico de linha de uma lista de valores
       {WavefunctionWolframSMODList, FastWaveSMODList},
       PlotStyle → {Blue, Red},
      estilo do gráfico azul vermelho
       Frame → True,
       quadro verdadeiro
       FrameLabel → {"n", "Runtime [ms]"},
       legenda do quadro
       PlotLabel →
      Letiqueta de gráfico
        Row[{Style["Wavefunction Wolfram1 vs Wavefunction Fast-Wave(sfsp; less fast)",
        linha estilo
            Bold, 13], "\n", Style["x: 20.0, to each value of n \n", 12]}],
       GridLines → Automatic,
       grade de linhas automático
       PlotLegends →
      Llegenda do gráfico
        Placed[{" avg[Wavefunction_Wolfram1] = " <> ToString[SetPrecision[Mean[
        situado
                                                        converte··· define precisão média
               WavefunctionWolframSMODList], 20], TraditionalForm] <> " ms;",
                                                     forma tradicional
           " avg[Fast-Wave(sfsp; less_fast)] = " <> ToString[
                                                       converte em cadeia de caracteres
             SetPrecision[Mean[FastWaveSMODList], 20], TraditionalForm] <> " ms"}, Below],
             define precisão _média
                                                          forma tradicional
                                                                                         abaixo
       ImageSize → Large ,
       tamanho da ··· grande
       PlotRange → {{Automatic, Automatic}, {0, 1.0}}
      intervalo do gráf··· automático automático
      1
      Functionality Test Passed: True
```

Out[32]=

## Wavefunction\_Wolfram1 vs Wavefunction\_Fast-Wave(sfsp; less\_fast)

x: 20.0, to each value of n



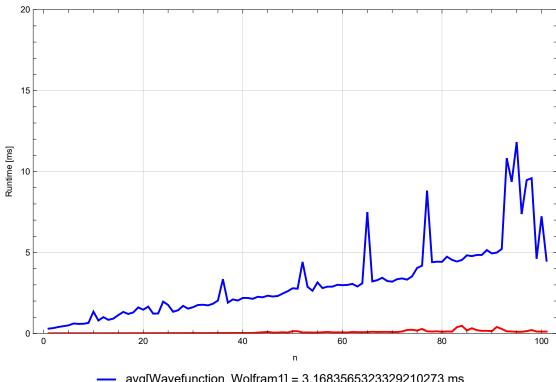
- avg[Wavefunction\_Wolfram1] = 0.10537896027517791586 ms;
- avg[Fast-Wave(sfsp; less\_fast)] = 0.0024588139603966374484 ms

### ★ Single-Mode and Multidimensional speed test

```
In[41]:= FastWaveSMMDList =
                                                        "import fast_wave.wavefunction_numba
        Normal[ExternalEvaluate["Python",
        normal execução externa
             as wn;import timeit;import numpy as np;N_max = 100;xmax =
             20.0;xmin=-20.0;xsize=100;X=np.linspace(xmin,xmax,xsize);[(timeit.timeit(
             lambda : wn.psi_n_single_fock_multiple_position(n,
             X) , number=10000) /10000) *1000 for n in range(N_max+1)];"]];
     WavefunctionWolframSMMDList = {};
      For[i = 1, i ≤ (Nmax + 1), i++, AppendTo[WavefunctionWolframSMMDList,
         RepeatedTiming[WavefunctionMathematica1[i - 1, Xvector, prec]][1] * 1000];]
         cronometra repetidamente
      ListLinePlot[
     gráfico de linha de uma lista de valores
       {WavefunctionWolframSMMDList, FastWaveSMMDList},
       PlotStyle → {Blue, Red},
       estilo do gráfico azul vermelho
       Frame → True,
       quadro verdadeiro
       FrameLabel → {"n", "Runtime [ms]"},
       legenda do quadro
       PlotLabel →
       etiqueta de gráfico
        Row[{Style["Wavefunction_Wolfram1 vs Wavefunction_Fast-Wave(sfmp)", Bold, 13],
        linha Lestilo
           "\n", Style["X: [(-20.0) \rightarrow 20.0 ; 100], to each value of n \n", 12]}],
                estilo
       GridLines → Automatic,
       grade de linhas automático
       PlotLegends → Placed[{" avg[Wavefunction_Wolfram1] = " <> ToString[
      legenda do gráfico situado
                                                                      converte em cadeia de caracteres
             SetPrecision[Mean[WavefunctionWolframSMMDList], 20], TraditionalForm] <> " ms",
             define precisão média
                                                                      forma tradicional
           " avg[Fast-Wave(sfmp)] = " <> ToString[
                                           converte em cadeia de caracteres
             SetPrecision[Mean[FastWaveSMMDList], 20], TraditionalForm] <> " ms"}, Below],
             define precisão média
                                                          forma tradicional
       ImageSize → Large , PlotRange → {{Automatic, Automatic}, {0, 20.0}}
      Lamanho da ··· Lgrande Lintervalo do gráf··· Lautomático Lautomático
      ]
      Functionality Test Passed: True
```

Out[44]=

# Wavefunction\_Wolfram1 vs Wavefunction\_Fast-Wave(sfmp) X: [(-20.0) $\rightarrow$ 20.0; 100], to each value of n



- avg[Wavefunction\_Wolfram1] = 3.1683565323329210273 ms
- avg[Fast-Wave(sfmp)] = 0.084915205544553590267 ms

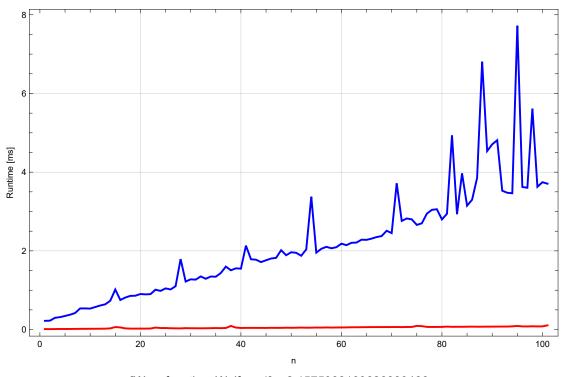
### ★ Single-Mode and Multidimensional speed test (less\_fast)

```
In[45]:= FastWaveSMMDList =
                                                        "import fast_wave.wavefunction_numba
        Normal[ExternalEvaluate["Python",
        Lnormal Lexecução externa
             as wn;import timeit;import numpy as np;N_max = 100;xmax =
             20.0;xmin=-20.0;xsize=100;X=np.linspace(xmin,xmax,xsize);[(timeit.timeit(
             lambda : wn.psi_n_single_fock_multiple_position(n,
             X, more_fast = False) , number=10000) /10000) *1000
             for n in range(N_max+1)];"]];
      WavefunctionWolframSMMDList = {};
      For [i = 1, i \le (Nmax + 1), i++, AppendTo[WavefunctionWolframSMMDList,]
     para cada
                                     adiciona a
         RepeatedTiming[WavefunctionMathematica1[i - 1, Xvector, prec]][1] * 1000];]
         cronometra repetidamente
      ListLinePlot[
     gráfico de linha de uma lista de valores
       {WavefunctionWolframSMMDList, FastWaveSMMDList},
       PlotStyle → {Blue, Red},
      estilo do gráfico azul
                          vermelho
       Frame → True,
       _quadro _verdadeiro
       FrameLabel → {"n", "Runtime [ms]"},
       legenda do quadro
       PlotLabel →
      etiqueta de gráfico
        Row[{Style["Wavefunction_Wolfram1 vs Wavefunction_Fast-Wave(sfmp; less_fast)", Bold,
            13], "\n", Style["X: [(-20.0) \rightarrow 20.0 ; 100], to each value of n \n", 12]}],
       GridLines → Automatic,
       grade de linhas automático
       PlotLegends → Placed[{" avg[Wavefunction_Wolfram1] = " <> ToString[
       legenda do gráfico situado
                                                                      converte em cadeia de caracteres
             SetPrecision[Mean[WavefunctionWolframSMMDList], 20], TraditionalForm] <> " ms",
             define precisão média
                                                                       forma tradicional
           " avg[Fast-Wave(sfmp; less_fast)] = " <> ToString[
                                                       converte em cadeia de caracteres
             SetPrecision[Mean[FastWaveSMMDList], 20], TraditionalForm] <> " ms"}, Below],
                                                          forma tradicional
             define precisão média
       ImageSize → Large ]
      tamanho da ··· grande
      Functionality Test Passed: True
```

Out[48]=

## Wavefunction\_Wolfram1 vs Wavefunction\_Fast-Wave(sfmp; less\_fast)

X:  $[(-20.0) \rightarrow 20.0$ ; 100], to each value of n



- avg[Wavefunction\_Wolfram1] = 2.1575988109626389466 ms
- avg[Fast-Wave(sfmp; less\_fast)] = 0.050787311188119750593 ms

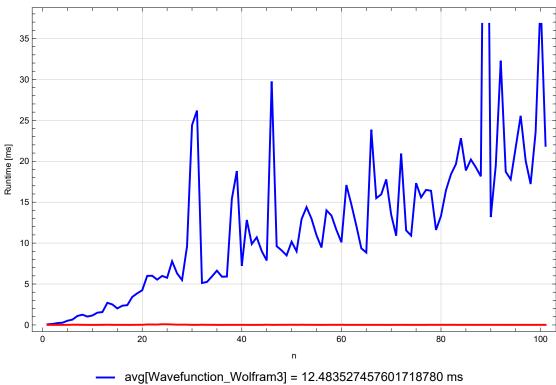
### ★ Multi-Mode and Onedimensional speed test

```
In[53]:= FastWaveMMODList = Normal[ExternalEvaluate["Python",
                         normal execução externa
           "import fast_wave.wavefunction_numba as wn;import timeit;N_max = 100;x =
             20.0;[(timeit.timeit(lambda : wn.psi_n_multiple_fock_single_position(n,
             x) , number=10000) /10000) *1000 for n in range(N max+1)];"]];
     WavefunctionWolframMMODList = {};
      For [i = 1, i \le (Nmax + 1), i++, AppendTo [WavefunctionWolframMMODList,]
         RepeatedTiming[WavefunctionMathematica3[i - 1, x, prec]] [1] * 1000];]
         cronometra repetidamente
      ListLinePlot[
     gráfico de linha de uma lista de valores
       {WavefunctionWolframMMODList, FastWaveMMODList},
       PlotStyle → {Blue, Red},
      Lestilo do gráfico Lazul Lvermelho
       Frame → True,
       _quadro _verdadeiro
       FrameLabel → {"n", "Runtime [ms]"},
      legenda do quadro
       PlotLabel →
       etiqueta de gráfico
        Row[{Style["Wavefunction_Wolfram3 vs Wavefunction_Fast-Wave(mfsp)", Bold, 13],
        linha estilo
                                                                                   negrito
           "\n", Style["x: 20.0, to each value of n \n", 12]}],
                estilo
       GridLines → Automatic,
       grade de linhas automático
       PlotLegends → Placed[{" avg[Wavefunction_Wolfram3] = " <> ToString[
       legenda do gráfico situado
                                                                      converte em cadeia de caracteres
             SetPrecision[Mean[WavefunctionWolframMMODList], 20], TraditionalForm] <> " ms",
             define precisão média
                                                                       forma tradicional
           " avg[Fast-Wave(mfsp)] = " <> ToString[
                                           converte em cadeia de caracteres
             SetPrecision[Mean[FastWaveMMODList], 20], TraditionalForm] <> " ms"}, Below],
             define precisão média
                                                           forma tradicional
                                                                                         labaixo
       ImageSize → Large ]
      tamanho da ··· grande
      Functionality Test Passed: True
```

Out[56]=

## Wavefunction\_Wolfram3 vs Wavefunction\_Fast-Wave(mfsp)

x: 20.0, to each value of n



- avg[Fast-Wave(mfsp)] = 0.017711036435646230341 ms

### ★ Multi-Mode and Multidimensional speed test

```
In[57]:= FastWaveMMMDList =
                                                        "import fast_wave.wavefunction_numba as
        Normal[ExternalEvaluate["Python",
        normal execução externa
             wn; import timeit;import numpy as np;N_max = 100;xmax = 20.0;xmin =
             -20.0;xsize=100;X=np.linspace(xmin,xmax,xsize);[(timeit.timeit(lambda
             : wn.psi_n_multiple_fock_multiple_position(n, X) ,
             number=10000) /10000) *1000 for n in range(N_max+1)];"]];
      WavefunctionWolframMMMDList = {};
      For[i = 1, i ≤ (Nmax + 1), i++, AppendTo[WavefunctionWolframMMMDList,
     para cada
                                     adiciona a
         RepeatedTiming[WavefunctionMathematica3[i - 1, Xvector, prec]][1] * 1000];]
         cronometra repetidamente
      ListLinePlot[
     gráfico de linha de uma lista de valores
       {WavefunctionWolframMMMDList, FastWaveMMMDList},
       PlotStyle → {Blue, Red},
      Lestilo do gráfico Lazul Lvermelho
       Frame → True,
       quadro verdadeiro
       FrameLabel → {"n", "Runtime [ms]"},
       Llegenda do quadro
       PlotLabel →
       etiqueta de gráfico
        Row[{Style["Wavefunction Wolfram3 vs Wavefunction Fast-Wave(mfmp)", Bold, 13],
           "\n", Style["X: [(-20.0) \rightarrow 20.0 ; 100], to each value of n \n", 12]}],
       GridLines → Automatic,
       grade de linhas automático
       PlotLegends → Placed[{" avg[Wavefunction_Wolfram3] = " <> ToString[
       legenda do gráfico situado
                                                                      converte em cadeia de caracteres
             SetPrecision[Mean[WavefunctionWolframMMMDList], 20], TraditionalForm] <> " ms",
             define precisão média
                                                                       forma tradicional
           " avg[Fast-Wave(mfmp)] = " <> ToString[
                                           converte em cadeia de caracteres
             SetPrecision[Mean[FastWaveMMMDList], 20], TraditionalForm] <> " ms"}, Below],
             define precisão | média
                                                          forma tradicional
                                                                                         abaixo
       ImageSize → Large ]
       Ltamanho da ··· Lgrande
      Functionality Test Passed: True
```

Out[60]=

## Wavefunction\_Wolfram3 vs Wavefunction\_Fast-Wave(mfmp)

X:  $[(-20.0) \rightarrow 20.0$ ; 100], to each value of n

