Global Variables

In[145]:=

```
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];
          (·· intervalo de valores
Nvector = Range[0, Nmax, 1];
          intervalo de valores
```

Wavefuntion_Wolfram_Mathematica_1

In[154]:=

```
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      número pi
   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[155]:=

```
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 ≤ n + 1, i++, wavefunction[[i]] = 2 x (wavefunction[[i - 1]] / Sqrt[2 (i - 1)]) -
   para cada                                                                   raiz quadrada
       Sqrt[(i - 2) / (i - 1)] wavefunction[[i - 2]];];
       raiz quadrada
   wavefunction[[n + 1]];
```

Wavefuntion_Wolfram_Mathematica_3

In[156]:=

```
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];
                       define precisão  número pi  exponencial
   For[i = 1, i ≤ n, i++,
   para cada
    wavefunction[[i + 1]] =
     SetPrecision[2 x (wavefunction[[i]] / Sqrt[2 (i)]) -
     define precisão                       raiz quadrada
       Sqrt[(i - 1) / i] wavefunction[[i - 1]], prec]];
       raiz quadrada

   wavefunction];
```

Tests

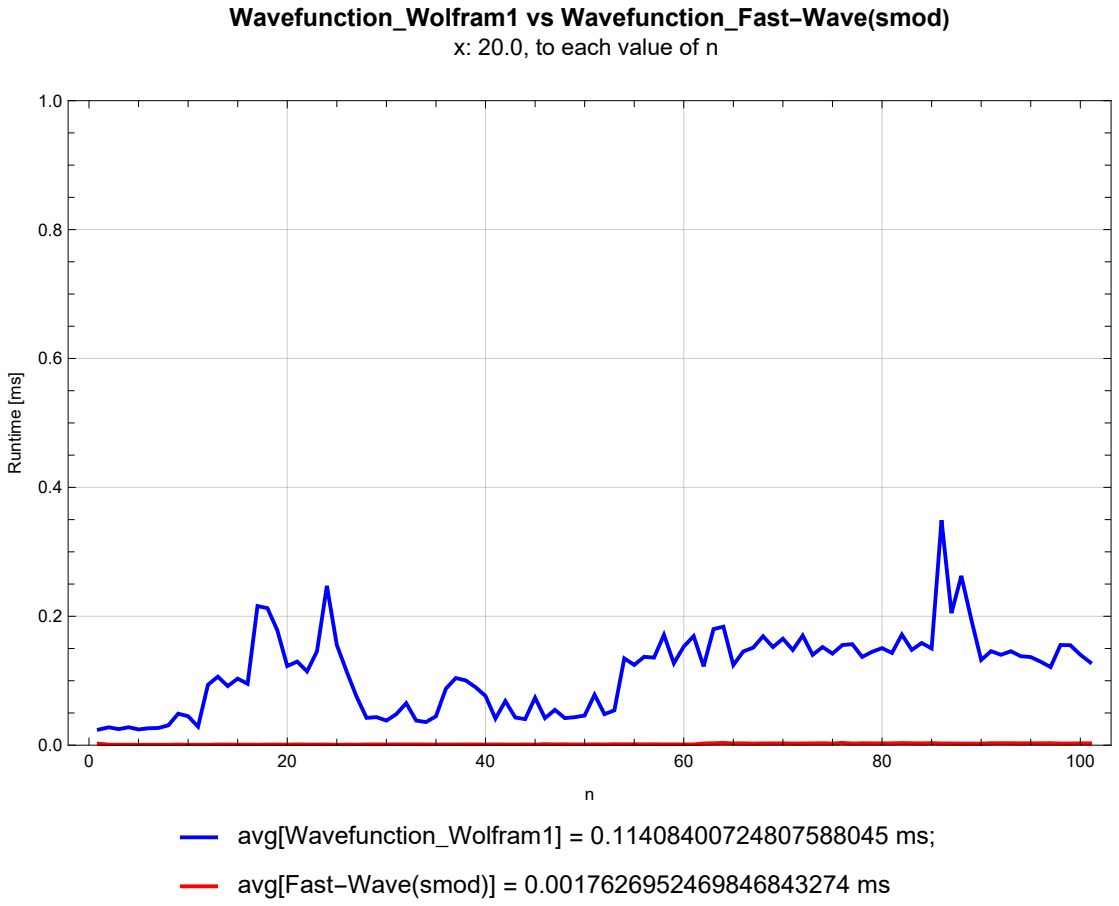
★ Single-Mode and Onedimensional speed test

In[157]:=

```
(*To use timeit.repeat in the Python is a option too*)

FastWaveSMODList = Normal[ExternalEvaluate["Python",
                   normal  execução externa
    "from fast_wave.wavefunction import wavefunction_smod;import timeit;N_max
      = 100;x = 20.0;[(timeit.timeit(lambda : wavefunction_smod(n,
      x) , number=10000)/10000)*1000 for n in range(N_max+1)];"]];

WavefunctionWolframSMODList = {};
For[i = 1, i ≤ (Nmax + 1), i++, AppendTo[WavefunctionWolframSMODList,
 para cada                      adiciona a
   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(smod)", 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 →
 legenda do gráfico
   Placed[{" avg[Wavefunction_Wolfram1] = " <> ToString[SetPrecision[Mean[
  situado                                  converte···  define precisão  média
         WavefunctionWolframSMODList], 20], TraditionalForm] <> " ms;",
                                                 forma tradicional
     " avg[Fast-Wave(smod)] = " <> 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
]
```

```
Functionality Test Passed: True
```

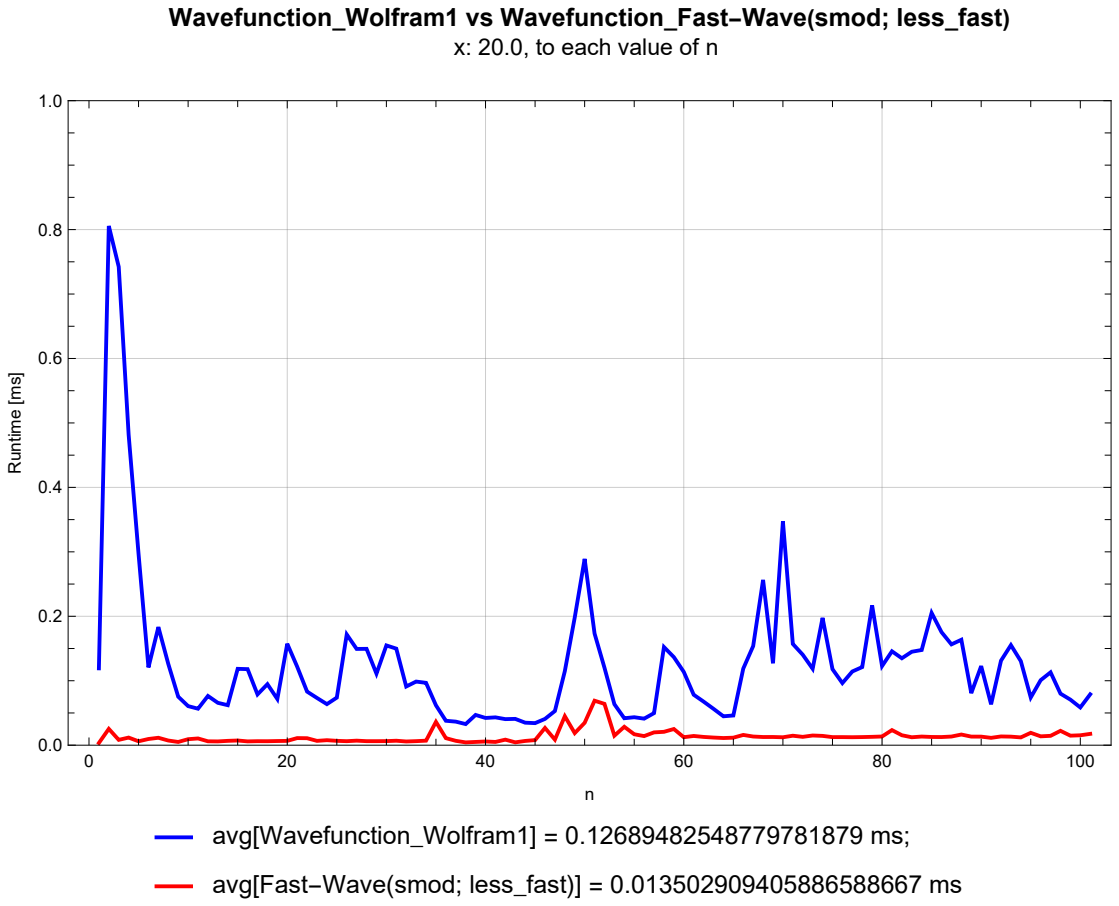
Out[160]=


Wavefunction_Wolfram1 vs Wavefunction_Fast−Wave(smod)
x: 20.0, to each value of n
Runtime [ms]
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
100
n
avg[Wavefunction_Wolfram1] = 0.11408400724807588045 ms;
avg[Fast−Wave(smod)] = 0.0017626952469846843274 ms

★ Single-Mode and Onedimensional speed test (less_fast)

```
In[•]:= FastWaveSMODList =
          Normal[ExternalEvaluate["Python",          "from fast_wave.wavefunction
          normal  execução externa
               import wavefunction_smod;import timeit;N_max = 100;x =
               20.0;[(timeit.timeit(lambda : wavefunction_smod(n, x, more_fast=False)
                                                                                falso
               , number=10000)/10000)*1000 for n in range(N_max+1)];"]];

        WavefunctionWolframSMODList = {};
        For[i = 1, i ≤ (Nmax + 1), i++, AppendTo[WavefunctionWolframSMODList,
        para cada                       adiciona a
            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(smod; less_fast)",
           linha  estilo
               Bold, 13], "\n", Style["x: 20.0, to each value of n \n", 12]}],
               negrito  estilo
          GridLines → Automatic,
          grade de linhas  automático
          PlotLegends →
          legenda do gráfico
           Placed[{" avg[Wavefunction_Wolfram1] = " <> ToString[SetPrecision[Mean[
           situado                                  converte···  define precisão  média
                  WavefunctionWolframSMODList], 20], TraditionalForm] <> " ms;",
                                                      forma tradicional
             " avg[Fast-Wave(smod; 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
        ]
        Functionality Test Passed: True
```

Out[•]=

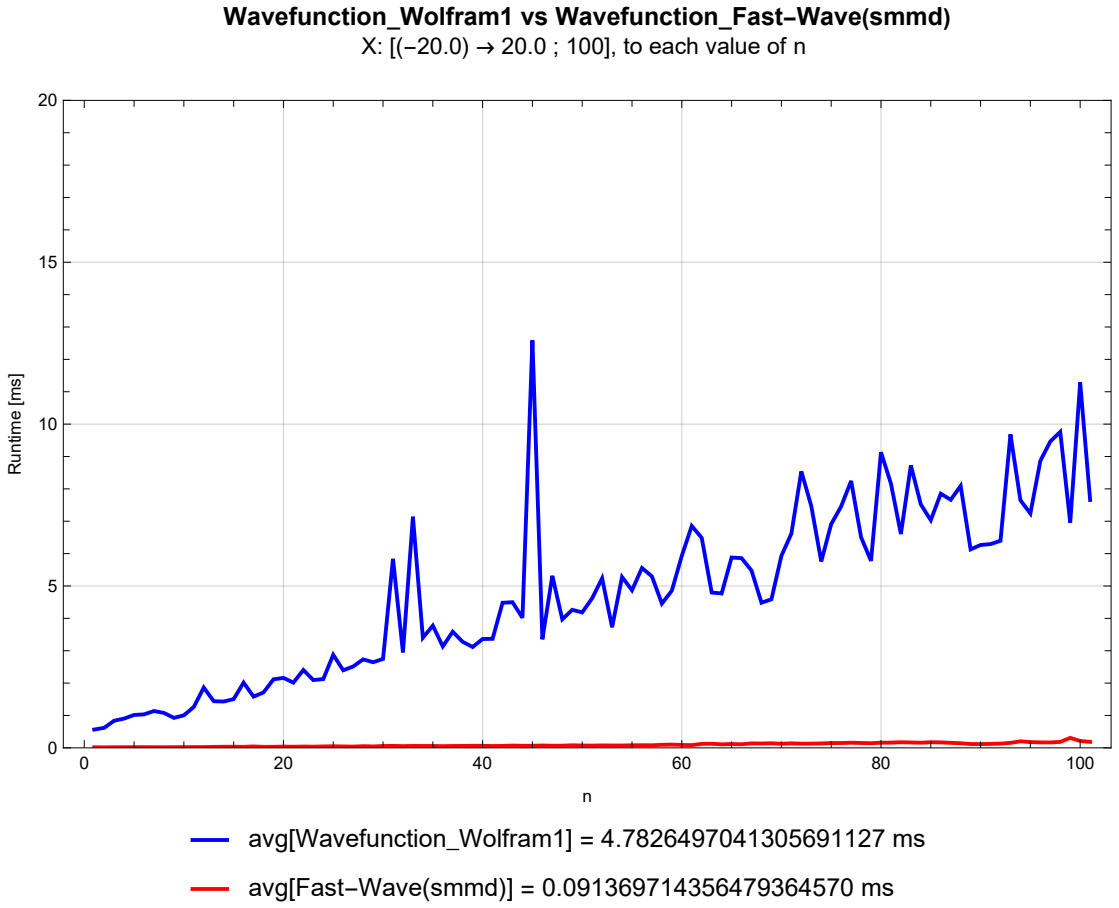

Wavefunction_Wolfram1 vs Wavefunction_Fast−Wave(smod; less_fast)
x: 20.0, to each value of n
Runtime [ms]
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
100
n
avg[Wavefunction_Wolfram1] = 0.12689482548779781879 ms;
avg[Fast−Wave(smod; less_fast)] = 0.013502909405886588667 ms

★ Single-Mode and Multidimensional speed test

In[161]:=

```
FastWaveSMMDList =
  Normal[ExternalEvaluate["Python",          "from fast_wave.wavefunction import
  normal  execução externa
      wavefunction_smmd;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 : wavefunction_smmd(n, X) ,
      number=10000)/10000)*1000 for n in range(N_max+1)];"]];

WavefunctionWolframSMMDList = {};
For[i = 1, i ≤ (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(smmd)", Bold, 13],
  linha  estilo                                                        negrito
     "\n", Style["X: [(-20.0) → 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 gráficc  situado                              converte em cadeia de caracteres
      SetPrecision[Mean[WavefunctionWolframSMMDList], 20], TraditionalForm] <> " ms",
      define precisão  média                               forma tradicional
    " avg[Fast-Wave(smmd)] = " <> ToString[
                                  converte em cadeia de caracteres
      SetPrecision[Mean[FastWaveSMMDList], 20], TraditionalForm] <> " ms"}, Below],
      define precisão  média                    forma tradicional          abaixo
 ImageSize → Large , PlotRange → {{Automatic, Automatic}, {0, 20.0}}
 tamanho da ···  grande  intervalo do gráf···  automático  automático
]
Functionality Test Passed: True
```

Out[164]=

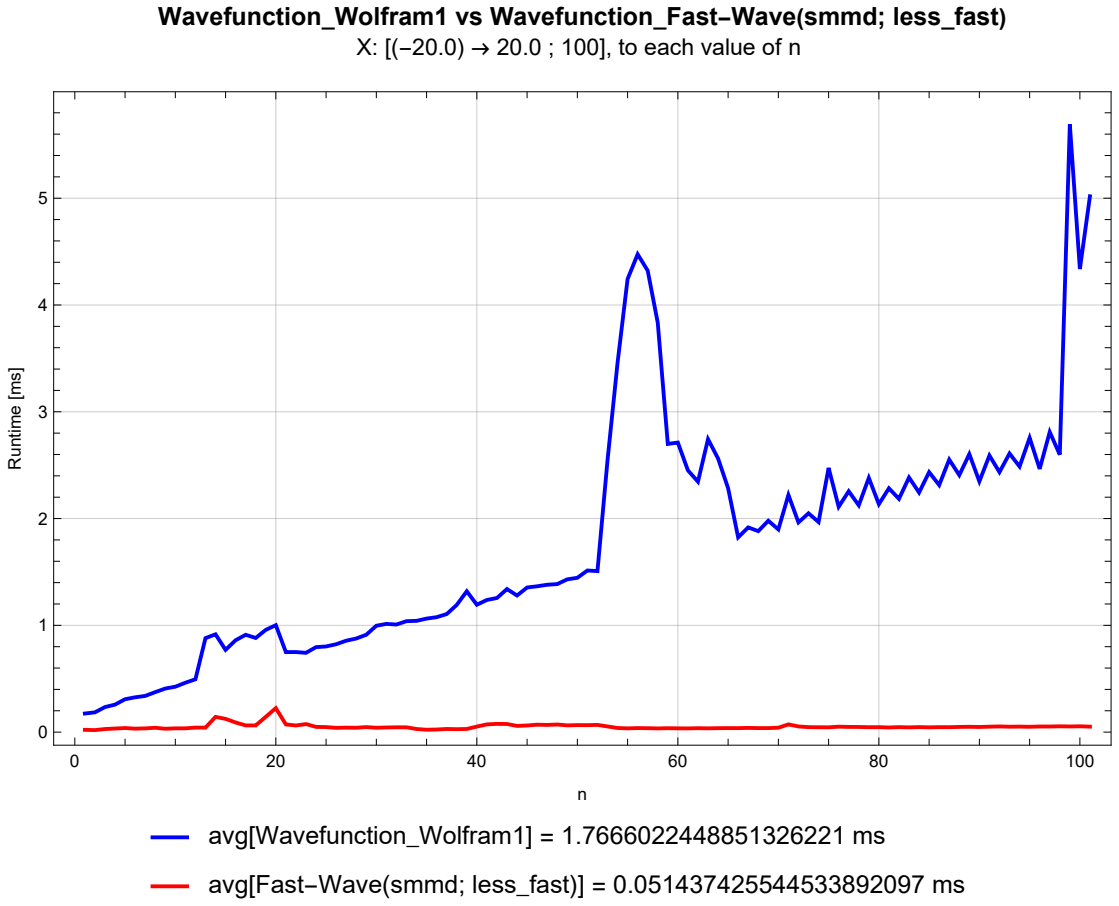

Wavefunction_Wolfram1 vs Wavefunction_Fast−Wave(smmd)
X: [(−20.0) → 20.0 ; 100], to each value of n
Runtime [ms]
n
0
5
10
15
20
0
20
40
60
80
100
avg[Wavefunction_Wolfram1] = 4.7826497041305691127 ms
avg[Fast−Wave(smmd)] = 0.091369714356479364570 ms

★ Single-Mode and Multidimensional speed test (less_fast)

In[•]:=
```
FastWaveSMMDList =
  Normal[ExternalEvaluate["Python",          "from fast_wave.wavefunction import
  normal  execução externa
      wavefunction_smmd;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 : wavefunction_smmd(n, X, more_fast = False)
                                                  falso
      , number=10000)/10000)*1000 for n in range(N_max+1)];"]];

WavefunctionWolframSMMDList = {};
For[i = 1, i ≤ (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(smmd; less_fast)", Bold,
  linha  estilo                                                                  negrito
     13], "\n", Style["X: [(-20.0) → 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 gráficc  situado                              converte em cadeia de caracteres
      SetPrecision[Mean[WavefunctionWolframSMMDList], 20], TraditionalForm] <> " ms",
      define precisão  média                               forma tradicional
    " avg[Fast-Wave(smmd; less_fast)] = " <> ToString[
                                          converte em cadeia de caracteres
      SetPrecision[Mean[FastWaveSMMDList], 20], TraditionalForm] <> " ms"}, Below],
      define precisão  média                    forma tradicional          abaixo
 ImageSize → Large ]
 tamanho da ···  grande
```

```
Functionality Test Passed: True
```

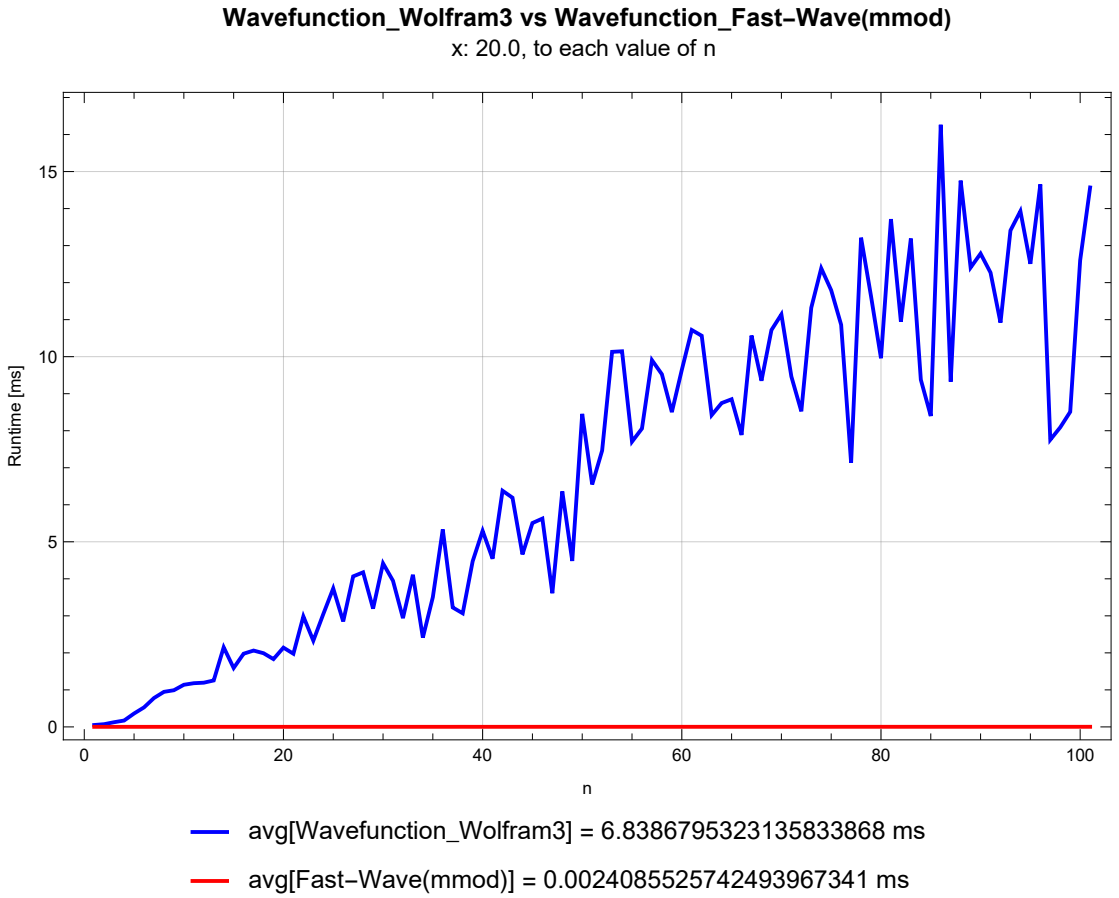
Out[•]=


Wavefunction_Wolfram1 vs Wavefunction_Fast−Wave(smmd; less_fast)
X: [(−20.0) → 20.0 ; 100], to each value of n
Runtime [ms]
n
0
1
2
3
4
5
0
20
40
60
80
100
avg[Wavefunction_Wolfram1] = 1.7666022448851326221 ms
avg[Fast−Wave(smmd; less_fast)] = 0.051437425544533892097 ms

★ Multi-Mode and Onedimensional speed test

In[•]:=
```
FastWaveMMODList = Normal[ExternalEvaluate["Python",
                  normal  execução externa
    "from fast_wave.wavefunction import wavefunction_mmod;import timeit;N_max
      = 100;x = 20.0;[(timeit.timeit(lambda : wavefunction_mmod(n,
      x) , number=10000)/10000)*1000 for n in range(N_max+1)];"]];

WavefunctionWolframMMODList = {};
For[i = 1, i ≤ (Nmax + 1), i++, AppendTo[WavefunctionWolframMMODList,
para cada                          adiciona a
   RepeatedTiming[WavefunctionMathematica3[i - 1, x, prec]][[1]] * 1000];]
   cronometra repetidamente

ListLinePlot[
gráfico de linha de uma lista de valores
 {WavefunctionWolframMMODList, FastWaveMMODList},
 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_Wolfram3 vs Wavefunction_Fast-Wave(mmod)", 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 gráficc  situado                              converte em cadeia de caracteres
      SetPrecision[Mean[WavefunctionWolframMMODList], 20], TraditionalForm] <> " ms",
      define precisão  média                               forma tradicional
    " avg[Fast-Wave(mmod)] = " <> ToString[
                                  converte em cadeia de caracteres
      SetPrecision[Mean[FastWaveMMODList], 20], TraditionalForm] <> " ms"}, Below],
      define precisão  média                    forma tradicional          abaixo
 ImageSize → Large ]
 tamanho da ···  grande
Functionality Test Passed: True
```

Out[•]=

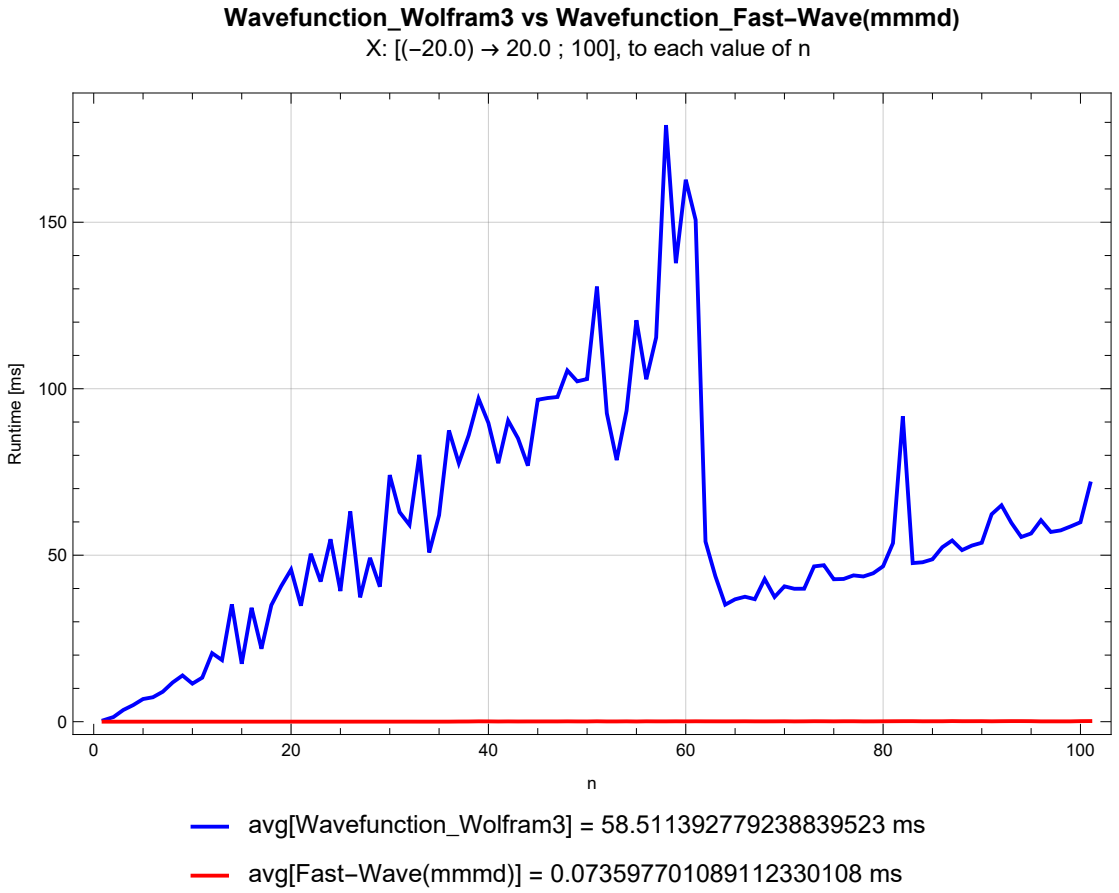

Wavefunction_Wolfram3 vs Wavefunction_Fast−Wave(mmod)
x: 20.0, to each value of n
Runtime [ms]
0
5
10
15
0
20
40
60
80
100
n
avg[Wavefunction_Wolfram3] = 6.8386795323135833868 ms
avg[Fast−Wave(mmod)] = 0.0024085525742493967341 ms

★ Multi-Mode and Multidimensional speed test

In[•]:=
```
FastWaveMMMDList = Normal[ExternalEvaluate["Python",
                   normal  execução externa
    "from fast_wave.wavefunction import wavefunction_mmmd;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
      : wavefunction_mmmd(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},
  estilo do gráfico  azul  vermelho
  Frame → True,
  quadro  verdadeiro
  FrameLabel → {"n", "Runtime [ms]"},
  legenda do quadro
  PlotLabel →
  etiqueta de gráfico
   Row[{Style["Wavefunction_Wolfram3 vs Wavefunction_Fast-Wave(mmmd)", Bold, 13],
    linha  estilo                                                      negrito
     "\n", Style["X: [(-20.0) → 20.0 ; 100], to each value of n \n", 12]}],
           estilo
  GridLines → Automatic,
  grade de linhas  automático
  PlotLegends → Placed[{" avg[Wavefunction_Wolfram3] = " <> ToString[
  legenda do gráficc  situado                              converte em cadeia de caracteres
       SetPrecision[Mean[WavefunctionWolframMMMDList], 20], TraditionalForm] <> " ms",
       define precisão  média                               forma tradicional
     " avg[Fast-Wave(mmmd)] = " <> ToString[
                                  converte em cadeia de caracteres
       SetPrecision[Mean[FastWaveMMMDList], 20], TraditionalForm] <> " ms"}, Below],
       define precisão  média                    forma tradicional          abaixo
  ImageSize → Large ]
  tamanho da ···  grande
```

```
Functionality Test Passed: True
```

Out[•]=


Wavefunction_Wolfram3 vs Wavefunction_Fast−Wave(mmmd)
X: [(−20.0) → 20.0 ; 100], to each value of n
Runtime [ms]
0
50
100
150
0
20
40
60
80
100
n
avg[Wavefunction_Wolfram3] = 58.511392779238839523 ms
avg[Fast−Wave(mmmd)] = 0.073597701089112330108 ms