

Global Variables

```
In[ ]:= prec = 100;

Nmax = 100;

x1 = 1.0;
x2 = 10.0;
x3 = 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[ ]:= 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[*]:= 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]];

```

Wavefuncton_Wolfram_Mathematica_3

```

In[*]:= 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[
        _define precisão
        2 x (wavefunction[[i]] / Sqrt[2 (i)]) - Sqrt[(i - 1) / i] wavefunction[[i - 1]], prec];
        _raiz quadrada _raiz quadrada
    wavefunction];

```

Tests

★ Single Fock and Single Position Function with $x = 1.0$ to the Normalized Hermite Coefficients Matrix

```

FastWaveSFSpN100x1 = SetPrecision[Normal[ExternalEvaluate["Python",
    [define precisão [normal [execução externa
    "import fast_wave.wavefunction_numba as wn;import numpy as np;N_max =
      100;x1 = 1.0;np.array([wn.psi_n_single_fock_single_position(n,x1)
      for n in range(N_max+1)])];"], prec];

(*WolframSFSpN100x1 = WavefunctionMathematica3[Nmax,x1,prec];*)
WolframSFSpN100x1 = {};
For[i = 1, i ≤ (Nmax + 1), i++,
  [para cada
    AppendTo[WolframSFSpN100x1, WavefunctionMathematica1[i - 1, x1, prec]]];
  [adiciona a

Residual = (WolframSFSpN100x1 - FastWaveSFSpN100x1) ^ 2;

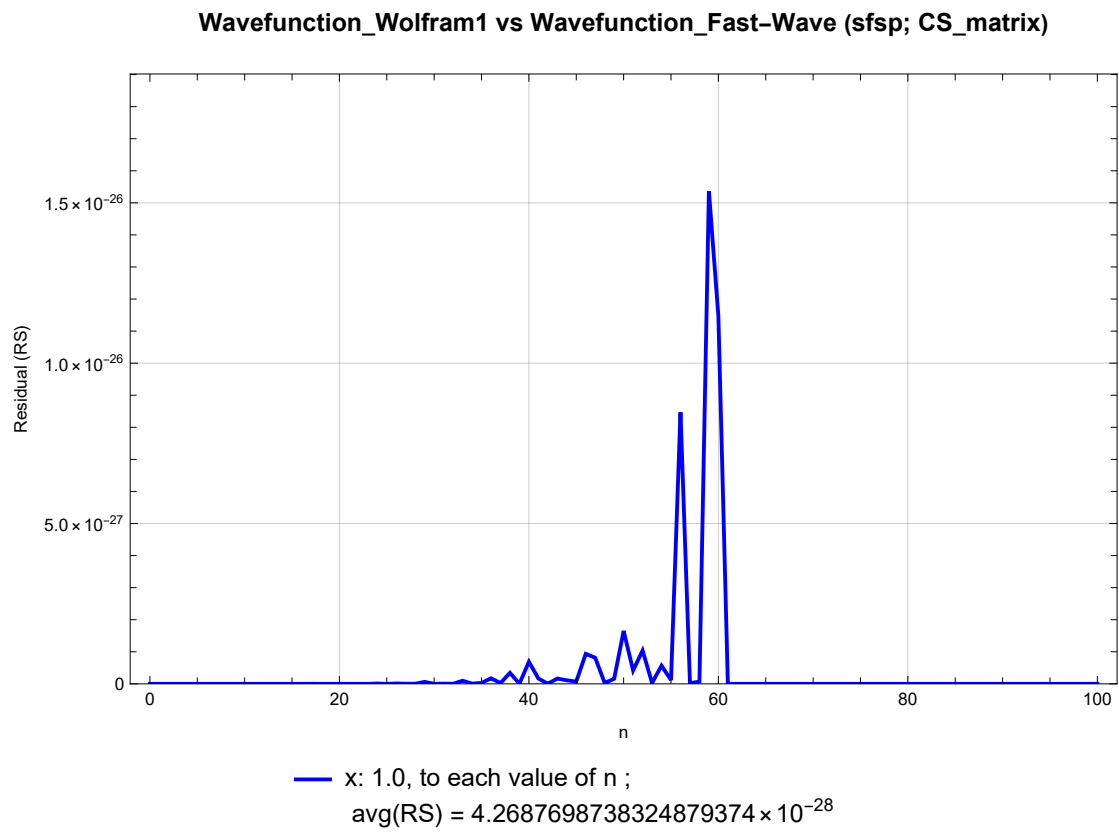
ListLinePlot[
  [gráfico de linha de uma lista de valores
    Transpose[{Nvector, Residual}],
    [transposição
    PlotStyle → {Thick, Blue},
    [estilo do gráfico [espessura [azul
    Frame → True,
    [quadro [verdadeiro
    FrameLabel → {"n", "Residual (RS)"},
    [legenda do quadro
    PlotLabel → Style[
    [etiqueta de gráfico [estilo
      "Wavefunction_Wolfram1 vs Wavefunction_Fast-Wave (sfsp; CS_matrix)\n", 13, Bold],
      [negrito

    GridLines → Automatic,
    [grade de linhas [automático
    PlotLegends → Placed[{"x: 1.0, to each value of n ; \n avg(RS) = " <>
    [legenda do gráfico [situado
      ToString[SetPrecision[Mean[Residual], 20],
      [converte... [define precisão [média
      TraditionalForm]], Below],
      [forma tradicional [abaixo

    ImageSize → Large,
    [tamanho da ... [grande
    PlotRange → {{Automatic, Automatic}, {0, 1.2 * 10^(-25.8)}}
    [intervalo do gráfico [automático [automático
  ]

Functionality Test Passed: True

```

Out[\ast]=

★ Single Fock and Single Position Function with $x = 1.0$

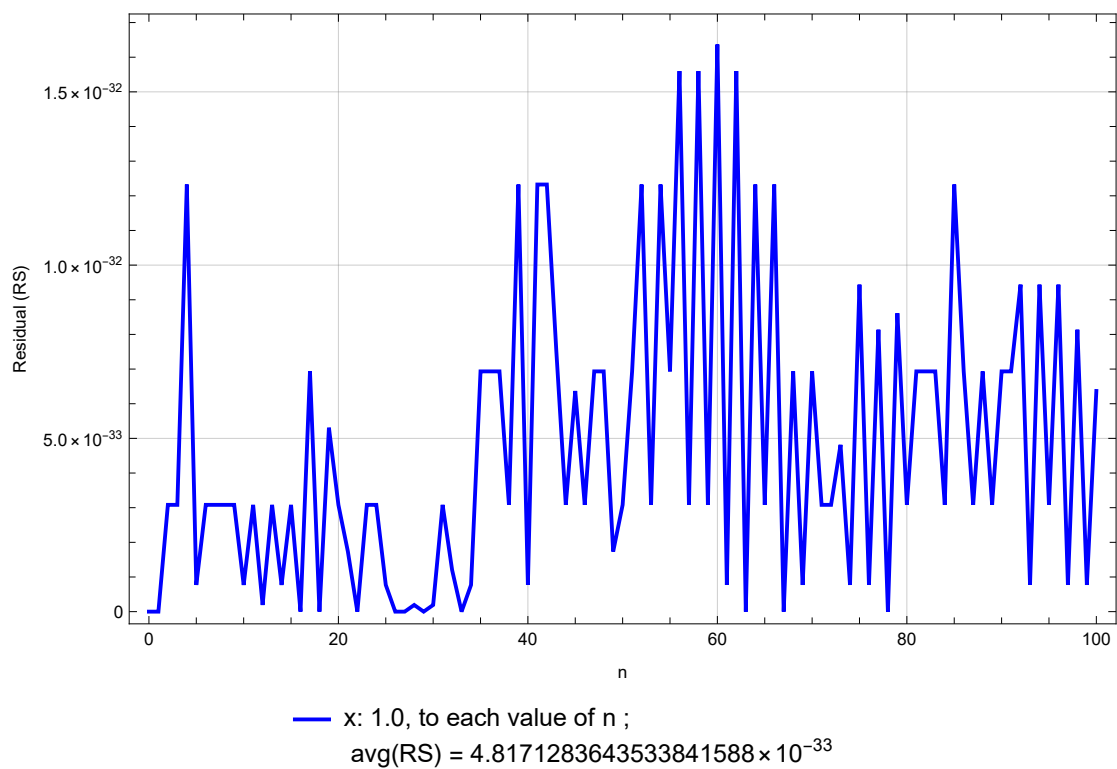
```
FastWaveSFSpN100x1 = SetPrecision[Normal[ExternalEvaluate["Python",
    "import fast_wave.wavefunction_numba as wn;import numpy as np;N_max = 100;x1 =
    1.0;np.array([wn.psi_n_single_fock_single_position(n,x1,CS_matrix=False)
    for n in range(N_max+1)])];"], prec];
```

```
(*WolframSFSpN100x1 = WavefunctionMathematica3[Nmax,x1,prec];*)
WolframSFSpN100x1 = {};
For[i = 1, i ≤ (Nmax + 1), i++,
    AppendTo[WolframSFSpN100x1, WavefunctionMathematica1[i - 1, x1, prec]]];
```

```
Residual = (WolframSFSpN100x1 - FastWaveSFSpN100x1) ^ 2;
```

```
ListLinePlot[
    Transpose[{Nvector, Residual}],
    PlotStyle → {Thick, Blue},
    Frame → True,
    FrameLabel → {"n", "Residual (RS)"},
    PlotLabel →
        Style["Wavefunction_Wolfram1 vs Wavefunction_Fast-Wave (sfsp)\n", 13, Bold],
    GridLines → Automatic,
    PlotLegends → Placed[{"x: 1.0, to each value of n ; \n avg(RS) = " <>
        ToString[SetPrecision[Mean[Residual], 20],
        TraditionalForm]], Below],
    ImageSize → Large
]
```

Functionality Test Passed: True

Out[*n*]=**Wavefunction_Wolfram1 vs Wavefunction_Fast-Wave (sfsp)**

★ Single Fock and Single Position Function with $x = 10.0$ to the Normalized Hermite Coefficients Matrix

```

FastWaveSFSpN100x2 = SetPrecision[Normal[ExternalEvaluate["Python",
    "import fast_wave.wavefunction_numba as wn;import numpy as np;N_max = 100;x2
    = 10.0;np.array([wn.psi_n_single_fock_single_position(n,x2)
    for n in range(N_max+1)])];"], prec];

(*WolframSFSpN100x2 = WavefunctionMathematica3[Nmax,x2,prec];*)

WolframSFSpN100x2 = {};
For[i = 1, i ≤ (Nmax + 1), i++,
    AppendTo[WolframSFSpN100x2, WavefunctionMathematica1[i - 1, x2, prec]];]

Residual = (WolframSFSpN100x2 - FastWaveSFSpN100x2) ^2;

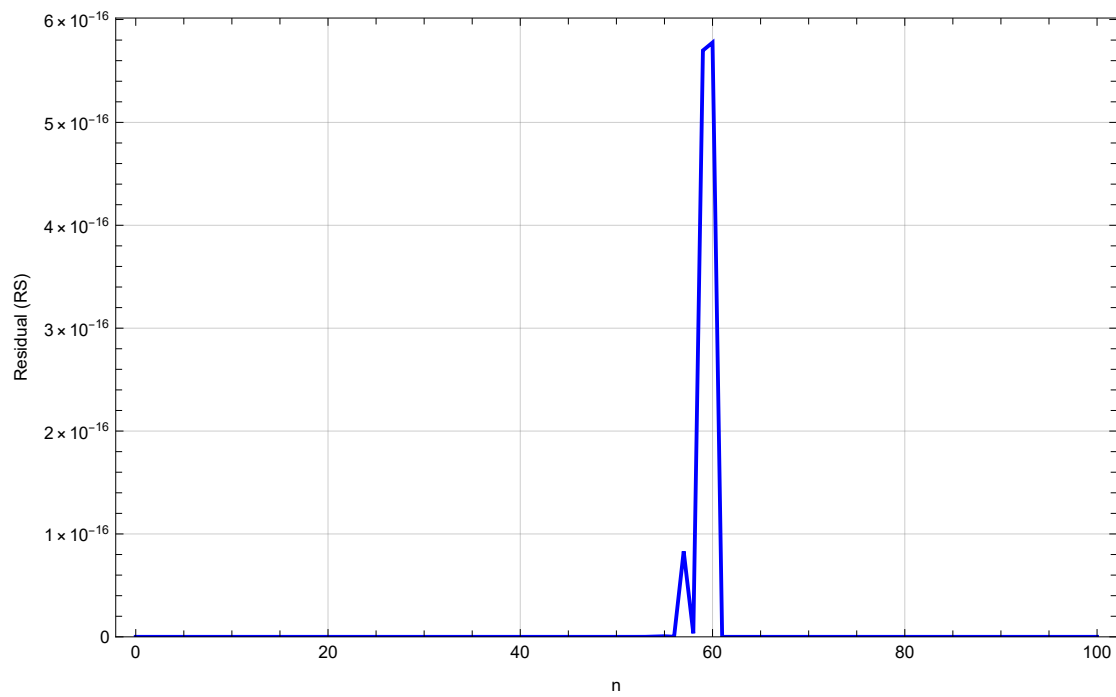
ListLinePlot[
    Transpose[{Nvector, Residual}],
    PlotStyle → {Thick, Blue},
    Frame → True,
    FrameLabel → {"n", "Residual (RS)"},
    PlotLabel → Style[
        "Wavefunction_Wolfram1 vs Wavefunction_Fast-Wave (sfsp; CS_matrix)\n", 13, Bold],
    GridLines → Automatic,
    PlotLegends → Placed[{" x: 10.0, to each value of n ; \n avg(RS) = [" <>
        ToString[SetPrecision[Mean[Residual], 20],
        TraditionalForm]} <> "]", Below],
    ImageSize → Large ,
    PlotRange → {{Automatic, Automatic}, {0, 1.2 * 10^(-15.3)}}]

```

Functionality Test Passed: True

Out[*n*]=

Wavefunction_Wolfram1 vs Wavefunction_Fast-Wave (sfsp; CS_matrix)



x: 10.0, to each value of n ;

avg(RS) = [$1.2227826509448020424 \times 10^{-17}$]

★ Single Fock and Single Position Function with $x = 10.0$

```
FastWaveSFSpN100x2 = SetPrecision[Normal[ExternalEvaluate["Python",
    "import fast_wave.wavefunction_numba as wn;import numpy as np;N_max = 100;x2 =
    10.0;np.array([wn.psi_n_single_fock_single_position(n,x2,CS_matrix=False
    ) for n in range(N_max+1)])];"], prec];
```

```
(*WolframSFSpN100x2 = WavefunctionMathematica3[Nmax,x2,prec];*)
```

```
WolframSFSpN100x2 = {};
For[i = 1, i ≤ (Nmax + 1), i++,
    AppendTo[WolframSFSpN100x2, WavefunctionMathematica1[i - 1, x2, prec]];]
```

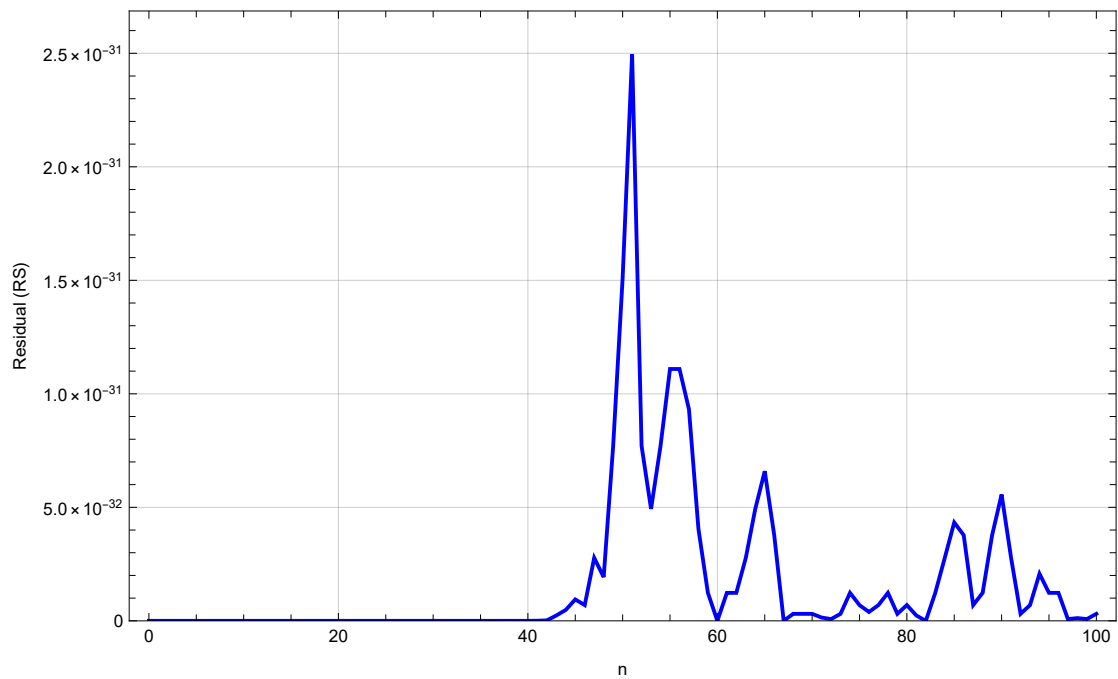
```
Residual = (WolframSFSpN100x2 - FastWaveSFSpN100x2) ^ 2;
```

```
ListLinePlot[
    Transpose[{Nvector, Residual}],
    PlotStyle → {Thick, Blue},
    Frame → True,
    FrameLabel → {"n", "Residual (RS)"},
    PlotLabel →
        Style["Wavefunction_Wolfram1 vs Wavefunction_Fast-Wave (sfsp)\n", 13, Bold],
    GridLines → Automatic,
    PlotLegends → Placed[{" x: 10.0, to each value of n ; \n avg(RS) = [" <>
        ToString[SetPrecision[Mean[Residual], 20],
        TraditionalForm]] <> "]" , Below],
    ImageSize → Large ,
    PlotRange → {{Automatic, Automatic}, {0, 1.2 * 10^(-30.65)}}
```

Functionality Test Passed: True

Out[*n*]=

Wavefunction_Wolfram1 vs Wavefunction_Fast-Wave (sfsp)



x: 10.0, to each value of n ;

avg(RS) = [$1.7001583826933030519 \times 10^{-32}$]

★ Single Fock and Single Position Function with $x = 20.0$ to the Normalized Hermite Coefficients Matrix

```

FastWaveSFSpN100x3 = SetPrecision[Normal[ExternalEvaluate["Python",
    [define precisão [normal [execução externa
    "import fast_wave.wavefunction_numba as wn;import numpy as np;N_max = 100;x3
      = 20.0;np.array([wn.psi_n_single_fock_single_position(n,x3)
      for n in range(N_max+1)])];"], prec];

(*WolframSFSpN100x3 = WavefunctionMathematica3[Nmax,x3,prec];*)
WolframSFSpN100x3 = {};
For[i = 1, i ≤ (Nmax + 1), i++,
  [para cada
    AppendTo[WolframSFSpN100x3, WavefunctionMathematica1[i - 1, x3, prec]];]
  [adiciona a

Residual = (WolframSFSpN100x3 - FastWaveSFSpN100x3) ^2;

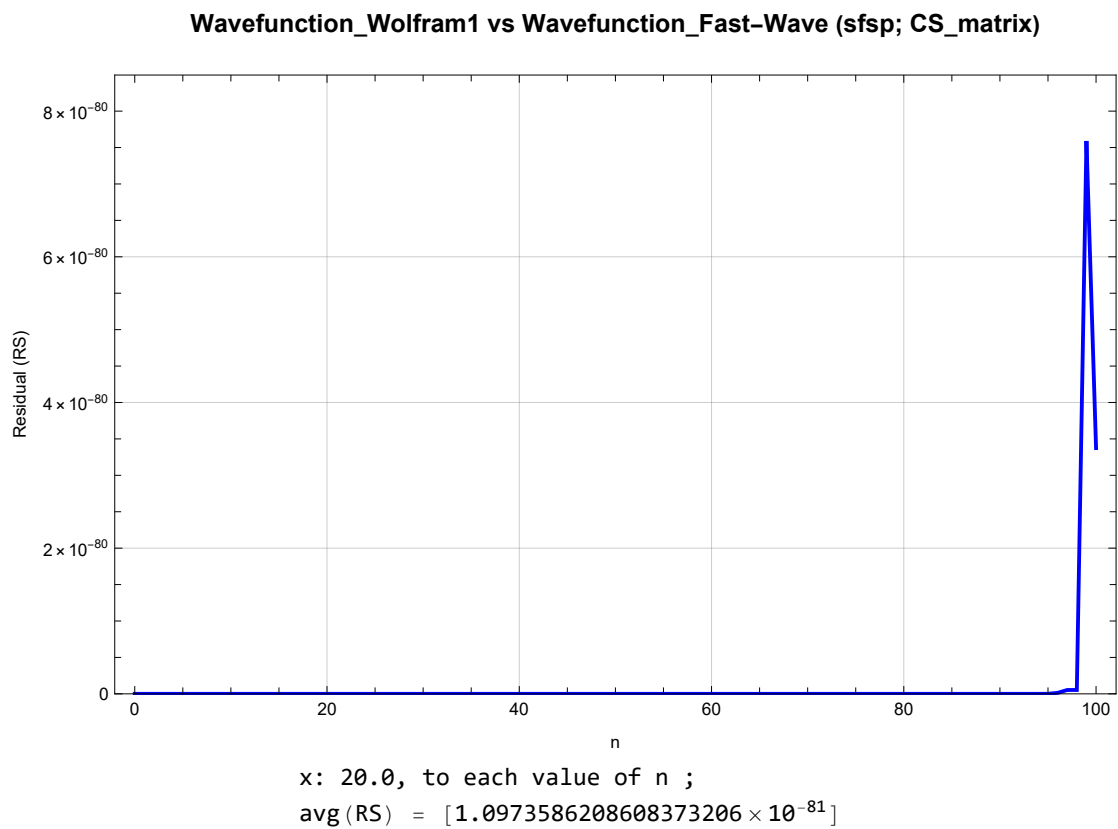
ListLinePlot[
  [gráfico de linha de uma lista de valores
    Transpose[{Nvector, Residual}],
    [transposição
    PlotStyle → {Thick, Blue},
    [estilo do gráfico [espessc [azul
    Frame → True,
    [quadro [verdadeiro
    FrameLabel → {"n", "Residual (RS)"},
    [legenda do quadro
    PlotLabel → Style[
    [etiqueta de gr· [estilo
      "Wavefunction_Wolfram1 vs Wavefunction_Fast-Wave (sfsp; CS_matrix)\n", 13, Bold],
      [negrito

    GridLines → Automatic,
    [grade de linhas [automático
    PlotLegends → Placed[{"x: 20.0, to each value of n ; \n avg(RS) = [" <>
    [legenda do gráfico [situado
      ToString[SetPrecision[Mean[Residual], 20],
      [converte· [define precisão [média
      TraditionalForm]] <> "]" , Below],
      [forma tradicional [abaixo

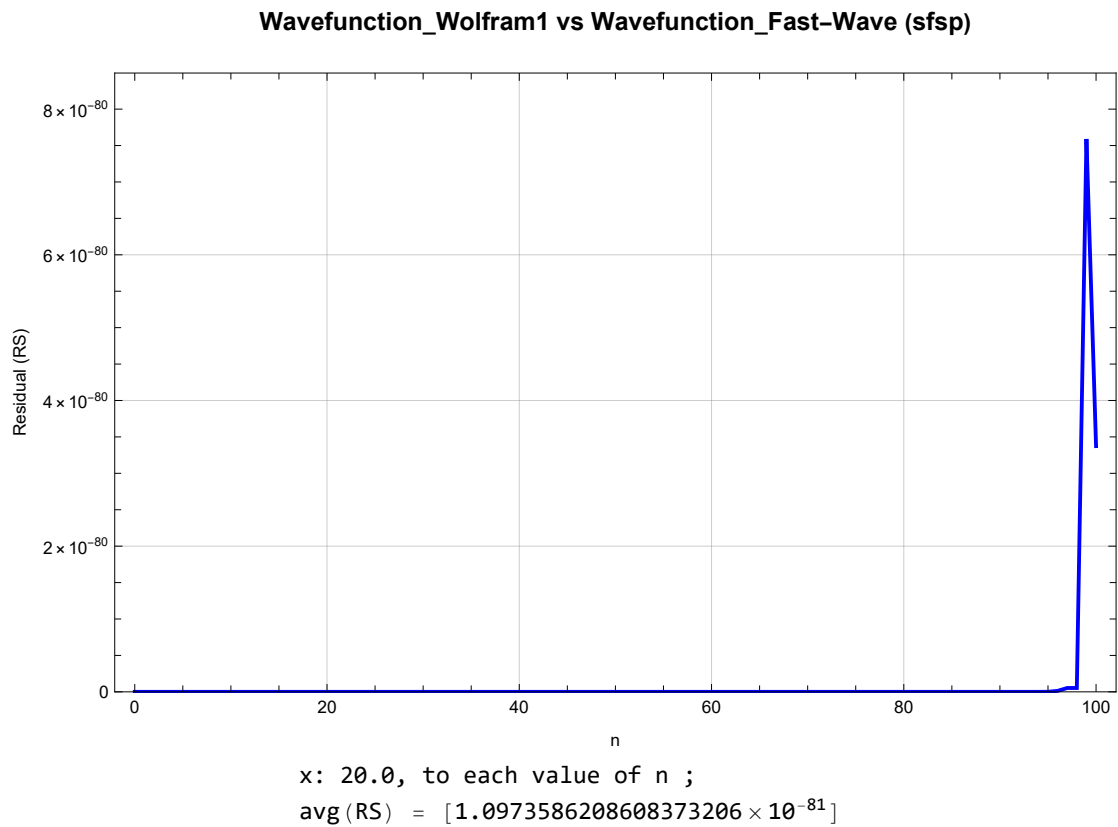
    ImageSize → Large ,
    [tamanho da · [grande
    PlotRange → {{Automatic, Automatic}, {0, 1.2 * 10^(-79.15)}}
    [intervalo do gráf· [automático [automático
  ]
]
Functionality Test Passed: True

```

Out[*n*]=



Out[*n*]=



★ Single Fock and Multiple Position Function with $X = [(-20) \rightarrow 20; 100]$ to the Normalized Hermite Coefficients Matrix

```
FastWaveSFmpN100X = SetPrecision[
    Normal[ExternalEvaluate["Python",
        "import fast_wave.wavefunction_numba
        as wn;import numpy as np;N_max = 100;xmax =
        20.0;xmin=-20.0;xsize=100;X=np.linspace(xmin,xmax,xsize);np.array([wn.
        psi_n_single_fock_multiple_position(n,X)
        for n in range(N_max+1)])];"], prec];

(*WolframSFmpN100X = WavefunctionMathematica3[Nmax,Xvector,prec];*)
WolframSFmpN100X = {};
For[i = 1, i ≤ (Nmax + 1), i++,
    AppendTo[WolframSFmpN100X, WavefunctionMathematica1[i - 1, Xvector, prec]];]

ResidualMatrix = (WolframSFmpN100X - FastWaveSFmpN100X) ^ 2;

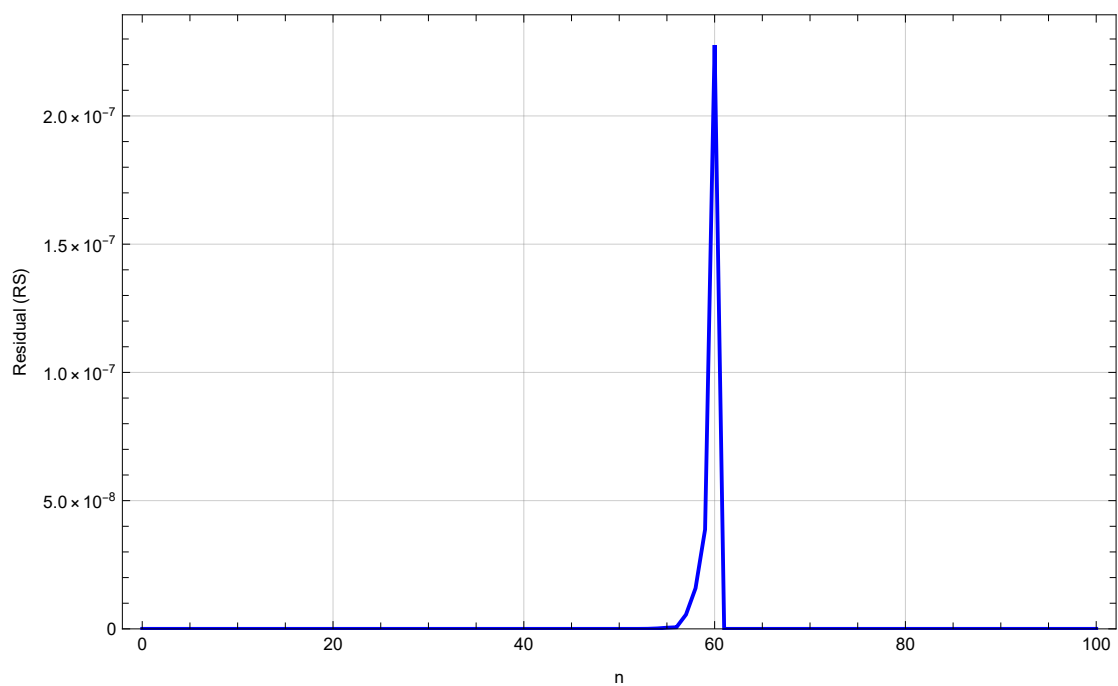
Residual = Mean /@ ResidualMatrix;

ListLinePlot[
    Transpose[{Nvector, Residual}],
    PlotStyle → {Thick, Blue},
    Frame → True,
    FrameLabel → {"n", "Residual (RS)"},
    PlotLabel → Style[
        "Wavefunction_Wolfram1 vs Wavefunction_Fast-Wave (sfmp, CS_matrix)\n", 13, Bold],
    GridLines → Automatic,
    PlotLegends → Placed[{" X: [(-20)→20;100], to each value of n ; \n avg(RS) = [" <>
        ToString[SetPrecision[Mean[Residual], 20],
        TraditionalForm] <> "]" , Below],
    ImageSize → Large,
    PlotRange → {{Automatic, Automatic}, {0, 1.2 * 10^(-6.7)}}
```

Functionality Test Passed: True

Out[*n*]=

Wavefunction_Wolfram1 vs Wavefunction_Fast-Wave (sfmp, CS_matrix)



X: $[(-20) \rightarrow 20; 100]$, to each value of n ;
 avg (RS) = $[2.8624974439968216501 \times 10^{-9}]$

★ Single Fock and Multiple Position Function with $X = [(-20) \rightarrow 20; 100]$

```

FastWaveSFMPN100X = SetPrecision[
    Normal[ExternalEvaluate["Python",
        "import fast_wave.wavefunction_numba
        as wn;import numpy as np;N_max = 100;xmax =
        20.0;xmin=-20.0;xsize=100;X=np.linspace(xmin,xmax,xsize);np.array([wn.
        psi_n_single_fock_multiple_position(n,X,CS_matrix=False)
        for n in range(N_max+1)])];"], prec];

(*WolframSFMPN100X = WavefunctionMathematica3[Nmax,Xvector,prec];*)
WolframSFMPN100X = {};
For[i = 1, i ≤ (Nmax + 1), i++,
    AppendTo[WolframSFMPN100X, WavefunctionMathematica1[i - 1, Xvector, prec]];]

ResidualMatrix = (WolframSFMPN100X - FastWaveSFMPN100X) ^ 2;

Residual = Mean /@ ResidualMatrix;

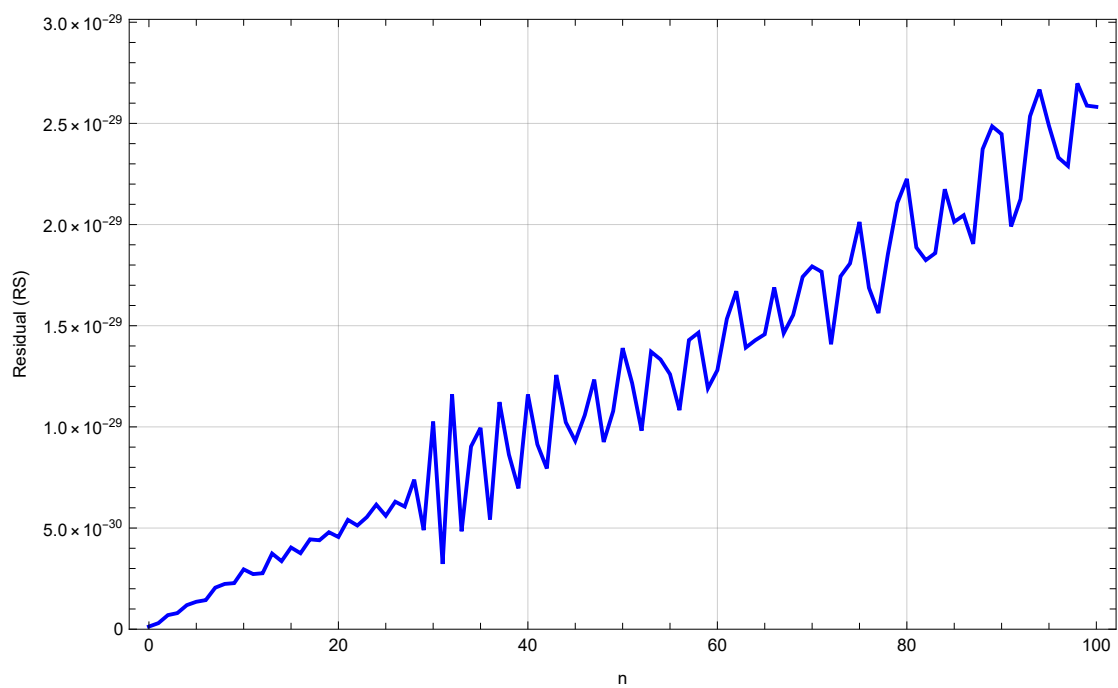
ListLinePlot[
    Transpose[{Nvector, Residual}],
    PlotStyle → {Thick, Blue},
    Frame → True,
    FrameLabel → {"n", "Residual (RS)"},
    PlotLabel →
    Style["Wavefunction_Wolfram1 vs Wavefunction_Fast-Wave (sfmp)\n", 13, Bold],
    GridLines → Automatic,
    PlotLegends → Placed[{"X: [(-20)→20;100], to each value of n ; \n avg(RS) = [" <>
    ToString[SetPrecision[Mean[Residual], 20],
    TraditionalForm] <> "]" , Below],
    ImageSize → Large,
    PlotRange → {{Automatic, Automatic}, {0, 1.2 * 10^(-28.6)}}}
]

```

Functionality Test Passed: True

Out[]=

Wavefunction_Wolfram1 vs Wavefunction_Fast-Wave (sfmp)



X: $[(-20) \rightarrow 20; 100]$, to each value of n ;
 avg(RS) = $[1.2113401822724537959 \times 10^{-29}]$

★ Multiple Fock and Single Position Function with $x = 1.0$

```

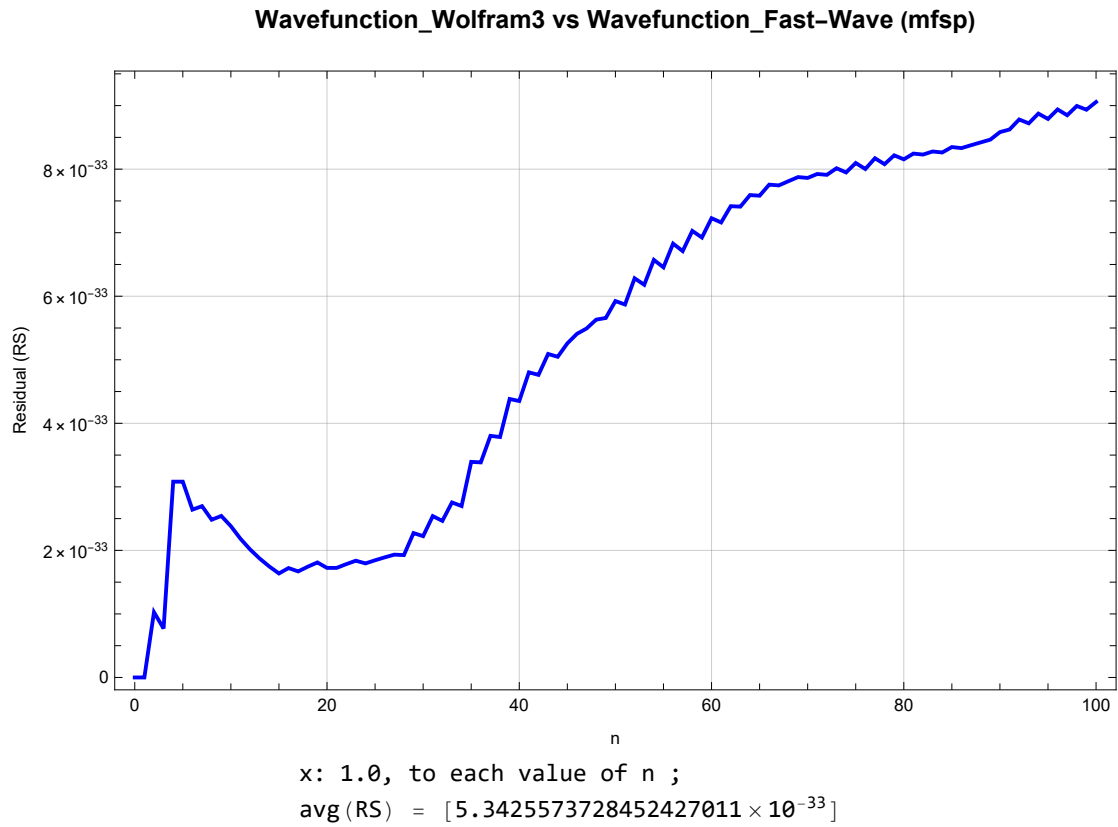
In[*]:= FastWaveMFSpN100x1 = SetPrecision[Normal[ExternalEvaluate["Python",
    [define precisão [normal [execução externa
    "import fast_wave.wavefunction_numba as wn;import numpy as np;N_max
      = 100;x1 =1.0;[wn.psi_n_multiple_fock_single_position(n,x1)
      for n in range(N_max+1)];"]], prec];

WavefunctionMFSpN100x1 = {};
For[i = 1, i ≤ (Nmax + 1), i++,
  [para cada
    AppendTo[WavefunctionMFSpN100x1, WavefunctionMathematica3[i - 1, x1, prec]]];
  [adiciona a
ResidualList = (WavefunctionMFSpN100x1 - FastWaveMFSpN100x1) ^2;

Residual = Mean /@ResidualList;
  [média

ListLinePlot[
  [gráfico de linha de uma lista de valores
    Transpose[{Nvector, Residual}],
    [transposição
    PlotStyle → {Thick, Blue},
    [estilo do gráfico [espessc [azul
    Frame → True,
    [quadro [verdadeiro
    FrameLabel → {"n", "Residual (RS)"},
    [legenda do quadro
    PlotLabel →
    [etiqueta de gráfico
    Style["Wavefunction_Wolfram3 vs Wavefunction_Fast-Wave (mfsf)\n", 13, Bold],
    [estilo [negrito
    GridLines → Automatic,
    [grade de linhas [automático
    PlotLegends → Placed[{" x: 1.0, to each value of n ; \n avg(RS) = [" <>
    [legenda do gráfico [situado
    ToString[SetPrecision[Mean[Residual], 20],
    [converte... [define precisão [média
    TraditionalForm]] <> "]" , Below],
    [forma tradicional [abaixo
    ImageSize → Large ]
    [tamanho da ... [grande
Functionality Test Passed: True

```

Out[*n*]=

★ Multiple Fock and Single Position Function with $x = 10.0$

```

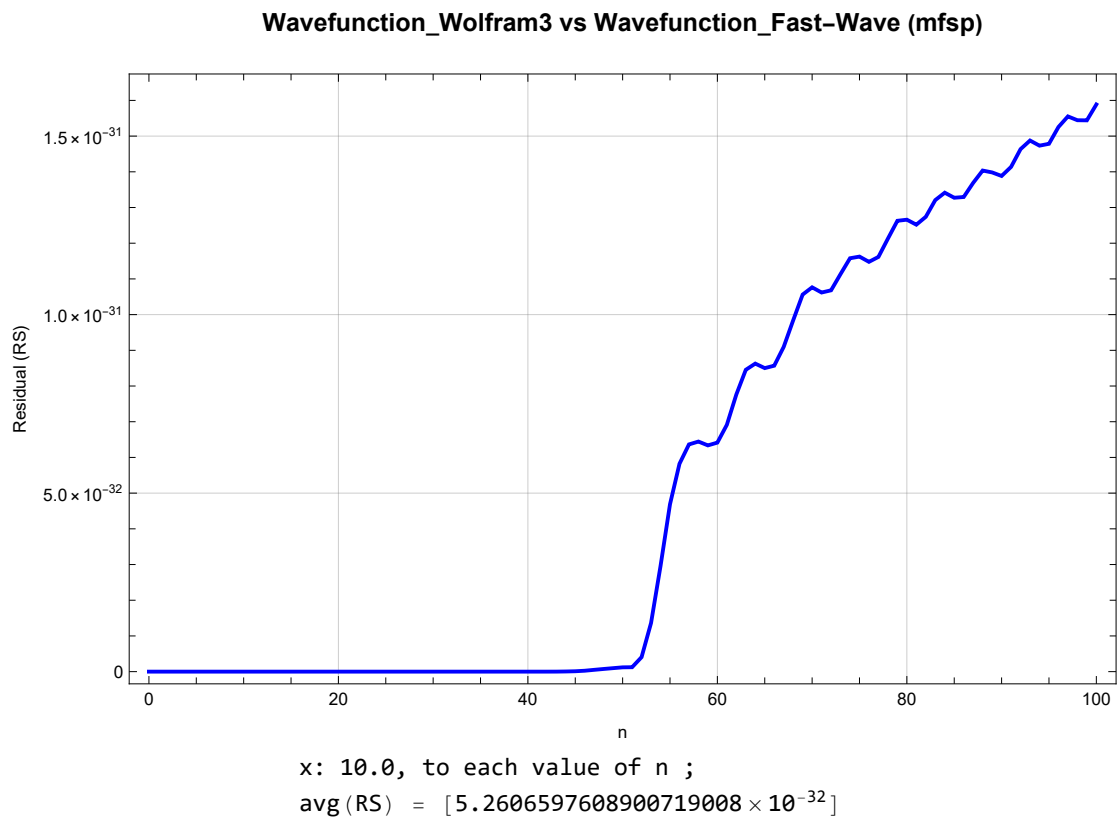
In[*]:= FastWaveMFSpN100x10 = SetPrecision[Normal[ExternalEvaluate["Python",
    [define precisão [normal [execução externa
    "import fast_wave.wavefunction_numba as wn;import numpy as np;N_max
      = 100;x2 =10.0;[wn.psi_n_multiple_fock_single_position(n,x2)
      for n in range(N_max+1)];"]], prec];

WavefunctionMFSpN100x10 = {};
For[i = 1, i ≤ (Nmax + 1), i++,
  [para cada
    AppendTo[WavefunctionMFSpN100x10, WavefunctionMathematica3[i - 1, x2, prec]]];
  [adiciona a
ResidualList = (WavefunctionMFSpN100x10 - FastWaveMFSpN100x10) ^ 2;

Residual = Mean /@ ResidualList;
  [média

ListLinePlot[
  [gráfico de linha de uma lista de valores
    Transpose[{Nvector, Residual}],
    [transposição
    PlotStyle → {Thick, Blue},
    [estilo do gráfico [espessc [azul
    Frame → True,
    [quadro [verdadeiro
    FrameLabel → {"n", "Residual (RS)"},
    [legenda do quadro
    PlotLabel →
    [etiqueta de gráfico
    Style["Wavefunction_Wolfram3 vs Wavefunction_Fast-Wave (mfsp)\n", 13, Bold],
    [estilo [negrito
    GridLines → Automatic,
    [grade de linhas [automático
    PlotLegends → Placed[{" x: 10.0, to each value of n ; \n avg(RS) = [" <>
    [legenda do gráfico [situado
    ToString[SetPrecision[Mean[Residual], 20],
    [converte... [define precisão [média
    TraditionalForm]] <> "]" , Below],
    [forma tradicional [abaixo
    ImageSize → Large ]
    [tamanho da ... [grande
Functionality Test Passed: True

```

Out[*n*]=

★ Multiple Fock and Single Position Function with $x = 20.0$

```

In[*]:= FastWaveMFSpN100x20 = SetPrecision[Normal[ExternalEvaluate["Python",
    [define precisão [normal [execução externa
    "import fast_wave.wavefunction_numba as wn;import numpy as np;N_max
      = 100;x3 =20.0;[wn.psi_n_multiple_fock_single_position(n,x3)
      for n in range(N_max+1)];"]], prec];

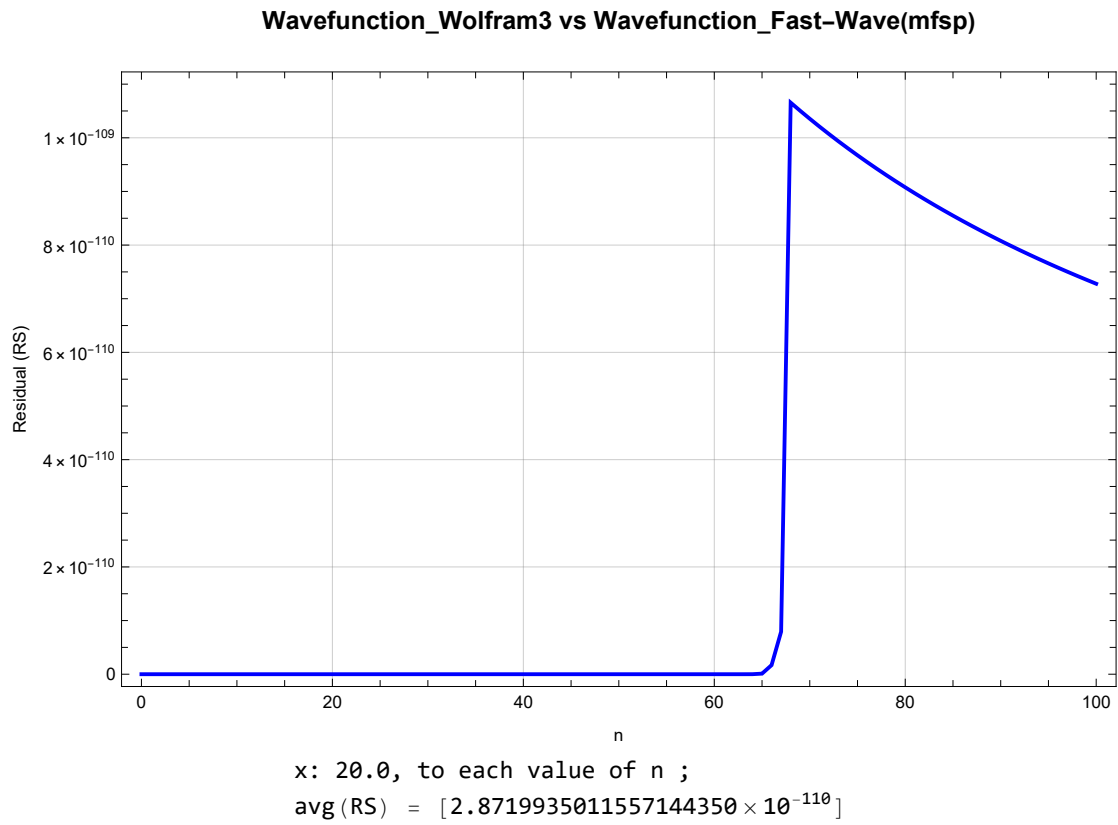
WavefunctionMFSpN100x20 = {};
For[i = 1, i ≤ (Nmax + 1), i++,
  [para cada
    AppendTo[WavefunctionMFSpN100x20, WavefunctionMathematica3[i - 1, x3, prec]]];
  [adiciona a
ResidualList = (WavefunctionMFSpN100x20 - FastWaveMFSpN100x20) ^2;

Residual = Mean /@ResidualList;
  [média

ListLinePlot[
  [gráfico de linha de uma lista de valores
    Transpose[{Nvector, Residual}],
    [transposição
    PlotStyle → {Thick, Blue},
    [estilo do gráfico [espessc [azul
    Frame → True,
    [quadro [verdadeiro
    FrameLabel → {"n", "Residual (RS)"},
    [legenda do quadro
    PlotLabel →
    [etiqueta de gráfico
    Style["Wavefunction_Wolfram3 vs Wavefunction_Fast-Wave(mfsp)\n", 13, Bold],
    [estilo [negrito
    GridLines → Automatic,
    [grade de linhas [automático
    PlotLegends → Placed[{" x: 20.0, to each value of n ; \n avg(RS) = [" <>
    [legenda do gráfico [situado
    ToString[SetPrecision[Mean[Residual], 20],
    [converte... [define precisão [média
    TraditionalForm]] <> "]" , Below],
    [forma tradicional [abaixo
    ImageSize → Large ]
    [tamanho da ... [grande
Functionality Test Passed: True

```

Out[]=



★ Multi Fock and Multiple Position Function with $X = [(-20) \rightarrow 20; 100]$

```

In[*]:= FastWaveMFmpN100X = SetPrecision[
    Normal[ExternalEvaluate["Python", "import fast_wave.wavefunction_numba
    as wn;import numpy as np;N_max = 100;xmax =
    20.0;xmin=-20.0;xsize=100;X=np.linspace(xmin,xmax,xsize);[wn.psi_n
    _multiple_fock_multiple_position(n,X)
    for n in range(N_max+1)]];"], prec];

WolframMFmpN100X = {};
For[i = 1, i ≤ (Nmax + 1), i++,
    AppendTo[WolframMFmpN100X, WavefunctionMathematica3[i - 1, Xvector, prec]];]

ResidualMatrixList = (WolframMFmpN100X - FastWaveMFmpN100X) ^ 2;

Residual = Mean /@ (Flatten /@ ResidualMatrixList);

ListLinePlot[
    Transpose[{Nvector, Residual}],
    PlotStyle → {Thick, Blue},
    Frame → True,
    FrameLabel → {"n", "Residual (RS)"},
    PlotLabel →
    Style["Wavefunction_Wolfram3 vs Wavefunction_Fast-Wave(mfmp)\n", 13, Bold],
    GridLines → Automatic,
    PlotLegends → Placed[{" X: [(-20)→20;100], to each value of n ; \n avg(RS) = [" <>
    ToString[SetPrecision[Mean[Residual], 20],
    TraditionalForm]] <> "]", Below],
    ImageSize → Large ]

Functionality Test Passed: True

```

Out[*n*]=