

Getting Started with Maple Toolboxes

Copyright © Maplesoft, a division of Waterloo Maple Inc.
2021

Getting Started with Maple Toolboxes

Copyright

Maplesoft and Maple are trademarks of Waterloo Maple Inc.

© Maplesoft, a division of Waterloo Maple Inc. 2021. All rights reserved.

No part of this book may be reproduced, stored in a retrieval system, or transcribed, in any form or by any means — electronic, mechanical, photocopying, recording, or otherwise. Information in this document is subject to change without notice and does not represent a commitment on the part of the vendor. The software described in this document is furnished under a license agreement and may be used or copied only in accordance with the agreement. It is against the law to copy the software on any medium except as specifically allowed in the agreement.

Linux is a registered trademark of Linus Torvalds.

Mac is a registered trademark of Apple, Inc.

MATLAB and Simulink are registered trademarks of The MathWorks, Inc.

Windows is a registered trademark of Microsoft Corporation.

Java and all Java based marks are trademarks or registered trademarks of Oracle and/or its affiliates.

Optimus is a registered trademark of Noesis Solutions.

All other trademarks are the property of their respective owners.

This document was produced using a special version of Maple and DocBook.

Printed in Canada

Contents

Preface	iv
1 BlockImporter	1
1.1 Introduction to BlockImporter	1
Overview	1
Requirements	1
1.2 Getting Started with BlockImporter	1
Establishing a Connection	1
Help with BlockImporter	2
1.3 Working with BlockImporter	2
2 Global Optimization Toolbox	4
2.1 Introduction to the Global Optimization Toolbox	4
Overview	4
Requirements	4
2.2 Getting Started with the Global Optimization Toolbox	4
Initialization	4
Help with the Global Optimization Toolbox	5
2.3 Working with the Global Optimization Toolbox	5
Example	7
3 Grid Computing Toolbox	10
3.1 Introduction to the Grid Computing Toolbox	10
Overview	10
Requirements	10
3.2 Getting Started with the Grid Computing Toolbox	10
Establishing a Server and Network	10
Help with Grid Computing	11
3.3 Working with the Grid Computing Toolbox	11
Example	12
4 Quantum Chemistry Toolbox	15
4.1 Introduction to the Quantum Chemistry Toolbox	15
Overview	15
Requirements	15
4.2 Getting Started with the Quantum Chemistry Toolbox	15
Initialization	15
Help with Quantum Chemistry	16
4.3 Working with the Quantum Chemistry Toolbox	16
Examples	16

Preface

Introduction to the Toolboxes

Maplesoft™ offers a rich selection of add-on products. These toolboxes enhance and extend the power of Maple™ by adding solutions in specialized application areas, enhanced computation and deployment options, and connectivity with other technical tools. When taking advantage of these advanced products, you continue to have access to Maple's computational power, easy-to-use smart document interface, and rich technical documentation features.

- **BlockImporter™** allows you to import a Simulink® model into Maple, and convert it to a set of mathematical equations. Maple provides the power to simplify and manipulate the model, before simulating it in Maple or exporting it back to Simulink® .
- The **Global Optimization Toolbox**, powered by Optimus® technology from Noesis Solutions, provides world-class global optimization technology to return the best answer to your optimization model, robustly and efficiently.
- The **Grid Computing Toolbox** provides tools for performing Maple computations in parallel, allowing you to distribute computations across a network of workstations, a supercomputer, or the CPUs of a multiprocessor machine. It includes a personal grid server, allowing you to simulate and test your parallel applications before running them on a real grid network.
- The **Quantum Chemistry™ Toolbox** allows you to: define molecules instantly from a database of more than 96 million molecules, run quantum computations, and analyze molecular energies and properties through 2-D and 3-D plots and animations.

In This Manual

This manual provides an introduction to each of these toolboxes. Each section contains an overview of the toolbox, set-up details, getting started information, and examples.

Trademarks

Maplesoft, Maple, and BlockImporter are trademarks of Waterloo Maple Inc.

Linux is a registered trademark of Linus Torvalds.

Mac is a registered trademark of Apple, Inc.

MATLAB and Simulink are registered trademarks of The MathWorks, Inc.

Java and all Java-based marks are trademarks or registered trademarks of Oracle and/or its affiliates.

Optimus is a registered trademark of Noesis Solutions.

All other trademarks are the property of their respective owners.

1 BlockImporter

1.1 Introduction to BlockImporter

Overview

BlockImporter allows you to import a Simulink® model into Maple, and convert it to a set of mathematical equations. Maple provides the power to simplify, manipulate, and simulate the model.

Features of this toolbox include:

- The ability to perform calculations and simplifications on your Simulink® models by using Maple's suite of tools.
- Perform advanced analysis on your systems by using Maple's built-in DynamicSystems package, including system object representation, graphical analysis, system manipulation procedures, signal generation tools, and system simulation.
- Reliable, tested computational routines to test the validity of your models, before performing simulations.
- Commands for performing frequency- and complex-domain analysis, stability and sensitivity analysis, and parameter optimization on your Simulink® models.
- Symbolic methods for eliminating algebraic loops, which can significantly improve the efficiency and execution speed of your Simulink® models.

Requirements

Before installing BlockImporter, you must install and activate Maple 2021. You must also install MATLAB® and Simulink® before using this toolbox. For details on supported Simulink® versions and installation instructions, see the Install.html file on the product disc.

You need a purchase code to activate BlockImporter. This code has been emailed to you. If you have not received your purchase code, contact Maplesoft Customer Service at custservice@maplesoft.com, or the Maplesoft office or reseller in your region (visit <http://www.maplesoft.com/contact/>).

After installation, the BlockImporter.mw file appears on your desktop (Windows® and Mac®) or in your home directory (Linux®). Open this file. Note that you can also access this file by entering **?BlockImporter,Tour** in Maple.

The document BlockImporter.mw contains links to getting started documentation, help system documentation, and more. The getting started documentation contains an overview of the tools in this product, and provides multiple examples. The examples illustrate how to define a model in Simulink®, import the mathematical model into Maple, and perform analyses such as stability, sensitivity, and parameter optimization.

1.2 Getting Started with BlockImporter

Establishing a Connection

To begin, open a new Maple window. Enter the following command to establish a connection with MATLAB®.

```
> Matlab[openlink]()
```

A MATLAB® command window should open. If one does not, follow the instructions in the **Matlab/setup** help page to configure the connection.

You are now ready to use BlockImporter.

Help with BlockImporter

For a list of commands in Maple to support BlockImporter, see the **BlockImporter** help page. Links to related Maple commands are also provided; many built-in Maple functions, especially the commands in the **Dynamic Systems** package, can be extremely helpful in generating and manipulating physical system models. For more information, refer to the **DynamicSystems** help page.

1.3 Working with BlockImporter

You can import any Simulink® system or subsystem model by using the **Import** command. For more information, refer to the **BlockImporter/Import** help page.

1. Set the directory in which the Simulink® files are located. For example, use the directory containing the pre-installed BlockImporter example models, which can be located by using the following command.

```
> datadir := BlockImporter[DataDirectory]() :
```

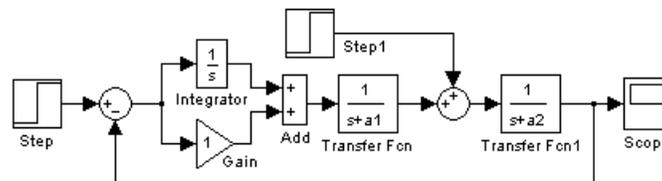
2. Using the **Import** command, specify the file to import. The *inplace* option indicates that the model will be converted in MATLAB® to a Maple **record**. For more information, refer to the **Record** help page.

```
> with(BlockImporter)
```

```
[BuildDE, Import, PrintSummary, SimplifyModel] (1.1)
```

```
> sys := Import("example", path = datadir, init
= "example_init", inplace = true) :
```

This particular model has the following model diagram in Simulink®.



3. A copy of the model is created, consisting of a list of mathematical equations. Use the **PrintSummary** command to display the equations, variables, and parameters. For more information, refer to the **BlockImporter/PrintSummary** help page.

```
> PrintSummary(sys) :
```

```
Equations [24]:
```

$$\begin{aligned}
& [u_{10,1,1} = y_{2,1,1}, u_{2,2,1} = y_{3,1,1}, u_{2,1,1} = y_{4,1,1}, u_{8,1,1} = y_{6,1,1}, \\
& u_{9,1,1} = y_{7,1,1}, u_{4,1,1} = y_{8,1,1}, u_{3,1,1} = y_{8,1,1}, u_{11,1,1} = y_{9,1,1}, \\
& u_{9,2,1} = y_{10,1,1}, u_{5,1,1} = y_{11,1,1}, u_{8,2,1} = y_{11,1,1}, y_{2,1,1} \\
& = u_{2,1,1} + u_{2,2,1}, y_{3,1,1} = u_{3,1,1}, D(x_{4,1}) = u_{4,1,1}, y_{4,1,1} \\
& = x_{4,1}, Sink_{Scope,5,1,1} = u_{5,1,1}, y_{6,1,1} = Source_{Step,6,1}, y_{7,1,1} \\
& = Source_{Step,7,1}, y_{8,1,1} = u_{8,1,1} - u_{8,2,1}, y_{9,1,1} = u_{9,1,1} \\
& + u_{9,2,1}, D(x_{10,1}) = u_{10,1,1} - K_{0,"a1"} x_{10,1}, y_{10,1,1} = x_{10,1}, \\
& D(x_{11,1}) = u_{11,1,1} - K_{0,"a2"} x_{11,1}, y_{11,1,1} = x_{11,1}]
\end{aligned}$$

State Variables [3]:

$$[[x_{4,1}, x_{10,1}, x_{11,1}]]$$

Initial Equations [3]:

$$[[x_{4,1}([0]) = 0, x_{10,1}([0]) = 0, x_{11,1}([0]) = 0]]$$

Source Equations [2]:

$$\left[\begin{array}{l} Source_{Step,6,1} = \begin{cases} 0 & t < 1 \\ 1 & otherwise \end{cases}, Source_{Step,7,1} = \\ \begin{cases} 0 & t < 4 \\ 0.1 & otherwise \end{cases} \end{array} \right]$$

Input Variables [2]:

$$[Source_{Step,6,1}, Source_{Step,7,1}]$$

Output Variables [1]:

$$[Sink_{Scope,5,1,1}]$$

Parameters [2]:

$$[K_{0,"a1"} = 2., K_{0,"a2"} = 1.] \quad (1.2)$$

4. Use Maple's built-in simplification and simulation routines, especially those in the DynamicSystems package, to manipulate the model.

With the basic tools outlined here, you are now ready to use BlockImporter to create many engineering design solutions. See the Maple help system for more information about the commands used in this guide, or more ways in which BlockImporter can help you.

2 Global Optimization Toolbox

2.1 Introduction to the Global Optimization Toolbox

Overview

The Global Optimization Toolbox, powered by Optimus technology from Noesis Solutions, provides world-class global optimization technology to return the best answer to your optimization model, robustly and efficiently.

Features of this toolbox include:

- Several solver modules for nonlinear optimization problems, including branch-and-bound global search, global adaptive random search, multi-start based global random search, and a generalized reduced gradient local search.
- The ability to solve models with thousands of variables and constraints, with Maple's arbitrary precision capabilities in their calculations, to greatly reduce numerical instability.
- Support for arbitrary objective and constraint functions, including those defined in terms of special functions (for example, Bessel or hypergeometric), derivatives and integrals, piecewise functions, and Maple procedures.
- The interactive GlobalOptimization Assistant, an easy-to-use interface for entering your problem and choosing the solving method.
- Maple's built-in model visualization capabilities for viewing one- or two-dimensional subspace projections of the objective function, with visualization of the constraints as planes or lines on the objective surface.

Requirements

Before installing the Global Optimization Toolbox, you must install and activate Maple 2021. For details and installation instructions, see the Install.html file on the product disc.

You need a purchase code to activate the Global Optimization Toolbox. This code has been emailed to you. If you have not received your purchase code, contact Maplesoft Customer Service at custservice@maplesoft.com, or the Maplesoft office or reseller in your region (visit <http://www.maplesoft.com/contact/>).

After installation, enter `?GlobalOptimization` in Maple to see an overview of the toolbox.

2.2 Getting Started with the Global Optimization Toolbox

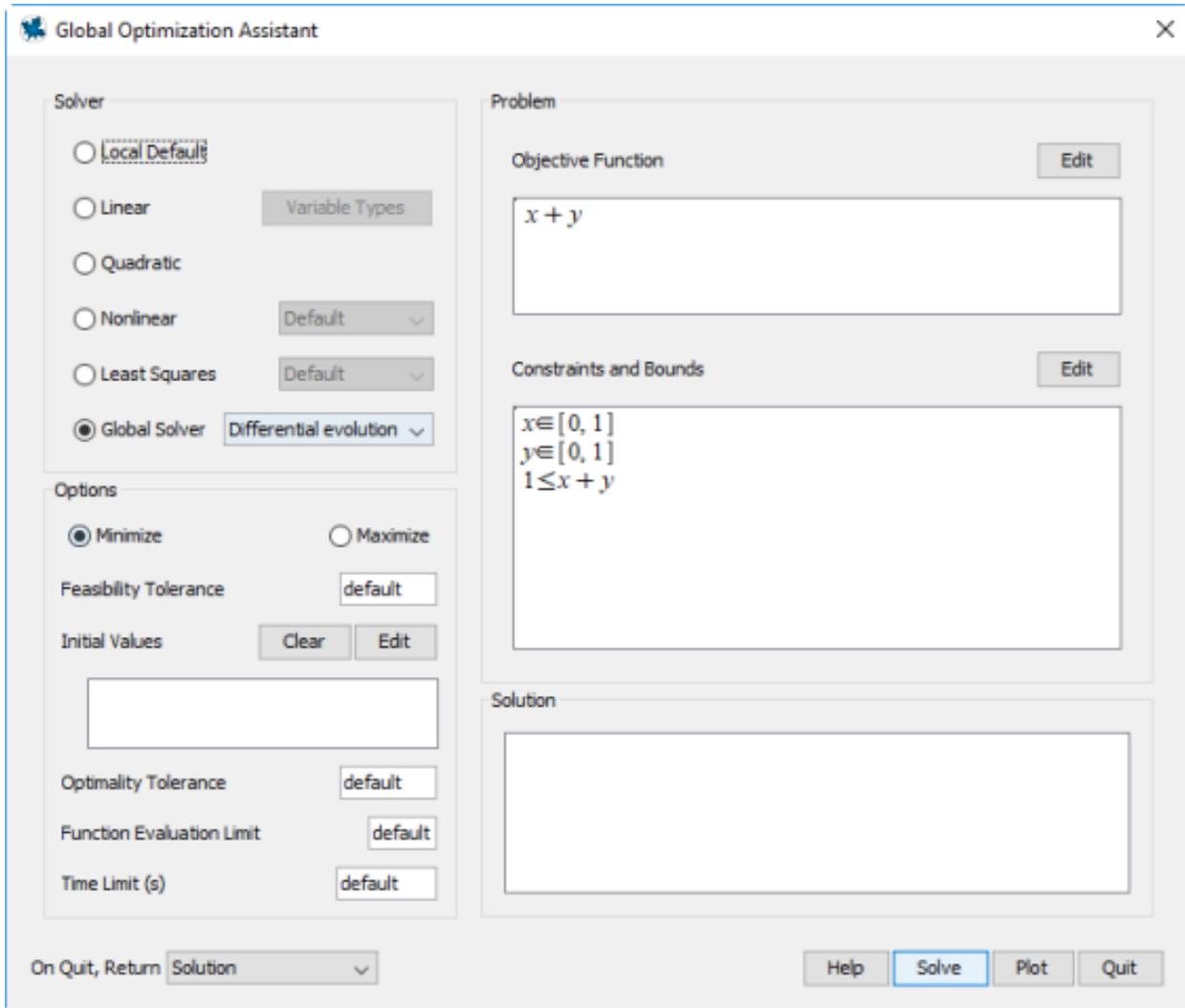
Initialization

To start using the Global Optimization Toolbox, open a new Maple window and load the **GlobalOptimization** package by using the following command.

```
> with(GlobalOptimization);
```

```
[GetLastSolution, GlobalSolve, Interactive] (2.1)
```

You can either use the commands to solve your pre-defined global optimization problem, or use the Global Optimization Assistant, shown below. The following examples demonstrate the use of the commands, but the assistant could also be used to solve any of the problems presented.



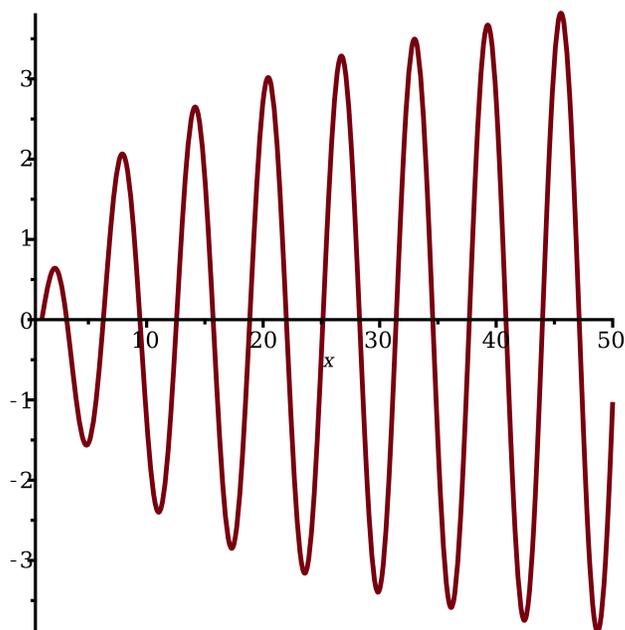
Help with the Global Optimization Toolbox

For help with the commands in the Global Optimization Toolbox, see the **GlobalOptimization** help page. You may also find the related commands in the built-in **Optimization** package helpful for solving optimization problems. For more information, refer to the **Optimization** help page.

2.3 Working with the Global Optimization Toolbox

In many optimization problems, simple methods are not sufficient to find the best solution. They will only find a local optimum, usually the one closest to the search starting point, which is often given by the user. For example, consider the expression $\ln(x) \cdot \sin(x)$.

```
> plot(ln(x)·sin(x), x = 1 ..50)
```



You could likely approximate the global minimum in the given domain, and find that minimum easily, by simply looking at the plot. But if you were unable to properly approximate it, or if you approximated incorrectly, you would not find the global minimum by using the usual optimization techniques.

```
> Optimization[Minimize](ln(x)·sin(x), x = 1 ..50)
```

```
[-3.39618690740209, [x = 29.8549920107437]] (2.2)
```

According to the **Minimize** command, the minimum is at approximately $x = 30$. However, you can see in the plot above that this is not the global minimum.

By using the global optimization equivalent of this command, you can be assured that you have found the global minimum in the specified interval.

```
> with(GlobalOptimization) :
```

```
> GlobalSolve(ln(x)·sin(x), x = 1 ..50)
```

```
[-3.88562416790700960, [x = 48.6999273727307]] (2.3)
```

To view the solving methods that were used to determine the global minimum, change the *infolevel* variable and re-execute the command. At *infolevel* = 3, the command displays the input model size and type, solver operational mode and parameter, and detailed runtime information.

```
> infolevel[GlobalOptimization] := 3 :
```

> `GlobalSolve(ln(x)·sin(x), x = 1 ..50)`

```
GlobalSolve: calling NLP solver
GlobalSolve: calling global optimization solver
GlobalSolve: number of problem variables 1
GlobalSolve: number of nonlinear inequality constraints 0
GlobalSolve: number of nonlinear equality constraints 0
GlobalSolve: method OptimusDEVOL
GlobalSolve: maximum iterations 80
GlobalSolve: population size 50
GlobalSolve: average stopping stepwidth 0.1e-3
GlobalSolve: time limit 100
GlobalSolve: trying evalhf mode
GlobalSolve: performing local refinement
```

`[-3.88562416790700960, [x = 48.6999273727307]]` (2.4)

Typically, the `inforevel` is set to 0, the default.

> `inforevel[GlobalOptimization] := 0 :`

The following is an example of a situation in which you cannot approximate the global minimum by using linear methods; however, the global solver finds the best solution.

Example

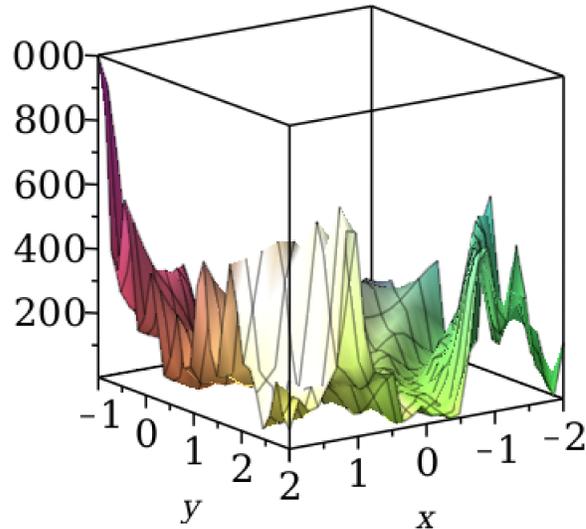
Consider a non-linear system of equations.

> `eq1 := sqrt(x^2 + y^4) + e^(x-y^2) + 5 sin(2 x - 4 x y) - 12 cos(x y) :`

> `eq2 := 5 ln(1 + x^2) + e^(-y+x) + 5 sin(6 x y) :`

The induced least-squares error function is highly multi-extremal, making it difficult to minimize the error of the least squares approximation.

```
> plot3d(eq12 + eq22, x = -2..2, y = -1..3, grid = [30, 30],
  lightmodel = light4, axes = boxed)
```



To determine the global minimum of the least-squares error, define the objective function and constraints to be optimized.

```
> objf := eq12 + eq22 :
```

```
> cons := {eq1, eq2} :
```

First, try to find a local solution by using Maple's built-in **Optimization** package. This system is sufficiently complex that linear optimization solvers cannot find a feasible solution.

```
> localsoln := Optimization[Minimize](objf, {eq1 = 0, eq2 = 0},
  x = -1..2, y = -2..1)
```

```
Error, (in Optimization:-NLPSolve) no improved point could be found
```

However, global optimization techniques can be used to find a global minimum.

```
> sol := GlobalSolve(objf, {eq1 = 0, eq2 = 0}, x = -1..2, y = -2
  ..1) :
  sol[1]; sol[2]
```

$6.31088724176809444 \cdot 10^{-30}$

$[x = -0.558972497939247, y = -1.58234523718254]$ (2.5)

Substitution into the constraints shows that the least squares approximation can be a fairly precise solution. That is, the error of the least squares approximation is very small at the minimum point.

```
> eval(cons, sol[2])
```

$\{1.77635683940025 \cdot 10^{-15}\}$ (2.6)

With the examples demonstrated here, you are now ready to use the Global Optimization Toolbox to solve many complex mathematical problems. See the Maple help system for more information about the commands used in this guide, or more ways in which the Global Optimization Toolbox can help you.

3 Grid Computing Toolbox

3.1 Introduction to the Grid Computing Toolbox

Overview

The **Grid Computing Toolbox** provides tools for performing Maple computations in parallel, allowing you to distribute computations across a network of workstations, a supercomputer, or the CPUs of a multiprocessor machine. It includes a personal grid server, allowing you to simulate and test your parallel applications before running them on a real grid network.

Features of this toolbox include:

- A self-assembling grid in local networks, with an easy-to-use interactive interface for launching parallel jobs.
- Integration with job scheduling systems, such as PBS.
- High-level parallelization operations, such as *map* and *seq*, as well as a generic, parallel divide-and-conquer algorithm.
- Automatic deadlock detection and recovery.

Requirements

Before installing the Grid Computing Toolbox, you must install and activate Maple 2021. For details and installation instructions, see the `Install.html` file on the product disc.

You need a purchase code to activate the Grid Computing Toolbox. This code has been emailed to you. If you have not received your purchase code, contact Maplesoft Customer Service at custservice@maplesoft.com, or the Maplesoft office or reseller in your region (visit <http://www.maplesoft.com/contact/>).

Note that if you do not have a valid Grid license, the Grid Computing Toolbox will run in a limited capacity, allowing at most one server per machine and eight nodes in a job.

After installation, the `GridComputing.mw` file appears on your desktop (Windows and Mac) or in your home directory (Linux). Open this file.

3.2 Getting Started with the Grid Computing Toolbox

Establishing a Server and Network

You can run a server on your desktop machine to develop and test your parallel applications. The **Personal Grid Server** worksheet is an interactive Maple document that can help you start a personal server with any number of nodes. For more information, refer to the **Grid/wks/PersonalGridServer** help page.

The following Maple commands are a guideline for configuring your computer for a personal server. The given broadcast mask should ensure that you will not be added to any Grid networks. Note that these settings can be set by default. See the **Install.html** file for instructions. Configuration details can be found on the **Grid/Properties** help page.

```
> gridhost := "localhost" :  
   gridport := 2000 :  
  
> Grid[Setup]( "hpc", host = gridhost, port = gridport )  
                                     2000                                     (3.1)
```

To run Grid Computing applications on a network of machines, you must start Grid servers on each machine that you want to be part of the network. The toolbox will automatically detect new machines as they are added to the network, or you can turn off auto-discovery for use in a controlled environment, such as a PBS setup.

You will need to re-configure the Grid so that you can create or be added to a Grid network. Change the *broadcastAddress* and *broadcastPort* to your network's settings, and then start a server with those settings.

A few simple interactive examples using multiple nodes over multiple machines are in the **Grid Computing** worksheet. For more information, refer to the **Grid/wks/Grid** help page.

You are now ready to use the Grid Computing Toolbox, either on your own computer as a test server, or on a network of computers to run parallel applications.

Help with Grid Computing

For a list of commands in Maple to support the Grid Computing Toolbox, see the **Grid** help page.

3.3 Working with the Grid Computing Toolbox

As mentioned in the previous section, a few simple examples using multiple nodes over multiple machines can be found in the **Grid Computing** worksheet. For more information, refer to the **Grid/wks/Grid** help page.

The following provides a sample of the commands required to execute such examples. To begin, start a personal server using the local settings from the previous section, or use your network settings to connect with other computers running servers in the Grid Computing Toolbox. The code for this example can be found in the Grid Computing worksheet.

> *with(Grid)* :

```
> Server[StartServer](port = 2000, numnodes = 4)
24417 (3.2)
```

Define the application or procedure that you want to perform, call it *sampleCode*. Then execute the following commands to deploy the application *sampleCode* over the network.

```
> fname := cat(kernelopts(toolboxdir = "Grid"),
"/samples/Simple.mpl") :
> sampleCode := FileTools[Text][ReadFile](fname) :
> AvailableNodes := Status()[2]
AvailableNodes := 4 (3.3)
```

```
> result := Launch(numnodes = AvailableNodes, sampleCode )
Node 2: This is node 2 out of 4
Node 3: This is node 3 out of 4
Node 0: This is node 0 out of 4
Node 1: This is node 1 out of 4
result := [foo0bar, foo1bar, foo2bar, foo3bar] (3.4)
```

When you are finished, make sure to close the connection before you close Maple, by executing the following command.

```
> Server[StopServer](port = 2000, numnodes = 4)
0 (3.5)
```

The following is a more detailed example of how you can use the Grid Computing Toolbox to create and perform parallel applications on a network of computers.

Example

Consider a fractal, specifically a Julia set, that you want to create and display in Maple. For any more than a few iterations, this can take a long time on a single computer. But you can divide the construction between an arbitrary sized network of computers by using the Grid Computing Toolbox.

First define a Julia set as a procedure, which will determine the color of the plot at point (a, b) . A Julia set is formally defined as

$$\{z \in \mathbb{C} \mid z_{i+1} = z_i^2 + c \text{ converges for } z_0 = z\}$$

where c is a constant.

```
> JuliaSet := proc(a, b) global c1, c2;
  local z1, z2, z1s, z2s, m;
  (z1, z2) := (a, b) :
  z1s := z1^2 : z2s := z2^2;
  for m from 1 to 30 while z1s + z2s < 4 do
    (z1, z2) := (z1s - z2s + c1, 2*z1*z2 + c2) :
    z1s := z1^2 : z2s := z2^2;
  end do;
  m;
end proc;
```

Here it is assumed that for m over 30, the sequence z converges. Increasing this number will make the computation more accurate, but take much more time. Define the constant $c = c1 + I \cdot c2$ and an appropriate view and grid size for this fractal. If c is changed, then v and $gridsize$ may also need to be changed for the fractal to display properly.

```
> c1, c2 := -1.1107, .3089 :
> v := [-1.7..1.6, -1..1] :
> gridsize := [250, 250] :
```

To display the fractal as a plot, use the Julia Set as the color. The procedure *plotsegment* displays the fractal, and is called by the nodes of the grid separately for each section of the plot.

```
> plotsegment := subs(js = eval(JuliaSet), proc(viewgrid)
  plot3d(0, viewgrid[1], viewgrid[2], orientation = [-90, 0],
  grid = viewgrid[3], style = patchnogrid,
  scaling = constrained, color = js) :
  end proc) :
```

Define the procedure to be run by the **Launch** command, which includes a procedure for splitting up the computation. For more information, refer to the **Grid/Launch** help page.

```

> code := proc( ) local msg, split;
    split := proc( view, gridsize, n)
        local i, gs, splitview, viewi, viewn; global vlength,
        vs;
        vs := op( view[1] )[1] :
        vlength := abs( op( view[1] )[2] - op( view[1] )[1] ) / n :
        gs := floor( gridsize[1] / n ) :
        splitview := [ vs .. vs + vlength, view[2], [ gs,
gridsize[2] ] ] :
        vs := vs + vlength :
        for i from 2 to n do
            if i = n then
                viewn := vs .. op( view[1] )[2] :
                splitview := splitview, [ viewn, view[2], [ gridsize[1]
- (n - 1) · gs, gridsize[2] ] ] :
            else
                viewi := vs .. vs + vlength :
                vs := vs + vlength :
                splitview := splitview, [ viewi, view[2], [ gs,
gridsize[2] ] ] :
            end if:
        end do:
        splitview;
    end proc:

    msg := Grid:-Map( plotsegment, [ split(v, gridsize, N) ] ) :
    msg;
end proc:

```

Restart the Grid with your computer as the server, as in the above example. Configure the server for your network to run this example over a Grid.

```

> Server[ StartServer ]( port = 2000, numnodes = 4)
                                24525                                     (3.6)

```

```

> N := Status( ) [2]
                                N := 4                                 (3.7)

```

Now you are ready to perform the computation and display the results. Ensure that you pass all assigned variables to the **Launch** command, or they will not be available on the other nodes of the grid.

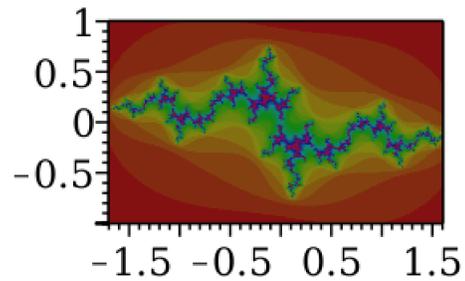
The printer is specified as *printf*, but could be any method of output, including writing to a text area component or a text file. The procedure provides a mechanism for you to stop the computation at any time, on all nodes. In this example, it is always false, so the computation cannot be stopped.

```

> picture := Launch( code, numnodes = N, imports
    = [ "plotsegment", "v", "gridsize", "JuliaSet", "c1", "c2",
"N" ] ) :

```

```
> plots[display](picture);
```



```
> Server[StopServer](port = 2000, numnodes = 4);
```

With the basic tools shown here, you are now ready to use the Grid Computing Toolbox to solve many large mathematical problems. See the Maple help system for more information about the commands used in this guide, or more examples illustrating how the Grid Computing Toolbox can help you.

4 Quantum Chemistry Toolbox

4.1 Introduction to the Quantum Chemistry Toolbox

Overview

The Maple Quantum Chemistry Toolbox is a comprehensive, easy-to-use environment for the parallel computation of the electronic energies and properties of molecules.

Features of this toolbox include:

- Define molecules instantly from a database of 96+ million molecules
- Run quantum computations with well-known electronic structure methods as well as recently developed, advanced methods for cutting-edge research
- Analyze molecular energies and properties through publication-quality, 2-D and 3-D plots and animations.

The Quantum Chemistry Toolbox is designed and implemented by RDMChem LLC, which was founded to develop the next generation of computational chemistry software with applications to engineering, molecular biology, and physics. While conventional wave function methods scale exponentially with the size of the molecule, the Toolbox achieves a low, polynomial computational scaling through recently developed reduced density matrix (RDM) methods. These methods enable the computation of strongly correlated molecules and materials that were previously inaccessible. They are capable of providing chemists, physicists, and materials scientists with the ability to predict and design novel molecules and materials for applications across the sciences.

Requirements

Before installing the Quantum Chemistry Toolbox, you must install and activate Maple 2021. For details and installation instructions, see the Install.html file on the product disc.

You need a purchase code to activate the Quantum Chemistry Toolbox. This code has been emailed to you. If you have not received your purchase code, contact Maplesoft Customer Service at custservice@maplesoft.com, or the Maplesoft office or reseller in your region (visit <http://www.maplesoft.com/contact/>).

4.2 Getting Started with the Quantum Chemistry Toolbox

Initialization

To start using the Quantum Chemistry Toolbox, open a new Maple window and load the Quantum Chemistry Toolbox commands by using the following command.

```
> with(QuantumChemistry);
      [AOLabels, ActiveSpaceCI, ActiveSpaceSCF, AtomicData,
       BondAngles, BondDistances, Charges, ChargesPlot,
       ContractedSchrodinger, CorrelationEnergy, CoupledCluster,
       DensityFunctional, DensityPlot3D, Dipole, DipolePlot, Energy,
       ExcitationEnergies, ExcitationSpectra, ExcitationSpectraPlot,
       ExcitedStateEnergies, ExcitedStateSpins, FullCI,
       GeometryOptimization, HartreeFock, Interactive, Isotopes,
       MOCoefficients, MODiagram, MOEnergies, MOIntegrals,
       MOOccupations, MOOccupationsPlot, MOSymmetries, MP2,
       MolecularData, MolecularDictionary, MolecularGeometry,
       NuclearEnergy, NuclearGradient, OscillatorStrengths,
       Parametric2RDM, PlotMolecule, Populations, Purify2RDM,
       RDM1, RDM2, RTM1, ReadXYZ, Restore, Save, SaveXYZ,
       SearchBasisSets, SearchFunctionals, SkeletalStructure,
       Thermodynamics, TransitionDipolePlot, TransitionDipoles,
       TransitionOrbitalPlot, TransitionOrbitals, Variational2RDM,
       VibrationalModeAnimation, VibrationalModes, Video]
```

(4.1)

Set the global variable, Digits to 15 (double precision) rather than 10 (default):

```
> Digits := 15 :
```

For an introduction to the Quantum Chemistry package, including detailed examples, see **QuantumChemistry,Tutorial**.

Help with Quantum Chemistry

For help with the commands in the Quantum Chemistry Toolbox, see the **QuantumChemistry,Overview** help page.

In addition, a video tutorial is available. See the **QuantumChemistry,Video** help page for details.

4.3 Working with the Quantum Chemistry Toolbox

The examples in the next section demonstrate some everyday uses of the Quantum Chemistry Toolbox, and the ways in which the commands work together. More examples are available on the **QuantumChemistry,Tutorial** page.

Examples

```
> with(QuantumChemistry) :
```

The geometry of the hydrogen fluoride (HF) molecule is entered as a Maple list of lists.

```
> hf := [{"H", 0, 0, - 0.48}, {"F", 0, 0, 0.48}];
      hf := [{"H", 0, 0, -0.48000000}, {"F", 0, 0, 0.48000000}]
```

(4.2)

Calculate the energy of hydrogen fluoride (HF), from the Hartree-Fock method using the **QuantumChemistry,Energy** command.

```
> Energy(hf, method = HartreeFock);  
-98.57282092 (4.3)
```

Use the **QuantumChemistry,PlotMolecule** command to visualize the geometry of hydrogen fluoride.

```
> PlotMolecule(hf)
```

