A Basic Introduction on Math-Link in Mathematica

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## Contents

Preface 3

1 Introduction 4

2 How to Start Mathematica ? 4
   2.1 How to Use a Mathematica Notebook ? . . . . . . . . . . . . . . . . . . 5
   2.2 How to Write a Program in Mathematica ? . . . . . . . . . . . . . . . . 5
       2.2.1 Characterization of Local and Global Variables . . . . . . . 7

3 How to Link External Programs in Mathematica by Using Proper Math-Link Commands ? 8
   3.1 Mathlink for XL Fortran-90 Source Files . . . . . . . . . . . . . . . . 8
       3.1.1 How to Compile and Optimize XL Fortran-90 Source Files ? . . 10
       3.1.2 Link of XL Fortran-90 Program with Mathematica . . . . . . . 11
       3.1.3 Link of other XL Fortran Programs with Mathematica . . . . . 13

Concluding Remarks 13

Acknowledgment 13

References 13
Preface

Starting from the basic ideas of mathematica, we give a detailed description about the way of linking of external programs with mathematica through proper mathlink commands. This article may be quite helpful for the beginners to start with and write programs in mathematica.

In the first part, we illustrate how to use a mathematica notebook and write a complete program in the notebook. Following with this, we also mention elaborately about the utility of the local and global variables those are very essential for writing a program in mathematica. All the commands needed for doing different mathematical operations can be found with some proper examples in the mathematica book written by Stephen Wolfram [1].

In the rest of this article, we concentrate our study on the most significant issue which is the process of linking of external programs with mathematica, so-called the mathlink operation. By using proper mathlink commands one can run very tedious jobs efficiently and the operations become extremely fast.
1 Introduction

Mathematica is a robust software development for doing mathematics. It has widespread applications in different fields and is often used for research, loading and analyzing data, giving technical presentations and seminars etc. Mathematica is extraordinary well-rounded. It is suitable for both numeric and symbolic work, and it has remarkable word-processing capabilities as well. Mathematicians can search for a working model, do intensive calculation, and write a dissertation on the project (including complex graphics) – all from within mathematica. It is mathematica’s complete consistency in design at every stage that gives it this multilevel capability and helps advanced usage evolve naturally.

Symbolic programming is the underlying technology that provides mathematica this unmatched range of abilities. Just a single line sometimes makes a meaningful program in mathematica—the syntax, documents and methodology used for input and output remaining as they are for immediate calculations. It supports every type of operation—be they data, functions, graphics, programs, or even complete documents—to be represented in a single, uniform way as a symbolic expression. This unification has many practical benefits to broadening the scope of applicability of each function. The raw algorithmic power of mathematica is magnified and its utility extended.

2 How to Start Mathematica?

We generally use mathematica through documents called notebooks. To start a mathematica notebook in Unix we write ‘mathematica &’ from a command line and then press the ‘Enter’ key from the keyboard. A typical notebook consists of cells that may contain graphics, texts, programs or calculations. Now to exit from a mathematica notebook we first go to the command ‘File’ and then press ‘Quit’ from the menu bar of the notebook. Without using a notebook one can also use mathematica by typing the command ‘math’ from a command line and all the jobs can also be done as well. To exit from mathematica for this particular case, we should write either ‘Exit’ or ‘Quit’ and then press the ‘Enter’ key. Thus one can run mathematica by using any one of the above two ways, but the most general way to do the interactive calculations in mathematica is the use of mathematica through notebook documents.
2.1 How to Use a Mathematica Notebook?

In a notebook, a job is performed in a particular cell and for different jobs we use different cells. One can also use a single cell for all the operations, but it is quite easy if different operations are performed in separate cells. A cell is automatically created when we begin to write anything in the notebook. After writing proper operation/operations, it is needed to run the jobs. For this purpose, we press the key ‘Shift’ and holding this key, we then press ‘Enter’ from the keyboard. The results for the inputs are evaluated and they are available immediately underneath in a separate cell, so-called the output cell.

In mathematica we can do all kinds of mathematical operations like numerical computation, algebraic computation, matrix manipulation, different types of graphics etc., and all these things are clearly described by several examples in key mathematica book of Wolfram Research [1]. So in this article we shall not give any such example further. Now to do large numerical computations, it is needed to write a complete program. For this purpose, here we describe something about the way of writing a complete program in a mathematica notebook.

2.2 How to Write a Program in Mathematica?

In mathematica, we can write a program efficiently compared to any other existing languages. As illustrative example, here we mention a very simple program which is: the generation of a list of two random numbers and the creation of a 2D plot from these numbers.

The program is:

```mathematica
sample[times_] := Block[{local variables},
numbers = Table[{Random[], Random[]}, {i, 1, times}];
figure = ListPlot[numbers, PlotJoined -> True, AxesLabel -> {xlabel, ylabel}]]
```

This is the complete program for the generation of a list of two random numbers and the creation of a 2D plot from these numbers. This program is written in a single cell. After the end of this program we run it by using the command ‘SHIFT’ + ‘ENTER’, and then the mathematica does the proper operations and executes the result in an output cell.

Now to understand this program, it is necessary to describe the meaning of the
different commands used in this program. To start a program it is necessary to specify a name for the particular program. In this case, we specify ‘sample’ as a program name, for the sake of simplicity. One can also use any other name in place of ‘sample’, since this is a dummy name. If there is any running variable, like ‘times’ (a dummy variable) in this particular case, then it has to be given within the bracket ‘[ ]’. After that the symbol ‘_’ is used, which indicates the variable as a functional variable. This is similar to define a functional variable, like $f[x]$ as $f[x_]$ in mathematica. Now all the mathematical commands those are used for calculating the job are inserted within ‘Block[...]. This is the central part of the program. This portion i.e., ‘Block[...’ is connected with ‘sample[times_]’ by the symbols ‘:=’. The symbol ‘:’ has an important role, and therefore it has to be taken into account properly. Inside the ‘Block’ the ‘local variables’ for the program are declared within the bracket ‘{ }’. There may also exist another type of variables called ‘global variables’. Later in this article, we will focus about these two different types of variables in detail. Now the rest part of the program differs from program to program depending on the nature of the particular operations. In this program, first we construct a list of two random numbers. In mathematica, a random number is generated simply by using the command ‘Random[]’. Therefore, a list of two such random numbers can be done very easily if we construct a table, which is performed by the command ‘Table’ as given in the program. The integer $i$ runs from 1 to ‘times’, where the value of ‘times’ can be put anything. So if we write ‘sample[10]’, here ‘times = 10’, then $i$ runs from 1 to 10 and if we take ‘sample[30]’, where ‘times = 30’, then $i$ goes from 1 to 30. Now it becomes quite user friendly if we
mention different variable names for the different mathematical operations which are *not exactly* identical with any built in function available in mathematica like ‘Random’, ‘Table’, ‘Plot’, etc. In this program we use the variable names ‘numbers’ and ‘figure’ for the two different operations. At the end of each mathematical operation, except the last operation which gives the final output of a program, we put the symbol ‘;’. This is also very crucial. Here we use the symbol ‘;’ at the end of the second line only, but not in the last operation since this is the final output of this program. The command ‘ListPlot’ plots the list of data points where the command ‘PlotJoined→True’ connects the lines between the data points. Finally, the command ‘AxesLabel’ in this line is an option for the graphics functions to specify the labels in the axes.

The output for this program is shown in Fig. 1 which appears in a separate cell just below the input cell of the program. So now we can easily write and compile a program in mathematica.

### 2.2.1 Characterization of Local and Global Variables

The local and global variables in mathematica play an important role, and therefore care should be taken about these two types of variables when we write a program in mathematica. We have already mentioned about the local variables in the previous section that these variables are introduced only inside the bracket ‘{ }’ at the beginning of the ‘Block[ ]’. In such a case, the values of these parameters are only *defined within the cell* where we write a particular program. Outside this cell, they are undefined and therefore, we may also use these same parameters for writing other programs without any trouble.

On the other hand, the global variables are those which are not used within the bracket ‘{ }’ of a program. For such a case, these variables are assigned throughout the notebook for all cells. Thus if we declare any value for a such parameter, then it will read this particular value whenever we use it in any program. Accordingly, it may cause a difficulty if we use the same variable in another program by mistake. So we should take care about these two types of variables. To make it clear, here we illustrate the behavior of these two different kinds of variables by giving proper examples.

```mathematica
sample[times_]:=Block[{t = 2.3, p = -1.5},
    numbers=Table[{{Random[]}, Random[]}, {i, 1, times}];
    figure=ListPlot[numbers, PlotJoined→True, AxesLabel→{xlabel, ylabel}]]
```
Let us consider the above program which is written in a particular cell in the mathematica notebook. In this program, we introduce two local variables \( t = 2.3 \) and \( p = -1.5 \). Both these two variables are given inside the bracket ‘\{ \}'. Now if we check the values outside the cell then the output will be simply \( t \) and \( p \) for these two variables. So these are the local variables and one can safely use these parameters again in other programs.

```mathematica
sample[times_] := Block[{t = 2.3, p = -1.5},
    q = 3.5;
    numbers = Table[{Random[], Random[]}, {i, 1, times}];
    figure = ListPlot[numbers, PlotJoined -> True, AxesLabel -> {xlabel, ylabel}]]
```

Now we refer to this program where we introduce an extra line for another variable \( q = 3.5 \) compared to the previous program of this section. Once we run this program, the value of \( q \) will be assigned for any cell of the notebook. Therefore, in this case \( q \) becomes the global variable, and if one uses it further in other program then the value of this parameter \( q \) will be assigned as 3.5. Hence a mismatch will occur, and thus we should be very careful about these two different types of parameters.

### 3 How to Link External Programs in Mathematica by Using Proper Math-Link Commands?

This section describes the most significant issue of this article which deals with the way of linking of an external program with mathematica through proper mathlink commands. The mechanism for the linking of external program written in C with mathematica has already been established [2]. But this will not work if one tries to link an external program written in other languages like F77, F90, F95, etc., with mathematica. This motivates us to find a way of linking an external program written either in any one of these later languages (F77, F90, F95) with mathematica. Here we illustrate it for the FORTRAN-90 source files [3, 4] only, but this mechanism will also work significantly for the other Fortran source files as well.

#### 3.1 Mathlink for XL Fortran-90 Source Files

In order to understand the basic mechanism for linking an external program with mathematica, let us begin by giving a simple example. Here we set the program as
follows:

1. Construct two square matrices in mathematica.

2. Take the product of these two matrices by using an external program written in F90.

3. Calculate the eigenvalues of the product matrix in mathematica.

The whole operations can be pictorially represented as,

![Diagram](image)

Figure 2: Schematic representation of mathlink operations.

The operations 1 and 3 are performed in mathematica, while the operation 2 is evaluated by the external program. The transformations of the datas from the mathematica notebook to the external program are done by using some proper commands, so-called mathlink operation. To complete this particular job (operations 1-3), we need two programs. One is written in mathematica for the operations 1 and 3, while the other program is written in F90 for the operation 2. Now we describe all these steps one by one. Let us first concentrate on the external program, given below, where the multiplication of the two square matrices (operation 2) is performed. The first line of the program corresponds to the command line where the symbol ‘!’ is used to make a statement as a command statement. The next line provides a specific name of the program which is described by the command ‘program multiplication’. This actually starts the program, and accordingly, the program is ended by the command ‘end program multiplication’. In F90, we can allocate and deallocate array variables in the programs which help us a lot to save memory and are very essential to run many jobs simultaneously. Here we use three array variables ‘a, b and c’ for the three different matrices whose dimensions are allocated by the order of the matrix ‘n’. Finally, the product of the two matrices ‘a’ and ‘b’ is determined by the command ‘matmul(a,b)’
and the datas are stored in the matrix ‘c’. This is the full program for the matrix multiplication of any two square matrices of order ‘n’.

![A program for matrix multiplication of two square matrices](image)

```fortran
program multiplication
  implicit double precision (a-h,o-z)
  double precision, allocatable :: a(:,:,),b(:,:,),c(:,:,)
  read *, n !(the order of the matrix)
  allocate (a(n,n),b(n,n),c(n,n))
  read *, ((a(i,j),j=1,n),i=1,n) ; read * , ((b(i,j),j=1,n),i=1,n)
  ! Calculation of matrix multiplication :
  c=matmul(a,b)
  print'(1(1x,f10.6))',((c(i,j),j=1,n),i=1,n)
end program multiplication
```

### 3.1.1 How to Compile and Optimize XL Fortran-90 Source Files?

After writing a program, first we need to compile it to check whether there is any syntax error or not to proceed for further operations. Several commands are accessible for the compilation and optimization of a program. The commands generally used to compile a F90 source file are: xlf90, xlf90\_r, xlf90\_r7, etc. Thus we can use anyone of these to compile this program, but different commands optimize a program in different ways which solely depends on the nature of the particular program. The simplest way for the compilation of a program is,

```
xlf90 filename.f
```

With this operation, an ‘executable file’ named ‘a.out’ is created, by default, in the present working directory (pwd). But if one uses several programs simultaneously then it would be much better to specify different names of different ‘executable files’ for separate programs. To do this we use the prescription,

```
xlf90 filename.f -o filename
```

Under this process, the ‘executive file’ named as ‘filename’ is created. Thus we can create proper ‘executive files’ for different jobs and all the jobs can be performed simultaneously without any difficulty.

For our illustrative purposes, below we mention some other optimization techniques for the Fortran source files.
-o : Optimizes code generated by the compiler.

-00 : Performs no optimizations. (It is the same as -qnoopt.)

-02 : Optimizes code (this is the same as -O).

-03 : Performs the -O level optimizations and performs additional optimizations that are memory or compile time intensive.

-04 : Aggressively optimizes the source program, trading off additional compile time for potential improvements in the generated code. This option implies the following options: -qarch=auto -qtune=auto -qcache=auto -qhot -qipa.

-05 : Same as -O4, but also implies the -qipa=level=2 option.

From these operations, we can make some flavors about the compilation and optimization technique for a Fortran source file. For a detailed description of each operation, we refer to the XL Fortran User’s Guide [5].

3.1.2 Link of XL Fortran-90 Program with Mathematica

This is the heart of this article. Below we set the mathematica program for the operations 1 and 3, incorporating the operation 2 by using the proper mathlink commands, and illustrate all the steps properly.

Let us suppose the external program, for the operation 2, is written in the directory `/allibmusers/santanu/files/test`. Generally we are habituated to see the working directory as `/user/santanu/...` or `/home/santanu/...` or `/allusers/santanu/...`, etc. So it can be anything like these. Thus knowing the directory where the external program is written, we enter into that particular directory and compile the external program properly to create an ‘executive file’ for further operations. For this particular case, we create the ‘executive file’ named as ‘mat’ which is used in the 13-th line of the following mathematica program. Now the external program is ready for the operation, and we enter into the directory where we will run the job in the mathematica notebook for the operations 1 and 3.

Sitting in the directory where the mathematica notebook is open, we need to connect the proper directory where the ‘executive file’ for the external program exists. The name of the pwd can be checked directly from the mathematica notebook by using the command ‘Directory[]’. Suppose the pwd is `/allibmusers/santanu/math`. Now If this
pwd is different from the directory where the file ‘mat’ exists, then we make a link to that particular directory through the command ‘SetDirectory’. Below we give an example to connect the directory ‘/allibmusers/santanu/files/test’, where the file ‘mat’ exists.

```
SetDirectory["/allibmusers/santanu/files/test"]
```

For this operation, the total path must be used within the double quotes “ ”. Using the command ‘ResetDirectory[]’, we can come back to the initial directory. Thus we can connect and disconnect any directory with the pwd from the mathematica notebook, and able to link external programs with mathematica very easily.

```
sample[ns_] := Block[{t = 0, s = 0, vacuum1 = {}, vacuum2 = {}},
  SetDirectory["/allibmusers/santanu/files/test"];  
Do[Do[a1 = If[i == j, t, 1.213];
    a2 = AppendTo[vacuum1, a1], {j, 1, ns}], {i, 1, ns}];
  mat1 = Partition[a2, ns];
  Do[Do[a3 = If[k == l, s, 2.079];
    a4 = AppendTo[vacuum2, a3], {l, 1, ns}], {k, 1, ns}];
  mat2 = Partition[a4, ns];
  mat3 = Partition[Flatten[{{mat1}, {mat2}}], ns];
  matrixorder = {ns};
  output = Insert[mat3, matrixorder, 1];
  Export["mat3.dat", output];
  matrix = Partition[Flatten[ReadList["!mat<mat3.dat", Number, 
RecordLists -> True]], ns];
  results = Eigenvalues[matrix]]
```

In the above program, the variables ‘t’ and ‘s’ are the local variables, and we have already discussed about these variables in the previous section. ‘vacuum1={}’ and ‘vacuum2={}’ are the two empty lists where the datas are stored for each operation of the two ‘DO’ loops given in the program to make the lists ‘a2’ and ‘a4’ respectively. The ‘Partition’ command makes the partition of a list. The parameter ‘ns’ gives the order of the two square matrices. By using the command ‘Export’ we send the file ‘mat3.dat’ which is treated as the input file for the external program kept in the directory ‘/allibmusers/santanu/files/test’. To perform the matrix multiplication by using the external program and get back the product matrix in the mathematica notebook we use the operation: ReadList["!mat<mat3.dat", Number, RecordLists->True]. Here
the command ‘ReadLeast’ is used to read the objects from a file and the commands ‘Number’ and ‘RecordLists→True’ are the options of the command ‘ReadList’. Finally, the eigenvalues of the matrix in the mathematica notebook are determined by using the command ‘Eigenvalues’.

3.1.3 Link of other XL Fortran Programs with Mathematica

Now we can also use the mathlink operations for other programs written either in F77 or F95 by the above mechanisms. For these programs, we should use proper commands for the compilations and optimizations. As representative example, here we mention some of the commands for the compilation of these XL Fortran source files those are: xlf, f77, fort77, xlf_r, xlf_r7, xlf95, xlf95_r and xlf95_r7.

So now we can able to use mathlink commands for any type of Fortran program.

Concluding Remarks

In conclusion, we have explored some significant issues of mathematica starting from its basic level i.e., how to start mathematica, open a mathematica notebook, write a program in mathematica, etc., and finally, illustrated the basic mechanism for the linking of external programs with mathematica notebook. This mathlink operation is the heart of this article, and it is extremely crucial for doing large numerical computations. In this article, we have concentrated the mathlink operations mainly for the XL Fortran 90 source files. But these operations can also be used for any other Fortran source files. Following with this, we have also illustrated very briefly about the optimization techniques for the Fortran source files which may help us to run very complicated jobs quite efficiently.

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