

MathCode F90

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First edition, 2006

Preface

Mathematica is a comprehensive numeric and symbolic programming system with applications in a wide range of areas. The *MathCode*[®] code generation system presented in this book adds very high performance, connectivity to external applications and easy-to-use matrix arithmetic to this system. The combined *Mathematica & MathCode* system becomes a very powerful environment that supports both design, prototyping, programming and documentation.

MathCode makes it possible to develop prototypes in the interactive *Mathematica* environment which can be automatically translated to fast production code in C++ or Fortran90 and, if necessary, linked to external applications. Generated code is typically about 1000 times faster than basic *Mathematica* code, and it is often close to 100 times faster than code generated by the standard *Mathematica Compile*. Both stand-alone code and connected code can be produced. Connectivity from *Mathematica* to C, C++, Fortran77 or Fortran90 code is obtained by automatically generating MathLink code for calling generated code and external applications.

Callbacks from external applications to *Mathematica* can be generated automatically. Generation of stand-alone external code is supported. Symbolic *Mathematica* code can be translated provided that the final result of symbolic operations are arithmetic expressions.

To summarize, *MathCode* opens up completely new possibilities for cost-effective development of high-performance computational applications in the highly productive *Mathematica* environment.

Several people have contributed to particular subject matters within this book and *MathCode*. Johan Gunnarsson contributed to the general design in a number of places, most of the chapter on array slice operations as well as their implementation in *Mathematica*, parts of the high-level code transformations, and several notebook examples. Vadim Engelson implemented parts of the low-level code generator and helped with the external functions and trouble shooting chapter, as well as contributed to the *MathCode* array package and the implementation of external functions and callbacks. Pontus Lidman made most of the index to this book, most of the installation instructions, and helped with editing and minor corrections. Mats Jirstrand gave useful comments regarding the manuscript.

Yelena Turetskaya checked the most recent version of this book. Many other people have read the manuscript and given valuable comments. Thank you!

The *MathCode* system is inspired by the code-generation facilities in an earlier research prototype called ObjectMath, intended for object-oriented mathematical modeling and efficient code generation. This prototype was developed between 1990-96 at the Programming Environments Laboratory, Department of Computer and Information Science, Linköping University, with contributions from myself, Dag Fritzon, Niclas Andersson, Vadim Engelson, Johan Herber, Patrik Hägglund, Lars Viklund, Rickard Westman, and Lars Willför. Vadim Engelson has maintained and further developed the system, including the most recent version. The development of ObjectMath was strongly influenced by the fruitful cooperation with SKF, where the system was used for applications in bearing modeling and simulation.

Linköping, Sweden, 2004

Peter Fritzon

How to Read this Book

This section gives a short reader's guide to the contents of this book. Before starting to read, note that installation instructions for *MathCode* are distributed together with installation media, See distribution CD and read the instructions before you start software installation. *MathCode* FAQ (frequently asked questions) as well as latest software updates are available at www.mathcore.com

Chapter 1 gives a quick introduction to the basic facilities in *MathCode*, including a small “hands-on” example for the reader to try out. This introduction is enough to be able to use *MathCode* on simple applications.

Chapter 2 provides more comprehensive examples of translation. This includes both symbolically expanded code and numeric code, how to organize your code into packages to be translated by *MathCode*, as well as performance measurements of compiled code and comparison with Matlab. After reading chapter 1 and looking at these examples you should be able to use *MathCode* on medium-sized applications, even though it is advisable to read appropriate additional chapters for more complete information.

Chapter 3 covers the convenient array, vector, and matrix operations made available in Mathematica by *MathCode*. This chapter should be read by anyone interested in array and matrix operations.

Chapter 4 explains the notions of type system and static/dynamic typing. The need for typing and some of the design decisions in *MathCode* are motivated. Reading this chapter is not necessary in order to use *MathCode* but gives useful background information.

Additional information concerning declarations of constants, variables, arrays, and functions is given in Chapter 5, which is more detailed than the quick overview in Chapter 1.

Chapter 6 presents an overview of data structure allocation and declaration, with special emphasis on arrays. Related array issues, such as array indexing, are also covered.

Chapter 7 gives a comprehensive description of commands and options for code generation, compilation, linking with compiled object modules and/or external libraries, and building executables.

Chapter 8 presents the *MathCode* call interface to external code written in languages such as C, C++, Fortran77 and Fortran90, as well as the callback mechanism to

Mathematica from code written in these languages.(Mathcode C++ only)

Chapter 9 presents system information, *MathCode* distribution structure and installation instructions.

Chapter 10 explains the *MathCode* translation structure and gives hints on troubleshooting.

The typed subset of *Mathematica* which can be compiled by *MathCode* is defined in Appendix A. Use this appendix as a short reference guide.

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Chapter 1 Quick Tour of *MathCode*

1.1 Introduction

MathCode is a *Mathematica* application package which includes the following:

- Translation of a subset of *Mathematica* to efficient **Fortran90** code
- Type annotations compatible with standard *Mathematica*
- Availability of Matlab-like matrix operations on array sections both in *Mathematica* and in compiled code
- Transparent calling of compiled executable code via MathLink or stand-alone execution

The performance of compiled generated **Fortran90** code is often approximately 1000 times better than standard interpreted *Mathematica*, and often 100 times better than code compiled using the internal *Mathematica* compiler.

1.2 Short Example

The following short example shows one way of using the *MathCode* system. It is recommended that you try it yourself! You must have a **Fortran90** compiler installed on your system in order for the generated code to be executable.

The following command will load *MathCode*:

```
Needs["MathCode`"]
```

You might want to set the working directory to a subdirectory such as ".../DemosF90/Simple" under the *MathCode* root directory. Otherwise all files produced by *MathCode* will be written to the current directory.

```
SetDirectory[$MCRoot<>"/DemosF90/Simple"];
```

Define a simple *Mathematica* function that sums the first n integers:

```
sumint[n_] := Module[{
  res = 0, i
},
  For[i=1, i<=n, i++,
    res = res+i
  ];
  res
];
```

Specify the types of the input parameters, function results, and local variables. This is done by a type markup syntax. The parameter, the result, and the local variables are declared as integers:

```
Declare[
  sumint[Integer x_]->Integer, {Integer, Integer}]
```

Instead of declaring the types using a separate `Declare`, you may put them directly inside the function definition:

```
sumint[Integer n_]->Integer := Module[{
  Integer res = 0,
  Integer i
},
  For[i=1, i<=n, i++,
    res = res+i
  ];
  res
];
```

Generate **Fortran90** code of the functions, including `sumint`, in the context "Global`"1. Then compile and link to an executable connected via *MathLink*:

```
BuildCode[]
```

Start and connect the generated external program seamlessly to *Mathematica*.

```
InstallCode[];
```

The external variant of `sumint` can now be called transparently in the same way as a function inside *Mathematica*:

1. Initially the default compiled package name is `Global` if the package name is not given explicitly as an argument to `BuildCode`. See also Section 7.3.1 on page 112.

```
sumint[10000]
```

The result is:

```
50005000
```

Give the command to look at the generated **Fortran90** source file:

```
!!Global.f90
```

The generated source code:

```
function sumint(n) result(mc_O1)
  use MathCodePrecision
  use MathCodeSheep
  implicit none
  integer(mc_int), intent(in) :: n
  integer(mc_int) mc_O1
  integer(mc_int) i
  integer(mc_int) res

  res = 0
  i = 1
  do while (i <= n)
    res = res+i
    i = i+1
  end do
  mc_O1 = res
end function sumint
```

Uninstall the external code and clean up the directory:

```
UnInstallCode[];

CleanMathCodeFiles[];
Remove["Global`"];
```

1.3 Using the *MathCode* System

The *MathCode* application can easily be made available by executing the following command in *Mathematica*:

```
Needs["MathCode`"]
```

Figure 1.1: Generating **Fortran90** code with *MathCode*, for a package called `foo`.

To generate code for short examples it is convenient to write the functions directly in the "Global`" context as we did with the short example function `sumint` above, which implies that the resulting name for the generated package will be "Global". However, from now on the package name "`foo`" is assumed.

If you are compiling your own package, e.g. called `foo`, using *MathCode*, you also need to mention `MathCodeContexts` within the path of the package as below:

```
BeginPackage["foo`", {MathCodeContexts}]
```

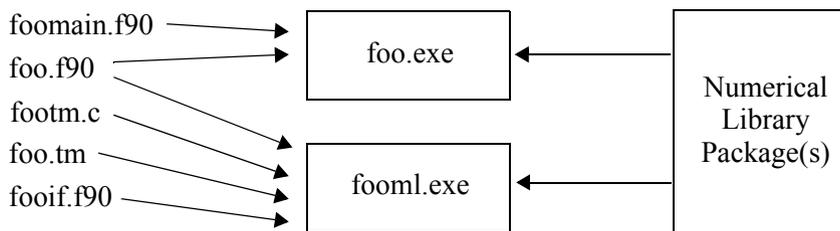


Figure 1.2: Building two executables from package `foo`, possibly including numerical libraries.

1.3.1 Code Generating Phase

The *MathCode* code generator translates a *Mathematica* package, here called `foo`, to a corresponding **Fortran90** source file, here called `foo.f90`. Additional files which are automatically produced are: the *MathCode* header file `foo.mh`, the MathLink related files `footm.c`, `foo.tm`, and `fooif.f90`. These files enable transparent calling of the **Fortran90** versions of functions in `foo` from *Mathematica*, and `foomain.f90` which con-

tains the `program` part needed when building a stand-alone executable for `foo` (Figure 1.3)

1.3.2 Building Phase

The generated file `foo.f90` created from the package `foo` together with additional files are compiled and linked into an executable: either `foo.exe` or `fooml.exe`. Numerical libraries may be included in the linking process by specifying inclusion of external libraries (Figure 1.2).

1.3.3 Executing Phase

The produced executable `foo.exe`¹ can be used for stand-alone execution, whereas `fooml.exe` is used when transparent calling from *Mathematica* via *MathLink* of the compiled **Fortran90** functions in `fooml.exe` is desired.

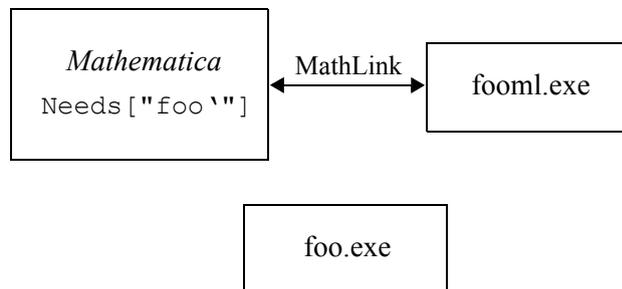


Figure 1.3: Executing compiled code. The executable `foo.exe` is used for stand-alone execution, whereas functions in `fooml.exe` are called interactively from *Mathematica* via *MathLink*.

1.4 *MathCode* Type System

The *MathCode* type system allows the user to associate static type information with *Mathematica* variables and functions. This information is needed in order to generate efficient code in strongly typed languages such as **Fortran90**. Future versions of *MathCode* may support inference of some type information, but the current version requires specification of types for all variables and functions to be translated to **Fortran90**.

1. The `.exe` extension is also used under Unix systems such as Solaris, Linux, etc.

1.4.1 Dual Type System

Standard *Mathematica* is dynamically typed; thus types may change during execution. For example a variable `x` may first be a symbol, next change into an expression and finally change into a real floating-point number during evaluation. In order to constrain dynamically changing types at run-time, *Mathematica* provides pattern-matching constructs. For example: to only allow certain dynamic types of arguments when a function `foo` is called:

```
foo[x_Real, y_Integer] := ...
```

The function `foo` above can only be called with the first argument being a floating-point value and the second an integer value. It cannot be called, for example, for variables which are still symbols, in which case the full expression is returned in unevaluated form.

On the other hand, in a static type system, one would like to express that a variable always has the static type `Real` even though it can be represented by a symbol, expression, or floating-point value. This is especially relevant for compiling to statically typed languages and for static type checking. Another need for static types is for user-defined types; for example a variable could have a static type `Voltage` even though it has a real value and would have matched the head `Real` in *Mathematica*.

Thus, to handle both needs we must a dual type system where we can express both dynamic and static types. We describe below how to declare static types as an extension of the existing dynamic type system in *Mathematica*.

1.4.2 Basic Types

The following basic types are supported by the current version of *MathCode*:

```
Integer, Real,
```

The `Real` type corresponds to IEEE double precision floating point types in generated code. Support for the following additional basic types is not yet implemented (except for a rudimentary support for `String` and `Boolean`, as specified in Appendix A):

```
Complex, Boolean, String
```

1.4.3 Declarations

The types of global variables can be declared as follows:

```
Declare[
  Real      r1,
  Integer   i2 = 3,
```

```
Integer i3
]
```

For convenience and compatibility in notation with most programming languages, one or more space characters are used to separate the type prefix¹ from the variable name.

Several `Declare[]` declarations may appear within the same *Mathematica* package and can be evaluated interactively. Local variables are declared in a similar fashion, but within the standard curly braces `{}` in a `Module[]`, `Block[]` or `With[]` body of a function definition:

```
... := Module[
{
Integer n,
Real {y,z,w},
Real w2,
Integer i = 1,
Integer j= 0
},
y = x+i+j;
y
]
```

Declared variables can be initialized by some initialization expression, just as in standard *Mathematica*. Initialization expressions for local variables are evaluated when the corresponding function is called, whereas initialization and allocation of global variables is performed when the `Declare[]` statement is evaluated, or optionally at a later point in time by a special initialization function.

1.4.4 Function Signatures

A *function signature* is the set of properties that uniquely identifies a specific function. Usually the signature is the function name and the number and types of input and output arguments. Function signatures of statically typed *Mathematica* functions are integrated into the function definitions, or can be provided in a separate `Declare` statement. The integration of function signatures into function definitions has been made possible by an extension of the standard `:=` and `->` operators. This does not change the behavior or performance of the *Mathematica* functions, when executed interpretively within *Mathematica*, and is thus completely backwards compatible. The syntax has the following structure:

1. Attaching the type in front of the variable is represented as a kind of prefix operator in the *Mathematica FullForm* internal representation.

```
func[type1 x1, ..., typen xn]-> ftype := ...
```

Both static types and “dynamic types” can be specified, as in:

```
func[statictype x1_dynamictype1,...] -> ftype := ...
```

The *static type* is only needed for code generation and does not influence the interpreted function definition within *Mathematica*, whereas the *dynamic type* is the traditional *Mathematica* pattern construct. For example, the function `vfunc` below will only match `Real` number arguments during execution in *Mathematica*:

```
vfunc[Voltage x1_Real, ...] -> Voltage := ...
```

Multiple function results are allowed and specified as such:

```
func[...] -> {ftype1, ..., ftypen} := ...
```

An example with one function result:

```
mytan[Real x_] -> Real := Sin[x]/Cos[x];
```

An example with two results:

```
sinandcos[Real x_] -> {Real, Real} := {Sin[x], Cos[x]};
```

When adding static type information to existing untyped *Mathematica* code, it may be more convenient to use the `Declare` method, as below, where the type information is provided separately:

```
Declare[mytan[Real x_] -> Real];
```

```
mytan[x_] := Sin[x]/Cos[x];
```

Apart from the function signatures, the types for the local variables are also needed in order to have full type information for a function. The keyword `Declare[]` can be used to specify both function signatures and types for local variables. The example below with a `Declare` statement combined with a function declaration, e.g.:

```
Declare[myfunc[Integer x_, Real y_] -> Real, {Real, Integer}]
```

```
myfunc[x_, y_] := Module[{myreal, myint}, ...
```

gives the same result as:

```
myfunc[Integer x_, Real y_]->Real := Module[{
  Real    myreal,
  Integer myint
}, ...
```

1.4.5 Arrays and Lists

A key data structure in *Mathematica* is the list structure. Nested list structures are commonly used to represent matrices and other arrays. For example, a nested list `{{2.1, 3.1}, {2.2, 3.2}}` is a two by two array of real numbers. The type of such (nested) list structures can be specified by array type declarations, as long as they have a matrix-like shape and are *homogenous*, i.e. all elements have the same type.

It is interesting to note that *Mathematica* internally implements lists as arrays. This has the advantage of providing constant time indexing operations.

Basic Array Static Type Definition

Array types are represented by a type name parameterized by one or more *dimension size specifiers*:

```
type[size1, ..., sizen]
```

Global array variables can be declared as below:

```
Declare[
  type[size1, ..., sizen] arr
]
```

Examples

A type for a three dimensional array of real numbers:

```
Real[3, 6, 4]
```

Such an array could be declared as follows:

```
Declare[ Real[3, 6, 4] arr]
```

The sizes of array dimensions can be specified by values of integer variables, e.g. *n* and *m* below:

```
Integer[n, m]
```

Unspecified Dimension Sizes

Typically, the sizes of arrays passed as function parameters or returned from a function are not known until the function is executed. Such unspecified array-dimension sizes are indicated by the underscore (`_`) unnamed dimension placeholder or (`ident_`) named dimension placeholder. The actual values of dimension sizes may, however, be accessed later at runtime. This new use of underscore is only valid within array type specifiers, as shown below:

```
type[_,_]
```

Named Dimension Placeholders

Named dimension placeholders like `n_` make it possible to express that the sizes of several dimensions are equal, as with square matrices. Such dimension placeholder names are local to the function where the type is used.

```
type[n_,n_]
```

This will give rise to a local variable `n`, which is initialized to the size of the array dimension as defined by the first occurrence of `n`. This variable can, for example, be used to declare local arrays of the same size.

Array Sizes in Function Signatures

Named dimension placeholders make it possible to express array-dimension size constraints in function signatures. For example, the following function signature is used for a matrix multiplication function, which multiplies two matrix parameters `amat` and `bmat`.

```
MatrixMult[Real[n_,k_] amat_, Real[k_,m_] bmat_] -> Real[n,m] :=  
...
```

This means that the dimension size parameters `n`, `k`, `m` are set to the dimension sizes of the input array arguments, and can be used in the function body or to specify output matrix type. No actual check is performed to verify that the second dimension of `amat` is equal to the first dimension of `bmat`.

Dimension Sizes of Array Parameters

Finding the dimension sizes at run time, e.g. for a function array parameter `mat`, can be done simply by placing named dimension size placeholders in the input array type specifying those sizes. The placeholder variables can later be used for declaring the local array `local-mat`:

```
func[Real[n_,m_] mat_]->Real := Module[{
  Real[n,m] localmat
},
  ...
]
```

The sizes given for the output type are currently for documentation purposes only; no actual checking is performed.

Initialization of Arrays in Declarations

Matrices can be initialized by a constant matrix, or elementwise by a scalar. Elementwise initialization of a matrix by a scalar constant (general expressions currently not allowed) can be done, for example, as below for locally or globally declared variables:

```
Real[2,3] mat = 5.0
```

which gives `mat` the following contents:

```
{ {5., 5., 5.},
  {5., 5., 5.} }
```

Initialization by a constant matrix can be done as follows:

```
Real[3,3] mat2 = { {1., 2., 3.},
                  {2., 3., 4.},
                  {3., 4., 5.} }
```

1.5 Compilation to Fortran90 code

MathCode provides facilities to compile statically typed *Mathematica* functions and variables to **Fortran90** code. Functions always reside in some package (or to be more precise, always in some context). If no package has been specified by the user, the default package `Global` is usually used. The compiler is invoked by calling `CompilePackage`. There are essentially two ways to compile functions:

- Straight compilation of the code as it is
- Compilation combined with symbolic evaluation

The second way is used primarily to handle symbolic operations, e.g. symbolic integration, simplification, substitution etc. which may be present in the function body to be compiled.

The default method of compiling typed functions is by *straight compilation*. Compilation with symbolic evaluation is used for functions mentioned in the list of names

to the optional parameter `EvaluateFunctions`, and should only be used for functions which contain symbolic operations, or when symbolic evaluation leads to increased performance.

1.5.1 Calling the Code Generator

CompilePackage

The code generation is started by the command `CompilePackage`, e.g.:

```
CompilePackage["foo"]
```

or

```
CompilePackage["foo`"]
```

which collects the variables and functions defined in the package context `foo``, i.e. corresponding to the symbols returned by:

```
Names["foo`*"]
```

All *MathCode* functions that take a package name as argument, can be called with or without the backtick, as in the example above. By default, *MathCode* compiles all typed functions and typed global variables within the package. Typed functions and global variables are those to which *MathCode* type information has been added, either together with their declaration or in a separate `Declare` statement.

SetCompilationOptions

Additional information needed to guide the compilation process can be specified using optional parameters to `CompilePackage`, or by inserting calls to `SetCompilationOptions` within the package to be compiled.

Below we briefly examine the different items to be compiled and some of the available options.

Compiling Different Items

Variable Declarations

All typed global variables declared in *Mathematica* to be compiled (e.g. within the package `foo`) are translated to declarations in **Fortran90**. Declarations and possible initialization code are put into the file `foo.f90`.

Functions

The default is to translate typed *Mathematica* functions into **Fortran90** without any symbolic evaluation. This produces target code similar to the original *Mathematica* code, i.e. loops in *Mathematica* become loops in **Fortran90**, if-statements are still if-statements, etc.

Functions With Symbolic Operations

Functions which contain symbolic operations cannot be directly translated to **Fortran90**. Fortunately, in many cases symbolic operations can be eliminated by symbolic expansion. In this way, symbolic operations such as symbolic integration, derivation, series expansion etc. can be performed by *Mathematica* before the final code generation stage. The resulting expression, which is assumed to contain only non-symbolic operations, is then passed to the code generator which performs common subexpression elimination to speed up and reduce the code size before finally translating to **Fortran90** code. For this to work reliably, the body of the “symbolic function” should not contain side effects such as assignments to global variables or input/output. Neither should it contain loop constructs such as `While`, `For` etc.

For example, the function below contains a symbolic series expansion and a symbolic substitution:

```
SymbSeriesSin[Real y_]->Real := Series[Sin[x],{x,0,10}] /. x->y;
```

Therefore, the function should be symbolically evaluated before final code generation, and it should be specified as a function for symbolic evaluation using the option `EvaluateFunctions`:

```
SetCompilationOptions[EvaluateFunctions->{"SymbSeriesSin"}]
```

Main Program Function

In case a stand-alone executable should be created, the option `MainFileAndFunction` can be used to specify the `program` part needed in such an executable. The argument string specifies the text from which the file `foomain.f90` is created (assuming the package name is `foo`). In the example below the function `f` is called and the result is printed by the program.

```
SetCompilationOptions[MainFileAndFunction->
  "PRINT *, f(5)"]
```

1.5.2 Building

The building process compiles all produced **Fortran90** files and links them into an execut-

able.

MakeBinary

```
MakeBinary["foo"]
```

The call `MakeBinary["foo"]` builds all the files for either the stand-alone version of the application (e.g. `foo.exe`), or for the interactively callable `MathLink` version (e.g. `fooml.exe`).

BuildCode

```
BuildCode["foo"]
```

The call `BuildCode["foo"]` calls `CompilePackage["foo"]` and then `MakeBinary["foo"]`. For example, a call to `BuildCode["foo"]` will make a complete code generation, compilation and linking of the *Mathematica* package “foo”. As mentioned earlier, the backtick is allowed as used in package context specifications in *Mathematica*:

```
BuildCode["foo`"]
```

1.5.3 Installing

For compiled functions to be directly callable from within *Mathematica*, the code must be installed.

InstallCode

The call:

```
InstallCode["foo"]
```

or, equivalently,

```
InstallCode["foo`"]
```

installs the binary `fooml.exe` into *Mathematica*. It first saves (in the *Mathematica* workspace, to be restored if uninstalled) the original interpreted functions and then creates function definition stubs out of the compiled package in *Mathematica*. This enables the calling of compiled functions from within *Mathematica* via `MathLink`.

1.5.4 Executing

Functions in the compiled and installed package can be executed by standard function calls just like functions in any standard *Mathematica* package. If stand-alone execution is desired, simply run the created stand-alone executable (which does not have an `m1` suffix in its name).

1.5.5 Uninstalling

When the compiled code is no longer to be accessible and the MathLink connection is to be closed down, `UninstallCode` should be called:

```
UninstallCode["foo"]
```

This will restore the original interpreted version of the package, (called `foo` in the example).

1.6 Matrix Operations

In many engineering applications, matrices and matrix manipulation are very common. The availability of an easy-to-use and short-handed notation for manipulating matrices is important for these application domains. Thus, we have extended the `Part ([[]])` operation in *Mathematica* to fulfill this objective.

The current basic set of matrix operations consists of operations on array sections. The syntax is inspired by the syntax used by Matlab and Fortran 90, and is supported by the *MathCode* code generator for up to 4-dimensional arrays and within *Mathematica* for an arbitrary number of dimensions.

As an example, create a small matrix `A` containing indexed symbols of the form `a[i,j]`:

```
A=Table[a[i,j],{i,4},{j,5}]; A//MatrixForm

{ {a[1,1], a[1,2], a[1,3], a[1,4], a[1,5]},
  {a[2,1], a[2,2], a[2,3], a[2,4], a[2,5]},
  {a[3,1], a[3,2], a[3,3], a[3,4], a[3,5]},
  {a[4,1], a[4,2], a[4,3], a[4,4], a[4,5]} }
```

Below we extract row 2 and 3, using the Matlab-style notation `A[[2|3, _]]`.

Compared to the standard Matlab syntax `A(2:3, :)` we have made a *Mathematica* compatible version by replacing colon as a binary range operator with vertical bar (`|`), and replacing colon as a placeholder for the whole range of a dimension with underscore (`_`).

```
A[[2|3, _]] // MatrixForm
      { {a[2,1], a[2,2], a[2,3], a[2,4], a[2,5]},
        {a[3,1], a[3,2], a[3,3], a[3,4], a[3,5]} }
```

Extract all but the first two columns, using `A[[_ , 3|_]]` which corresponds to standard Matlab syntax `A(:, 3:)`. The notation `3|_` here means the range from the 3rd to the last column.

```
A[[_ , 3|_]] // MatrixForm
      { {a[1,3], a[1,4], a[1,5]},
        {a[2,3], a[2,4], a[2,5]},
        {a[3,3], a[3,4], a[3,5]},
        {a[4,3], a[4,4], a[4,5]} }
```

Assign values to a submatrix of A:

```
A[[2|3, 2|3]] = {{1, 2},
                 {3, 4}};
```

```
A // MatrixForm
      { {a[1,1], a[1,2], a[1,3], a[1,4], a[1,5]},
        {a[2,1], 1,      2,      a[2,4], a[2,5]},
        {a[3,1], 3,      4,      a[3,4], a[3,5]},
        {a[4,1], a[4,2], a[4,3], a[4,4], a[4,5]} }
```

1.7 Implementing Missing *Mathematica* Functions

The *MathCode* system directly supports translation of a set of basic *Mathematica* functions and operations, as defined in Appendix A. There are still quite a number of standard *Mathematica* functions not yet included in this set.

-

Standard functions can be re-implemented by hand.

1.7.1 An Example *systemF90.nb* Notebook

This particular notebook `system.nb` contains an example `system` package (note lower-case!) with an alternative implementation of the standard function `RotateLeft`, which earlier was not in the standard subset supported by the *MathCode* translator.

Initialization Needed to use *MathCode*

```
Needs["MathCode`"]
```

Package Header

```
BeginPackage["system`", {MathCodeContexts}]
```

Public Exported Global Symbols

```
Begin["system`"];
Off[General::shdw]
```

Introduce symbols that should be exported outside the package (there exist some other symbols in this package as well).

```
system`RotateRight;
```

End Public Section

```
On[General::shdw] (* avoid shadowing messages from Mathematica *)
End[];
```

Private Implementation Section

```
Begin["`Private`"];
```

Define implementations of the functions and variables.

RotateRight

Definition of RotateRight for integer vectors:

```
RotateRight[ Integer[_] a_]->Integer[_] :=
Module[{
  Integer m=Dimensions[a][[1]]
},
Module[{
  Integer[m] res
},
res[[2|m]]=a[[1|m-1]];
res[[1]]=a[[m]];
res
```

```
]];
```

End of Private Section

```
End[];
```

End of Package

```
EndPackage[];
```

Compiling

Compile the `system` package into **Fortran90** code:

```
CompilePackage["system"];
```

Building

Compile the **Fortran90** files to binaries and possibly link into an executable:

```
MakeBinary["system"];
```

Install and Test

```
InstallCode["system"];
```

`RotateRight` test example.

```
RotateRight[{1,2,3,4}]=={4, 1, 2, 3}]  
True
```

Note that the *MathCode* compiled version of `system`RotateRight` is executed (via `MathLink`) because it is earlier in the context path than the *Mathematica* built-in function `RotateRight`.

1.8 Interfacing With External Libraries

This option is not implemented in the current version of `MathCode F90`.

1.9 *MathCode* Limitations

The main limitation of *MathCode* is of course that it cannot compile the full *Mathematica* language. The compilable subset is defined in Appendix A. This subset will grow in future releases of *MathCode*, but will never include the full *Mathematica* language since that would entail a complete reimplementaion of most of *Mathematica*.

Chapter 2 Getting Started by Examples

The purpose of this chapter is to walk through some aspects of the *MathCode* system by showing complete application examples in order to help the user become acquainted with some of the type and code generation facilities. Recall that a very simple example of the use of *MathCode* has already been presented in Section 1.2 at the beginning of Chapter 1. The two examples in this chapter are slightly more advanced, showing the use of packages, symbolic expansion and array slices.

The following applications will be presented below:

- *SinSurface*, which computes and plots a *Sin*-like surface function on a 2D grid, using symbolic series expansion to create the symbolic expression which is the body of the surface function.
- *Gauss*, which solves a linear equation system by a textbook Gauss elimination algorithm, programmed using both for-loops and Matlab-like array slice matrix operations.

Additional examples can be found in the `DemosF90` directory of the *MathCode* distribution.

The performance of the generated code is measured for the presented applications. The performance figures shown have been obtained for *Mathematica* 5.0 for Windows. You should re-run these examples to obtain the correct performance figures for your platform; when running *MathCode* compiled applications it is particularly the speedup figures which vary between platforms.

This description is valid for execution under Windows95/98/NT/2000/XP.

Other facilities, such as type declarations and array slice operations, work on all *Mathematica* supported platforms.

In order to run the system, there must be a valid *Mathematica* license on your computer. Also, you must have installed the *MathCode* system. See installation description in Chapter 9.

2.1 Compilation and Code Generation

As briefly mentioned in the introductory overview chapter, there are several options concerning the compilation and code-generation facilities provided by *MathCode* for translation of typed *Mathematica* code:

- *Target code.* Specifies which type of code should be produced. Currently, only C++ or Fortran90 code generation is supported, depending on whether *MathCode* C++ or *MathCode* F90 is installed on your computer.
- *Execution integration.* The compiled code can either be directly callable from within *Mathematica*, or simply be placed in an external file.
- *Symbolic expansion.* The *Mathematica* code may contain symbolic operations which should be evaluated and expanded in conjunction with code generation.

These options are explained in more detail in Chapter 7 which covers code generation. In this chapter we present a few small application examples which illustrate some of these aspects.

To use typed declarations and code-generation facilities for functions and data structures in your own package, you always need to refer to the *MathCode* application by evaluating a `Needs` statement:

```
Needs["MathCode`"]
```

In order to invoke code-generation functions from within your package, you also need to include the *MathCode* contexts in the search path of your package, as below:

```
BeginPackage["myPackage`", {MathCodeContexts, ...}]
```

2.2 Two Modes of Code Generation

The first example application is a rather contrived small *Mathematica* program called *Sin-Surface*, which is designed to illustrate the two basic modes of the code generator: compilation *without* symbolic evaluation, which is default, and compilation preceded by symbolic expansion, which is indicated by setting the option `EvaluateFunctions` (see Section 2.3.5).

- *Standard code generation.* This is the default for generating procedural code from a typed *Mathematica* function. The function body is translated, e.g. to **Fortran90**, as it is, without applying any symbolic transformations. Such a function may only contain non-symbolic operations, typically numeric computations over arrays and scalars. When translating to external code, e.g. in **Fortran90**, emitted code will be rather close to the

original *Mathematica* code in structure.

- *Code generation preceded by symbolic evaluation.* This is used to generate code from a function that may contain symbolic operations, e.g. series expansion, symbolic integration, symbolic derivation, etc. It is not useful to perform such symbolic operations in languages like C++ or Fortran90, so they are therefore performed in *Mathematica* before the final translation.

The symbolic operations result in expressions that should contain only non-symbolic, typically numeric operations. This is typically the case since *Mathematica* always evaluates as far as possible. Thus, the function body is expanded (and simplified) into a usually huge symbolic expression before being transformed into **Fortran90** code, for example. The result is rather unrecognizable compared to the original *Mathematica* function since both symbolic expansion and optimizations such as common subexpression elimination have been performed.

The following two sections present the actual application examples.

2.3 The SinSurface Application Example

Below we describe the *SinSurface* program example. It is structured as a standard *Mathematica* package within a notebook file `SinSurface.nb`. The actual computation is performed by the functions `calcPlot`, `sinFun2` and their help functions.

The two functions `calcPlot` and `sinFun2` in the *SinSurface* package will be translated to **Fortran90** together with the declaration of the global array `xyMatrix`.

- The array `xyMatrix` represents a 21x21 grid on which the numeric function `sinFun2` will be computed.
- The function `calcPlot` accepts four arguments which are coordinates that describe a square in the x-y plane, and one counter (`iter`) to make the function repeat the computation as many times as necessary for measuring execution time. For each point on a 21x21 grid in that square, the numeric function `sinFun2` is called to compute a value that is stored as a matrix element in the matrix representing the grid.
- The function `sinFun2` computes essentially the same values as $\text{Sin}[x+y]$, but in a more complicated manner. This function uses a rather large expression obtained through conversion of the arguments into polar coordinates (through `arcTan`) and then uses series expansion of both `Sin` and `Cos` in 10 terms. The resulting large symbolic expression (more than a page) becomes the body of `sinFun2`, and is then used as input to `CompilePackage[]` with the `EvaluateFunction` option (see Section 7.5) to generate efficient **Fortran90** code.

2.3.1 Introduction

The *SinSurface* example application computes a function (here `sinFun2`) over a 2-D grid. The function values are first stored in the matrix `xyMatrix` before being plotted. The execution of compiled **Fortran90** code for the function `sinFun2` is approximately 1000 times faster than evaluating the same function interpretively within *Mathematica*.

To run this example, start *Mathematica*, open the notebook file “`SinSurface.nb`”, and either evaluate it cell by cell or all at once.

2.3.2 Initialization

Check Current Directory

Check the current directory, since a number of files will be placed there during the code-generation process. This particular example shows directories from a computer with the Windows platform.

```
Directory[]  
"C:\MathCode\DemosF90\SinSurface\"
```

You might want to place the directory somewhere where all generated files are put, e.g. the directory below, or another location.

```
SetDirectory["C:\MathCode\DemosF90\SinSurface\  
"C:\MathCode\DemosF90\SinSurface\"
```

2.3.3 Start of the SinSurface Package

First give a Needs statement, to make sure that the *MathCode* application is loaded:

```
Needs["MathCode`"]
```

The *SinSurface* package starts in the usual way by a `BeginPackage` declaration which references other packages. The `MathCodeContexts` variable is needed in order to call the code-generation related functions.

```
BeginPackage["SinSurface`", {MathCodeContexts}];  
Clear["SinSurface`*"];
```

Exported Symbols

Define possibly exported symbols. Even though it is not necessary here, we enclose these names within a `Begin["SinSurface`"] ... End[]` type of “context bracket”, since this can be put into a cell in the notebook and conveniently re-evaluated (only this cell!) if new names are added to the list below.

```
Begin["SinSurface`"]  
  xyMatrix;  
  calcPlot;  
  sinFun1;  
  sinFun2;  
  arcTan;  
  sin;  
  cos;  
  plot;  
  cplus;  
  plotfile;  
End[]
```

Setting Compilation Options

This defines how the functions and variables in the *SinSurface* package should be compiled to **Fortran90**. By default, all typed variables and functions are compiled. However, the compilation process can be controlled in a more detailed manner by giving compilation options to `CompilePackage` or via `SetCompilationOptions`. For example, in this package the function `sinFun2` should be symbolically evaluated before being translated to code since it contains symbolic operations; the functions `sin`, `cos`, and `arcTan` should not be compiled at all since they are expanded within the body of `sinFun2`. The remaining typed function, `calcPlot`, will be compiled in the normal way.

```
SetCompilationOptions[
  EvaluateFunctions->{sinFun2},
  UnCompiledFunctions->{sin, cos, arcTan},
  MainFileAndFunction->""
]
```

2.3.4 The Body of the SinSurface Package

Begin with the implementation section of the *SinSurface* package, where functions are defined. This is usually private to avoid accidental name shadowing due to identical local variables in several packages.

```
Begin["SinSurface`Private`"];
```

2.3.5 Functions and Declarations to be Translated to Fortran90

Global Variables

Declare public global variables and private package-global variables:

```
Declare[
  Real[21,21] xyMatrix
];
```

sin, cos

Taylor-expanded `sin` and `cos` functions called by `sinFun2`. In the normal order of evaluation of function `Sin[]` the actual parameter is replaced, `Sin[]` is evaluated and series expansion is performed. To reorder this sequence of operations, `z` must be substituted with `x` after the series expansion.

```

sin[Real x_] -> Real := Normal[Series[Sin[z], {z, 0, 10}]]
/. z -> x ;
cos[Real x_] -> Real := Normal[Series[Cos[z], {z, 0, 10}]]
/. z -> x ;

```

arcTan

Conversion of grid point to an angle, called by `sinFun2`.

```

arcTan[Real x_, Real y_] -> Real := (
  If[x < 0, Pi, 0] + If[x == 0, Sign[y]*Pi/2, ArcTan[y/x] ]
);

```

sinFun2

The function `sinFun2` is the function to be computed and plotted, called by `calcPlot`. It provides a more complicated and computationally heavier way (series expansion) to calculate approximately the same result as `Sin[x+y]`. This gives an example of a combination of symbolic and numeric operations as well as a rather standard mix of arithmetic operations. The expanded symbolic expression which comprises the body of `SinFun2` is between 1 and 2 pages long when printed.

Note that the types of local variables to `sinFun2` need not be declared since setting the `EvaluateFunctions` option will make the whole function body symbolically expanded before translation to **Fortran90** code.

Note also that in order for a function to be symbolically expanded before final code generation it should be without side effects, e.g. no assignment to global variables or input/output. This is because the relative order between these actions when executing the code often changes when the symbolic expression is created and later rearranged and optimized by the code generator.

```

sinFun2[Real x_, Real y_] -> Real := Block[
  {
    Real {r, xx, yy}
  },
  r = Sqrt[x^2+y^2];
  xx = r*cos[arcTan[x, y]];
  yy = r*sin[arcTan[x, y]];
  sin[xx+yy]
];

```

calcPlot

The function `calcPlot` calculates data for a plot of `sinFun2` over a 21x21 grid, which is returned as a 21x21 array.

```
calcPlot[Real xmin_, Real xmax_, Real ymin_,
         Real ymax_, Integer iter_] -> Real[21,21] :=
Module[{
  Integer n = 20,
  Real {x,y},
  Integer {i,j,count}
},
For[count=1, count<=iter, count=count+1,
  For[i=1, i<=(n+1), i=i+1,
    For[j=1, j<=(n+1), j=j+1,
      x = xmin+(xmax-xmin)*(i-1)/n;
      y = ymin+(ymax-ymin)*(j-1)/n;
      xyMatrix[[i,j]] = sinFun2[x,y]
    ]
  ]
];
xyMatrix
];
```

End of SinSurface Package

```
End[];
EndPackage[];
```

2.3.6 Execution

We first execute the application interpretively within *Mathematica*, and then compile the key function and execute the application again. Next we compile the application to **Fortran90**, build an executable, and call the same functions from *Mathematica* via Math-Link.

Mathematica Evaluation

Let *Mathematica* calculate a plot.

```
meval = Timing[plot = calcPlot[-2., 2., -2., 2., 1] ][[1]]
0.672 Second
```

Perform the plot:

```
ListPlot3D[plot];
```

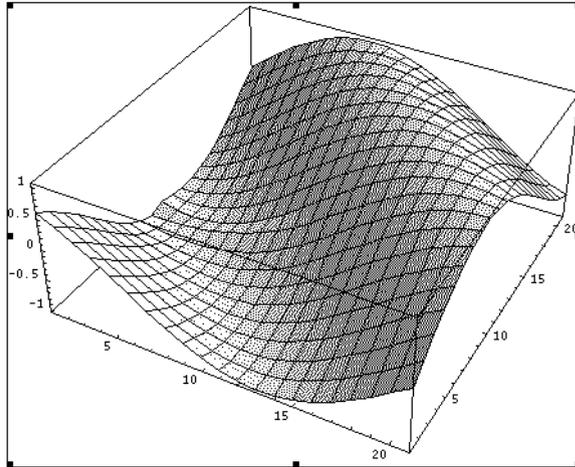


Figure 2.1: Plot of the 21×21 grid in the SinSurface example.

Using *Mathematica* Standard Compile[]

We redefine `sinFun2` to become a compiled version, using *Mathematica* standard `Compile[]`:

```
sinFun2 = Compile[{x, y}, Evaluate[sinFun2[x, y]]];

compeval = Timing[plot = calcPlot[-2., 2., -2., 2., 1]; ]
{0.078 Second, Null}

compeval = compeval[[1]];
sinFun2 =.
```

2.3.7 Using the *MathCode* Code Generator

Compile the SinSurface package:

```
CompilePackage["SinSurface"]
```

Successful compilation to Fortran90: 2 function(s)

The Generated Fortran90 Code

The generated **Fortran90** code from the `SinSurface` program follows below. Notice that the package name is used to create a Fortran90 module. Thus the *Mathematica* package `SinSurface` becomes `mc_SinSurface` in Fortran90.

The generated code from `SinSurface`sinFun2` is produced from a large expression by the `EvaluateFunctions` option. Therefore, common subexpression elimination is performed by the code generator, producing many temporary variables and subexpressions which can be seen in the body of the **Fortran90** function `sinFun2`.

By contrast, the **Fortran90** code in the body of function `calcPlot` produced from the *Mathematica* function `SinSurface`calcPlot`, without being specified by the `EvaluateFunctions` option, follows the structure of the original code quite closely.

We give a command to type out the text of the generated **Fortran90** file:

```
!!SinSurface.f90
```

The generated `SinSurface.f90` file is included below. Note that the exact appearance of this file is very dependent on the exact *MathCode* version and may differ slightly on your system.

```
module mc_SinSurface

  use MathCodePrecision
  use MathCodeSheep
  implicit none

  real(mc_real) xyMatrix(21,21)

contains

  function calcPlot(xmin, xmax, ymin, ymax, iter) result(mc_O1)

    use MathCodePrecision
    use MathCodeSheep
    implicit none
    real(mc_real), intent(in) :: xmin
    real(mc_real), intent(in) :: xmax
    real(mc_real), intent(in) :: ymin
    real(mc_real), intent(in) :: ymax
    integer(mc_int), intent(in) :: iter
    real(mc_real), pointer :: mc_O1(:, :)
    integer(mc_int) count
    integer(mc_int) j
```

```
integer(mc_int) i
real(mc_real) y
real(mc_real) x
integer(mc_int) n

n = 20

count = 1
do while (count <= iter)

  i = 1
  do while (i <= n+1)

    j = 1
    do while (j <= n+1)
      x = xmin+(((xmax+(-xmin))* (i+(-1))))/n
      y = ymin+(((ymax+(-ymin))* (j+(-1))))/n
      xyMatrix(j, i) = sinFun2 (x, y)

      j = j+1
    end do

    i = i+1
  end do

  count = count+1

end do

if (associated(mc_O1)) nullify(mc_O1)
allocate(mc_O1(21, 21))
mc_O1 = xyMatrix
end function calcPlot

subroutine SinSurfaceInit()

  use MathCodePrecision
  use MathCodeSheep
  implicit none
end subroutine SinSurfaceInit

function sinFun2(x, y) result(mc_O1)
```

```
use MathCodePrecision
use MathCodeSheep
implicit none
real(mc_real), intent(in) :: x
real(mc_real), intent(in) :: y
real(mc_real) mc_O1
real(mc_real) mc_T1
real(mc_real) mc_T2
real(mc_real) mc_T3
real(mc_real) mc_T4
real(mc_real) mc_T5
logical mc_T6
integer(mc_int) mc_T7
real(mc_real) mc_T8
real(mc_real) mc_T9
real(mc_real) mc_T10
real(mc_real) mc_T11
real(mc_real) mc_T12
logical mc_T13
real(mc_real) mc_T14
real(mc_real) mc_T15
real(mc_real) mc_T16
real(mc_real) mc_T17
real(mc_real) mc_T18
real(mc_real) mc_T19
real(mc_real) mc_T20
real(mc_real) mc_T21
real(mc_real) mc_T22
real(mc_real) mc_T23
real(mc_real) mc_T24
real(mc_real) mc_T25
real(mc_real) mc_T26
real(mc_real) mc_T27
real(mc_real) mc_T28
real(mc_real) mc_T29
real(mc_real) mc_T30
real(mc_real) mc_T31
real(mc_real) mc_T32
real(mc_real) mc_T33
real(mc_real) mc_T34
real(mc_real) mc_T35
real(mc_real) mc_T36
real(mc_real) mc_T37
real(mc_real) mc_T38
```

```
real(mc_real) mc_T39
real(mc_real) mc_T40
real(mc_real) mc_T41
real(mc_real) mc_T42
real(mc_real) mc_T43
real(mc_real) mc_T44
real(mc_real) mc_T45
real(mc_real) mc_T46
real(mc_real) mc_T47
real(mc_real) mc_T48
real(mc_real) mc_T49
real(mc_real) mc_T50
real(mc_real) mc_T51
real(mc_real) mc_T52

mc_T1 = x**2
mc_T2 = y**2
mc_T3 = mc_T1+mc_T2
mc_T4 = real(1)/2
mc_T5 = mc_T3*mc_T4
mc_T6 = x == 0
mc_T7 = sign(1.0D0, y)
mc_T8 = 3.1415926535897932_mc_real*mc_T7
mc_T9 = mc_T8/2
mc_T10 = y/x
mc_T11 = atan(mc_T10)
if (mc_T6) then
    mc_T12 = mc_T9
else
    mc_T12 = mc_T11
end if
mc_T13 = x < 0
if (mc_T13) then
    mc_T14 = 3.1415926535897932_mc_real
else
    mc_T14 = 0
end if
mc_T15 = real((-1))/6
mc_T16 = mc_T12+mc_T14
mc_T17 = mc_T16**3
mc_T18 = mc_T15*mc_T17
mc_T19 = mc_T16**5
mc_T20 = mc_T19/120
mc_T21 = real((-1))/5040
```

```

mc_T22 = mc_T16**7
mc_T23 = mc_T21*mc_T22
mc_T24 = mc_T16**9
mc_T25 = mc_T24/362880
mc_T26 = mc_T12+mc_T14+mc_T18+mc_T20+mc_T23+mc_T25
mc_T27 = mc_T5*mc_T26
mc_T28 = real((-1))/2
mc_T29 = mc_T16**2
mc_T30 = mc_T28*mc_T29
mc_T31 = mc_T16**4
mc_T32 = mc_T31/24
mc_T33 = real((-1))/720
mc_T34 = mc_T16**6
mc_T35 = mc_T33*mc_T34
mc_T36 = mc_T16**8
mc_T37 = mc_T36/40320
mc_T38 = real((-1))/3628800
mc_T39 = mc_T16**10
mc_T40 = mc_T38*mc_T39
mc_T41 = 1+mc_T30+mc_T32+mc_T35+mc_T37+mc_T40
mc_T42 = mc_T5*mc_T41
mc_T43 = mc_T27+mc_T42
mc_T44 = mc_T43**3
mc_T45 = mc_T15*mc_T44
mc_T46 = mc_T43**5
mc_T47 = mc_T46/120
mc_T48 = mc_T43**7
mc_T49 = mc_T21*mc_T48
mc_T50 = mc_T43**9
mc_T51 = mc_T50/362880
mc_T52 = mc_T27+mc_T42+mc_T45+mc_T47+mc_T49+mc_T51
mc_O1 = mc_T52
end function sinFun2

end module mc_SinSurface

```

Compiling and Linking the Fortran90 Code

The command `MakeBinary` compiles the generated **Fortran90** code using a **Fortran90** compiler (e.g. Digital Visual Fortran). The object code is by default linked into the executable: `SinSurface.m1.exe` for calling the compiled code via *MathLink*.

```
MakeBinary[];
```

If any problems are encountered during code compilation, the warning and error messages are shown in the notebook. Otherwise no messages are shown. When `MakeBinary` is called without arguments, the call applies to the current package.

Installing and Connecting to *Mathematica*

The command `InstallCode` installs and connects the external process containing the compiled and linked SinSurface code.

```
InstallCode["SinSurface"]
```

Define an elapsed time-measurement function called `AbsTime` with a resolution of 1 second:

```
SetAttributes[AbsTime, HoldFirst];

AbsTime[x_] := Module[{
  start, res
},
  start = AbsoluteTime[];
  res=x;
  {(AbsoluteTime[]-start) Second, res}
];
```

Execution of generated Fortran90 Code

Perform the computation and the plot:

```
(plot = calcPlot[-2.0, 2.0, -2.0, 2.0, 3000];) // AbsTime
{0.7816 Second, Null}
```

Since the external computation was performed 3000 times, the time needed for one external computation is:

```
externaleval = %[[1]]/3000
0.0002603867 Second
```

Check that the result appears graphically identical:

```
ListPlot3D[plot];
```

Figure 2.2: Plot of the SinSurface function computed by generated **Fortran90** code.

2.3.8 Performance Comparison

The performances between the three forms of execution are compared in the table below. The generated **Fortran90** code for this example is roughly 2580 times faster than standard interpreted *Mathematica* code, and almost 300 times faster than expression code compiled by the internal *Mathematica* `Compile[]` command. This test is performed on a 2.6 Ghz Pentium 4 running Windows XP, *Mathematica* 5.0, Digital Visual Fortran 6.0 .

| Execution form | Time consumed | Relative |
|---|----------------------|-----------------|
| Standard <i>Mathematica</i> | 0.672 | 2580.78. |
| Compile[] | 0.078 | 299.555 |
| External Fortran90 via Math-Link | 0.0002603867 | 1.00 |

2.4 The Gauss Application Example

The Gauss application example uses a textbook Gauss elimination algorithm to solve a linear equation system. Two versions of the Gauss elimination algorithm are presented:

- *GaussSolveArrayslice*. This algorithm is largely coded using the Matlab-like array slice operations.
- *GaussSolveForLoops*. This algorithm is coded using traditional for-loops.

Both versions of the algorithm are compiled to **Fortran90** code. The performance is measured both with and without MathLink overhead.

2.4.1 The Gauss Package

Initialization of the Package

```
Needs["MathCode`"]
```

You might want to check which directory you are in and set where you want to be, since some files are generated during the compilation process. You can use the `$MCRoot` variable that points to the root directory of your *MathCode* installation.

```
SetDirectory[$MCRoot<>"/DemosF90/Gauss"]
```

Start the Package

```
BeginPackage["Gauss`", {MathCodeContexts}];
```

Define Exported Symbols

```
Begin["Gauss`"]
  GaussSolveArrayslice;
  GaussSolveForLoops;
End[]
```

Define the Functions and Variables

Begin the “private” implementation section:

```
Begin["`Private`"];
```

GaussSolveArrayslice

The GaussSolveArrayslice function

```

GaussSolveArrayslice[
  Real[n_,n_] ain_,
  Real[n_,m_] bin_,
  Integer iterations_]-> Real[n,m] :=
Module[{
  Real[n]      dumc,
  Real[n,n]    a,
  Real[n,m]    b,
  Integer[n]   {ipiv, indxr, indxc},
  Integer      {i,k,l,irow,icol},
  Real         {pivinv, amax, tmp},
  Integer      {beficol, afticol, count}
},

For[count=1,count<=iterations,count=count+1,(
  a=ain;
  b=bin;
  For [k=1,k<=n, k=k+1,
    ipiv[[k]]=0
  ];

  For [i=1,i<=n, i=i+1,
    (* Algorithm first finds absolutely largest matrix element *)
    amax=0.0;
    For [k=1,k<=n, k=k+1,
      If [ ipiv[[k]]==0 ,
        For [l=1,l<=n, l=l+1,
          If [ ipiv[[l]]==0 ,
            If [ Abs[a[[k,l]]] > amax,
              amax= Abs[a[[k,l]]];
              irow=k;
              icol=l
            ]]]];
  ]]]];

  ipiv[[icol]]=ipiv[[icol]]+1;
  If[ipiv[[icol]]>1,
    Print["*** Gauss2 input data error ***"];
    Break];
  If[ irow!=icol ,
    For [k=1,k<=n, k=k+1,

```

```

        tmp=a[[irow,k]] ;
        a[[irow,k]]=a[[icol,k]];
        a[[icol,k]]=tmp];
    For [k=1,k<=m, k=k+1,
        tmp=b[[irow,k]] ;
        b[[irow,k]]=b[[icol,k]];
        b[[icol,k]]=tmp]
    ];
    indxr[[i]]=irow;
    indxc[[i]]=icol;
    If [ a[[icol,icol]]==0,
        Print["*** Gauss2 input data error 2 ***"];
        Break];

    pivinv=1.0 / a[[icol,icol]];
    a[[icol,icol]]=1.0;

    a[[icol,_]]=a[[icol,_]]*pivinv;
    b[[icol,_]]=b[[icol,_]]*pivinv;
    dumc=a[[_,icol]];
    For [k=1,k<=n, k=k+1, a[[k,icol]]=0];

    a[[icol,icol]]= pivinv;

    For [k=1,k<=n, k=k+1,
        If[ k != icol,
            a[[k,_]]= a[[k,_]]- dumc[[k]]*a[[icol,_]];
            b[[k,_]]= b[[k,_]]- dumc[[k]]*b[[icol,_]]
        ]
    ]
];

For [l=n,l>=1, l=l-1,
    For [k=1,k<=n, k=k+1,
        tmp= a[[k,indxr[[l]]]];
        a[[k,indxr[[l]]]]=a[[k,indxc[[l]]]];
        a[[k,indxc[[l]]]]=tmp
    ]
];
b
];

```

GaussSolveForLoops

The GaussSolveForLoops function:

```
GaussSolveForLoops[
  Real[n_,n_] ain_,
  Real[n_,m_] bin_,
  Integer iterations_ ]-> Real[n,m] :=
Module [{
  Real[n]      dumc,
  Real[n,n]    a,
  Real[n,m]    b,
  Integer[n]   {ipiv, indxr, indxc},
  Integer      {i, k, l, irow, icol},
  Real         {pivinv, amax, tmp},
  Integer      {beficol, afticol, count}
},
For[count=1, count<=iterations, count=count+1, (
  a=ain;
  b=bin;
  For [k=1, k<=n, k=k+1,
    ipiv[[k]]=0
  ];

  For [i=1, i<=n, i=i+1,
    (* Algorithm first finds absolutely largest matrix element *)
    amax=0.0;
    For [k=1, k<=n, k=k+1,
      If [ ipiv[[k]]==0 ,
        For [l=1, l<=n, l=l+1,
          If [ ipiv[[l]]==0 ,
            If [ Abs[a[[k,l]]] > amax,
              amax= Abs[a[[k,l]]];
              irow=k;
              icol=l
            ]]]];
          ]]]];

    ipiv[[icol]]=ipiv[[icol]]+1;
    If[ipiv[[icol]]>1,
      Print["*** Gauss2 input data error ***"];
      Break];
    If[ irow!=icol ,
      For [k=1, k<=n, k=k+1,
        tmp=a[[irow,k]] ;
```

```

        a[[irow,k]]=a[[icol,k]];
        a[[icol,k]]=tmp];
    For [k=1,k<=m, k=k+1,
        tmp=b[[irow,k]] ;
        b[[irow,k]]=b[[icol,k]];
        b[[icol,k]]=tmp]
    ];
indxr[[i]]=irow;
indxc[[i]]=icol;
If [ a[[icol,icol]]==0,
    Print["*** Gauss2 input data error 2 ***"];
    Break];

pivinv=1.0 / a[[icol,icol]];
a[[icol,icol]]=1.0;

For [k=1,k<=n, k=k+1,
    a[[icol,k]]=a[[icol,k]]*pivinv];
For [k=1,k<=m, k=k+1,
    b[[icol,k]]=b[[icol,k]]*pivinv];
For [k=1,k<=n, k=k+1,
    dumc[[k]]=a[[k,icol]];a[[k,icol]]=0];

a[[icol,icol]]= pivinv;

For [k=1,k<=n, k=k+1,
    If [ k != icol,
        For [l=1,l<=n, l=l+1,
            a[[k,l]]= a[[k,l]]- dumc[[k]]* a[[icol,l]]];
        For [l=1,l<=m, l=l+1,
            b[[k,l]]= b[[k,l]]- dumc[[k]]* b[[icol,l]]]
        ]
    ];

For [l=n,l>=1, l=l-1,
    For [k=1,k<=n, k=k+1,
        tmp= a[[k,indxr[[l]]]];
        a[[k,indxr[[l]]]]=a[[k,indxc[[l]]]];
        a[[k,indxc[[l]]]]=tmp
    ]
];
b
];

```

The Compiled GaussSolveForLoops function, using Compile[]

```

GaussSolveForLoopsC=
Compile[{{ain,_Real,2},{bin,_Real,2},{iterations,_Integer}},
Module[{
n=Dimensions[ain][[1]],
m=Dimensions[bin][[2]],
dumc=Table[0.0,{n}],
a=Table[0.0,{n},{n}],
b=Table[0.0,{n},{m}],
ipiv=Table[0,{n}],
    indxr=Table[0,{n}],
    indxk=Table[0,{n}],
    i=0, k=0, l=0, irow=0, icol=0,
    pivinv=0.0, amax=0.0, tmp=0.0,
    beficol=0, afticol=0, count=0
}],
For[count=1,count<=iterations,count=count+1,(
    a=ain; (* The arguments are always generated as const references
           and therefore cannot be changed.Actuall we get waste
           of space and time here when they are copied. *)
    b=bin;
    For [k=1,k<=n, k=k+1,ipiv[[k]]=0];
    For [i=1,i<=n, i=i+1,
        (* Algorithm first finds absolutely largest matrix element *)
        amax=0.0;
        For [k=1,k<=n, k=k+1,
            If [ ipiv[[k]]==0 ,
                For [l=1,l<=n, l=l+1,
                    If [ ipiv[[l]]==0 ,
                        If [ Abs[a[[k,l]]] > amax,
                            amax= Abs[a[[k,l]]];
                            irow=k;
                            icol=l
                        ]]]];
        ipiv[[icol]]=ipiv[[icol]]+1;
        If[ipiv[[icol]]>1,
            Print["*** Gauss2 input data error ***"];
            Break];
        If[ irow!=icol ,

```

```

    For [k=1,k<=n, k=k+1,
        tmp=a[[irow,k]] ;
        a[[irow,k]]=a[[icol,k]];
        a[[icol,k]]=tmp];
    For [k=1,k<=m, k=k+1,
        tmp=b[[irow,k]] ;
        b[[irow,k]]=b[[icol,k]];
        b[[icol,k]]=tmp]
];
indxr[[i]]=irow;
indxc[[i]]=icol;
If [ a[[icol,icol]]==0,
    Print["*** Gauss2 input data error 2 ***"];
    Break];
pivinv=1.0 / a[[icol,icol]];
a[[icol,icol]]=1.0;
For [k=1,k<=n, k=k+1,
    a[[icol,k]]=a[[icol,k]]*pivinv];
For [k=1,k<=m, k=k+1,
    b[[icol,k]]=b[[icol,k]]*pivinv];
For [k=1,k<=n, k=k+1,
    dumc[[k]]=a[[k,icol]];a[[k,icol]]=0];
a[[icol,icol]]= pivinv;
For [k=1,k<=n, k=k+1,
    If [ k != icol,
        For [l=1,l<=n, l=l+1,
            a[[k,l]]= a[[k,l]]- dumc[[k]]* a[[icol,l]]];
        For [l=1,l<=m, l=l+1,
            b[[k,l]]= b[[k,l]]- dumc[[k]]* b[[icol,l]]]
        ]]]];
];
For [l=n,l>=1, l=l-1,
    For [k=1,k<=n, k=k+1,
        tmp= a[[k,indxr[[l]]]];
        a[[k,indxr[[l]]]]=a[[k,indxc[[l]]]];
        a[[k,indxc[[l]]]]=tmp
        ]]]];
b
]];

```

End of the Gauss Package

End of the package:

```
End[];
EndPackage[];
```

2.4.2 Executing the Interpreted Version in *Mathematica*

First we need to create two arrays to be used as input for the solver.

```
a=Table[Random[],{10},{10}];
b=Table[Random[],{10},{2}];
```

Run GaussSolveArrayslice

The loop time may be too short for reliable measurements. It is only 3- 4 seconds combined with a resolution of 1 second. The relevant factor for a 1.5 GHz computer is 10.

```
factor=10;
loops=1*factor;
```

Call the solver:

```
s=(c=GaussSolveArrayslice[a,b,loops];)//Timing;
meval=s[[1]];
Print["TIMING FOR NON-COMPILED VERSION=",meval];
```

```
TIMING FOR NON-COMPILED VERSION= 0.1672 Second
```

Run the For-loop Version

Execute the version with for-loops:

```
s=(c=GaussSolveForLoops[a,b,loops];)//Timing;
mevalFor=s[[1]];
Print["TIMING FOR NON-COMPILED VERSION (FOR-LOOPS)=",mevalFor];
```

```
TIMING FOR NON-COMPILED VERSION (FOR-LOOPS)= 0.1094 Second
```

2.4.3 Generation of Fortran90 code

The command `CompilePackage` translates the package to **Fortran90** code:

```
CompilePackage["Gauss"]
```

```
Successful compilation to Fortran90: 2 function(s)
```

The Produced Fortran90 Code for Gauss

To save space, we only show the **Fortran90** code of the translated `GaussSolveArraySlice` function (which in fact also contains a few for-loops). The actual code generated on your system may differ slightly, as it is very dependent on the exact version of *MathCode* used.

```
function GaussSolveArraySlice(ain,bin,iterations) result(mc_O1)

    use MathCodePrecision
    use MathCodeSheep
    implicit none
    real(mc_real), intent(in) :: ain(:, :)
    real(mc_real), intent(in) :: bin(:, :)
    integer(mc_int), intent(in) :: iterations
    real(mc_real) mc_O1(SIZE(bin, 3-2), SIZE(ain, 3-1))
    integer(mc_int) count
    integer(mc_int) afticol
    integer(mc_int) beficol
    real(mc_real) tmp
    real(mc_real) amax
    real(mc_real) pivinv
    integer(mc_int) icol
    integer(mc_int) irow
    integer(mc_int) l
    integer(mc_int) k
    integer(mc_int) i
    integer(mc_int) indx( SIZE(ain, 3-1) )
    integer(mc_int) indxr( SIZE(ain, 3-1) )
    integer(mc_int) ipiv( SIZE(ain, 3-1) )
    real(mc_real) b( SIZE(bin, 3-2), SIZE(ain, 3-1) )
    real(mc_real) a( SIZE(ain, 3-1), SIZE(ain, 3-1) )
    real(mc_real) dumc( SIZE(ain, 3-1) )
    integer(mc_int) m
    integer(mc_int) n

    m = SIZE(bin, 3-2)
    n = SIZE(ain, 3-1)

    count = 1
    do while (count <= iterations)
```

```
a = ain
b = bin

k = 1
do while (k <= n)
  ipiv(k) = 0
  k = k+1
end do
i = 1
do while (i <= n)
  amax = 0.D0
  k = 1
  do while (k <= n)
    if (ipiv(k) == 0) then
      l = 1
      do while (l <= n)
        if (ipiv(l) == 0) then
          if (abs(a(l, k)) > amax) then
            amax = abs(a(l, k))
            irow = k
            icol = l
          end if
        end if
        l = l+1
      end do
    end if
    k = k+1
  end do
  ipiv(icol) = ipiv(icol)+1
  if (ipiv(icol) > 1) then
    PRINT *, "**** Gauss2 input data error ****"
  exit
end if

if (irow /= icol) then
  k = 1
  do while (k <= n)
    tmp = a(k, irow)
    a(k, irow) = a(k, icol)
    a(k, icol) = tmp
    k = k+1
  end do
  k = 1
```

```
do while (k <= m)
    tmp = b(k, irow)
    b(k, irow) = b(k, icol)
    b(k, icol) = tmp

    k = k+1
end do
end if
indxr(i) = irow
indxc(i) = icol
if (a(icol, icol) == 0) then
    print *, "*** Gauss2 input data error 2 ***"
    exit
end if
pivinv = 1.D0/a(icol, icol)
a(icol, icol) = 1.D0
a(:, icol) = a(:, icol)*pivinv
b(:, icol) = b(:, icol)*pivinv
dumc = a(icol, :)
k = 1
do while (k <= n)
    a(icol, k) = 0
    k = k+1
end do
a(icol, icol) = pivinv
k = 1
do while (k <= n)
    if (k /= icol) then
        a(:, k) = a(:, k)+((-dumc(k)*a(:, icol)))
        b(:, k) = b(:, k)+((-dumc(k)*b(:, icol)))
    end if
    k = k+1
end do
i = i+1
end do
l = n
do while (l >= 1)
    k = 1
    do while (k <= n)
        tmp = a(indxr(l), k)
        a(indxr(l), k) = a(indxc(l), k)
        a(indxc(l), k) = tmp
        k = k+1
    end do
```

```

        l = l+(-1)
    end do
    count = count+1

end do
mc_O1 = b
end function GaussSolveArraySlice

```

2.4.4 Building the Executable

Call `MakeBinary` to compile the generated **Fortran90** code and build the executable(s).

```
MakeBinary[]
```

Here, no package is given to `MakeBinary`. This means that the current package should be used.

2.4.5 Installing Compiled Code

Interpreted versions are removed, and compiled ones are used instead by using the `InstallCode` function:

```
InstallCode["Gauss"];
```

2.4.6 Prepare for Execution

Define a time measurement function, `AbsTime`:

```

SetAttributes[AbsTime, HoldFirst];
AbsTime[x_] := Module[{start, res},
    start = AbsoluteTime[];
    res=x;
    {(AbsoluteTime[]-start) Second, res}
];

```

2.4.7 External Execution

External Execution of Array Slice Version

Call the version of `GaussSolve` which contains array slice operations. Repeat the solution

process several thousand times in order to get a measurable time. The external compiled `GaussSolveArrayslice` function is called via `MathLink`, in the same way an internal *Mathematica* function is called. Recall that we defined test matrices `a` and `b` earlier. The same matrices will be used for this test.

```
loops=8000 * factor;
externaleval=((cc=GaussSolveArrayslice[a,b,loops]; )
  //AbsTime)[[1]]/loops
0.000015019427 Second
```

External Array Slice Version, MathLink in each Iteration

Call the `GaussSolve` externally-compiled code via `MathLink` as before, but perform the solution process only once per call. This causes the `MathLink` communication overhead to dominate (almost by a factor of 80) over the time needed to perform the actual solution process.

```
loops=100*factor;
externalevalPass=(Do[cc=GaussSolveArrayslice[aa,bb,1],{loops}];)
  //AbsTime)[[1]]/loops
0.000013124328 Second
```

External Execution of For-Loop Version

The for-loop version of `GaussSolve` is executed externally several thousand times, which is sufficient to get an execution time long enough for reliable measurements. The compiled code is slightly faster than the array slice version, since the generated code avoids some overhead in creating array objects. On the other hand, the array slice code is almost as fast and is more concise and convenient to write and understand.

```
loops=8000* factor;
externalevalFor=((cc=GaussSolveForLoops[aa,bb,loops]; )
  //AbsTime)[[1]]/loops
0.000013437156 Second
```

External For-loop Version, MathLink in each Iteration

As before with the array slice version, if a call via `MathLink` is performed in each iteration, the `MathLink` communication overhead will dominate over the actual computation time.

```
loops=100;
externalevalPassFor=
```

```

      ((Do[cc=GaussSolveForLoops[aa,bb,1],{loops}]);)
      //AbsTime)[[1]]/loops
0.0012497360 Second

```

Internal Execution of LinearSolve as a Comparison

As a comparison, we call the built-in *Mathematica* function `LinearSolve` for a solution of a linear equation system. `LinearSolve` uses an efficient solution algorithm from the `Lin-Pack` library, which has been linked into the *Mathematica* kernel.

```

loops=800*factor;
internalEval=((Do[cc=LinearSolve[a,b]; {loops}]);)
  //AbsTime)[[1]]/loops
0.000154021472 Second

```

Internal execution of Compiled version

```

loops=200*factor;
s=(c=GaussSolveForLoopsC[a,b,loops];)//Timing;

mevalForC=s[[1]]/loops;
Print["TIMING FOR VERSION (FOR-LOOPS) with Compile[]=",mevalForC];
Dot[a,c] - b // MatrixForm

TIMING FOR VERSION (FOR-LOOPS) with Compile[]=0.000989667 Second

```

2.4.8 Cleanup

The calls below uninstall the `MathLink` package and remove temporary files produced during the code-generation process.

```

UninstallCode["Gauss"]
CleanMathCodeFiles[]

```

`CleanMathCodeFiles` can also be given an argument to specify which package to clean up. The default is to clean up the last package compiled, which is used above.

Chapter 3 Matrix and Vector Operations

In many engineering applications, matrices and matrix manipulation operations are very common. The availability of an easy-to-use and short-handed notation for manipulating matrices is important for these application domains. Thus, we have extended the `Part ([[]])` operation in *Mathematica* to fulfill this objective.

The basic set of matrix operations in typed *Mathematica* presented in this chapter is currently limited to operations on array sections. Declaration of array variables is described in Chapter 5 and dynamic array allocation and initialization in Chapter 6.

The syntax is inspired by the syntax used by Matlab, Fortran90 and Modelica. This syntax is supported by the *MathCode* code generator for up to 4-dimensional arrays and within *Mathematica* for an arbitrary number of dimensions.

Only operations on homogenous arrays, i.e. where all elements have the same type, are supported by the code generator. Also, arrays must have a matrix-like shape, i.e. there must be the same number of elements in each row or column of a matrix. This constraint applies to generated code, but not necessarily within *Mathematica*.

3.1 Examples of Array Operations

Before going into detail about the index notation, the differences between vectors and matrices, and operations on those, we show below a few array-slice operations to give you an intuitive understanding of the process. First create a small matrix A with symbolic components of the form `a[i,j]`:

```
A=Table[a[i,j], {i,4},{j,5}]
```

Result:

```
{{a[1,1], a[1,2], a[1,3], a[1,4], a[1,5]},  
 {a[2,1], a[2,2], a[2,3], a[2,4], a[2,5]},  
 {a[3,1], a[3,2], a[3,3], a[3,4], a[3,5]},  
 {a[4,1], a[4,2], a[4,3], a[4,4], a[4,5]}}
```

Extract row 2 and 3:

```
A[[2|3, _]]
{{a[2,1], a[2,2], a[2,3], a[2,4], a[2,5]},
 {a[3,1], a[3,2], a[3,3], a[3,4], a[3,5]}}
```

Extract all but the first two columns, i.e. from the 3rd to the last column:

```
A[[_, 3|_]]
{{a[1,3], a[1,4], a[1,5]},
 {a[2,3], a[2,4], a[2,5]},
 {a[3,3], a[3,4], a[3,5]},
 {a[4,3], a[4,4], a[4,5]}}
```

3.2 Index Range Notation

When manipulating sections of arrays, it is important to have a concise and readable notation for index ranges. Such a notation is currently missing from standard *Mathematica*. There is a standard colon (:) notation used both by Matlab and Fortran90, which unfortunately was not possible to employ directly in *Mathematica* due to parsing problems. Instead we chose the vertical bar (|) which has a graphical layout similar to that of a colon and parses without problems in *Mathematica*. For example, an index range from 2 to n is expressed as follows in Matlab and Fortran90:

```
2:n
```

and in our *Mathematica* notation as:

```
2|n
```

3.2.1 Omitting End of Index Range

There are index-range colon expressions in Matlab and Fortran90 without a right-hand side, which implies that the largest value implied by the context should be used. For example:

```
2:
```

The $2 :$ in Matlab or Fortran90 means the same as $2 : n$ if there are at most n elements in the matrix dimension where this range is used, since n is then the largest value implied by context.

In *Mathematica* the vertical bar is always a binary operator, which means that a placeholder must be provided for the missing right-hand side. We use underscore (`_`) as this placeholder, since that notation is already used for placeholders in *Mathematica* patterns. Thus the Matlab and Fortran90 example $2 :$ is represented by the following *Mathematica* syntax:

```
2 | _
```

3.2.2 Omitting Start of Index Range

Alternatively, the left-hand side of the colon can be omitted in Matlab and Fortran90, for example:

```
: n-1
```

This means that the lowest index value should be used, which is always 1 in Matlab and Fortran90, as well as in *Mathematica*. The *Mathematica* counterpart then becomes:

```
1 | n-1
```

3.2.3 Omitting Both Start and End of a Range

It is possible to omit both the start and the end of an index range, which in Matlab and Fortran90 becomes a single colon and is equivalent to $1 : n$ for a dimension of size n :

```
:
```

In *Mathematica* this can be represented by:

```
1 | _
```

This is a very common special case denoting the whole range of a matrix dimension. Therefore we also provide the compact notation of a single underscore (`_`) to represent the whole range of a dimension:

```
_
```

3.3 Vectors Versus Rows and Columns

In Matlab all arrays including rows or columns of matrices are 2-dimensional matrices, whereas in *Mathematica* and Fortran90 either 1-dimensional vectors or 2-dimensional row vectors or column vectors are possible.

3.3.1 One-dimensional Vectors

One-dimensional vector variables are type declared using one index dimension, e.g.:

```
Declare[
  Real[5]  x;
]
```

A one-dimensional vector (i.e. a 1×5 array value with symbolic components might appear as follows in *Mathematica*:

```
{x[1], x[2], x[3], x[4], x[5]}
```

3.3.2 Row Vectors

A row vector extracted from a matrix is always a two-dimensional (e.g. $1 \times n$) array in Matlab, whereas in *Mathematica* and Fortran90 it can be either a two-dimensional or a one-dimensional entity. Most operations in *Mathematica* and Fortran90 accept either representation by performing automatic type conversion to the appropriate vector type, but certain operations such as dot product can be sensitive to the type of vector. An extracted *Mathematica* row-vector with symbolic components can appear as follows:

```
{ {a[2,1], a[2,2], a[2,3], a[2,4], a[2,5]} }
```

or with numeric components:

```
{ {1.1, 3.5, 2.3, 5., 6.2} }
```

The corresponding type is:

```
Real[1,5]
```

Thus, a more appropriate term for row vector would be row matrix, since it really is a matrix.

3.3.3 Column Vectors

Analogous to the case for row vectors, a column vector extracted from a matrix is always a

two-dimensional (e.g. $n \times 1$) array in Matlab, whereas in *Mathematica* and Fortran90 it can be either two-dimensional or one-dimensional. An extracted *Mathematica* column-vector (i.e. an 1×4 array) with symbolic components can appear as follows:

```
{ {a[1,2]},
  {a[2,2]},
  {a[3,2]},
  {a[4,2]} }
```

or with numeric components:

```
{ {5.5},
  {6.7},
  {8.98},
  {9.35} }
```

The corresponding type is:

```
Real[4,1]
```

In line with the previous case, a more appropriate term for column vector would be column matrix, since it also is a matrix.

3.4 Extracting or Assigning Vectors From Vectors

A range of elements forming a vector can be extracted or assigned from/to another vector. For example, first we create a vector X containing symbolic elements:

```
X = Table[x[i], {i,1,4}]
```

```
{x[1], x[2], x[3], x[4]}
```

Extract the two middle elements:

```
X[[2|3]]
```

```
{x[2], x[3]}
```

Assign the last three elements:

```
x[[2|4]] = {22,33,44}
```

```
{x[1], 22, 33, 44}
```

3.5 Extracting Vectors From Matrices

Either one-dimensional vectors or two-dimensional row- or column vectors can be extracted from rows and columns of matrices. However, in almost all cases the one-dimensional version is desired when programming in *Mathematica* or Fortran90. This results in slightly more efficient code and allows for indexing the vector using one index instead of two.

3.5.1 Extracting One-dimensional Vectors

Extraction operators using a single number or expression, e.g. 2 below, will always produce 1-dimensional vectors. For example:

Extraction of a row as a 1-dimensional vector:

```
A[[2, _]]
{a[2,1], a[2,2], a[2,3], a[2,4], a[2,5]}
```

Extraction of a column as a 1-dimensional vector:

```
A[[_ , 2]]
{a[1,2], a[2,2], a[3,2], a[4,2]}
```

3.5.2 Extracting Vectors as Submatrices of Shape $1 \times n$ or $n \times 1$

The index-range notations $\{i2\}$ and $i1|i2$ always produce vectors as two-dimensional submatrices, whereas just $i2$ results in one-dimensional vectors as presented in Section 3.5.1. For example:

Extraction of a column as a column-vector, i.e. as an $n \times 1$ submatrix:

```
A[[_ , {2}]]
{{a[1,2]},
 {a[2,2]},
 {a[3,2]},
 {a[4,2]}}
```

The $n1|i2$ syntax always gives a submatrix. Here it is used to extract a column-vector which is an $n \times 1$ submatrix as in the previous example:

```
A[[_ , 4|4]]
```

```
{ {a[1,4]},
  {a[2,4]},
  {a[3,4]},
  {a[4,4]}}
```

Extraction of a row as a 1xn submatrix:

```
A[{{2},_]}
{ {a[2,1],a[2,2],a[2,3],a[2,4],a[2,5]} }
```

The notation {2} is equivalent to 2|2.

3.6 Assigning Vectors to Rows or Columns of Matrices

The examples in this section assume that A is re-initialized as shown in section 3.1 before execution of each example.

The following sets the contents of a row to the contents of a vector. For example, setting row 2 to another value:

```
A[[2,_]] = {11, 22, 33, 44, 55}
{{a[1,1], a[1,2], a[1,3], a[1,4], a[1,5]},
 {11, 22, 33, 44, 55},
 {a[3,1], a[3,2], a[3,3], a[3,4], a[3,5]},
 {a[4,1], a[4,2], a[4,3], a[4,4], a[4,5]}}
```

Due to the list representation of arrays in *Mathematica*, it is possible to get identical results by only giving a row dimension, e.g.:

```
A[[2]] = {11, 22, 33, 44, 55}
```

A column can be assigned the value of a one-dimensional vector:

```
A[[_,3]] = {11, 22, 33, 44}
```

Result:

```
{{a[1,1], a[1,2], 11, a[1,4], a[1,5]},
 {a[2,1], a[2,2], 22, a[2,4], a[2,5]},
 {a[3,1], a[3,2], 33, a[3,4], a[3,5]},
 {a[4,1], a[4,2], 44, a[4,4], a[4,5]}}
```

Row- and column vectors or two-dimensional shapes $1 \times n$ or $n \times 1$ can also be assigned to rows or columns of a matrix. However, be sure to also specify such shapes on the left-hand side. For example, assigning a $1 \times n$ row vector:

```
A[[_ , 2 | 2]] = {{11, 22, 33, 44, 55}}
```

Assigning an $n \times 1$ column vector:

```
A[[_ , 3 | 3]] = {{11},
                 {22},
                 {33},
                 {44}}
```

3.7 Extracting and Assigning Arbitrary Submatrices

Arbitrary submatrices can be extracted or assigned by using complete range specifications. For example:

Extracting a 2×2 submatrix from A:

```
A[[2 | 3, 2 | 3]]
```

Result:

```
{ {a[2,2], a[2,3]},
  {a[3,2], a[3,3]}}
```

Assigning values to a submatrix of A:

```
A[[2 | 3, 2 | 3]] = {{1, 2},
                   {3, 4}};
```

Result:

```
A // MatrixForm1
{ {a[1,1], a[1,2], a[1,3], a[1,4], a[1,5]},
  {a[2,1], 1,      2,      a[2,4], a[2,5]},
  {a[3,1], 3,      4,      a[3,4], a[3,5]},
  {a[4,1], a[4,2], a[4,3], a[4,4], a[4,5]} }
```

1. Actually, a matrix formatted using `MatrixForm` in a real notebook looks nicer than what is shown in this text.

3.8 Promotion of Scalars to Vectors or Matrices

The standard *Mathematica* assignment operation will allow the assigning of a scalar value to a matrix variable even though it has been declared and initialized as a matrix:

```
A = 5
```

A has now been converted to a scalar integer variable with the value 5:

```
A
```

```
5
```

Such assignments will give rise to a type error in generated **Fortran90** code. However, it is possible to perform elementwise initialization of arrays by scalar values both in *Mathematica* and in generated code by specifying the dimensions in the left-hand side. Then the scalar value will automatically be promoted to constant array of compatible shape when performing the assignment.

For example, the two last columns (from 4 to the end) of A should be set to zero. The scalar 0 in the example below can be regarded as being promoted to a 4×2 constant array of zeroes before performing the actual assignment.

```
A[[_ , 4|_]] = 0;
```

```
A // MatrixForm
```

```
{ {a[1, 1], a[1, 2], a[1, 3], 0, 0 },
  {a[2, 1], 1, 2, 0, 0 },
  {a[3, 1], 3, 4, 0, 0 },
  {a[4, 1], a[4, 2], a[4, 3], 0, 0 } }
```

It is possible to set all elements of the array to the same scalar value:

```
A[[_ , _]] = 555;
```

```
A // MatrixForm
```

```
{ {555, 555, 555, 555, 555 },
  {555, 555, 555, 555, 555 },
  {555, 555, 555, 555, 555 },
  {555, 555, 555, 555, 555 } }
```

3.9 An Example Matrix Function

This example function, called `matrixtestfunc`, is completely meaningless from a computational point of view, but still illustrates how matrices can be declared as formal parameters and local arrays, returned as function values, and operated on by a number of assignment and value-extraction array section operations. The local variables `a`, `b`, `c` and `d` are simply initialized to integer constants. The syntax used for declaring arrays is explained in more detail in Chapter 5.

```
matrixtestfunc[Real[n_,n_] ain_]->Real[n,n] := Module[{
  Real[n,n] y;
  Integer {a=2,b=3,c=2,d=4};
},
  y[[_ ,2]] = ain[[_ ,2]];
  y[[_ ,a|_]] = ain[[_ ,a|_]];
  y[[_ ,c|d]] = ain[[_ ,c|d]];
  y[[a,_]] = ain[[a,_]];
  y[[a|_ ,_]] = ain[[a|_ ,_]];
  y[[a|b,_]] = ain[[a|b,_]];
  y[[a|_ ,c|_]] = ain[[a|_ ,c|_]];
  y[[a|_ ,c|d]] = ain[[a|_ ,c|d]];
  y[[a|b,c|_]] = ain[[a|b,c|_]];
  y[[a|b,c|d]] = ain[[a|b,c|d]];
  y[[_ ,b]] = ain[[_ ,b]];
  y[[a,_]] = ain[[a,_]];
  y
];
```

3.10 Current Limitations

The current *MathCode* code generator is limited to array section operations on up to 4-dimensional homogenous arrays. Also, it is currently not possible to specify a different stride (i.e. step size) than the default 1, as can be done in both Matlab and Fortran90.

Chapter 4 Rationale for Type Declarations in *Mathematica*

Previously, in Chapter 1, we presented some examples of static type declarations in *Mathematica* code needed to use the *MathCode* code generator. In this chapter, the *type declaration* notation, or “type system”, is motivated and presented in broader perspective—a type system can be used for more purposes than just to provide the necessary typing needed for a code generator.

The main reason to introduce static typing in *Mathematica* is to be able to generate efficient code in languages such as C++ and Fortran90.

The static type system presented here is designed to be well integrated into *Mathematica*. The syntax is *Mathematica* compatible, which makes it possible to use the type extensions in ordinary *Mathematica* code.

The type declarations are treated as code annotations within *Mathematica*, i.e. loosely associated additional information. Thus, they have no effect on execution and symbolic transformations within *Mathematica* apart from introducing the names of declared types and variables in the current *Mathematica* context. The only exceptions are typed array variable declarations with or without initialization parts, where the declared variable is allocated automatically to the specified dimensions and size.

Certain advanced features of the type system such as class declarations, records, etc., which sometimes are briefly hinted at in the text, are not implemented in the current version of *MathCode*, but are planned to become available in a future version.

4.1 Why Type Declarations?

There are several reasons why a static type system is a useful extension to *Mathematica*:

- Precise static type information is needed for generation of efficient executable code.
- A type checker is useful for finding errors during software development in *Mathematica*.
- Object-oriented typing is useful to handle complexity when building large applications

and equation-based simulation models.

Additional requirements of a type system are:

- *Ease of use.* The type system should be easy to understand and use.
- *Readability and standardization.* The type notation should be readable and conform to common program language standards, as well as to relevant *Mathematica* conventions.
- *Compatibility.* Typed *Mathematica* code should be able to be executed together with untyped code. Adding type information should be a pure extension—existing code should, for the most part, not need to be changed.

We discuss below the motivation behind a static type system in more detail.

4.2 Types for Code Generation

Precise static type information is needed for translating *Mathematica* into efficient code in strongly typed languages such as C++, Fortran90 and Java. It is also needed for more efficient internal compilation of *Mathematica* to efficient code as evidenced by the type information parameters to the standard *Mathematica* `Compile` function.

Experience from research on code generation to C++ and Fortran90 from the ObjectMath¹ extension to *Mathematica* made it clear that precise static type information could not always be automatically deduced from dynamically typed *Mathematica* code, especially when list structures (arrays) were involved. Therefore explicit declaration of static type information was introduced. However, in many cases it is possible to automatically derive static type information through type inference.

Precise static typing is especially important to provide *consistent handling of arrays* between *Mathematica*, C++, Fortran90, Java, etc., including compatibility with array representations used in common numerical subroutine libraries.

4.3 The Need for Type Checking

Debugging *Mathematica* programs can be hard. Simple spelling errors and other mistakes may cause pattern matching to fail, which causes huge unevaluated expressions to be returned to the user. It is usually not so easy to realize where the source of the error is located. Partial dynamic type checking of function parameters can be turned on, but will only be able to catch errors for the particular test cases which are used during debugging and testing.

A static type checker can be of great help in finding simple mistakes such as spelling

1. Article in IEEE Software, July 1995.

errors of variables or function names, wrong number of arguments to functions, mismatch of actual argument types and formal parameter types, etc. Concerning parameter types, most built-in *Mathematica* functions have numeric parameters which will be assigned the type `Real` in the static type system. The static type `Real` is, of course, an approximation, since there are several numeric forms in *Mathematica* such as infinite precision numbers and fractions. However, the approximation to `Real` fits well with code generation to statically typed languages such as C++ or Fortran90 as well as being a reasonable static type approximation for execution within *Mathematica*, since the exact numeric type may change dynamically during execution.

A relevant question is whether the static type system would be able to detect enough errors, since most functions in *Mathematica* are numeric anyway, and declaring the type `Real` for function parameters and results will not add considerable information. There are however many functions which accept parameters that are vectors and arrays of different forms and for which precise type information is quite useful for type checking. Other functions accept parameters which are records represented as tagged tuples. Additionally, checking the number of function parameters and whether a function or variable has been declared would catch many common mistakes by *Mathematica* programmers.

4.4 Types for Object Oriented Simulation Modeling

Simulation models are usually constructed to simulate a model of aspects of the external world. This is precisely where object orientation is most useful. For example, typical mechanical systems consist of a number of mechanical components which can be described by classes containing equations that describe motion, forces, material properties, etc. Simulation models of mechanical and other systems can be put together by connecting such objects from class libraries.

For example, a car contains connected objects such as a motor, transmission, wheels, etc. Inheritance provides reuse of equations and function definitions when inheriting from general classes to more application-specific instances. Thus, object-oriented type and class mechanisms provide structuring and reuse when building mathematical simulation models of physical systems. A future extension of the *MathCode* system will provide object-oriented typing for simulation applications.

4.5 Introducing Declarations in *Mathematica*

When introducing declarations and static typing as an extension of *Mathematica*, some keywords and names need to be reserved. The chosen keywords should be intuitive and easy to understand, correspond to common practice in other programming languages, and preferably not be used for other purposes within *Mathematica*.

The same requirements hold for the syntax of typed definitions. This syntax should be readable, easy to use, compatible with *Mathematica* syntax, and correspond to common programming language conventions.

4.6 Declarations in *Mathematica* Packages

The notion of declaration is already present in standard *Mathematica*, although it is not very pronounced. A *Mathematica* package can be regarded as a sequence of untyped variable and function declarations. For example:

```
BeginPackage["ExamplePackage`"]

varname1;
varname2=35;

func1[a_,b_] := ...;
func2[x_,y_] := ...;

EndPackage[]
```

The untyped “declarations” of variables `varname1` and `varname2` introduce these names into the name context of the package. The “declaration” of `varname2` also initializes the variable. The “declarations” of functions `func1` and `func2` define these functions.

4.7 Basic Types

The basic type names `Real`, `Integer`, `Complex`, `Symbol`, `String` etc. are already defined by *Mathematica* to be used in patterns and as head tags of basic objects. However, since the meanings of these words are essentially the same when used in a static type system, there should not be a problem with continuing to use these type names. To choose other names would be confusing to the user.

We introduce the type name `Boolean` as the type for values `True` or `False`, and `Null` to indicate the empty type or absence of type, e.g. for a procedure that does not return any data value.

The type name `AnyType` indicates that an object may have any type, which is useful to describe the type of certain objects, e.g. the element type of an array that may contain a mixture of objects such as real numbers, integers, strings etc. See section 5.1 that explains which basic types are actually implemented in *MathCode F90*

4.8 Dual Type System

Are *Mathematica* patterns the same as *types*? One might be tempted to answer yes to this question since both notions describe sets of objects which fulfill a pattern or type constraint. There are however certain differences between patterns and types, as evident in languages such as C++ or Fortran90:

- A pattern language is designed to express structural properties to be dynamically tested during execution, whereas a static type system describes properties to be checked statically before execution starts. This tends to influence the pattern or type notation.
- Certain aspects of the static type system, e.g. user-defined type names, record types, arrays, classes, etc. do not fit well into the *Mathematica* pattern language.
- Static type information can be approximate when used for type checking. For example, our `Real` type is an annotation that tells the system that a certain object (e.g. a function call) has a potential numeric non-integer (`Real` or `Rational`) value if all arguments to such an object are numeric and not symbolic.
- Precise static type information is needed for generation of efficient code in statically compiled languages. Sometimes this information must be provided by the user to obtain the precise intended meaning for generated code.

Mathematica patterns is in fact a mechanism to describe *dynamic* types — i.e. types that can change during execution. For example a variable `x` may be a symbol, then change into an expression and finally change into a real floating-point number during evaluation.

On the other hand, in a static type system, one would like to express that a variable always has the static type `Real` even though it is sometimes represented by a symbol, sometimes by an expression and sometimes by a floating-point value. This is especially needed for compiling to statically typed languages and for static type checking. Another use for static types is in user-defined types; for example a variable could have a static type `Voltage` even though it has a real value and would have matched the head `Real` in *Mathematica*.

Hence, we need *static typing*. Combined with the *Mathematica* patterns, *MathCode* thus provides a *dual type system*, fulfilling both requirements.

4.9 Typed Function Declarations

Consider the following four variants of the same untyped function `f2` in *Mathematica*, for which the second and third rules are attempts to include some dynamic type information; the variable `x` could be a symbol, an expression, a floating-point number etc.:

```
f2[x_] := x+2;

f2[x:_Integer] := x+2;

f2[x:(_ | _Integer)] := x+2;

f2 = Function[{x}, x+2];
```

The first definition of `f2` works for both symbolic and numeric arguments, which is often what the user intends, e.g. when producing symbolic expressions that will eventually be computed numerically. If an `_Integer` pattern is provided as a parameter “type” in the second definition, the function will unfortunately no longer work for symbolic arguments such as names of variables with potential integer values. The third definition can both handle symbolic arguments and provide some type information, but may collide with some uses of `Alternative()` and still does not specify a function-return type. The fourth version does not include any type information at all, analogous to the first version.

Therefore, for reasons mentioned in the previous section, we provide static argument types and the function type in a function signature integrated into the function head. Type prefixes are separated from formal parameter names by one or more spaces, which are represented by a special kind of prefix operator in the *Mathematica* FullForm representation¹. An arrow in the signature indicates mapping from input argument types to output result types. Some examples are shown below.

```
sin2[Real x_] -> Real := Sin[x]+2.0;

myprint[Real x_] -> Null := Print[x];

myrandom[] -> Real := Random[];

myfunc[Integer x_, Real y_] ->Real := x+y*y;

sincos3[Real x_, Real y_] -> Integer :=
    Floor[Sin[x]+Cos[y]+myfunc[x,y]];
```

Notice that the `:=` must be on the same line as the function head. Otherwise the *Mathematica* parser will read the first line separately and the type information will not become associated with the declared function. The following is not allowed:

```
sincos3[Real x_, Real y_]->Integer
```

1. The exact form of this FullForm prefix operator will change in future MathCode releases. Users should not make themselves dependent on the current FullForm representation of the prefix operator.

```
:= Floor[Sin[x]+Cos[y]+myfunc[x,y]];
```

Below is the `FullForm` of the first definition (`sin2`). As shown, the arrow from the function prototype to the result type becomes a `Rule[]` node.

```
SetDelayed[
  Rule[sin2[Real[Pattern[x,Blank[]]]],Real],Plus[Sin[x],2.]
]
```

Since `Rule[]` nodes are essentially never used as function names in normal *Mathematica* code (they are expressions, not names), the `:=` operator (`SetDelayed`) can for `Rule[]` nodes be redefined to perform the special action of storing type information in a symbol table, as well as defining an untyped `sin2` function as usual. This stored type information is then used for type checking and code generation. The untyped `sin2` function can be executed interpretively within *Mathematica*, which gives full compatibility with interpreted *Mathematica* code.

4.9.1 Type Arguments to the *Mathematica* Compile Function

The example below illustrates the rather drastic changes that would need to be made to a typical user-defined function such as `sincos3`, in order to use the standard *Mathematica* `Compile` function. This violates our requirements of compatibility and co-existence with interpreted *Mathematica* code and makes the function definition much less readable. Therefore this notation is not a viable option for typed *Mathematica* function definitions.

```
sincos3 = Compile[{{x, _Real}, {y, _Real}},
  Floor[Sin[x]+Cos[y]+myfunc[x,y]],
  {{myfunc[_], _Integer}}
```

4.10 Typed Declarations

There are several kinds of declarations where static type information can be supplied. For example, the type signatures of functions and the types of global variables need to be declared. We introduce the `Declare[]` declarator for declaring global variables, as shown in the example package below. Declared variables may be initialized, as in the variable `varname2` below:

```
BeginPackage["TypedExamplePackage`"]

Declare[
  Real    varname1;
  Integer varname2 = 35;
```

```
];  
  
myfunc[Real x_, Real y_]->Real := x+y*y;  
  
sincos[Real x_, Real y_]->Real := Sin[x]+Cos[y]+myfunc[x,y];  
  
EndPackage[]
```

Declare can also be used to declare function signatures, i.e. provide separate static type information for previously untyped *Mathematica* functions:

```
BeginPackage["TypedExamplePackage`"]  
  
Declare[  
  Real varname1;  
  Integer varname2 = 35;  
  myfunc[Real x_, Real y_]->Real;  
  sincos[Real x_, Real y_]->Real  
];  
  
myfunc[x_, y_] := x+y*y;  
  
sincos[x_, y_] := Sin[x]+Cos[y]+myfunc[x,y];  
  
EndPackage[]
```

Chapter 5 More on Typing and Declarations

As previously mentioned, the typed extension to *Mathematica* provides language extensions for declaring static types of *Mathematica* variables, arrays and functions. It also augments the pattern facilities for functions already present in *Mathematica*. This static typing scheme is general enough to provide a consistent, strong typing of the compilable *Mathematica* subset, described in more detail in Appendix A. This is the basic subset of *Mathematica* handled by the code generator. This subset is extensible via definitions provided by the `system` package (see Section 7.8 on page 125).

5.1 Basic Types

As mentioned in the previous chapter, the basic type names `Real`, `Integer`, `Complex`, `Symbol`, `String`, etc. are already defined by *Mathematica* to be used in patterns and as head tags of basic objects. We continue to use some of these type names in the static type system.

- `Real`—In generated code the `Real` type is represented by the IEEE double precision floating point type (`REAL(8)`). When executing within *Mathematica* the `Real` type has a wider range, including infinite precision rational numbers.
- `Integer`—In generated code the `Integer` type is represented by a standard integer type, `INTEGER(4)`. When executing within *Mathematica*, integers with unlimited numbers of digits are supported. This may lead to differences in numerical results.
- `Null`—This represents the absence of a typed value, e.g. for functions which do not return any value. In standard *Mathematica* `Null` is used in several circumstances to indicate the absence of an item, e.g. a non-existent value, a missing expression or statement, etc. There is no such type in Fortran. *Mathematica* functions that return a value are translated to Fortran functions. *Mathematica* functions that do not return any value are translated to Fortran subroutines.
-

All other types are not part of the compilable subset

5.2 Declarations

There are several kinds of declarations where type information can be supplied, including declarations of constants, variables, and user-defined types.

5.2.1 Variable Declarations

The types of variables need to be declared for reasons previously mentioned, although type inferencing techniques can be introduced to deduce the types of some, but not all, variables.

Earlier we introduced the `Declare[]` declarator for declaring global variables, as shown in the example *Mathematica* package below. Declared variables may be initialized, as for the variable `i2` below.

```
Declare[
  Real    r1,
  Integer i2 = 35
];
```

The `Declare[]` declarator is not needed for declarations of local variables in `Module[]`, `Block[]` or `With[]` bodies of *typed* functions, as in the contrived example below. This example also shows the syntax of simultaneous declaration of several variables (here: `y, z, w`) with the same type. Note that the variable `y` is returned as the value of the function `f` by being the last expression (which thus must be without the ending semicolon) at the end of the function body.

```
f[Real x_]->Real := Module[{
  Integer n,
  Real    {y, z, w},
  Integer i = 1,
  Integer j = 0
},
  y = x+i+j;
  y
];
```

The following example shows how both function signatures and global variables can be declared separately using `Declare`:

```

Declare[
  mytan[Real x_]->Real,
  Real[3,3] myarr
]

mytan[x_] := Sin[x]/Cos[x];

```

You might ask how typed local variable declarations can work, since such declarations are not allowed by *Mathematica* for `Module[]` or `Block[]` sections within ordinary untyped functions. The reason that these declarations work is that the *MathCode* type analyzer during the analysis of typed function declarations removes and stores elsewhere all type information from local variable declarations and simultaneously produces an ordinary untyped version of the function that can execute as usual within *Mathematica*. This is done just once during declaration elaboration, before the function is called, so that the *Mathematica* code is not slowed down by any additional type checking at run-time.

5.2.2 Constant Declarations

Named compile-time constants are available in several languages such as C, C++, Fortran, etc. When translating from *Mathematica* to those languages, it is useful to be able to generate declarations of such symbolic constants since this guarantees that generated code and hand-written code referring to such a constant references exactly the same constant value. Symbolic constants are also quite useful when specifying the dimension sizes in declarations of fixed sized arrays. Currently the constants used in symbolically evaluated functions are replaced by their values. All declared constants are represented as global variables in the generated code and are initialized by corresponding constant expressions.

The constant declaration sets the `Constant` attribute for the constant name in *Mathematica*, which is relevant for symbolic derivatives, as well as setting the attribute `Protected` which prevents accidental assignment of a new value to the constant. Some examples are shown below.

```

Declare[
  Constant one = 1,
  Constant age = 5.5,
  Constant Integer vsize = 100,
  Constant Real Pi,
  Constant Real[10] constvec = {1,2,3,4,5,6,7,8,9,10}
];

```

As can be seen from the examples, a constant may or may not be initialized, and can have an associated optional type. If no type is specified, the type is inferred from the type of the initialization expression, if possible. If no value is supplied, the constant is either used only

for symbolic computations where the value is not needed, or the value has already been pre-defined as in the case of `Pi`.

5.3 Type Constructors and Data Constructors

A *type constructor* is a function that can create types and may have types or other entities as arguments. Essentially any type name can be used as a type constructor.

For example, `Real` is a 0-ary (i.e. nullary—no arguments) type constructor that creates the `Real` type. By contrast, a *data constructor* is a function or tag that creates and marks a data value.

5.3.1 List Structures and Array Types

Arrays in the compilable *Mathematica* subset are homogenous, ordered collections of elements, all belonging to a common base type (e.g. `Real`, `Integer`). In standard *Mathematica*, arrays are known as list structures. However, these are internally implemented as dynamically extensible arrays.

Arrays can be declared as one-dimensional, two-dimensional or multi-dimensional. If the *Mathematica* program is going to be translated to Fortran90, there is a limitation of 7 dimensions. For translation to C++ there is currently a limitation of 4 dimensions.

Arrays can be passed as arguments to *Mathematica* functions and returned as function values.

5.3.2 Array Type Constructors

Compared to the previous example where `Real` was a nullary type constructor, in `Real[10]` the name `Real` is a unary (one argument) type constructor that creates the type: *array of ten real numbers*. In `Integer[5, 5]`, the name `Integer` is a binary (two argument) type constructor that creates the type: *square 5 by 5 matrices of integers*. Thus, the element type with one or more arguments is used as a type constructor for arrays of one or more dimensions. Some examples:

```
Real[3]           (* A type for one-dimensional arrays of 3 real numbers *)
Real[5, 4, 10]   (* A three-dimensional real array type *)
Integer[4, 4]    (* A type for 4x4 arrays of integers *)
Integer[_, _]    (* A type for 2-dim arrays of integers with
                  unspecified number of rows/columns *)
```

The symbols `m` and `n` in the array type below can be named integer constants or global variables assigned only once, in which case they are sometimes referred to as *execution param-*

eters (see page 97), or local variables which have been initialized to the dimension sizes of the array:

```
Integer[m,n]
```

5.3.3 Data Constructors

In contrast to type constructors, data constructors are functions or tags which build or mark data values. For example, the tag `Complex` in *Mathematica* is a data constructor that builds and tags complex numbers.

The basic type names `Real`, `Integer`, `Symbol`, `String` might also be regarded as types of basic data constructors, since `Head[3.2353]` returns `Real`, and `Head[55]` returns `Integer`, `Head["a string"]` returns `String` and `Head[MyX]` returns `Symbol`.

`Complex` is a data constructor as well. `Complex[2.0, 3.0]` creates a complex number. An expression `2.0 + i 3.0` when evaluate returns this complex number.

5.4 Array Variable Declarations

Below is an example of declaring global array variables, enclosed within the `Declare[]` declarator needed to specify global variables:

```
Declare[
  Real[10]      x,
  Integer[n,m] y
]
```

Local array variables in functions are declared within the list of local variables in a `Module[]`, `Block[]` or `With[]`:

```
Module[{
  Real[10]      x,
  Integer[n,m] y
},
  ...
]
```

5.4.1 Declaring Multiple Array Variables

The syntax for declaring multiple array variables of the same type is the same as that for declaring several scalar variables of the same type, as in the declaration of the scalar variables `x`, `y`, `z` and the array variables `xvec`, `yvec`, `zvec` below:

```
Real      {x, y, z }
Real[2]   {xvec, yvec, zvec }
```

Initialization parts are possible in both cases:

```
Real      {x=value1, y=value2, z=35.4 }
Real[2]   {xvec={1.,1.}, yvec={3.,4.}, zvec={10.,5.5} }
```

5.5 Functions

Functions can be declared with zero or more argument types and a return type which might be `Null` to indicate the absence of a return value. The first example shows a function `DoubleSix` which accepts one integer parameter and returns a real result:

```
DoubleSix[Integer x_]->Real := 6.0+x+x;
```

Static type signatures of functions can also be specified in a separate `Declare` statement as shown below:

```
Declare[DoubleSix[Integer x_]->Real ];
DoubleSix[x_] := 6.0+x+x;
```

Both static and dynamic types¹ (e.g. see Section 4.8 on page 81) can be specified as below:

```
Declare[DoubleSix[Integer x_]->Real ];
DoubleSix[x_Integer] := 6.0+x+x;
```

5.5.1 Functions with No Input Parameters

Functions without input parameters are specified with an empty `[]` representing the empty list of input parameter types, e.g.:

```
Six[]->Real := 6.0
```

1. The “dynamic type” is an ordinary Mathematica pattern like `_Integer` or `_Real` that is used for ordinary dynamic pattern matching.

5.5.2 Functions with Multiple Return Values

An example of a function with multiple return values is shown below. This function accepts one real parameter value and returns two real values. When translating to C++ or Fortran90, multiple return values are handled by adding additional output parameters in the code of the translated functions.

```
SinCos[Real x_]->{Real, Real} := { Sin[x], Cos[x] };
```

Functions with multiple return values should be called on the right-hand side of an assignment statement with several variables on the left-hand side, e.g.:

```
{y,z} = SinCos[5.5];
```

Note that from a typing point of view this is different than a function returning an array of two elements, which can be declared as follows:

```
SinCos2Vec[Real x_]->Real[2] := { Sin[x], Cos[x] };
```

and called as below:

```
y2vec = SinCos2Vec[5.5];
```

5.5.3 Functions Returning Arrays

Arrays can be passed as parameters to functions, as in the function `AddThree` below:

```
AddThree[Real[3] vec_]->Real := vec[[1]]+vec[[2]]+vec[[3]];
```

and arrays can be returned as function values:

```
OneTwoThree[]->Real[3] := { 1., 2., 3. };
```

5.5.4 Functions with No Return Value

Some functions (usually called procedures) do not return any values. They simply perform computations and side effects, such as assigning values to global variables or performing input/output.

The function `AssignIntvar` below is an imperative function (really a procedure) that does not return anything (just `Null`) but has a side effect of changing the declared global integer variable `Intvar`:

```
AssignIntvar[Integer x_]->Null := ( Intvar = x+5; );
```

An example of a function lacking both input parameters and result value:

```
AssignIntvar[]->Null := ( Intvar = 5; );
```

In standard *Mathematica* `Null` is used in several circumstances to indicate the absence of an item, e.g. a non-existent value, a missing expression or statement, etc.

5.5.5 Functions with Local Variables

The type information for local variables uses the same syntax as that of globally declared variables but with the keyword `Declare[]` omitted. For example the function body creates

```
foo[Real x_]->Real := Module[
{
  Integer    n,
  Real      w2,
  Integer    i = 1
},
...
]
```

the local variables `n`, `w2`, and `i` with the types `Integer`, `Real`, and `Integer` respectively.

The `Declare[]` command can be used to separately specify the types for the local variables in combination with function signatures as follows:

```
Declare[function signature, {local variable types}]
```

The list of local variable types must be given immediately after the corresponding function signature. Several function signatures can be given in a `Declare[]` statement combined with local variable type specifications. If the function body consists of several nested blocks the types for the local variables are assumed to match the topmost block.

The previous example appears as follows when local variable type specifications are separated from the function itself as in the `Declare[]` statement below:

```
Declare[ foo[Real x_]->Real, {Integer, Real, Integer}]

foo[x_] := Module[
{ n, w2, i = 1},
...
]
```

5.5.6 Structure of a Small Example Package with Typed Functions

The following small package example shows the recommended structure of a typical package using constructs in typed *Mathematica*. More complete package examples have already been presented in Chapter 2.

There are two sections containing names here. The first contains publicly visible names that can be referenced outside the package. The second contains global names that should only be visible within the package. There are several reasons to have these as separate sections. For example, if the package is stored in a notebook, you can have each of these sections in a separate cell. It is then easy to add a new public or private global name just by adding it to the appropriate list and re-evaluating the corresponding cell. It is also beneficial to have a private global name list for documentation purposes and to make it easier to move names between the public and private global name lists as needed.

```
Needs["MathCode`"]

BeginPackage["TypedExamplePackage`"]

(* Interface section with exported, publicly visible names *)
Begin["TypedExamplePackage`"]
  r1;
  extfunc;
End[]

(* Private global names, only visible within the package *)
Begin["TypedExamplePackage`Private`"]
  i2;
  b3;
  sincos;
End[]

(* Implementation section *)
Begin["TypedExamplePackage`Private`"]

(* Global variables *)
Declare[
  Real    r1,
  Integer i2 = 35,
  Boolean b3 = False
];

(* Typed function definitions *)

extfunc[Real x_, Real y_]->Real := x+y*y;
```

```
sincos[Real x_, Real y_]->Real := Sin[x]+Cos[y]+extfunc[x,y];

(* End of implementation section *)
End[]

(* End of Package *)
EndPackage[];
```

Chapter 6 Data Allocation and Initialization

The standard *Mathematica* semantics of variable declarations *separates* the declaration of the variable, i.e. the introduction of the *name* of the variable, from the allocation/initialization of a *value* for that variable. This makes sense, since many computations in *Mathematica* are symbolic and thus involve symbolic *names* rather than (numerical) values.

Thus the *separation* of type declaration and memory allocation for a variable means that allocation is specified by a separate *explicit* allocation/initialization part. This is different from languages with implicit allocation. *Complete separation* goes even further—declaration of the type for a variable is completely separated from allocation and initialization which can occur later, even in a separate part of the program.

Below we compare *Mathematica* with possible target languages for generated code.

- *Mathematica*. Declaration of type is *separate* from allocation/initialization. Allocation and initialization are *explicitly* specified in an initialization part. Allocation and initialization are coupled, i.e. always occur together. The initialization part of declarations is *optional*. *Complete separation* of type declaration and allocation is possible by leaving out the initialization part.
- *Fortran90*. Declaration of variables with simple types (*Real*, *Integer*,...) implicitly allocates memory. Regarding the declaration of variables with structured types (arrays, records), *both* explicit and implicit models are possible. Declarations can either cause implicit allocation or require separate explicit allocation depending on how constructor functions are defined and used. The *MathCode* library used by the *MathCode* code generator supports *implicit* allocation in conjunction with variable declaration. Initialization is *optional*. Complete separation of type declaration and allocation is possible in Fortran90 via pointer variables.

Implicit allocation of declared variables is a safer programming practice and usually gives better performance of the compiled code than *complete separation* of declaration and allocation. Therefore, *Mathematica* variable declarations with or without the initialization part are compiled to variable declarations with implicit allocation whenever possible.

6.1 When Should Allocation and Initialization be Performed?

The rules for variable allocation and initialization are specific for each programming language. Here we are primarily interested in the comparison between transparent allocation/initialization behavior in typed *Mathematica* and generated code behavior in **Fortran90**, i.e. initialization code should execute in essentially the same way.

For typical computing applications there is often a set of global variables which, in a sense, are *execution parameters* for the whole application and thus should obtain their values quite early. We need a way to structure the computation so that these execution parameters obtain their values before the actual computation occurs and before the allocation of non-constant sized data structures.

6.1.1 Initialization of Global Variables

There are three cases of declarations of global variables to consider:

- Global variables with *statically known size*. Examples are scalar variables or array variables with constant dimension sizes, e.g. in a declaration such as:

```
Declare[Real[3,3] xmat = initializer]
```

Such variables can be allocated and initialized statically before execution. This is usually done automatically in Fortran90. For typed *Mathematica*, allocation is performed when the declaration statement is first encountered and evaluated.

However, if the initializer contains a non-constant expression that refers to some variables whose values are not yet defined, the initialization should be done later when these variables have received their values, e.g. as in the `Electrons` example in the next paragraph. This should be done via a user-specified call to the function `packagenameInit[]`. This function is generated automatically when `CompilePackage` is called. For example, for a package `mypack` this function would be called `mypackInit[]`.

- Global array variables for which the *allocated sizes are not fixed until runtime* and for which dependency on the values of one or more integer variables is possible. Such integer variables are sometimes called *execution parameters* since they may parameterize array allocation for the whole computation.

An example of this is the simulation of an atom, for which the value `n` of the number of electrons needs to be read in before descriptive array variables like `Electrons` in the following declaration are allocated:

```
Declare[ Real[n] Electrons = initializer]
```

The desired behavior is to allocate such array variables *after* the relevant execution parameters have received their values but *before* the array variables are first used.

Therefore the system generates a function called `packagenameInit[]` in each compiled package. This function *allocates and initializes global variables declared in that package*. For *Mathematica* code intended to be translated to stand-alone code, a call to this allocation/initialization function should be inserted explicitly by the user at the appropriate point in the code, usually quite early in the computation. This function is automatically called to perform initialization at the start of a C++ computation when the application is installed by `InstallCode[]` from the *Mathematica* environment.

- Global variables with *unknown sizes* and *explicit* initialization code. Allocation occurs when the relevant explicit allocation/initialization user-written code is executed. Such allocations and initializations which are part of the declaration initializer are performed when the package specific `packagenameInit[]` function is called.

Local Variables

Declared local variables are allocated and possibly initialized when the function body is entered and these declarations are elaborated. This is done both for *Mathematica* and for target languages like C++ and Fortran90. Thus, such variables pose no special problems.

6.1.2 Execution Parameters

For typical applications such as simulations and numerical experiments there are certain global or class variables that might be called *execution parameters* since they, in a sense, are parameters for each execution of the whole application.

These variables should be assigned values only once, quite early during execution, before the allocation of all “static” variable-sized data structures and before execution of non-constant initializers. An example is the parameter `n`, which determines the size of allocated arrays for the atom simulation mentioned in Section 6.1.1.

6.2 Array Allocation and Initialization

A declared array usually needs to be allocated and initialized in order to be used for further numeric or symbolic computations. *Mathematica* always initializes arrays when they are allocated, whereas languages like C++ and Fortran90 allow the (sometimes error prone) practice of allocating without initialization.

There are two situations in which an array variable does not need to be allocated; the first is when it is a formal parameter to a function and thus already has been allocated. The second case is when declaring an un-allocated array variable which eventually obtains its allocated value by assigning the results from some function that returns array values.

6.2.1 Array Usage and Representation in *Mathematica*

In *Mathematica* several options are available for creating and storing arrays, e.g., homogeneous list structures. It is necessary to have several variants of array storage and representation due to different needs in different situations. For example, there might be a need to work either symbolically or numerically, to evaluate as soon as possible, or to defer evaluation. Additional aspects concern storage allocation and initialization at array allocation time. The four most important aspects are:

- Symbolic or numeric array elements
- Immediate or deferred evaluation
- Storage allocation and representation
- Initialization

By comparison, languages like Fortran90 and C++ always perform numeric computation, have immediate evaluation, usually allocate storage immediately, and may or may not initialize data at array creation.

6.2.2 Array Initialization by Promoted Scalar Values

It is often the case that a numeric array needs to be allocated and each element initialized to zero. This can be expressed rather clumsily by explicit initialization to a constant array value as in the declaration below:

```
Real[3,3] mat = {{0.,0.,0.}, {0.,0.,0.}, {0.,0.,0.}}
```

A more elegant way to express this is to introduce promotion of scalar values like 0.0 to array values of appropriate size and dimension. This is possible since the element type, size and dimension information is available within the declaration. Such promotion is already standard in *Mathematica* for arithmetic expressions consisting of mixed scalars and arrays, since arithmetic operations have the `Listable` attribute. Thus, the following concise and readable notation is supported in typed *Mathematica*:

```
Real[3,3] mat = 0.0
```

What actually happens is that the system replaces 0.0 by the call `Table[0.0, {3}, {3}]` which allocates the desired zero-initialized array. The above example will give the array variable `mat` the following initial value:

```
{{0.,0.,0.}, {0.,0.,0.}, {0.,0.,0.}}
```

A declaration and initialization of such a global variable can be expressed as follows:

```
Declare[  
  Real[3,3] mat = 0.0  
];
```

Remember that the `Declare[]` declarator is only used for the declaration of global variables—not for local variables.

Initialization of Runtime Sized Arrays

It is common that the sizes of array dimensions are not known until runtime. Essentially all code in general numerical libraries is written in that way. The variable names `n` and `m` are used instead of constants for array dimension sizes in the example below:

```
Real[n,m] mat = 0.0
```

In this case, the symbolic names `n` and `m` will still be part of the type specification of `mat`, and the values of `n` and `m` will be used when creating an array of appropriate size.

Dimension size variables like `n` and `m` can be any local variable, function parameter or global variable, all of which must be of type integer. Good programming practice is to regard these variables as *single assignment*, i.e. they should be assigned the dimension sizes just once and not changed afterwards to avoid making the values of dimension size variables inconsistent with the actual dimension sizes of the array. If `n` and `m` have not been assigned integer values, a run-time error will occur in *Mathematica*.

Also regard the declaration of a square matrix below:

```
Real[n,n] squaremat = 0.0
```

This declaration expresses two type constraints. The first is that both dimension sizes are equal, i.e. a square matrix. The second constraint is that the sizes of both dimensions are *equal* to the value of the integer variable `n` at the point in time when the array is allocated and initialized—and hopefully also afterwards.

Allocation Without Initialization

Type declaration of an array together with allocation without requiring initialization can be specified for an array variable by simply leaving out the initialization part. When executing in typed *Mathematica* the array variable is in effect initialized to an array of unspecified content—often an array filled with an unspecified internal value (e.g. -999), in order to catch possible access-before-definition errors.

Generated code in C++ and Fortran90 becomes slightly faster when using this

alternative since initialization to zero is not required. The first example below shows allocation of a fixed-sized array without explicit initialization:

```
Real[3,3] mat
```

The second version declares and allocates an array for which the sizes of the dimensions are determined by two variables `n` and `m`, whose values are not known until runtime:

```
Real[n,m] mat
```

General Initializers

Explicit initialization of array elements to an arbitrary value or expression, e.g. the value 150 below, is also possible, using one of *Mathematica*'s array data constructors `Array` or `Table`, or any other *Mathematica* function that returns an array with the appropriate dimensions and sizes. For example:

```
Real[3,3] mat = Array[150.&,{3,3}]
```

or

```
Real[3,3] mat = Table[150.,{3},{3}]
```

which both initializes `mat` to the same array value:

```
{{150.,150.,150.}, {150.,150.,150.}, {150.,150.,150.}}
```

The `Array` form is more general than `Table`, but slower when running interpretively in *Mathematica* (by more than a factor of ten) for large arrays, since `Array` computes a supplied function (in the above example the constant anonymous function `150.&`) for each element, whereas `Table` just computes an expression for each array element.

Two examples of allocation and initialization of matrices with special structure are the calls to `IdentityMatrix` and `DiagonalMatrix` below, where `n` is a global or local integer variable.

```
Real[n,n] mati = IdentityMatrix[n]
```

```
Real[n,n] matd = DiagonalMatrix[Range[n]]
```

Unspecified Dimension Sizes

It is also possible to declare the type of arrays for which dimension sizes are not known even when the declaration is elaborated. In such cases, the size indicator of each dimension is replaced by an underscore (`_`) placeholder, as in the example below:

```
Real[_,_] mat
```

Since the dimension sizes are not known in the type, no implicit allocation of the array variable is possible. Initialization by promoting scalar values to such an array is also not possible. However, initialization by an array value with well-defined dimension sizes like `Array[150.&, {3, 3}]` is of course possible.

This kind of declaration is seldom needed in new code apart from the common case of adding static array types to variables in previously untyped *Mathematica* code. One possible use for this kind of declaration is, however, to declare an array variable which (later) is assigned an array value of unknown size returned by a function:

```
Real[_,_] mat = FuncUnknownSizedArr[]
```

Either an underscore (`_`) or a symbolic name followed by underscore (`n_`) can be used when denoting an unknown size of a single dimension.

Named size placeholders like `n_` have an advantage in that some type constraints can be expressed in a general way. For example, the fact that both dimensions of square matrices are always equal can be expressed without limiting the square matrix type to any specific size variable or constant:

```
Real[n_,n_] squaremat
```

The scope of named dimension-size placeholders (like `n_`, `k_`, `m_`) is limited to the body of the function in which they are declared as formal parameters. This is convenient for expressing size constraints on array parameters and function results. For example, the matrix multiplication function signature below expresses that multiplication of an $n \times k$ matrix by a $k \times m$ matrix gives an $n \times m$ matrix as a result.

```
MatMult[Real[n_,k_] amat_, Real[k_,m_] bmat_]->Real[n,m] := ...
```

Note that a placeholder variable that occurs more than once is initialized according to the first occurrence, and that no equality checking for the different occurrences is currently performed.

6.2.3 Summary of Array Dimension Specification

In the two subsequent sections we summarize the different forms of specifying dimension information in array types. There are two main cases to consider:

- Arrays which are passed as function parameters or returned as function values, where the actual array value has been previously allocated.
- Declaration of array variables, usually specifying both the type and the allocation of the declared array.

Array Dimensions for Function Parameters and Results

There are five forms allowed for specifying array dimension sizes in array types for function arguments and results:

- *Integer constant* dimension sizes, e.g. `Real [3, 4]`.
- *Symbolic constant* dimension sizes, e.g. `Real [three, four]`.
- Unknown dimension sizes with *unnamed placeholders*, e.g. `Real [_ , _]`.
- Unknown dimension sizes with *named placeholders*, e.g. `Real [n_ , m_]`.
- Unknown dimension sizes with variables as dimension sizes, e.g. `Real [n, m]`.

The dimension sizes can be *constant*, in which case the size information is part of the type. Alternatively, the sizes are *unknown* and thus fixed later at runtime when the array is allocated. Such unknown dimension sizes are specified through named (e.g. `n_`) or unnamed (`_`) placeholders.

All array values which are passed as arguments at function calls have already been allocated at runtime. Thus their sizes are already determined. These sizes may, however, be different for different calls. Therefore specification of conflicting dimension sizes through integer variables in array types of function parameters or results is not allowed, though it is allowed for ordinary declared variables. Only constants and named or unnamed placeholders are allowed.

Array Dimensions for Declared Variables

Below are the five different kinds of forms for expressing array dimension information in variable declarations. The example shows a global variable declaration using the `Declare[]` declarator, which can also be used for local declarations in functions.

The fifth case is where sizes are specified through integer variables. This is needed to handle declaration and allocation of arrays for which the sizes are not determined until runtime.

- *Integer constant* dimension sizes, e.g., for an example array `arr`:

```
Declare[Real[3,4] arr];
```

- *Symbolic constant* dimension sizes, e.g.,

```
Declare[Real[three,four] arr];
```

- Unknown dimension sizes with *unnamed placeholders*, e.g.,

```
Declare[Real[_,_] arr];
```

- Unknown dimension sizes with *named placeholders*, e.g.,

```
Declare[Real[k_,m_] arr];
```

- Unknown dimension sizes which are specified by *integer variables* such as function parameters, and local or global variables that are *visible* from the declaration, e.g.,

```
Declare[Real[n,m] arr];
```

Note that `Declare` is not needed for local variables.

Such integer variables, e.g., `n`, `m`, are assumed to be assigned once, i.e. their values are not changed after the initial assignment so that the declared sizes of allocated arrays are kept consistent with the values of those variables. This *single-assignment* property is not checked by the current version of the system, however. You, the user, are therefore responsible for maintaining such consistency.

6.3 Array Index Bounds

Obtaining and using array index bounds and dimension sizes is important in general array-based programming. Below we examine how to obtain and use index bounds in *Mathematica* and briefly discuss these issues for the target languages of the code generator.

6.3.1 Array Index Lower Bounds

In *Mathematica* the lower bound for array indexing is always 1, which is compatible with traditional mathematical indexing and enumeration notation. The lower bound for indexing in a numeric array processing language such as Fortran90 is also 1.

Unfortunately the C language and languages derived from C, e.g. C++ and Java, use zero as the lower bound for indexing of the built-in array type, which is incompatible with *Mathematica*. There is, however, no standard object-based array type defined for C++ — only the old C array construct which is too static and inconvenient to be used for serious numerical computing. The efficient *MathCode* array library in C++ is, however, designed

with a lower index bound of 1 in order to be compatible with both *Mathematica* and with standard Fortran subroutine libraries. However, when generating Fortran90 code the *MathCode* array library is not needed since the array functions are built into the language.

Thus, we have the following situation:

- *Mathematica*—lower index bound is 1.
- *MathCode* array library in C++—lower index bound is 1.
- Fortran90—lower index bound is 1.
- Matlab —lower index bound is 1.
- Java—lower index bound is 0. All index expressions must be converted by adding "1" to these expressions in generated code. An alternative would be a special *MathCode* array library in Java, designed to have a lower index bound of 1.

6.3.2 Dimension Sizes and Upper Index Bounds

The actual sizes of the dimensions of variable-sized arrays can be obtained through a call to the standard *Mathematica* function `Dimensions`, by passing the array as an argument and returning one or more results depending on the dimensions of the array. The size of a dimension is the same as the upper index bound of the corresponding dimension for a *Mathematica* array. The following example shows how to obtain the dimension sizes for a two-dimensional array `mat`:

```
dim1 = Dimensions[mat][[1]]
dim2 = Dimensions[mat][[2]]
```

6.3.3 Declaring Local Arrays with Variable Dimension Sizes

There is a special problem in obtaining and using array parameter dimension sizes which are needed to declare and allocate local arrays of compatible sizes (this is necessary when implementing general size-independent algorithms for arrays).

The problem stems from the fact that the *Mathematica* `Module[]` construct initializes all local variables at the same time. Therefore, it is not intrinsically possible to obtain the dimension sizes from the first variables in the list in order to declare and initialize array variables later in the list. The following example shows how a typed *Mathematica* function can be written, within which values of `n` and `m` must be available for declaration of the two local arrays `ipiv` and `Rx`:

```
foo[Real[n_,k_] ain_, Real[k_,m_] bin_]->Real[n,m]:=
Module[{
```

6.4 When x in $a[[x]]$ is negative, a range check error will be triggered if range checking is

```
Integer[n] ipiv,  
Real[m,m] Rx  
},  
...  
]
```

The example below shows the solution to this problem used by the *MathCode* compiler, by using a *double* Module[] structure. The variables *n* and *m* are initialized to appropriate dimension sizes in the outer Module, and are subsequently used for declaring and allocating variables in the inner Module. The above code fragment is thus expanded internally to:

```
foo[Real[n_,k_] ain_, Real[k_,m_] bin_]->Real[n,m]:=  
Module[{  
  Integer n= Dimensions[ain][[1]],  
  Integer m= Dimensions[bin][[2]]  
}, Module[{  
  Integer[n] ipiv,  
  Real[m,m] Rx  
},  
...  
]  
]
```

Negative Indices

In *Mathematica* negative indices may occur, which is not allowed in Fortran90 or C++. The use of negative indices in *Mathematica* indicates access relative to the end of an array.

6.4 When x in $a[[x]]$ is negative, a range check error will be triggered if range checking is turned on using `SetCompilationOptions[CompilerOptions->"/CB"]`. If range check is turned off (default), the result is unpredictable.

Array Constructor Functions

There are two general data constructor functions for creating arrays in *Mathematica*, `Array` and `Table`. There are also a few more specialized array constructors.

- `Array[elemfunc, {dim1,dim2, ...}]`. The `Array` function creates an array object of the specified dimensions, calling the user-supplied *elemfunc* function on the indices of each array element in order to initialize each element. If *elemfunc* is an undefined function symbol, e.g. `f`, symbolic array elements like `f[1,3]` etc. are left in unevaluated form. In the current *MathCode* version *elemfunc* is restricted to constant functions. One common special case for *elemfunc* is `0.0&`, which means that each

element is initialized with the real constant 0.0.

- `Table[expr, {dim1}, {dim2}, ...]`. The `Table` function creates an array object of the specified dimensions, initializing each array element by evaluating the expression `expr`. A more general form is, for example, `Table[expr, {i, imin, imax, istep}, {j, jmin, jmax, jstep}, ...]`, in which `expr` often contains the iterator variables `i` and `j`. The special case `Table[0.0, {dim1}, {dim2}]` creates arrays approximately 10 times faster than the corresponding `Array` call when executed interpretively in *Mathematica*.
- `IdentityMatrix[n]`. This creates a 2D $n \times n$ `Integer` identity matrix of integers, with integer constants 1 along the diagonal and zeros elsewhere.
- `DiagonalMatrix[vec]`. This creates a 2D matrix with elements from the vector `vec` along the diagonal.
- `Range[]`. The `Range` function occurs in three forms. `Range[n]` creates a vector of integer values in the range 1..n, e.g. `Range[2]` gives `{1, 2}`. `Range[start,end]` creates an array (real or integer depending on the start value) of elements starting at `start` with stride 1, e.g. `Range[2.5, 4.5]` gives `{2.5, 3.5, 4.5}`. The three-parameter version `Range[start,end,stride]` also specifies the stride when generating the range, e.g. `Range[2.5, 10, 2]` gives `{2.5, 4.5, 6.5, 8.5}`.

6.4.1 Array Dimension Size Functions

Sizes of array dimensions are obtained by calling the `Dimensions` function in *Mathematica*, which returns a short array of integers giving the sizes of each array. The `Length` function in *Mathematica* returns the number of rows when applied to a matrix. Since arrays are statically typed in C++ and Fortran90, calls like `TensorRank`, `Depth` etc. become compile-time constants in generated code. Using `Dimensions[]` in *Mathematica* is usually the most efficient choice, except for 1-dimensional arrays, where `Length[]` is slightly more efficient.

- *Size of dimension i for an array arr* . The size of dimension i of an array `arr` is usually expressed as `Dimensions[arr][[dim]]` in *Mathematica*. An alternative way is to use `Length`, where, for example, `Length[arr]` gives the size of dimension 1 and `Length[arr][[1]]` gives the size of dimension 2 for a matrix. Thus, `Length[Array[0&, {4, 3}]]` gives 4.

For example, the process for obtaining the size of the second dimension of a 2Dmatrix is compiled to a Fortran90 call `size(t, 1)`. The numbering of dimensions in Fortran90 code is the opposite of numbering in *Mathematica*. Analogously for dimensions up to 4.

- `TensorRank[arr]`. This is equivalent to `Length[Dimensions[arr]]` and returns the number of dimensions of a homogenous array object. Remember that homogenous

6.4 When x in $a[[x]]$ is negative, a range check error will be triggered if range checking is

array objects, i.e. array objects where all elements have the same type, may be compiled to C++ or Fortran90.

- `Depth[arr]`. This is essentially `TensorRank[arr]+1` for homogenous array objects, i.e. the function gives the number of dimensions+1.
- `VectorQ[arr]`. Gives `True` for 1-dimensional arrays.
- `MatrixQ[arr]`. Gives `True` for 2-dimensional arrays.

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Chapter 7 Compilation and Code Generation

MathCode provides a flexible programming interface that controls code generation and execution facilities. This chapter presents this interface in more detail. An easy-to-use subset of these facilities was presented earlier in Chapters 1 and 2. As briefly described in Chapter 1, typed variable declarations and function definitions can either be directly translated into efficient target code (e.g. **Fortran90**), or function bodies can first be symbolically evaluated and then translated during the first phase of the code generation process.

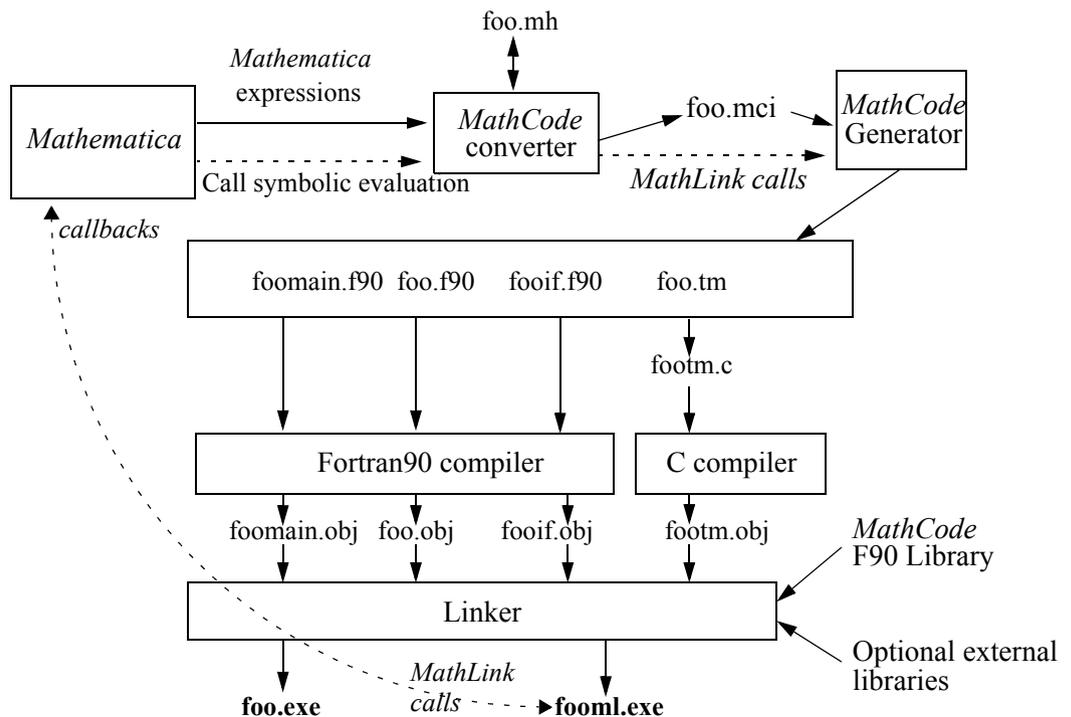


Figure 7.1: Generating **Fortran90** code with *MathCode*, for a package called `foo`.

7.1 Overall System Structure

Compilation and code generation in the *MathCode* context can be described from the perspective of a number of largely orthogonal dimensions. For example, to which *type* of *target code* should the *Mathematica* code be translated? What is the *compilation scope*, i.e. which parts of the *Mathematica* program should be translated? Should the *Mathematica* code be *symbolically evaluated* as the first step of code generation or not? Should the compiled code be *integrated*, i.e. be set up to be transparently callable from *Mathematica*, or should it just be placed in an external file? Others issues concern how to invoke the code generator.

The typical case of generating **Fortran90** code from a *Mathematica* package (e.g. called `f00`), is depicted in Figure 7.1. Some parts of the *MathCode* code generator run within *Mathematica* (*MathCode* converter), but most of it resides in a separate process called via MathLink (*MathCode* generator). This is invisible to the user, for whom the code generator appears to be an ordinary *Mathematica* package.

Partially translated *Mathematica* expressions analyzed by the *MathCode* converter are written to the intermediate form in the file `f00.mci` which is sent over to the external process, *MathCode* generator. Sometimes the *MathCode* generator needs to call back to *Mathematica* to perform symbolic evaluation of expressions. In this case the result of the symbolic evaluation is sent to the *MathCode* generator via Mathlink calls.

The package `f00` is translated to **Fortran90** code in the file `f00.f90`. A MathLink template file `f00.tm`, together with MathLink interfacing code in files `f00if.f90` are also produced. The `mprep` tool from the standard *Mathematica* distribution is used by *MathCode* to generate the file `footm.c` from `f00.tm`. A main program file `foomain.f90` is produced for the case when the user wants to build a stand-alone executable from the generated code. The *MathCode* header file `f00.mh` is a *Mathematica* package file which lists all functions generated by *MathCode* from the package `f00` and as well as types referenced by those function signatures. The compilation options used when the `f00` package was compiled to **Fortran90** are also stored in the file `f00.mh`. The information in the *MathCode* header file is used by `InstallCode`, and in situations when code is generated for packages using typed functions from other packages.

7.2 Compilation and Code Generation Aspects

There are four main aspects of code generation in *MathCode* which are largely orthogonal, i.e. they describe independent properties that can be combined in almost any way.

7.2.1 Target Code Type

The target code option specifies which type of code should be produced by the code generator. The only available choices at this time are C++ and Fortran90, but other options such

as Java, or *Mathematica* byte code might become available in the future.

The code generator produces efficient code in Fortran90 that is often 1000 times faster than interpreted *Mathematica* code, or 100 times faster than internally compiled code.

7.2.2 Evaluation of Symbolic Operations

Many *Mathematica* operations are symbolic in nature, i.e. they produce symbolic *Mathematica* expressions. Examples are symbolic integration and differentiation, simplification, substitution of expressions, etc. Such symbolic operations are not useful to translate to strongly typed languages, e.g. C++ or Fortran90, since this would entail reimplementing a large part of the functionality of a computer algebra system, and would probably not give better performance than the original system.

However, most symbolic operations eventually produce symbolic expressions which are (numerically) computable when symbolic variable names are replaced by data values. This makes it useful to perform all symbolic operations *before* generating the target code, since the result of the symbolic operations in most cases will be executable expressions without symbolic operations. It is of course also possible to partially evaluate expressions with a mixture of symbolic and numeric operations before passing those on to the code generator.

The code generator is informed about which functions should be symbolically evaluated/expanded in conjunction with code generation by setting the `EvaluateFunctions` option, see Section 7.3.2 on page 113.

7.2.3 Integration

The *integration* property determines whether the compiled code will be integrated for direct execution with *Mathematica*, or whether the generated code should simply be stored in an external file. Such *integrated* functions are callable in exactly the same way as internal interpreted *Mathematica* functions.

There are several aspects of code integration:

- *Compiled code integration.* Compiled function definitions can be integrated to be directly callable from *Mathematica*. Alternatively, they are simply linked into an executable for stand-alone execution.
- *External code integration.* Function definitions in external libraries or software modules can be integrated to be callable from *Mathematica* and/or from generated code. This option is not available in the current release of *MathCode F90*.
- *Callbacks.* Some *Mathematica* functions cannot be translated to external code. Such function calls can be evaluated by *callbacks* to *Mathematica*. This option is not available in the current release of *MathCode F90*.

7.3 Invoking the Code Generator

The code generation facilities can be invoked by calling a number of *Mathematica* functions, defined in the *Mathematica* package *MathCode*. Some of these functions are actually just stubs which call corresponding routines in the *MathCode* code generator process via MathLink. Below we describe the available code generation functions. Note that in all *MathCode* functions taking a package argument, the package name can be given with or without backtick (`).

7.3.1 CompilePackage[]—the Primary Code Generation Function

The function `CompilePackage` controls the compilation of entire *Mathematica* packages which contain typed and/or untyped function definitions, variable declarations etc. However, only typed definitions are compiled. Untyped definitions will be ignored.

CompilePackage[*packagename*]

This function generates code for a *Mathematica* package. For example:

```
CompilePackage["mypackage"]
```

It can also be called with the customary backtick:

```
CompilePackage["mypackage`"]
```

Note! The package name `"mypackage`"` (or `"mypackage"`) refers to the context name rather than the package itself. `CompilePackage["mypackage`"]` searches typed variables and function in the context `"mypackage`"`. `CompilePackage["Global`"]` is therefore generating code for all types of variables and functions belonging to the default context `"Global`"`.

If no package name is provided as an argument to `CompilePackage` (or to `BuildCode`, `MakeBinary`), the most recent package name used in calls to these functions is used as default. The initial default is `"Global"`. For example:

```
CompilePackage[]
```

Different Items to be Compiled

`CompilePackage` compiles the different items in the package as follows:

- *Variable declarations*

All typed global variables declared in a *Mathematica* package to be compiled (e.g.

package `foo`) are translated to declarations in **Fortran90**.

- *Functions*

The default is to translate typed *Mathematica* functions into **Fortran90** without any symbolic evaluation. This produces target code similar to the original *Mathematica* code, i.e. loops in *Mathematica* become loops in **Fortran90** etc.

- *Functions with symbolic operations*

Functions which contain symbolic operations such as symbolic integration, substitution etc. should be symbolically expanded (see Section 7.5) before final code generation. Those functions should be indicated using the option `EvaluateFunctions` described in Section 7.3.2 below.

- *Main program function*

In the case that a stand-alone executable is to be created, the option `MainFileAndFunction` described on page 114 can be used to specify the `program` part needed in such an executable.

7.3.2 Optional Parameters to Control Code Generation

There are several optional parameters to `CompilePackage` that provide more detailed control over the code generation process. However, instead of passing such parameters to `CompilePackage` it is usually more convenient to set these options via calls to `SetCompilationOptions` which are placed at the beginning of the package to be compiled.

SetCompilationOptions

Additional information needed to guide the compilation process can be specified using optional parameters to `CompilePackage` and/or `MakeBinary`, or by inserting calls to `SetCompilationOptions` within the package to be compiled. Section 7.4 on page 118 shows the recommended placement of such calls.

Below we briefly examine the available options.

Priority of Parameter Settings

Options passed directly to `CompilePackage` and `MakeBinary` have the highest priority, i.e. they override the settings made via `SetCompilationOptions`. If a compilation option is cleared, any existing individual attribute settings will apply.

Option *EvaluateFunctions*

As mentioned above, `CompilePackage` automatically compiles all typed functions and variables in the package. The default assumption is that those functions should be compiled without symbolic evaluation using `CompileFunction`.

However, side-effect free function bodies which contain symbolic operations (see Section 7.5 on page 119) should be compiled using `CompileEvaluateFunction` instead of `CompileFunction`. The set of functions which should be compiled in this way can be specified using the `EvaluateFunctions` option. For example:

```
CompilePackage["mypackage", EvaluateFunctions->{func1, func2}]
```

or defining `SetCompilationOptions` in the package context:

```
mypackage`SetCompilationOptions[EvaluateFunctions->{func1, func2}]
```

Option *UnCompiledFunctions*

This option prevents some *typed* functions in the package from being compiled. This might be the case for functions which are only meant to be expanded within the body of another symbolically evaluated function. For example:

```
SetCompilationOptions[UnCompiledFunctions->{sin, cos, arcTan}]
```

See Section 2.3.5 on page 42 for an example where this option is used.

Option *DisabledMathLinkFunctions*

This option (used in very rare cases) prevents some typed functions of the package from being called via `MathLink`. By default all functions in the package given as argument to `MakeBinary` can be called by `MathLink` from the *Mathematica* environment. This option might be useful in the case that the installed `MathLink` function confuses *Mathematica*, or if its call template is generated with errors. This is primarily intended as a temporary workaround in case of errors. Example:

```
SetCompilationOptions[DisabledMathLinkFunctions->{foo1, foo2}]
```

Option *MainFileAndFunction*

In the case that a stand-alone executable is to be created, the option `MainFileAndFunction` can be used to specify the `program` part needed in such an executable. The argument string specifies the text of the `program` part in the file `foomain.f90`. (see section 7.6.1 regarding the `StandAloneExecutable` option). For example:

```
SetCompilationOptions[
  MainFileAndFunction->"i = i+1"]
```

or

```
CompilePackage["foo",
  MainFileAndFunction->"i = i+1"]
```

Note that *MathCode* generates the contents of the `foomain.f90` file. The example above will generate the following Fortran90 code:

```
PROGRAM MathCodeStandaloneMain
USE mc_Global
IMPLICIT NONE
i = i+1
END PROGRAM MathCodeStandaloneMain
```

Option *NeedsExternalLibrary*

This option informs about the need for external libraries where called external functions may be defined. This is an option to `SetCompilationOptions` and `MakeBinary`.

```
MakeBinary[NeedsExternalLibrary->{"extlib1", "extlib2"},
  NeedsExternalObjectModule->{"file3"} ]
```

Option *NeedsExternalObjectModule*

This option informs about the need for external modules where called external functions may be defined. This is an option to `SetCompilationOptions` and `MakeBinary`.

```
MakeBinary[NeedsExternalObjectModule->{"file3"} ]
```

Note that an object module `fee.obj` produced by *MathCode* corresponding to a package `fee` that is used (by e.g. calling `Needs["fee"]`) within another package `foo`, is automatically linked into the binaries for `foo` by `MakeBinaries["foo"]`, if `fee.obj` is in the current directory. The option `NeedsExternalObjectModule` is not needed in that case.

Option *MacroRules*

This option specifies a set of rules that are applied to the right-hand side of every function before compilation. Example:

```
SetCompilationOptions[MacroRules->{Sin[x_]/Cos[x_]->Tan[x_]}]
```

The above basically causes the following Mathematica replacement rule to be applied to every function body to yield the code to compile:

```
funcbody /. {Sin[x_]/Cos[x_]->Tan[x_]}
```

Option *DebugFlag*

The option `DebugFlag` (value `True` or `False`) controls whether or not a debugging trace of the code converter is printed. This flag is mainly intended for internal use by the *MathCode* developers.

```
SetCompilationOptions[DebugFlag->True]
```

Option *Language*

The `Language` option (currently only `C++` and `Fortran90` is supported) controls which target language *MathCode* will generate code for. *MathCode* will use the default compiler for the specified language, which is chosen at the installation of *MathCode*. In order to use a certain language, you need a *MathCode* license for that language. Examples of selecting the language:

```
CompilePackage[Language->"Fortran90"]
```

```
CompilePackage[Language->"C++"]
```

The system can reject the request if generating code in the chosen language is not permitted by the license check.

Option *Compiler*

The `Compiler` option makes it possible to select which compiler should be used to compile generated code in a given target language. The option value should be one of the symbolic names (strings) of compilers defined during *MathCode* installation and stored in the `MathCodeConfig.m` configuration file. The `Compiler` option to `MakeBinary` overrides the default compiler specified for the selected language. Example:

```
MakeBinary[Compiler->"df60"]
```

As usual, `BuildCode[]` can be given both `CompilePackage[]` and `MakeBinary[]` options. The following example will generate **Fortran90** code and use the "df60" compiler to compile this code, overriding any default specification:

```
BuildCode[Language->"Fortran90", Compiler->"df60"]
```

Option *CompilerOptions*

`CompilerOptions` is an option to `MakeBinary[]`. `CompilerOptions->"opts"` adds the string `"opts"` to the set of options given to the **Fortran90** compiler. The default value of this option is `""`. The makefile variable `CCOPT` in the makefile is assigned the string `"opts"`. The file `MathCodeConfig.m` contains a string with the name of the makefile used by `MathCode` to produce executable binaries. See also Section 7.6.1 about `MakeBinary` for further information. Example:

```
SetCompilationOptions[CompilerOptions->"/CB"]
```

or

```
MakeBinary["Foo", CompilerOptions->"/CB"]
```

This assigns the string `"/CB"` as the value of the makefile variable `CCOPT`, which subsequently can be used within compilation and linking commands, as seen below:

```
ifort -c Global.f90 /CB
```

The option `/CB` tells the computer to perform range checking for array indexes at runtime

Option *LinkerOptions*

`LinkerOptions` is an option to `MakeBinary[]`. `LinkerOptions->"opts"` adds the string `"opts"` to the set of options given to the linker. The default value of this option is `""`. The makefile variable `LINKOPT` in the actual makefile is assigned the string `"opts"`. See also Section 7.6.1 about `MakeBinary` for further information. An example:

The option `-lm` requests linking with `libm.a` library on Unix systems and for GCC compilers

```
SetCompilationOptions[LinkerOptions->"/MAP"]
```

The option `/MAP` tells to the linker to create a map file

Option *MathCodeMakeFile*

`MathCodeMakeFile` is an option to `MakeBinary[]` that makes it possible to replace the standard makefile with a user specified one. `MathCodeMakeFile->"filename"` specifies the makefile template to be used for building the executables. The file `MakefileConfig.m` contains a string with the name of the makefile used by `MathCode` to produce bina-

ries.

```
MakeBinary["Foo",MathCodeMakeFile->"/home/putte/mymake.mak"]
```

This command results in the use of the makefile `mymake.mak` instead of the default makefile.

7.4 Standard Layout of a Package to be Compiled

Before going into more detail about code generation we present the layout of a typical *Mathematica* package (named by the dummy name `foo`) to be compiled by *MathCode*. All example packages in Chapter 2 have this structure.

The call to `SetCompilationOptions` regarding functions is best placed after the sections for public names and package global names since those names need to be declared first, as in the example package `foo` below. The information about external libraries, on the other hand, can be specified in the same place or closer to the beginning of the package. Note that the object module for `feel.obj` is automatically passed to the linker if the package `feel` has been compiled before.

The typical recommended package layout is as follows:

```
Needs["MathCode`"]

BeginPackage["foo`",{MathCodeContexts,"feel`",...}]
...

(* Public, exported names *)
...

(* Private, package-global names *)
...

(* Possible setting of compilation options for certain functions*)
SetCompilationOptions[EvaluateFunctions->{func1,func2}];
...

(* Private implementation section *)
Begin["`foo`Private"]
...

End[];
EndPackage[];
```

7.5 Code Generation of Symbolically Evaluated Expressions

The following example illustrates code generation for (usually very large) symbolic expressions that are created by *Mathematica* during symbolic evaluation when calling `CompilePackage` with the `EvaluateFunctions` option. Common subexpression elimination is performed on such code in order to break it into pieces and to make it execute more efficiently.

Common Subexpression Elimination

The code generator takes advantage of the fact that pure (i.e. side-effect free) functions like *sin*, *cos*, and *tan* are devoid of side-effects in order to eliminate common subexpressions that the **Fortran90** compiler sometimes cannot optimize since it normally cannot assume that all library functions are side effect free. Note that it is necessary to eliminate all common subexpressions (even if the compiler can handle the ones involving only arithmetic operators) so that we do not miss any opportunities for further optimizations. Temporary variables which hold the results of subexpressions are also introduced. Thus the code generator must derive the type of each subexpression, including the types of intermediate arrays.

Even without the common subexpression elimination, some partitioning of the symbolic expressions would be necessary since the expressions may otherwise become so large that the target language compiler cannot handle them—many compilers have a built-in hard limit on the size of expressions.

A Short Example

As an example, consider the following *Mathematica* function.

```
func[Real a_] -> Real :=
Cos[a+5] * Sin[a]*Sin[a+5] + Sin[a]*Cos[a]*Cos[a]*(a+5);
```

The code generator invoked by

```
CompilePackage[EvaluateFunctions->{func}].
```

The following Fortran90 code is generated:

```
function func(a) result(mc_O1)
use MathCodePrecision
use MathCodeSheep
implicit none
real(mc_real), intent(in) :: a
real(mc_real) mc_O1
real(mc_real) mc_T1
real(mc_real) mc_T2
real(mc_real) mc_T3
```

```
real(mc_real) mc_T4
real(mc_real) mc_T5
real(mc_real) mc_T6
real(mc_real) mc_T7
real(mc_real) mc_T8
real(mc_real) mc_T9
mc_T1 = 5+a
mc_T2 = sin(mc_T1)
mc_T3 = sin(a)
mc_T4 = cos(mc_T1)
mc_T5 = mc_T4*mc_T3*mc_T2
mc_T6 = cos(a)
mc_T7 = mc_T6**2
mc_T8 = mc_T1*mc_T7*mc_T3
mc_T9 = mc_T8+mc_T5
mc_O1 = mc_T9
end function func
```

The only common subexpressions in this example are $5+a$ (stored in `mc_T1` and used three times) and $\text{Sin}[a]$ (stored in `mc_T3` and used twice). For complicated expressions in realistic applications, the common subexpression elimination often reduces the size of the generated code by a factor of ten or more.

Different numerical programs can be generated from the same *Mathematica* program depending on how much information is supplied before generating and compiling the code. If *Mathematica* variables are declared as constants and initialized to constant numerical values before such code generation, symbolic simplification usually results in a more efficient but *less general* program. This can be viewed as a form of *partial evaluation* of the program.

7.6 Building Executables

The building process compiles all produced **Fortran90** files and links them into one (or two) executables. An overview is presented in figure 7.2

Figure 7.2: Building two executables from package `foo`, possibly including numerical libraries.

7.6.1 `MakeBinary["packagename"]`

The call `MakeBinary["foo"]` builds all the files for the stand-alone version of the application (e.g. `foo.exe` if the package is called `foo`), or for the interactively callable MathLink version (e.g. `fooml.exe`). This process includes compiling the generated **Fortran90** source code using an externally available **Fortran90** compiler which should already be installed on the computer being used. See Chapter 9 regarding system specific information about computer platforms and compilers.

If no arguments are supplied to `MakeBinary`, it will assume that all packages translated to **Fortran90** by the most recent calls to `CompilePackage` should be compiled using the external **Fortran90** compiler and linked into a MathLink callable executable (e.g. `fooml.exe`).

Setting Compilation Options for the Fortran90 Compiler

Usually there is no need to use `CompilerOptions->"opts"` to manually specify the options given to the **Fortran90** compiler. The default value of this option is `""`, which is the normal case. An example:

```
MakeBinary["Foo", CompilerOptions->"/CB"]
```

This assigns the string `"/CB"` as the value of the makefile variable `CCOPT`, which subsequently can be used within compilation commands within the makefile. See page 117 for more information.

Controlling Type of Binary Executable

By default, the MathLink version of the binary executable is built by a call such as `MakeBinary[]`. This is equivalent to the call:

```
MakeBinary[StandAloneExecutable->False]
```

However, the following call instead builds a stand-alone executable:

```
MakeBinary[StandAloneExecutable->True]
```

Both versions can be built by two successive calls to `MakeBinary`:

```
MakeBinary[StandAloneExecutable->False]
```

```
MakeBinary[StandAloneExecutable->True]
```

7.6.2 `BuildCode["packagename"]`

The call `BuildCode["foo"]` calls `CompilePackage["foo"]` and then `MakeBinary["foo"]`, i.e. a call to `BuildCode["foo"]` will make a complete code generation, compilation and linking of the *Mathematica* package "foo".

```
BuildCode["foo"]
```

7.7 Integration

As already mentioned, the *integration* property determines if compiled or external code will be integrated for direct execution with *Mathematica*. Such integrated functions are callable in exactly the same way as internal interpreted *Mathematica* functions.

7.7.1 Calling Compiled Generated Code via MathLink

Integrated functions are compiled and linked into an executable, e.g. as `fooml.exe` in Figure 7.3 below, which is connected to *Mathematica* via MathLink.

Generated code to be executed stand-alone, i.e. in a non-integrated fashion, is linked into a stand-alone executable, for example `foo.exe` in Figure 7.3.

Figure 7.3: Integrating generated code from the package `foo` with *Mathematica*. Functions in `fooml.exe` can be called interactively from *Mathematica* via MathLink. The binary file `foo.exe` can be used for non-integrated stand-alone execution.

The following *MathCode* functions control the integration of compiled code with *Mathematica*. It is possible to switch back and forth between executing the compiled versions of *Mathematica* functions and the original interpreted versions by successively calling `ActivateCode[]` and `DeactivateCode[]`. This is useful for testing purposes and performance comparisons. The names of both interpreted and compiled functions are always kept within the original context.

Only the functions within the package specified as an argument to `MakeBinary` or `BuildCode` will be made callable via MathLink. If multiple compiled packages are linked together, functions in other packages are currently not made automatically available via MathLink. The workaround is to insert stub functions into the main package whose only purpose is to call those functions you want to access interactively.

- `InstallCode[]`. Installs compiled code for possible execution from within *Mathematica* through stub functions for calls via MathLink. MathLink stub¹ functions to generated code are stored under `ExternalDownValues`. Each interpreted function definition in the relevant package is moved from `DownValues[funcname]` to `SourceDownValues[funcname]`. Then an `ActivateCode[]`, see below, is performed. Thus, `InstallCode[]` performs the following actions:
 - Reads the *MathCode* header file corresponding to the package, to find the list of functions for which there is external code generated and compiled.
 - Saves interpreted function definitions for the relevant functions under

1. A stub function is an interface function that performs no action of its own apart from possibly re-ordering/re-packaging the function arguments before passing them on to the function that performs the actual work.

SourceDownValues, and clears DownValues for these functions.

- Performs `Mathematica Install[]` if the generated code is callable via MathLink, and saves the stub functions under `ExternalDownValues[]`.
- Saves the MathLink descriptor to the open MathLink connection, so that it can be closed later by `UninstallCode[]`. In the case of compiled bytecode this is not necessary.
- `ActivateCode[]`. When the compiled code is activated, the interpreted function definitions are removed and saved under `SourceDownValues[funcname]` for each function. Instead the compiled function definitions are activated for possible execution by setting `DownValues[f]` to `ExternalDownValues[f]`.
- `DeactivateCode[]`. Deactivates previously installed and activated compiled code, by restoring the interpreted function versions if available, i.e. resetting `DownValues` to `SourceDownValues`.
- `UninstallCode[]`. First perform a `DeactivateCode[]`. Then close possible open MathLink connections and remove MathLink stub functions.

Code Storage Places

Where is compiled Mathematica code stored? We have already seen (Figure 7.1) that generated code in languages like C++ or Fortran90 is placed in external files, which are then further compiled and linked into a binary executable file.

However, internal storage places within *Mathematica* are needed both for storing the original interpreted definitions of compiled *Mathematica* functions, the stub functions needed for possible communication with compiled code via MathLink, and compiled bytecode in case *Mathematica* functions are compiled to bytecode. Information about these storage places is not necessary to know in order to use *MathCode*, but might be of some help for the advanced *Mathematica* programmer.

The following code storage places are employed by *MathCode* within *Mathematica*:

- `DownValues`. The currently active definition rules for a *Mathematica* function *f* are obtained through `DownValues[f]`, or assigned by `DownValues[f]=...`
- `SourceDownValues`. The standard interpreted *Mathematica* source versions of the functions are saved here when the interpreted versions are replaced by stub functions or compiled versions.
- `ExternalDownValues`. Function definitions which are `ExternalCall` expressions calling external executable code via MathLink. `ExternalCall` is a built-in *Mathematica* function used to call external MathLink objects.

7.7.2 Integration of External Libraries and Software Modules

The integration of external software means that external code, available in libraries or object modules and originally implemented in languages like Fortran, C, C++, is integrated with the *Mathematica* execution environment so that functions in the external code can be transparently called from within *Mathematica*. Such code is typically implemented manually and has not been generated by the *MathCode* code generator. See Section 7.7.1 regarding interactive calling via MathLink for functions in other modules than the main module.

7.7.3 Callbacks to *Mathematica*

Currently this option is available in MathCode C++ only

7.8 Providing Missing *Mathematica* Functions

The *MathCode* translator directly supports a set of basic *Mathematica* functions and operations, as defined in Appendix A. There are still a number of standard *Mathematica* functions not yet included in this set.

Standard functions can be re-implemented by hand.

7.8.1 The *system* Package

The user can supply his or her own implementations of missing functions by providing alternative *Mathematica* function implementations in the `system` package. It is intentionally named `system` (lower-case!) to mimic the *Mathematica* `System` context which contains most standard functions. The `system` package is by default translated and, if needed, included in built executables.

The available array slice operators in *MathCode* simplify re-implementation of certain list-operations, which are not directly supported by *MathCode* but are indirectly supported as array slice operators.

The object module `system.obj` (`system.o` under Unix) is included by default when linking executables if the compiled package uses a *Mathematica* function not in the compilable subset of *MathCode* but implemented in the `system` package. However, the intention is to use the `system` for such standard functions which have already been implemented and tested. This is to avoid unnecessary recompilation of already implemented functions while the user is developing implementations of additional functions. At delivery, the *MathCode* system contains a `system` package and a `system` object module containing a number of *Mathematica* functions which have been re-implemented in this way.

The header file `system.h` is automatically included, if needed, in produced **Fortran90**

code so that system functions can be called from generated code. Additionally, the code generator performs the special action of creating *MathCode* header files when compiling `system`. This file, which is always loaded when *MathCode* is started, is called `system.mh`, and contains only typed *Mathematica* external declarations of the compiled functions.

An example of a system package is provided as a `system.nb` notebook file. It currently resides in "`MathCode/lib/stdpackages/src/`". See `UsingSystem.nb` demo which explains how functions from `System.nb` should be used. The contents of this file depend on *MathCode* version, used language (C++ or Fortran) and attached libraries.

7.9 Fortran90 Fortran Code Compilation from Command Shell

Instead of using `MakeBinary[]` call every time, you can also use the standard command shell for compilations.

7.9.1 Command Shell Compilation in Windows using make

`MakeBinary` creates the command script named `packagename.cmd`. The shell command:

```
make -f packagename.cmd
```

invokes the `make` utility, which in turn invokes the **Fortran90** compiler and linker.

7.9.2 Command Shell Compilation in Windows using nmake

The shell command:

```
nmake @packagename.cmd
```

invokes the `nmake` utility, which in turn invokes the **Fortran90** compiler and linker. Either the stand-alone or the `MathLink` version of the executable file is created depending on the setting of the option `StandAloneExecutable`. System requirements are described in the *MathCode* distribution.

7.9.3 Command Shell Compilation in UNIX

`MakeBinary` creates the make file `packagename.unx`. The UNIX command

```
make -f packagename.unx
```

invokes the `make` utility, which in turn invokes the **Fortran90** compiler and linker. Either the stand-alone or the `MathLink` version of the executable file is created depending on the

setting of the `StandAloneExecutable` option. UNIX system requirements are described in the *MathCode* distribution.

Chapter 8 Interfacing to External Libraries

Currently interfacing to external libraries is available in MathCode C++ only.

Chapter 9 System and Installation Information

MathCode F90 is currently available only for Windows.

9.1 Files in the *MathCode* Distribution

The following files and directories should appear within the Mathcode directory after installation:

| File or directory | Explanation |
|--------------------------|---|
| DemosF90 | A directory of notebook files of runnable demo examples. |
| System | A directory of system executable files, both <i>Mathematica</i> .m files and binary files. The binary files are platform dependent. |
| lib | A directory of system libraries necessary for compilation and linking generated code. |
| lib/stdpackages | Pre-compiled packages containing re-implementations of standard <i>Mathematica</i> functions absent in the <i>MathCode</i> library or the standard Fortran90 library. |
| lib/stdpackages/src | Notebook and Fortran90 source code of the <code>system</code> and other packages. |
| Doc | This directory contains the PDF version of the <i>MathCode</i> manual. |
| Doc/ReleaseNotes.nb | Release notes with additional information since this manual was printed. |

9.2 System-specific installation information

Specific information on the installation procedure for each platform is distributed separately with *MathCode*. See special leaflets and the distribution CD, as well as electronically avail-

able information.

9.3 ReadMe Information and Release Notes

ReadMe information and release notes on changes and additions to *MathCode* since this manual was printed are available in the notebook `ReleaseNotes.nb`.

Chapter 10 Trouble Shooting

When using *MathCode* to compile a typed *Mathematica* package, you will occasionally encounter errors in your package, or you might have used commands and constructs not supported by *MathCode*.

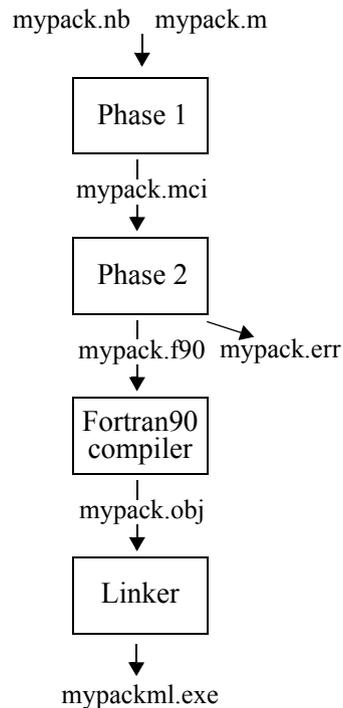


Figure 10.1: Phases of generating **Fortran90** code for a *Mathematica* package `mypack` and compiling into binary code. Object file and executable file extensions are shown according to Windows conventions.

When the compiler finds errors and/or constructs that it cannot understand, certain error messages are reported immediately, whereas other error messages are written out into spe-

`cial.err` and `.clog` files. For example, if you compile a package called `mypack`, and the compilation terminates for some reason, you can look for error messages in both files `mypack.err` and `mypack.clog`.

Before going into more detail about different categories of errors and how to find and correct them, it is useful to gain some insight into the different translation phases of the code generator and their relation to different classes of errors.

10.1 Code Generation Phases

The process of compiling typed *Mathematica* packages to **Fortran90** code and executable binary code consists of several phases, depicted in Figure 10.1. This figure shows an example package `mypack` translated to be executed via a MathLink connection.

The first phase performs a preliminary analysis and transforms some *Mathematica* constructs into combinations of simpler constructs. This phase currently performs almost no type checking, so most type errors will be passed on and reported in the next phase. The emitted *MathCode* intermediate code file `mypack.mci` is in many cases quite close to the original *Mathematica* package.

The second phase performs the bulk of the code generation to **Fortran90**. Type checking needed for code generation is also performed. However, not all static type errors will be detected here—some will be passed on and detected by the **Fortran90** compiler. The emitted code will be stored in `mypack.f90`. Syntax errors in the intermediate file `mypack.mci` are reported in the file `mypack.err`.

Finally, the **Fortran90** compiler will compile `mypack.f90` into object code, which is linked into a binary executable together with possible external library files and object modules. Compilation errors are collected in `mypack.clog`.

It is helpful to perform more error checking in earlier phases to be able to report errors in a form more closely related to the original *Mathematica* program. Still, most error messages are rather easy to understand since both the intermediate file `mypack.mci` and the **Fortran90** file `mypack.f90` are quite recognizable in terms of the original source code.

10.2 Error Categories

Different categories of errors can be detected by *MathCode*, such as errors in the syntactic form of expressions (syntax errors), undeclared functions/variables and type inconsistencies (semantic errors), and missing object code modules when linking object code into a binary executable.

10.2.1 Packaging Errors - Missing Functions

`CompilePackage` should always report the number of functions you expect to compile *plus one*. The extra function `packagenameInit` is an initialization function for global variables, which is always generated even for empty packages.

If this is not the case, some functions are missing. Compile using `DebugFlag->True` and look for a line similar to the following:

```
Found generateFunctions={Hold[faa], Hold[fee], Hold[foo],
Hold[fxx], Hold[ObjfilesInit]}
```

If one of your functions is missing there, you may have forgotten to write the function name after `BeginPackage`. If all of your functions are missing you may have specified the wrong package name somewhere. Package names should always be spelled identically and are case-sensitive.

10.2.2 Syntactic Errors

Most syntax errors are checked immediately by the *Mathematica* parser when reading function or variable definitions. However, typed *Mathematica* is more restrictive than standard untyped *Mathematica*. Also, many “syntax” errors and type errors that would go undetected in *Mathematica* until the erroneous function is executed will be reported by *MathCode* already during code generation.

For example, the function `func2` presented below is a typed *Mathematica* function definition causing syntax errors, since the function argument `n` must have type `MyType` which is not a valid type:

```
func2[MyType n_] -> Integer:= Module[{Integer k}, k = k + 1; k]
```

The presence of syntax errors is reported by `CompilePackage`, e.g. as follows:

```
Ccompiler::MathCode: MathCode:Error messages:
7 lines of messages found. See listing in Global.err . Inter-
mediate code in Global.mci.
```

Detailed error messages from the syntax analysis are stored in the file `Global.err`, (this name depends on your package name) and may appear as follows:

```
6, 18: Error syntax error
6, 18: Information expected tokens:, [ ]
6, 18: Repair token inserted: ]
6, 18: Repair token inserted: ;
```

```
6, 19: Error syntax error
6, 19: Information expected tokens: ; [ :=
6, 22: Information restart point
```

Note that the line number (6) and character number within the line (18) are given with respect to the file Global.mci. This intermediate file is the result of transformations of functions in packages submitted for compilation. These transformations are usually local with respect to the original code. Therefore, the meaning of these somewhat cryptic messages can easily be found by inspecting Global.mci at the indicated line number and character positions.

10.2.3 Semantic Errors

If there are semantic errors during code generation, e.g. type inconsistencies and references to undeclared variables or undeclared functions within a function, this will cause an error message from CompilePackage. If a function is defined as

```
func3[Real n_] -> Integer :=
  Module[{Integer[3] k}, k = p; k]
```

then the messages produced are:

```
Ccompiler::MathCode: MathCode:Error messages:
7 lines of messages found. See listing in Global.erf.
Intermediate code in Global.mci. These errors may cause
Fortran90 compiler messages.
```

```
0, 0: Note In function Global`func3:
0, 0: Error Incompatible types in return statement :
0, 0: Error Assigned to "Output (return) parameter no. 1"
0, 0: Error Of type Integer
0, 0: Error Assigned from k
0, 0: Error Of type Array [ 3 ] of Integer
0, 0: Error Un-defined symbol: p
```

The type inconsistency occurs between the returned expression and the return type of the function.

The variable `p` is used but it is never defined.

10.2.4 Errors During Fortran Compilation and Linking

Sometimes errors occur during the compilation and linking of generated Fortran90 code, which is performed by `MakeBinary[]`. These messages are presented to the user in the following form:

```
Ccompiler::error: Executable file is not produced due to an
error.The following command returned an error: nmake
@Global.cmd > Global.clog. See file Global.clog for more
details.
```

Messages from compiler appear, for example, if the Fortran90 compiler recognizes syntactic or semantic error in the generated code, and can be considered as internal errors of *MathCode* since the system should have performed more complete error checking before emitting erroneous Fortran90 code.

10.2.5 Internal Code Generator Errors

Occasionally internal errors in the *MathCode* code generator may occur, e.g., the executable `om.exe` crashes or stops waiting for a message. In this case you should interrupt evaluation, e.g. via the menu command *Kernel/Quit Kernel* (this stops all processes linked with *Math-link*), and inspect the files `Global.mci` and `Global.err` for error messages.

Such situations can be caused by errors in your *Mathematica* functions, but can be considered internal errors of *MathCode* since the system should have detected and reported such errors without crashing.

10.2.6 Long Compilation Times

In certain situations, using *MathCode* to compile *Mathematica* functions with very large bodies containing numerous array slice operations, e.g. on the order of many thousands of lines, may incur unacceptably long times for code generation. A temporary pragmatic fix for this problem is to divide the large function into several smaller functions and call these functions from the original function.

10.2.7 Internal Errors During Execution of Generated Code

Occasionally internal errors occur in the generated code. This happens when, for instance, an array index in an operation is out of bounds and the *MathCode* array library is used with array-bounds checking turned on.

In the *stand-alone* mode the application issues the message to the “*standard error*” output unit (i.e. shown in the terminal window, like xterm in Unix or Command Prompt window in Windows) including the line number (in the *MathCode* library source code) where the error occurs.

In MathLink mode the "LinkConnect ... is dead" message appears.

In the Unix version (both *stand-alone* and *MathLink* versions) the application also dumps core where the call stack can be analyzed by running `gdb`, `dbx` or any other appropriate debugger.

In the Unix version (*MathLink* mode) a debugging tool (for example, `gdb`) can also be attached to the running process after it has been installed by `InstallCode`. By this means the code can be debugged in its dynamic behavior (note that this may require considerable computer memory and processor time resources).

In the Windows version (*MathLink* mode), if the application is compiled with `/Zi /DEBUG` flags

```
MakeBinary[CompilerOptions->"/Zi", LinkerOptions->"/DEBUG"]
```

It is possible to use the `Tools/Debug Process` option in Microsoft Visual Studio environment. After the process is installed by `InstallCode[]`, it can be debugged. In `Globaltm.c` file it is convenient to set up the break within `_MLDoCallPacket()` function and then follow C++ interface functions and your generated Fortran90 function step by step.

If the answer is never returned to *Mathematica* from a MathLink-mode call, you may suspect an infinite loop in your generated code. If disk access is heavy, you may suspect infinite recursive calls in your generated code.

When modifying and searching for the cause of an error in the generated code it is typically more convenient to use stand-alone mode. Debugging under Unix is generally easier. You should also consider command line compilation under Windows and Unix as described in Section 7.9 on page 126.

10.3 Appendix

Appendix A The Compilable *Mathematica* Subset

This chapter of MathCode User Guide describes the *MathCode F90* release 1.2, September 2007 .

Note that the Compilable Subset varies from one release to another. Please read the Release Notes attached to your *MathCode* installation for the most actual information

The *MathCode* system provides facilities to translate a subset of the *Mathematica* language to compiled programs in strongly typed languages such as C++ or Fortran90. This subset includes most elementary functions and operators that compute numeric values, but excludes symbolic and computer algebra-related functions that compute symbolic expressions.

However, it is possible to evaluate a symbolic expression (which may contain operations such as simplification, symbolic differentiation, substitution etc.) and generate executable numeric code from the symbolic expression resulting from this evaluation, provided that the resulting expression(s) only contain operators and functions in the compilable *Mathematica* subset described here.

The arithmetic model used in the compilable *Mathematica* subset is specified by the IEEE Standard for Binary Floating Point Arithmetic, IEEE Standard 754. Operations on complex numbers are currently not supported, but are planned in the near future.

A.1 Operations not in the Compilable Subset

The following is a short list of those *Mathematica* operations and functions not in the compilable subset. Since the primary reason to generate compiled code is to get high performance of numeric computing code, the operations in the compilable subset are oriented towards efficient computing on numbers and arrays.

- Pattern matching is not supported, except for the simple case of function argument patterns like `arg1_Integer` or `arg2_Real`, which are handled by the static type

system of the target language. However, overloading of functions is not supported by the current version of the code generator, e.g., there may not be two functions with the same name and arguments, one having `Integer` typed arguments and the other having `Real` typed arguments.

- When a function is declared, its arguments must be specified as single-variable names, separated with commas. As an example, node patterns like `Name[a_, b_]` below are not permitted.

```
foo [Real[2] a_, Real c_]->Real[2] := ...      correct
fie [Real[2] Name[a_, b_], Real c_]->Real[2] := ... incorrect
```

- Arbitrary precision numbers and arithmetic are not supported. Numbers and arithmetic operations are converted to either IEEE double precision floating-point arithmetic or 32-bit (or better) integer arithmetic.
- Symbolic operations that give symbolic expressions as results are not included. However, such operations can be compiled if they are expanded to expressions in the compilable subset before code generation. Such expansion can handle many common cases of symbolic operations.
- Negative array indexing, relative to the end of arrays, is not in the compilable subset, String operations are not included. Input/Output operations are not included, apart from a simple `Print` operation.
- Certain list (i.e. array) operations, specifically those that change the size of arrays or are very inefficient, are not included in the set of functions mentioned in this appendix. Such functions can be added by the user e.g. in the `system` module.
- The `Return[]` function is not included. Therefore loop constructs like `For`, `While` cannot be used as expressions returning values.
- Some procedural style statements cannot be used within a `CompoundExpression` used in value context within arithmetic expressions. For instance, `a=a+(While[i<10, i=i+1]; 5)` cannot be translated.

The expression `a=a+(c=3; 5)`, however, can be translated to C++. More details on nested constructs are given below.

A.2 Predefined Functions and Operators

Expression operators listed in this section are predefined by the code generator and will be translated correctly from *Mathematica* into the target language (e.g. C++ or Fortran90) without any additional type declarations.

Almost all operators belong to the *compilable expression subset*, e.g., all value-returning

operators and predefined or user-defined functions without *side effects* (i.e. functions that do not change global variables or perform input/output).

The reason for imposing the condition of calls to side-effect free functions is that expressions can be re-ordered and common subexpressions removed in the generated code, in order to make execution more efficient. Another order in assigning and referencing global variables or performing input/output usually results in different, often unintended, program behavior. However, some restricted cases of side-effects can be re-ordered without changing the meaning of the program. One such case is when the elements of an array are assigned once, independently of each other, and are not used in the same expression. Such restricted side-effects are allowed for functions in the compilable expression subset. The code generator does not check the condition of side-effect freeness—this is the user’s responsibility.

All operators and functions in the compilable expression subset also belong to the compilable subset, which contains control expressions (`If`, `While`, `For`, etc.), assignment statements and functions with side effects. All real and integer constants naturally belong to the compilable expression subset, except for the special case of arbitrary-precision values. Some operators and functions can be applied to arrays or return arrays as values.

The current version of the compilable subset is oriented toward operations on real numbers and integers, and arrays containing such numbers. The basic mathematical functions usually found in C/C++ or Fortran are provided. In *Mathematica* there are also a number of special mathematical functions such as `BesselJ[]`, `Gamma[]`, etc. If the user has access to an implementation of such a function in C/C++ or Fortran, or a linkable object code library containing this function, it can be declared as an external function and thus automatically included in the compilable subset. Since efficient computation based on mathematical models has been the main application of MathCode so far, the compilable *Mathematica* subset does not include string operations, file input, formatted file output and certain mapping and list operations.

A.2.1 Statements and Value Expressions

In standard *Mathematica*, all predefined and user-defined functions can appear as an argument of another function. Accuracy of such constructs is tested during code interpretation.

In procedural languages, such as C++ and Fortran, procedural statements cannot be used within expressions. Also, the type of allowed expressions is restricted.

In order to compile *Mathematica* code to procedural language, some restrictions in using statements and expressions are introduced.

In the descriptions below “*stmt*” means that corresponding *Mathematica* expressions are used as statements. In the compiled subset they do not return values, their returned values cannot be used, and they cannot be applied where values are expected. In the compiled set there is no `Null` value.

In descriptions below “*expr*” means that corresponding *Mathematica* expressions are used as values (l-value or r-value). These expressions must return some value when evaluated. This value cannot be `Null`. The word “*exprs*” means one or more expressions separated by a comma.

Some *Mathematica* constructs - `Set`, `If`, `Which`, `CompoundExpression` - can appear both as statements and as values. Some specific restrictions on their use are described below.

A.2.2 Function Call

| Spec syntax | Operator | Arg type(s) | Result type(s) |
|-------------|-------------------------------------|-------------|----------------|
| | <code>funcname[<i>exprs</i>]</code> | ... | ... |

All user-defined functions which have been *type* declared according to the typing rules for typed *Mathematica* belong to the compilable subset. Compilable subset functions may only contain operations that belong to the compilable subset, or may contain non-subset operations inside bodies of functions compiled with the `EvaluateFunction` option, which will expand into compilable subset operations.

Functions with *multiple* return arguments can be compiled if they are type declared. Such a function can only be used on the right-hand side of an assignment statement in which the left-hand side has to be a list of variables. Thus, a call that returns multiple values can look like this:

```
{a, b, c} = F[x+y, 3.4];
```

Calls to functions with *no return arguments* and functions with *more than one* return arguments are to be considered statements (*stmt*).

Calls to functions returning one argument are considered to be expressions (*expr*).

A.2.3 Function Definition

A function returning values can be defined as follows:

```
function_name[arg_type1 arg1, ..., arg_typen argn]->result_types :=
  expr
```

```
function_name [arg_type1 arg1, ..., arg_typen argn]->
  result_types := Module[variables, expr]
```

```
function_name [arg_type1 arg1, ..., arg_typen argn]->
  result_types := Module[variables, stmt1;stmt2;...;expr]
```

A function that does not return values can be defined as follows:

```
function_name[arg_type1 arg1, ..., arg_typen argn]->Null := stmt
```

```
function_name[arg_type1 arg1, ..., arg_typen argn]->Null :=
  Module[variables, stmt;]
```

```
function_name[arg_type1 arg1, ..., arg_typen argn]->Null :=
  Module[variables, stmt1; stmt2;...;stmtn;]
```

Block or With can be used instead of Module.

A.2.4 Scope Constructs

| Spec syntax | Operator | Arg type(s) | Result type(s) |
|-------------|---------------------------------|-------------|----------------|
| | Module[<i>variables,body</i>] | special | none/(fnbody) |
| | Block[<i>variables, body</i>] | special | none/(fnbody) |
| | With[<i>variables,body</i>] | special | none/(fnbody) |

A value can be returned from one of the above scope constructs when it occurs as a function body or when it is used in a value context within an expression. The *body* is restricted as follows:

- If a function does not return any value, the *body* is a statement. If it is a `CompoundExpression` statement, then all (possibly nested) elements in `CompoundExpression` must be statements.

In the following example two nesting levels of `CompoundExpression` are demonstrated:

```
foo[Real a_]->Null := Module[{ Real t},
  (t=a+1;t=t+1); (t=t+2;t=t+3)]
```

- If a function returns one or more values, the *body* is an expression. If it is a `CompoundExpression` construct, then the last (possibly nested) element in the `CompoundExpression` must be an expression. All other components must be

statements.

In the following example two nesting levels of `CompoundExpression` are demonstrated; note that `t+4` is an expression.

```
foo[Real a_]->Real := Module[{ Real t },
  (t=a+1;t=t+1); (t=t+2;t=t+3;t+4) ]
```

A.2.5 Control Statements

The control statements can appear wherever a statement is allowed, in which case they do not return any value.

| Spec syntax | Operator | Arg type(s) | Result type(s) |
|-------------------|--|-------------|----------------|
| $s_1; s_2; \dots$ | <code>CompoundExpression [stmts]</code> | statements | none |
| | For [<i>start-stmt</i> , <i>boolean-test-expr</i> , <i>incr-stmt</i> , <i>body-stmt</i>] | special | none |
| | While [<i>boolean-test-expr</i> , <i>body-stmt</i>] | special | none |
| | If [<i>boolean-test-expr</i> , <i>true-stmt</i> , <i>false-stmt</i>] | special | none |
| | Which [<i>boolean-test-expr</i> ₁ , <i>stmt</i> ₁ <i>boolean-test-expr</i> ₂ , <i>stmt</i> ₂ ,...]] | special | none |
| | Break [] | - | none |
| | Do [<i>expr</i> , iterators] | special | none |

The `CompoundExpression` (a sequence of expressions separated by semicolons) `Which` and `If` can also appear as an arithmetic expression. See “Arithmetic expression” for details.

A.2.6 Mapping Operations

Map expressions can be compiled in the following cases:

```
var=Map[f, expr]
var=Map[f, expr, {n}]
```

The result must be directly assigned to a variable as shown. The function f can be:

- A function symbol of the compilable subset
- An anonymous function, also called pure function in *Mathematica*
- A user defined typed function for which code has been generated

n must be an integer constant. The `var=Map[...]` statement will be converted to a corresponding assignment statement with a call to `Table` on the right-hand side.

A.2.7 Iterator Expressions

Computing operations in *Mathematica* such as `Do`, `Sum`, `Product` and `Table` use iterators. Additionally there are a number of plotting functions such as `Plot`, `ContourPlot`, `DensityPlot`, `Plot3D` and `ParametricPlot`, which also use iterators but with some limitations in form and usually constructing sets of real values for the purpose of plotting. These plotting functions are not part of the compilable subset.

An iterator can take on one of the following forms:

| Form | Explanation |
|--|--|
| <code>{imax}</code> | iterate <i>imax</i> times |
| <code>{i,imax}</code> | <i>i</i> goes from 1 to <i>imax</i> in steps of 1 |
| <code>{i,imin,imax}</code> | <i>i</i> goes from <i>imin</i> to <i>imax</i> in steps of 1 |
| <code>{i,imin,imax,di}</code> | <i>i</i> goes from <i>imin</i> to <i>imax</i> in steps of <i>di</i> |
| <code>{i,imin,imax},{j,jmin,jmax}</code> | Two iterators: <i>i</i> controls the outer iteration loop, <i>j</i> controls the inner loop |

Iterators in *Mathematica* can use either integer or real values for the iteration variables in the iteration. The compilable subset of iteration functions is limited to integer iteration variables. The iteration variables in *Mathematica* are declared in a local scope consisting of the body (the *expr* below) of the iteration function. Thus, translated code in **Fortran90** needs to declare those iteration variables in a way that does not clash with other local variables. Typically, these iteration constructs will be translated to (nested) `for` loops in the target language.

Iteration functions in *Mathematica* may or may not return a value. The functions `Sum`, `Product`, `Table` and `Range` always return a value from the iteration. Loop-terminating constructs like `Return`, `Break`, `Continue`, or `Throw` can be used inside `Do`. However, `Do` in *Mathematica* does not return a value except in the case of an explicit `Return` of a value.

The compilable subset currently does not support return of a value from a `Do` loop. Another constraint of the compilable subset is that the constructs `Sum`, `Product` and `Table` may currently only occur on the right-hand side of an assignment statement. Concerning `Table`, see also Section A.2.12.

| Spec syntax | Operator | Arg type(s) | Result type(s) |
|-------------|--|--------------|----------------|
| | <code>Do[expr,iter1,iter2,...]</code> | special | none |
| | <code>Sum[expr,iter1,iter2,...]</code> | Real,Integer | Real, Integer |
| | <code>Product[expr,iter1,iter2,...]</code> | Real,Integer | Real, Integer |

| Spec syntax | Operator | Arg type(s) | Result type(s) |
|-------------|--|--------------|----------------|
| | Table[<i>expr</i> , <i>iter1</i> , <i>iter2</i> ,...]] | Real,Integer | Array |

A.2.8 Input/Output Operations

(*Export and Import are new in MathCode 1.4*)

| Operator | Arg type(s) | Result type(s) |
|-----------------------|------------------------------|----------------|
| Print[<i>exprs</i>] | Real, Integer, Array, String | none |

When **Print[]** is performed the output is placed on the standard output stream of the external process where the generated code is executing. For some operating environments (e.g. with MathLink) this stream is not available.

A.2.9 Standard Arithmetic and Logic Expressions

| Spec syntax | Operator | Arg type(s) | Result type(s) |
|-------------|---|--------------------|--------------------|
| == | Equal[<i>e</i> ₁ , <i>e</i> ₂] | Real,Integer,Array | Boolean |
| != | Unequal[<i>e</i> ₁ , <i>e</i> ₂] | Real,Integer,Array | Boolean |
| > | Greater[<i>e</i> ₁ , <i>e</i> ₂] | Real, Integer | Boolean |
| < | Less[<i>e</i> ₁ , <i>e</i> ₂] | Real, Integer | Boolean |
| >= | GreaterEqual[<i>e</i> ₁ , <i>e</i> ₂] | Real, Integer | Boolean |
| <= | LessEqual[<i>e</i> ₁ , <i>e</i> ₂] | Real, Integer | Boolean |
| | Inequality[<i>exprs</i> ...]] | <i>special</i> | Boolean |
| ! | Not[<i>e</i>] | Boolean | Boolean |
| | Or[<i>exprs</i> ...]] | Boolean | Boolean |
| && | And[<i>exprs</i> ...]] | Boolean | Boolean |
| + | Plus[<i>exprs</i> ...]] | Real,Integer,Array | Real,Integer,Array |
| - | Subtract[<i>e</i> ₁ , <i>e</i> ₂] | Real,Integer,Array | Real,Integer,Array |
| - | Minus[<i>exprs</i> ...]] | Real,Integer,Array | Real,Integer,Array |
| * | Times[<i>e</i> ₁ , <i>e</i> ₂] | Real,Integer,Array | Real,Integer,Array |
| / | Divide[<i>e</i> ₁ , <i>e</i> ₂] | Real,Integer,Array | Real, Array |
| | Mod[<i>e</i> ₁ , <i>e</i> ₂] | Real,Integer,Array | Real, Array |
| | Rational[<i>e</i> ₁ , <i>e</i> ₂] | Real,Integer | Real |

| Spec syntax | Operator | Arg type(s) | Result type(s) |
|-------------|---|--|--------------------|
| ^ | Power[e_1, e_2] | Real,Integer,Array | Real,Integer,Array |
| | Abs[e] | Real,Integer,Array | Real,Integer,Array |
| | If[<i>boolean-test-expr</i> , <i>true-expr</i> , <i>false-expr</i>] | 1st arg Boolean; Real,Integer,Array | Real,Integer,Array |
| | Sign[e] | Real,Integer | Integer |
| | Floor[e] | Real,Array | Integer |
| | Ceiling[e] | Real,Array | Integer |
| | Round[e] | Real,Array | Integer |
| | Sqrt[e] | Real,Integer,Array | Real, Array |
| | Exp[e] | Real,Integer,Array | Real, Array |
| | Log[e] | Real,Integer,Array | Real, Array |
| | Sin[e] | Real,Integer,Array | Real, Array |
| | Cos[e] | Real,Integer,Array | Real, Array |
| | Tan[e] | Real,Integer,Array | Real, Array |
| | Cot[e] | Real,Integer,Array | Real, Array |
| | Sec[e] | Real,Integer,Array | Real, Array |
| | Csc[e] | Real,Integer,Array | Real, Array |
| | ArcSin[e] | Real,Integer,Array | Real, Array |
| | ArcCos[e] | Real,Integer,Array | Real, Array |
| | ArcTan[e] | Real,Integer,Array | Real, Array |
| | ArcTan[e_1, e_2] | Real,Integer,Array | Real, Array |
| | ArcSinh[e] | Real,Integer,Array | Real, Array |
| | ArcCosh[e] | Real,Integer,Array | Real, Array |
| | ArcTanh[e] | Real,Integer,Array | Real, Array |
| | ArcCoth[e] | Real,Integer,Array | Real, Array |
| | IntegerPart[e] | Real,Integer,Array | Integer, Array |
| | FractionalPart[e] | Real,Integer,Array | Real,Integer,Array |
| | Quotient[e_1, e_2] | Real,Integer,Array | Integer,Array |
| | Max[m, n] | Real,Integer | Real,Integer |
| | Min[m, n] | Real,Integer | Real,Integer |
| | Max[e] | Array of Real | Real |

| Spec syntax | Operator | Arg type(s) | Result type(s) |
|-------------------------------------|---|-------------------|--------------------|
| | Max[e] | Array of Integer | Integer |
| | Min[e] | Array of Real | Real |
| | Min[e] | Array of Integer | Integer |
| | Outer[e ₁ ,e ₂] | 1D-Array,1D-Array | Array |
| | Cross[e ₁ ,e ₂ ,...,e _n] | Arrays | Array |
| | Transpose[e] | 2D-Array | 2D-Array |
| e ₁ . e ₂ ... | Dot[e ₁ ,e ₂ ,...] | Array | Real,Integer,Array |
| | CompoundExpression[stmt ₁ , ..., stmt _n , expr] | statements | expr |

For functions with two arguments, the following rule applies: one argument can be Array and another argument can be either scalar (of the same type as the base type of the array) or Array of the same dimension. This does not apply to == and !=.

Those functions that return an integer value converted from real: Sign, Floor, Ceiling and Round, give an undefined value or an exception (depending on the underlying target language, e.g. Fortran90) when trying to fit too large a number into an integer.

The following functions are implemented according to *Mathematica* semantics¹:

- IntegerPart returns (int)x for Reals
- FractionalPart returns x-IntegerPart(x)
- Quotient[m,n] returns Floor(m/n) for Reals. Mod[m,n] returns m%n if m and n have the same sign and m%n+n if they have opposite signs. If m or n is a Real then m-n*floor(m/n) is returned.
- The Rational function is part of the compilable subset. It is treated exactly like Divide and converted to Divide during code generation.
- The special purpose Cross function computes the cross product of n-1 vectors of length n and returns a vector of length n. For example, Cross[{2, 3, 4}, {5, 6, 7}] returns the vector {-3, 6, -3} which is orthogonal to the two argument vectors. The function Cross is implemented for n= 3, 4, 5 according to the generalized *Mathematica* definition.

The CompoundExpression construct when used as a value within another statement

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or expression (but not as a function definition) has the following limitation: the statements ($stmt_1, \dots, stmt_n$) allowed within `CompoundExpression` are assignments (`Set`), `Print` or `Put` only.¹ Assignment to list cannot be used there. For instance:

```
a=b+(While[i<10,i=i+1] ; c); (* not allowed *)
a=Foo[{d,f}={3,5} ; c]; (* not allowed *)
a=b+(Print[x];c); (* allowed *)
foo[Real a_]->Real=(i=i-1;(While[i<10,i=i+1] ; c)) // allowed
```

A.2.10 Named Constants

| Spec syntax | Operator | Arg type(s) | Result type(s) |
|-------------|----------|-------------|----------------|
| | True | - | Boolean |
| | False | - | Boolean |
| | E | - | Real |
| | Pi | - | Real |

Variables of type `Boolean` are not supported in the compilable subset. If boolean values are assigned to integer variables, `False` becomes 0, `True` becomes non-zero. Named constants are expressions (*expr*).

A.2.11 Assignment Expressions

| Spec syntax | Operator | Arg type(s) | Result type(s) |
|----------------------|--|-------------|----------------|
| $var := e$ | <code>SetDelayed[<i>var</i>,<i>e</i>]</code> | all types | value |
| $var = expr$ | <code>Set[<i>var</i>,<i>expr</i>]</code> | all types | value |
| $\{vars\} = funcall$ | <code>Set[List[<i>vars</i>],<i>funcall</i>]</code> | - | none |
| $\{vars\} = expr$ | <code>Set[List[<i>vars</i>],<i>expr</i>]</code> | - | none |

The supported main assignment functions, `Set` and `SetDelayed`, have return types. Therefore these can be used both as statements and as expressions.

The arguments (left- and right-hand side of the assignment) must be of compatible types.

Left- and right-hand side arguments are compatible if they can be made into the same type by performing standard type promotion (e.g. promoting integer to real, or a scalar or lower-dimensional array to a higher-dimensional array), provided that this promotion does not change the type of the left-hand side. If it does, then the assignment is illegal. This means

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that an expression of a real type cannot be assigned to a variable of integer type without using explicit conversion of the right-hand side (e.g. using `Floor[]`).

In the case of simultaneous assignment to a list of variables `{vars}`, *funcall* must be a call to a function returning a list of the same length as the list on the left-hand side of the assignment. Also, the *vars* list on the left-hand side may only contain variables.

A.2.12 Array Data Constructors

| Spec syntax | Operator | Arg type(s) | Result type(s) |
|-------------|--|--------------------------|----------------|
| | <code>Array[<i>exprfunc</i>, {<i>dim1</i>, <i>dim2</i>, ...}]</code> | <i>exprfunc</i> constant | Array |
| | <code>Table[<i>expr</i>, {<i>dim1</i>}, {<i>dim2</i>}, ...]</code> | | Array |
| | <code>Table[<i>expr</i>, {<i>i</i>, <i>imin</i>, <i>imax</i>, <i>istep</i>}, {<i>j</i>, <i>jmin</i>, <i>jmax</i>, <i>jstep</i>}, ...]</code> | | Array |
| | <code>IdentityMatrix[<i>n</i>]</code> | Integer | Array (2D) |
| | <code>DiagonalMatrix[<i>vec</i>]</code> | Array (1D) | Array (2D) |
| | <code>Range[<i>n</i>]</code> | Real or Integer | Array (1D) |
| | <code>Range[<i>start</i>, <i>end</i>]</code> | Real or Integer | Array (1D) |
| | <code>Range[<i>start</i>, <i>end</i>, <i>step</i>]</code> | Real or Integer | Array (1D) |

See also section A.2.7 concerning iterator expressions. The following limitations currently apply to compilation of `Array`, `Table`, `IdentityMatrix` and `DiagonalMatrix` calls: the *exprfunc* used by `Array` may only be a constant function; local iteration variables used in iterators to `Table` are automatically created but are always of type `Integer`; calls to `Array`, `Table`, `IdentityMatrix` and `DiagonalMatrix` may only occur on the right-hand side of an assignment statement, for example:

```
arrvariable = Table[3.1+i+j, {i,5}, {j,1,10,2}]
```

A.2.13 Array Data Manipulation

A.2.14 Statistics and sorting functions

The command `Median[]` does not work with Complex numbers in Mathematica.

A.2.15 Array Dimension Functions

| Spec syntax | Operator | Arg type(s) | Result type(s) |
|-------------|---|-------------|----------------|
| | <code>Dimensions[<i>arr</i>][[<i>i</i>]]</code> | Array | Integer |

| | | |
|--------------------------|-------|-------------------|
| Dimensions[<i>arr</i>] | Array | Array of Integers |
| Length[<i>arr</i>] | Array | Integer |

A.2.16 Array Indexing

| Spec syntax | Operator | Arg type(s) | Result type(s) |
|-----------------------------|-------------------------|----------------------------|-----------------------|
| <i>arr</i> [[<i>ind</i>]] | Part[<i>arr,ind</i>] | Integer | Integer,Real,Array |
| | Extract[<i>a1,a2</i>] | Array of Integer constants | Array of Element Type |

Extract[*a, i*] takes an array of rank 1,2,3, or 4 as the first argument and a vector of integers as the second argument. It returns the base element of the first array. If the size of the vector *i* is not equal to the rank of *a* then a runtime error may occur.

The Part construct can be used in both the left and right parts of an assignment. The number of indices should be less than or equal to the rank of the array. For instance, these operations are allowed:

```
Declare[
  Real[3,3,3,3] a4;
  Real[3,3,3] a3;
  Real[3,3] a2;
  Real[3] a1;
  Real x;
  ...
]

a3[1]=a2; a3[2,1]=a1; a3[3,1,2]=5.5;
a2[1]=a1; a2[2,2]=7.7;
a4[2,3,1,2] = 6.6;

x=Extract[a4,{2,3,1,2}]

a4[1,2,3]=a1;a4[1,2]=a2;a4[1]=a3;
```

This operation is not permitted:

```
a1=Extract[a4,{2,3,1}] (* Wrong rank. May cause run time error *)
```

A.2.17 Array Section Operations

| Spec syntax | Operator | Arg type(s) | Result type(s) |
|--|------------------------|-------------|----------------|
| <i>arr</i> [[<u> </u>]] | Part[<i>arr,...</i>] | special | Array |
| <i>arr</i> [[<i>n</i> ₁ <u> </u>]] | Part[<i>arr,...</i>] | special | Array |
| <i>arr</i> [[<i>n</i> ₁ <i>n</i> ₂]] | Part[<i>arr,...</i>] | special | Array |

These are extensions to standard *Mathematica*. See Chapter 3 for more information. These operations are currently supported for up to four dimensions by the code generator and for arbitrary dimensions within *Mathematica* and can be used on both the left- and right-hand sides of assignment statements.

A.2.18 Other Expressions

| Spec syntax | Operator | Arg type(s) | Result type(s) |
|-----------------------|-------------------------------------|-------------|----------------|
| $\{e_1, e_2, \dots\}$ | List[expressions] Apply[f, args] | all types | Array |

List

List is partially implemented when appearing within expressions, for instance when used as an actual parameter to a function. The arguments of List can be:

- Real expressions (creates an Array of Real)
- Integer expressions (creates an Array of Integer)
- Arrays of Real (creates a 2-, 3-, 4-dimensional Array of Real). Can be nested.
- Arrays of Integer (creates a 2-, 3-, 4-dimensional Array of Integer). Can be nested.

List is also implemented when it appears on the left-hand side of an assignment. In this case Part is applied to the right-hand side, and all types should match¹:

```
{a,b,{c,d}}=x (* is the same as
                a=x[[1]];b=x[[2]];c=x[[3,1]];d=x[[3,2]]; *)
```

A runtime error may occur if a matrix appears to be non-rectangular.

These special cases are implemented:

```
variable={expr1, ..., exprn}
```

```
{var1, ..., varn}=expression
```

```
{var1, ..., varn}={expr1, ..., exprn}
```

Apply

The following cases of Apply are implemented:

1. Read Release Notes for more information

- Plus, Power and Times applied to an expression with assignment to a typed variable:

```
var=Apply[Plus, expression]      var = Plus @@ expression
var=Apply[Power, expression]    var = Power @@ expression
var=Apply[Times, expression]    var = Times @@ expression
```

- Apply of typed functions, for example

```
var=Apply[function, expression]  function @@ expression
```

The number of arguments to the function must match the length of the expression.

- Apply of anonymous (pure) functions, for example

```
var=Apply[Sin[#1+#2]&, expression] Sin[#1+#2]& @@ expression
```

The code `Apply[foo, expr]`, equivalent to `foo @@ expr`, will be converted to `foo[expr[[1]], expr[[2]], ...]`. Therefore the behavior will be different from that of *Mathematica* (and hence probably unexpected) if the number of parameters is not the same as the length of the expression `expr`.

It is the user's responsibility to ensure that the number of arguments to the pure function is the same as the length of the expression. The number of arguments is taken as the maximum slot number (for `Function[body]`) or the length of the variable list (for `Function[{vars...}, body]`).

The expression given to `Apply` may be computed many times which may be a performance issue. If the expression is large, it is better to assign the expression to a temporary variable before using `Apply`.

No level specification is supported for `Apply`.

A.2.19 Operators Which May Have Side-effects

| Spec syntax | Operator | Arg type(s) | Result type(s) |
|---|---|-------------|-------------------------|
| <code>var := e</code> | <code>SetDelayed[var, e]</code> | all types | none |
| <code>var = expr</code> | <code>Set[var, expr]</code> | all types | none |
| <code>{vars}=funcall</code> | <code>Set[List[vars], funcall]</code> | special | none |
| | <code>For[start, test, incr, body]</code> | special | none |
| | <code>While[test, body]</code> | special | none |
| | <code>Do[expr, {iter1...}, {iter2...}..]</code> | special | none |
| | <code>If[test, true-expr, false-expr]</code> | special | none/expr |
| | <code>If[test, true-expr]</code> | special | none/expr |
| | <code>Which[test₁, val₁, test₂, val₂, ...]</code> | special | none |
| | <code>Break[]</code> | - | none |
| <code>e₁; e₂; ..</code> | <code>CompoundExpression[exprs]</code> | special | type of last expression |

| | | |
|---------------------------------|---------|---------------------|
| Module[<i>variables,body</i>] | special | none/function value |
| Block[<i>variables, body</i>] | special | none/function value |
| With[<i>variables,body</i>] | special | none/function value |

A.3 Predefined Types

As already mentioned, there are a number of predefined basic types included in the compilable subset of *Mathematica*. There is also a set of predefined types, primarily array types, which are included for convenience.

A.3.1 Basic Types

| Name | Comment |
|---------|---|
| Real | IEEE double precision floating point |
| Integer | 32 bit integer |
| String | 8-bit byte string. May contain '\0' characters. |
| Null | Absence of type |

A.3.2 Array Type Constructors

| Name | Comment |
|-------------------------------|---|
| <i>eltype</i> [dim1,dim2,...] | Here <i>eltype</i> is the array type constructor. |

Maximal rank of arrays is 4 in the current implementation. The base type should be Real or Integer.

A.4 Predefined Constants

The following constants are available within *Mathematica*, and are predefined to the following values with 18 decimal digits within generated C++ or Fortran90 code. A standard double precision floating-point value can hold slightly less than 16 digits of precision.

| Name | Value |
|------|---------------------|
| Pi | 3.14159265358979324 |
| E | 2.718 281 828 46 |

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