MathCode: A System for C++ or Fortran Code Generation from Mathematica

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MathCode is a package that translates a subset of Mathematica into a compiled language like Fortran or C++. The chief goal of the design of MathCode is to add extra performance and portability to the symbolic prototyping capabilities offered by Mathematica. This article discusses several important features of MathCode, such as adding type declarations, examples of functions that can be translated, ways to extend the compilable subset, and generating a stand-alone executable, and presents a few application examples.

Introduction

MathCode is a Mathematica add-on that translates a Mathematica program into C++ or Fortran 90. The subset of Mathematica that MathCode is able to translate involves purely numerical operations, and no symbolic operations. In the following sections we provide a variety of examples that show precisely what we mean. The code that is generated can be called and run from within Mathematica, as if you were running a Mathematica function.

There are two important purposes that are served by MathCode. Firstly, the C++/Fortran 90 code runs faster, typically by a factor of about a few hundreds (or about 50 to 100) over interpreted (compiled) Mathematica code, resulting in considerable performance gains, while still requiring hardly any knowledge of C++/Fortran 90 on the part of the user. Secondly, the generated code can also be executed as a stand-alone program outside Mathematica, offering a portability otherwise not possible. You should note, however, that these advantages come at some loss of generality since integer and floating point overflow are not trapped and switched to arbitrary precision as in standard Mathematica code. Here the user is responsible for ensuring an appropriate choice of scaling and input data to
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There are situations in which having a system such as MathCode can be particularly helpful and effective, like when a certain calculation involves a symbolic phase followed by a numerical one. In such a hybrid situation, Mathematica can be employed for the symbolic part to give a set of expressions involving only numerical operations that can be made part of a Mathematica function, which can then be translated into C++/Fortran 90 using MathCode.

In this article, we describe some of the more important features of MathCode. For a more detailed discussion the reader is referred to [1]. For brevity, we simply say C++ when we actually mean C++ or Fortran 90: MathCode can generate code in both C++ and Fortran, although we illustrate C++ code generation in this article.

In Section 2, we show how to quickly get started with MathCode using a simple example of a function to add integers.

Section 3 presents many useful features of MathCode. In Section 3.1, we discuss the way the system works, the various auxiliary files generated and what to make of them, and how to build C++ code and install the executable. We then compare the execution times of the interpreted Mathematica code and the compiled C++ code. This section also illustrates how MathCode works with packages.

Section 3.2 briefly makes a few points about types and type declarations in MathCode. There are two ways to declare argument types and return types of a function mentioned in this section.

In Section 3.3, we show how to generate a stand-alone C++ executable. This executable can be run outside of Mathematica. We illustrate how to design a suitable main program that the executable runs.

It should be emphasized that MathCode can generate C++ for only that subset of Mathematica functions referred to as the compilable subset. Section 3.4 gives a sample of this subset, while Section 3.5 presents three ways to extend it with the already-available features of MathCode: Sections 3.5.1 through 3.5.3 discuss, respectively, symbolic expansion of function bodies, callbacks to Mathematica, and handling external functions. Each of these extensions has its own strengths and limitations.

Section 3.6 discusses common subexpression elimination, a feature that is aimed at enhancing the efficiency of generated code.

Section 3.7 presents some shortcuts available in MathCode to extract and make assignments to elements of matrices and submatrices, while Section 3.8 is about array declarations.

In Section 4, we present several examples of effectively using MathCode. Section 4.1 provides a summary of the examples.

Section 4.2 discusses an essentially simple example, that of computing the function \( \sin(x+y) \) over a grid in the \( x\)-\( y \) plane, but done in a somewhat roundabout manner so as to illustrate various features of MathCode.

Section 4.3 discusses an implementation of the Gaussian elimination algorithm [2] to solve matrix systems of the type \( A.X = B \), where \( A \) is a square matrix of size \( n \) and \( X \) (the solution vector) and \( B \) are vectors of size \( n \). In this section, we make a detailed performance study by computing the solution of a matrix...
system by turning on a few compilation options available in *MathCode*, and also make comparisons with *LinearSolve*.

In Section 4.4, we show how to call external libraries and object files from a C++ program that is automatically generated by *MathCode*. We take the example of a well-known matrix library called SuperLU [3], and demonstrate how to solve, using one of its object modules, a sparse matrix system arising from a partial differential equation.

The *MathCode* User Guide that is available online discusses more advanced aspects, like a detailed account of types and declarations, the numerous options available in *MathCode* with the aid of which the user can control code generation and compilation, and other features. We refer interested readers to [1].

In Section 5, we summarize the salient aspects of *MathCode* and discuss the kinds of applications for which *MathCode* is particularly useful. We conclude the article with a brief summary of various points made. The first version of *MathCode*, released in 1998, was partly developed from the code generator in the Object-Math environment [4, 5]. The current version is almost completely rewritten and very much improved.

### 2. Getting Started with *MathCode*

#### 2.1. An Example Function

In this section we take the reader on a quick tour of *MathCode* using the simple example of a function to add integers.

The following command loads *MathCode*.

```
In[1]:= Needs["MathCode"]
```

```
MathCode C++ 1.4.0 for mingw32 loaded from C:\MathCode
```

*MathCode* works by generating a set of files in the current directory (see Section 3.1). We can set the directory in the standard way as follows; here, $MCRoot$ is the *MathCode* root directory. The user can, however, use any other directory to store the files.

```
In[2]:= SetDirectory[MCRoot <> "/Demos/SimplestExample"];
```

Let us now define a *Mathematica* function sumint to add the first $n$ natural numbers.

```
In[3]:= sumint[n_] :=
   Module[{res = 0, i}, For[i = 1, i <= n, i++, res = res + i]; res]
```

Note that the body of this function has purely numerical operations, like incrementing the loop index $i$, adding two numbers, and assigning the result to a variable.
2.2. Declaration of Types

We must now declare the data types of the parameter \( n \) and the local variables \( res \) and \( i \); we must also specify the return type of the function. We do this using the function `Declare` that `MathCode` provides.

\[
\text{In[4]:=} \quad \text{Declare[sumint[Integer n_] \to \text{Integer}, \{\text{Integer, Integer}\}];}
\]

Note that `Integer n_` does not mean `Integer*n_`; the function `Declare` creates an environment in which this is interpreted as a type declaration, that is, an integer variable \( n \) is being declared in the example. The type `Integer` is translated to a native C `int` type, and the type `Real` to a native C `double` type.

2.3. C++ Code

To generate and compile the C++ code, we execute the following command.

\[
\text{In[5]:=} \quad \text{BuildCode["Global"];}
\]

Successful compilation to C++: 1 function(s)

Since we have not specified the context of `sumint`, its default context is `Global`. We could, therefore, have simply executed the following command instead.

\[
\text{In[6]:=} \quad \text{BuildCode[];}
\]

Successful compilation to C++: 1 function(s)

With the following command, we seamlessly integrate an external program with `Mathematica`.

\[
\text{In[7]:=} \quad \text{InstallCode[];}
\]

Global is installed.

We can now run the external program in the same way that we would execute a `Mathematica` command.

\[
\text{In[8]:=} \quad \text{sumint[1000]}
\]

\[
\text{Out[8]=} \quad 500 \ 500
\]

If we want to run the `Mathematica` code (and not the generated C++ code) for `sumint`, we must first uninstall the C++ executable.

\[
\text{In[9]:=} \quad \text{UninstallCode[];}
\]

Now the `Mathematica` code for `sumint` will run.

\[
\text{In[10]:=} \quad \text{sumint[1000]}
\]

\[
\text{Out[10]=} \quad 500 \ 500
\]
3. A Tour of MathCode

3.1. How the MathCode System Works

MathCode works by generating a set of files in the home directory. In the example of `sumint`, the default context is `Global` and the files generated by MathCode are: `Global.cc` (the C++ source file), `Global.h` and `Global.mh` (the header files), `Globaltm.c`, `Global.tm` and `Globalif.cc` (the MathLink-related files that enable transparently calling C++ versions of the function `sumint` from Mathematica), and `Globalmain.cc`, which contains the function `main()` needed when building a stand-alone executable.

We can also create a package (let us call it `foo`) that defines its own context `foo` instead of the default context `Global`. See Figure 1 for a block diagram of the way the overall system works. The MathCode code generator translates the Mathematica package to a corresponding C++ source file `foo.cc`. Additional files are automatically generated: the header file `foo.h`, the MathCode header file `foo.mh`, the MathLink-related files `footm.c`, `foo.tm`, `foo.icc`, and `fooif.cc`, which enable calling the C++ versions from Mathematica, and `foomain.cc`, which contains the function `main` that is needed when building a stand-alone executable for `foo` (see Section 3.3). The generated file `foo.cc` created from the package `foo`, the header file `foo.h`, and additional files are compiled and linked into two executables. In the case of MathCode F90, Fortran 90 is generated and a file `foo.f90` is created. No header file is generated in that case since Fortran 90 provides directives for the use of module. External numerical libraries may be included in the linking process by specifying their inclusion (Sections 3.5.3 and 4.5). The executable produced, `foo.exe`, can be used for stand-alone execution, whereas `fooml.exe` is used when calling on the compiled C++ functions from Mathematica via MathLink.

Let us see how to work with a package again using the same `sumint` example.

```
In[1]:= Needs["MathCode"];
MathCode C++ 1.4.0 for mingw32 loaded from C:\MathCode

In[2]:= SetDirectory["$MCRoot <> "/Demos/SimplestExample"];
```
If we are compiling the package foo using MathCode, we also need to mention MathCodeContexts within the path of the package.

```
In[3]:= BeginPackage["foo", {MathCodeContexts}];
```

We define the function sumint

```
In[4]:= sumint[n_] :=
    Module[{res = 0, i}, For[i = 1, i \[LessEqual] n, i++, res = res + i]; res];
```

and close the context foo.

```
In[5]:= EndPackage[];
```

We next declare the types, and then build and install as before.

```
In[6]:= Declare[sumint[Integer x_] \rightarrow Integer, {Integer, Integer}];
In[7]:= BuildCode["foo"];
```

Successful compilation to C++: 1 function(s)

Again, since the package foo has been defined, it is the default context, and so we could simply have executed the following command.

```
In[8]:= BuildCode[];
```

Successful compilation to C++: 1 function(s)

To run the executable from the notebook, we must install it.

```
In[9]:= InstallCode[];
```

foo is installed.

Now the following command runs the C++ executable fooml.exe. The call to sumint via MathLink is executed 1000 times. The timing measurement includes MathLink overhead, which typically for small functions is much more than the execution time for the compiled function. This can be avoided if the loop is executed within the external function itself, as in the example in Section 4.2.5.

```
In[10]:= Timing[Do[res = sumint[1000], {1000}]; res]
```

```
Out[10]= {1.392, 500500}
```
Here is the C++ code that was generated.

```cpp
#include "foo.h"
#include "foo.icc"
#include <math.h>
void foo_TfooInit ()
{
;
}

int foo_Tsumint ( const int &n)
{
  int res = 0;
  int i;
  i = 1;
  while (i <= n)
  {
    res = res+i;
  i = i+1;
  }
  return res;
}
```

Note that the function `sumint` appears as `foo_Tsumint` in the generated code. This is because the full name of the function is in fact `foo`sumint, and `MathCode` replaces the backquote `""` by `"_T"` in the C++ code.

To run the `Mathematica` function (and not its C++ equivalent) `sumint`, we must use the following command to uninstall the C++ code.

```mathematica
In[12]:= UninstallCode[];
```

Now it is the `Mathematica` code that runs when you execute `sumint`.

```mathematica
In[13]:= Timing[Do[res = sumint[1000], {1000}]; res]
```

```
Out[13] = {22.161, 500 500}
```

You can see that the C++ executable together with the `MathLink` overhead runs about 15 times faster than the `Mathematica` code. The factor by which the performance is enhanced is problem dependent, however. The performance of the `Mathematica` code could also have been improved by using the built-in `Compile` function. In Section 4 we will see many more examples, some quite involved, where we get a range of performance enhancements, also including usage of the `Compile` function.

We clean up the current directory by removing the files automatically generated by `MathCode`.

```mathematica
In[14]:= CleanMathCodeFiles[Confirm -> False, CleanAllBut -> {}];
```
3.2. Types and Declarations

To be able to generate efficient code, the types of function arguments and return values must be specified, as we have seen in the preceding examples. The basic types used by MathCode are

\{Real, Integer, Null\}

Arrays (vectors and matrices) of these types can also be declared.

\{Real[5], Real[3, 4], Real[_], Integer[m, n], Integer[2, 3, n_]\}

Type declarations can be given in two different ways:

- Directly in the function definition
  \[ f[\text{Real \_}] \rightarrow \text{Real} := x^2 \]

- In a separate command
  \[ g[\text{\_}] := \text{Sin}[\text{x}] \]
  \[ \text{Declare}[g[\text{Real \_}] \rightarrow \text{Real}] \]

The latter construction can be useful if you want to separate already existing Mathematica code with the type information needed to be able to generate C++ code using MathCode.

3.3. Generating a Stand-Alone Program

So far we have only seen examples in which the installed C++ code can be run within Mathematica. However, we can also produce a stand-alone executable. This offers a degree of portability that can be useful in practice.

To illustrate, we take the same example function \texttt{sumint} that we discussed in the previous sections. The sequence of commands is very much as in the previous section, except for the option \texttt{StandAloneExecutable \rightarrow True} for the MathCode function \texttt{MakeBinary}, and an appropriate option \texttt{MainFileAndFunction} for the function \texttt{SetCompilationOptions} immediately after \texttt{BeginPackage}. Figure 2 illustrates the process of building the two kinds of executable, namely fooml.exe (on some systems foomain.exe) from a package called \texttt{foo}.

\begin{verbatim}
in[15]:= Needs["MathCode\"];
in[16]:= SetDirectory[$MCRoot <> "/Demos/SimplestExample"];
in[17]:= BeginPackage["foo", \{MathCodeContexts\}];
\end{verbatim}

The option \texttt{MainFileAndFunction} is used to specify the main file. The functions defined in Mathematica must have the prefix \texttt{Global_T} (\texttt{packagename_T} in general) to be recognized in the main file.
Figure 2. Building two executables from the package foo, possibly including numerical libraries.

```
In[18]:= SetCompilationOptions[
   MainFileAndFunction -> "#include <stdio.h>
   int main()
   {int n;printf("give an integer:");scanf("%d",\n   );printf("the
   sum is %d.\n",foo_Tsumint(n));return 0;}
   
   ];

In[19]:= sumint[n_] := Module[{res = 0, i}, For[i = 1, i <= n, i++ , res = res + i]; res];

In[20]:= EndPackage[];

In[21]:= Declare[sumint[Integer x_] -> Integer, {Integer, Integer}];

Now we are ready to generate and compile the C++ code for the package foo. We can do this in two ways: we can either employ the MathCode function BuildCode, as in the previous examples, or first execute CompilePackage (which generates the C++ source and header files) and then the function MakeBinary (which creates the executable).

In[22]:= CompilePackage["foo"];

Successful compilation to C++: 1 function(s)

In[23]:= MakeBinary["foo", StandAloneExecutable -> True];

The last command generates the stand-alone executable foo.exe that can be executed from a command line, or, alternatively, by using the Mathematica function Run.

In[24]:= Run["foo.exe"]

Out[24]= 0

If you desire, you can, in addition to the stand-alone executable foo.exe, also generate fooml.exe that can be run from within Mathematica, just like before.

In[25]:= MakeBinary["foo"];"
foo is installed.

Now the following command runs the C++ program foo.cc.

\begin{verbatim}
in[27]:= sumint[1000]
\end{verbatim}

\textbf{3.3.1. Generating a DLL}

Here we briefly mention the possibility of generating a DLL, without giving a full example. To generate a DLL from a package, you have to write a file containing one simple wrapper function in order to make a generated function visible outside the DLL. You write a wrapper function for each generated function. The flags used are as follows:

\begin{verbatim}
CompilePackage[NeedsExternalObjectModule \rightarrow "ext"];
MakeBinary[StandaloneExecutable \rightarrow True, LinkerOptions \rightarrow "/DLL"]
\end{verbatim}

Here "ext.cpp" is a C++ file with wrapper functions, and "/DLL" is a flag for the Visual C++ linker. For other C++ compilers this procedure is not automatic and requires several operating system commands, but the wrapper functions are not needed.

\section*{3.4. The Compilable Subset}

\textit{MathCode} generates C++ code for a subset of \textit{Mathematica} functions, called the \textit{compilable subset}. The following items give a sample of the compilable subset. For a complete list of \textit{Mathematica} functions in the compilable subset, see [1].

- Statically typed functions, where the types of function arguments and return values are given by the types discussed in Section 3.2
- Scoping constructs: \texttt{BeginPackage[ ], EndPackage[ ], Module[ ], Block[ ], With[ ]}
- Procedural constructs: \texttt{For[ ], While[ ], If[ ], Which[ ], Do[ ]}
- Lists and tables: \texttt{List[ ], Table[ ], Array[ ], Range[ ], Identity[ ], Matrix[ ]}
- Size functions: \texttt{Dimensions[ ], Length[ ]}
- Arithmetic and logical expressions, for example: +, -, *, /, ==, !=, >, <, &&, ||, and so forth
- Elementary functions and some others, for example: \texttt{Sin[ ], Exp[ ], ArcSin[ ], Sqrt[ ], Round[ ], Max[ ], Cross[ ], Transpose[ ], Dot[ ]}
- Constants: True, False, E, Pi
- Assignments: :=, =
Functional commands: Map[], Apply[]

Some special commands: Sum[], Product[]

Functions not in the compilable subset can be used in external code by callbacks to Mathematica (see Section 3.5.2 for an example).

Examples of functions that are not a part of the compilable subset include: Integrate[], Solve[], FindRoot[], LinearSolve[], Expand[], Factor[].

These functions can be used if Mathematica can evaluate them at compile time to expressions that belong to the compilable subset. In general, Mathematica functions that perform symbolic operations are not in the compilable subset. Also, many functions in the subset are implemented with limitations, that is, more difficult cases are not always supported. However, MathCode currently provides several ways to extend the compilable subset, as we discuss in the next section.

3.5 Ways to Extend the Compilable Subset

3.5.1. Symbolic Expansion of Function Bodies

Functions not entirely written using Mathematica code in the compilable subset, but whose definitions can be evaluated symbolically to expressions that belong to the compilable subset, can be handled by MathCode.

\[ f[a_\_, b_\_] \rightarrow \text{Real} := \text{Integrate}[x \sin x, \{x, a, b\}] \]

Generate C++ code and compile it to an executable file.

\[ \text{Integrate}[x \sin x, \{x, a, b\}] \]

\[ a \cos[a] - b \cos[b] - \sin[a] + \sin[b] \]
The generated executable is connected to *Mathematica*:

```
In[8]:= InstallCode[];
Global is installed.
```

```
In[9]:= f[1., 2.]
Out[9]= 1.44042
```

### 3.5.2. Callbacks to Mathematica

Consider the following function whose definition includes the Zeta function, which does not belong to the compilable subset.

```
In[1]:= Needs["MathCode"]
```

```
MathCode C++ 1.4.0 for mingw32 loaded from C:\MathCode
```

```
In[2]:= SetDirectory[$MCRoot <> "\Demos\SimplestExample"]
Out[2]= C:\MathCode\Demos\SimplestExample
```

```
In[3]:= f[x_] := Sin[x] Cos[x] e^{-x^2} Zeta[x]
```

Let us plot the function:

```
In[4]:= Plot[f[x], {x, 2, 4}, PlotRange -> All]
```

![Plot of the function](image)

We now make the declarations:

```
In[5]:= Declare[f[Real x_] -> Real]
In[6]:= Declare[Zeta[Real x_] -> Real]
```

These declare statements do not change the way *Mathematica* computes the function.

```
In[7]:= {f[2.5], f[5/2]}
Out[7]= {-0.000796932, \[
\cos\left(\frac{5}{2}\right) \sin\left(\frac{5}{2}\right) \zeta\left(\frac{5}{2}\right) \]
\[e^{25/4} \left(1 + \tan\left(\frac{5}{2}\right)^2\right)\]}
```
Let us now generate C++ code and compile it to an executable file. The option `CallBackFunctions` tells `MathCode` which functions have to be evaluated by `Mathematica`. As a result, although the function `Zeta` is not in the compilable subset, an executable is still generated and communicates with the kernel to evaluate `Zeta`.

```mathematica
In[8]= BuildCode[CallBackFunctions -> {Zeta}]
```

Successful compilation to C++: 2 function(s)

The generated executable is connected to `Mathematica`:

```mathematica
In[9]= InstallCode[];
```

Global is installed.

Now it is the external code that is used to compute the function:

```mathematica
In[10]= {f[2.5], f[5/2]}
```

```mathematica
Out[10]= {-0.000796932, f[5/2]}
```

In this case the external code calls `Mathematica` when the `Zeta` function has to be evaluated. After the evaluation the computation proceeds in the external code.

Note that it is the installed code for the function `f` that is executed above, and not the original `Mathematica` function. In the installed code, the argument of `f` must be real, according to our declaration. As a result, `f[5/2]`, in which we pass a rational number as an argument, is left unevaluated.

We again plot the function, but this time using the external code to evaluate it:

```mathematica
In[11]= Plot[f[x], {x, 2, 4}, PlotRange -> All]
```

3.5.3. External Functions

We can have references to external objects in C++ code generated by `MathCode`. Let us consider three very simple external functions that compute $x^2$, $e^x$, and $\sin(x)$ to illustrate the idea. These must be defined as follows in an external source file that must be in the working directory.
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```
In[1]:= Needs["MathCode"]

MathCode C++ 1.4.0 for mingw32 loaded from C:\MathCode

In[2]:= SetDirectory[$MCRoot <> "/Demos/Overview"];

In[3]:= FilePrint["external1.cc"]

#include <math.h>
extern double extsqr(const double &x) {
    return x*x;
}
extern double extexp(const double &x) {
    return exp(x);
}
extern double extoscillation(const double &x) {
    return sin(x);
}

Observe here that each function definition, which is in C language syntax, is followed by a “wrapper” that enables MathCode to recognize the object as external. We can then create an object file corresponding to these functions and link the object as follows.

```
In[4]:= extsqr[Real x_] -> Real := ExternalFunction[];
    extexp[Real x_] -> Real := ExternalFunction[];
    extoscillation[Real x_] -> Real := ExternalFunction[];

We define a function to create a list of numbers using the external functions.

```
In[7]:= Makeplot[Integer n_] -> Real[n] := Module[{Integer i, Real[_] arr},
    arr = Table[extsqr[extoscillation[0.1 i]],
    extexp[-extsqr[0.03 i]], {i, n}]; arr]

We now compile the package. Since this is a very small example, we do not bother to create a special package for the code.

```
In[8]:= CompilePackage[]

Successful compilation to C++: 4 function(s)

Let us now create the MathLink binary; to do this when there are external functions, we must specify the option NeedsExternalObjectModule as follows.

```
In[9]:= MakeBinary[NeedsExternalObjectModule -> {"external1"]

Here, as we noted above, external1 and external2 represent the external object modules external1.o and external2.o. Install the MathCode-compiled code so it is called using MathLink.
```
When we make the following plot, it is the external code for extsqr, extexp, and extoscillation that is used.

\begin{align*}
\text{In[11]}:= \text{ListPlot[Makeplot[100], Joined → True]} \\
\text{Out[11]}=
\end{align*}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{plot.png}
\caption{Plot of extsqr, extexp, and extoscillation}
\end{figure}

\section{3.6. Common Subexpression Elimination}
Consider the following function whose definition contains a number of common subexpressions (e.g., $1 + x^2$ and $\sqrt{1 + x^2}$).

\begin{align*}
\text{In[1]}:= \text{Needs["MathCode"]}; \\
\text{MathCode C++ 1.4.0 for mingw32 loaded from C:\MathCode}
\end{align*}

\begin{align*}
\text{In[2]}:= g[\text{Real } x_\_] \rightarrow \text{Real} := \\
\frac{x \cos[x] \cos[\sqrt{1 + x^2}]}{(1 + x^2)^{3/2} (1 + \cos[x]^2)} - \frac{2 x \cos[x] \sin[\sqrt{1 + x^2}]}{(1 + x^2)^2 (1 + \cos[x]^2)} + \\
\frac{2 \cos[x]^2 \sin[x] \sin[\sqrt{1 + x^2}]}{(1 + x^2) (1 + \cos[x]^2)^2} - \frac{\sin[x] \sin[\sqrt{1 + x^2}]}{(1 + x^2) (1 + \cos[x]^2)}
\end{align*}

There are very efficient algorithms to evaluate functions containing common subexpressions. The basic idea is to evaluate common subexpressions only once and put the results in temporary variables.

Now we generate C++ code using MathCode and run it.

\begin{align*}
\text{In[3]}:= \text{BuildCode[]} \\
\text{Successful compilation to C++: 1 function(s)}
\end{align*}

\begin{align*}
\text{In[4]}:= \text{InstallCode[]} \\
\text{Global is installed.}
\end{align*}
MathCode does common subexpression elimination (CSE) when the option EvaluateFunctions is given to CompileCode[] or BuildCode[]. This basic strategy could be further improved for special cases in future versions of MathCode. Moreover, since mathematical expressions are intrinsically free of side effects and do not have a specific evaluation order, the CSE optimization may change the order of computing subexpressions if this improves performance. Changing the order can sometimes have a small influence on the result when floating-point arithmetic is used.

We take a look at the generated C++ file.

```c++
#include "Global.h"
#include "Global.icc"

#include <math.h>
void Global_TGlobalInit ()
{
    ;
}

double Global_Tg ( const double &x)
{
    double mc_T1;
    double mc_T2;
    double mc_T3;
    double mc_T4;
    double mc_T5;
    double mc_T6;
    double mc_T7;
    double mc_T8;
    double mc_T9;
    double mc_T10;
    double mc_T11;
    
    mc_T1 = (x*x);
    mc_T2 = 1+mc_T1;
    mc_T3 = cos(x);
    mc_T4 = (mc_T3*mc_T3);
    mc_T5 = 1+mc_T4;
    mc_T6 = mc_T5*mc_T2;
    mc_T7 =                        0.5;
    mc_T8 = pow(mc_T2, mc_T7);
    mc_T9 = sin(mc_T8);
    mc_T10 = sin(x);
    mc_T11 = mc_T10*mc_T9;
    mc_T12 = mc_T11/mc_T6;
    mc_T13 = -mc_T12;
    mc_T14 = pow(mc_T5, -2);
    mc_T15 = 2*mc_T4*mc_T14*mc_T10*mc_T9;
    mc_T16 = mc_T15/mc_T2;
    mc_T17 = pow(mc_T2, -2);
    mc_T18 = -2*x*mc_T17*mc_T3*mc_T9;
    mc_T19 = mc_T18/mc_T5;
    mc_T20 = cos(mc_T8);
    mc_T21 =                       -1.5;
    mc_T22 = pow(mc_T2, mc_T21);
    mc_T23 = x*mc_T22*mc_T3*mc_T20;
    mc_T24 = mc_T23/mc_T5;
    mc_T25 = mc_T24+mc_T19+mc_T16+mc_T13;
    return mc_T25;
}
```c
void Global_TGlobalInit()
{
    double mc_T1;
    double mc_T2;
    double mc_T3;
    double mc_T4;
    double mc_T5;
    double mc_T6;
    double mc_T7;
    double mc_T8;
    double mc_T9;
    double mc_T10;
    double mc_T11;
    double mc_T12;
    double mc_T13;
    double mc_T14;
    double mc_T15;
    double mc_T16;
    double mc_T17;
    double mc_T18;
    double mc_T19;
    double mc_T20;
    double mc_T21;
    double mc_T22;
    double mc_T23;
    double mc_T24;
    double mc_T25;
    mc_T1 = (x*x);
    mc_T2 = 1+mc_T1;
    mc_T3 = cos(x);
    mc_T4 = (mc_T3*mc_T3);
    mc_T5 = 1+mc_T4;
    mc_T6 = mc_T5*mc_T2;
    mc_T7 = 0.5;
    mc_T8 = pow(mc_T2, mc_T7);
    mc_T9 = sin(mc_T8);
    mc_T10 = sin(x);
    mc_T11 = mc_T10*mc_T9;
    mc_T12 = mc_T11/mc_T6;
    mc_T13 = -mc_T12;
    mc_T14 = pow(mc_T5, -2);
    mc_T15 = 2*mc_T4*mc_T14*mc_T10*mc_T9;
    mc_T16 = mc_T15/mc_T2;
    mc_T17 = pow(mc_T2, -2);
    mc_T18 = -2*x*mc_T17*mc_T3*mc_T9;
    mc_T19 = mc_T18/mc_T5;
    mc_T20 = cos(mc_T8);
    mc_T21 = -1.5;
    mc_T22 = pow(mc_T2, mc_T21);
    mc_T23 = x*mc_T22*mc_T3*mc_T20;
    mc_T24 = mc_T23/mc_T5;
    mc_T25 = mc_T24+mc_T19+mc_T20+mc_T13;
    return mc_T25;
}
```

Note how the computation of the function has been divided into small subexpressions that are evaluated only once and then stored in temporary variables for future use. This gives very efficient code for large functions. The speed enhancement of roughly 150% brought about by CSE in this example is not appreciable because the example itself is rather small.

### 3.7. Extended Matrix Operations

When dealing with matrices, it is very convenient to have a short notation for part extraction. *MathCode* extends the functionality of `Part[ ]` or `[[ ]]` to achieve this.
Consider the following $4 \times 5$ matrix:

\begin{verbatim}
In[12]:= A = Table[a[i, j], {i, 1, 4}, {j, 5}]; A // MatrixForm
\end{verbatim}

\begin{verbatim}
Out[12]//MatrixForm=
\begin{pmatrix}
a[1,1] & a[1,2] & a[1,3] & a[1,4] & a[1,5] \\
\end{pmatrix}
\end{verbatim}

We can extract rows 2 to 4 as follows, with the shorthand available in MathCode.

\begin{verbatim}
In[13]:= A[[2, 4]] // MatrixForm
\end{verbatim}

\begin{verbatim}
Out[13]//MatrixForm=
\begin{pmatrix}
\end{pmatrix}
\end{verbatim}

We can extract the elements in all rows that belong to column 3 and higher:

\begin{verbatim}
In[14]:= A[_, 3 ;;] // MatrixForm
\end{verbatim}

\begin{verbatim}
Out[14]//MatrixForm=
\begin{pmatrix}
a[1,3] & a[1,4] & a[1,5] \\
\end{pmatrix}
\end{verbatim}

We can assign values to a submatrix of A.

\begin{verbatim}
In[15]:= A[[2, 3], 2 ;;] = {{1, 2}, {3, 4}};

In[16]:= A // MatrixForm
\end{verbatim}

\begin{verbatim}
Out[16]//MatrixForm=
\begin{pmatrix}
a[1,1] & a[1,2] & a[1,3] & a[1,4] & a[1,5] \\
\end{pmatrix}
\end{verbatim}

All these operations belong to the compilable subset and can result in compact code. Note: A[[2|4]] denotes the same Mathematica computation as Take[A, {2, 4}, All], and A[[_, 3|_]] is equivalent to Take[A, All, {3,-1}].

### 3.8. Array Declaration and Dimension

In this subsection, we give a few examples of array declarations. There are two main cases to consider.

- Arrays that are passed as function parameters or returned as function values, where the actual array size has been previously allocated
- Declaration of array variables, usually specifying both the type and the allocation of the declared array
There are five allowed ways to specify array dimension sizes in array types for function arguments and results.

- Integer constant dimension sizes, for example: `Real[3,4]`
- Symbolic-constant dimension sizes, for example: `Real[three, four]`
- Unknown dimension sizes with unnamed placeholders, for example: `Real[_ ,_]`
- Unknown dimension sizes with named placeholders, for example: `Real[n_, m_]`
- Unknown dimension sizes with variables as dimension sizes, for example: `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 arrays that are passed as arguments to functions have already been allocated at runtime. Thus, their sizes are already determined. These sizes might, however, be different for different calls. Therefore it is not allowed to specify conflicting dimension sizes through integer variables (e.g., `Real[n, m]`) in array types of function parameters or results, as can be done for ordinary declared variables. Only constants and named, or unnamed, placeholders are allowed.

We now give examples of the five different ways of specifying array dimension information in variable declarations. The examples show a global variable declaration using `Declare`, but the same kinds of declarations 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 using the array `arr`:
  ```mathematica
  Declare[Real[3, 4] arr];
  ```
- Symbolic constant dimension sizes:
  ```mathematica
  Declare[Real[three, four] arr];
  ```
- Unknown dimension sizes with unnamed placeholders:
  ```mathematica
  Declare[Real[_ ,_] arr];
  ```
- Unknown dimension sizes with named placeholders:
  ```mathematica
  Declare[Real[k_, m_] arr];
  ```
- Unknown dimension sizes that are specified and fixed to the values of integer variables, for example, `n, m` (e.g., function parameters, local or global variables that are visible from the declaration):
  ```mathematica
  Declare[Real[n, m] arr];
  ```
Integer variables, such as \( n \) and \( m \), are assumed to be assigned once; that is, 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. Thus, the user is responsible for maintaining such consistency.

### 4. Application Examples

#### 4.1. Summary of Examples

In the following we present a few complete application examples using MathCode. The first example application is a small Mathematica program called SinSurface (Section 4.2), which has been designed to illustrate two basic modes of the code generator: compiling without symbolic evaluation (the default mode, in which the function body is translated into C++ as it is), and compilation preceded by symbolic expansion, which is indicated by setting the option `EvaluateFunctions`\( \rightarrow \)True (the function body is expanded using symbolic operations, simplified, and then translated).

The second example, presented in Section 4.3, is an implementation of the Gaussian elimination procedure to solve a linear algebraic system of equations (see any standard text on numerical techniques for a discussion of the procedure, e.g., [2]). Here we compile generated C++ code with various options and do a detailed performance analysis.

In Section 4.4, we discuss the example of SuperLU, an external library [3] that performs efficient sparse matrix operations. We give an example of a program useful in solving partial differential equations that calls the SuperLU library and some of its object modules to solve a matrix equation of the type \( A \cdot X = B \), where \( A \) is a very sparse square matrix.

#### 4.2. The SinSurface Application Example

Here we describe the SinSurface program example. The actual computation is performed by the functions `calcPlot`, `sinFun2`, and their helper functions. The two functions `calcPlot` and `sinFun2` in the SinSurface package will be translated into C++ and are declared together with a global array `xyMatrix`.

The array `xyMatrix` represents a \( 21 \times 21 \) grid on which the numerical function `sinFun2` will be computed. The function `calcPlot` accepts five arguments: four of these are coordinates describing a square in the \( x \)-\( y \) plane and one is a counter (`iter`) to make the function repeat the computation as many times as necessary in order to measure execution time. For each point on a \( 21 \times 21 \) grid, the numeric function `sinFun2` is called to compute a value that is stored as an element in the matrix representing the grid.

##### 4.2.1. Introduction

The SinSurface example application computes a function (here `sinFun2`) over a two-dimensional grid. The function values are stored in the matrix `xyMatrix`. The execution of compiled C++ code for the function `sinFun2` is over 500 times faster than evaluating the same function interpretively within Mathematica.
The function \( \text{sinFun2} \) computes essentially the same values as \( \sin(x + y) \), but in a more complicated way, using a rather large expression obtained through converting the arguments into polar coordinates (through \( \text{ArcTan} \)) and then using a series expansion of both \( \sin \) and \( \cos \), up to 10 terms. The resulting large symbolic expression (more than a page) becomes the body of \( \text{sinFun2} \), and is then used as input to \( \text{CompileEvaluateFunction} \) to generate efficient C++ code. The symbolic expression and the call to \( \text{CompileEvaluateFunction} \) is initiated by using the \( \text{EvaluateFunctions} \) option.

### 4.2.2. Initialization

We first set the directory in which \( \text{MathCode} \) will store the auxiliary files, the C++ code, and executable, and then load \( \text{MathCode} \).

\[
\text{In[1]:=} \quad \text{Needs["MathCode"]}
\]

MathCode C++ 1.4.0 for mingw32 loaded from C:\MathCode

\[
\text{In[2]:=} \quad \text{SetDirectory[\$MCRoot <> "/test"]};
\]

The \( \text{SinSurface} \) package starts in the usual way with a \( \text{BeginPackage} \) declaration that references other packages. \( \text{MathCodeContexts} \) is needed in order to call the code generation related functions.

\[
\text{In[3]:=} \quad \text{BeginPackage["SinSurface", \{MathCodeContexts\}]};
\]

\[
\text{Clear["SinSurface\#"]};
\]

Next we define possibly exported symbols. Even though it is not necessary here, we enclose these names within \( \text{Begin["SinSurface"]} \) ... \( \text{End[ ]} \) as a kind of context bracket, since this can be put into a cell, which can be conveniently re-evaluated by itself if new names are added to the list.

\[
\text{In[5]:=} \quad \text{Begin["SinSurface"]}
\]

\[
\text{xyMatrix;}
\]

\[
\text{calcPlot;}
\]

\[
\text{sinFun1;}
\]

\[
\text{sinFun2;}
\]

\[
\text{arcTan;}
\]

\[
\text{sin;}
\]

\[
\text{cos;}
\]

\[
\text{plot;}
\]

\[
\text{cplus;}
\]

\[
\text{plotfile;}
\]

\[
\text{End[]}
\]

\[
\text{Out[5]= \text{SinSurface'}
\]

Now we set compilation options as follows. This defines how the functions and variables in the package should be compiled to C++. By default, all typed variables and functions are compiled. However, the compilation process can be controlled in a more detailed way by giving compilation options to \( \text{Compile\'} \). \( \text{Package} \) or via \( \text{SetCompilationOptions} \). For example, in this package the function \( \text{sinFun2} \) should be symbolically evaluated before being translated to code, because it contains symbolic operations; the functions \( \sin \), \( \cos \), and \( \text{arcTan} \)...
should not be compiled at all, because they are expanded within the body of sinFun2. The remaining typed function, calcPlot, will be compiled in the normal way.

```
In[6]:= SetCompilationOptions[
   EvaluateFunctions -> {sinFun2},
   UnCompiledFunctions -> {sin, cos, arcTan},
   MainFileAndFunction -> "int main() {return 0;"}];
```

### 4.2.3. The Body of the SinSurface Package

We begin 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.

```
In[7]:= Begin["SinSurface`Private"];
```

Declare public global variables and private package-global variables:

```
In[8]:= Declare[Real[21, 21] xyMatrix];
```

Taylor-expanded sin and cos functions called by sinFun2 are now defined, just for the sake of the example, even though such a series gives lower relative accuracy close to zero. A substitution of the symbol z for the actual parameter x is necessary to force the series expansion before replacing with the actual parameter.

```
In[9]:= sin[Real[x_]] \rightarrow Real := Normal[Series[Sin[z], {z, 0, 10}]] /. z \rightarrow x;
   cos[Real[x_]] \rightarrow Real := Normal[Series[Cos[z], {z, 0, 10}]] /. z \rightarrow x;
```

Define arcTan, which converts a grid point to an angle, called by sinFun2:

```
In[11]:= arcTan[Real[x_], Real[y_]] \rightarrow Real :=
   If[x < 0, \pi, 0] + If[x == 0, \frac{1}{2} Sign[y] \pi, ArcTan[y/x]]; 
```

sinFun2 is the function to be computed and plotted, called by calcPlot. It provides a computationally heavy (series expansion) and complicated way of calculating an approximation to \(\sin(x + y)\). 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 about two 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 be symbolically expanded before translation.

Note also that a function should be without side effects in order to be symbolically expanded before final code generation. For example, there should be no assignments to global variables or input/output, since the relative order of these actions when executing the code often changes when the symbolic expression is created and later rearranged and optimized by the code generator.
The function calcPlot calculates data for a plot of \( \sinFun2 \) over a \( 21 \times 21 \) grid, which is returned as a \( 21 \times 21 \) array.

\[
\begin{align*}
\text{calcPlot}[\text{Real } \text{xmin}_-, \text{Real } \text{xmax}_-, \text{Real } \text{ymin}_-, \text{Real } \text{ymax}_-, \text{Integer } \text{iter}_-] & \to \text{Real}[21, 21] := \\
\text{Module}[(\text{Integer } n = 20, \text{Real } \{x, y\}, \text{Integer } \{i, j, \text{count}\}), \\
\text{For}[\text{count} = 1, \text{count} \leq \text{iter}, \text{count} = \text{count} + 1, \\
\text{For}[i = 1, i \leq n + 1, i = i + 1, \\
\text{For}[j = 1, j \leq n + 1, j = j + 1, \\
x = \text{xmin} + \frac{(\text{xmax} - \text{xmin}) (i - 1)}{n}; \\
y = \text{ymin} + \frac{(\text{ymax} - \text{ymin}) (j - 1)}{n}; \\
\text{xyMatrix}[[i, j]] = \sinFun2[x, y]]; \\
\text{xyMatrix}]
\end{align*}
\]

### 4.2.4. Execution

We first execute the application interpretively within *Mathematica*, and then use `Compile` on the key function and execute the application again. Then we compile the application to C++, build an executable, and call the same functions from *Mathematica* via MathLink.

Let us first do the *Mathematica* evaluation and plot.

\[
\begin{align*}
\text{meval} & = \text{Timing}[\text{plot} = \text{calcPlot}[-2., 2., -2., 2., 20]][[1]] / 20 \\
\text{Out[16]} & = 0.1305
\end{align*}
\]
In[17]:= ListPlot3D[plot]

Out[17]=

Next, we redefine \texttt{sinFun2} to become a compiled version, using \textit{Mathematica}'s standard \texttt{Compile}.

\begin{verbatim}
In[18]:= sinFun2 = Compile[{x, y}, Evaluate[sinFun2[x, y]]];
In[19]:= compeval = Timing[plot = calcPlot[-2., 2., -2., 2., 100];]
Out[19]= {7.109, Null}
In[20]:= compeval = compeval[[1]] / 100
Out[20]= 0.07109
In[21]:= sinFun2 =.
\end{verbatim}

4.2.5. \textbf{Using the MathCode Code Generator}

Compile the \texttt{SinSurface} package.

\begin{verbatim}
In[22]:= CompilePackage["SinSurface"]
\end{verbatim}

\begin{quote}
\texttt{MathCodeConv\_defConv::untypedlocalvars: Warning: Untyped local variable(s): (SinSurface\_Private\_r, SinSurface\_Private\_xx, SinSurface\_Private\_yy) in function with head sinFun2\_[SinSurface\_Private\_x, SinSurface\_Private\_y]. Real type(s) assumed}

\text{Successful compilation to C++: 2 function(s)}
\end{quote}

The warnings concern local variables in \texttt{sinFun2} that have no type information. This is not important because those variables disappear upon symbolic expansion.

The command \texttt{MakeBinary} compiles the generated code using a compiler (g++ in the present case). The object code is by default linked into the executable \texttt{SinSurface\_ml.exe} for calling the compiled code via \textit{MathLink}.

\begin{verbatim}
In[23]:= MakeBinary[];
\end{verbatim}

If any problems are encountered during code compilation, then warning and error messages are shown. Otherwise no messages are shown. When \texttt{Make\_Binary} is called without arguments, the call applies to the current package.
The command `InstallCode` installs and connects the external process containing the compiled and linked `SinSurface` code.

```
In[24]:= InstallCode["SinSurface"]
SinSurface is installed.
```

Execute the generated C++ code for `calcPlot`.

```
In[25]:= AbsoluteTiming[plot = calcPlot[-2.0, 2.0, -2.0, 2.0, 3000];]
Out[25]= {3.6408347, Null}
```

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

```
In[26]:= externeval = %[[1]]/3000
Out[26]= 0.0012136116
```

Check that the result appears graphically the same.

```
In[27]:= ListPlot3D[plot]
```

### 4.2.6. Performance Comparison

Let us now compare the running times for the three cases, the standard Mathematica, compiled Mathematica, and the generated C++ code.

```
In[28]:= {meval / externeval, compeval / externeval}
Out[28]= {107.53, 58.5772}
```

The performance between the three forms of execution are compared in Table 1. The generated C++ code for this example is roughly 100 times faster than standard interpreted Mathematica code, and 50 times faster than code compiled by the internal Mathematica Compile command. This is on a Toshiba Satellite-2100, 400 Mhz AMD-K6, running Windows XP Pro SP2 and Mathematica 6, without inline and norange optimization. If the inline is specified,
The performance between the three forms of execution are compared in Table 1.

- The inline directive is passed to the C++ compiler for all functions to be compiled. If norange is specified, array element index range checking is turned off in the code generated by the C++ compiler, resulting in faster but less safe code.

We should emphasize that the comparisons in Table 1 are rather crude for several reasons. From a separate measurement, the loop part of calcPlot excluding the call to sinFun2 comprises 25% of the total calcPlot time executed in interpreted Mathematica. The calcPlot function itself cannot be compiled using Compile, since it contains an assignment to a global matrix variable that cannot currently be handled by Compile. This might be regarded as unfair to Compile. On the other hand, a MathLink overhead (divided by 500) in returning the $21 \times 21$ matrix is embedded in the figure for MathCode, which can be regarded as unfair to MathCode. A better comparison for another small application example is available in Section 4.3.6.

```
in[29]:= TableForm[{
  {"Execution Form", "Time consumed", "Relative"},
  {"Standard Mathematica", meval, meval / externaleval},
  {"Compile[]", compeval, compeval / externaleval},
  {"External C++ via MathLink", externaleval, 1}}]
```

```
Out[29]//TableForm =

<table>
<thead>
<tr>
<th>Execution Form</th>
<th>Time consumed</th>
<th>Relative</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard Mathematica</td>
<td>0.1305</td>
<td>107.53</td>
</tr>
<tr>
<td>Compile[]</td>
<td>0.07109</td>
<td>58.5772</td>
</tr>
<tr>
<td>External C++ via MathLink</td>
<td>0.0012136116</td>
<td>1</td>
</tr>
</tbody>
</table>
```

Table 1. Approximate performance comparison for the calcPlot example.

### 4.3. Gauss Application Example

#### 4.3.1. Introduction

In this section, we present a textbook algorithm, Gaussian elimination (e.g., [2]), to solve a linear equation system. The given linear system, represented by a matrix equation of the type $A.X = B$, is subjected to a sequence of transformations involving a pivot, resulting in the solution to the system, contained in the matrix $X$.

The following subsections illustrate the various aspects of the application.

#### 4.3.2. Initialization

```
in[1]:= Needs["MathCode"]
```

```
MathCode C++ 1.4.0 for mingw32 loaded from C:\MathCode
```

```
in[2]:= SetDirectory[$MCRoot <> $PathnameSeparator <> "Demos" <> $PathnameSeparator <> "Gauss"];
```

```
in[3]:= BeginPackage["Gauss", {MathCodeContexts}];
```
Define exported symbols:

\begin{verbatim}
In[4]:= Begin["Gauss"];
GaussSolveArraySlice;
End[];
\end{verbatim}

4.3.3. Body of the Package

We now define the function GaussSolveArraySlice, based on the Gaussian elimination algorithm.

\begin{verbatim}
In[7]:= Begin["Private"];
GaussSolveArraySlice[Real[n_, m_] ain_, Real[n_, m_] bin_,
   Integer iterations_] :=
Module[{Real[n] dumc, Real[n, n] a, Real[n, m] b,
   Integer[n] {ipiv, indx, indcx}, Integer {i, k, l, irow, icol},
   Real {pivinv, amax, tmp}, Integer {beficol, afticol, count}]
For[count = 1, count \leq iterations, count = count + 1, (a = ain;
   b = bin;
   For[k = 1, k \leq n, k = k + 1, ipiv[[k]] = 0];
   For[i = 1, i \leq n, i = i + 1,
     (*find the matrix element with largest absolute value*)
     amax = 0.0;
     For[k = 1, k \leq n, k = k + 1,
       If[ipiv[[k]] == 0,
         For[l = 1, l \leq 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, "*** Gauss2 input data error ***" >> ";
     Break];
   (*if irow \neq icol,
   then interchange rows irow and icol in both a and b*)
   If[irow \neq icol, For[k = 1, k \leq n, k = k + 1, tmp = a[[irow, k]];
     a[[irow, k]] = a[[icol, k]]; a[[icol, k]] = tmp];
   For[k = 1, k \leq m, k = k + 1, tmp = b[[irow, k]];
     b[[irow, k]] = b[[icol, k]]; b[[icol, k]] = tmp];
   indx[[i]] = irow;
   indxc[[i]] = icol;
   If[a[[icol, icol]] == 0,
     Print["*** Gauss2 input data error 2 ***"];
     Break];
   (*prepare to divide by the
   pivot and subsequent row transformations*)
   pivinv = 1.0 / a[[icol, icol]];
   a[[icol, icol]] = 1.0;
\end{verbatim}
In[10]:= 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, indx[[l]]]];
a[[k, indx[[l]]]] = tmp]]
];
b];
End[];
EndPackage[];

This function accepts three arguments in an attempt to solve a matrix equation of the form $A.X = B$. The first two arguments are essentially the matrices $A$ and $B$. The third argument specifies the number of times the body of the function must run; this is useful for an accurate measurement of the running time. The function output ($X$) has the same shape as the second argument ($B$).

4.3.4. Mathematica Execution
Let us create two random matrices.

\[
\begin{align*}
\text{In}[10]:= & \quad a = \text{RandomReal}[\{0, 1\}, \{10, 10\}] ; \\
& \quad b = \text{RandomReal}[\{0, 1\}, \{10, 2\}] ; \\
\end{align*}
\]

In the following, loops factor specifies the number of times the body of GaussSolveArraySlice runs. The appropriate value of loops for reliable estimates of running time is system dependent. A reasonable value of factor for a 1.5 GHz computer is about 10. The output checks that the solution obtained is correct.
\begin{verbatim}
In[12]:= factor = 30; loops = 2 factor;
s = Timing[c = GaussSolveArraySlice[a, b, loops];];
meval = s[[1]] / loops;
Print["TIMING FOR NON-COMPiled VERSION= ", meval];
MatrixForm[a.c - b]
\end{verbatim}

\begin{verbatim}
Out[16]//MatrixForm=
\begin{pmatrix}
0. & 0. \\
-1.33227 \times 10^{-15} & 0. \\
2.22045 \times 10^{-16} & -1.11022 \times 10^{-16} \\
6.66134 \times 10^{-16} & -2.22045 \times 10^{-16} \\
2.22045 \times 10^{-15} & -3.33067 \times 10^{-16} \\
2.22045 \times 10^{-16} & -1.249 \times 10^{-16} \\
-2.22045 \times 10^{-15} & 5.55112 \times 10^{-17} \\
1.77636 \times 10^{-15} & -1.11022 \times 10^{-16} \\
-2.66454 \times 10^{-15} & 0. \\
-1.77636 \times 10^{-15} & -1.66533 \times 10^{-16} \\
\end{pmatrix}

4.3.5. Generating and Running the C++ Code

The command BuildCode translates the package and produces an executable.

\begin{verbatim}
In[17]:= BuildCode["Gauss"]
\end{verbatim}

Successful compilation to C++: 1 function(s)

Interpreted versions are removed, and compiled ones are used instead.

\begin{verbatim}
In[18]:= InstallCode["Gauss"]
\end{verbatim}

Gauss is installed.

\begin{verbatim}
Out[18]= LinkObject["\.
Gaussml.exe", 14, 7]
\end{verbatim}

\begin{verbatim}
In[19]:= c = GaussSolveArraySlice[a, b, 1];
\end{verbatim}

We now make two runs of the C++ code for the package Gauss. The first run evaluates the body of GaussSolveArraySlice \texttt{loops} times, and returns the solution only once. The second run evaluates the body of GaussSolveArraySlice only once, but does this inside a Do-loop for \texttt{loops} times, returning the solution \texttt{loops} times as a result. Clearly, there is overhead in the second run, and the time taken is expected to be higher, as can be seen from the following.
\textbf{4.3.6. Performance Comparison}

We present the performance analysis in Table 2. As we observe from the table, a performance enhancement by a factor of approximately 500 can be obtained for the compiled C++ code over interpreted \textit{Mathematica}. More importantly, we are able to get a performance close to \textit{LinearSolve}, although we have implemented a simple version of a Gaussian elimination algorithm directly from a textbook as straight-line code without any attempts at tuning or optimization. Also note that \textit{LinearSolve} is more general in that it can also handle sparse arrays efficiently using the \textit{SuperLU} package linked into the \textit{Mathematica} kernel. To achieve similar generality with the \textit{MathCode} package, the example would need to be extended and a \textit{SuperLU} routine, for example, called as an external function from the generated code. In general, it is better to use already implemented robust and reliable routines from packages like \textit{LAPACK} and \textit{SuperLU}, which also can be called as external functions from \textit{MathCode}-generated code. The Gauss example in this article is not intended to replace such routines but to be a simple example of using \textit{MathCode}. 
\[4.4. \text{External Libraries and Functions}\]

We now demonstrate how to call external functions and libraries using MathCode. We have already presented an example of how to do this for three very simple functions, \(x\), \(\exp(x)\), and \(\sin(x)\), in Section 3.5.3. In this section we present a more realistic application example that illustrates how to employ an external library for handling sparse matrix systems that arise in the solution of partial differential equations [6].

We take as our example the problem of solving the one-dimensional diffusion equation using the method of finite differences.

\[
\frac{\partial u(x, t)}{\partial t} = \frac{\partial^2 u(x, t)}{\partial x^2}
\]

In this method, the continuous \(x\) domain is approximated by a set of discrete points called a grid, and each derivative is replaced by a certain linear function of values of the dependent variables, called a finite difference. For the previous equation, a variant of this method gives

\[
\frac{u(x, t + 1) - u(x, t)}{k} = \frac{u(x - 1, t) - 2u(x, t) + u(x + 1, t)}{h^2},
\]

where now \(x\) and \(t\) are assumed to take integer values, and \(k\) and \(h\) are step sizes along \(x\) and \(t\) directions, respectively. The algebraic equation must be solved at each grid point, thus resulting in a simultaneous system of equations, which is essentially a matrix system of the form \(A.X = B\). Since the matrix system in this case is very sparse, we solve it using the sparse matrix library called SuperLU [3].

The rest of this section assumes that the SuperLU library has been compiled. We now explain how to call the external objects based on this library using MathCode.

Here is the Mathematica code to solve the one-dimensional diffusion equation.

```mathematica
SolveDiffusion1D[Nx_, dt_, nnz_, xasize_, U_] :=
  Module[{k, x, dx, kt, rhsmat, colmat, rowmat, valmat, amat, asubmat, xamat},
    (*initialize variables and arrays*)
    kt = 0; dx = 1/(Nx - 1); rhsmat = Table[0., {Nx}];
    colmat = Table[0, {nnz}]; rowmat = Table[0, {nnz}];
    valmat = Table[1., {nnz}]; amat = Table[1., {nnz}];
    asubmat = Table[0, {nnz}]; xamat = Table[0, {xasize}];
    (*define the matrices*)
    For[x = 1, x < 2, x = 1 + x, rhsmat[[x]] = 0.; (++kt; colmat[[kt]] = x);
      rowmat[[kt]] = x; valmat[[kt]] = 1];
    For[x = 2, x < Nx, x = 1 + x,
      rhsmat[[x]] = U[[x]]/dt + (U[[1 + x]] - 2 U[[x]] + U[[1 + x]])/dx^2;
      (++kt; colmat[[kt]] = x; rowmat[[kt]] = x; valmat[[kt]] = 1/dt)];
    For[x = Nx, x < 1 + Nx, x = 1 + x, rhsmat[[x]] = 0.;
      (++kt; colmat[[kt]] = x; rowmat[[kt]] = x; valmat[[kt]] = 1)];
    (*transform the matrices into SuperLU format*)
    kt = 0; Do[Do[If[colmat[[k1]] == k, ++kt; amat[[kt]] = valmat[[k1]];
        asubmat[[kt]] = -1 + rowmat[[k1]], {k1, 1, nnz}], {k, 1, Nx}];
      kt = 0; Do[Do[If[colmat[[k1]] == k, ++kt], {k1, 1, nnz}],
        {k, 1, Nx}];
      xamat[[1 + k]] = kt, {k, 1, Nx}];
    (*call SuperLU-based function to solve the matrix system A.x=B*)
    linsolvepp[Nx, Nx, nnz, 1, amat, asubmat, xamat, rhsmat]
  ]
```
Note that this source file is somewhat different from the one in Section 3.5.3, mainly because arrays are involved here. This wrapper function makes a reference to a C function linsolve() that is defined in the following source file.
void linsolve(int m, int n, int nnz, int nrhs, double *a, int *asub, int *xa, double *rhs)
{
    SuperMatrix A, L, U, B;
    int info, permc_spec;
    int *perm_r; /* row permutations from partial pivoting */
    int *perm_c; /* column permutation vector */
    superlu_options_t options;
    SuperLUStat_t stat;

    /* Create matrices A and B in the format expected by SuperLU. */
    dCreate_CompCol_Matrix(&A, m, n, nnz, a, asub, xa, SLU_NC, SLU_D, SLU_GE);
    dCreate_Dense_Matrix(&B, m, nrhs, rhs, m, SLU_DN, SLU_D, SLU_GE);

    if ( !(perm_r = intMalloc(m)) ) ABORT("Malloc fails for perm_r[].");
    if ( !(perm_c = intMalloc(n)) ) ABORT("Malloc fails for perm_c[].");

    /* Set the default input options. */
    set_default_options(&options);
    options.ColPerm = NATURAL;

    /* Initialize the statistics variables. */
    StatInit(&stat);

    dgssv(&options, &A, perm_c, perm_r, &L, &U, &B, &stat, &info);

    /* De-allocate storage */
    SUPERLU_FREE (rhs);
    SUPERLU_FREE (perm_r);
    SUPERLU_FREE (perm_c);
    Destroy_CompCol_Matrix(&A);
    Destroy_SuperMatrix_Store(&B);
    Destroy_SuperNode_Matrix(&L);
    Destroy_CompCol_Matrix(&U);
    StatFree(&stat);
}

It is the function linsolve() that solves the matrix equation $A X = B$ by calling other object modules of the SuperLU library; from these two C/C++ source codes, object files must be generated using suitable makefiles.
It is the function linsolve() that solves the matrix equation \( A.X = B \) by calling other object modules of the SuperLU library; from these two C/C++ source codes, object files must be generated using suitable makefiles.

The matrices are expected to be in a special format called “column-compressed storage format,” so as to minimize storage space. Thus, the \( N_x \times N_x \) matrix elements of \( A \) need not all be specified, since only a small number, \( nnz \), of them are nonzero; here \( N_x \) is the number of spatial grid points. The matrix \( A \) is specified through three row matrices \( \text{amat} \) and \( \text{asubmat} \) (that have a length \( nn \)), and \( \text{xamat} \) (that has a length \( xasize = N_x + 1 \)). Our function takes these integers \( N_x, \) \( nnz \), and \( xasize \) as parameters; in addition, we must pass as parameters the time step \( dt \) and the solution vector of the PDE at time \( t \); the function then returns the solution vector at time \( t + dt \).

The function \text{linsolvepp} must now be defined as an external procedure using the following command.

```mathematica
In[7]:= linsolvepp[ nx_, nx1_, nx2_, one_,
   expamat_, expasubmat_, expxamat_, exprhsmat_ ] :=
   ExternalProcedure[nx, nx1, nx2, one, expamat,
   expasubmat, expxamat, InOut exprhsmat];
```

Note the keyword InOut preceding the last argument of \text{ExternalProcedure}: in the calling function \text{SolveDiffusion1D}, the array \text{rhsmat} is passed to \text{linsolvepp} as input, but \text{linsolvepp} also returns the solution vector by destroying \text{rhsmat} and using it to store the solution vector. As a result, the array \text{rhsmat} is both an input and an output. The way to declare this is by using the keyword InOut.

```mathematica
In[8]:= EndPackage[];
```

We next declare the types, and then build and install.

```mathematica
In[9]:= Declare[SolveDiffusion1D[Integer Nx_, Real dt_, Integer nnz_,
   Integer xasize_, Real[_] U_] -> Real [Nx], {Integer, Integer,
   Real, Integer, Real[Nx], Integer[nnz], Integer[nnz],
   Real[nnz], Real[nnz], Integer[nnz], Integer[xasize]}];
```

```mathematica
In[10]:= Declare[
   linsolvepp[Integer nx_, Integer nx1_, Integer nx2_,
   Integer one_, Real[_] expamat_, Integer[_] expasubmat_,
   Integer[_] expxamat_, Real[_] exprhsmat_] -> Real[nx];
] ;
```

```mathematica
In[11]:= CompilePackage["foo" ];
```

Successful compilation to C++: 2 function(s)
We now create the executable. Note that an additional option `NeedsExternalLibrary` must also be specified in this example, since the external objects depend on other objects of the SuperLU library.

```mathematica
In[12]:= MakeBinary["foo", NeedsExternalObjectModule ->
    {MCRoot <> "\Demos\ExternalFunction\linsolve", MCRoot <> 
      "\Demos\ExternalFunction\linsolvepp"}, NeedsExternalLibrary ->
    {MCRoot <> "/PDESOLVER/MathPDE2/SuperLU_3.0/superlu_cygwin.a", 
      MCRoot <> "/PDESOLVER/MathPDE2/SuperLU_3.0/blas_cygwin.a"}];
```

```mathematica
In[13]:= InstallCode[];
```

foo is installed.

We take the following initial conditions.

```mathematica
In[14]:= soln = Table[(x - 1) * (-x + 100) / (99.0 * 99.0), {x, 1, 100}];
```

Now the following command runs the C++ executable fooml.exe. We evolve from $t = 0$ to $t = 1000$ with $dt = 0.00001$.

```mathematica
In[15]:= Timing[
    Do[soln = SolveDiffusion1D[100, 0.00001, 100, 101, soln], {1000}];]
```

```mathematica
Out[15]= {6.8 Second, Null}
```

5. Summary and Conclusions

`MathCode` is an application package that generates optimized Fortran/C++ code for numerical computations. The code can be either compiled and run from within a notebook environment, or ported, and typically runs several hundred times faster than original `Mathematica` code.
MathCode is easy to use, since only the following three simple steps are involved for most applications:

- Add type declarations.
- Execute `BuildCode[]` to generate C++ code and an executable program.
- Execute `InstallCode[]` to connect the executable program to `Mathematica`.

It must be remembered that only a subset of `Mathematica` functions and operations are translated into C++ by `MathCode`. However, `MathCode` also provides these ways to extend the subset:

- Symbolic evaluation
- Callbacks to `Mathematica`
- Use of external code

To conclude, we remark that `MathCode` can turn `Mathematica` into a powerful environment for prototyping advanced numerical algorithms and production code development. Since it can generate stand-alone code, applications that use `Mathematica` as an environment for development and need to automatically generate efficient C++ code as embedded code in large software systems can greatly benefit.

`MathCode` is a product available both for purchase and free trial (see the website of MathCore Engineering, [1]). Currently, both the C++ and Fortran 90 versions of the code generator are available.

### References


[3] The `SuperLU` package is available for download at crd.lbl.gov/~xiaoye/SuperLU.


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