C++ for Scientific Computing

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Introduction

Why C++?

Why not Matlab?

- Matlab is a high level language, e.g. provides many functions/algorithms allowing rapid developement.
- But Matlab is limited to dense and (to some degree) sparse matrices, therefore not flexible enough, especially for large problems.

Why not Fortran?

- Fortran is one of the main programming language in many areas including numerics.
- Many excellent software libraries are written in Fortran, e.g. LAPACK.
- Fortran 77 quite dated in terms of language features.
- Recent updates of Fortran (90, 95, 2000) modernised the language, but still somewhat dated.

Why C++?

So, Why C++ (and not C) ?

- C is a subset of C++.
- C++ provides many features which make programming easier.
- C++ can be as fast as C (and sometimes faster).
- C++ (like C) can use all software libraries written in Fortran or C.
- Many new software libraries are written in C++.

Why not C++?

- C++ can be complicated as opposed to C.
- If you do not follow strict programming rules, you can make many errors (unlike Matlab, or Fortran).

Hello World

Like every programming course, we start with something simple:

```
#include <iostream>

using namespace std;

int
main ( int argc, char ** argv )
{
    // print welcome message
    cout << "Hello World" << endl;
    return 0;
}
```

Even this small example contains:

- modules and namespaces,
- functions and blocks and
- variables and datatypes

Remark

Comments in C++ begin with a “//” and span the rest of the line.

Hello World

C++ is a compiler based language, i.e. one has to translate the source code of the program into a machine executable format using another program, called the *compiler*.

Source code files, or just *source files*, typically have a filename suffix like ".cc", ".C" or ".cpp".

There are many different C++ compilers available even for one operating system. On Linux, the GNU Compiler Collection provides the `g++` compiler. Alternatively, Intel offers another compiler named `icpc`.

As an example, to compile the source file `hello.cc` for "Hello World" into an executable binary using the GCC compiler, you'll have to enter

```
g++ -o hello hello.cc
```

and afterwards run the program via "`./hello`".

Variables and Datatypes

Variables and Datatypes

In C++, all variables have to be of some specific datatype, which is, once defined, fixed and can not be changed, e.g. unlike in Matlab.

Integer Datatypes

characters :

- `char`: 'c', '/', '\n', '\\', 'π' (with Unicode)
- also numbers: from $-2^7 \dots 2^7 - 1$, e.g. 0, −128, 127

signed integers :

- `short`: from $-2^{15} \dots 2^{15} - 1$, e.g. 0, −32768, 1000
- `int`: from $-2^{31} \dots 2^{31} - 1$, e.g. 0, −100, 2147483647
- `long`: from $-2^{31} \dots 2^{31} - 1$, or $-2^{63} \dots 2^{63} - 1$

unsigned integers :

- `unsigned short`: from $0 \dots 2^{16} - 1$
- `unsigned int` or `unsigned`: from $0 \dots 2^{32} - 1$
- `unsigned long`: from $0 \dots 2^{32} - 1$, or $0 \dots 2^{64} - 1$

Variables and Datatypes

Integer Datatypes: Overflow and Underflow

When doing arithmetic with integer types, the range of the types has to be considered. If the result is bigger than the maximum value, the result becomes negative, e.g. using `short`:

$$32760 + 100 = -32676$$

Here, an overflow occured.
Similar behaviour can be observed if the result is less that the minimum (underflow):

$$-32760 - 100 = 32676$$

Variables and Datatypes

Floating Point Datatypes

Floating point numbers x are represented as

$$x = s \cdot m \cdot 2^e$$

with the sign s, the mantissa m and the exponent e.
In C++, like in many other languages, we have two floating point types

- `float`: single precision, 23 bits for mantissa, 8 bits for exponent, $x \in [-3 \cdot 10^{38} \ldots -10^{-38}, 0, 10^{-38} \ldots, 3 \cdot 10^{38}]$,
- `double`: double precision, 52 bits for mantissa, 11 bits for exponent, $x \in [-2 \cdot 10^{308} \ldots -10^{-308}, 0, 10^{-308} \ldots, 2 \cdot 10^{308}]$.

Floating point numbers are entered with a *dot*:

`4.0` (`double`) or `4.0f` (`float`) instead of just `4` (`int`)

Exponent is defined using scientific notation via 'E' or 'e':
$4.25 \cdot 10^{-4}$ is "`4.25E-4`" or "`4.25e-4`"

Variables and Datatypes

Floating Point Datatypes: Rounding

Since number of bits for representing numbers is limited, real numbers are rounded, e.g. π:

- `float`: $\tilde{\pi} = 3.141592741$,
- `double`: $\tilde{\pi} = 3.141592653589793116$

This might also lead to wrong results:

$$\pi - 3.1415926 \approx 5.36 \cdot 10^{-8}$$

but in single precision one obtains

$$\pi - 3.1415926 = 1.41 \cdot 10^{-7}.$$

This effect is also known as cancellation

Variables and Datatypes

Floating Point Datatypes: Absorption

When adding two numbers with a large difference in the exponent, the result might be equal to the larger of the two addend, e.g. in single precision for $x \in \mathbb{R}$:

$$x + 1 \cdot 10^{-8} = x$$

For any floating point type, the smallest number ε, such that $1 + \varepsilon \neq 1$ is known as the machine precision:

- for `float`: $\varepsilon \approx 1.2 \cdot 10^{-7}$,
- for `double`: $\varepsilon \approx 2.2 \cdot 10^{-16}$.

Coding Principle No. 1

Always check if the range and the precision of the floating point type is enough for your application. If in doubt: use double precision.

Variables and Datatypes

Boolean Datatype

Integer and floating point types are also available in C. In C++ one also has a boolean type `bool`, which can be either **true** or **false**.

Missing Types

C++ does not have datatypes for strings or complex numbers. Those have to be implemented by special ways.

Variables and Datatypes

Variables

Variables can be declared at (almost) any position in the source file. The declaration follows the scheme:

$\langle$*typename*$\rangle$ $\langle$*variablename*$\rangle$*;*

or

$\langle$*typename*$\rangle$ $\langle$*variablename1*$\rangle$, $\langle$*variablename2*$\rangle$, *...;*

Remark

Every statement in C++ is finished with a semicolon.

A name for a variable can contain any alphanumerical character plus '_' and must not begin with a number. Also, they can not be identical to a reserved name used by C++. Variable names are case sensitive.

Variables and Datatypes

Variables

Examples:

```
int     n;
int     i, j, k;
float   pi, Pi, PI;
double  1_over_pi;      // ERROR
double  _1_over_pi;     // Ok
```

Coding Principle No. 2

Give your variables a reasonable name.

Variables: Initial Values

When declaring a variable, one can provide an initial value:

```
int     n           = 10;
int     i, j, k;
float   pi          = 3.1415926;
double  _1_minus_pi = 1.0 - pi;
double  max         = 1.8e308;
```

Variables and Datatypes

Variables: Initial Values

Coding Principle No. 3

Resource allocation is initialisation (RAII):
Whenever a resource, e.g. variable, is allocated/declared, it should be initialised with some reasonable value.

Otherwise, strange things might happen, e.g. what is wrong with:

```
int     n           = 10;
int     i, j, k;
float   pi;
double  _1_minus_pi = 1.0 - pi;
double  max         = 1.8e308;
```

The value of `_1_minus_pi` is not defined, but only some compilers will give you a warning about that.

Variables and Datatypes

Variables: Usage

Variables can only be used after they have been declared:

```
const double  _1_minus_pi = 1.0 - pi;    // ERROR: "pi" is unknown
const float   pi          = 3.1415926;
const double  _2_plus_pi  = 2.0 + pi;    // Ok: "pi" is defined
```

Type Modifiers

Each type can be modified with one of the following modifiers:

- `const`: the value of the variable is fixed,
- `static`: the variable is declared only once in the whole program (we'll come back to that later),

The modifiers can be combined:

```
const int            n           = 10;
int                  i, j, k;
const float          pi          = 3.1415926;
const double         _1_minus_pi = 1.0 - pi;
static const double  max         = 1.8e308;
```

Type Modifiers

Coding Principle No. 4

Use `const` as much as possible.

You avoid errors, e.g. by mistakenly changing the value and the compiler can optimise more, e.g. replace every occurence by the actual value.

Variables and Datatypes

Pointers and References

A *pointer* is a special datatype derived from a base type, where the variable contains the memory position of another variable. The syntax is:

⟨*base type*⟩ ***** ⟨*pointer name*⟩*;*

The memory position, i.e. the address, of a standard variable is obtained by the *address operator* "**&**", e.g.

& ⟨*variable*⟩

To obtain the value of the memory position, the pointer directs to, the (unary) *dereference operator* "*****", e.g.

***** ⟨*variable*⟩

is available (not to be mistaken with the binary multiplication operator!).

Variables and Datatypes

Pointers and References

Example for the usage of pointers:

```
int    n  = 5;
int *  p  = & n;
int    m1, m2;

m1 = n  + 3;
m2 = *p + 3;   // m2 equal to m1
*p = 6;        // this changes the value of n to 6!
m2 = n + 4;    // evaluates to 10!
```

The value of a pointer, e.g. the address, can be assigned to another pointer:

```
int *  q = p;  // q now points to the same position
               // as p, hence, to n

n  = 2;
m1 = *p + *q   // is equivalent to n+n
```

Variables and Datatypes

Pointers and References

A special pointer value, **NULL**, exists, for the case, that no standard variable is available to point to:

```
int *  p = NULL;
```

Dereferencing a **NULL** pointer is illegal and leads to a program abort.

Coding Principle No. 5

Always initialise a pointer with the address of an existing variable or with **NULL***.*

Remark

RAII is even more important when working with pointers than with standard variables, since undefined pointers almost always lead to hard to find errors.

Variables and Datatypes

Pointers and References

A *reference* is a special form of a pointer, which can only be initialised with the address of an existing variable. The syntax is:

> ⟨*base type*⟩ **&** ⟨*pointer name*⟩*;*

One does not need to dereference references:

```
int    n = 5;
int &  r = n;
int    m;

m = r + 3;  // m == n + 3
r = m;      // r still points to n and n == m
m = 0;      // r and n are unchanged
```

And you can not change the address where a reference points to:

```
int &  s = m;

r = s;      // r still points to n and n == m (== 0)
```

Variables and Datatypes

Pointers and References

Pointers and references can also be combined with **const** in various forms:

```
      int *         pn1;  // non-const pointer to non-const var.
const int *         pn2;  // non-const pointer to const var.
      int * const   pn3;  // const pointer to non-const var.
const int * const   pn4;  // const pointer to const var.
```

If the pointer is constant, the address it is directing to can not be changed. If the variable is constant, the value of it can not be modified:

```
int          n   = 0;
const int    m   = 1;

int *        pn1 = & n; // Ok
const int *  pn2 = & n; // ERROR
int * const  pn3 = & n; // Ok
```

Arithmetic Operators

Arithmetic and Assignment Operators

Arithmetic

For integer and floating point types:

```
x + y;
x - y;
x * y;
x / y;
```

For integer types, the modulus operator:

```
x % y;
```

Remark

No operator for power, like `^` *in Matlab.*

Arithmetic and Assignment Operators

Assignment

Standard assignment (as with initial values)

```
x = y;
```

Assignment can be combined with arithmetic, so

```
x = x + y;  x = x - y;
x = x * y;  x = x / y;
x = x % y;              // for integers
```

is the same as

```
x += y;  x -= y;
x *= y;  x /= y;
x %= y;                 // for integers
```

Arithmetic and Assignment Operators

Increment and Decrement

In C++ (like in C) exist special versions for variable increment/decrement:

```
int  n = 0;

++n; // same as n = n + 1 or n += 1
n++;
--n; // same as n = n - 1 or n -= 1
n--;
```

Difference between preincrement and postincrement, e.g.

```
int  n = 5, m = 5 * n++;
```

results in $n = 6$ and $m = 25$, whereas

```
int  n = 5, m = 5 * ++n;
```

results in $n = 6$ and $m = 30$.

Arithmetic and Assignment Operators

Examples

```
int  n1 = 3, n2 = 4;
int  n3;

n3  = 2 * n1 - n2 + n1 / 2;
n2 *= 6;
n1 -= 8;

const double  approx_pi = 355.0 / 113.0;
double        f1        = approx_pi / 2.0;
double        f2;

f2  = approx_pi * approx_pi + 10.0 * f1;
f1 /= 5.0;
```

Arithmetic and Assignment Operators

Division by Zero and other undefined Operations

With floating point types:

$$x/0.0 = \texttt{INF}$$

for $x \neq 0.0$. INF is a special floating point number for infinity.
For $x = 0.0$:

$$x/0.0 = \texttt{NAN}$$

NAN (not-a-number) is another special floating point number for invalid or not defined results, e.g. square root of negative numbers. Both operations are (usually) performed without notification, i.e. the program continues execution with these numbers. NANs often occur with uninitialised variables, therefore RAII.
In integer arithmetic, $x/0$ leads to an exception, i.e. the program (usually) aborts.

Relational and Logical Operators

Comparison

Standard comparison for integer and floating point types:

```
x >  y;   // bigger than
x <  y;   // less than
x >= y;   // bigger or equal
x <= y;   // less or equal
x == y;   // equal
x != y;   // unequal
```

Logic

Logical operators and, or and not for boolean values:

```
b1 && b2;  // and
b1 || b2;  // or
! b1;      // not
```

Relational and Logical Operators

Minimal Evaluation

Logical expressions are only evaluated until the result is known. This is important if the expression contains function calls (see later), or a sub expression is only allowed if a previous sub expression is `true`.

```cpp
int  x = 2;
int  y = 4;
int  z = 4;
bool b;

// z == 4 is not tested
b = ( x == 2 && y == 3 && z == 4 );

// only x == 2 is tested
b = ( x == 2 || y == 3 || z == 4 );

// correct, since x != 0 in "y/x"
b = ( x != 0 && y/x > 1 );
```

Relational and Logical Operators

Floating Point Comparison

Coding Principle No. 6

For floating point types, avoid equality/inequality checks due to inexact arithmetic.

Better is interval test:

```
double  f1  = sqrt( 2.0 );
double  f2  = f1 * f1;
bool    b;

b = ( f2 == 2.0 );  // unsafe

const double  eps = 1e-14;

b = ( f2 > 2.0 - eps && f2 < 2.0 + eps );  // safe
b = ( abs( f2 - 2.0 ) < eps );             // even better
```

Precedence and Associativity of Operators

Precedence

When evaluating complex expressions, what is evaluated first, and in which order? Example:

```
int    n1 = 2 + 3 * 4 % 2 - 5;
int    n2 = 4;
bool   b  = n1 >= 4 && n2 != 3 || n1 < n2;
```

Precedence of arithmetics follows algebraic/logical precedence, e.g. * before +, $\wedge$ (&&) before $\vee$ (||). Increment (++) and decrement (--) have higher, assignment (=, +=, ...) has lower priority. Parentheses have highest priority.

```
int    n1 = (2 + ((3 * 4) % 2) - 5);
int    n2 = 4;
bool   b  = (((n1 >= 4) && (n2 != 3)) || (n1 < n2));
```

Precedence and Associativity of Operators

Associativity

Arithmetic and logical operators are left associative, whereas assignment operators are right associative:

```
int  n1 = 1 + 2 + 3 + 4;
int  n2 = 1 * 2 * 3 * 4;
int  n3, n4 , n5;

n3 = n4 = n5 = 0;
```

is the same as

```
int  n1 = (((1 + 2) + 3) + 4);
int  n2 = (((1 * 2) * 3) * 4);
int  n3, n4 , n5;

(n3 = (n4 = (n5 = 0)));
```

Precedence and Associativity of Operators

Summary

Priority	Associativity	Operators
highest	left	()
	right	++, --, - (unary), !, & (address), * (dereference)
	left	* (multiplication), /, %
	left	+, -
	left	>, <, >=, <=
	left	==, !=
	left	&&
	left	||
lowest	right	=, +=, -=, *=, /=, %=

Precedence of Operators

Usage of Parentheses

Example:

```
int   n1 = 4;
int   n2 = 2 + 5 * n1 / 3 - 5;
bool  b  = n2 >= 4 && n1 != 3 || n2 < n1;
```

vs.

```
int   n1 = 4;
int   n2 = 2 + (5 * n1) / 3 - 5;
bool  b  = ( n2 >= 4 ) && (( n1 != 3 ) ||
                           ( n2 < n1 ));
```

Coding Principle No. 7

When in doubt or to clarify the expression: use parentheses.

Type Casting

Type Casting

Implicit Type Conversion

Up to now, we have only had expressions with either integer or floating point types. Often, these types are mixed:

```
const double  pi = 3.14159265358979323846;
double        f  = 1 / ( 2 * pi );
```

Here, implicit type conversion occurs: the `int` numbers `1` and `2` are automatically converted to the `double` numbers `1.0` and `2.0`, respectively.

```
const double  pi = 3.14159265358979323846;
int           n  = 2 * pi;
```

is also allowed. Here, `2` is first converted to `double` and the result is finally converted back to `int`.

Type Casting

Explicit Type Conversion

Explicit conversion between data types is performed via

typename(value)

Examples:

```
const float  pi = float(3.14159265358979323846);
int          n  = 2 * int(pi);
bool         b  = bool(n);
```

Remark

A non-zero value is interpreted as `true`, a zero value as `false`.

The old C syntax *(typename) value*, e.g.

```
int  n = 2 * (int) pi;
```

is also allowed, but not recommended.

Type Casting

Problems while Casting

Problem 1: Different ranges:

```
int            n1 = 5 - 6;
unsigned int   n2 = n1;    // underflow
```

Problem 2: Different precision:

```
const double   pi = 3.14159265358979323846;
float          f1 = 2.1;
float          f2 = 4 * f1 / pi;
```

The last expression is computed in double precision. Using `float(pi)` instead, would result in pure single precision arithmetic, which is (usually) faster.

Coding Principle No. 8

Avoid implicit type conversion.

Type Casting

Cast Operators

C++ defines four cast operators for various purposes:

- const_cast⟨T⟩(v) : remove `const` qualifier of a variable `v`,
- static_cast⟨T⟩(v) : classic, compile time type conversion with type checking
- reinterpret_cast⟨T⟩(v) : type conversion with correct handling of variable value and
- dynamic_cast⟨T⟩(v) : runtime type conversion with type checking

Since these operators are usually used in connection with *classes*, we will come back to them later.

Blocks and Scope

Blocks and Scope

Blocks

Statements in a C++ program are part of a block, which is enclosed by '{' and '}':

```
{ // ...
}
```

Remark

The trivial block is defined by a single statement.

Blocks can be arbitrarily nested or otherwise put together:

```
{ // block 1
    { // subblock 1.1
    }
    { // subblock 1.2
        { // sub subblock 1.2.1
        }
    }
}
```

Blocks and Scope

Variable Scope

Variables can be declared in each block individually, even with the same name:

```
{ // block 1
    int     n1 = 1;
    double  f1 = 0.0;
}
{ // block 2
    int     n1 = 2;    // n1 has value 2 in this block
}
```

but not twice in the same block:

```
{
    int  n1 = 1;
    // ...
    int  n1 = 2;   // ERROR
}
```

Blocks and Scope

Variable Scope

A variable is declared in the local block and all enclosed blocks:

```
{ // block 1:             n1 declared
    int  n1 = 1;

    { // block 1.1:       n1, n2 declared
        int  n2 = 2;

        { // block 1.1.1: n1, n2 declared
        }
    }

    int  n4 = 4;

    { // block 1.2:       n1, n4, n3 declared
        int  n3 = 3;
    }
}
```

Blocks and Scope

Variable Scope

Variables with the same name can also be declared in nested blocks.

```
{ // block 1
    int  n1 = 1;       // n1 == 1

    { // block 1.1
        int  n1 = 2;   // n1 == 2
    }
                       // n1 == 1
    { // block 1.2
        int  n1 = 3;   // n1 == 3
    }
    { // block 1.3
        n1 = 4;
    }
                       // n1 == 4 !!!
}
```

Blocks and Scope

Variable Scope

A reference to a variable will always be made to the first declaration found when going up the hierarchy of enclosing blocks.

```cpp
{ // block 1
    int  m, n1 = 1;

    { // block 1.1
        int  n2 = 2;

        { // block 1.1.1
            m = n1 + n2;   // evaluates to m = 3
        }
    }
    { // block 1.2
        int  n2 = 3;

        m = n1 + n2;       // evaluates to m = 4
    }
}
```

Variable Scope

Remark

Using variables with same name in nested blocks is not recommended, since that often leads to erroneous programs.

Blocks and Scope

Variable Lifetime

The scope of a variable also defines their *lifetime*, e.g. the time where resources are needed for the variable. For non-**static** variables, memory is allocated if a declaration is encountered and released, when the leaving the block holding the declaration:

```
{
    int  n = 0;          // memory for an integer is allocated

    {
        double f = 1.2;  // memory for a double is allocated
        ...
    }                    // memory for "f" is released
}                        // memory for "n" is released
```

For **static** variables, the memory will never be released and only allocated once per program run:

```
{
    static int m = 10;   // allocate memory once
}                        // memory for "m" is not released
```

Control Structures

Control Structures

Conditional Structure

A condition is defined by

> **if** *(* ⟨*condition*⟩ *)* ⟨*block*⟩

where ⟨*block*⟩ is executed if ⟨*condition*⟩ is **true** or

> **if** *(* ⟨*condition*⟩ *)* ⟨*if_block*⟩
> **else** ⟨*else_block*⟩

where additionally ⟨*else_block*⟩ is executed if ⟨*condition*⟩ is **false**, e.g.

```
int  n = 1;

if ( n > 0 )
{
    n = n / n;
}

if ( n < 0 ) n += 5;  // NOTE: trivial block!
else         n -= 6;
```

Control Structures

C++ supports three different loops: *for loops*, *while loops* and *do-while loops*.

For Loops

> **for** *(⟨start stmt.⟩ ; ⟨loop condition⟩ ; ⟨loop stmt.⟩)*
> *⟨block⟩*

The *start statement* is executed before the loop is entered. Before each iteration, the *loop condition* is evaluated. If it is **false**, the loop is finished. After each iteration, the *loop statement* is executed.

Example for factorial:

```
int  n = 1;

for ( int i = 1; i < 10; ++i )
{
    n = n * i;
}
```

Control Structures

While Loops

while *(⟨loop condition⟩)*
⟨block⟩

The loop iterates until the loop condition is no longer **true**, i.e. evaluates to **false**. The condition is checked before each iteration. Example for factorial:

```
int  n = 1;
int  i = 1;

while ( i < 10 )
{
    n *= i;
    ++i;
}
```

Control Structures

Do-While Loops

```
do
    ⟨block⟩
while ( ⟨loop condition⟩ );
```

The loop condition is tested after each iteration. Hence, the block is at least executed once.

Example for factorial:

```
int  n = 1;
int  i = 1;

do
{
    n *= i;
    ++i;
} while ( i < 10 );
```

Control Structures

Breaking out of Loops

To finish the current loop immediately, e.g. without first testing the loop condition, the keyword **break** can be used:

```
int  n = 1;

for ( int i = 1; i < 20; ++i )
{
    // avoid overflow
    if ( n > 21474836 )
        break;

    n = n * i;
}
```

Control Structures

Breaking out of Loops

Only the current loop is finished, not all enclosing loops:

```
for ( int j = 1; j < 20; ++j )
{
    int  n = 1;

    for ( int i = 1; i < j; ++i )
    {
        if ( n > 21474836 )      // break here
            break;

        n = n * i;
    }

    cout << n << endl;           // and continue here
}
```

Control Structures

Finish current Iteration

To immediately finish the current iteration of a loop use the keyword **continue**:

```
int  n2 = 0;

for ( int i = 0; i < 1000; i++ )
{
    // skip odd numbers
    if ( i % 2 == 1 )
        continue;

    n2 += i;
}
```

After **continue**, the loop condition of a loop is tested. In for-loops, the loop statement is first evaluated.

Remark

Again, **continue** *effects only the current loop.*

Control Structures

Selective Statement

To directly switch between several cases, the **switch** structure can be used:

```
switch ( ⟨value⟩ ) {
    case ⟨CASE 1⟩ : ⟨statements⟩; break;
    case ⟨CASE 2⟩ : ⟨statements⟩; break;
    ⋮
    case ⟨CASE n⟩ : ⟨statements⟩; break;
    default : ⟨statements⟩
}
```

The type of ⟨value⟩ must be some integral typ, i.e. it can be mapped to an integer type. Hence, floating point or more advanced types (later) are not possible.

Control Structures

Selective Statement

Example for a **switch** statement:

```
unsigned int  i = 3;
unsigned int  n;

switch ( i )
{
case  0 : n = 1;  break;
case  1 : n = 1;  break;
case  2 : n = 2;  break;
case  3 : n = 6;  break;
case  4 : n = 24; break;
default : n = 0;  break;
}
```

Coding Principle No. 9

> *Always implement the* **default** *case to avoid unhandled cases.*

Control Structures

Selective Statement

If **break** is missing after the statements for a specific case, the statements of the next case are also executed:

```
unsigned int  i = 3;
unsigned int  n;

switch ( i )
{
case  0 :
case  1 : n = 1;  break; // executed for i == 0 and i == 1
case  2 : n = 2;  break;
case  3 : n = 6;  break;
case  4 : n = 24; break;
default : n = 0;  break;
}
```

Control Structures

Selective Statement

A **switch** statement can be implemented via **if** and **else**:

```
unsigned int  i = 3;
unsigned int  n;

if        ( i == 0 ) { n = 1;  }
else if ( i == 1 ) { n = 1;  }
else if ( i == 2 ) { n = 2;  }
else if ( i == 3 ) { n = 6;  }
else if ( i == 4 ) { n = 24; }
else                 { n = 0;  }  // default statement
```

Remark

> *Using* **switch** *is faster than* **if-else***, among other things since less comparisons are performed!*

Functions

Functions

Function Definition

The definition of a function in C++ follows

⟨*return type*⟩
⟨*function name*⟩ *(* ⟨*argument list*⟩ *)*
⟨*block*⟩

When a function does not return a result, e.g. a procedure, then the return type is `void`.
To return a value from a function, C++ provides the keyword **return**.

```
double
square ( const double x )
{
    return x*x;
}
```

Functions

Function Call

A function is called by

⟨function name⟩ (⟨argument1⟩, ⟨argument2⟩, . . .);

Example:

```
double y = square( 4.3 );
```

One can not define a function in the body of another function:

```
double cube ( const double  x )
{
    // ERROR
    double square ( const double  y ) { return y*y; }

    return square( x ) * x;
}
```

Functions

Function Examples

Previous computation of factorial in functional form:

```
int
factorial ( const int  n )
{
    int  f = 1;

    for ( int i = 1; i <= n; i++ )
        f *= i;

    return f;
}
```

Coding Principle No. 10

Make all function arguments **const***, except when changing value (see later).*

Functions

Function Examples (Cont.)

Power function with positive integer exponents:

```
double
power ( const double  x, const unsigned int  n )
{
    switch ( n )
    {
        case 0 : return 1;
        case 1 : return x;
        case 2 : return square( x );
        default:
        {
            double  f = x;
            for ( int i = 0; i < n; i++ ) f *= x;
            return f;
}   }   }
```

Coding Principle No. 11

Make sure, that a function has a call to **return** *in every execution path.*

Functions

Main Function

The main function is the first function called by the operating system in your program. Every program must have exactly one main function.

In principle, only code in main and functions called directly or indirectly from main will be executed.

The main function may be implemented without arguments and has a return type of int:

```
int
main ()
{
    ... // actual program code
    return 0;
}
```

The value returned from main is supplied to the operating system. As a standard, a value of 0 signals no error during program execution.

Functions

Call by Value

In previous examples, only the *value* of a variable (or constant) is used as the argument of a function, e.g. changing the value of the argument does not change the value of the original variable:

```
int
f ( int m )      // non const argument!
{
    m = 4;       // explicitly changing the value of argument m
    return m;
}

int  m = 5;
int  n = f( m ); // m is unchanged by f
```

This is known as call-by-value.

Remark

It is nevertheless advised to use **const** *arguments.*

Functions

Call by Reference

If the original variable should be changed in a function, a pointer or reference to this variable has to be supplied:

```
int
f ( int & m )    // reference argument
{
    m = 4;       // changing m, changes the variable pointed to
    return m;
}

int  m = 5;
int  n = f( m ); // m is changed by f to 4
```

This is known as call-by-reference.

Functions

Call by Reference

The same function with pointers:

```
int
f ( int * m )      // reference argument
{
    *m = 4;        // changing m, changes the variable pointed to
    return *m;
}

int  m = 5;
int  n = f( & m ); // m is changed by f to 4
```

Functions

Call by Reference

When using references to *constant* variables, the value can not be changed:

```
int
f ( const int & m )
{
    m = 4;          // ERROR: m is constant
    return m;
}
```

Therefore, this is (almost) equivalent to call-by-value and needed for advanced datatypes (see later).
For basic datatypes, using call-by-reference, even with **const**, is usually not advisable, except when changing the original variable.

Functions

Call by Reference

Example for multiple return values

```cpp
void
min_max ( const int n1, const int n2, const int n3,
          int & min, int & max )
{
    if ( n1 < n2 )
        if ( n1 < n3 )
        {
            min = n1;

            if ( n2 < n3 ) max = n3;
            else           max = n2;
        }
        else
        {
            min = n3;
            max = n2;
        }
    else
        ...
}
```

Functions

Recursion

Calling the same function from inside the function body, e.g. a *recursive* function call, is allowed in C++:

```
unsigned int
factorial ( const unsigned int  n )
{
    if ( n <= 1 )
        return 1;
    else
        return n * factorial( n-1 );
}
```

Remark

The recursion depth, i.e. the number of recursive calls, is limited by the size of the stack*, a special part of the memory. In practise however, this should be of no concern.*

Functions

Recursion

It is also possible to perform recursive calls multiple times in a function:

```
unsigned int
fibonacci ( const unsigned int  n )
{
    unsigned int  retval;

    if ( n <= 1 ) retval = n;
    else          retval = fibonacci( n-1 ) +
                           fibonacci( n-2 );

    return retval;
}
```

Remark

Remember, that variables belong to a specific block and each function call has it's own block. Therefore, variables, e.g. `retval`*, are specific to a specific function call.*

Functions

Function Naming

A function in C++ is identified by it's name and the number and type of it's arguments. Hence, the same name can be used for different argument types:

```
int     square ( const int    x ) { return x*x; }
float   square ( const float  x ) { return x*x; }
double  square ( const double x ) { return x*x; }
```

Coding Principle No. 12

> *Functions implementing the same algorithm on different types should be named equal.*

This can significantly reduce the number of different functions you'll have to remember und simplifies programming.

Functions

Function Naming

If only the return type is different between functions, they are identified as equal:

```
float  f ( int x ) { ... }
double f ( int x ) { ... }  // ERROR: "f" already defined
```

Functions

Default Arguments

Arguments for a function can have default arguments, which then can be omitted at calling the function:

```
void
f ( int n, int m = 10 )
{
    // ...
}

{
    f( 5 );    // equivalent to f( 5, 10 )
    f( 5, 8 );
}
```

Only limitation: after the first default value, all arguments must have default values:

```
void g1 ( int n, int m = 10, int k );      // ERROR
void g2 ( int n, int m = 10, int k = 20 ); // Ok
```

Functions

Default Arguments and Function Names

Two functions with the same name must differ by their arguments without default values:

```cpp
void f ( int n1, int n2, int n3 = 1 ) { ... }
void f ( int n1, int n2 )             { ... }

...

{
    f( 1, 2, 3 );   // Ok: call to f(int, int, int)
    f( 1, 2 );      // Error: call of "f(int, int)" is ambiguous
}
```

Functions

Function Name Scope

A function can only be called, if it was previously implemented:

```
void f ( int x )
{
    g( x );        // ERROR: function "g" unknown
}

void g ( int y )
{
    f( y );        // Ok: function "f" already defined
}
```

or *declared*, i.e. definition of function without function body:

```
void g ( int y );  // forward declaration

void f ( int x )
{
    g();           // Ok: "g" is declared
}
```

This is known as forward declaration.

Functions

Function Name Scope

Of course, every function with a forward declaration has to be implemented eventually:

```
void g ( int y );  // forward declaration

void f ( int x )
{
    g();
}

...

void g ( int y )   // implementation
{
    f( y );
}
```

Functions

Inline Functions

Calling a function involves some overhead. For small functions, this overhead might exceed the actual computation:

```
double  square ( const double x ) { return x*x; }

{
    double  f = 0;

    for ( int i = 0; i < 100; i++ )
        f += square( double(x) );
}
```

Here, simply calling `square` takes a significant part of the runtime. Some compilers automatically replace the function call by the function body:

```
...
    for ( int i = 0; i < 100; i++ )
        f += double(x) * double(x);
...
```

Functions

Inline Functions

Replacing the function call by the function body is called inlining. To help the compiler with such decisions, functions can be marked to be inlined by the keyword **inline**:

```
inline double
square ( const double x )
{
    return x*x;
}
```

Especially for small functions, this often dramatically increases program performance.

Remark

> *If the function body is too large, inlining can blow up the program since too much code is compiled, e.g. every occurence of the function, and therefore decreases performance!*

Functions

Function Pointers

A function, like a variable, is stored somewhere in the memory and therefore, also has an address. Hence, a pointer can be aquired for it. For a function

> *⟨return type⟩ ⟨function name⟩ (⟨argument list⟩);*

a pointer is defined by

> *⟨return type⟩ (* ⟨variable name⟩) (⟨argument list⟩);*

Example:

```
int f ( const int  n, int &  r );

{
    int ( * pf ) ( const int n, int & r );  // function ptr named "pf"

    pf = f;
}
```

Functions

Function Pointers

A variable holding the address of a function can be used as a function by itself:

```
int  n = 0;

pf = f;      // pf holds address to f
pf( 2, n );  // call to f
```

Since function pointers are normal variables, they can be supplied as function arguments:

```
double  f1 ( const double x )           { return  x*x; }

double  f2 ( double ( * func ) ( const double x ),
             const double x )           { return func( x ); }

int main ()
{
    f2( f1, 2.0 );  // returns f1( 2.0 )
}
```

Functions

Function Pointers

Example: apply Simpson rule to various functions

```
double
simpson_quad ( const double a, const double b,
               double ( * func ) ( const double ) )
{
    return (b-a) / 6.0 * ( func(a) +
                           4 * func( (a+b) / 2.0 ) +
                           func(b) );
}

double f1  ( const double  x ) { return x*x; }
double f2  ( const double  x ) { return x*x*x; }

int main ()
{
    cout << simpson_quad( -1, 2, f1 ) << endl;
    cout << simpson_quad( -1, 2, f2 ) << endl;
}
```

Functions

Functions and Minimal Evaluation

As discussed, C++ uses minimal evaluation when looking at logical expressions, e.g. only evalutates until results is known. If functions are used in the expressions, it can imply, that they are not called at all:

```
double f ( const double  x ) { ... }

...
    // f is not called if x >= 0.0
    if (( x < 0.0 ) && ( f( x ) > 0.0 ))
    {
        ...
    }
```

For the programmer this means:

Coding Principle No. 13

Never rely on a function call in a logical expression.

Functions

Functions and static Variables

In contrast to standard variables in a function, which are specific to a specific function call, for **static** variables in all function calls the same instance, e.g. memory position, is referenced:

```
double
f ( const double x, long & cnt )
{
    static long  counter = 0;     // allocated and initialised
                                  // once per program
    cnt = ++counter;

    return 2.0*x*x - x;
}

int main ()
{
    long  cnt = 0;

    for ( double x = -10; x <= 10.0; x += 0.1 )
        f( x, cnt );

    cout << cnt << endl;          // print number of func. calls
}
```

Arrays and Dynamic Memory

Arrays and Dynamic Memory

Array Definition

So far, we had only datatypes with one entry per variable. Arrays with a fixed number of entries are defined as:

⟨*datatype*⟩ ⟨*variablename*⟩**[**⟨*number of entries*⟩**]***;*

where the number of entries is a constant, e.g.

```
int        n[ 5 ];
double     f[ 10 ];
const int  len = 32;
char       str[ len ];
```

Arrays can also be preinitialised. In that case, the array size can be omitted:

```
int  n1[5] = { 0, 1, 2, 3, 4, 5 };
int  n2[]  = { 3, 2, 1, 0 };       // automatically size of 4
```

Arrays and Dynamic Memory

Array Access

A single entry in an arrays is accessed by the index operator $[\cdot]$:

```
double  f[5];
int     i;

f[0] = -1.0;
f[1] =  3.0;
f[4] =  f[1] * 42.0;

i    = 3;
f[i] = f[0] + 8.0;
```

In C++, indices are counted from zero. The valid index range is therefore:

$$[0, \dots, \text{array size} - 1]$$

```
for ( int i = 0; i < 5; i++ )
    f[i] = 2*i;
```

Arrays and Dynamic Memory

Array Access

There are normally no array boundary checks in C++, i.e. you can specify arbitrary, even negative indices, resulting in an undefined program behaviour.

Typical error:

```
double  f[5];

for ( int i = 0; i < 5; i++ )    // Ok
    f[i] = 2*i;

for ( int i = 0; i <= 5; i++ )   // Bug
    f[i] = 2*i;
```

Coding Principle No. 14

Always make sure, that you access arrays within the valid index range.

Arrays and Dynamic Memory

Array Operations

Unfortunately, there are no operators for arrays, e.g. no assignment, elementwise addition or multiplication like in other languages. All of these have to be programmed by yourself:

```
void  copy ( const double x[3], double y[3] )
{
    for ( int i = 0; i < 3; i++ )
        y[i] = x[i];
}

void  add ( const double x[3], double y[3] )
{
    for ( int i = 0; i < 3; i++ )
        y[i] += x[i];
}
```

Remark

Arrays can be used as function arguments like all basic datatypes. But not as function return types!

Arrays and Dynamic Memory

Multidimensional Arrays

So far, all arrays have been onedimensional. Multidimensional arrays are defined analogously by appending the corresponding size per dimension:

```
int     M[3][3];
double  T3[10][10][10];
long    T4[100][20][50];
```

The access to array elements in multidimensional arrays follows the same pattern:

```
M[0][0] =  1.0; M[0][1] = 0.0; M[0][2] = -2.0;
M[1][0] =  0.0; M[1][1] = 4.0; M[1][2] =  1.0;
M[2][0] = -2.0; M[2][1] = 1.0; M[2][2] = -1.5;

for ( int i = 0; i < 100; i++ )
    for ( int j = 0; j < 20; j++ )
        for ( int k = 0; k < 50; k++ )
            T3[i][j][k] = double(i+j+k);
```

Arrays and Dynamic Memory

Multidimensional Arrays

Example: Matrix-Vector multiplication

```
void
mulvec ( const double  M[3][3],
         const double  x[3],
         double        y[3] )
{
    for ( int i = 0; i < 3; i++ )
    {
        y[i] = 0.0;

        for ( int j = 0; j < 3; j++ )
            y[i] += M[i][j] * x[j];
    }
}
```

Arrays and Dynamic Memory

Arrays and Pointers

C++ does not support variable sized arrays as an intrinsic datatype. Hence, arrays with an unknown size at compile time are not possible with previous array types in C++.

But, in C++, there is no distinction between a pointer and an array. A pointer not only directs to some memory address, it is also the base point, e.g. index 0, of an array.

```
int   n[5] = { 2, 3, 5, 7, 11 };
int * p    = n;

cout << p[0] << endl;  // yields n[0]
cout << p[1] << endl;  // yields n[1]
cout << p[4] << endl;  // yields n[4]
```

The index operator **[i]** of a pointer `p` gives access to the `i`'th element of the array starting at address `p`.

Arrays and Dynamic Memory

Dynamic Memory

Since pointers and arrays are equivalent, one needs to initialise a pointer with the address of a memory block large enough to hold the wanted array. This is accomplished by dynamic memory management:

> *Memory of arbitrary size can be allocated and deallocated at runtime.*

In C++ this is done with the operators **new** and **new[·]** to allocate memory and **delete** and **delete[·]** to deallocate memory.
For a single element:

> ⟨*datatype*⟩ ***** *p* = **new** ⟨*datatype*⟩*;*
> **delete** *p;*

For more than one element:

> ⟨*datatype*⟩ ***** *p* = **new** ⟨*datatype*⟩**[**⟨*size*⟩**]***;*
> **delete[]** *p;*

Arrays and Dynamic Memory

Dynamic Memory

Examples:

```
char *   s = new char[ 100 ];
int      n = 1024;
double * v = new double[ n ];
float *  f = new float;

for ( int i = 0; i < n; i++ )
    v[i] = double( square( i ) );

*f = 1.41421356237; // dereference f

...

delete[] v;  // new[] => delete[]
delete[] s;
delete   f;  // new   => delete
```

Remark

The size parameter to **new** *does not need to be a constant.*

Arrays and Dynamic Memory

Problems with Pointers

The corresponding array to a pointer has no information about the array size. Remember, that C++ performs no boundary checks. That opens the door to many errors (see Coding Principle No. 14).

```
double * v = new double[ 1000 ];

...

v[2000] = 1.0;
```

With the last instruction, you overwrite a memory position corresponding to completely other data. The program will only terminate, if the memory does not belong to the program (segmentation fault).

Arrays and Dynamic Memory

Problems with Pointers

The programmer does not know if the memory was allocated or deallocated, except if the pointer contains **NULL** (see Coding Principle No. 5).

```
double * v = new double[ 1000 ];

...

delete[]  v;

...

v[100] = 2.0;      // Bug: memory for v is deallocated
```

Again, the last instruction will be executed and will only result in an immediate error, if the memory is no longer part of the program.

Coding Principle No. 15

*After calling **delete**, reset the pointer value to **NULL**.*

Arrays and Dynamic Memory

Problems with Pointers

Memory addressed by forgotten pointers is lost for the program. C++ does not automatically delete memory with no references to it (garbage collection).

```
void f ()
{
    double * v = new double[ 1000 ];
    ...  // no delete[] v
}
// v is no longer accessible, memory is lost
```

This bug is not directly a problem, since no other data is overwritten. But if a lot of memory is not deleted after use, the program will have no available memory left.

Coding Principle No. 16

Always make sure, that allocated memory is deallocated after using.

Arrays and Dynamic Memory

Problems with Pointers

Remark

The aftermath of a pointer related bug, e.g. array boundary violation or accessing deleted memory, may show up much later than the actual position of the error.

Summary: pointers are dangerous and require careful programming. But we have no choice ☹.

Problems with Pointers

Remark

The aftermath of a pointer related bug, e.g. array boundary violation or accessing deleted memory, may show up much later than the actual position of the error.

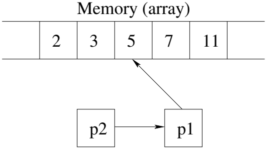
Summary: pointers are dangerous and require careful programming. But we have no choice ☹. Well, almost ☺ (see later).

Arrays and Dynamic Memory

Multidimensional Arrays with Pointers

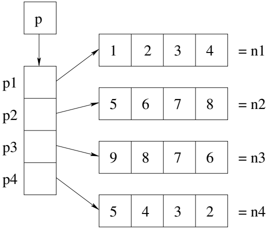
The analog of multidimensional arrays are pointers of pointers, i.e. pointers which direct to a memory address containing a pointer to another memory address:

```
int     n[5] = { 2, 3, 5, 7, 11 };
int *   p1   = & n[2];
int **  p2   = & p1;
```



This can be generalised to multiple dimensions:

```
int   n1[4], n2[4], n3[4], n4[4];
int * p1   = n1;
int * p2   = n2;
int * p3   = n3;
int * p4   = n4;

int * p[4] = { p1, p2, p3, p4 };

cout << p[1][3] << endl; // yields 8
```

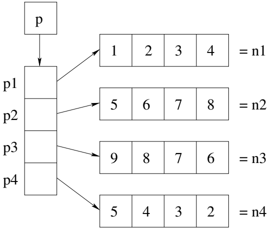


Arrays and Dynamic Memory

Multidimensional Arrays with Pointers

The same example with dynamic memory:

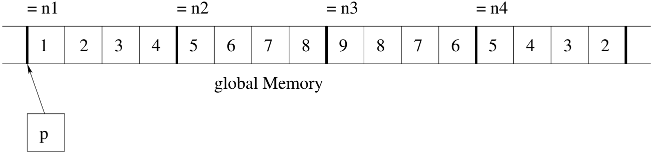
```
int *  p1 = new int[4];
int *  p2 = new int[4];
int *  p3 = new int[4];
int *  p4 = new int[4];

int ** p  = new int*[4];

p[0] = p1;
p[1] = p2;
p[2] = p3;
p[3] = p4;

p[0][0] = 1;
p[0][1] = 2;
...
p[2][2] = 7;
p[2][3] = 6;
p[3][0] = 5;
...
```



Arrays and Dynamic Memory

Multidimensional Arrays with Mappings

Working with pointers to pointers is only one way to implement multidimensional arrays. You can also map the multiple dimensions to just one:



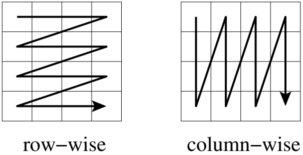
```
int  * p = new int[4*4];

p[ 2 * 4 + 1 ] = 8;  // p[2][1]
p[ 0 * 4 + 2 ] = 3;  // p[0][2]
```

Arrays and Dynamic Memory

Multidimensional Arrays with Mappings

In theory, one could use any mapping. In practise, two different mappings are standard:

- row-wise: standard in C, C++
- column-wise: standard in Fortran, Matlab



For a two-dimensional array, e.g. a matrix, with dimensions $n \times m$, the mappings are for index (i, j):

- row-wise: $i \cdot m + j$,
- column-wise: $j \cdot n + i$.

It is up to you, which mapping you prefer.

Arrays and Dynamic Memory

Example: $n \times m$ Matrix (row-wise)

```
void
set_entry ( const double * M,
            const int i, const int j,
            const int m, const double f )
{
    M[ i*m + j ] = f;
}

int
main ()
{
    int      n = 10;
    int      m = 20;
    double * M = new double[ n * m ];

    set_entry( M, 3, 1, m, 3.1415 );
    set_entry( M, 2, 7, m, 2.7182 );
}
```

Arrays and Dynamic Memory

Comparison: Pointers vs. Mapping

Two approaches have been introduced for multidimensional arrays: pointers of pointers and user defined mapping. Which is to be preferred?

A user defined mapping is faster since only simple arithmetic is performed for a memory access. The pointer based approach needs to follow each pointer individually, resulting in many memory accesses.

Pointers are more flexible, e.g. for triangular matrices, whereas a special mapping has to be defined for each shape.

My recommendation: use mappings, especially if you want fast computations.

Arrays and Dynamic Memory

Application: BLAS

Properties and requirements:

- vectors are onedimensional arrays, matrices implemented via mapping (row-wise),
- should provide functions for all standard operations, e.g. creation, access, linear algebra

Initialisation:

```
inline double *
vector_init ( const unsigned  i )
{
    return new double[i];
}

inline double *
matrix_init ( const unsigned  n, const unsigned  m )
{
    return new double[ n * m ];
}
```

Arrays and Dynamic Memory

Application: BLAS

Vector Arithmetic:

```
void fill  ( const unsigned  n, const double f, double * y );
void scale ( const unsigned  n, const double f, double * y );

void add   ( const unsigned  n, const double f, const double * x,
             double * y )
{ for ( unsigned i = 0; i < n; i++ ) y[i] += f * x[i]; }

double
dot ( const unsigned  n, const double * x, const double * y )
{
    double  d = 0.0;

    for ( unsigned i = 0; i < n; i++ ) d += x[i] * y[i];
    return d;
}

inline double
norm2 ( const unsigned  n, const double * x )
{ return sqrt( dot( n, x, x ) ); }
```

Arrays and Dynamic Memory

Application: BLAS

Matrix Arithmetic:

```
void
fill ( const unsigned  n, const unsigned  m,
       const double f, double * M )
{ fill( n*m, f, M ); }       // use vector based fill

void
scale ( const unsigned  n, const unsigned  m,
        const double f, double * M );

void
add ( const unsigned  n, const unsigned  m,
      const double f, const double * A, double * M );

inline double
normF ( const unsigned  n, const unsigned  m,
        double * M )
{ return norm2( n*m, M ); }  // use vector based norm2
```

Arrays and Dynamic Memory

Application: BLAS

Matrix-Vector Multiplication $y := y + \alpha A \cdot x$:

```
void
mul_vec ( const unsigned  n, const unsigned  m,
          const double alpha, const double * M, const double * x,
          double * y )
{
    for ( unsigned i = 0; i < n; i++ )
    {
        double  f = 0.0;

        for ( unsigned j = 0; j < m; j++ )
            f += get_entry( n, m, i, j, M ) * x[j];
        // alternative: f = dot( m, & M[ i * m ], x );

        y[i] += alpha * f;
    }
}
```

Remark

Compute dot product in local variable to minimize memory accesses.

Arrays and Dynamic Memory

Application: BLAS

Matrix-Matrix Multiplication $C := C + \alpha A \cdot B$:

```
void
mul_mat ( const unsigned n, const unsigned m, const unsigned k,
          const double alpha, const double * A, const double * B,
          double * C )
{
    for ( unsigned i = 0; i < n; i++ )
        for ( unsigned j = 0; j < m; j++ )
        {
            double  f = 0.0;

            for ( unsigned l = 0; l < k; l++ )
                f += get_entry( n, k, i, l, A ) *
                     get_entry( k, m, l, j, B );

            add_entry( n, m, i, j, f, M );
        }
}
```

Arrays and Dynamic Memory

Application: BLAS

```
double * M = matrix_init( 10, 10 );
double * x = vector_init( 10 );
double * y = vector_init( 10 );

fill( 10, 1.0, x );
fill( 10, 0.0, y );

...  // fill matrix M

cout << normF( 10, 10, M ) << endl;

mul_vec( 10, 10, -1.0, M, x, y );
```

Arrays and Dynamic Memory

Strings

One important datatype was not mentioned up to now: strings. Strings are implemented in C++ as *arrays of characters*, e.g.

`char str[]` *or* `char * str`

As arrays have no size information, there is no information about the length of a string stored. To signal the end of a string, by convention the character '0' is used (as an integer, not the digit), entered as '\0':

```
char  str[] = { 'S', 't', 'r', 'i', 'n', 'g', '\0' };
```

Constant strings can also be defined and used directly with ‘‘...’’:

```
char  str[] = "String";  // array initialisation
```

Here, '\0' is automatically appended.

Arrays and Dynamic Memory

Strings

If a string is too long for one input line, it can be wrapped by a backslash '\':

```
const char *  str = "This is a very long \
string";
```

C++ does not provide operators for string handling, e.g. concatenation or searching for substrings. All of that has to be implemented via functions:

```
char * concat ( const char * str1, const char * str2 )
{
    const unsigned  len1 = strlen( str1 );
    const unsigned  len2 = strlen( str2 );
    char *          res  = new char[ len1 + len2 + 1 ];
    int             pos  = 0, pos2 = 0;

    while ( str1[pos]  != ’\0’ ) { res[pos]   = str1[pos]; pos++; }
    while ( str2[pos2] != ’\0’ ) { res[pos++] = str2[pos2++]; }
    res[pos] = ’\0’;

    return res;
}
```

Arrays and Dynamic Memory

Strings

Usage:

```
const char * str1 = "Hallo ";
char *       str2 = concat( str1, "World" );

cout << str2 << endl;

delete[] str2;  // don't forget to deallocate!
```

It can not be emphasised too much:

Coding Principle No. 17

Always ensure, that strings are terminated by '\0'.

Otherwise, operations on strings will fail due to array boundary violations.

Arrays and Dynamic Memory

Strings

'\0' is one example of a special character in C++ strings. Others are

Character	Result
'\n'	a new line
'\t'	a tab
'\r'	a carriage return
'\b'	a backspace
'\′'	single quote '′'
'\ “'	double quote '“'
'\\'	backslash '\'

Examples:

```
cout << "First \t Second"  << endl;
cout << "line1 \n line2"   << endl;
cout << "special \"word\"" << endl;
cout << "set1 \\ set2"     << endl;
```

Advanced Datatypes

Advanced Datatypes

Type Definition

Often you do not always want to care about the actual datatype used in your program, e.g. if it is `float` or `double` or if strings are `char *`, but instead give the types more reasonable names, e.g. `real` or `string`. In C++ you can do this via **typedef**:

> **typedef** ⟨*data type*⟩ ⟨*name*⟩*;*

Afterwards, ⟨name⟩ can be used like any other datatype:

```
typedef  double      real_t;
typedef  char *      string_t;
typedef  real_t **   matrix_t;  // pointers of pointers

const string_t  str = "String";
matrix_t        A   = new real_t*[ 10 ];
real_t          f   = real_t( 3.1415926 );
```

Advanced Datatypes

Type Definition

Remark

A `real_t` datatype allows you to easily change between `float` and `double` in your program.

To simplify the destinction between variables and datatypes, the following is strongly advised:

Coding Principle No. 18

Follow a strict convention in naming new types, e.g. with special prefix or suffix.

Advanced Datatypes

Predefined Types

The C++ library and the operating system usually define some abbreviations for often used types, e.g.

- `uint`: unsigned integer, sometimes special versions `uint8`, `uint16` and `uint32` for 8, 16 and 32 bit respectively,
- similar `int8`, `int16` and `int32` are defined for signed integers,
- `size_t` : unsigned integer type for holding size informations best suited for the local hardware
- `ssize_t` : analog to `size_t` but signed integer (not always available)

Advanced Datatypes

Records

Working with vectors and matrices always involved several variables, e.g. the size and the arrays. That results in many arguments to functions and hence, to possible errors. It would be much better to store all associated data together. That is done with records:

```
struct ⟨record name⟩ {
    ⟨datatype 1⟩ ⟨name 1⟩;
    ⋮
    ⟨datatype n⟩ ⟨name n⟩;
};
```

By defining a **struct**, also a new type named ⟨record name⟩ is defined.

Advanced Datatypes

Records

Example:

```
struct vector_t {
    size_t    size;
    real_t *  coeffs;
};

struct matrix_t {
    size_t    nrows, ncolumns;
    real_t *  coeffs;
};

void
mul_vec ( const real_t      alpha,
          const matrix_t &  A,
          const vector_t &  x,
          vector_t &        y );

struct triangle_t {
    int     vtx_idx[3];  // indices to a vertex array
    real_t  normal[3];
    real_t  area;
};
```

Advanced Datatypes

Access Records

The individual variables in a record are accessed via “.”, e.g.:

```
vector_t  x;

x.size   = 10;
x.coeffs = new real_t[ x.size ];
```

If a pointer to a record is given, the access can be simplified. Instead of “*” (dereference) and “.”, the operator “->” is provided:

```
vector_t *  x = new vector_t;

x->size = 10;
x->data = new real_t[ x->size ];

cout << (*x).size << endl; // alternative
```

Advanced Datatypes

Access Records

In case of a reference, e.g. `vector_t &`, the standard access has to be used, e.g. via "`.`":

```
vector_t  x;

x.size   = 10;
x.coeffs = new real_t[ x.size ];

vector_t & y = x;

cout << y.size << endl;
cout << y.coeffs[5] << endl;
```

Advanced Datatypes

Records and Functions

Records can be supplied as normal function arguments, either as call-by-value or call-by-reference:

```
double dot  ( const vector_t  x, const vector_t    y );
void   fill ( const real_t    f, vector_t &        y );
void   add  ( const real_t    f, const vector_t &  x,
              vector_t &      y );
```

When using call-by-value, a copy of the complete record is actually created. For large records, this can be a significant overhead:

```
struct quadrule_t {
    real_t   points[  100 ];
    real_t   weights[ 100 ];
};

double quadrature ( const quadrule_t  rule,
                    double ( * func ) ( const double x ) );
```

Advanced Datatypes

Records and Functions

In such cases, call-by-reference with a **const** argument is necessary to avoid this overhead:

```
double quadrature ( const quadrule_t &  rule,
                    double ( * func ) ( const double x ) );
```

Here, only a single pointer is supplied to the function instead of 200 `real_t` values.

Application: BLAS (Version 2)

Modified BLAS function set using the previous record types for vectors and matrices:

```
inline vector_t *
vector_init ( const unsigned  i )
{
    vector_t *  v = new vector_t;

    v->size = i;
    v->coeffs = new real_t[ i ];

    for ( unsigned i = 0; i < n; i++ )  // RAII
        v->coeffs[i] = 0.0;

    return v;
}

inline matrix_t *
matrix_init ( const unsigned  n, const unsigned  m )
{ ... }
```

Application: BLAS (Version 2)

```
// vector functions
void fill  ( const double f, vector_t & x );
void scale ( const double f, vector_t & x );

void add   ( const double f, const vector_t & x, vector_t & y )
{
    for ( unsigned i = 0; i < n; i++ )
        y.coeffs[i] += f * x.coeffs[i];
}

double        dot   ( const vector_t & x, const vector_t & y );
inline double norm2 ( const vector_t & x )
{ return sqrt( dot( x, x ) ); }

// matrix functions
void fill  ( const double f, matrix_t & M );
void scale ( const double f, matrix_t & M );
void add   ( const double f, const matrix_t & A, matrix_t & M );

inline double
normF ( double & M )
{ ... }  // can not use vector based norm2!
```

Advanced Datatypes

Application: BLAS (Version 2)

```
void
mul_vec ( const double       alpha,
          const matrix_t &   M,
          const vector_t &   x,
          vector_t &         y )
{
    for ( unsigned i = 0; i < M.nrows; i++ )
    {
        double  f = 0.0;

        for ( unsigned j = 0; j < M.ncolumns; j++ )
            f += get_entry( M, i, j ) * x.coeffs[j];

        y.coeffs[i] += alpha * f;
    }
}

void
mul_mat ( const double       alpha,
          const matrix_t &   A,
          const matrix_t &   B,
          matrix_t &         C );
```

Advanced Datatypes

Application: BLAS (Version 2)

```
matrix_t * M = matrix_init( 10, 10 );
vector_t * x = vector_init( 10 );
vector_t * y = vector_init( 10 );

fill( 1.0, x );
fill( 0.0, y );

...  // fill matrix M

cout << normF( M ) << endl;

mul_vec( -1.0, M, x, y );
```

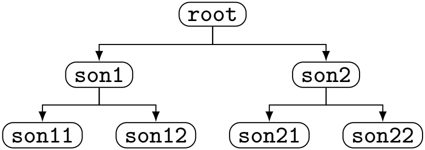
Advanced Datatypes

Recursive Records

Records can have variables of it's own type in the form of a pointer. That way, recursive structures can be defined, e.g. a binary tree:

```
struct node_t {
    int       val;
    node_t *  son1, * son2;
};

node_t  root;
node_t  son1, son2;
node_t  son11, son12, son21, son22;

root.son1 = & son1;  root.son2 = & son2;
son1.son1 = & son11; son1.son2 = & son12;
son2.son1 = & son21; son2.son2 = & son22;
```

The above code yields:



Advanced Datatypes

Recursive Records

Insert new value in binary tree:

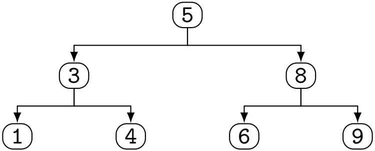
```
void
insert ( const node_t & root, const int val )
{
    if ( val < root.val )
    {
        if ( root.son1 != NULL )
            insert( * root.son1, val );
        else
        {
            root.son1       = new node_t;
            root.son1->val  = val;
            root.son1->son1 = NULL;
            root.son1->son2 = NULL;
        }
    }
    else
    {
        if ( root.son2 != NULL )
            insert( * root.son2, val );
        else
            ...
}   }
```

Recursive Records

Example for insertion:

```
int     values[7] = { 5, 3, 1, 4, 8, 6, 9 };
node_t  root;

root.son1 = root.son2 = NULL;
root.val  = values[0];

for ( int i = 1; i < 7; i++ )
    insert( root, values[i] );
```

yields:



Advanced Datatypes

Recursive Records

Looking for value in binary tree:

```
bool
is_in ( const node_t & root, const int val )
{
    if ( root.val == val )
        return true;

    return is_in( * root.son1, val ) ||
           is_in( * root.son2, val );
}

...

    cout << is_in( root, 6 ) endl;  // yields true
    cout << is_in( root, 7 ) endl;  // yields false
```

Advanced Datatypes

Arrays of Records

Like any other datatype, records can also be allocated in the form of an array:

```
struct coord_t {
    real_t  x, y, z;
};

coord_t   coordinates[ 10 ];
```

for fixed sized array or

```
coord_t * coordinates = new coord_t[ 10 ];
```

using dynamic memory management.

Advanced Datatypes

Arrays of Records

The access to record variables then comes after addressing the array entry:

```
for ( unsigned i = 0; i < 10; i++ )
{
    coordinates[i].x = cos( real_t(i) * 36.0 * pi / 180.0 );
    coordinates[i].y = sin( real_t(i) * 36.0 * pi / 180.0 );
    coordinates[i].z = real_t(i) / 10.0;
}
```

If instead, an array of pointers to a record is allocated:

```
coord_t ** coordinates = new coord_t*[ 10 ];

for ( int i = 0; i < 10; i++ )
    coordinates[i] = new coord_t;
```

the access if performed with the arrow operator ->:

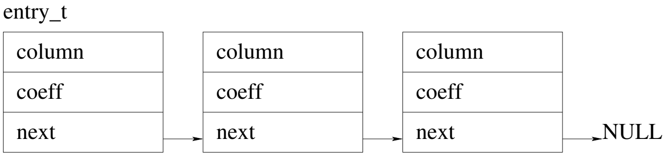
```
    coordinates[i]->x = cos( real_t(i) * 36.0 * pi / 180.0 );
```

Record Application: Sparse Matrices

We only want to store nonzero entries in a sparse matrix. For this, each entry is stored in a record type, containing the column index and the coefficient:

```
struct entry_t {
    unsigned   column;  // column of the entry
    real_t     coeff;   // actual coefficient
    entry_t *  next;    // next entry in row
};
```

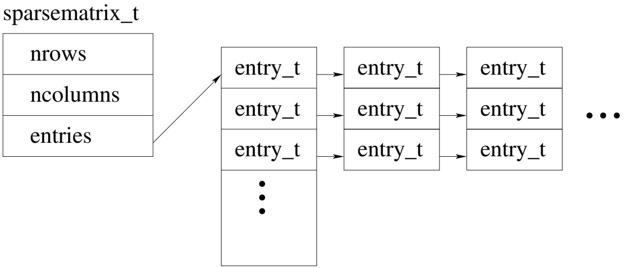
All entries in a row are stored in a list, provided by the `next` pointer in an entry type. A **NULL** value of `next` signals the end of the list.



Record Application: Sparse Matrices

A sparse matrix is then allocated as an array of entry lists per row:

```
struct sparsematrix_t {
    unsigned   nrows, ncolumns;
    entry_t *  entries;
};
```

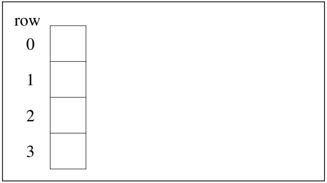


Advanced Datatypes

Record Application: Sparse Matrices

As an example, consider the matrix

$$\begin{pmatrix} 1 & & 3 & \\ & 2 & & -1 \\ -4 & -1 & 1 & \\ 1 & & & 3 \end{pmatrix}$$



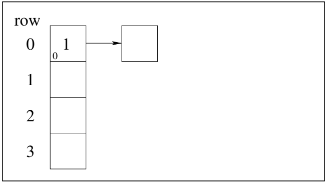
```
sparsematrix_t  S;
entry_t *       entry;

S.nrows = 4; S.ncolumns = 4;
S.entries = new entry_t[4];

// first row
entry = & S.entry[0];
entry->column = 0;  entry->coeff = 1.0; entry->next = new entry_t;

entry = entry->next;
entry->column = 2;  entry->coeff = 3.0; entry->next = NULL;
...
```

Advanced Datatypes

Record Application: Sparse Matrices

As an example, consider the matrix

$$\begin{pmatrix} 1 & & 3 & \\ & 2 & & -1 \\ -4 & -1 & 1 & \\ 1 & & & 3 \end{pmatrix}$$

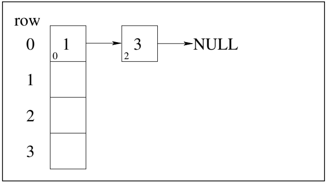


```
sparsematrix_t  S;
entry_t *       entry;

S.nrows = 4; S.ncolumns = 4;
S.entries = new entry_t[4];

// first row
entry = & S.entry[0];
entry->column = 0;  entry->coeff = 1.0; entry->next = new entry_t;

entry = entry->next;
entry->column = 2;  entry->coeff = 3.0; entry->next = NULL;
...
```

Record Application: Sparse Matrices

As an example, consider the matrix

$$\begin{pmatrix} 1 & & 3 & \\ & 2 & & -1 \\ -4 & -1 & 1 & \\ 1 & & & 3 \end{pmatrix}$$

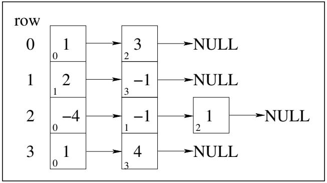


```
sparsematrix_t  S;
entry_t *       entry;

S.nrows = 4; S.ncolumns = 4;
S.entries = new entry_t[4];

// first row
entry = & S.entry[0];
entry->column = 0;  entry->coeff = 1.0; entry->next = new entry_t;

entry = entry->next;
entry->column = 2;  entry->coeff = 3.0; entry->next = NULL;
...
```

Record Application: Sparse Matrices

As an example, consider the matrix

$$\begin{pmatrix} 1 & & 3 & \\ & 2 & & -1 \\ -4 & -1 & 1 & \\ 1 & & & 3 \end{pmatrix}$$



```
sparsematrix_t  S;
entry_t *       entry;

S.nrows = 4; S.ncolumns = 4;
S.entries = new entry_t[4];

// first row
entry = & S.entry[0];
entry->column = 0;  entry->coeff = 1.0; entry->next = new entry_t;

entry = entry->next;
entry->column = 2;  entry->coeff = 3.0; entry->next = NULL;
...
```

Advanced Datatypes

Record Application: Sparse Matrices

Matrix-Vector multiplication:

```
void
mul_vec ( const real_t   alpha, const sparsematrix_t & S,
          const vector_t x, vector_t & y )
{
    for ( unsigned i = 0; i < S.nrows; i++ )
    {
        real_t    f     = 0.0;
        entry_t * entry = & S.entries[i];

        while ( entry != NULL )
        {
            f     += entry->coeff * x[ entry->column ];
            entry  = entry->next;
        }

        y[ i ] += alpha * f;
    }
}
```

Advanced Datatypes

Record Application: Sparse Matrices (Version 2)

We can store sparse matrices even more memory efficient, without pointers. For this, we'll use three arrays:

- `colind`: stores column indices for all entries, sorted by row,
- `coeffs`: stores all coefficients in same order as in `colind` and
- `rowptr`: stores at `rowind[i]` the position of the first values corresponding to row i in the arrays `colind` and `coeffs`. The last field, contains the number of nonzero entries.

This format is known as the *compressed row storage* format.

```
struct crsmatrix_t {
    unsigned    nrows, ncolumns;
    unsigned *  rowptr;
    unsigned *  colind;
    real_t *    coeffs;
};
```

Advanced Datatypes

Record Application: Sparse Matrices (Version 2)

For the matrix

$$\begin{pmatrix} 1 & & 3 & \\ & 2 & & -1 \\ -4 & -1 & 1 & \\ 1 & & & 3 \end{pmatrix}$$

the corresponding source code is:

```
crsmatrix_t  S;
unsigned     rowptr[] = { 0, 2, 4, 7, 9 };
unsigned     colind[] = { 0, 2,   1,  3,    0,  1, 2,   0, 3 };
real_t       coeffs[] = { 1, 3,   2, -1,   -4, -1, 1,   1, 3 };

S.nrows = 4; S.ncolumns = 4;
S.rowptr = rowptr;
S.colind = colind;
S.coeffs = coeffs;
```

Record Application: Sparse Matrices (Version 2)

Matrix-Vector multiplication:

```
void
mul_vec ( const real_t   alpha, const crsmatrix_t & S,
          const vector_t x, vector_t & y )
{
    for ( unsigned row = 0; row < S.nrows; row++ )
    {
        real_t         f  = 0.0;
        const unsigned lb = S.rowptr[ row ];
        const unsigned ub = S.rowptr[ row+1 ];

        for ( unsigned j = lb; j < ub; j++ )
            f += S.coeffs[ j ] * x[ S.colind[ j ] ];

        y[ i ] += alpha * f;
    }
}
```

Advanced Datatypes

Enumerations

A special datatype is available to define enumerations:

> **enum** ⟨*enum name*⟩ {
>   ⟨*name 1*⟩, ⟨*name 2*⟩, . . ., ⟨*name n*⟩
> };

Example:

```
enum matrix_type_t { unsymmetric, symmetric, hermitian };

matrix_type_t  t;

if ( t == symmetric ) { ... }
```

Enumerations are handled as integer datatypes by C++. By default, the members of an enumeration are numbered from 0 to $n-1$, e.g. <name 1>$= 0$, <name 2>$= 1$, etc..

Advanced Datatypes

Enumerations

One can also define the value of the enumeration members explicitly:

```
enum matrix_size_t { small = 10, middle = 1000, large = 1000000 };

if      ( nrows < small  ) { ... }
else if ( nrows < middle ) { ... }
else if ( nrows < large  ) { ... }
else                       { ... }
```

Since enumerations are equivalent to integer types, they can also be used in **switch** statements:

```
switch ( type )
{
case symmetric:   ...; break;
case hermitian:   ...; break;

case unsymmetric:
default:          ...;
}
```

Advanced Datatypes

Unions

A union is a special record datatype where all variables share the same memory, i.e. changing one variable changes all other variables.

```
union ⟨union name⟩ {
    ⟨datatype 1⟩ ⟨name 1⟩;
    ⋮
    ⟨datatype n⟩ ⟨name n⟩;
};
```

Example:

```
union utype_t {
    int    n1;
    int    n2;
    float  f;
};
```

```
utype_t  u;

u.n1 = 2;
cout << u.n2 << endl;  // yields 2
cout << u.f  << endl;  // ???
```

Advanced Datatypes

Unions

Unions can also be used inside records:

```
enum smat_type_t { ptr_based, crs_based };

struct general_sparse_matrix_t {
    smat_type_t  type;

    union {
        sparsematrix_t  ptrmat;
        crsmatrix_t     crsmat;
    } matrix;
};

general_sparse_matrix_t  S;

S.type = ptr_based;
S.matrix.ptrmat.nrows = 10;
```

Remark

Typical usage for unions: save memory for different representations.

Advanced Datatypes

Unions

The name matrix of the **union** can be omitted. The access is then as if it were a direct member of the **struct**.

```
enum smat_type_t { ptr_based, crs_based };

struct general_sparse_matrix_t {
    smat_type_t  type;

    union {
        sparsematrix_t  ptrmat;
        crsmatrix_t     crsmat;
    };
};

general_sparse_matrix_t  S;

S.type = ptr_based;
S.ptrmat.nrows = 10;
```

Modules and Namespaces

Modules and Namespaces

Header Files

Up to now, all source code was placed into one file. For reasonable programs, this is not desirable, especially if functions are reused by different programs.

Unfortunately, C++ has no real module system like, e.g. Pascal or Java, to group similar functions or types. Instead, header files are used to make C++ objects known to different source files.

As you remember, functions can be used if they were previously declared or implemented. By separating declaration and implementation into header and source file:

```
// header file: f.hh

void f ( int n, double f );
```

```
// source file: f.cc

void f ( int n, double f )
{ ... }
```

the function can be reused by just including the header file.

Modules and Namespaces

Header Files

Including another file into the current source code is performed by the **include** directive:

#include *“filename”* *or*
#include <*filename*>

The first version is usually used for files in the same project, whereas the second version is for files from other projects, e.g. the operating system or the C++ compiler.

```
#include "f.hh"   // contains decl. of "f"

int main ()
{
    f( 42, 3.1415926 );
}
```

Modules and Namespaces

Header Files

Remark

By convention, the filename suffix of the header file should be either "h" (like in C), "H", "hh" or "hpp".

Modules and Namespaces

C++ Library

The C++ compiler comes with a set of standard include files containing declarations of many functions:

`cstdlib`: standard C functions, e.g.

- `exit`: stop program,
- `atoi` and `atof`: string to `int` and `double` conversion,
- `qsort`: sort arrays,
- `malloc` and `free`: C-style dynamic memory management,

`cmath`: mathematical functions, e.g.

- `sqrt`: square root,
- `abs`: absolute value,
- `sin` and `cos`,
- `log`: natural logarithm

Modules and Namespaces

C++ Library

`cstdio`: C-style IO functions, e.g.

- `printf`: print variables to standard output,
- `fopen`, `fclose`, `fread` and `fwrite`: file IO

`cstring`: string functions, e.g.

- `strlen`: string length,
- `strcat`: string concatenation,
- `strcmp`: string comparison,
- `strcpy`: string copy

`cctype`: character tests, e.g.

- `isdigit`: test for digit,
- `islower`: test for lower case,
- `isspace`: test for white-space

etc.: `cassert`, `cerrno`, `cinttypes`, `climits`, `ctime`.

Modules and Namespaces

C++ Library

Specific C++ functionality usually comes in the form of the *standard template library*. It is implemented via classes (see later) and provided by the following header files:

- `iostream`: file input/output functions and classes,
- `vector`: dynamic containers similar to arrays,
- `valarray`: similar to `vector` but better suited for numerics,
- `limits`: functions for determining type limits, e.g. minimal or maximal values,
- `map`: associative array, e.g. indices are arbitrary types,
- `list`: provides standard list and iterators,
- `complex`: provides complex datatype,
- etc.

The specific classes and their usage will be discussed later.

Modules and Namespaces

Libraries without Headers (LAPACK)

LAPACK is written in Fortran and no header files exist for C++. Therefore, we will have to write them ourselves. Consider

```
 SUBROUTINE DGESVD( JOBU, JOBVT, M, N, A, LDA, S, U, LDU, VT, LDVT,
$                   WORK, LWORK, INFO )

 CHARACTER          JOBU, JOBVT
 INTEGER            INFO, LDA, LDU, LDVT, LWORK, M, N
 DOUBLE PRECISION   A( LDA, * ), S( * ), U( LDU, * ),
$                   VT( LDVT, * ), WORK( * )
```

To define a C++ function corresponding to the above Fortran function the datatypes have to be mapped to C++ types. In Fortran, every variable is provided as a pointer, hence:

CHARACTER → char *,
INTEGER → int * and
DOUBLE PRECISION → double *.

Modules and Namespaces

Libraries without Headers (LAPACK)

Fortran function names are in lower case and end with and underscore '_', when seen from C or C++. Hence, the name of the above Fortran function is dgesvd_:

```
void dgesvd_ ( char * jobu, char * jobv, int * n, int * m,
               double * A, int * lda, double * S, double * U,
               int * ldu, double * V, int * ldv, double * work,
               int * lwork, int * info );
```

Furthermore, there is a difference between C and C++ functions. Fortran only provides C-style functions, whereas the above is a C++ function. To tell the compiler, that a C-style function should be declared, the **extern "C"** instruction is provided:

```
extern "C" {
void dgesvd_ ( char * jobu, char * jobv, int * n, int * m,
               double * A, int * lda, double * S, double * U,
               int * ldu, double * V, int * ldv, double * work,
               int * lwork, int * info );
}
```

Modules and Namespaces

Libraries without Headers (LAPACK)

Afterwards, the function `dgesvd_` can be used like any other C++ function. To compute the SVD $M = U \cdot S \cdot V^T$ of a matrix M, the code looks like:

```
int          n     = 10;
double *     M     = new double[ n*n ];
char         jobu  = ’O’;                  // overwrite M with U
char         jobv  = ’S’;                  // store V^T in VT
int          info  = 0;
int          lwork = 10*n*n;
double *     work  = new double[ work ]; // workspace for dgesvd
double *     S     = new double[ n ];
double *     VT    = new double[ n*n ];

... // fill M

dgesvd_( & jobu, & jobv, & n, & n, M, & n, S, M, & n, V, & ldv,
         work, & lwork, & info );
```

Modules and Namespaces

Header File Recursion

The **include** directive can be seen as simple text replacement: the directive is replaced by the content of the corresponding file.

```
#include "f.hh"

int main ()
{
    f( 42, 3.1415926 );
}
```

```
void f ( int n, double f );

int main ()
{
    f( 42, 3.1415926 );
}
```

This might lead to infinite loops, if you have recursive **include** directives in different files, e.g. “file1.hh” includes “file2.hh”, which by itself includes “file1.hh”.

```
// FILE: file1.hh

#include "file2.hh"

...
```

```
// FILE: file2.hh

#include "file1.hh"

...
```

Modules and Namespaces

Header File Encapsulation

To prevent infinite loops, two other directives are provided:

> **#ifndef** ⟨*NAME*⟩
> ⋮
> **#endif**

tests, if the symbol ⟨NAME⟩ was previously defined by the directive

> **#define** ⟨*NAME*⟩

If it was not defined, all source code between the **ifndef** directive and the corresponding **endif** will be included by the C++ compiler. Otherwise, the source code will be omitted.

Remark

> *It is recommended to name the symbol ⟨NAME⟩ after the name of the header file.*

Modules and Namespaces

Header File Encapsulation

Now, for the recursive example:

```
// FILE: file1.hh

#ifndef __FILE1_HH
#define __FILE1_HH

#include "file2.hh"

#endif
```

```
// FILE: file2.hh

#ifndef __FILE2_HH
#define __FILE2_HH

#include "file1.hh"

#endif
```

If “file1.hh” is included by a source file, the symbol “__FILE1_HH” will be defined and the content of the header file included. Similar, `#include ‘‘file2.hh’’` will be replaced by the content of “file2.hh”. If now again “file1.hh” should be included, “__FILE1_HH” is already defined and the content of “file1.hh” is omitted, stopping the recursion.

Modules and Namespaces

Header File Encapsulation

Coding Principle No. 19

Always encapsulate your header files by an **ifndef-define-endif** *construct.*

Modules and Namespaces

Inline Functions

It is also possible to implement a function in a header file. In that case, it has to be declared **inline**, because otherwise, the function is defined in each source file, where the header is included. If you than compile all source files together, you would have multiple instances of the same function, which is not allowed.

```
#ifndef __SQUARE_HH
#define __SQUARE_HH

inline
double
square ( const double x )
{
    return x*x;
}

#endif
```

Modules and Namespaces

Variables

Beside functions, you can also declare variables in header files. For non-const data, the declaration and definition has to be separated to prevent multiple instances. In the header file, the variables have to be declared with the keyword **extern**:

```
// header file: real.hh

#ifndef  __REAL_HH
#define  __REAL_HH

typedef double  real_t;

const  real_t  PI = 3.1415926;   // const: "extern" not needed
extern real_t  eps;
extern int     stepwidth;

#endif
```

Modules and Namespaces

Variables

The definition than has to be made in a source file:

```
// source file: real.cc

#include "real.hh"  // for real_t

real_t  eps       = 1e-8;
int     stepwidth = 1024;
```

Afterwards, every module including the corresponding headerfile has access to the variables `eps` and `stepwidth`:

```
#include "real_t.hh"

int
main ()
{
    eps = 1e-4;
    cout << stepwidth << endl;

    return 0;
}
```

Modules and Namespaces

Module Scope

If a function or variable is declared in a header file, it is globally visible by all other parts of the program. It is in global scope.
For variables, that simplifies access, e.g. global variables do not need to be supplied as function parameters. But it has a major drawback: every function can change the variable, independent on possible side effects.
Better approach: define a function for changing the variable. That way, the access can be controlled:

```
// header
void
set_eps ( const real_t  aeps );

real_t
get_eps ();
```

```
// source
static real_t eps = 1e-8;

void
set_eps ( const real_t  aeps )
{
  if      ( aeps < 0.0 ) eps = 0.0;
  else if ( aeps > 1.0 ) eps = 1.0;
  else                   eps = aeps;
}
```

Modules and Namespaces

Module Scope

Therefore:

Coding Principle No. 20

Only if absolutely neccessary make non-const variables global.

Remark

The **static** *declaration of a variable or function in a source file prevents other modules from using that variable or function, respectively.*

Modules and Namespaces

Namespaces

Following situation: we have written datatypes and functions for dense matrices in a module, e.g.

```
struct matrix_t {
    size_t    nrows, ncolumns;
    real_t *  coeffs;
};

matrix_t *  init    ( ... );
void        mul_vec ( ... );
```

and you want to join that with another module for sparse matrices:

```
struct matrix_t {
    size_t    nrows, ncolumns, nnzero;
    size_t *  rowptr, * colind;
    real_t *  coeffs;
};

matrix_t * init    ( ... );
void       mul_vec ( ... );
```

Modules and Namespaces

Namespaces

Problem: although functions with the same name are allowed, two datatypes must not have the same name.

Solution 1: rename all occurences of `matrix_t` for sparse matrices, and change all functions, or

Solution 2: put each type and function set into a different namespace.

A namespace is a mechanism in C++ to group types, variables and functions, thereby defining the scope of these objects, similar to a block. Till now, all objects were in the global namespace.

Namespace definition:

```
namespace ⟨namespace name⟩ {
    ⋮
}
```

Modules and Namespaces

Namespaces

Applied to the two matrix modules from above:

```
namespace Dense {

struct matrix_t {
  unsigned  nrows, ncolumns;
  real_t *  coeffs;
};


matrix_t *  init    ( ... );
void        mul_vec ( ... );

}
```

```
namespace Sparse {

struct matrix_t {
  unsigned    nrows, ncolumns, nnzero;
  unsigned *  rowptr, * colind;
  real_t *    coeffs;
};

matrix_t * init    ( ... );
void       mul_vec ( ... );

}
```

This defines two namespaces `Dense` and `Sparse`, each with a definition of `matrix_t` and corresponding functions.

Modules and Namespaces

Namespace Access

The access to functions or types in a namespace is performed with the namespace operator "**::**" :

```
Dense::matrix_t *   D = Dense::init(  10, 10 );
Sparse::matrix_t *  S = Sparse::init( 10, 10, 28 );

Dense::mul_vec(  1.0, D, x, y );
Sparse::mul_vec( 1.0, S, x, y );
```

Modules and Namespaces

Namespace Access

To make all objects in a namespace visible to the local namespace, the keyword **using** is provided:

```
using namespace Dense;
using namespace Sparse;

Dense::matrix_t *   D = init( 10, 10 );     // call to Dense::init
Sparse::matrix_t *  S = init( 10, 10, 28 ); // call to Sparse::init

mul_vec( 1.0, D, x, y );                    // call to Dense::mul_vec
mul_vec( 1.0, S, x, y );                    // call to Sparse::mul_vec
```

Remark

Remember, that types must have different names.
Hence, the types for `D` *and* `S` *have to be named with their namespaces.*

Modules and Namespaces

Namespace Access

Restrict the usage of **using** to source files and avoid **using** directives in header files, because all modules including the header would also include the corresponding **using** instruction:

```cpp
// header file: vector.hh

#include "dense.hh"

using namespace Dense;

...  // vector definitions
```

```cpp
// source file: module.cc

#include "vector.hh"
#include "sparse.hh"

using namespace Sparse;

void  f ( matrix_t & M );
```

Here, `matrix_t` is ambiguous, e.g. either `Dense::matrix_t` or `Sparse::matrix_t`.

Modules and Namespaces

Namespace Aliases

It is also possible to define an alias for a namespace, e.g. to abbreviate it:

```
namespace De = namespace Dense;
namespace Sp = namespace Sparse;

De::matrix_t *  D = De::init( 10, 10 );
Sp::matrix_t *  S = Sp::init( 10, 10, 28 );

De::mul_vec( 1.0, D, x, y );
Sp::mul_vec( 1.0, S, x, y );
```

Modules and Namespaces

Nested Namespaces

Namespaces can also be nested and different parts of a namespace can be defined in different modules:

```
namespace LinAlg {
    namespace Dense {
        ...
    }
}
```

```
namespace LinAlg {
    namespace Sparse {
        ...
    }
}
```

```
LinAlg::Dense::matrix_t *  D = LinAlg::Dense::init(  10, 10 );
LinAlg::Sparse::matrix_t * S = LinAlg::Sparse::init( 10, 10, 28 );

LinAlg::Dense::mul_vec(  1.0, D, x, y );
LinAlg::Sparse::mul_vec( 1.0, S, x, y );
```

Modules and Namespaces

Anonymous Namespaces

Namespaces can also be defined without a name:

```
namespace {
    void f ()
    {
        ...
    }
}
```

The C++ compiler will then automatically assign a unique, hidden name for such a namespace. This name will be different in different modules.

Functions in an anonymous namespace can be used without specifying their namespace name:

```
namespace {
    void f () { ... }
}

void g () { f(); }
```

Modules and Namespaces

Anonymous Namespaces

On the other hand, since the automatically assigned name is unique per module, only functions in the same module as the anonymous namespace can access the functions within:

```
// module 1

namespace {
    void f () { ... }
}

void g ()
{
    f(); // Ok: same module
}
```

```
// module 2

void h ()
{
    f(); // Error: unknown
         // function "f"
}
```

Such functions are therefore hidden for other modules and purely local to the corresponding module.

Modules and Namespaces

Anonymous Namespaces

Remark

If an anonymous namespace is defined in a header file, each module including the header would define a new, local namespace!

Coding Principle No. 21

Put module local functions into an anonymous namespace.

This approach is different from the previous C-style version using **static** functions and variables and should be preferred.

Modules and Namespaces

The std Namespace

All functions (and classes) of the C++ standard library, e.g. `sqrt` or `strcpy` are part of the std namespace. Previous use always assumed a corresponding **using** command:

```
using namespace std;

const real_t  PI     = 3.14159265358979323846;
const real_t  sqrtPI = sqrt( PI );

cout << sqrtPI << endl;
```

is equivalent to

```
const real_t  PI     = 3.14159265358979323846;
const real_t  sqrtPI = std::sqrt( PI );

std::cout << sqrtPI << std::endl;
```

Classes

Classes

Records with Functions

Records were previously introduced only as a way to group data. In C++, records can also be associated with functions.

```
struct vector_t {
    unsigned  size;
    real_t *  coeffs;

    void init  ( const unsigned  n );
    void fill  ( const real_t    f );
    void scale ( const real_t    f );
};
```

For the implementation of these functions, the function name is prefixed by the record name:

```
void vector_t::init ( const uint n )
{
    ...
}
```

Classes

Records with Functions

A record function is called specifically for an instance of a record, using the same dot operator '.' as for record variables:

```
int main ()
{
    vector_t  x;

    x.init( 10 );
    x.fill( 1.0 );
    x.scale( 5.0 );

    return 0;
}
```

Classes

Record Function Implementation

Inside a record function, one has implicit access to all record variables of the specific record object, for which the function was called. Therefore, the following two functions are equivalent:

```
void
vector_t::init ( const uint n )
{
    size   = n;
    coeffs = new real_t[n];
}


...

    x.init( 10 );
```

```
void
init ( vector_t *  x,
       const uint  n )
{
    x->size   = n;
    x->coeffs = new real_t[n];
}

...

    init( x, 10 );
```

Classes

Record Function Implementation

A pointer to the corresponding record object is actually available in C++. It is called **this**. Hence, one can also write:

```
void vector_t::init ( const uint n )
{
    this->size   = n;
    this->coeffs = new real_t[n];
}
```

Record member functions can also be implemented in the definition of the **struct**. They are then automatically declared as **inline** functions:

```
struct vector_t {
    ...
    void init  ( const unsigned  n )   // inline function
    {
        size   = n;
        coeffs = new real_t[n];
    }
    ...
};
```

Classes

Records: const functions

Member functions not changing the record data should be defined as **const** functions:

```
struct vector_t {
    ...
    void    scale ( const real_t  f );
    real_t  norm2 () const;
    ...
};
```

When calling record functions for **const** objects, e.g.

```
const vector_t  x( 10 );
```

only such **const** functions are allowed to be called, since all non-**const** functions potential change the object:

```
cout << x.norm2() << endl;  // Ok: vector_t::norm2 is const
x.scale( 2 );               // ERROR: vector_t::scale is non-const
```

Classes

Records: Constructors and Destructors

There are special functions for each record:

constructors: functions automatically called when a record type is instantiated, e.g. by **new**, and

destructor: a function automatically called when a record variable is destroyed, e.g. by **delete**.

The name of a constructor function is identical to the name of the record, whereas the name of the destructor is the record name prefixed by '~':

```
struct vector_t {
    unsigned  size;
    real_t *  coeffs;

    vector_t  ();                    // constructor 1
    vector_t  ( const unsigned n );  // constructor 2
    ~vector_t ();                    // destructor
};
```

Classes

Records: Constructors and Destructors

By definition, constructors should create necessary resources for the object, whereas destructors should free all record object resources:

```
vector_t::vector_t ()
{
    size   = 0;
    coeffs = NULL;
}

vector_t::vector_t ( const uint  n )
{
    size   = n;
    coeffs = new real_t[n];
}
```

```
vector_t::~vector_t ()
{
    delete[] coeffs;
}
```

Remark

Constructors and the destructor have no return type. Furthermore, destructors must not have function arguments.

Classes

Records: Constructors and Destructors

Example 1: instantiated and destroyed explicitly by **new** and **delete**:

```
vector_t * x = new vector_t();        // calling constructor 1
vector_t * y = new vector_t( 10 );    // calling constructor 2

y->fill( 1.0 );

delete x;                             // calling destructor
```

Remark

> *If the constructor has no arguments, the corresponding parentheses can be omitted:*

```
vector_t * x = new vector_t;          // calling constructor 1
```

Classes

Records: Constructors and Destructors

Example 2: instantiated and destroyed implicitly by block scope:

```
{
    vector_t  x;         // calling constructor 1
    vector_t  y( 10 );   // calling constructor 2

    y.fill( 1.0 );
}                        // destructor called automatically
```

Here, the record objects are not pointers. When leaving the block, the destructors of all record objects are called automatically! Thereby, it is ensured, that all resources are released.

Classes

Records: Special Constructors

By default, each record type has two constructors already implemented by the C++ compiler: the default constructor and the copy constructor.

The default constructor is a constructor without arguments, e.g. constructor 1 in the previous example. The copy constructor is a constructor with one argument being a constant reference to an object of the same type as the record itself:

```
struct vector_t {
    ...
    vector_t ( const vector_t & x );  // copy constructor
    ...
};
```

This is used for

```
vector_t  x( 10 );
vector_t  y( x );     // call copy constructor
vector_t  z = y;      // usually converted to z( y )
```

Classes

Records: Special Constructors

The default constructor implemented by the C++ compiler does nothing, e.g. it does not initialise the member variables. Hence, without a user implemented default constructor, the values of the member variables are random (ref. Coding Principle No. 3).

The C++ generated copy constructor simply copies the data in each member variable of the record:

```
vector_t *  x = new vector_t( 10 );
vector_t *  y = new vector_t( & x ); // now: x.coeffs == y.coeffs,
                                     // e.g. equal pointers
```

Here, changing `y` also changes `x`:

```
x->coeffs[ 5 ] = 2;   // also changes y.coeffs[ 2 ]
y->coeffs[ 3 ] = 4;   // also changes x.coeffs[ 3 ]
```

Classes

Records: Special Constructors

For vectors, instead of the pointers, the content of the array should be copied:

```
vector_t::vector_t ( const vector_t & v )
{
    size   = v.size;
    coeffs = new real_t[ size ];

    for ( uint i = 0; i < size; i++ ) coeffs[i] = v.coeffs[i];
}
```

Now, the instructions

```
vector_t *  x = new vector_t( 10 );
vector_t *  y = new vector_t( & x );

x->coeffs[ 5 ] = 2;
y->coeffs[ 3 ] = 4;
```

only effect either x or y, not both.

Records: Special Constructors

To sum this up:

Coding Principle No. 22

Always make sure, that the C++ generated default and copy constructors behave as expected. If in doubt: implement constructors by yourself.

Classes

Records: Visibility

All member variables and functions of a record were visible and accessible from any other function or datatype in C++. This makes illegal changes to the data in a record possible, e.g. change the `size` variable of `vector_t` without also changing the `coeffs` variable.

To prevent this behaviour, one can change the visibility of variables and functions using one of the following keywords:

public: variables or functions can be accessed without restrictions,

protected: variables or functions can only be accessed by member functions of the record type or by derived records (see later),

private: variables or functions can only be accessed by member functions of the record type.

Classes

Records: Visibility

Example 1:

```
struct vector_t {
private:                       // all following variables and functions
    size_t    size;    // are private
    real_t *  coeffs;

public:                        // all following variables and functions
                       // are public
    vector_t ( const size_t  n );
...
    size_t  get_size () const { return size; }
};

...

{
    vector_t  x( 10 );

    cout << x.size << endl;        // ERROR: <size> is private
    cout << x.get_size() << endl;  // Ok: <get_size> is public
}
```

Records: Visibility

Example 2:

```
struct vector_t {
private:
    size_t    size;
    real_t *  coeffs;

public:

...

protected:
    void init ( const size_t  n )
    {
        size   = n;    // Ok: <size> is visible to member functions
        coeffs = new real_t[n];
    }
};

{
    vector_t  x( 10 );

    x.init( 20 );      // ERROR: <init> is protected
}
```

Classes

Records: Visibility

Illegal states of member variables can be prevented by making them **private** and allowing modifications only via **public** member functions:

```
struct vector_t {
private:
    size_t    size;
    real_t *  coeffs;

public:
    ...
    size_t  get_size () const            { return size; }
    void    set_size ( const size_t  n ) { init( n ); }
    ...
};
```

Coding Principle No. 23

Make all member variables of a record **private** *and allow read-/write-access only via member functions.*

Records: Operator Overloading

In C++, operators, e.g. **+**, *****, **=** or **[·]**, can be defined for record datatypes to simplify access or to ensure correct behaviour.
Depending on the operator, it can be defined inside or outside the record definition, e.g. operators changing the object like **=** or **+=** in the record definition and binary operators working on two objects typically outside the record.
In terms of syntax, operator functions are treated like any other function. The name of the operator is defined by

operator ⟨*operator name*⟩

e.g.

operator =
operator +
operator *
operator []

Records: Operator Overloading (Example)

```
struct vector_t {
    ...
    // provide index operator for vectors
    real_t  operator [] ( const size_t i ) { return coeffs[i]; }

    // arithmetics
    vector_t &  operator += ( const vector_t & v )
    {
        for ( size_t i = 0; i < size; i++ ) coeffs[i] += v.coeffs[i];
        return *this;
    }
    vector_t &  operator -= ( const vector_t & v ) { ... }
    vector_t &  operator *= ( const real_t  f )
    {
        for ( size_t i = 0; i < size; i++ ) coeffs[i] *= f;
        return *this;
    }
    ...
};

{ ...
    x += y;
    y *= 2.0;
}
```

Classes

Records: Operator Overloading

Be very careful when overloading the standard arithmetic operators, e.g. + or *, since that can lead to very inefficient code:

```
// vector addition
vector_t  operator + ( const vector_t &  v1, const vector_t &  v2 )
{
    vector_t  t( v1 );
    return ( t += v2 );
}
```

Here, a temporary object t has to be created. Furthermore, usually another temporary object is created by the compiler since the lifetime of t ends when returning from the function. Each of these temporary objects needs memory and performs a copy operation. Hence, the addition is very inefficient.

Coding Principle No. 24

Only overload operators if necessary and reasonable.

Records: Special Operators

The analog to the copy constructor is the copy operator '=', e.g. used in

```
x = y;
```

It is also generated by the C++ compiler by default, simply copying the individual member variables of the record. Thereby, the same problems occur, e.g. copying pointers instead of arrays.
Coding principle for copy operators (see Coding Principle No. 22):

Coding Principle No. 25

> *Always make sure, that the C++ generated copy operator behaves as expected. If in doubt: implement operator by yourself.*

Classes

Records: Special Operators

Copy operator for vectors:

```
struct vector_t {
    ...
    vector_t &  operator = ( const vector_t &  v )
    {
        init( v.size );

        for ( uint i = 0; i < size; i++ ) coeffs[i] = v.coeffs[i];

        return *this;
    }
    ...
};
```

Now, when assigning record objects to each other, e.g.

```
x = y;
```

the user implemented copy operator is used, ensuring correctness.

Classes

Records: Special Operators

The copy operator also allows a simplified copy constructor:

```
vector_t::vector_t ( const vector_t & v )
{
    *this = v;
}
```

Classes

Classes

Records provide all mechanisms for object-oriented programming. What about classes?

C++ also provides a **class** type, e.g.

```
class ⟨class name⟩ {
        ⋮
};
```

Classes in C++ are identical to records, except for one little difference: if the visibility specifiers, e.g. **public**, **protected** and **private**, are missing, by default all member variables and functions are **private** in a class and **public** in a record.

Therefore, it is up to you, which form you prefer: classes or records.

One possible rule: for simple records without functions use a **struct**, otherwise use a **class**. But remember Coding Principle No. 22, Coding Principle No. 25 and Coding Principle No. 3 (RAII).

Application: BLAS (Version 3)

Vector type:

```
class vector_t {
private:
    size_t    size;
    real_t *  coeffs;

public:
    vector_t ( const size_t      n = 0 );
    vector_t ( const vector_t &  x );
    ~vector_t ();

    size_t  get_size () const;

    real_t   operator [] ( const size_t  i ) const;
    real_t & operator [] ( const size_t  i );

    void fill  ( const real_t  f );
    void scale ( const real_t  f );
    void add   ( const real_t  f, const vector_t & x );

    vector_t & operator = ( const vector_t & x );
};
```

Classes

Application: BLAS (Version 3)

Remarks to the vector class:

- The constructor

  ```
      vector_t ( const size_t      n = 0 );
  ```

  also serves as a default constructor since it can be called without an argument.

- The index operator

  ```
      real_t & operator [] ( const size_t  i )
      {
          return  coeffs[i];
      }
  ```

  provides write access to the coefficients since a reference to the corresponding entry is returned. Therefore, it is defined non-**const**.

Classes

Application: BLAS (Version 3)

Matrix type:

```
class matrix_t {
private:
    size_t    nrows, ncolumns;
    real_t *  coeffs;

public:
    matrix_t  ( const size_t  n, const size_t  m );
    matrix_t  ( const matrix_t &  M );
    ~matrix_t ();

    size_t  get_nrows    () const;
    size_t  get_ncolumns () const;

    real_t    operator [] ( const size_t i, const size_t j ) const;
    real_t & operator [] ( const size_t i, const size_t j );

    void fill  ( const real_t  f );
    void scale ( const real_t  f );
    void add   ( const real_t  f, const matrix_t & M );
```

Classes

Application: BLAS (Version 3)

```
    void mul_vec ( const real_t  alpha, const vector_t & x,
                   vector_t &    y ) const;

    real_t normF () const;

    matrix_t & operator = ( const matrix_t & M );

private:
    matrix_t ();
};

void
mul_mat ( ... );
```

Remarks:

- The private default constructor prevents accidental matrices of dimension 0, since it can not be called.
- The function `mul_mat` is not part of the matrix class, since the algorithm can not be connected with a specific matrix.

Classes

Application: BLAS (Version 3)

```
matrix_t * M = new matrix_t( 10, 10 );
vector_t * x = new vector_t( 10 );
vector_t * y = new vector_t( 10 );

x.fill( 1.0 );
y.fill( 0.0 );

...
M[3,4] = ... // fill matrix M
...

cout << M.normF() << endl;

M.mul_vec( -1.0, x, y );

delete x;
delete y;
delete M;
```

Generic Programming

Generic Programming

Generic Programming

Consider

```
int     square ( const int    x ) { return x*x; }
float   square ( const float  x ) { return x*x; }
double  square ( const double x ) { return x*x; }
```

The same algorithm is implemented for different datatypes. For more complicated algorithms, this potentially leads to a lot of programming overhead. If one aspect of the algorithm should be changed, all other implementations have to be changed as well.

A similar overhead is involved with record datatypes used with multiple base types, e.g. lists or dynamic arrays. The record has to be reprogrammed whenever a new type should be placed in the list or array, respectively.

Alternative: write source code for the record or function once and leave out the specific datatype to operate on. That is called generic programming.

Generic Programming

Templates

C++ supports generic programming in the form of templates.

A template function is defined as

> **template** < **typename** ⟨*name*⟩ >
> ⟨*return type*⟩ ⟨*function name*⟩ *(* ⟨*argument list*⟩ *)*
>   ⟨*function body*⟩

e.g.

```
template <typename T>
T square ( const T f ) { return f*f; }
```

If the C++ compiler detects the usage of a template function, e.g.

```
double  sq2 = square( 2.0 );
```

it will automatically generate the corresponding function:

```
double square ( const double f ) { return f*f; }
```

Generic Programming

Templates

Similar defined are template record (or class) types:

```
template < typename ⟨name⟩ >
struct ⟨record name⟩ {
    ⋮
}
```

Example for a simple list:

```
template <typename T>
struct list {
    T       element;
    list *  next;
};
```

Generic Programming

Templates

Template datatypes are used by explicitly defining the corresponding type to be used in the template. The syntax is:

⟨*record name*⟩< ⟨*type*⟩ >

For the list type, this looks as:

```
int main ()
{
    list< int >        ilist;
    list< double > *  dlist = new list< double >;

    ilist.element  = 2;
    ilist.next     = NULL;

    dlist->element = 2.0;
    dlist->next    = NULL;
}
```

Generic Programming

Templates

The template type can be a template by itself:

```
int main ()
{
    list< list< float > >  fllist;

    fllist.element.element = 2.0f;
    fllist.element.next    = NULL;
    fllist.next            = NULL;
}
```

Here, the list can be extended in two dimensions, either by the `next` pointer or the `element.next` pointer.

Generic Programming

Templates

Template functions can also be explicitly typed using the same syntax:

```
float  sq2 = square< float  >( 2.0f );
double sq3 = square< double >( 3.0 );
```

This is necessary, if the compiler can not automatically determine the type used for a template function:

```
template <typename T>
T min ( const T a, const T b )
{
    if ( a < b ) return a;
    else         return b;
}

...

    int        n1 = 10;
    unsigned   n2 = 20;
    int        n3 = min( n1, n2 );      // ambiguous: int or unsigned?
    int        n4 = min<int>( n1, n2 ); // ok: int explictly chosen
```

Generic Programming

Templates

Since template functions or types are generated at compile time, the full specification, e.g. function header and body, has to be available whenever such a function is used. Therefore, template functions must always be implemented in a header file.

Remark

> *If many template types and functions are used for many different datatypes, this significantly can bloat the resulting compiled program. Also, the compilation time can be much higher.*

Generic Programming

Templates: Example (CG iteration for $Ax = b$)

```
template <typename T_MAT> void
cg ( const T_MAT &  A, vector_t & x, const vector_t & b )
{
    vector_t  r( b ), p, a( x.get_size() );

    mul_vec( -1.0, A, x, r );           // r = b - A x
    p = r;                              // p = r

    for ( size_t it = 0; it < 1000; it++ ) {
        real_t  lambda;

        a.fill( 0.0 );
        mul_vec( 1.0, A, p, a );        // a = A p
        lambda = dot( r, p ) / dot( a, p ); // lambda = <r,p>/<Ap,p>
        x.add(  lambda, p );            // x = x + lambda p;
        r.add( -lambda, a );            // r = r - lambda a
        p.scale( - dot( r, a ) / dot( a, p ) );
        p.add( 1.0, r );                // p = r - (<r,a> / <a,p>) p

        if ( r.norm2() < 1e-10 )        // stop crit.: |r|_2 < 1e-10
            break;
}   }
```

Generic Programming

Templates: Example (CG iteration for $Ax = b$)

Remark

Works for arbitrary matrix types, e.g. dense and sparse, as long as `mul_vec` is implemented for each type:

```
Dense::matrix_t   M( n, n );
vector_t          x( n );
vector_t          b( n );

cg( M, x, b );

Sparse::matrix_t  S( n, n, nnonzero );

cg( S, x, b );
```

Generic Programming

Templates: Multiple Template Arguments

Template functions and datatypes are also possible with more than one argument type:

```
template <typename T_MAT, typename T_VEC> void
cg ( const T_MAT &  A, T_VEC & x, const T_VEC & b )
{
    ...
}
```

Generic Programming

Templates: Value Templates

Previous templates were used to leave out the type to work on. One can also predefine the type and leave out the specific value:

```
template <int N>
struct smallvector_t {
    real_t  coeffs[N];   // constant size array

    smallvector_t ()
    {
        for ( size_t i = 0; i < N; i++ )
            coeffs[i] = 0.0;
    }

    smallvector_t & operator += ( const smallvector_t & v ) { ... }
    smallvector_t & operator -= ( const smallvector_t & v ) { ... }
    smallvector_t & operator *= ( const real_t          f ) { ... }
};

template <int N>
smallvector<N> operator + ( const smallvector_t<N> & v1,
                            const smallvector_t<N> & v2 ) { ... }
```

Generic Programming

Templates: Value Templates

```
smallvector_t<3>  x, y, z;

x += y;
y *= 2.0;

z = x -= z + y;
```

Remark

As long as `N` *is small, e.g.* ≤ 5, *the arithmetic operators are still very efficient.*

Templates: Conclusion

Templates are a very powerful tool to simplify programming. Furthermore, they are *Turing complete*, i.e. you can program every computable program by only using templates.
Unfortunately, templates are also quite complex and involve a sginificant overhead in terms of programming, compilation time and (possibly) program size. Therefore, it is suggested to use them sparsely.

Error Handling

Error Handling

General Thoughts

Consider

```
vector_t  x( 10 );
vector_t  y( 20 );

y = x;
```

The copy operator of `vector_t` simply copies all elements up to the size of the vector:

```
for ( size_t i = 0; i < size; i++ )
    (*this)[i] = x[i];
```

but the argument `x` only has 10 elements. Hence, memory is overwritten, which is not part of the vector.

Error Handling

General Thoughts

Another typical error involves NULL pointers:

```
bool is_in ( const node_t & root, const int val )
{
    if ( root.val == val ) return true;
    else                   return is_in( * root.son1, val ) ||
                                  is_in( * root.son2, val );
}
```

Here, the recursive call to `is_in` for the sons is only possible, if the sons are not **NULL**, which is not tested.

Error Handling

General Thoughts

The following example for a LU factorisation of a dense matrix shows another problem:

```
for ( uint j = 0; j <= min(nrows,ncolumns); ++j )
{
    if ( j < n-1 )
        scale( nrows-1-j, 1.0 / A[j, j], & A[j + 1, j] );

    if ( j < mrc )
        // rank-1 update
        geru( nrows-1-j,  ncolumns-1-j, -1.0,
              & A[j + 1, j], 1,
              & A[j, j + 1], n,
              & A[j + 1, j + 1], n );
}
```

The division by the diagonal element is not guarded against division by zero, which would result in **INF** numbers.

Error Handling

General Thoughts

Obviously, we need some protection against possible errors. Even more important is, that errors are detected and reported.

For detecting errors:

Coding Principle No. 26

- *Always check function arguments, especially pointers for illegal values (pre condition of a function).*
- *If a critical situation is possible by an instruction, check the operands of the instruction.*
- *Check, whether the results of a function are as expected (function post condition).*

Error Handling

General Thoughts

For reporting errors different strategies are possible:

by message: Detect the error and print a (detailed) message that a problem occured, but otherwise continue the program. This is usuable for non-critical errors.

by abort: Detect the error and abort the program, possibly with a detailed description of the error. This behaviour is acceptable for short running programs.

by exception: Detect the error and throw an exception and let the programmer either catch the exception or not, in which case the program is aborted.

Error Handling

Assertions

Assertions fall into the category "error handling by abort". An assertions is defined using the function `assert` defined in the module `cassert`.

Remark

> *Assertions are also possible in C, therefore the filename cassert.*

The `assert` function expects a logical expression as it's function argument. If the expression is **false**, the program is terminated, printing the definition of the failed assertion together with the file name and line number, where the assertion failed.

Error Handling

Assertions

For the copy operator of `vector_t` this looks as:

```
#include <cassert>

struct vector_t {
...

    vector_t & operator = ( const vector_t & x )
    {
        assert( get_size() == x.get_size() );

        for ( size_t i = 0; i < size; i++ )
            (*this)[i] = x[i];
    }
}
```

Now, if `x` has a different size than the local vector, the application will immediately abort.

Error Handling

Assertions and Optimisation

When using optimisation to translate the source code into machine code, assertions are usually omitted. This is an advantage and a disadvantage:

- one can put quite expensive tests into assertions, which are only executed when running the program without optimisation, e.g. in *test mode*,
- but the optimised program will not detect those errors.

Therefore, it should be used only if one can test all cases without optimisation and simply want to have a fast program for such known and tested cases.

Error Handling

Assertion Usage

The size of the logical expression in the assertion is not limited, but large expressions do not give the programmer the information, he seeks:

```
void
mul_mat ( const real_t  alpha, const matrix_t & A, const matrix_t & B,
          matrix_t & C )
{
    assert( A.get_nrows()    == C.get_nrows()    &&
            B.get_ncolumns() == C.get_ncolumns() &&
            A.get_ncolumns() == B.get_nrows() );

    ...
}
```

Although the function will only be executed, if the prerequisite for matrix multiplaction are fulfilled, in case of an error, the programmer does not know, which matrix was wrong.

Error Handling

Assertion Usage

Alternatively the assertion can be split, resulting in more information if some incompatible matrices are used:

```
void
mul_mat ( const real_t  alpha, const matrix_t & A, const matrix_t & B,
          matrix_t & C )
{
    assert( A.get_nrows()    == C.get_nrows()    );
    assert( B.get_ncolumns() == C.get_ncolumns() );
    assert( A.get_ncolumns() == B.get_nrows()    );

    ...
}
```

Error Handling

Assertion Conclusion

Assertions are suitable for

- non-critical programs or programs with a short runtime,
- for errors, which can be detected in a previous test mode of the program.

Assertions are not suitable for

- programs which shall not terminate or have a very long runtime,
- programs with many different input data.

Although not suitable for all programs:

Remark

Assertions are better than nothing!

Error Handling

By Return Value

In C, the error status of a function was typically reported by the return value, e.g. if non-zero, an error occured (see `main`). This is not encouraged:

- Since the return code of every function has to be tested, the resulting source code is very complex:

```
if ( f1( ... ) != 0 ) { ... }  // Error
else                  { ... }  // Ok
if ( f2( ... ) != 0 ) { ... }  // Error
else                  { ... }  // Ok
if ( f3( ... ) != 0 ) { ... }  // Error
else                  { ... }  // Ok
```

- One can simply ignore the return value of called functions, bypassing error handling.
- Local objects, e.g. records, can not be deleted if an error occures and a **return** is instructed.

Error Handling

Exceptions

C++ allows to **try** to execute portions of the source code and **catch** detected errors by special handlers. Furthermore, the error information is supplied in the form of an arbitrary datatype, thereby allowing to provide further information about the error. This mechanism is called exception handling and the error objects (or the errors) are exceptions.
The syntax for exception handling is:

```
try
    ⟨block⟩
catch ( ⟨error type⟩ ⟨error⟩ )
    ⟨block⟩
```

Here, ⟨error type⟩ can be any datatype and ⟨error⟩ is the corresponding error variable.

Error Handling

Throwing Exceptions

Example:

```
vector_t  x( 10 );
vector_t  y( 20 );

try
{
    y = x;
}
catch ( VectorSizeErr &  e )
{
    ... // handle error
}
```

Of course, one can not catch an error, if it is not *thrown*. C++ provides the keyword **throw** to generate an error object:

```
vector_t & operator = ( const vector_t & x )
{
    if ( get_size() == x.get_size() )
        throw VectorSizeErr;
    ...
}
```

Error Handling

Exception Types

The type of the exception can be defined according to the needs of the programmer, no limitations are set. Example with a class:

```
class VectorSizeErr
{
public:
    const char *  what () const
    {
        return "vector sizes differ";
    }
};
```

Here, only a simple information is provided about the type of the error. The error handler could therefore simply print this information:

```
try { y = x; }
catch ( VectorSizeErr &  e )
{
    cout << e.what() << endl;
}
```

Error Handling

Exception Types

Alternatively, the error can be more described:

```
class VectorSizeErr
{
    const char *  err_function;

public:
    VectorSizeErr ( const char * err_fn )
    {
        err_function = err_fn;
    }

    const char *  what  () const { return "vector sizes differ"; }
    const char *  where () const { return err_function; }
};
```

Error Handling

Exception Types

Now, the function where the error occured is stored while throwing the exception:

```
vector_t & operator = ( const vector_t & x )
{
    if ( get_size() == x.get_size() )
        throw VectorSizeErr( "vector::operator =" );
    ...
}
```

and the exception handler can use that information:

```
try { y = x; }
catch ( VectorSizeErr &  e )
{
    cout << "in function "
         << e.where()
         << " : "
         << e.what() << endl;
}
```

Error Handling

Multiple Exception Handlers

C++ permits to implement multiple exception handlers for a single **try** block:

```
try
{
    y     = x;
    x[30] = 1.0;  // throws ArrayBoundErr
}
catch ( VectorSizeErr & e )
{
    ...
}
catch ( ArrayBoundErr & e )
{
    ...
}
```

If no exception handler is implemented for a specific exception type, it will be handled by the default handler implemented by C++. By default, this handler aborts the program.

Error Handling

General Exception Handlers

To catch all exceptions with a single handler, the following construct is allowed:

```
try
{
    y     = x;
    x[30] = 1.0;
}
catch ( ... )
{
    cout << "exception occured" << endl;
}
```

By specifying "`...`", all exceptions are catched. Of course, no further information is then available about the type of error.

The general exception handler can be combined with other handlers, thereby providing a *fallback* in the case of an unexpected exception.

Error Handling

Exceptions and Functions

For a C++ function one can define the exception types the function and all directly or indirectly called functions can throw by using

⟨*function header*⟩ **throw***(* ⟨*exception list*⟩ *);*

e.g.:

```
void mul_mat ( ... ) throw( MatrixSizeErr, ArrayBoundErr );
```

Here, `mul_mat` is expected to throw `MatrixSizeErr` or `ArrayBoundErr`, which can be catched by a handler. All other exceptions will cause the program to abort.
The exception list can also be empty:

```
void f ( ... ) throw();
```

in which case the function is expected to not throw an exception at all.

Error Handling

Predefined Exceptions

Some exceptions are already defined by the C++ library, e.g.

bad_alloc: thrown by **new** if no memory is left to serve the allocation request

bad_exception: thrown, if no exception handler is found for a previously thrown exception.

These exceptions are defined in the module `exception` of the `std` namespace.

Error Handling

Rethrow an Exception

A catched exception can be thrown again by the exception handler, thereby forwarding the handling of the error to another exception handler:

```
try
{
    ...
}
catch ( ArrayBoundErr & e )
{
    ...
    throw;  // rethrow exception
}
```

Remark

The instruction **throw;** *is only allowed in an exception handler.*

Error Handling

Stack Unwinding

Suppose that an error occures inside a complicated recursive function, which allocates many variables, e.g.

```
void f ( ... )
{
    record1_t  r1;
    ...
    f( ... );
    ...
    record2_t  r2;
    ...
    f( ... );
    ...
}
```

If the error is thrown in the form of an exception, all of these record types will be automatically deallocated. This is known as *stack unwinding*.

This mechanism ensures, that no memory is left allocated in the case of an error.

Stack Unwinding

Remark

Unfortunately, this does not hold for objects allocated by **new***. But that can be fixed (see later).*

Exceptions: Conclusion

Exceptions a superior to all other form of error handling, e.g.

- they do not interfere with the normal algorithm like the usage of return values,
- the program does not need to terminate as with assertions,
- specific handling can be implemented for specific errors,
- the cleanup of record objects is provided,
- etc.

Hence:

Coding Principle No. 27

Use exceptions for all error handling.

In the simplest case, implement the **throw** instructions for all errors and wrap your main function in a **try-catch** construct.

Standard Template Library

Standard Template Library

C++ and STL

The standard library of C++, e.g. the standard set of functions and types, is provided by the *Standard Template Library* or *STL* for short.

Most of these functions and types are implemented using generic programming, e.g. with templates.

The set of functionality in the STL includes

- dynamic arrays and associative arrays,
- lists and iterators,
- strings and complex numbers

Remark

Unfortunately, although the individual functions and types are defined by the C++ standard, not all compilers support all features.

Standard Template Library

Streams

Input and output in C++ is implemented in the form of streams. A C++ stream can be considered to be a sequential stream of bytes to which one can write or from which one can read data.

Writing to a stream is provided by the operator $<<$:

```
cout << 42 << endl;
```

The stream defined by the object `cout`, which is of type `std::ostream` and provides the function:

```
class ostream {
    ...
    std::ostream & operator << ( const int n );
    ...
};
```

`endl` is a constant, which is equivalent to '\n', new line.

Standard Template Library

Output Streams

We also have already made use of the successive calling of the operator $<<$:

```
cout << 42 << 3.1415 << '5' << "Hello World" << endl;
```

For new datatypes, special stream functions have to written, which always follows the same scheme, e.g. for a vector:

```
#include <ostream>

std::ostream &
operator << ( std::ostream & os, const vector_t & v )
{
    for ( size_t i = 0; i < v.get_size(); ++i )
        os << v[i] << endl;

    return os;
}
```

Standard Template Library

Output Streams

The corresponding stream output function for a matrix is declared as:

```
std::ostream &
operator << ( std::ostream & os, const matrix_t & M );
```

Remark

Remember to split declaration and implementation into header and source file or to use the **inline** *keyword.*

Standard Template Library

Input Streams

Reading from a stream is provided by the operator $>>$:

```
int  n;

cin >> n;
```

Here, `cin` is the equivalent to `cout` and represents the standard input, e.g. keyboard input, and is of type `std::istream`.

Again, the operator $>>$ can be used multiple times in a single statement:

```
int     n1, n2;
double  f1;
float   f2;

cin >> n1 >> f1 >> n2 >> f2;
```

The order in which the elements are read from the stream is defined by the order at which the appear in the statement, e.g. `n1` first and `f2` last.

Standard Template Library

Input Streams

Input stream functions are provided for all basic datatypes. For user defined types, they have to be implemented similar to stream output:

```
std::istream &
operator >> ( std::istream & is, vector_t & v )
{
    ... // vector input
    return is;
}
```

Standard Template Library

File Streams

The advantage of streams is, that one can switch between different output media, e.g. standard output or a file, and use the same functions. As an example, the output of a vector to a file looks like:

```
#include <fstream>

...

vector_t       x;
std::ofstream  file( "output" );

file << x << endl;
```

Here, `file` is an object of type `std::ofstream` provided by the module `fstream` for file output. The constructor of the stream expects the name of the file to write to.

Standard Template Library

File Streams

Similar, file input is used:

```
vector_t        x;
std::ifstream  file( "input" )

file >> x;
```

Now, `file` is of type `std::ifstream` for file input, provided by the same module.
Closing an open file, being either an input or output file, is implemented by the member function `close`:

```
file.close();
```

Standard Template Library

File Streams

Another member function of file streams is `is_eof`, which tests, whether the end of the stream (or file) was reached:

```
// read whole file
while ( ! file.is_eof() )
{
    char  c;

    file >> c;
}
```

If a file is open or not can be tested with `is_open`:

```
std::ifstream  file( "input" );

if ( ! file.is_open() )
    throw "could not open file";
```

Standard Template Library

Stream Manipulators

The output format of data and, to some degree, also the input format of data can be modified by manipulator objects. These are provided by the file `iomanip`:

setw(n): set the minimal width of a data field in the stream to n, e.g. each output item will at least use n characters (default: $n = 0$).

setprecision(n): set the precision of the number output to n (default: $n = 6$),

setfill(c): set the character to be used to fill the remaining characters for an entry (default: whitespace),

```
#include <iomanip>
...
    cout << setw( 8 ) << 5
         << setprecision( 4 ) << pi << endl;
         << setfill( '#' ) << "pi" << endl;
```

Standard Template Library

Stream Manipulators

fixed: use fixed point format, e.g. “100.432”,

scientific: use scientific notation, e.g. “1.00432e2”,

flush: immediately write all output to stream if buffers are used,

endl: write new line character.

```
cout << fixed      << 2.718281828459045235 << endl
     << scientific << 2718.281828459045235 << endl;
```

Standard Template Library

Containers and Iterators

Several *container* datatypes are implemented in the STL, e.g. lists, vectors and sets. All of these types are template types, hence the type of data that can be stored by container types is not fixed.

All containers in the STL implement the following functions:

insert(x): insert `x` into the container,

clear(): remove all elements in container,

size(): return number of elements in container.

empty(): return **true**, if the container is empty and **false** otherwise.

Remark

The complexity of `size` is not $\mathcal{O}(1)$ for all container classes and depends in the implementation of the STL.

Standard Template Library

Containers and Iterators

Furthermore, all of these container types can be accessed in the same way: through iterators.

Suppose that `container` is such a type from the STL. Then, `container` provides a *subclass* `container::iterator`, e.g.

```
container            cont;
container::iterator  iter;
```

and functions `begin` and `end` to return iterators corresponding to the first and last element in the container, respectively.

```
container::iterator  first = cont.begin();
container::iterator  last  = cont.end();
```

Standard Template Library

Containers and Iterators

That can be used to iterate through the container in the same way as previously was done with arrays:

```
for ( container::iterator  iter = cont.begin();
      iter != cont.end();
      ++iter )
{
    ...
}
```

To access the actual data element to which the current iterator points, the derefence operator is overwritten by the iterator class:

```
for ( container::iterator  iter = cont.begin();
      iter != cont.end();
      ++iter )
{
    cout << *iter << endl;
}
```

Standard Template Library

Container Classes: Lists

Lists in C++ are implemented in list by the std::list template class:

```
template <typename T>
class list
{
    ...
};
```

e.g.:

```
#include <list>

...

std::list< int >                  list1;
std::list< double * >             list2;
std::list< std::list< double > >  list3;
```

Standard Template Library

Container Classes: Lists

In addition to the standard container functions, the following member functions are implemented in the list class:

front()/back(): return first/last element in list,

push_front(x): insert `x` at the front of the list,

push_back(x): insert `x` at the end of the list,

pop_front(): remove first element in list,

pop_back(): remove last element in list,

Standard Template Library

Container Classes: Lists

Example:

```
list< int >  ilist;

ilist.push_front( 1 );
ilist.push_front( 2 );
ilist.push_back(  3 );
ilist.push_back(  4 );

for ( list<int>::iterator  it = ilist.begin();
      it != ilist.end();
      ++it )
    cout << *it << endl;

int  sum = 0;

while ( ! ilist.empty() )
{
    sum += ilist.front();
    ilist.pop_front();
}
```

Standard Template Library

Container Classes: Vectors

A vector is a container class providing a dynamic array, which can grow or shrink with respect to the number of elements.

Furthermore, a vector provides $\mathcal{O}(1)$ access to elements in the array.

Again, `vector` is a template class:

```
template <typename T>
class vector
{
    ...
};
```

implemented in the module `vector`.

```
#include <vector>

...

std::vector< int >                    vector1;
std::vector< double * >               vector2;
std::vector< std::vector< double > >  vector3;
```

Standard Template Library

Container Classes: Vectors

To make resizing more efficient, vectors usually allocate more memory than neccessary and do not immediately deallocate memory if the number of elements is reduced.

The following functions are implemented in `vector` beside the standard container functions:

front()/back(): return first/last element in vector,

resize(n): set new size for vector,

push_back(x): insert `x` at the end of the vector,

pop_back(): remove last element in vector,

operator **[]** (i): return i'th element of vector (read/write).

Remark

By default, elements in the vector are initialised with 0, or the corresponding equivalent of the stored type, e.g. **NULL**.

Standard Template Library

Container Classes: valarray

Whereas `vector` is a container suitable for changing the size of the container efficiently, in numerical applications the size is usually fixed. For that, the class `valarray` is provided:

```
template <typename T>
class valarray
{
    ...
};
```

Examples:

```
#include <valarray>

...


std::valarray< int >      array1( 10 );
std::valarray< double >   array1( 1000 );
```

Standard Template Library

Container Classes: valarray

`valarray` provides all functions also defined by `vector` but furthermore, overloads all standard arithmetics operators, e.g. `+`, `-`, `*`, `/`, etc., with element wise versions. In addition to that, the class also provides the following methods:

- min(): return minimal element in array,
- max(): return maxmial element in array,
- sum(): return sum of elements in array,

Standard Template Library

Container Classes: valarray

Example for a vector class in linear algebra without pointers:

```
#include <valarray>

class vector_t
{
private:
    std::valarray< real_t >  coeffs;

public:
    vector_t ( const size_t      n ) { coeffs.resize( n ); }
    vector_t ( const vector_t &  v );

    real_t operator [] ( const size_t i ) const
    { return coeffs[i]; }

    vector_t & operator = ( const vector_t &  v )
    {
        coeffs = v.coeffs;
        return *this;
    }
};
```

Standard Template Library

Other Container Classes

Not described here are:

map: class for an associative array, e.g. indexed by arbitrary types,

multimap: similar to `map` but allows different elements with same index,

set: stores unique elements, indexed by the elements themselves,

queue: container for FIFO (first-in first-out) access,

stack: container for LIFO (last-in first-out) access,

priority_queue: a container type, where the first element is always the greatest with respect to some defined order.

Standard Template Library

Strings

Previous strings were implemented as null terminated character arrays with all their limitations. The STL also provides a string class which provides a much more convenient way of handling strings.

The class is implemented in the module `string` and is not a template class (although implemented with such):

```
#include <string>

...

    std::string   str1;                  // empty string
    std::string   str2( "Hello World" ); // preinitialised string

    cout << str2 << endl;
```

Standard Template Library

Strings

The `string` class implements operators for standard string handling, e.g. assignment (=), concatenation (+ and +=) and comparison (== and !=):

```
std::string  str1( "Hello" );
std::string  str2( "World" );
std::string  str3;

str3  = str1 + ’ ’ + str2;
str3 += " Example";

if ( str1 == str2 )
    str3 = str1;

if ( str1 != str2 )
    str3 = str2;
```

Standard Template Library

Strings

It also provides functions for string operations:

- find(substr): return position of `substr` in the string or `string::npos` if not contained,
- rfind(substr): similar to `find`, but start search at the end of the string,
- substr(pos, n): return substring starting at position `pos` with length `n`,
- c_str(): return traditional character array for the string.

Remark

The pointer returned by `c_str` is actually the internal representation of the string. So do not delete that pointer!

Standard Template Library

Complex Numbers

As mentioned before, C++ does not support complex numbers as part of the language. Fortunately, there is an implementation of a class for complex numbers in the STL.
The complex class is again a template class, thereby enabling single and double precision complex numbers:

```
#include <complex>

std::complex< float >   c1;
std::complex< double >  c2;
```

Complex objects store the real and the imaginary part in two **public** member variables: `re` and `im`.

```
c1.re =  1.0;
c1.im = -2.0;
```

Standard Template Library

Complex Numbers

The constructors for complex numbers provide initialisation of both data fields:

```
std::complex< double >  I( 0.0, 1.0 );
std::complex< double >  r( 5.0 );        // == 5 + 0i
std::complex< double >  z;               // == 0 + 0i
std::complex< double >  i = I;
```

Furthermore, all standard arithmetical operators are provided and all standard mathematical functions are implemented:

```
std::complex< double >  c1, c2, c3;

c1 = c2 * c3;
c2 = 2.0 + c3;
c3 = std::sqrt( -3.0 * c1 + c2 / c3 );
```

Standard Template Library

Auto Pointers

When a block is left or an exception occurs in a function, all normal record variables are destroyed. Unfortunately, this is not true for record variables allocated by **new**, e.g.

```
{
    vector_t   x( 10 );
    vector_t * y = new vector_t( 10 );

}// "x" is deallocated, but not "y"
```

The STL provides a solution for this problem: the class `auto_ptr`. An auto pointer is a class with a single data element, a pointer of the specified type:

```
template <typename T>
class auto_ptr
{
private:
    T *  ptr;
...
};
```

Standard Template Library

Auto Pointers

Furthermore, `auto_ptr` provides operators, such that a `auto_ptr` variable behaves like a standard pointer:

```
#include <memory>

...

std::auto_ptr< vector_t >  x( new vector_t( 10 ) );

x->fill( 2.0 );
cout << x->norm2() << endl;
```

One can even access the pointer stored in the auto pointer:

```
vector_t * y = x.get();
```

Standard Template Library

Auto Pointers

But what makes auto pointers so special?
Remember, that all normal record variables are automatically deleted at the end of a block. Auto pointers are *normal record variables*:

```
std::auto_ptr< vector_t >  x( new vector_t( 10 ) );
```

Hence, upon leaving the block, the destructor of `auto_ptr` is called. But the destructor of `auto_ptr` is implemented as follows:

```
~autoptr () { delete ptr; }
```

Therefore, if the auto pointer is destroyed, so is the stored pointer.

```
{
    vector_t                   x( 10 );
    auto_ptr< vector_t >  y( new vector_t( 10 ) );

}// "x" and "y" are deallocated
```

Standard Template Library

Auto Pointers

The class auto_ptr also provides two other functions for handling the local pointer:

reset(ptr): Exchange the local pointer by ptr. If the previous pointer was not **NULL**, it will be deleted.

release(): Set the local pointer value to **NULL** and return the previous pointer, but do not delete it.

Especially release can be used to program exception safe:

```
vector_t *
f ( ... )
{
    auto_ptr< vector_t >  v( new vector_t( 10 ) );

    ...

    return v.release(); // a previous exception would delete v
}
```

Class Inheritance

Class Inheritance

Inheritance

In an earlier section, generic programming was used to provide a single implementation of an algorithm for multiple types. There is another way to do that in C++: by using object oriented programming or OOP.

In OOP one defines a hierarchy of classes, connected via inheritance, sharing a set of functions, which then can be called for all members of the hierarchy.

As an example, we will consider matrices. Up to now we had:

matrix_t: a dense matrix,

sparsematrix_t: a sparse matrix using lists and pointers and

crsmatrix_t: a sparse matrix using arrays.

Class Inheritance

Inheritance

All of these matrix types had similar functions:

```
size_t  get_nrows    () const;
size_t  get_ncolumns () const;

void fill  ( const real_t  f );
void scale ( const real_t  f );
void add   ( const real_t  f, const matrix_t & x );

void mul_vec ( const real_t  alpha, const vector_t & x,
               vector_t &    y ) const;

real_t normF () const;
```

but also different functions:

```
// sparse matrices
size_t  get_nnonzero () const;

// dense matrices
real_t  operator [] ( const size_t i, const size_t j ) const;
```

Class Inheritance

Base Classes

Now, let us define a general matrix type, with only the set of common functions and data to all other matrix types:

```
class matrix_t {
private:
    size_t  nrows, ncolumns;
public:
    matrix_t  ( const size_t  n, const size_t  m );
    matrix_t  ( const matrix_t &  M );

    size_t  get_nrows    () const { return nrows };
    size_t  get_ncolumns () const { return ncolumns };

    void   fill    ( const real_t  f );
    void   scale   ( const real_t  f );
    void   add     ( const real_t  f, const matrix_t & x );
    void   mul_vec ( const real_t  alpha, const vector_t & x,
                     vector_t &    y ) const;
    real_t normF   () const;
};
```

This class is the start of the inheritance hierarchy, a so called base class.

Class Inheritance

Base Classes

Although the base class defines all functions that can be used with a general matrix, it can not provide the corresponding implementation since no data is provided. Therefore, most functions, which are called methods in the terminology of OOP, are actually empty, i.e. have no body.
In C++ this can be define by using

$$\langle \textit{function header} \rangle = \textit{0;}$$

e.g.

```
void  fill ( const real_t  f ) = 0;
```

Such methods are called abstract. Classes with abstract methods are also called abstract and can not be instantiated, e.g. one can not define objects of that type.

Class Inheritance

Base Classes

The base class for matrices now looks like:

```
class matrix_t {
private:
    size_t  nrows, ncolumns;
public:
    matrix_t  ( const size_t  n, const size_t  m );
    matrix_t  ( const matrix_t &  M );

    size_t  get_nrows    () const { return nrows };
    size_t  get_ncolumns () const { return ncolumns };

    void   fill    ( const real_t  f ) = 0;
    void   scale   ( const real_t  f ) = 0;
    void   add     ( const real_t  f, const matrix_t & x ) = 0;
    void   mul_vec ( const real_t  alpha, const vector_t & x,
                     vector_t &    y ) const = 0;
    real_t normF   () const = 0;
};
```

Class Inheritance

Derived Classes

To really work with matrices, functionality has to be provided. Since that is specific to specific matrix formats, one needs to define new classes for each special matrix type.

But, since all matrix types can also be considered to be general matrix, they are matrices in the end, this should also be described in C++. For that, the new classes are derived from the base class:

```
class densematrix_t : matrix_t {
    ...
};

class sparsematrix_t : matrix_t {
    ...
};
```

Here, `matrix_t` is provided as a base class in the definition of the derived classes using '`:`'.

Class Inheritance

Derived Classes

A derived class inherits all methods and variables of the base class, e.g. the variables nrows and ncolumns and the methods get_nrows and get_ncolumns. Objects of the derived classes can therefore use all methods which were already implemented in the base class without providing an implementation:

```
densematrix_t  M;

cout << M.get_nrows() << " x " << M.get_ncolumns() << endl;
```

Abstract methods can not be called.

Class Inheritance

Derived Classes

The derived classes now need to provide functionality, e.g.

```
class densematrix_t : matrix_t {
private:
    std::valarray< real_t >   coeffs;

public:
    ...
    void  scale ( const real_t  f );
    ...
};

void densematrix_t::scale ( const real_t  f )
{
    coeffs *= f;
}
```

They overload the corresponding methods of the base class.

Class Inheritance

Derived Classes

The same can be done for sparse matrices:

```
class sparsematrix_t : matrix_t {
private:
    std::valarray< size_t >   rowptr;
    std::valarray< size_t >   colind;
    std::valarray< real_t >   coeffs;

public:
    ...
    void  scale ( const real_t  f );
    ...
};

void sparsematrix_t::scale ( const real_t  f )
{
    coeffs *= f;
}
```

Class Inheritance

Polymorphism

Now, if objects of each derived class are created:

```
densematrix_t   M( 10, 10 );
sparsematrix_t  S( 10, 10, 28 );
```

the overloaded methods can be called like for any other class previously presented:

```
M.scale( -1.0 );
S.scale( 10.0 );
```

Here, OOP comes into play:

> *Every object of a derived class is also an object of the base class.*

```
matrix_t  * A;

A = & M;      // A now points to the dense  M
A = & S;      // A now points to the sparse S
```

Class Inheritance

Polymorphism

But what happens when one calls

```
A = & M; A->scale( 1.5 );
A = & S; A->scale( 0.5 );
```

Here, although `A` is a pointer to a base class, the object to which it points is a derived class and OOP ensures, that the overloaded methods are called. This is called polymorphism.

So, the previous instructions are equivalent to

```
M.scale( 1.5 );
S.scale( 0.5 );
```

Class Inheritance

Polymorphism

This allows us to define a general algorithm, e.g. CG iteration, to work only with the base class:

```
void cg ( const matrix_t &  A, vector_t & x, const vector_t & b )
{
    vector_t  r( b ), p, a( x.get_size() );

    A.mul_vec( -1.0, x, r );   p = r;

    for ( size_t it = 0; it < 1000; it++ ) {
        real_t  lambda;

        a.fill( 0.0 );
        A.mul_vec( 1.0, p, a );
        lambda = dot( r, p ) / dot( a, p );
        x.add(  lambda, p );
        r.add( -lambda, a );
        p.scale( - dot( r, a ) / dot( a, p ) );
        p.add( 1.0, r );

        if ( r.norm2() < 1e-10 )
            break;
}   }
```

Class Inheritance

Polymorphism

But since all objects of derived classes are also objects of the base class, the general algorithm can be used for these derived classes too:

```
densematrix_t   D( n, n );
vector_t        x( n );
vector_t        b( n );

cg( D, x, b );

sparsematrix_t  S( n, n, nnonzero );

cg( S, x, b );
```

Class Inheritance

Virtual Methods

For polymorphism to actually work in C++, one thing has to be added to the definition of methods in classes. Consider

```
class matrix_t {
    ...
    void nullify () { scale( 0.0 ); }
}
```

Here, the method `nullify` in the base class `matrix_t` makes use of the method `scale`, which is only implemented in a derived class. Such functions in a base class would not call the function in the derived class:

```
densematrix_t  M( 10, 10 );

M.nullify();  // does not call densematrix_t::scale( 0.0 )
```

Class Inheritance

Virtual Methods

For polymorphism to work in such situations, these functions have to be virtual:

```
class matrix_t {
private:
    size_t  nrows, ncolumns;
public:
    matrix_t  ( const size_t  n, const size_t  m );
    matrix_t  ( const matrix_t &  M );

    size_t  get_nrows    () const { return nrows };
    size_t  get_ncolumns () const { return ncolumns };

    virtual void   fill    ( const real_t  f ) = 0;
    virtual void   scale   ( const real_t  f ) = 0;
    virtual void   add     ( const real_t  f, const matrix_t & x ) = 0;
    virtual void   mul_vec ( const real_t  alpha, const vector_t & x,
                             vector_t &    y ) const = 0;
    virtual real_t normF   () const = 0;
};
```

Class Inheritance

Virtual Methods

The same holds for derived classes:

```
class densematrix_t : matrix_t {
    ...
    virtual void  scale ( const real_t  f );
    ...
};

class sparsematrix_t : matrix_t {
    ...
    virtual void  scale ( const real_t  f );
    ...
};
```

Remark

The keyword **virtual** *is only neccessary in the method declaration, not the implementation.*

Class Inheritance

Virtual Methods

Now, the call to `scale(0.0)` in the function `nullify` of the base class will be handled by the corresponding methods in the derived classes:

```
densematrix_t  M( 10, 10 );

M.nullify();  // call to densematrix_t::scale( 0.0 )
```

Remark

If a class has a virtual function, it also must have a virtual destructor. Constructors can not be virtual and polymorphism does not work in constructors.

Remark

Abstract methods must also be virtual.

Class Inheritance

Extending the Hierarchy

In the beginning we had two different classes for a sparse matrix but have implemented only the CRS version.
Instead of that, sparsematrix_t should only serve as a base class for sparse matrices. Hence, it should only implement common functions and data:

```
class sparsematrix_t : matrix_t
{
private:
    size_t  nnonzero;

public:
    sparsematrix_t ( const size_t  n, const size_t  m,
                     const size_t  nnzero );

    size_t  get_nnonzero () const { return nnonzero; }
}
```

Note that it does not overload any method from matrix_t and is therefore also an abstract class.

Class Inheritance

Extending the Hierarchy

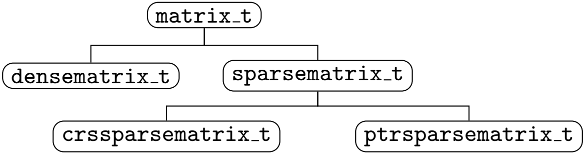
The special sparse matrix types are then derived from the base sparse matrix class:

```
class crssparsematrix_t : sparsematrix_t
{
private:
    std::valarray< size_t >   rowptr, colind;
    std::valarray< real_t >   coeffs;
public:
    ...
    virtual void mul_vec ( ... ) const;
    ...
};

class ptrsparsematrix_t : sparsematrix_t
{
private:
    std::valarray< entry_t >   entries;
public:
    ...
    virtual void mul_vec ( ... ) const;
    ...
};
```

Class Inheritance

Extending the Hierarchy

The complete class hierarchy now is:



matrix_t

densematrix_t

sparsematrix_t

crssparsematrix_t

ptrsparsematrix_t

Due to inhertance, each object of the new classes crssparsematrix_t and ptrsparsematrix_t is not only an object of sparsematrix_t, but also of matrix_t:

```
crssparsematrix_t   S( 10, 10, 28 );
matrix_t *          A = & S;

A->scale( 5.0 );  // call to crssparsematrix_t::scale

cg( S, x, b );
```

Class Inheritance

Visibility

Remember the visibily keywords **public**, **protected** and **private** for variables and functions in a record or class, respectively. The last only differ in the context of inheritance:

> *One can access* **protected** *variables or functions of base class in a derived class but not* **private** *members.*

```
class densematrix_t
{
    ...
    void print ()
    {
        // Error: nrows and ncolumns are private in matrix_t
        cout << nrows << " x " << ncolumns << endl;
    }
}
```

Class Inheritance

Visibility

Visibility can also be defined during inheritance. The previous examples always assumed:

```
class densematrix_t : public matrix_t
{
    ...
};

class sparsematrix_t : public matrix_t
{
    ...
};

class crssparsematrix_t : public sparsematrix_t
{
    ...
};

class ptrsparsematrix_t : public sparsematrix_t
{
    ...
};
```

Class Inheritance

Visibility

One can also define **private** inheritance:

```
class densematrix_t : private matrix_t
{
    ...
};

class sparsematrix_t : private matrix_t
{
    ...
};
```

The difference is, that all methods in the base class are now private in the derived class and can not be called from outside.

Class Inheritance

Constructors

A constructor of a base class can also be called in the constructor of a derived class:

```
class densematrix_t : public matrix_t
{
    ...
    densematrix_t ( const size_t  n, const size_t  m )
            : matrix_t( n, m )
    {
        coeffs.resize( n*m );
    }
    ...
}
```

By default, the default constructor of the base class is called.

Remark

Constrcutors are not inherited, they have to be implemented in each derived class.

Class Inheritance

Calling overloaded Functions

Methods of a base class can also be called in the derived class even though they were overloaded:

```
class densematrix_t : public matrix_t
{
    ...
    virtual void nullify ()
    {
        matrix_t::nullify();  // call nullify of base class
        ...
    }
    ...
}
```

All methods in all base classes are available for that, not only the direct ancestor.

Class Inheritance

Type Casting

We have discussed type casting operators, e.g. **const_cast**, **static_cast** and **dynamic_cast**. Especially the last one is important for classes, as it uses *runtime type information* and respects class hierarchy:

```
densematrix_t *      M  = new densematrix_t( 10, 10 );
crssparsematrix_t *  S1 = new crssparsematrix_t( 10, 10, 28 );
ptrsparsematrix_t *  S2 = new ptrsparsematrix_t( 10, 10, 28 );

matrix_t *           A  = M;

// cast a pointer of a base class to a derived class
densematrix_t *      M2 = dynamic_cast< densematrix_t * >( A );

A = S1;

// cast a pointer of a base class to a derived class
crssparsematrix_t *  S3 = dynamic_cast< crssparsematrix_t * >( A );

A  = S2;
S3 = dynamic_cast< crssparsematrix_t * >( A ); // returns NULL
M2 = dynamic_cast< densematrix_t * >( A );     // returns NULL
```

Class Inheritance

Type Casting

A dynamic cast will only return the requested pointer value, i.e. perform the cast, if the object to which the pointer directs is of that type, e.g. explicitly of that type or implicitly due to inheritance. Otherwise a **NULL** pointer is returned.

Remark

The complexity of a dynamic cast is not $\mathcal{O}(1)$, because the class hierarchy has to be parsed up to the specific datatype.

Coding Principle No. 28

Use dynamic casts for type casting of derived datatypes as much as possible.

Appendix

Coding Principles

1. choice of floating point type
2. variable names
3. RAII
4. **const** usage
5. pointer init to **NULL**
6. float equality test
7. parentheses
8. implicit casts
9. default case in **switch**
10. **const** function arguments
11. return in function
12. function naming
13. functions and minimal evaluation
14. array boundaries
15. pointer reset to **NULL**
16. deallocate pointer
17. string termination
18. type naming
19. header encapsulation
20. global variables
21. anonymous namespaces
22. default copy constructor

Coding Principles

23 data access in a record

24 operator overloading

25 default copy operator

26 detecting errors

27 use exceptions

28 dynamic casts

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