

C++ Programming for Scientists

C++ templates

The template facility in C++ essentially allows one to write functions and classes with variable *types*.

Remember our function for `max`?

```
inline double max(double a, double b)
{
    return (a > b ? a : b);
```

Lecture # 6

We noticed that was better than the macro

```
#define MAX(a,b)  ( a > b ? a : b)
```

because of type checking and evaluating its arguments only once. But our `inline` function only works for variables of type `double`.
C++ developers realized this problem and came up with a `template` mechanism to solve it.

```
template <class Type>
inline Type max(Type a, Type b)
{
    return (a > b ? a : b);
```

This is just like the previous function, but with `double` replaced by a variable name `Type` and the extra line
`template <class Type>`
in the function declaration.

C++ templates (cont'd.)

Now we can call `max()` with any matching pair of types:

```
i = max( 31, 56 );           // calls int max(int, int)
x = max( 5.6, 9.2 );        // calls double max(double, double)
c = max( 'c', 'A' );         // call char max(char, char)
```

even user-defined types

```
i = max(BigInt('209209832'), BigInt("283745343"));
```

all that is required of a user-defined class is that `operator>` and
`operator=` be defined on it. (You can see this directly from the definition
of `max()`).

Notice however, that the types must match the templated function
exactly, i.e.

```
max(3.1, 4)
```

won't work since the compiler would look for a template description of
`max(double, int)`.

```
template < class Matrix, class Vector, class Preconditioner, class Real >
int
CG(const Matrix &A, Vector &x, const Vector &b,
    const Preconditioner &M, int &max_iter, Real &tol)
{
    Real resid;
    Vector p, z, q;
    Vector alpha(1), beta(1), rho(1), rho_1(1);

    Real normb = norm(b);
    Vector r = b - A*x;
    /* ... */
}
```

- Same source (`cg.h`) works for *any* matrix, vector or preconditioner consistent with the above interface.
- These types need to be known at compile-time.
- Argument classes (`Matrix`, `Vector`, `Preconditioner`, `Real`) have to satisfy the operators used in function `CG()`.
 - matrices and vector need operators '`+`', '`*`', etc
 - preconditioner `M`; `M` requires only two methods, those for finding the solution `z` to $Mz = r$ or $M^Tz = r$.

A Template Example for PCG

Vector, Matrix Interface requirements

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Templated C++ Vector Class

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```

scalar ← dot( Vector, Vector )
Vector ← Matrix operator* Vector
Vector ← MatrixT operator* Vector

Vector ← Scalar * Vector
Vector ← Vector +/- Vector
scalar ← Vector::norm()

Vector ← Preconditioner::solve(Vector)
Vector ← Preconditioner::trans_solve(Vector)
Vector ← operator=(Vector)

```

```

class Vector<Type>

template <class Type>
class Vector
{
private:
    int dim_; // size of vector
    Type *p_; // memory where data is kept.

public:
    Vector(); // constructors
    Vector(unsigned int, Type t=0.0);
    Vector(unsigned int, const Type* );
    Vector(const Vector &); // destructor

    Type& operator[](int i){return p_[i];} // access functions
    int size() const { return dim_; }
    int null() const { return dim_== 0; }

    Vector& operator=(const Vector&); // assignment
    Vector& operator=(Type); // assignment

};


```

Templated C++ Vector Class

Just like `Vector` declaration before, except that rather than holding just `doubles`, it can hold any declared type:

```
Vector<double> A(10);           // a vector of doubles
Vector<int>  B(5);             // a vector of ints
Vector<Book> L(1000);          // a vector Books
B[3] = 178;                     // looks and acts like any other Vector

L[64].set_title("The Firm");
A[0] = sin(A[1] / 3.14159);
```

Everything you didn't want to know about errors...

Structured programming actually *impedes* the management of errors

Three common ways to handle them:

1. existentialist: assume no errors (i.e. do nothing).
2. bureaucratic: encode an error in return value, let someone else worry about it.

```
f(x, y, z, N, k);

becomes

errno = f(x, y, z, N, k);
if (errno ==1) call MyErrorHandler();
else
if (errno >= 2 && errno < 10) call MyErrorHandler2();
...

```

- clutters up application code.
- returned error codes often cryptic.
- programmers often ignore them. (How many times are `malloc()` and `fopen()` used without checking return value?)
- do not “scale” well, particularly in multi-level software components. Have to be handled immediately, or become lost.

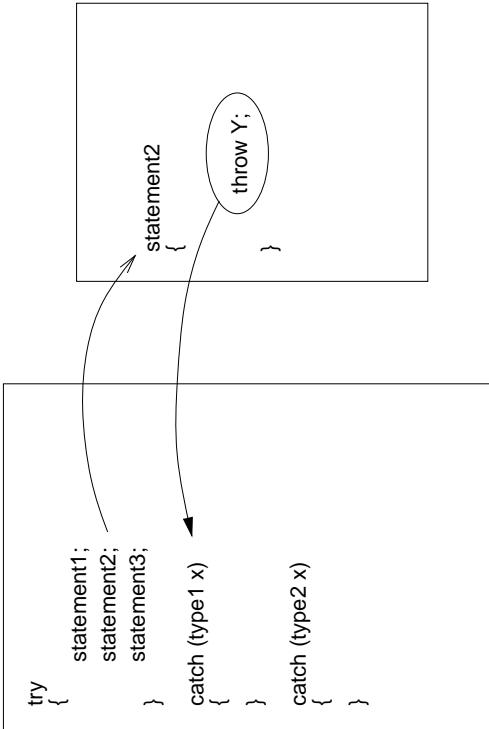
3. fascist: shut program down (i.e. `exit()`)

- OK, *only* in `main()` level of application
- not great for interactive applications (e.g. X apps), control applications (e.g. robotics), compilers, OS, etc.

C++ Exception Handling

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- ANSI C++ provides a better mechanism for handling errors. It introduces three new keywords:
- **try**, catch and throw.
 - **throw** is used to signal an error.
 - **catch** is used to process errors.
 - **try** is used to group the executable statements in your code that are treated by a **catch** statement.



Examples of Exception Handling

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```
#include <iostream.h>

int main()
{
    try
    {
        throw 17;
        cout << "This statement will never execute.\n";
        cout << "Nor will this one.\n";
    }
    catch (int i)
    {
        cout << "Caught error #" << i << "\n";
    }

    return 0;
}
```

Produces the output:

```
Caught error #17
```

● Exceptions need not be processed immediately. They are caught by the catch clause which may occur several levels above.

● C++ exceptions are like `setjmp()`/`longjmp()` in C, except that they properly handle class destructors.

● supported by standard functions, e.g. `new` throws a `bad_alloc` exception (ANSI C++) that can be later tested. (Otherwise, returns 0, or `NULL`.)

Wrap-Up

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Overview of C++: What we've learned

- Typesafe C
- C Enhancements
 - const, inline, references, function overloading
- Memory Management
 - new, delete, constructors/destructors
- Data Abstraction
 - classes, exceptions, operator overloading, templates
- OO Programming
 - inheritance, virtual functions

Overview, general comments, and
observations after several years
of C++ hacking...

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Issues in C++ Library Design

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- what are the basic objects?
- how should they interact?
- how general an interface?
- concrete data types, or abstract base classes?

Two ways to make code generic

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- inheritance
 - describe operations in terms of abstract base class(es)
 - foundation of classic OO design
 - * describe algorithms in terms of base class
 - * create similar (derived) classes
 - * apply existing algorithm to new class
 - use virtual function calls
 - some run-time overhead (3x regular function call)
- templates
 - describe skeletal code segments where “types” are arguments
 - no runtime costs
 - support varies among compilers
 - * no nested templates
 - * different linking semantics
 - * some compilers expect separate declaration and implementations
 - static arguments must match exactly to trigger

What has worked in Scientific C++

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- concrete data types
- reusing legacy Fortran kernels
- breaking application into separate computational levels
 - expressing mathematical transformations at higher levels
- reference semantics to reduce copying of large data structures (e.g. `const &`)

Common Pitfalls

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- over-generalizing
- deep, specialized, non-resuable hierarchies
- inconsistent assignment semantics
 - copy constructor must match operator=
- trying to derive off concrete classes
- development driven by “features” rather than good design

C++ Class Libraries

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Some Available Software

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- General
 - LEDA
 - NIH
 - Gnu C++ Libs
 - Standard Templates Library (STL)
 - Booch
 - Microsoft Foundation Classes (MFC)

- Scientific
 - adaptive grid refinement (A++/P++)
 - linear algebra (LAPACK++)
 - sparse matrices (SparseLib++)
 - iterative methods (IML++)
 - finite element PDEs (Diffpack)
 - general math (Math.h++)
 - arrays, matrices (M++)



<http://math.nist.gov/acmd/Staff/RPozo/>

References

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