C++ object oriented programming for scientific computing

Jamshed Anwar
Institute of Pharmaceutical Innovation
University of Bradford

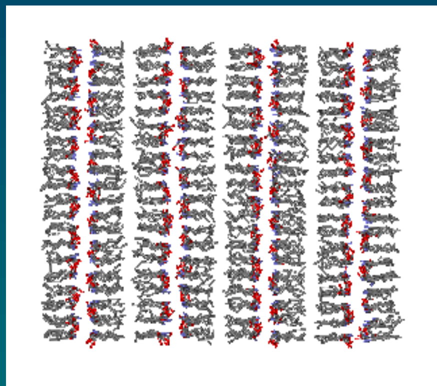
C++ object oriented programming for scientific computing

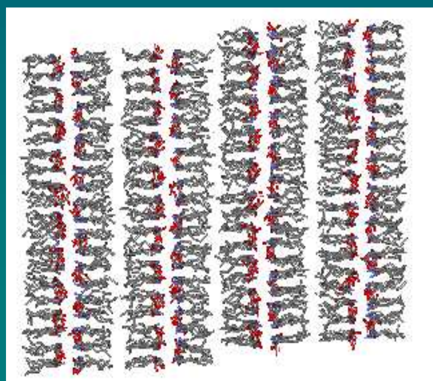
- Problems with traditional structured programming
- Object oriented programming (OOP)
- Objects: e.g. CAtom
- OOP languages for scientific computing & OOP features of C++
- Atomh++: Objects for molecular simulation
- Elegance & efficiency
- 'Unbiased' assessment of C++ OOP
- Testing of code
- Concluding remarks

Problems with traditional structured programming

angfrc.f
bndfrc.f
cfgscan.f
corshl.f
coul0.f
coul4.f
coul2.f
coul3.f
conscan.f
dblstr.f
dcell.f
diffsn0.f
diffsn1.f
dlpoly.f
duni.f
error.f
ewald1.f
…

DLPOLY 2.13
> 150 files





Mental image of subroutine interaction
Difficult to grasp;
Difficult to retain over an extended period.
Problems modifying and maintaining code

- 20,000 lines Hardwork!
- 50,000 lines Nightmare
- 100,000 lines Impossible; lose confidence

Graphics, games etc less of a problem

Large number of variables (typically reals) being passed in arguments→scope for errors

Defects rates 5-6/1000lines in production code
50-100 defects/1000 lines in new programs

Large (esp. number-crunching) codes → object-oriented

Object-oriented programming (OOP)

Model system close to ‘tangible’ reality
Easier to comprehend and retain in memory

Traditional programming
VERB-based
Emphasis on doing (action)
e.g. subroutine invert_matrix()

Noun: word referring to person, place or thing
Verb: word expressing idea of action or being

OOP
NOUN-based Emphasis on object

```
object Matrix
{
    function invert()
    function transpose()
    function multiply(Matrix2)
    ....
}
```

What comprises an object?

1. Attributes that define the object
   => data members
2. What can the object do?
   => functions

Object CAtom

```
{
        // Variables defining characteristics
        int           Index
        string        Label
        double        Charge
        double        Mass
        bool          IsFrozen
        CVectorDouble R
        CVectorDouble V
        CVectorDouble F

        // Behaviour/action/functions/procedure
        Get..
        Set..
        BondAngle(CAtom2&,CAtom3)
        TranslateTo(R)
        TranslateBy(R)
        VerletStep(timestep)
        WritePDB
}
```

Object-oriented programming: Languages

- C++
  Numerous features; unnecessary complexity;
  operator overloading

- Java
  Designed to minimise run-time errors
  ‘Subset’ of C++ (?)
  All memory allocated dynamically; garbage collection

  No operator overloading (Java Grande → no progress)
  cannot do MatrixC = MatrixA * MatrixB * VectorV
  instead MatrixC = MatrixA.multiply(MatrixB.multipy(VectorV))

  Multi-threading is part of language
  Built-in graphics (front end easy to develop)

- Smalltalk
  Not for scientific codes

- C# (?)

OOP features of C++ (1 of 3)

- Objects
- Encapsulation & implementation hiding
  Data and functions cannot be accessed without object; Less chance of changes in one part of code causing inadvertent problems elsewhere; Strong type-casting;
  First encounter: difficult to get objects to talk!
  Separate implementation from interface
  Can change implementation without changes to interface
- Polymorphism
  Same name for functions→consistent interface
  function force(Atom1, Atom2, cutoff)
  function force(Atom1, Molecule2, cutoff)
  function force(Molecule1, Molecule2, cutoff)

OOP features of C++ (2 of 3)

- Inheritance
  Reuse code – extend code

  CMolecule

  CRigidMolecule   CFlexibleMolecule

  CPartiallyRigidMolecule

- Operator overloading
  + - * / MatrixC = VectorA * MatrixB

- Dynamic memory allocation
  Complicated (messy!);
  No garbage collection: need to explicitly delete allocated memory

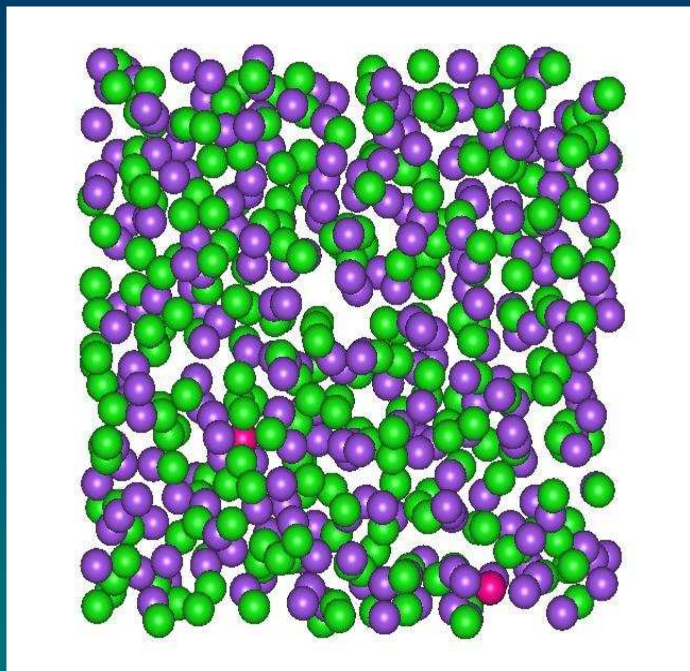
OOP features of C++ (3 of 3)

- Templates
  Same code, different object
  Minimise code

```
CVector<int>
CVector<double>
CVector<bool>

V<>   function + (V2<>)
{
   CVector<> VT
   for (i=0; i<size; i++)
   VT.E[I] = E[I] + V2.E[I];
   return VT;
}
```

Molecular dynamics simulation



1. Initial configuration
2. Equilibration
3. Production (averages)

NPT ↓G

Simulate time evolution of a system of atoms/molecules

$$\mathbf{f}_i = -\sum_j \nabla_{\mathbf{r}_i} U(\mathbf{r}_{ij})$$

$$\mathbf{r}_i(t+\Delta t) = 2\mathbf{r}_i(t) - \mathbf{r}_i(t-\Delta t) + \frac{\mathbf{f}_i(t)}{m_i}\Delta t$$

Periodic boundaries & minimum image convention

NVE, NVT, NPT & NσT
Employ extended Lagrangian
e.g. L(**r**,**p**,**H**,s)

Limitations

Limited system size
Cpu time (100ps -> 10ns)
Accuracy of interaction potential

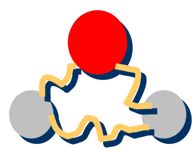
Interaction potential

$$U = \sum_{i<j} \sum 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] + \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}}$$

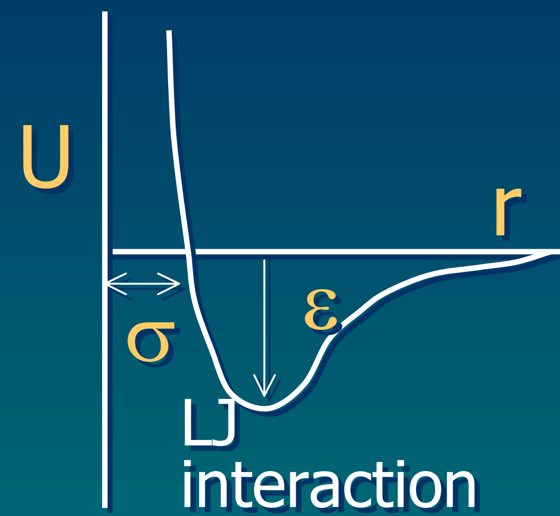
$$+ \sum_{bonds} \frac{1}{2} k_b (r - r_0)^2$$

$$+ \sum_{angles} \frac{1}{2} k_a (\theta - \theta_0)^2$$

$$+ \sum_{torsions} k_\phi \left[1 + \cos(n\phi - \delta)\right]$$



Ball & spring



Pair-interactions
N(N-1)/2

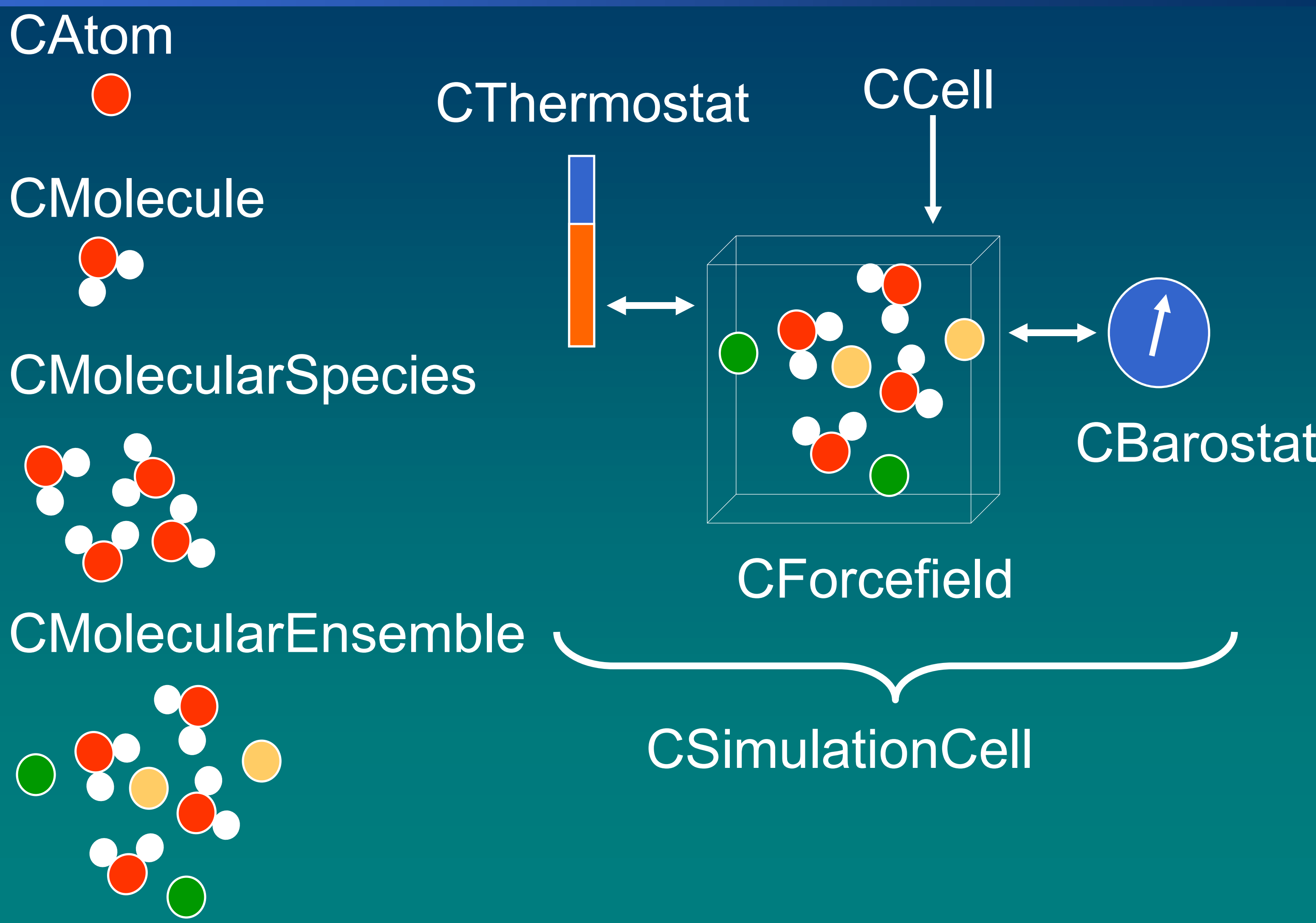
LJ: short ranged R_c
qq: long-ranged
(Ewald summation)

Parameters
empirical; from experiment
and optimised

Atom.h++ : objects for molecular simulation

Bond
Angle
Torsion
Constraint

CMatrix
CVector



CMolecule object

High memory requirement
Million particle systems

Data members
{
Name
Index

CAtoms[] // array of atoms

CentreOfMassR
Mass
DegreesOfFreedom

CBonds[]
CAngles[]
CTorsions[]
CBondConstraints[]
….
}

Functions
{
Align..()
Force()
Force(Molecule2)
Energy()
GetAtom(index)
GetCoordinates()
SetVelocity(V)
IncrementVelocity(dV)
TranslateTo(R)
TranslateBy(dR)
RotateTo(..)
RotateBy(..)
WritePDB(file)
….
}

CSimulationCell object

Data members

{

CMolecularEnsemble
CCell
CForcefield
CBarostat
CThermostat
CMonitor
CController

....

}

Functions

{

Energy
Force()
ConstraintForce()
Verlet..()
MCCycle()
MC()
MD()
ChemicalPotWidom()
...
MC_ThermodynamicInt.
MD_ThermodynamicInt.

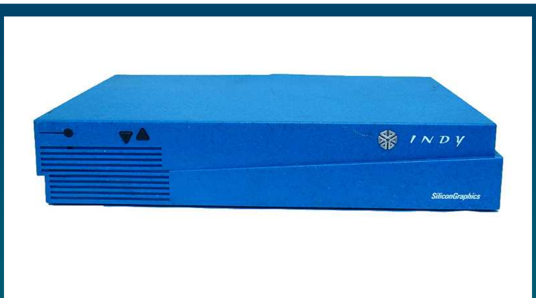
WriteConfig()
....

}

Dynamic memory allocation

Memory leaks: allocation of memory but no deletion

SGI Irix 5.1 (1993/94)
Indy with 16MB memory: completely unusable in 3-4 days. Transformed R4000 processor into an intel 386SX.
SGI solution: give away free additional memory



Object Vector Double* E=new double [Size] Vectors A & B
Copy object operation A = B {A.E = B.E}
Since E is a pointer, A.E → B.E
Pointer E of object A is pointing to the same memory location as that pointer E of object B

The original memory location of A.E has been dereferenced.
Delete B → delete B.E
Delete A → delete B.E (again) ERROR
Solution: Explicit copy constructor

Tools/code to check heap before & after running code

Elegance

$$\mathbf{v}\left(t+\frac{1}{2}\delta t\right)=\mathbf{v}\left(t-\frac{1}{2}\delta t\right)+\delta t.\mathbf{a}(t)$$

$$\mathbf{r}(t+\delta t)=\mathbf{r}(t)+\delta t.\mathbf{v}\left(t+\frac{1}{2}\delta t\right)$$

$$\mathbf{v}(\mathbf{t})=\frac{1}{2}\left[\mathbf{v}\left(t+\frac{1}{2}\delta t\right)+\mathbf{v}\left(t-\frac{1}{2}\delta t\right)\right]$$

```
// Advance velocity to V(t+0.5dt)
Velocity_fDT = Velocity_bDT + (Timestep * Force)/Mass;

// Advance position R(t+dt) using new velocity
R_fDT = R + Timestep * Velocity_fDT;

// Calculate Velocity(t)
Velocity = CConstant::HALF * (Velocity_fDT +Velocity_bDT);
```

Obscure programming by design

Citation Classics

Sheldrick G M. *SHELX76, program for crystal structure determination.* Cambridge, England: University of Cambridge, 1976. (Computer program.)

→ 4260 citations! SCI 1989

Sheldrick G M. *SHELX-90 computer program for determining crystal structures*, *Acta Cryst. A*, 46:467-73, 1990

→ cited 2,870 times ISI

Obscure programming by design: Achieving immortality in SCI rankings

(a) Program be robust; produce sensible numbers even when used for purposes for which it was not intended by someone who has lost the instructions (if there were any).

(b) “Comments” in a program and “structured programming” are superfluous and make it easy for users to “improve” the program and re-issue it as their own.

(c) Never publish the original algorithms employed (if any), or you will encourage cheap imitations.

(d) Make sure that the program contains one or two undocumented “features” or even “bugs” → user dependency and expectation of getting final/enhanced version will encourage users to cite you.

(e) By definition, the final version is always six months from completion, and so it never can be released.

Current Contents, 41, ISI, Oct 9, 1989

Obscure programming by design: Copyright issues

Scatter ‘do-nothing code’ throughout the program. Define some important looking variables, alter their contents in if-statements and within loops.

→Your signature

Post copies (x2) of the code (at significant stages of development) to yourself by special delivery. Keep certificates of posting and DO NOT open the packages until the lawyers need to,

Efficiency

Speed of execution

C and C++ should be identical – a design specification
Java ~80-90% of C/C++; in principle Java could be faster due lack of pointers and garbage collection.

Memory usage

To comply with the idea of objects, all variables defining the object's characteristics need to be defined in the class. Every molecule has info (variables) re atoms involved in bonds, angles and torsions; some variables may be redundant for a particular application; No scope for using variables transiently. → High memory requirement

Object-oriented programming: 'unbiased' assessment

Code is significantly more accessible

Easy to maintain & modify; Confidence

Major design issues

Spend 5 days pondering;
Implement in ½ day!

Obsession with elegance →
break design (again & again!)

Not good for small codes.
Superfluous code: functions coded for complete object characterization may never be used

Steep learning curve

> 1 year to write elegant (intuitive) code

Testing of code (1 of 2)

```
do 10 I=1,10
        a(I) = b(I,10) * sqrt(..)
C       write(5,*) print a(I);
        ....
10 continue
```

At some later stage, may even remove commented line!

Correct behaviour before efficiency

Testing of code (2 of 2)

Philosophy: test code is part & parcel of production code

Follow bottom up approach

Test each and every function

```
Function test()
{
   x1=10; y1=-6; z1=25;
   x2=7;   y2=7;  z2=7;
   d = distance(x1,x2,y1,y2,z1,z2)
   print  d, {22.4054}
   ..
   //test angle()
   …
   //test torsion()
   …
}
```

Test code is typically1/3
of real code;
Takes longer!

Use tools e.g. Mathematica;
Debugger to follow flow & values

If file has been modified
or further functions incorporated,
just run test code to check if
inadvertent editing occurred

Further reading

Beginners

Teach Yourself C++ by Herbert Schildt

Advanced

1. *Effective C++: 50 specific ways to improve your programs and design*, Scott Meyers
2. *The C++ programming language* Bjarne Stroustrup (Specification)

Free online resources

http://www.freeprogrammingresources.com/cppbooks.html

Thinking in C++, Bruce Eckel for C programmers

Concluding remarks

1. Consider OOP for large projects
   Be prepared to spend time in the design phase

   Don't forget the end goal:
   Simulation => results => publications

2. Test each and every function of your code using appropriate input data

   Test code is part & parcel of the production code

   Employ debuggers to follow flow and values of variable => confidence