Siena Computational Crystallography School 2005

Spectrum of languages

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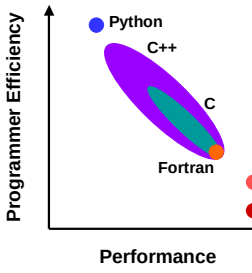
Spectrum of implementation languages

- Python
  - Interpreted, Object Oriented, Exception handling
- C++
  - Compiled, Object Oriented, Exception handling
- C
  - Compiled, User defined data types, Dynamic memory management
- Fortran
  - Compiled, Some high-level data types (N-dim arrays, complex numbers)
- Assembler
  - Computer program is needed to translate to machine code
- Machine code
  - Directly executed by the CPU

Matrix of language properties

	Dynamically typed -> convenience	Statically typed -> speed
Interpreted -> convenience	Python	Java
Compiled to machine code -> speed	Psyco	C++

Programmer Efficiency & Performance



- Maintainability
- Reusability
- Modularity

Choice of implementation languages

- Python
  - \+ Very high-level programming
  - \+ Easy to use (dynamic typing)
  - \+ Fast development cycle (no compilation required)
  - – Too slow for certain tasks
- C++
  - \+ High-level or medium-level programming
  - – Many arcane details (strong static typing)
  - \+ Largely automatic dynamic memory management (templates)
  - \+ Much faster than Python
  - \+ With enough attention, performance even rivals that of FORTRAN

Happy marriage: Python and C++

- Syntactic differences put aside, Python and C++ objects and functions are very similar.
- Flexibility (interpreted, dynamically typed) and Efficiency (compiled, statically typed) are complementary.
- Boost.Python (C++ library) provides the link:
  - Non-intrusive on the C++ design
  - Pseudo-automatic wrapping using C++ template techniques
  - No external tools needed
  - Creates sub-classable Python types
  - Python bindings are very maintainable
  - Tutorial and reference documentation

```
class_<unit_cell>("unit_cell")
  .def("volume", &unit_cell::volume)
  .def("fractionalize", &unit_cell::fractionalize)
;
```

Vector operations

- Computer Science wisdom:
  - Typically 90% of the time is spent in 10% of the code
- Similar to idea behind vector computers:
  - Python = Scalar Unit
  - C++ = Vector Unit
- Loading the vector unit: (8.7 seconds)

```
miller_indices = flex.miller_index()
for h in xrange(100):
  for k in xrange(100):
    for l in xrange(100):
      miller_indices.append((h,k,l))
```

- Go! (0.65 seconds)

```
space_group = sgtbx.space_group_info("P 41 21 2").group()
epsilons = space_group.epsilon(miller_indices)
```

Computing 1 million epsilons takes only 0.65 seconds!

Compiled vs. Interpreted

- Compiler
  - generates fast machine code
- Interpreter (Python, Perl, TCL/TK, Java)
  - may generate byte-code but not machine code

Compiled vs. Interpreted

- Compiler
  - generates fast machine code
  - needs arcane compilation commands
  - needs arcane link commands
  - generates object files (where?)
  - may generate a template repository (where?)
  - generates libraries (where?)
  - generates executables (where?)
  - needs a build tool (make, SCons)
  - all this is platform dependent
- Interpreter (Python, Perl, TCL/TK, Java)
  - may generate byte-code but not machine code

Conclusion languages

- It is important to know the modern concepts
  - Especially for ambitious projects
- Syntax is secondary
  - Anything that does the job is acceptable
    - Python, C++, csh, sh, bat, Perl, Java
- There is no one size fits all solution
  - But Python & C++ covers the entire spectrum
- Carefully weigh programmer efficiency vs. runtime efficiency
  - Prefer a scripting language unless runtime efficiency is essential

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http://www.phenix-online.org/ http://cctbx.sourceforge.net/