NORTHWEST INSTITUTE for ADVANCED COMPUTING

Modern C++ for High Performance Computing

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Backstory

- Group at Indiana University (Jaakko Jarvi, Jeremy Siek, Jeremiah Willock, Doug Gregor, et al)
- Contributed numerous features to C++11 (variadic templates, lambda, decltype, enable_if, &c.)
- (But not “concepts”)

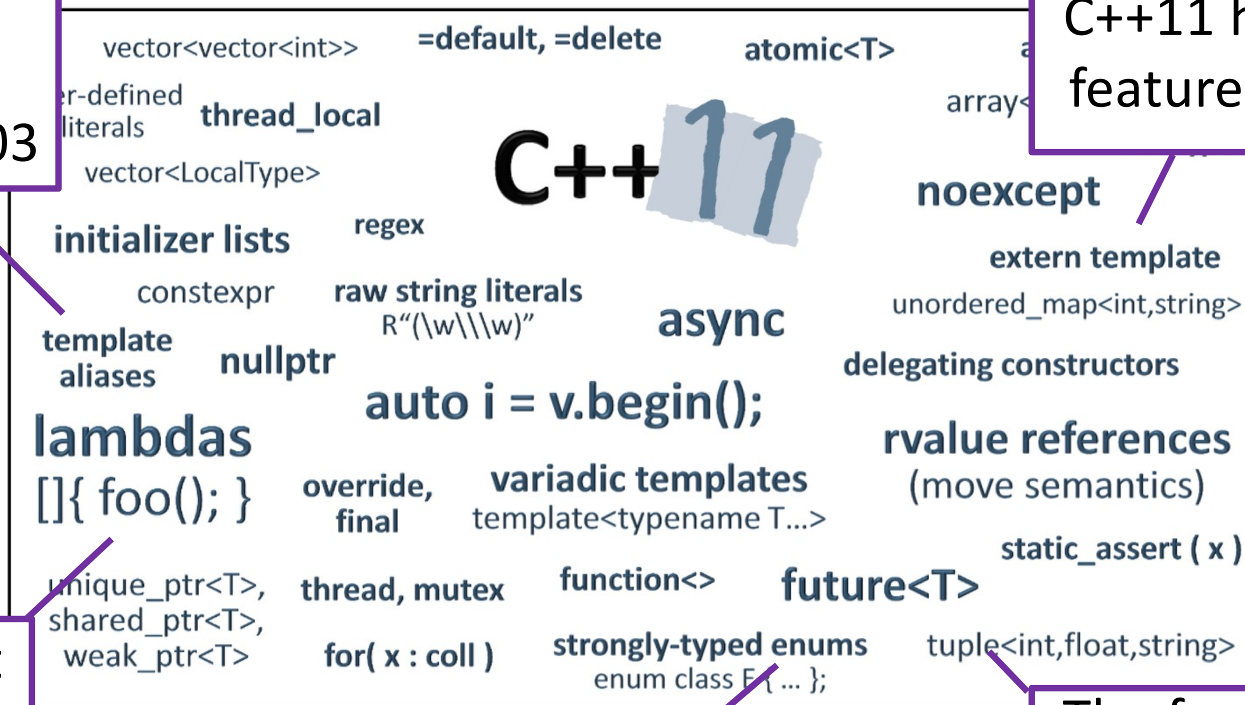
(Thank You BSSW)

- New institution, new course, new approach
- C++11 is a new language
- Clang is awesome
- Visual studio code is awesome

What this webinar is not about: Language Features

C++11 has many new features compared to C++03

C++11 has many features, period

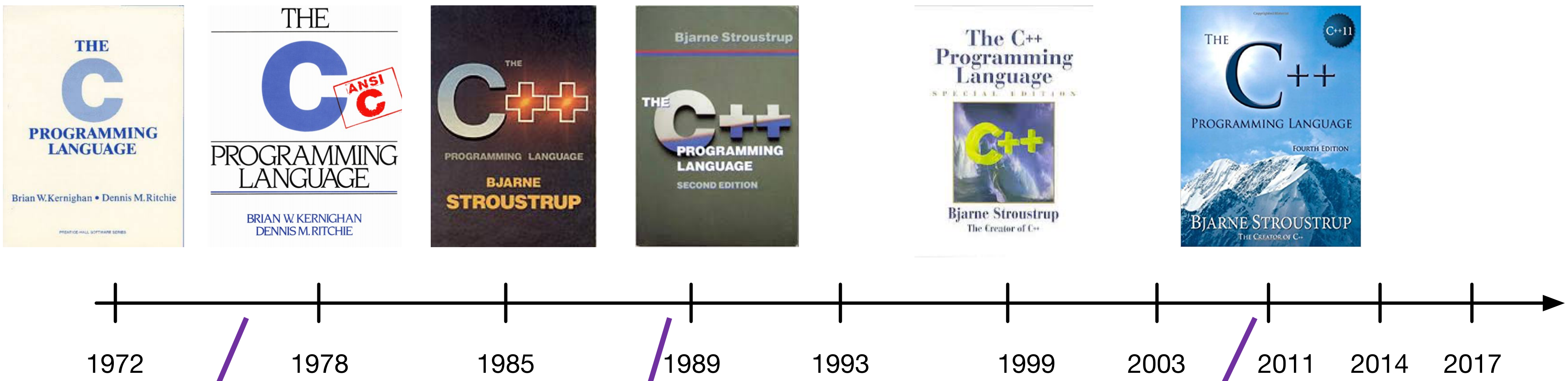


C++11 is not just C++03 with more features

A language is not just its features

The features per se aren't the source of power

Pedagogy recapitulates ontogeny considered harmful



Maturation of languages over time (ontogeny)

Features added, etc

Unfortunately, C++11 is taught as C plus 45 years of new features

Pedagogy recapitulates ontogeny

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1: A Tutorial Introduction.
2: Types, Operators, and Expressions.
3: Control Flow.
4: Functions and Program Structure.
5: Pointers and Arrays.
6: Structures.
7: Input and Output.
8: The UNIX System Interface.
Appendix A.
Appendix B.

Anonymous modern C++ book

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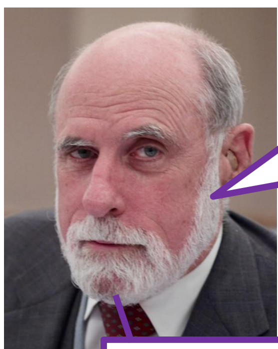
1: Introduction to Computers and C++
2: Introduction to C++ Programming, Input/Output and Operators
3: Introduction to Classes, Objects, Member Functions and Strings
4: Algorithm Development and Control Statements: Part 1
5: Control Statements: Part 2; Logical Operators
6: Functions and an Introduction to Recursion
7: Class Templates array and vector; Catching Exceptions
8: Pointers
9: Classes: A Deeper Look
10: Operator Overloading; Class string
11: Object-Oriented Programming: Inheritance
12: Object-Oriented Programming: Polymorphism
13: Stream Input/Output: A Deeper Look
14: File Processing
15: Standard Library Containers and Iterators
16: Standard Library Algorithms
17: &c.

What this webinar is about: Tasteful programming

- How to write your programs in C++11
- Not how to write C++11 in your programs
- Code is a medium for communication (a language)
- Any language has syntax and vocabulary – and style

With other developers

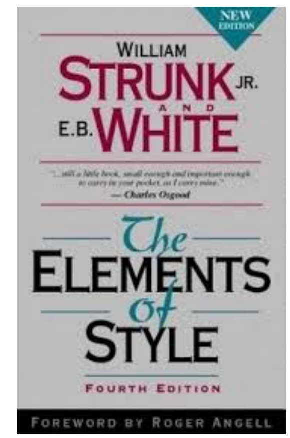
And with yourself



A language that doesn't affect the way you think about programming, is not worth knowing

Alan Perlis

CORE GUIDELINES



What is a programming language for?

- Managing (not causing) complexity
- What is the most powerful mental tool for managing complexity?

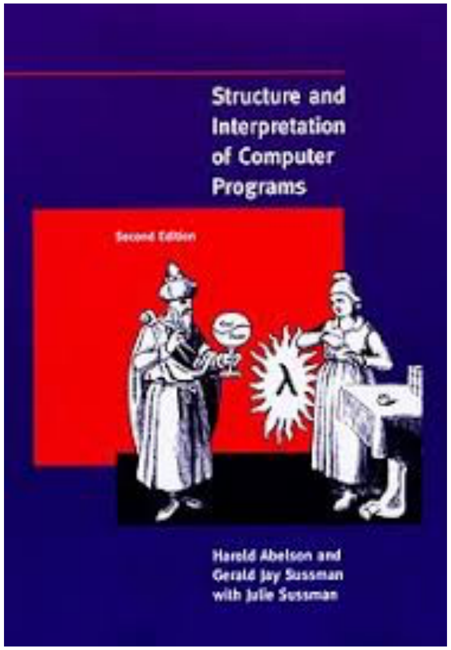
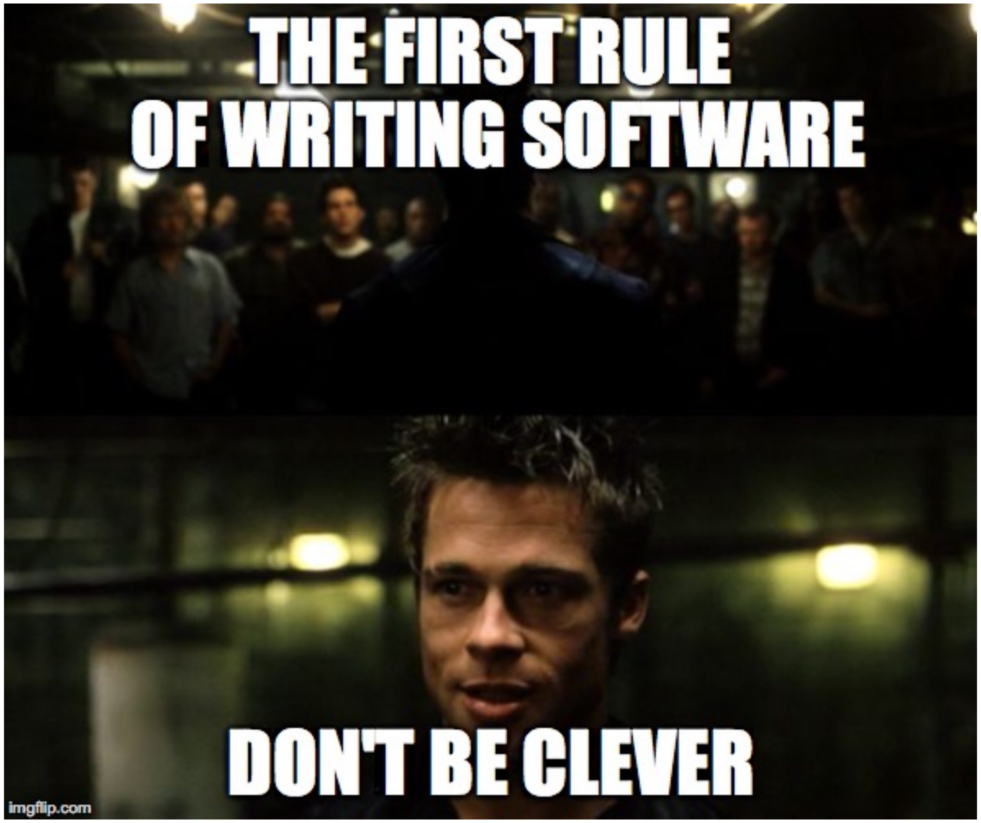
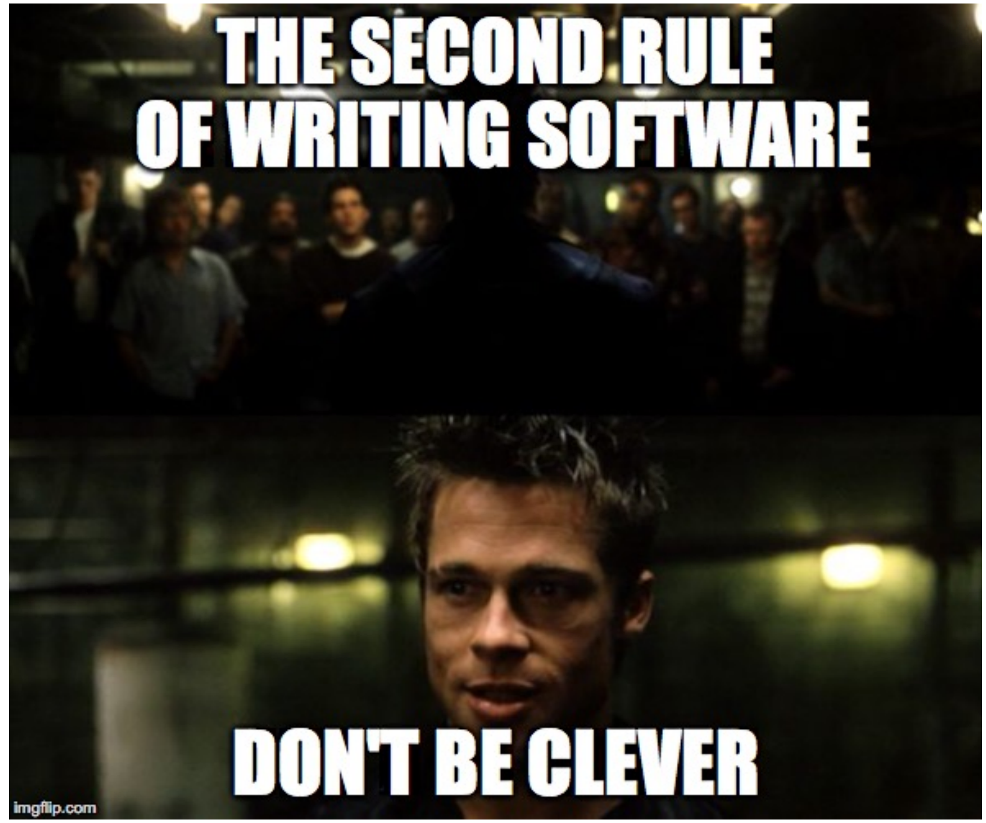


Table of Contents

Two simple rules for writing (tasteful) software





C++ core guidelines development philosophy

P.1: Express ideas directly in code
P.2: Write in ISO Standard C++
P.3: Express intent
P.4: Ideally, a program should be statically type safe
P.5: Prefer compile-time checking to run-time checking
P.6: What cannot be checked at compile time should be checkable at run time
P.7: Catch run-time errors early
P.8: Don't leak any resources
P.9: Don't waste time or space
P.10: Prefer immutable data to mutable data
P.11: Encapsulate messy constructs, rather than spreading through the code
P.12: Use supporting tools as appropriate
P.13: Use support libraries as appropriate

https://github.com/isocpp/CppCoreGuidelines/blob/master/CppCoreGuidelines.md#S-philosophy

C++ Core Guidelines

In: Introduction
P: Philosophy
I: Interfaces
F: Functions
C: Classes and class hierarchies
Enum: Enumerations
R: Resource management
ES: Expressions and statements
Per: Performance
CP: Concurrency
E: Error handling
Con: Constants and immutability
T: Templates and generic programming
CPL: C-style programming
SF: Source files
SL: The Standard library

A: Architectural Ideas
N: Non-Rules and myths
RF: References
Pro: Profiles
GSL: Guideline support library
NL: Naming and layout
FAQ: Frequently asked questions
Appendix A: Libraries
Appendix B: Modernizing code
Appendix C: Discussion
Appendix D: Tools support
Glossary
To-do: Unclassified proto-rules

GSL: Guidelines support library.

C++ Performance Core Guidelines (selected)

“Don’t”

Per.1: Don’t optimize without reason

Per.2: Don’t optimize prematurely

Per.3: Don’t optimize something that’s not performance critical

Per.4: Don’t assume that complicated code is necessarily faster than simple code

Per.5: Don’t assume that low-level code is necessarily faster than high-level code

Per.6: Don’t make claims about performance without measurements

Per.14: Minimize the number of allocations and deallocations

Per.19: Access memory predictably

Case Study: Numerical Linear Algebra

- Building abstractions with data: A Vector class
- Building abstractions with procedures: A Matrix class

P.1: Express ideas directly in code

P.2: Write in ISO Standard C++

P.3: Express intent

P.8: Don't leak any resources

P.9: Don't waste time or space

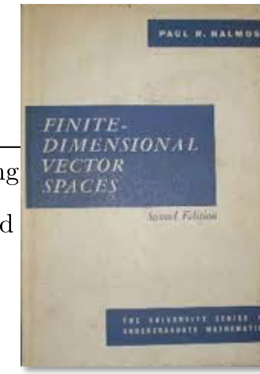
P.11: Encapsulate messy constructs, rather than spreading through the code

P.12: Use supporting tools as appropriate

P.13: Use support libraries as appropriate

Vector Desiderata

- Math
- $x \in \mathbb{R}^N$
- Access with subscript x_i
- $\alpha(x+y) = \alpha x + \alpha y$
- Code
- `Vector x(N);`
- Access elements with “subscript” `x(i)`
- `a * x(i)`



Definition. (Halmos) A vector space is a set V of elements called *vectors* satisfying

1. To every pair x and y of vectors in V there corresponds a vector $x+y$ called … such a way that
   - (a) addition is commutative, $x+y=y+x$
   - (b) addition is associative, $x+(y+z)=(x+y)+z$
   - (c) there exists in V a unique vector 0 (called the origin) such that $x+0=x$ for ever vector x, and
   - (d) to every vector x in V there corresponds a unique vector $-x$ such that $x+(-x)=0$
2. To every pair a and x where a is a scalar and x is a vector in V, there corresponds a vector ax in V called the product of a and x in such a way that
   - (a) multiplication by scalars is associative $a(bx)=(ab)x$, and
   - (b) $1x=x$ for every vector x.
3. (a) Multiplications by scalar is distributive with respect to vector addition. $a(x+y)=ax+ay$
   - (b) multiplication by vetors is distributive with respect to scalar addition $(a+b)x=ax+by$

Class Vector

```
class Vector {
public:
  Vector(size_t M) : num_rows_(M), storage_(num_rows_) {}

        double& operator()(size_t i)       { return storage_[i]; }
  const double& operator()(size_t i) const { return storage_[i]; }

  size_t num_rows() const { return num_rows_; }

private:
  size_t              num_rows_;
  std::vector<double> storage_;
};
```

Constructor

Accessors

Internal state

Class Vector

```
class Vector {
public:
  Vector(size_t M) : num_rows_(M), storage_(num_rows_) {}

        double& operator()(size_t i)       { return storage_[i]; }
  const double& operator()(size_t i) const { return storage_[i]; }

  size_t num_rows() const { return num_rows_; }

private:
  size_t              num_rows_;
  std::vector<double> storage_;
};
```

C.41: A constructor should create a fully initialized object

C.49: Prefer initialization to assignment in constructors

F.5: If a function is small and time-critical, declare it inline

C.4: Make a function a member only if it needs direct access to the representation of the class

C.9: Minimize exposure of members

Class Vector

C.20: If you can avoid defining any default operations, do

C.31: All resources acquired by a class must be released by the class's destructor

```
class Vector {
public:
  Vector(size_t M) : num_rows_(M), storage_(num_rows_) {}

        double& operator()(size_t i)       { return storage_[i]; }
  const double& operator()(size_t i) const { return storage_[i]; }

  size_t num_rows() const { return num_rows_; }

private:
  size_t              num_rows_;
  std::vector<double> storage_;
};
```

C.31: All resources acquired by a class must be released by the class's destructor

Class Vector

```
class Vector {
public:
  Vector(size_t M) : num_rows_(M), storage_(num_rows_) {}

        double& operator()(size_t i)       { return storage_[i]; }
              operator()(size_t i) const { return storage_[i]; }

              s() const { return num_rows_; }

private:
  size_t              num_rows_;
  std::vector<double> storage_;
};
```

ES.2: Prefer suitable abstractions to direct use of language features

SL.con.1: Prefer using STL array or vector instead of a C array

SL.con.2: Prefer using STL vector by default unless you have a reason to use a different container

[1] https://godbolt.org/z/9eNyFh

Using Vector class

```
int main() {
  const size_t size = 1024;

  Vector x(size), y(size);
  for (size_t i = 0; i < x.size(); ++i) {
    x(i) = i;
  }

  Vector z = add(x, y);

  Vector w(size);
  add(x, y, w);

  Vector u = x + y;
}
```

ES.20: Always initialize an object

ES.20: Always initialize an object

ES.21: Don't introduce a variable before you need it

ES.22: Don't declare a variable until you have a value to initialize it with

[1] https://godbolt.org/z/h80vg8

Copy constructors (before)

```cpp
Vector operator+(Vector& x, Vector& y) {
  Vector z(x.num_rows());
  // ...
  return z;
}

int main() {
  Vector u(1024), v(1024), w(1024);

  u = v;
  u = v + w;

  Vector x = u + v;
}
```

Constructor

Return by ***value***

Copy assignment

Copy assignment

Call operator+
Calls constructor (for temporary)
Return by value: copy constructor
(compiler tricks: NVRO)

Copy constructor

[1] https://godbolt.org/z/e7t60N

Move: Overload on value class

```
class Vector {
public:
  Vector(size_t);
  Vector();
  Vector(const Vector&);
  Vector(Vector&&);
  Vector& operator=(const Vector&);
  Vector& operator=(Vector&&);
  ~Vector();
  // ...
};
```

Copy constructor

Move constructor

Copy Assignment

Move assignment

Takes const reference

Takes ***rvalue reference***

Takes const reference

Takes ***rvalue reference***

Overload on whether parameter is temporary or not

Move and rvalue references

```
Vector operator+(Vector& x, Vector& y) {
  Vector z(x.num_rows());
  // ...
  return z;
}

int main() {
  Vector u(1024), v(1024), w(1024);

  Vector x = u + v;

  u = v;
  u = v + w;
}
```

Constructor

Return by ***value***

Move (or elided move)

Copy constructor not called

Returned by value from function

Copy assignment

Not copy assignment

Move from temporary

[1] https://godbolt.org/z/e7t60N

Swap

```cpp
template<typename T>
void old_swap(T& a, T& b) {
  T tmp = a;
  a = b;
  b = tmp;
}
```

Old generic swap template: 3 deep copies

Specialized (class specific) overload for efficient swap

New generic swap template: 3 moves (shallow copies)

```cpp
template<typename T>
void new_swap(T& a, T& b) {
  T tmp = std::move(a);
  a = std::move(b);
  b = std::move(tmp);
}
```

a is left uninitialized after move

Ready for(move) assignment

```cpp
int main() {
  Vector u(1024), v(1024);

  old_swap(u, w);
  new_swap(u, w);
}
```

Keep It Simple: Argument Passing

	Cheap or impossible to copy (e.g., int, unique_ptr)	**Cheap to move** (e.g., vector<T>, string) or **Moderate cost to move** (e.g., array<vector>, BigPOD) or **Don't know** (e.g., unfamiliar type, template)	**Expensive to move** (e.g., BigPOD**[]**, array<BigPOD>)
Out	X f()		
In/Out	f(X&)		
In	f(X)	f(const X&)	
In & retain "copy"			

"Cheap" ≈ a handful of hot int copies
"Moderate cost" ≈ memcpy hot/contiguous ~1KB and no allocation

** or return unique_ptr<X>/make_shared_<X> at the cost of a dynamic allocation*

Keep It Simple: Argument Passing

<table>
<tr><th></th><th>Cheap or impossible to copy (e.g., int, unique_ptr)</th><th>Cheap to move (e.g., vector<T>, string)
or Moderate cost to move (e.g., array<vector>, BigPOD)
or Don't know (e.g., unfamiliar type, template)</th><th>Expensive to move
(e.g., BigPOD[], array<BigPOD>)</th></tr>
<tr><td>Out</td><td colspan="2">X f()</td><td></td></tr>
<tr><td>In/Out</td><td colspan="3">f(X&)</td></tr>
<tr><td>In</td><td rowspan="2">f(X)</td><td colspan="2">f(const X&)</td></tr>
<tr><td>In & retain copy</td><td>f(const X&) + f(X&&) & move **</td><td>f(const X&)</td></tr>
<tr><td>In & move from</td><td colspan="3">f(X&&) **</td></tr>
</table>

** or return unique_ptr<X>/make_shared_<X> at the cost of a dynamic allocation*

*** special cases can also use perfect forwarding (e.g., multiple in+copy params, conversions)*

Resource Acquisition is Initialization (RAII)

```
int main() {

  Vector x(1024), y(1024);

  Vector u = foo(x);

  Vector v = bar(x);

  v = foo(x);

  u = bar(x);

  return 0;
}
```

```
int main() {

  int x = 1024, y = 1024;

  int u = foo(x);

  int v = bar(x);

  v = foo(x);

  u = bar(x);

  return 0;
}
```

We are using Vectors just like built-in types

And Vectors are non-trivial compound types

Resource Acquisition is Initialization (RAII)

- The "big six" (plus ordinary constructor) give us complete control over the lifetime of the resources contained in the object
- Resource Acquisition Is Initialization (RAII)
- Let each resource have an owner in some scope and by default be released at the end of its owners scope
- Note ***we never use "new" or "delete"*** (or, worse, malloc() and free()) – and never should use them
- Vector is a "resource handle"
- No abstraction penalty (no funny business with copies)

R.11: Avoid calling new and delete explicitly

R.10: Avoid malloc() and free()

Stroustrup, Bjarne. A Tour of C++ (C++ In-Depth Series) (p. 54).

Arithmetic operators

```
Vector operator+(const Vector& x,const Vector& y) {

  Vector z(x.num_rows());
  for (size_t i = 0; i < x.num_rows(); ++i
    z(i) = x(i) + y(i);
  }

  return z;
}
```

Returns a Vector

Free function

Takes two Vectors as input

Construct

Add elements

Returns a Vector

All access is through public member functions

Arithmetic operators

```
Vector operator*(const double& a,const Vector& x) {

  Vectory(x.num_rows());
  for (size_t i = 0; i < x.num_rows(); ++i) {
     y(i) = a * x(i);
  }

  return y;
}
```

Returns a Vector

Construct

Return by value

Arithmetic operators

Return by reference

```
Vector& operator+=(Vector& y, const Vector& x) {

  for (size_t i = 0; i < x.num_rows(); ++i) {
    y(i) += x(i);
  }

  return y;
}
```

Note no construction

Timing comparisons

```
Vector x(size), y(size);
double a = 3.14159;

for (size_t j = 0; j < iter; ++j) {
  y += a*x;
}
```

```
Vector x(size), y(size);
double a = 3.14159;

for (size_t j = 0; j < iter; ++j) {
  y += x;
}
```

Operator notation

```
double *x = (double*) malloc(size * sizeof(double));
double *y = (double*) malloc(size * sizeof(double));
double a = 3.14159;

for (size_t j = 0; j < iter; ++j) {
  for (size_t i = 0; i < size; ++i) {
    y[i] += a*x[i];
  }
}
```

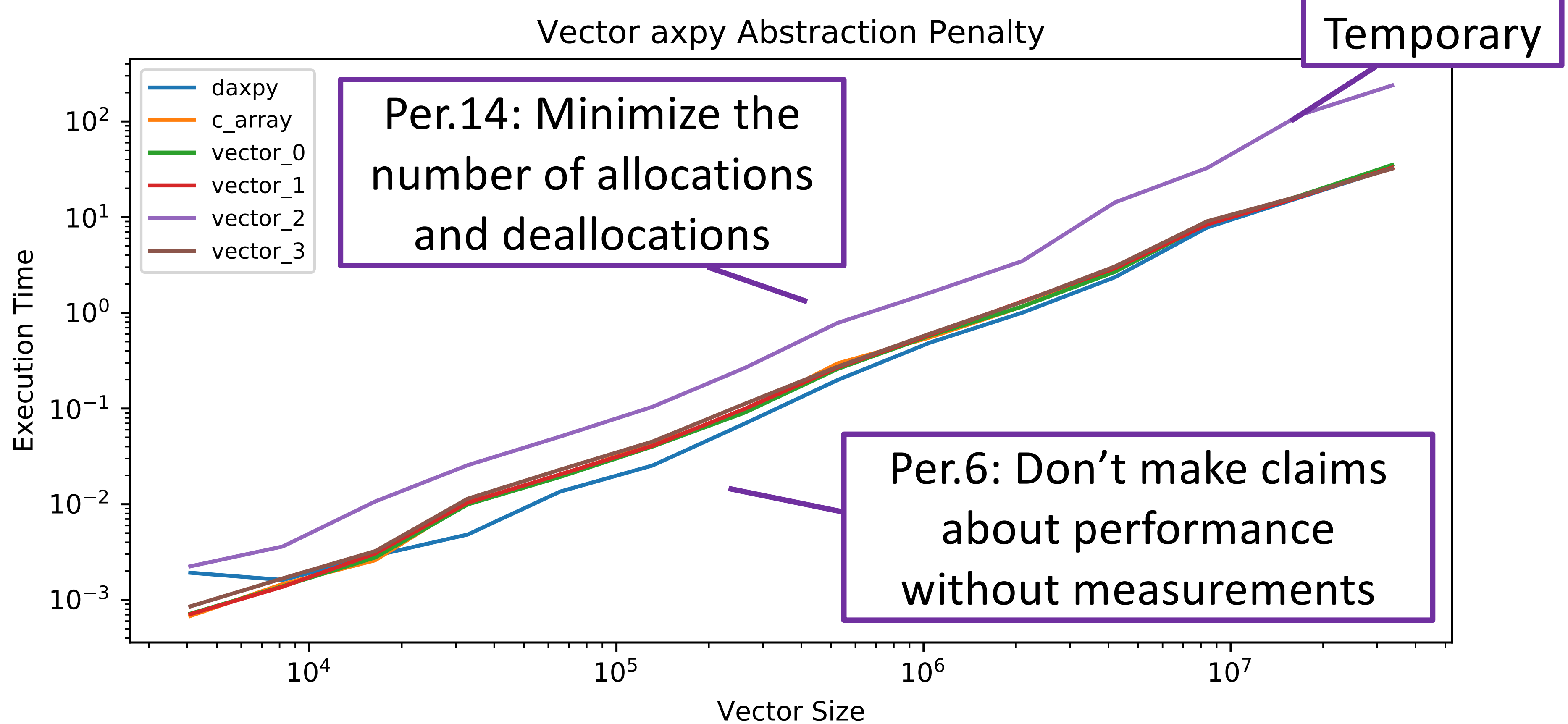
C

```
Vector x(size), y(size);
double a = 3.14159;

for (size_t j = 0; j < iter; ++j) {
  for (size_t i = 0; i < size; ++i) {
    y(i) += a*x(i);
  }
}
```

C++

Raw loop

Performance



Vector axpy with no temporary

```
Vector x(size), y(size);
scalar a = 3.14159;

for (size_t j = 0; j < iter; ++j) {
  y += a*x;
}
```

No temporary

As fast as hand-written

As fast as daxpy()

Lazy evaluation

Cf: MTL

Wrap up vector and scalar for later

```
struct scaledVector {
public:
  scaledVector(const double& a, const Vector& v) : scalar_(a), vector_(v) {}
  const double& scalar_;
  const Vector& vector_;
};

scaledVector operator*(const double& a, const Vector& x) {
  return scaledVector(a, x);
}

Vector& operator+=(Vector& y, const scaledVector& x) {
  for (size_t i = 0; i < y.num_rows(); ++i) {
    y(i) += x.scalar_ * x.vector_(i);
  }

  return y;
}
```

Scalar times vector doesn't do anything but wrap up scalar and vector

When we use the scaled vector, we do the scaling

Resist urge to be clever

Class Matrix

You should be able to explain the design decisions of this class

```
class Matrix {
public:
  Matrix(size_t M, size_t N) : num_rows_(M), num_cols_(N), storage_(num_rows_ * num_cols_) {}

        double& operator()(size_t i, size_t j)       { return storage_[i * num_cols_ + j]; }
  const double& operator()(size_t i, size_t j) const { return storage_[i * num_cols_ + j]; }

  size_t num_rows() const { return num_rows_; }
  size_t num_cols() const { return num_cols_; }

private:
  size_t              num_rows_, num_cols_;
  std::vector<double> storage_;
};
```

Note 1D storage

LU factorization

Partial pivoting takes two more lines of code

```cpp
void lu(Matrix& A) {
  size_t m = A.numRows(), n = A.numCols();

  for (size_t k = 0; k < m - 1; ++k) {
    for (size_t i = k + 1; i < m; ++i) {
      double z = A(i, k) / A(k, k);
      A(i, k) = z;

      for (size_t j = k + 1; j < n; ++j)
        A(i, j) -= z * A(k, j);
    }
  }
}
```

LU implemented only with Matrix accessors

```cpp
void lu(Matrix& A, std::vector<size_t>& perm) {
  size_t m = A.numRows(), n = A.numCols();

  std::iota(perm.begin(), perm.end(), 0);

  for (size_t k = 0; k < m - 1; ++k) {

    pivot(A, k, perm);

    for (size_t i = k + 1; i < m; ++i) {
      double z = A(i, k) / A(k, k);
      A(i, k) = z;

      for (size_t j = k + 1; j < n; ++j)
        A(i, j) -= z * A(k, j);
    }
  }
}
```

Again, only need specified interface (we will generalize this)

Matrix-matrix product

Free function

```
void multiply(const Matrix& A, const Matrix&B, Matrix&C) {
  for (size_t i = 0; i < A.num_rows(); ++i) {
    for (size_t j = 0; j < B.num_cols(); ++j) {
      for (size_ k = 0; k < A.num_cols(); ++k) {
        C(i,j) += A(i,k) * B(k,j);
      }
    }
  }
```

Written with external interface of Matrix class

Hoisting and tiling

```
void hoistedTiledMultiply2x2(const Matrix& A, const Matrix&B, Matrix&C) {
  for (size_t i = 0; i < A.num_rows(); i += 2) {
    for (size_t j = 0; j < B.num_cols(); j += 2) {
      double t00 = C(i,   j);     double t01 = C(i,   j+1);
      double t10 = C(i+1,j);     double t11 = C(i+1,j+1);
      for (size_t k = 0; k < A.num_cols(); ++k) {
        t00 += A(i   , k) * B(k, j   );
        t01 += A(i   , k) * B(k, j+1);
        t10 += A(i+1, k) * B(k, j   );
        t11 += A(i+1, k) * B(k, j+1);
      }
      C(i,   j) = t00;  C(i,   j+1) = t01;
      C(i+1,j) = t10;  C(i+1,j+1) = t11;
    }
  }
}
```

Well known optimization

Written with external interface of Matrix class

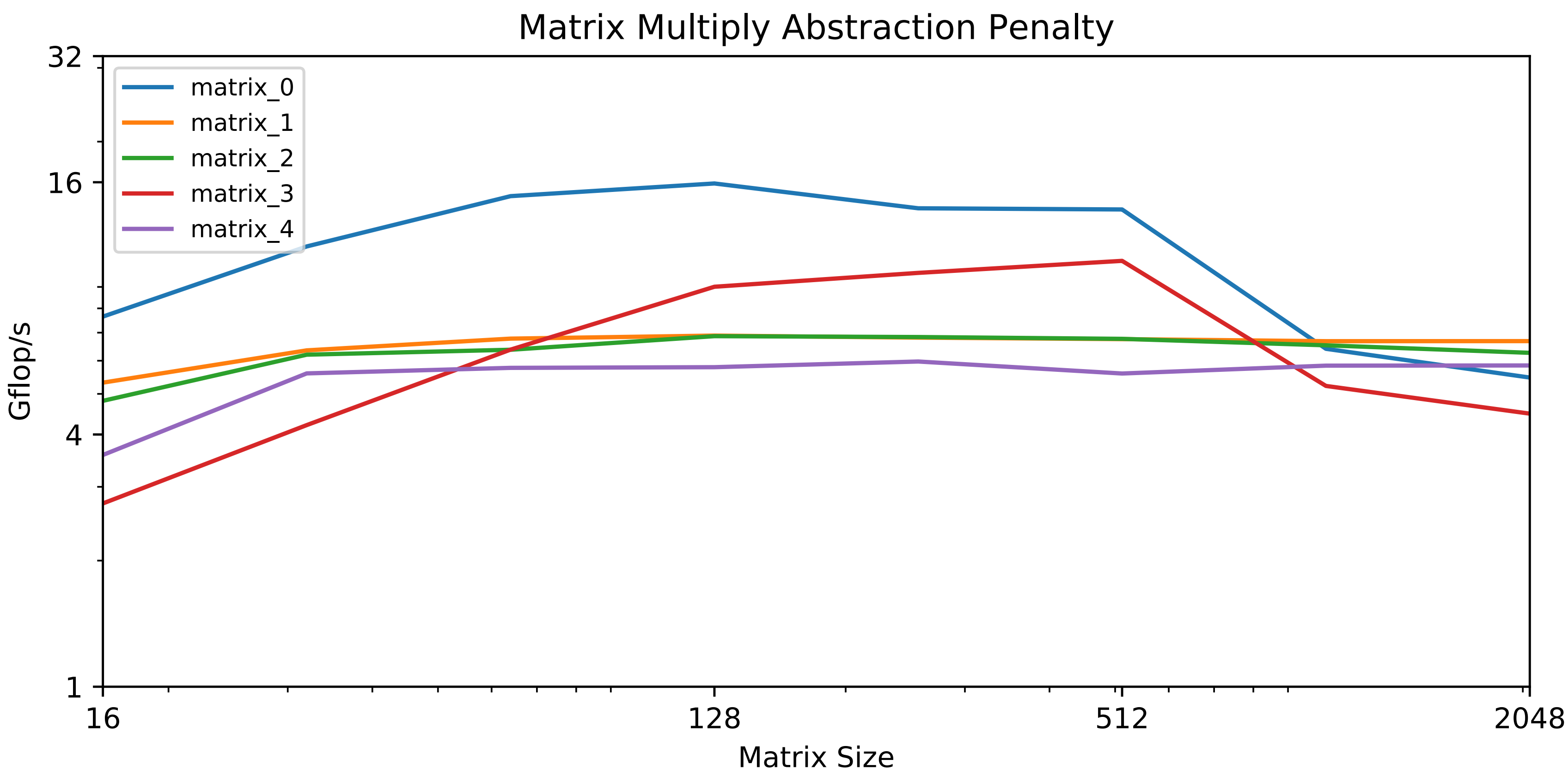
Blocking and tiling

```
void blockedTiledMultiply2x2(const Matrix& A, const Matrix&B, Matrix&C) {
  const int blocksize = std::min(A.num_rows(), 32);

  for (size_t ii = 0; ii < A.num_rows(); ii += blocksize) {
    for (size_t jj = 0; jj < B.num_cols(); jj += blocksize) {
      for (size_t kk = 0; kk < A.num_cols(); kk += blocksize) {

        for (size_t i = ii; i < ii+blocksize; i += 2) {
          for (size_t j = jj; j < jj+blocksize; j += 2) {
            for (size_t k = kk; k < kk+blocksize; ++k) {
              C(i  , j  ) += A(i  , k) * B(k, j  );
              C(i  , j+1) += A(i  , k) * B(k, j+1);
              C(i+1, j  ) += A(i+1, k) * B(k, j  );
              C(i+1, j+1) += A(i+1, k) * B(k, j+1);
            }
          }
        }
      }
    }
  }
}
```

Well known optimization

Written with external interface of Matrix class

Hierarchical memory optimizations



Vectorization with intrinsics

```
for (int i = ii; i < ii+blocksize; i += 4) {
  for (int j = jj, jb = 0; j < jj+blocksize; j += 4, jb += 4) {

    __m256d t0x = _mm256_load_pd(&C(i,  j));
    __m256d t1x = _mm256_load_pd(&C(i+1,j));
    __m256d t2x = _mm256_load_pd(&C(i+2,j));
    __m256d t3x = _mm256_load_pd(&C(i+3,j));

    for (int k = kk, kb = 0; k < kk+blocksize; ++k, ++kb) {

     __m256d bx = _mm256_setr_pd(BB(jb,kb), BB(jb+1,kb), BB(jb+2,kb), BB(jb+3,kb));

     __m256d a0 = _mm256_broadcast_sd(&A(i   ,k));
      a0  = _mm256_mul_pd(bx,  a0);
      t0x = _mm256_add_pd(t0x, a0);

      __m256d a1 = _mm256_broadcast_sd(&A(i+1,k));
      a1  = _mm256_mul_pd(bx,  a1);
      t1x = _mm256_add_pd(t1x, a1);

      __m256d a2 = _mm256_broadcast_sd(&A(i+2,k));
      a2  = _mm256_mul_pd(bx,  a2);
      t2x = _mm256_add_pd(t2x, a2);

      __m256d a3 = _mm256_broadcast_sd(&A(i+3,k));
      a3  = _mm256_mul_pd(bx,  a3);
      t3x = _mm256_add_pd(t3x, a3);
    }

    _mm256_store_pd(&C(i,  j), t0x);
    _mm256_store_pd(&C(i+1,j), t1x);
    _mm256_store_pd(&C(i+2,j), t2x);
    _mm256_store_pd(&C(i+3,j), t3x);
  }
}
```

X86 Assembly

AVX instructions

256 bit register

```
vbroadcastsd    (%rdx,%r8,8), %ymm3
vfmadd213pd     %ymm4, %ymm8, %ymm3
vbroadcastsd    (%rsi,%r8,8), %ymm2
vfmadd213pd     %ymm5, %ymm8, %ymm2
vbroadcastsd    (%rbx,%r8,8), %ymm1
vfmadd213pd     %ymm6, %ymm8, %ymm1
vbroadcastsd    (%rdi,%r8,8), %ymm0
vfmadd213pd     %ymm7, %ymm8, %ymm0
```

Fused Multiply-Add

Multiply-Add are separate here

Clang can do it better

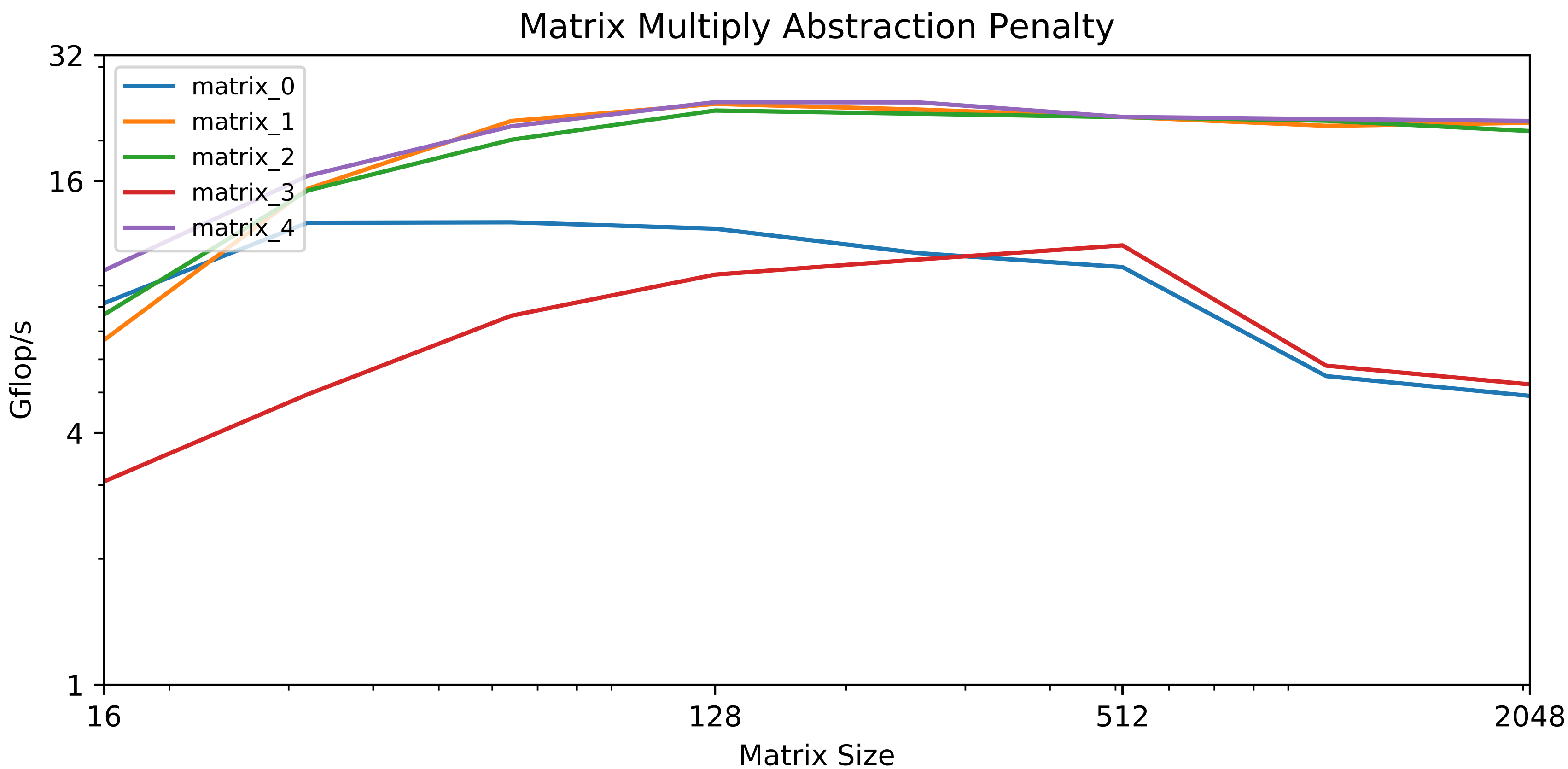
```
for (int i = ii; i < ii+blocksize; i += 2) {
  for (int j = jj, jb = 0; j < jj+blocksize; j += 2, jb += 2) {
    double t00 = C(i,j);        double t01 = C(i,j+1);
    double t10 = C(i+1,j);      double t11 = C(i+1,j+1);

    for (int k = kk, kb = 0; k < kk+blocksize; ++k, ++kb) {
      t00 += A(i  , k) * BB(jb  , kb);
      t01 += A(i  , k) * BB(jb+1, kb);
      t10 += A(i+1, k) * BB(jb  , kb);
      t11 += A(i+1, k) * BB(jb+1, kb);
    }

    C(i,  j) = t00;  C(i,  j+1) = t01;
    C(i+1,j) = t10;  C(i+1,j+1) = t11;
  }
}
```

Fused Multiply-Add

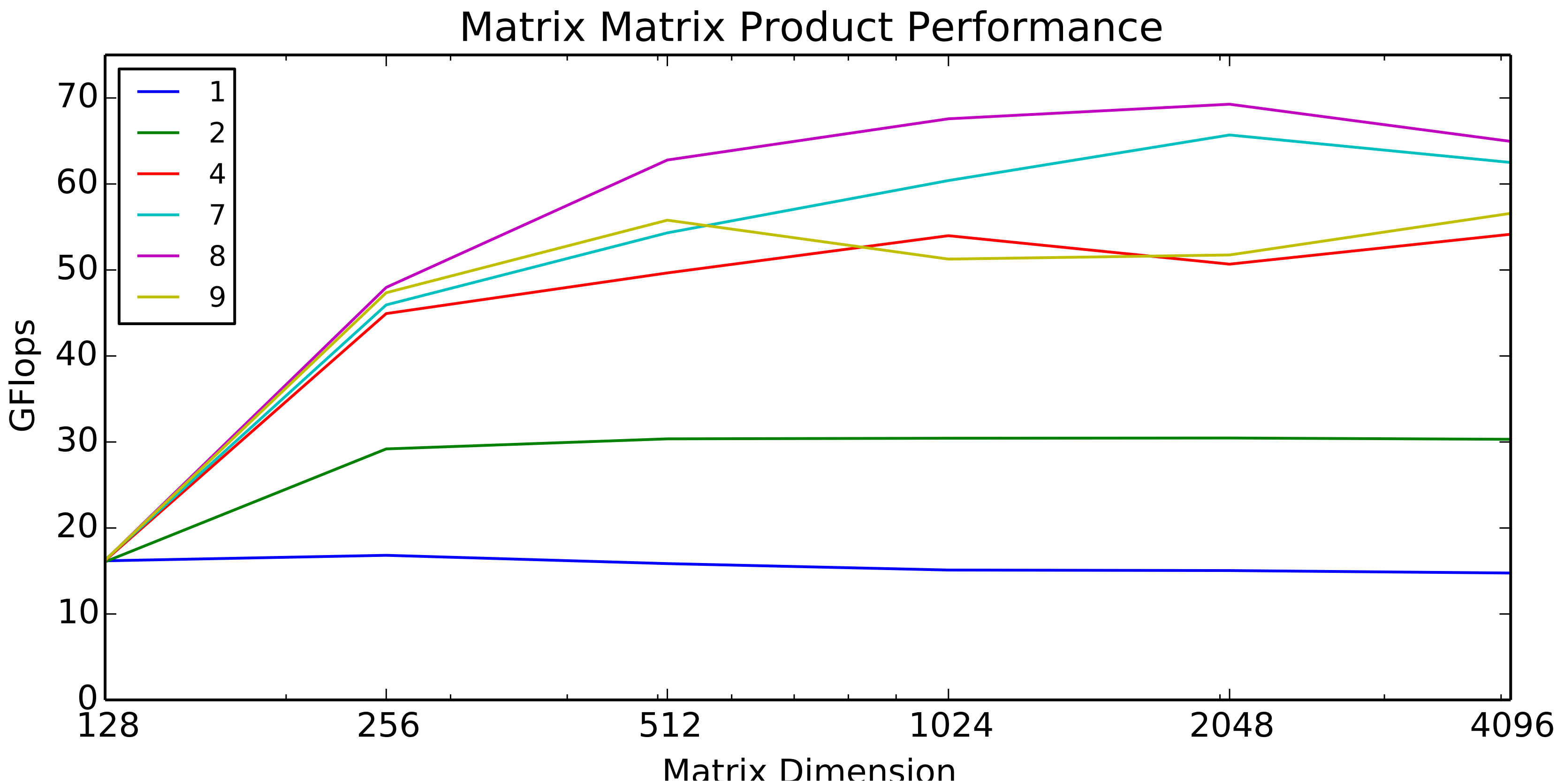
256 bit registers

```
vmovupd         (%r8,%r13,8), %ymm4
vmovupd         (%r11,%r13,8), %ymm5
vfmadd231pd     %ymm4, %ymm5, %ymm3
vmovupd -32     (%r9,%r13,8), %ymm6
vfmadd231pd     %ymm4, %ymm6, %ymm2
vmovupd         (%rdx,%r13,8), %ymm4
vfmadd231pd     %ymm5, %ymm4, %ymm1
vfmadd231pd     %ymm6, %ymm4, %ymm0
vmovupd         (%rcx,%r13,8), %ymm4
vmovupd 32      (%r11,%r13,8), %ymm5
vfmadd231pd     %ymm4, %ymm5, %ymm3
vmovupd         (%r9,%r13,8), %ymm6
vfmadd231pd     %ymm4, %ymm6, %ymm2
vmovupd         (%rbx,%r13,8), %ymm4
vfmadd231pd     %ymm5, %ymm4, %ymm1
vfmadd231pd     %ymm6, %ymm4, %ymm0
```

With clang optimizations



Parallelization with tasks



NORTHWEST INSTITUTE for ADVANCED COMPUTING

Pacific Northwest NATIONAL LABORATORY Proudly Operated by Battelle for the U.S. Department of Energy

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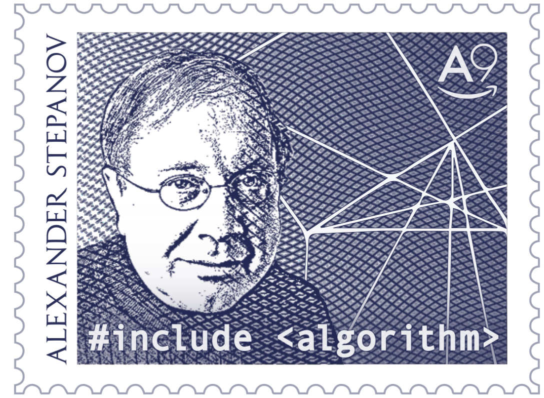
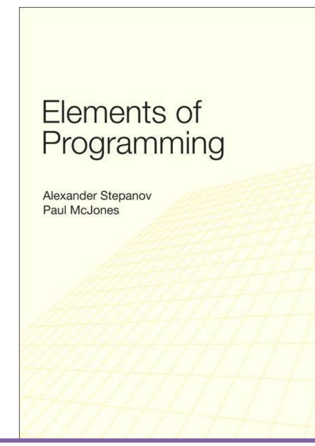
The Standard Template Library

- In early-mid 90s Stepanov, Musser, Lee applied principles of ***generic programming*** to C++
- Leveraged templates / parametric polymorphism



Containers	Iterators	Algorithms
`std::set`		`std::for_each`
`std::list`	ForwardIterator	`std::sort`
`std::map`	ReverseIterator	`std::accumulate`
`std::vector`	RandomAccessIterator	`std::min_element`
...		...



Alexander Stepanov and Paul McJones. 2009. *Elements of Programming* (1st ed.). Addison-Wesley Professional.

Generic LU factorization

Use with any type

```
template <typename Matrix>
void lu(Matrix& A) {
  size_t m = A.numRows(), n = A.numCols();

  for (size_t k = 0; k < m - 1; ++k) {
    for (size_t i = k + 1; i < m; ++i) {
      double z = A(i, k) / A(k, k);
      A(i, k) = z;

      for (size_t j = k + 1; j < n; ++j)
        A(i, j) -= z * A(k, j);
    }
  }
}
```

That has this interface

That models this ***concept***

```
template <typename Matrix>
void lu(Matrix& A, std::vector<size_t>& perm) {
  size_t m = A.numRows(), n = A.numCols();

  std::iota(perm.begin(), perm.end(), 0);

  for (size_t k = 0; k < m - 1; ++k) {

    pivot(A, k, perm);

    for (size_t i = k + 1; i < m; ++i) {
      double z = A(i, k) / A(k, k);
      A(i, k) = z;

      for (size_t j = k + 1; j < n; ++j)
        A(i, j) -= z * A(k, j);
    }
  }
}
```

A cautionary tale

"I've assigned this problem in courses at Bell Labs and IBM. Professional programmers had a couple of hours to convert the description into a programming language of their choice; a high-level pseudo code was fine… Ninety percent of the programmers found bugs in their programs (and I wasn't always convinced of the correctness of the code in which no bugs were found)."

- Jon Bentley, Programming Pearls, 1986

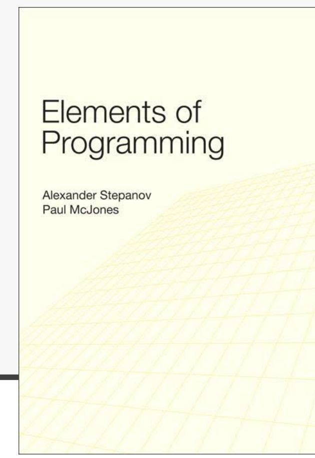
This must be a complicated algorithm!

(Example thanks to Sean Parent)

Binary search solution

```
int* lower_bound(int* first, int* last, int x)
{
  while (first != last)
  {
  int* middle = first + (last - first) / 2;

  if (*middle < x) first = middle + 1;
  else last = middle;
  }

  return first;
}
```

```
template<typename ForwardIterator, typename T>
ForwardIterator
lower_bound(ForwardIterator first,
            ForwardIterator last, const T& x) {

  while (first != last) {
    auto middle = first + (last - first) / 2;

    if (*middle < x)
      first = middle + 1;
    else
      last = middle;
  }

  return first;
}
```



Not an indictment of “kids these days”

Programming is really hard

When you get it right, make it generic

Generic accumulate

We use name “InputIt” to hint to programmer that this should be an InputIterator

Concepts (finally) with C++20

std::accumulate

Defined in header `<numeric>`

```
template< class InputIt, class T >
T accumulate( InputIt first, InputIt last, T init );                    (1)

template< class InputIt, class T, class BinaryOperation >
T accumulate( InputIt first, InputIt last, T init,                      (2)
              BinaryOperation op );
```

Computes the sum of the given value `init` and the elements in the range `[first, last)`. The first version uses `operator+` to sum up the elements, the second version uses the given binary function `op`, both applying `std::move` to their operands on the left hand side (since C++20).

`op` must not have side effects.	(until C++11)
`op` must not invalidate any iterators, including the end iterators, or modify any elements of the range involved.	(since C++11)

Type requirements

- `InputIt` must meet the requirements of `InputIterator`.
- `T` must meet the requirements of `CopyAssignable` and `CopyConstructible`.

Sort

std::sort

Defined in header <algorithm>

```
template< class RandomIt >
void sort( RandomIt first, RandomIt last );
```

```
template< class ExecutionPolicy, class RandomIt >
void sort( ExecutionPolicy&& policy, RandomIt first, RandomIt las
```

```
template< class RandomIt, class Compare >
void sort( RandomIt first, RandomIt last, Compare comp );
```

```
template< class ExecutionPolicy, class RandomIt, class Compare >
void sort( ExecutionPolicy&& policy, RandomIt first, RandomIt last, Compare comp );
```

Wait, what's this?

Defaultx

Customizable

Type requirements

- RandomIt must meet the requirements of ValueSwappable and RandomAccessIterator.
- The type of dereferenced RandomIt must meet the requirements of MoveAssignable and MoveConstructible.
- Compare must meet the requirements of Compare.

Execution Policies

std::execution::seq, std::execution::par, std::execution::par_unseq

Defined in header <execution>

```
inline constexpr std::execution::sequenced_policy seq { /* unspecified */ };
```

```
inline constexpr std::execution::parallel_policy par { /* unspecified */ };
```

```
inline constexpr std::execution::parallel_unsequenced_policy par_unseq { /* unspecified */ };
```

Parallel standard library algorithms

- std::adjacent_difference
- std::adjacent_find
- std::all_of
- std::any_of
- std::copy
- std::copy_if
- std::copy_n
- std::count
- std::count_if
- std::equal
- std::fill
- std::fill_n
- std::find
- std::find_end
- std::find_first_of
- std::find_if
- std::find_if_not
- std::generate
- std::generate_n
- std::includes
- std::inner_product
- std::inplace_merge
- std::is_heap
- std::is_heap_until
- std::is_partitioned
- std::is_sorted
- std::is_sorted_until
- std::lexicographical_compare
- std::max_element
- std::merge
- std::min_element
- std::minmax_element
- std::mismatch
- std::move
- std::none_of
- std::nth_element
- std::partial_sort
- std::partial_sort_copy
- std::partition
- std::partition_copy
- std::remove
- std::remove_copy
- std::remove_copy_if
- std::remove_if
- std::replace
- std::replace_copy
- std::replace_copy_if
- std::replace_if
- std::reverse
- std::reverse_copy
- std::rotate
- std::rotate_copy
- std::search
- std::search_n
- std::set_difference
- std::set_intersection
- std::set_symmetric_difference
- std::set_union
- std::sort
- std::stable_partition
- std::stable_sort
- std::swap_ranges
- std::transform
- std::uninitialized_copy
- std::uninitialized_copy_n
- std::uninitialized_fill
- std::uninitialized_fill_n
- std::unique
- std::unique_copy

Where is accumulate?

There is no parallel accumulate

Why not?

New parallel algorithms

Instead of accumulate

for_each	similar to std::for_each except returns void (function template)
for_each_n	applies a function object to the first n elements of a sequence (function template)
Defined in header <experimental/numeric>	
reduce (parallelism TS)	similar to std::accumulate, except out of order (function template)
exclusive_scan	similar to std::partial_sum, excludes the ith input element from the ith sum (function template)
inclusive_scan	similar to std::partial_sum, includes the ith input element in the ith sum (function template)
transform_reduce (parallelism TS)	applies a functor, then reduces out of order (function template)
transform_exclusive_scan	applies a functor, then calculates exclusive scan (function template)
transform_inclusive_scan	applies a functor, then calculates inclusive scan (function template)

Reduce

std::experimental::parallel::reduce

Defined in header <experimental/numeric>

```
template<class InputIt>
typename std::iterator_traits<InputIt>::value_type reduce(
    InputIt first, InputIt last);
```

```
template<class ExecutionPolicy, class InputIterator>
typename std::iterator_traits<InputIt>::value_type reduce(
    ExecutionPolicy&& policy, InputIt first, InputIt last);
```

```
template<class InputIt, class T>
T reduce(InputIt first, InputIt last, T init);
```

```
template<class ExecutionPolicy, class InputIt, class T>
T reduce(ExecutionPolicy&& policy, InputIt first, InputIt last, T init);
```

```
template<class InputIt, class T, class BinaryOp>
T reduce(InputIt first, InputIt last, T init, BinaryOp binary_op);
```

```
template<class ExecutionPolicy, class InputIt, class T, class BinaryOp>
T reduce(ExecutionPolicy&& policy,
         InputIt first, InputIt last, T init, BinaryOp binary_op);
```

Example

```
{ Timer t; t.start();
for (size_t k = 0; k < loops; ++k)
  result = std::accumulate(&v(0), &v(v.num_rows()), 0.0);
t.stop();
std::cout << "std::accumulate result " << result << " took " << t.elapsed()
          << " ms\n"; }

{ Timer t; t.start();
for (size_t k = 0; k < loops; ++k)
  result = std::reduce(pstl::execution::seq, &v(0), &v(v.num_rows()), 0.0);
t.stop();
std::cout << "std::reduce result " << result << " took " << t.elapsed()
          << " ms\n"; }
```

Regular accumulate

Sequential execution

Example

```
{ Timer t; t.start();
for (size_t k = 0; k < loops; ++k)
  result = std::reduce(pstl::execution::par, &v(0), &v(v.num_rows()), 0.0);
t.stop();
std::cout << "std::reduce result " << result << " took " << t.elapsed()
          << " ms\n"; }

{ Timer t; t.start();
for (size_t k = 0; k < loops; ++k)
  result = std::reduce(pstl::execution::par_unseq, &v(0), &v(v.num_rows()), 0.0);
t.stop();
std::cout << "std::reduce result " << result << " took " << t.elapsed()
          << " ms\n"; }
```

Parallel execution

Parallel execution

Results

```
std::accumulate result -2310.8 took 1155 ms
std::reduce result -2310.8 took 1167 ms
std::reduce result -2310.8 took 329 ms
std::reduce result -2310.8 took 337 ms
```

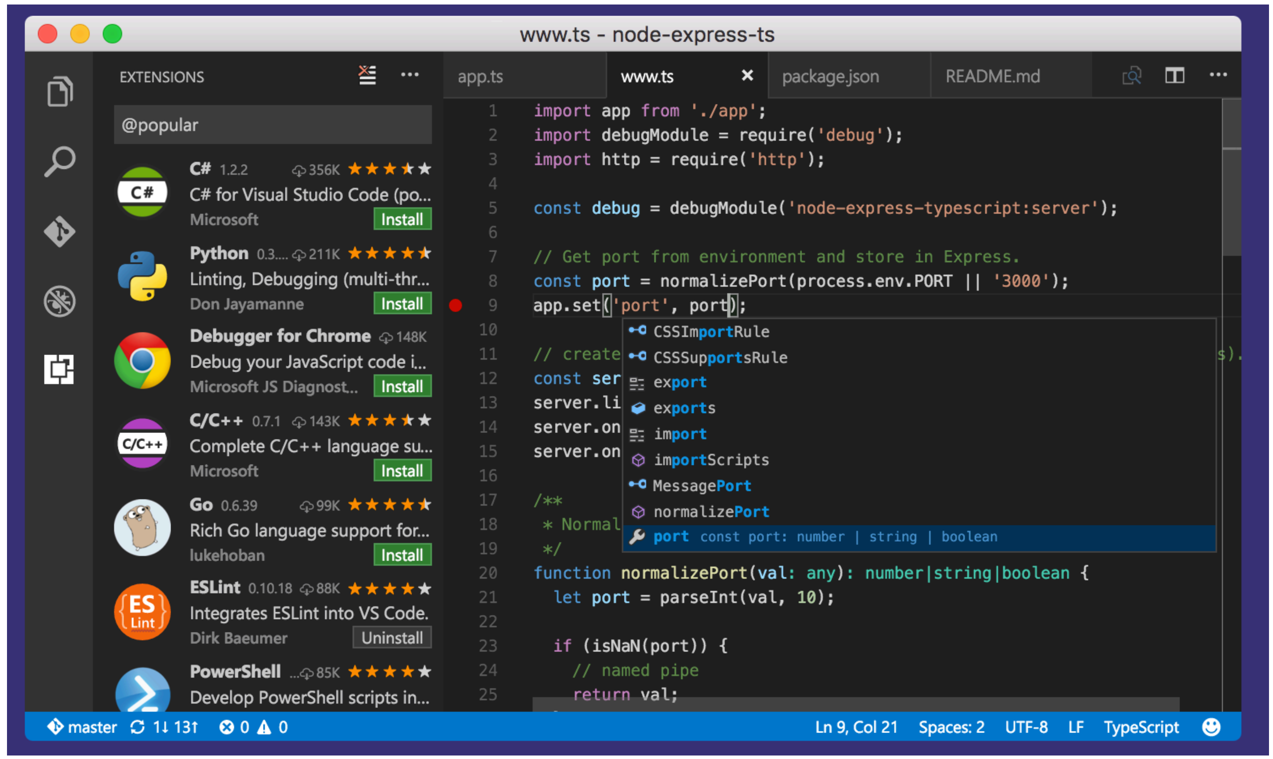
Accumulate

Sequential reduce

Parallel execution

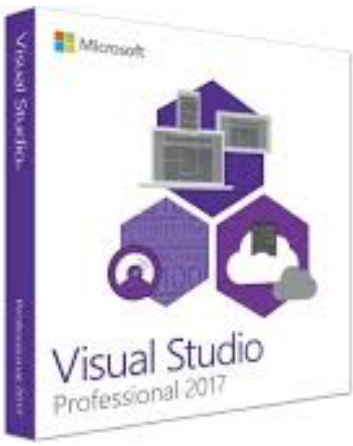
Parallel execution

Developing your code



- That includes (especially) mental labor
- Use productivity tools
- ***VS code***
- Intellisense

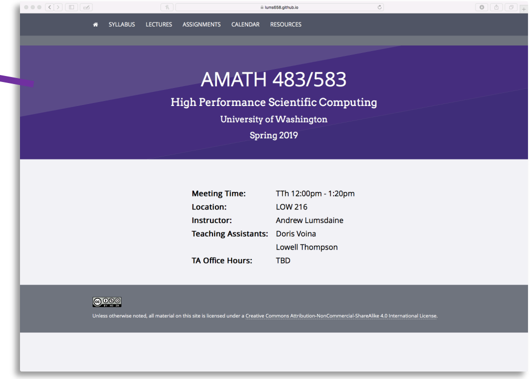
What about …?



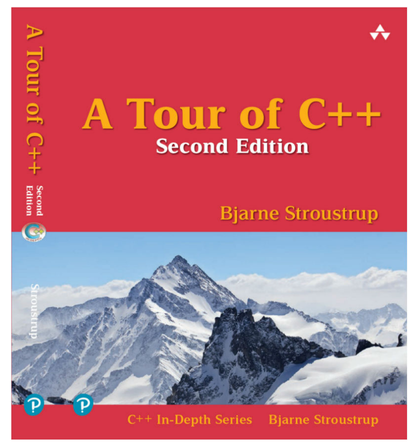
- Muscle memory for typing is not the same as productivity (know the difference)
  - Stretch yourself

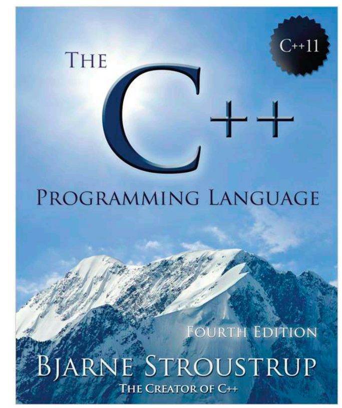
For More Information

Insomnia? There is a podcast



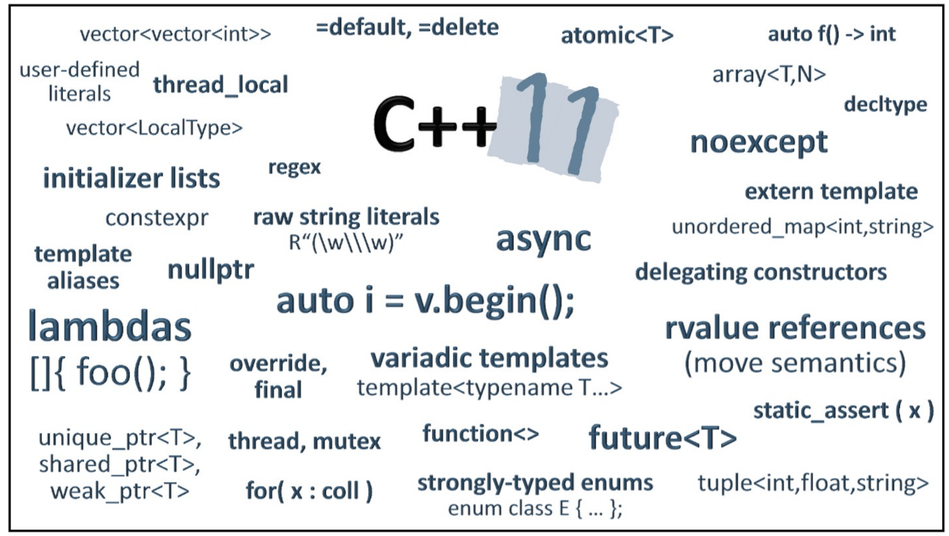
- AMATH 483/583 web site (shameless plug)
  - https://lums658.github.io/amath583s19/
- C++ Core Guidelines
  - http://isocpp.github.io/CppCoreGuidelines/CppCoreGuidelines
- Tour of C++
  - http://www.stroustrup.com/tour2.html
- C++ Programming Language (4th edition)
  - http://www.stroustrup.com/4th.html
- http://cppreference.com
- andrew.lumsdaine@pnnl.gov



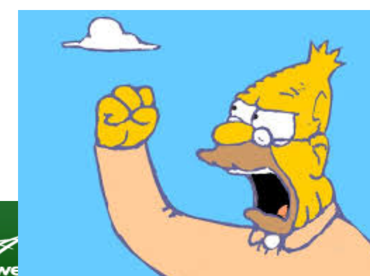


Sequels (again, about writing tastefully)

- C++ threads, tasks, futures
- C++ lambda
- constexpr
- ranges / range-based for
- Generic programming, templates, concepts
- decltype
- Tuples, array, variadic templates
- shared_ptr<T>, et al



- C++ and OpenMP
- C++ and MPI
- Thrust



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- Students of AMATH 483/583 (and CSEP 524)

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