AMATH 483/583
High Performance Scientific Computing

Lecture 5:
Classes, vectors, matrices

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Academic Integrity

- You are being evaluated in this course for how much **you** learn
- Not for someone else's work
- You may not claim someone else's work as your own (plagiarism)
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- But ***you must cite your sources***
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  - (Though you may not get full credit, you won't get the plagiarism zero)
- Fail this class for the 2nd plagiarism

Overview

- Last episode
  - class Vector
  - Member functions
  - Constructor
  - Accessor
  - Operator functions
  - Overloading
- Tour of computer architecture
- Class Matrix
- Matrix matrix product

C++ Core Guidelines related to classes

- C.1: Organize related data into structures (structs or classes)
- C.3: Represent the distinction between an interface and an implementation using a class
- C.4: Make a function a member only if it needs direct access to the representation of a class
- C.10: Prefer concrete types over class hierarchies
- C.11: Make concrete types regular

http://isocpp.github.io/CppCoreGuidelines/CppCoreGuidelines

Anatomy of a C++ class

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

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

  size_t num_rows() const { return num_rows_; }

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

Declares interface

Hides definition

Public accessors

Private data

Maintain invariants

Anatomy of a C++ class

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

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

  size_t num_rows() const { return num_rows_; }

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

Declares interface

Hides

Encapsulation

Public accessors

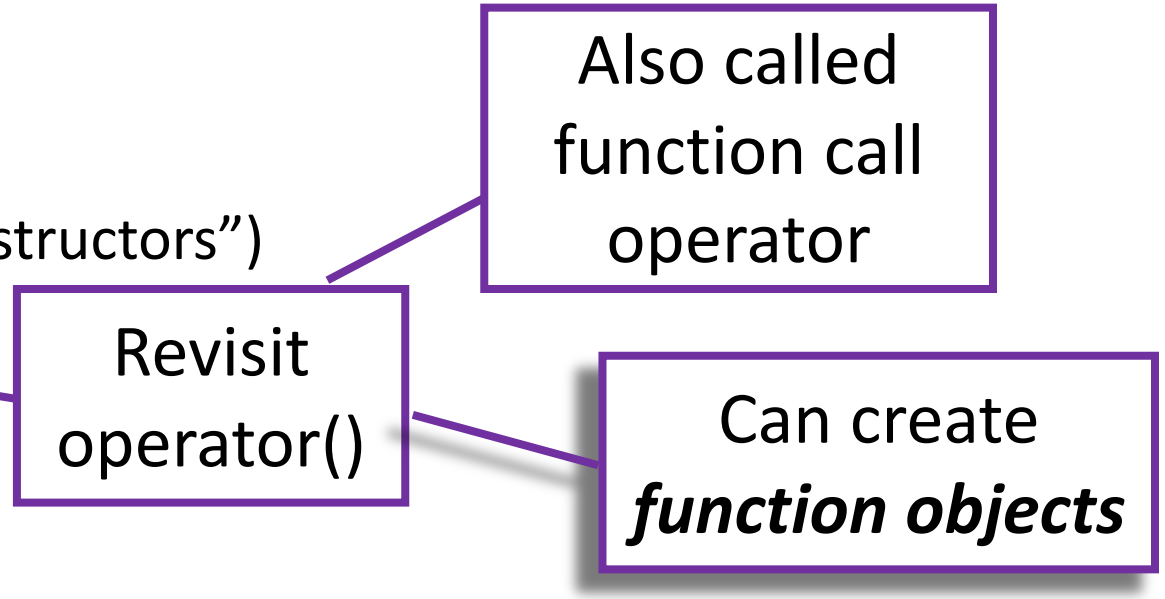
Private data

Maintain invariants

The Vector class so Far

- Encapsulates vector data
- Member data for dimensions (rows) and for storing elements
- Member function to get number of rows
- Separate interface and implementation via public / private

- Three more things:
  - How to bring a Vector into being (“constructors”)
  - Function for getting vector data
  - Function for setting vector data



Constructors

- The C++ compiler “knows” about built-in types
- When a variable of a built-in type is declared, the compiler just needs to allocate space for it
- C++ classes are user-defined
- Compiler can do its best (default constructor), but usually we need to do more to create a well-defined object

- For example, a well-defined vector should be given its (positive) dimension ***when it is created***. (And the data initialized.)

Constructors

```
int x = 42;


Vector x;

Vector x(27);


std::cout << "x is " << x.num_rows() << " in length." << std::cout;
```

Built-in type, compiler allocates known amount of space

Default constructor is invoked when variable is declared with no arguments

Compiler creates x with ***default constructor***

In this case, the constructor that takes an integer argument

Compiler creates x by making a call to a specific constructor

Create a Vector x with 27 elements

Because that is how we defined the constructor

Declaring Constructors

```
#include <vector>

class Vector {
public:
  Vector();
  Vector(size_t M);

  size_t num_rows() const  { r

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

A constructor is defined using the name of the class

And then the arguments

Can be ***overloaded*** (different functions distinguished by argument types)

Where have we already seen overloading?

Defining Constructors

Vector.hpp

```
#include <vector>

class Vector {
public:
  Vector();
  Vector(size_t M);

  size_t num_rows() const  { return num_rows; }

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

Vector.cpp

```
#include "Vector.hpp"

Vector::Vector(size_t M) {
  num_rows_ = M;
  storage_ = std::vector<double>(num_rows);
}

Vector::Vector() {
  num_rows_ = 1;
  storage_ = std::vector<double>(num_rows_);
}
```

Defining Constructors

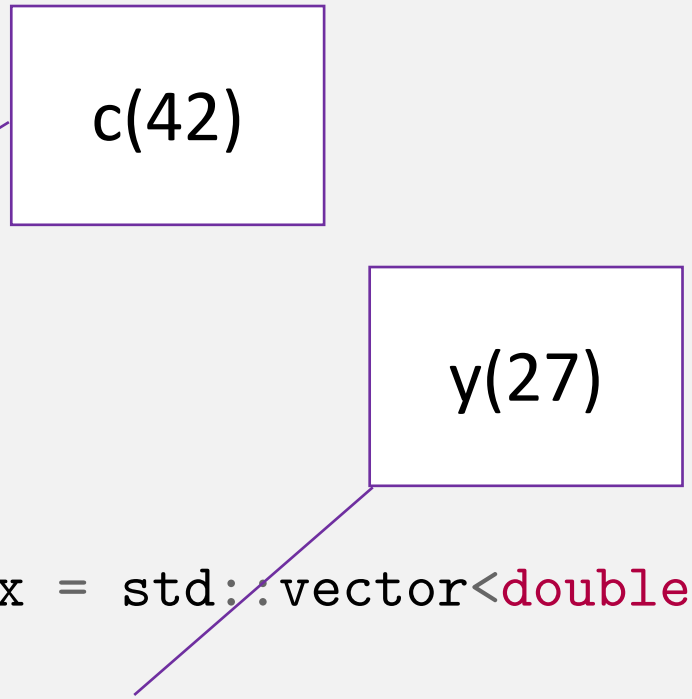
Vector.hpp

```cpp
#include <vector>

class Vector {
public:
  Vector() {
    num_rows_ = 1;
    storage_  = std::vector<double>(num_rows);
  }
  Vector(size_t M) {
    num_rows_ = M;
    storage_  = std::vector<double>(num_rows);
  }

  size_t num_rows() const { return num_rows; }

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

Initialization

- We have said that variables should always be initialized
- Different syntaxes

```
int a = 42;

int b = int(42);

int c(42);

int d = { 42 };

std::vector<double> x = std::vector<double>(27);

std::vector<double> y(27);
```



Defining Constructors

Vector.hpp

```
#include <vector>

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

  size_t num_rows() const { return num_rows_; }

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

Note order of initialization

Initialization syntax
Introduce with :
Construct data members

Omit default constructor (why?)

Note order of declaration

Defining Constructors

Vector.hpp

```
#include <vector>

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

  size_t num_rows() const { return num_rows_; }

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

Initialization

Primordial

Object doesn't yet exist

Object exists

What Should operator() return?

```
class Vector
public:
  double& operator()(size_t i);

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

Return a ***reference*** to internal member data

```
Vector x(5);

double foo = x(3);
x(2) = 0.0;
```

Can assign to internal data through the reference

Can read from internal data through the reference

```
Vector x(5);
```

All Together

Vector.hpp

```cpp
#include <vector>

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

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

  size_t num_rows() const { return num_rows_; }

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

Reprise operator+()

```
#include <vector>

class Vector {
public:
  Vector operator+(const Vector& y);

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

Reprise operator+()

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

```
#include <vector>

class Vector {
public:
  Vector operator+(const Vector& y) {
    Vector z(num_rows_);
    for (size_t i = 0; i < num_rows_; ++i) {
      z.storage_[i] = storage_[i] + y.storage[i];
    }
  }

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

Does this need to be a member? Why or why not?

Data for z

Data for “x”

Data for y

All Together

Vector.hpp

```cpp
#include <vector>

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

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

  size_t num_rows() const { return num_rows_; }

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

Can access via operator()

Don't need access to internals

Amath583.cpp

```cpp
#include "Vector.hpp"

Vector operator+(const Vector& x, const Vector& y) {
  Vector z(x.num_rows());
  for (size_t i = 0; i < z.num_rows(); ++i) {
    z(i) = x(i) + y(i);
  }
}
```

Return a Vector

Take args by const reference

Nicely symmetric

All Together

Vector.hpp

```cpp
#include <vector>

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

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

  size_t num_rows() const { return num_rows_; }

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

Amath583.hpp

```cpp
#include "Vector.hpp"

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

Amath583.cpp

```cpp
#include "Vector.hpp"
#include "amath583.hpp"

Vector operator+(const Vector& x, const Vector& y) {
  Vector z(x.num_rows());
  for (size_t i = 0; i < z.num_rows(); ++i) {
    z(i) = x(i) + y(i);
  }
}
```

Not quite finished

```cpp
#include "Vector.hpp"

int main() {

  Vector x(100), y(100), z(100), w(100);

  z = x + y;

  return 0;
}
```

```
% c++ constness.cpp
constness.cpp:20:12: error: no matching function for call to object of type 'const Vector'
    z(i) = x(i) + y(i);
           ^
constness.cpp:7:11: note: candidate function not viable: 'this' argument has type
      'const Vector', but method is not marked const
  double& operator()(size_t i) { return storage_[i]; }
          ^
constness.cpp:20:19: error: no matching function for call to object of type 'const Vector'
    z(i) = x(i) + y(i);
                  ^
constness.cpp:7:11: note: candidate function not viable: 'this' argument has type
      'const Vector', but method is not marked const
  double& operator()(size_t i) { return storage_[i]; }
          ^
2 errors generated.
```

Constness

Vector.hpp

```cpp
#include <vector>

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

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

  size_t num_rows() const { return num_rows_; }

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

x and y are defined to be const

Amath583.hpp

```cpp
#include "Vector.hpp"

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

"this" is not const

Amath583.cpp

```cpp
#include "Vector.hpp"
#include "amath583.hpp"

Vector operator+(const Vector& x, const Vector& y) {
  Vector z(x.num_rows());
  for (size_t i = 0; i < z.num_rows(); ++i) {
    z(i) = x(i) + y(i);
  }
}
```

Overloading

```
void foo(size_t i) {
  std::cout << "foo(size_t i)" << std::endl;
}

void foo(double d) {
  std::cout << "foo(double d)" << std::endl;
}
```

Takes a size_t

Takes a double

```
int main() {

  size_t a = 0;
  double b = 0.0;

  foo(a);
  foo(b);

  return 0;
}
```

```
% ./a.out
foo(size_t i)
foo(double d)
```

Overloading

```
void foo(size_t i) {
  std::cout << "void foo(size_t i)" << std::endl;
}

size_t foo(size_t i) {
  std::cout << "size_t foo(size_t i)" << std::endl;
}
```

Returns void

Returns size_t

```
% c++ overload.cpp
overload.cpp:7:8: error: functions that differ only in their return type cannot be overloaded
size_t foo(size_t i) {
~~~~~~ ^
overload.cpp:3:6: note: previous definition is here
void foo(size_t i) {
~~~~ ^
```

```
int main() {

  size_t a = 0;
  size_t b = 0;

  foo(a);
  double c = foo(a);

  return 0;
}
```

Have to pick the function then call it

No overloading on return values

```
size_t foo(size_t i) {
  std::cout << "size_t foo(size_t i)" << std::

  return i;
}


int main() {

  size_t a = 0;

  foo(a);
  size_t b = foo(a);
  double c = foo(a);

  return 0;
}
```

What happens to the return value is not the concern of the function

Ignore return value

Assign to size_t

Assign to double

Constness

```
double parens(double& x, size_t i) {
  std::cout << "called non const parens" << std::endl;
  double y = x;
  // .. some things
  return y;
}
```

x is a ref

```
int main() {

  double x = 5.0;
  double y = parens(x);

  const double z = 5.0;
  double w = parens(z);

  double a = parens(5.0);
  double b = parens(x + y);

  const double c = parens(x + y + z +

  return 0;
}
```

Okay,

```
c++ const3.cpp
const3.cpp:27:14: error: no matching function for call to 'parens'
  double w = parens(z, 27);
             ^~~~~
const3.cpp:13:8: note: candidate function not viable: 1st argument ('const double') would lose const
      qualifier
double parens(double& x, size_t i) {
       ^
const3.cpp:29:14: error: no matching function for call to 'parens'
  double a = parens(5.0, 27);
             ^~~~~
const3.cpp:13:8: note: candidate function not viable: expects an l-value for 1st argument
double parens(double& x, size_t i) {
       ^
```

Not okay to reference, z is read only

```
const3.cpp:32:20: error: no matching function for call to 'parens'
  const double c = parens(x + y + 5.0, 27);
                   ^~~~~
const3.cpp:13:8: note: candidate function not viable: expects an l-value for 1st argument
double parens(double& x, size_t i) {
       ^
```

Not okay, x+y is a rvalue

Not okay, x+y+z+5.0 is a rvalue

Constness

```
double parens(const double& x, size_t i) {
  std::cout << "called const parens" << std::endl;
  double y = x;
  // .. some things
  return y;
}
```

x is a const ref

Assign value of x to y

```
int main() {

  double x = 5.0;
  double y = parens(x);

  const double z = 5.0;
  double w = parens(z);

  double a = parens(5.0);
  double b = parens(x + y);

  const double c = parens(x + y + z + 5.0);

  return 0;
}
```

okay

okay

okay

okay

```
./a.out
called const parens
called const parens
called const parens
called const parens
called const parens
```

Constness

```cpp
double parens(const double& x, size_t i) {
  std::cout << "called const parens" << std::endl;
  double y = x;
  // .. some things
  return y;
}
```

x is a const ref

```cpp
double parens(double& x, size_t i) {
  std::cout << "called non const parens" << std::endl;
  double y = x;
  // .. some things
  return y;
}
```

x is a ref

```cpp
int main() {

  double x = 5.0;
  double y = parens(x);

  const double z = 5.0;
  double w = parens(z);

  double a = parens(5.0);
  double b = parens(x + y);

  const double c = parens(x + y + z + 5.0);

  return 0;
}
```

x is lvalue

z is read only

5.0 is a rvalue

x + y is a rvalue

```
./a.out
called non const parens
called const parens
called const parens
called const parens
called const parens
```

Rvalue can be referenced if read only

Why not always pass const reference?

```cpp
double parens(const double& x, size_t i) {
  std::cout << "called const parens" << std::endl;
  double y = x;
  // .. some things
  return x;
}
```

Return double

```cpp
int main() {
  double y = 0.5;
  double p = 3.14;

  double x = 5.0;
  parens(x, 27) = p;

  const double z = 5.0;
  parens(z, 27) = p;

  parens(5.0, 27) = p;
  parens(x + y, 27) = p;

  return 0;
}
```

```
c++ const4.cpp
const4.cpp:23:17: error: expression is not assignable
  parens(x, 27) = p;
  ~~~~~~~~~~~~~ ^
const4.cpp:26:17: error: expression is not assignable
  parens(z, 27) = p;
  ~~~~~~~~~~~~~ ^
const4.cpp:28:19: error: expression is not assignable
  parens(5.0, 27) = p;
  ~~~~~~~~~~~~~~~ ^
const4.cpp:29:21: error: expression is not assignable
  parens(x + y, 27) = p;
  ~~~~~~~~~~~~~~~~~ ^
```

Before

```
double parens(const double& x, size_t i) {
  std::cout << "called const parens" << std::endl;
  double y = x;
  // .. some things
  return x;
}
```

After

```
double& parens(const double& x, size_t i) {
  std::cout << "called const parens" << std::endl;
  double y = x;
  // .. some things
  return x;
}
```

Why not always pass const reference?

```
double& parens(const double& x, size_t i) {
  std::cout << "called const
  double y = x;
  // .. some things
  return x;
}
```

But x is const

Return ref to double

Can't return const

```
int main() {
  double y = 0.5;
  double p = 3.14;

  double x = 5.0;
  parens(x, 27) = p;

  const double z = 5.0;
  parens(z, 27) = p;

  parens(5.0, 27) = p;
  parens(x + y, 27) = p;

  return 0;
}
```

```
c++ const5.cpp
const5.cpp:9:10: error: binding value of type 'const double' to reference to type 'double' drops
      'const' qualifier
  return x;
         ^
```

Before

```
double& parens(const double& x, size_t i) {
  std::cout << "called const parens" << std::endl;
  double y = x;
  // .. some things
  return x;
}
```

After

```
const double& parens(const double& x, size_t i) {
  std::cout << "called const parens" << std::endl;
  double y = x;
  // .. some things
  return x;
}
```

Why not always pass const reference?

```cpp
const double& parens(const double& x, size_t i) {
  std::cout << "called const parens" << std::endl;
  double y = x;
  // .. some things
  return x;
}
```

```cpp
int main() {
  double y = 0.5;
  double p = 3.14;

  double x = 5.0;
  parens(x, 27) = p;

  const double z = 5.0;
  parens(z, 27) = p;

  parens(5.0, 27) = p;
  parens(x + y, 27) = p;

  return 0;
}
```

```
c++ const5.cpp
const5.cpp:26:17: error: cannot assign to return value because function 'parens' returns a const value
  parens(x, 27) = p;
  ~~~~~~~~~~~~~ ^
const5.cpp:5:7: note: function 'parens' which returns const-qualified type 'const double &' declared
      here
const double& parens(const double& x, size_t i) {
      ^~~~~~~
const5.cpp:29:17: error: cannot assign to return value because function 'parens' returns a const value
  parens(z, 27) = p;
  ~~~~~~~~~~~~~ ^
const5.cpp:5:7: note: function 'parens' which returns const-qualified type 'const double &' declared
      here
const double& parens(const double& x, size_t i) {
      ^~~~~~~
const5.cpp:31:19: error: cannot assign to return value because function 'parens' returns a const value
  parens(5.0, 27) = p;
  ~~~~~~~~~~~~~~~ ^
const5.cpp:5:7: note: function 'parens' which returns const-qualified type 'const double &' declared
      here
const double& parens(const double& x, size_t i) {
      ^~~~~~~
const5.cpp:32:21: error: cannot assign to return value because function 'parens' returns a const value
  parens(x + y, 27) = p;
  ~~~~~~~~~~~~~~~~~ ^
const5.cpp:5:7: note: function 'parens' which returns const-qualified type 'const double &' declared
      here
const double& parens(const double& x, size_t i) {
      ^
```

Before

```
double& parens(const double& x, size_t i) {
  std::cout << "called const parens" << std::endl;
  double y = x;
  // .. some things
  return x;
}
```

After

```
double& parens(double& x, size_t i) {
  std::cout << "called const parens" << std::endl;
  double y = x;
  // .. some things
  return x;
}
```

How about no const at all?

```cpp
double& parens(double& x, size_t i) {
  std::cout << "called const parens" << std::endl;
  double y = x;
  // .. some things
  return x;
}
```

```cpp
int main() {
  double y = 0.5;
  double p = 3.14;

  double x = 5.0;
  parens(x, 27) = p;

  const double z = 5.0;
  parens(z, 27) = p;

  parens(5.0, 27) = p;
  parens(x + y, 27) = p;

  return 0;
}
```

```
c++ const5.cpp
const5.cpp:30:3: error: no matching function for call to 'parens'
  parens(z, 27) = p;
  ^~~~~~
const5.cpp:14:9: note: candidate function not viable: 1st argument ('const double') would lose const
      qualifier
double& parens(double& x, size_t i) {
        ^
const5.cpp:32:3: error: no matching function for call to 'parens'
  parens(5.0, 27) = p;
  ^~~~~~
const5.cpp:14:9: note: candidate function not viable: expects an l-value for 1st argument
double& parens(double& x, size_t i) {
        ^
const5.cpp:33:3: error: no matching function for call to 'parens'
  parens(x + y, 27) = p;
  ^~~~~~
const5.cpp:14:9: note: candidate function not viable: expects an l-value for 1st argument
double& parens(double& x, size_t i) {
        ^
```

How about no const at all?

```
int main() {
  double y = 0.5;
  double p = 3.14;

  double x = 5.0;
  parens(x, 27) = p;

  const double z = 5.0;
  parens(z, 27) = p;

  parens(5.0, 27) = p;
  parens(x + y, 27) = p;

  return 0;
}
```

This makes sense

This ***should*** be an error

This ***should*** be an error

This ***should*** be an error

More sensible

```
int main() {
  double y = 0.5;
  double p = 3.14;

  double x = 5.0;
  parens(x, 27) = p;

  const double z = 5.0;
  double q = parens(z, 27);

  double r = parens(5.0, 27);
  double s = parens(x + y, 27);

  return 0;
}
```

This makes sense

This makes sense

This makes sense

This makes sense

More sensible

```
double& parens(double& x, size_t i) {
  std::cout << "called non const parens" << std::endl;
  double y = x;
  // .. some things
  return x;
}
```

```
int main() {
  double y = 0.5;
  double p = 3.14;

  double x = 5.0;
  parens(x, 27) = p;

  const double z = 5.0;
  double q = parens(z, 27);

  double r = parens(5.0, 27);
  double s = parens(x + y, 27);

  return 0;
}
```

```
c++ const6.cpp
const6.cpp:30:14: error: no matching function for call to 'parens'
  double q = parens(z, 27);
             ^~~~~~
const6.cpp:14:9: note: candidate function not viable: 1st argument ('const double') would lose const
      qualifier
double& parens(double& x, size_t i) {
        ^
const6.cpp:32:14: error: no matching function for call to 'parens'
  double r = parens(5.0, 27);
             ^~~~~~
const6.cpp:14:9: note: candidate function not viable: expects an l-value for 1st argument
double& parens(double& x, size_t i) {
        ^
const6.cpp:33:14: error: no matching function for call to 'parens'
  double s = parens(x + y, 27);
             ^~~~~~
const6.cpp:14:9: note: candidate function not viable: expects an l-value for 1st argument
double& parens(double& x, size_t i) {
        ^
```

Oops, need to be const

Going in circles?

More sensible

```
const double& parens(const double& x, size_t i) {
  std::cout << "called non const parens" << std::endl;
  double y = x;
  // .. some things
  return x;
}

int main() {
  double y = 0.5;
  double p = 3.14;

  double x = 5.0;
  parens(x, 27) = p;

  const double z = 5.0;
  double q = parens(z, 27);

  double r = parens(5.0, 27);
  double s = parens(x + y, 27);

  return 0;
}
```

```
c++ const6.cpp
const6.cpp:27:17: error: cannot assign to return value because function 'parens' returns a const value
  parens(x, 27) = p;
  ~~~~~~~~~~~~~ ^
const6.cpp:6:7: note: function 'parens' which returns const-qualified type 'const double &' declared
      here
const double& parens(const double& x, size_t i) {
      ^~~~~~~
```

Oops, need to be non const

Going in circles?

Overloading to the rescue

```
const double& parens(const double& x, size_t
  std::cout << "called non const parens" <<
  double y = x;
  // .. some things
  return x;
}
```

const

```
double& parens(double& x, size_t i) {
  std::cout << "called non const parens" << std::endl;
  double y = x;
  // .. some things
  return x;
}
```

Not const

Not const

const

```
int main() {
  double y = 0.5;
  double p = 3.14;

  double x = 5.0;
  parens(x, 27) = p;

  const double z = 5.0;
  double q = parens(z, 27);

  double r = parens(5.0, 27);
  double s = parens(x + y, 27);

  return 0;
}
```

Call Not const

```
./a.out
called non const parens
called const parens
called const parens
called const parens
```

What does this have to do with operator()

```
const double& parens(const double& x, siz
  std::cout << "called non const parens" <
  double y = x;
  // .. some things
  return x;
}
```

const

const

```
double& parens(double& x, size_t i) {
  std::cout << "called non const parens" << std::endl;
  double y = x;
  // .. some things
  return x;
}
```

Not const

Not const

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

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

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

Where is the const or non-const thing to overload on?

What does this have to do with operator()

```
const double& parens(const double& x, siz
  std::cout << "called non const parens"
  double y = x;
  // .. some things
  return x;
}
```

const

const

```
double& parens(double& x, size_t i) {
  std::cout << "called non const parens" << std::endl;
  double y = x;
  // .. some things
  return x;
}
```

Not const

Not const

```
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) { return storage_[i]; }

private:
  si                um_rows_;
  st                torage_;
};
```

Only differing by return type

Where is the const or non-const thing to overload on?

There is a secret argument

```
const double& parens(const double& x, siz
  std::cout << "called non const parens"
  double y = x;
  // .. some things
  return x;
}
```

const

```
double& parens(double& x, size_t i) {
  std::cout << "called non const parens" << std::endl;
  double y = x;
  // .. some things
  return x;
}
```

Not const

const

Not const

```
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) { return storage_[i]; }

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

Called “this”

There is a secret argument

There is a secret argument

There is a secret argument

```
const double& parens(const double& x, siz
  std::cout << "called non const parens"
  double y = x;
  // .. some things
  return x;
}
```

const

const

```
double& parens(double& x, size_t i) {
  std::cout << "called non const parens" << std::endl;
  double y = x;
  // .. some things
  return x;
}
```

Not const

Not const

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

        double& operator()(Vector *this, size_t i) { return storage_[i]; }
  const double& operator()(Vector *this, size_t i) { return storage_[i]; }

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

How would we fix our const problem?

Before

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

        double& operator()(Vector *this, size_t i) { return storage_[i]; }
  const double& operator()(Vector *this, size_t i) { return storage_[i]; }

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

After

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

        double& operator()(Vector *this, size_t i) { return storage_[i]; }
  const double& operator()(const Vector *this, size_t i) { return storage_[i]; }

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

const “this”

Finally

```
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]; }

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

const “this”

Matrix in Math

- Matrix is an array of numbers, 2 rows by 2 columns $\begin{bmatrix}1 & 2\\3 & 4\end{bmatrix}$
- Add two matrices: C = A + B

$$\begin{bmatrix}1 & 2\\3 & 4\end{bmatrix} + \begin{bmatrix}4 & 3\\2 & 1\end{bmatrix} = \begin{bmatrix}5 & 5\\5 & 5\end{bmatrix}$$

- Subtract two matrices: C = A – B

$$\begin{bmatrix}1 & 2\\3 & 4\end{bmatrix} - \begin{bmatrix}1 & 2\\3 & 4\end{bmatrix} = \begin{bmatrix}0 & 0\\0 & 0\end{bmatrix}$$

- Multiply one matrix by another matrix: C = A × B
- Transpose a matrix: A -> A^T

$$\begin{bmatrix}1 & 2\\3 & 4\end{bmatrix} \rightarrow \begin{bmatrix}1 & 3\\2 & 4\end{bmatrix}$$

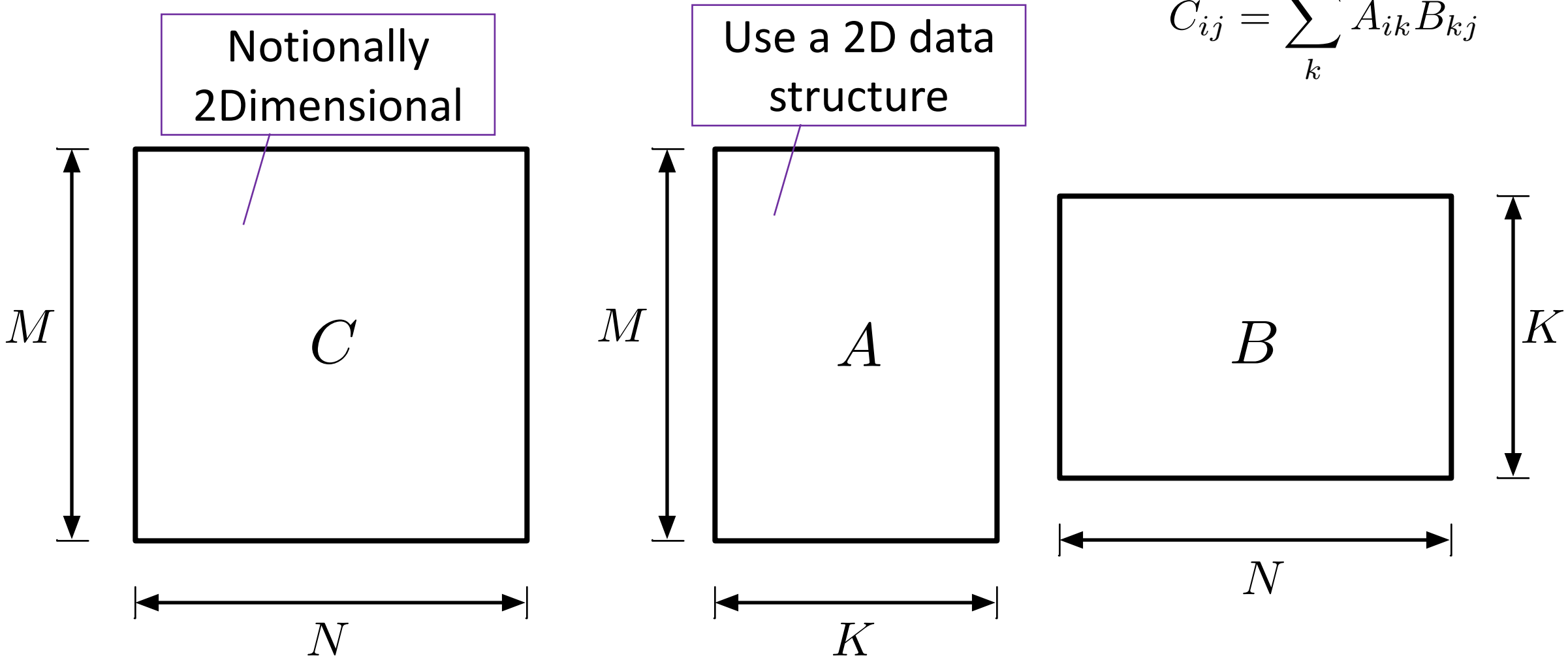
Matrix Representation in Computer

- Two issues
  - Interface (what is the abstraction we want to present?)
  - Implementation (how is the abstraction realized?)
- Sometimes there are tradeoffs
  - Evaluate relative to end user
  - In HPC – performance is most important
  - Elsewhere – safety, ease of use, standards compliance, etc

```
Matrix A(M,K), B(K,N), C(M,N);
...
for (int i = 0; i < N; ++i)
  for (int j = 0; j < N; ++j)
    for (int k = 0; k < N; ++k)
      C(i,j) += A(i,k) * B(k,j)
```

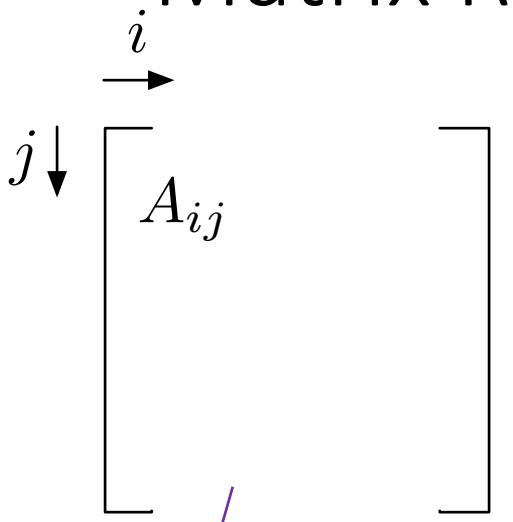
Matrix Matrix Product

$$C_{ij} = \sum_k A_{ik} B_{kj}$$



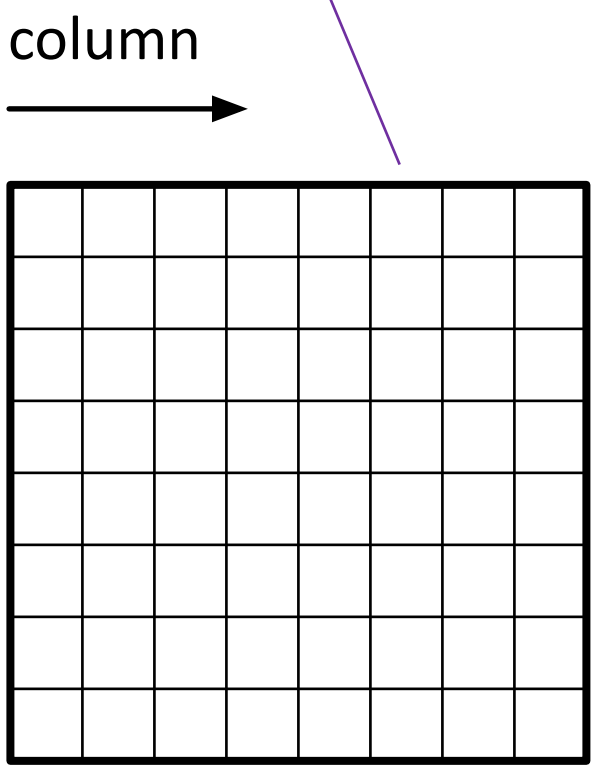
Matrix Representation

$$C_{ij} = \sum_k A_{ik} B_{kj}$$



A matrix is a doubly indexed set

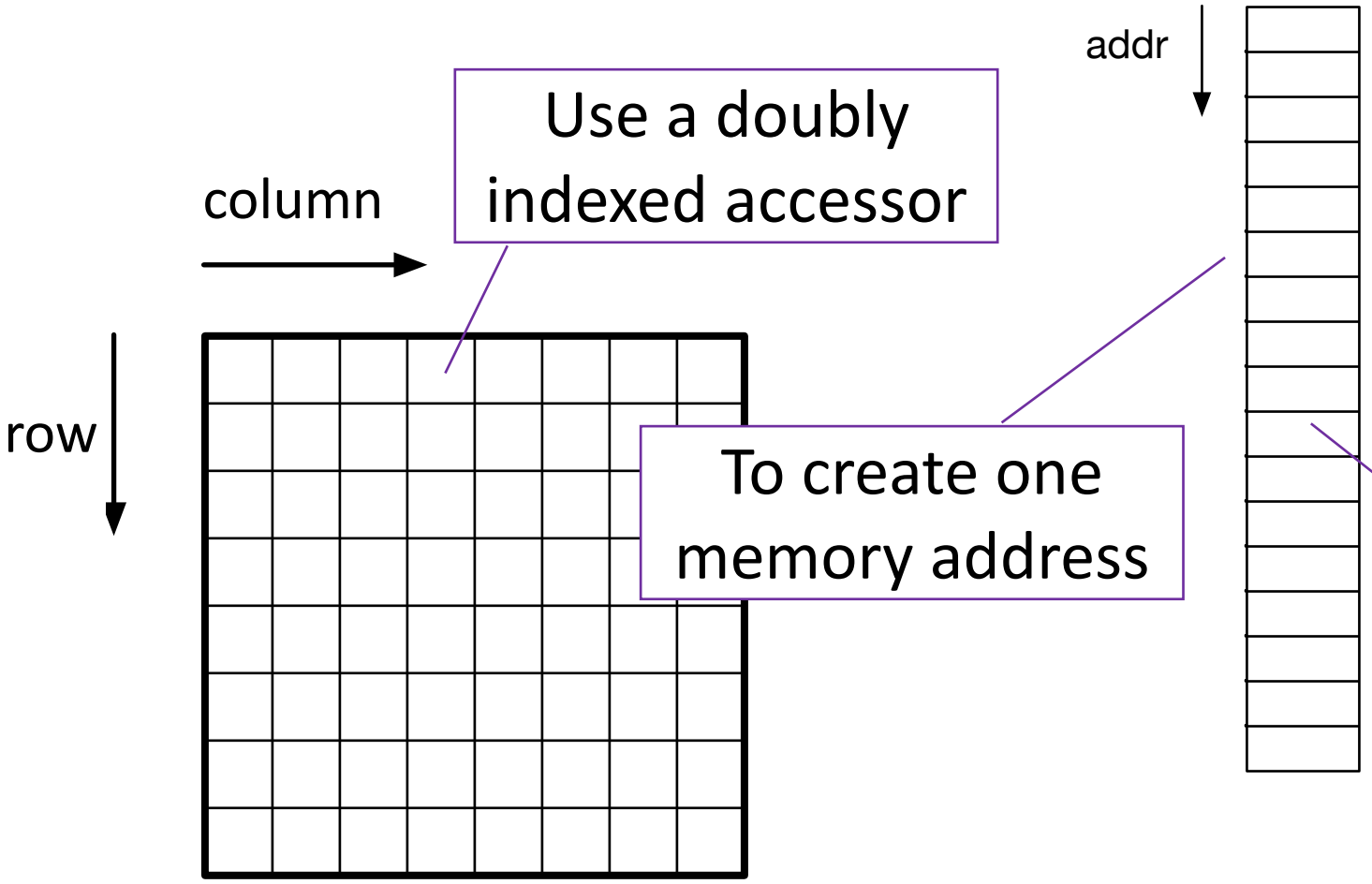
Use a doubly indexed data structure




```
Matrix A(M,K), B(K,N), C(M,N);
...
for (int i = 0; i < N; ++i)
  for (int j = 0; j < N; ++j)
    for (int k = 0; k < N; ++k)
      C(i,j) += A(i,k) * B(k,j)
```

Use a doubly indexed accessor

Matrix Representation



Use a doubly indexed accessor

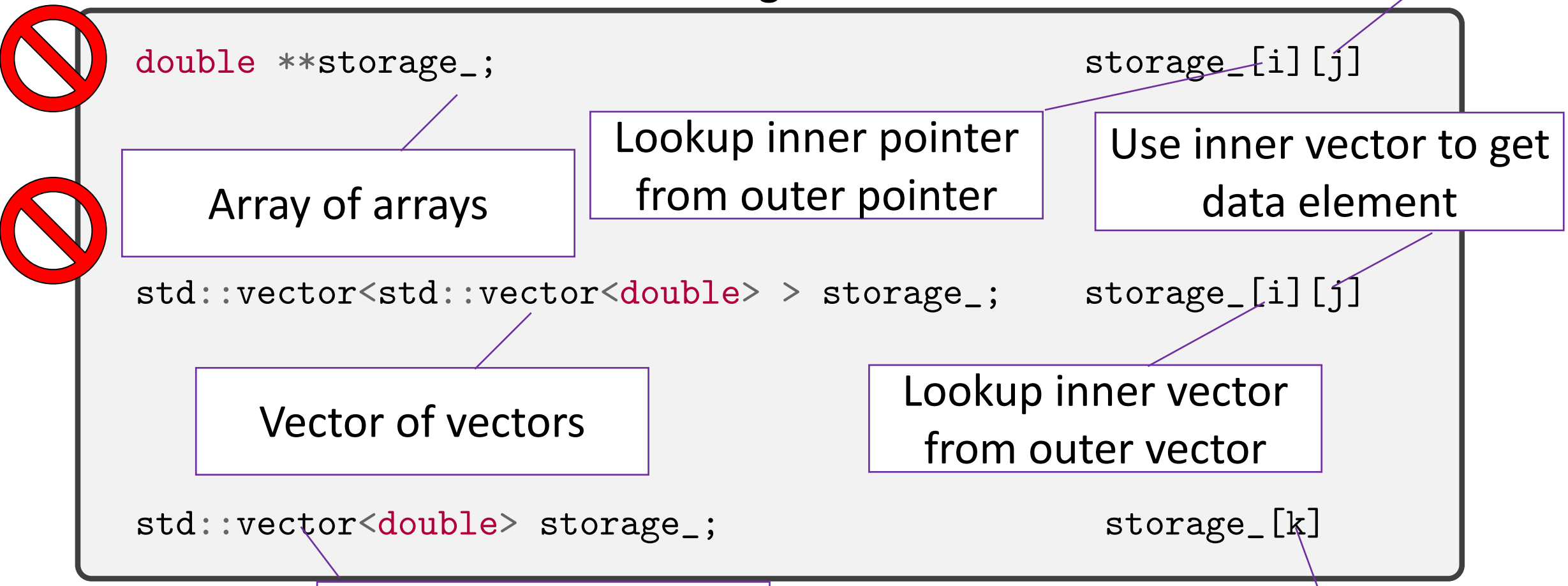
To create one memory address

Memory is a contiguous address space

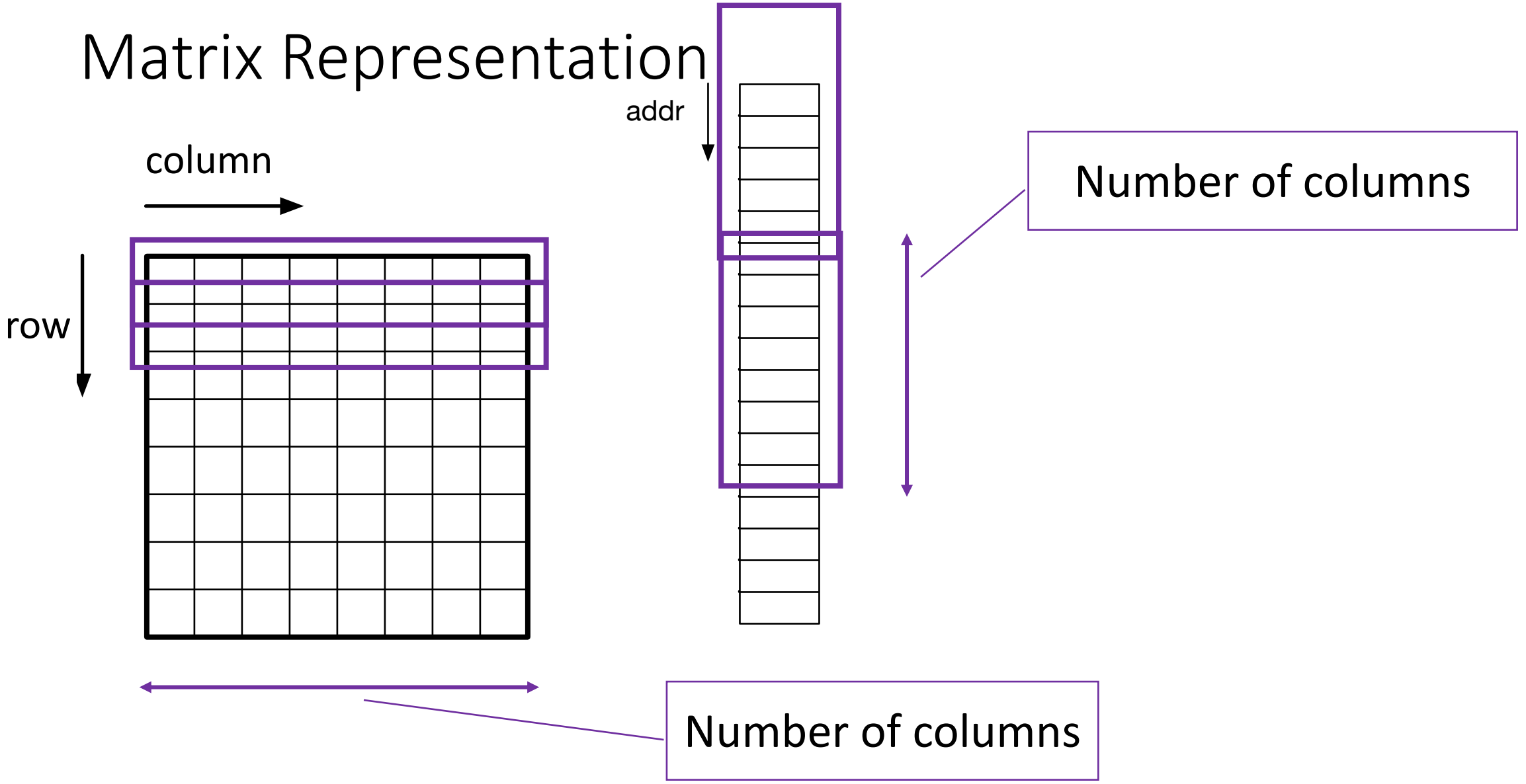
```
Matrix A(M,K), B(K,N), C(M,N);
...
for (int i = 0; i < N; ++i)
  for (int j = 0; j < N; ++j)
    for (int k = 0; k < N; ++k)
      C(i,j) += A(i,k) * B(k,j)
```

Matrix Representation

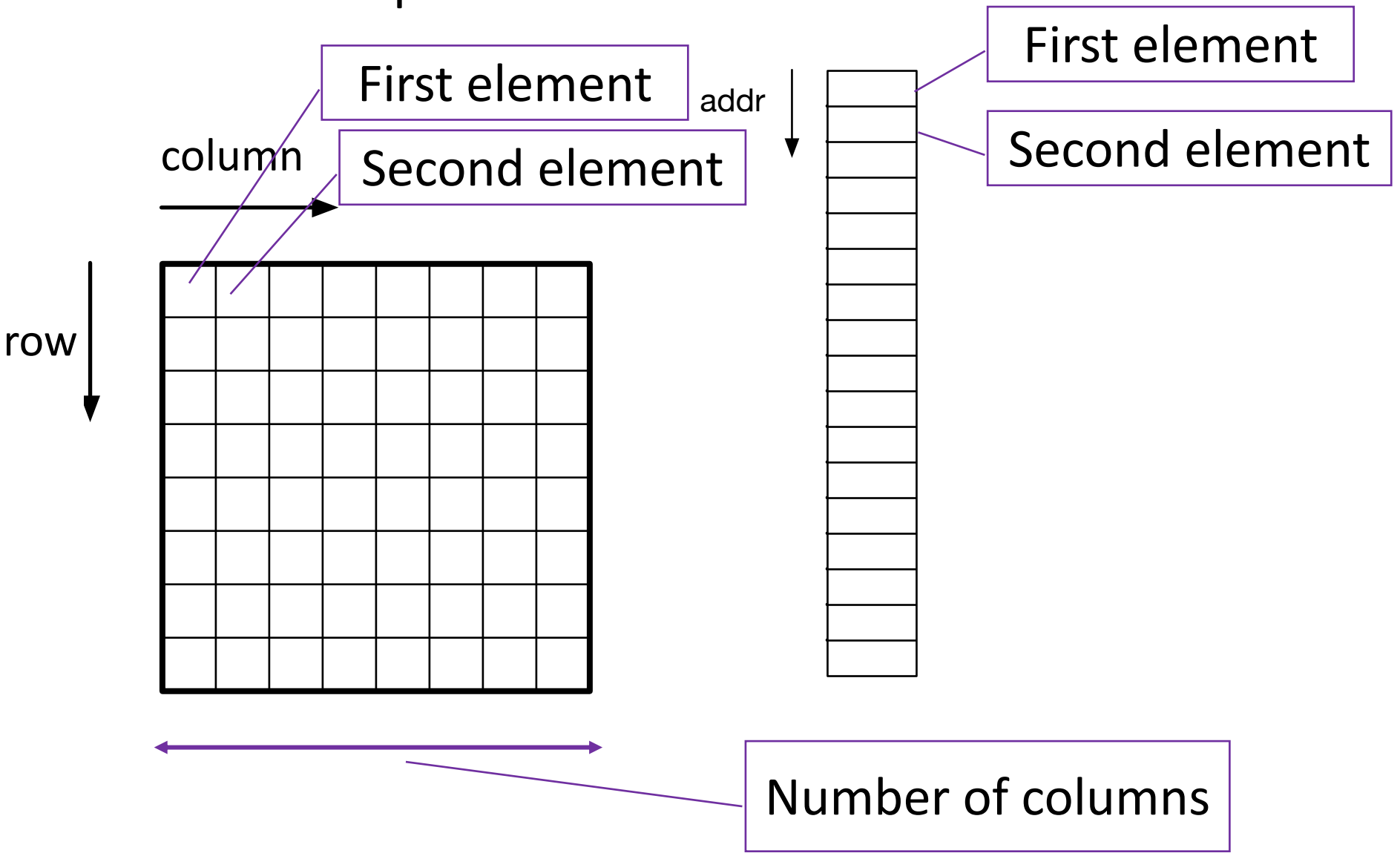
- To translate double index to single address



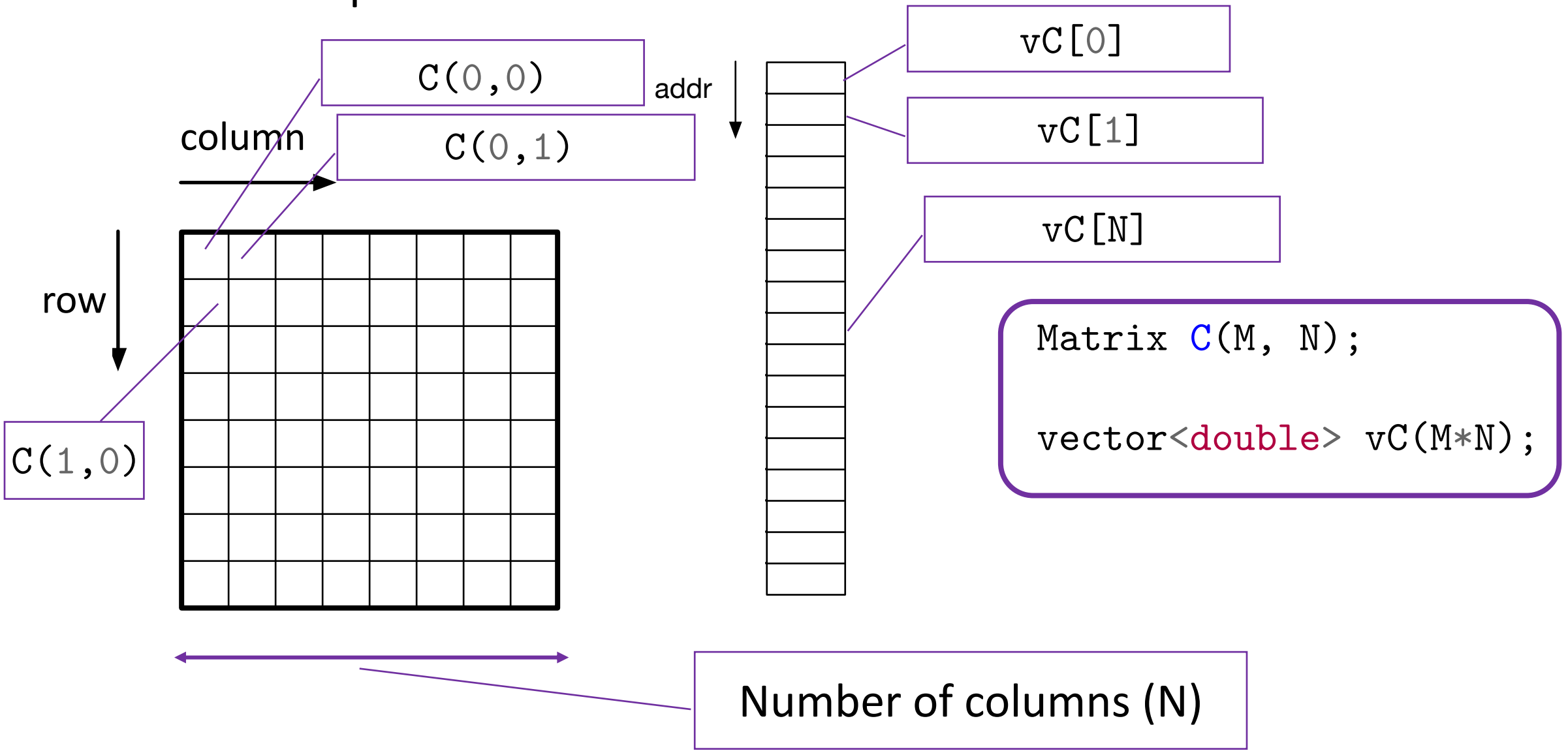
Matrix Representation



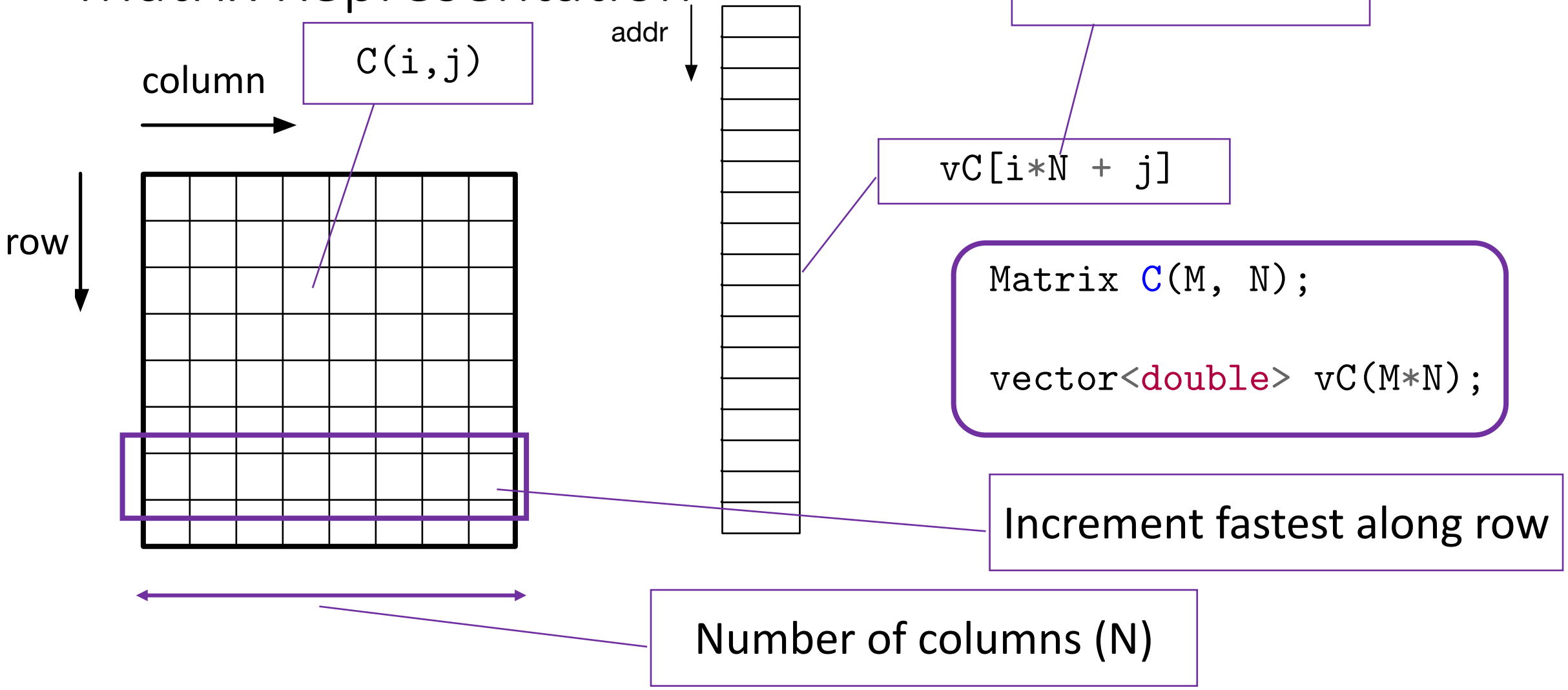
Matrix Representation



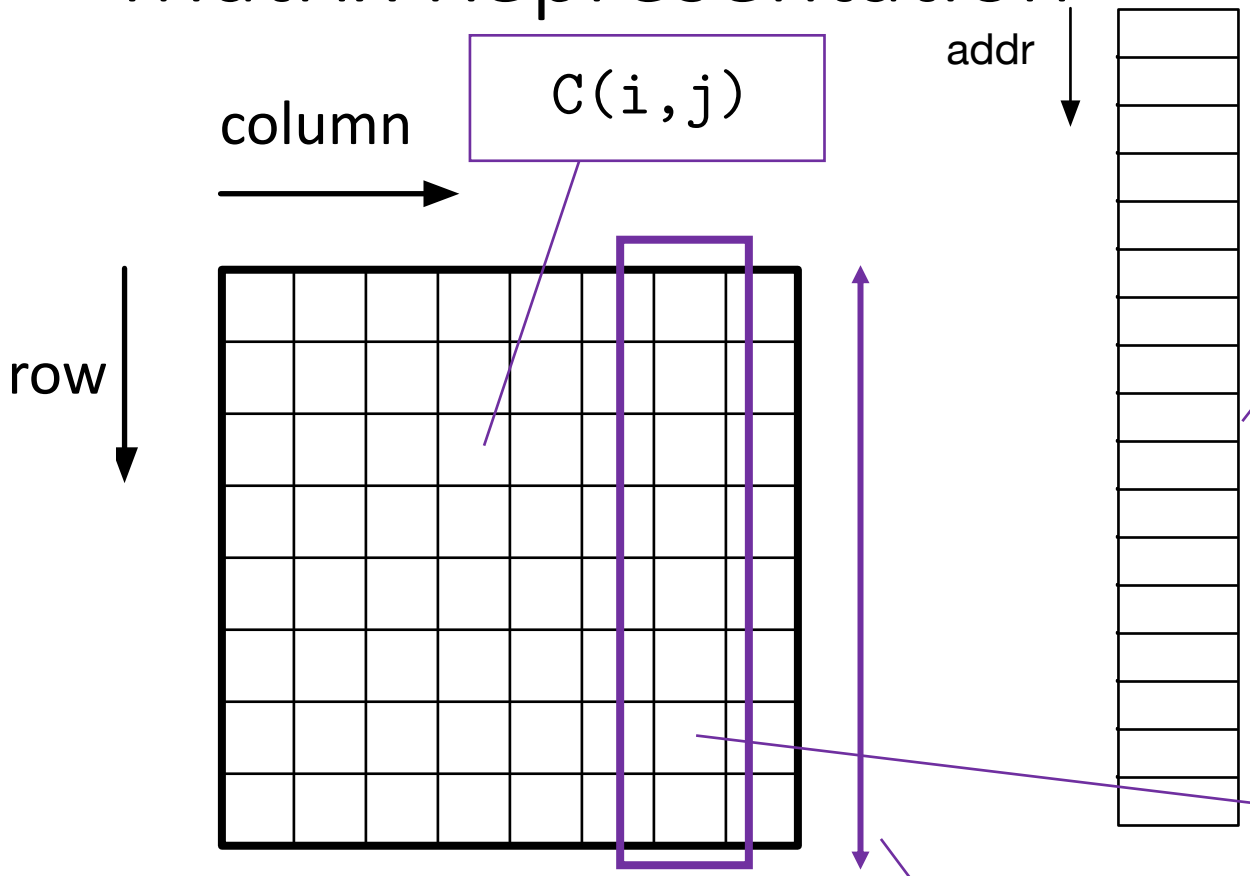
Matrix Representation



Matrix Representation



Matrix Representation



Column-Oriented

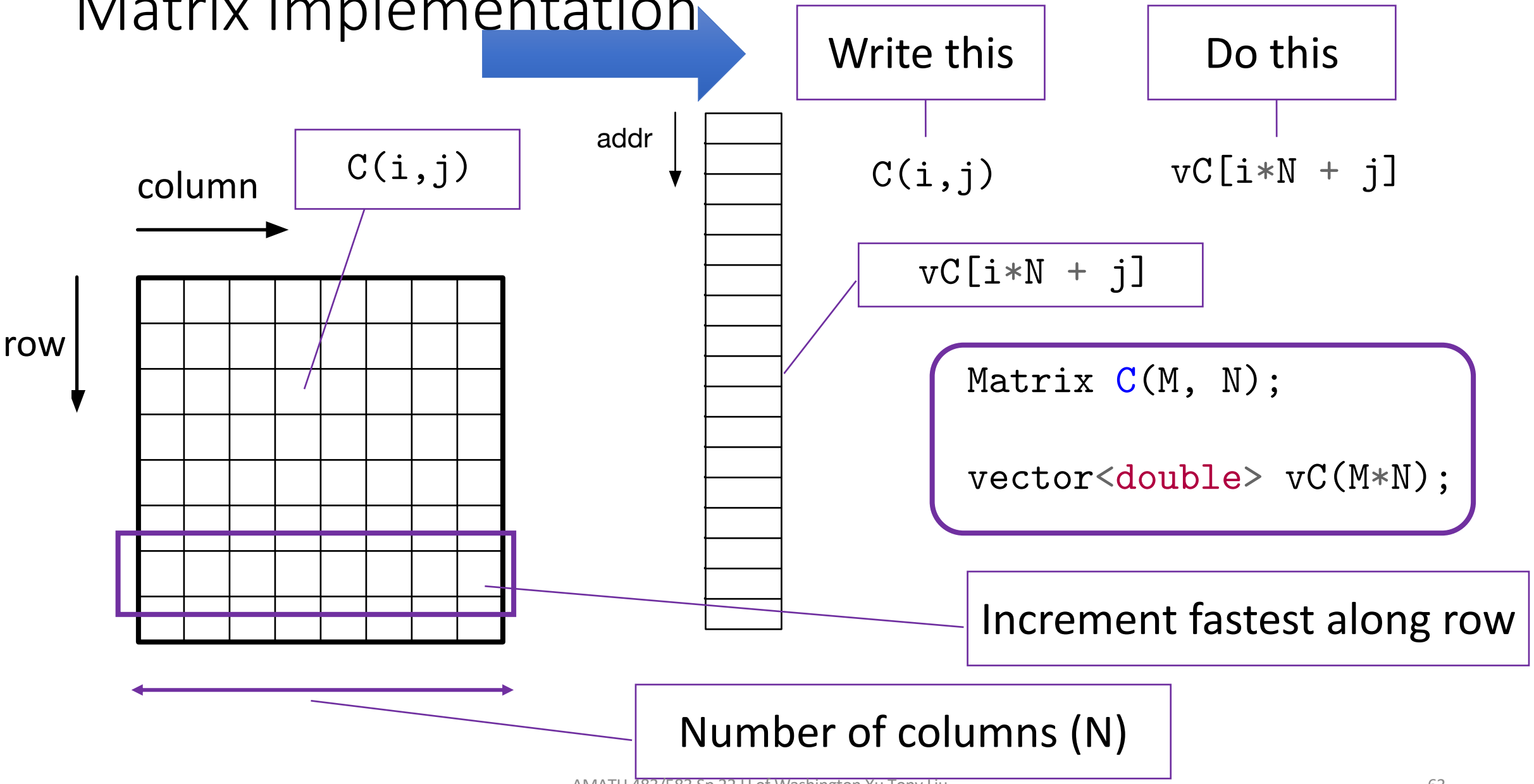
```
vC[j*M + i]
```

```
Matrix C(M, N);

vector<double> vC(M*N);
```

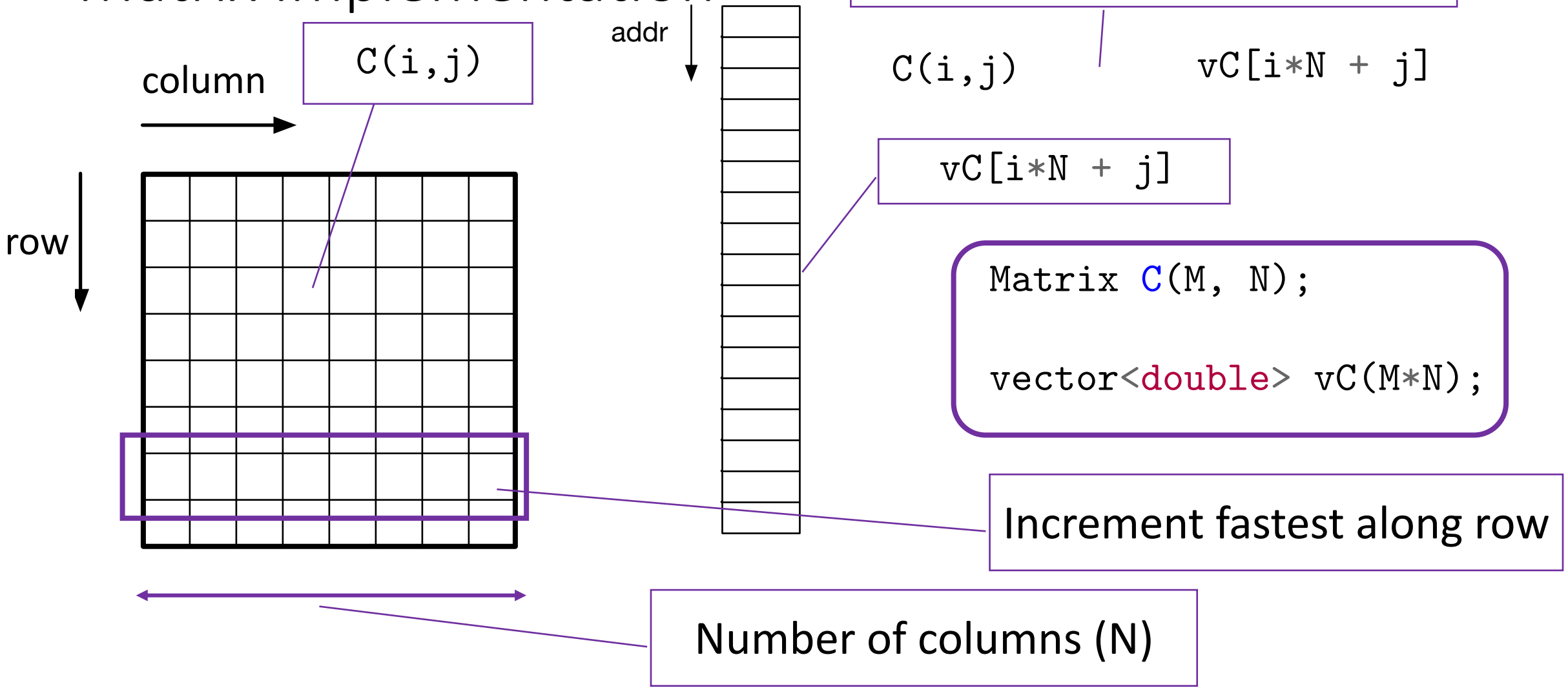
Increment fastest along column

Number of rows (M)

Matrix Implementation



Matrix Implementation



Matrix in C++

- Two dimensional accessor `C(i,j)`
- One dimensional access `vC[i*N + j]`

- Simultaneously (and safely) need matrix with
  - (i,j) two dimensional accessor
  - Transparent translation to one dimensional accessor

- Preprocessor? `#define C(i,j) vC[i*N+j]`

Only works for C and vC

Where does N come from

Matrix in C++

- Two dimensional accessor `C(i,j)`
- One dimensional access `vC[i*N + j]`

- A `Matrix` needs to
  - Have its "own" `vector<double> vC`
  - Have its "own" `N`
  - Have a doubly indexed accessor

Class Matrix

```cpp
#include <vector>

class Matrix {
public:
  Matrix(size_type M, size_type N)
      : num_rows_(M), num_cols_(N), storage_(num_rows_ * num_cols_) {}
  Matrix(size_type M, size_type N, double init)
      : num_rows_(M), num_cols_(N), storage_(num_rows_ * num_cols_, init) {}

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

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

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

Class Matrix

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

  Matrix(size_type M, size_type N, double init)
      : num_rows_(M), num_cols_(N), storage_(num_rows_ * num_cols_, init) {}

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

Class Matrix

```
class Matrix {
public:
  double &operator()(size_type i, size_type j) {
    return storage_[i * num_cols_ + j];
  }




  size_type num_rows() const { return num_rows_; }
  size_type num_Cols() const { return num_cols_; }

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

Class Matrix

```
class Matrix {
public:
  double &operator()(size_type i, size_type j) {
    return storage_[i * num_cols_ + j];
  }
  const double &operator()(size_type i, size_type j) const {
    return storage_[i * num_cols_ + j];
  }

  size_type num_rows() const { return num_rows_; }
  size_type num_Cols() const { return num_cols_; }

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

Class Matrix

```
class Matrix {
public:
  double &operator()(size_type i, size_type j) {
    return storage_[i * num_cols_ + j];
  }
  const double &operator()(size_type i, size_type j) const {
    return storage_[i * num_cols_ + j];
  }

  size_type num_rows() const { return num_rows_; }
  size_type num_Cols() const { return num_cols_; }

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

How would we write the other orientation?

What is the orientation?

Does it matter which?

Before

```
class Matrix {
public:
  double &operator()(size_type i, size_type j) {
    return storage_[i * num_cols_ + j];
  }
  const double &operator()(size_type i, size_type j) const {
    return storage_[i * num_cols_ + j];
  }

  size_type num_rows() const { return num_rows_; }
  size_type num_Cols() const { return num_cols_; }

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

After

```
class Matrix {
public:
  double &operator()(size_type i, size_type j) {
    return storage_[j * num_rows_ + i];
  }
  const double &operator()(size_type i, size_type j) const {
    return storage_[j * num_rows_ + i];
  }

  size_type num_rows() const { return num_rows_; }
  size_type num_Cols() const { return num_cols_; }

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

Finally

```
class Matrix {
public:
  double &operator()(size_type i, size_type j) {
    return storage_[j * num_rows_ + i];
  }
  const double &operator()(size_type i, size_type j) const {
    return storage_[j * num_rows_ + i];
  }

  size_type num_rows() const { return num_rows_; }
  size_type num_Cols() const { return num_cols_; }

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

Example: Matrix-Matrix Product

- For matrices $\mathbf{A} \in \mathbb{R}^{M \times K}$ and $\mathbf{B} \in \mathbb{R}^{K \times N}$, compute $\mathbf{C} \in \mathbb{R}^{M \times N}$

$\mathbf{C} \leftarrow \mathbf{A} \times \mathbf{B}$ Defined according to $C_{ij} = \sum_k A_{ik} B_{kj}$

Locality! (Data reuse)

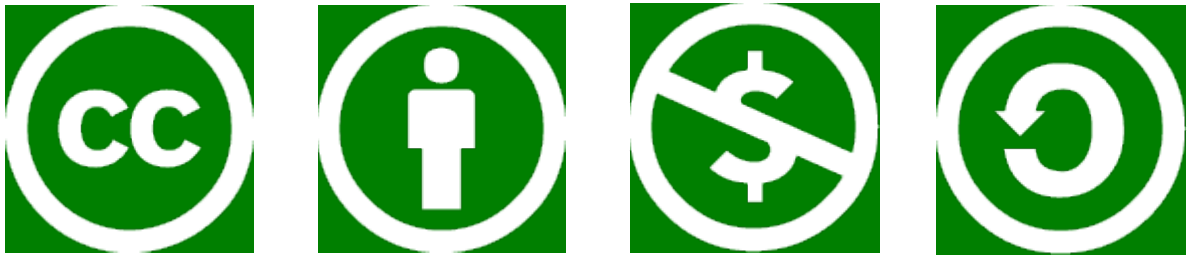
- Workhorse computational kernel (underlying LINPACK, HPL)
- Compute-intensive: $O(N^3)$ work with $O(N^2)$ data
- Basic algorithm in C++

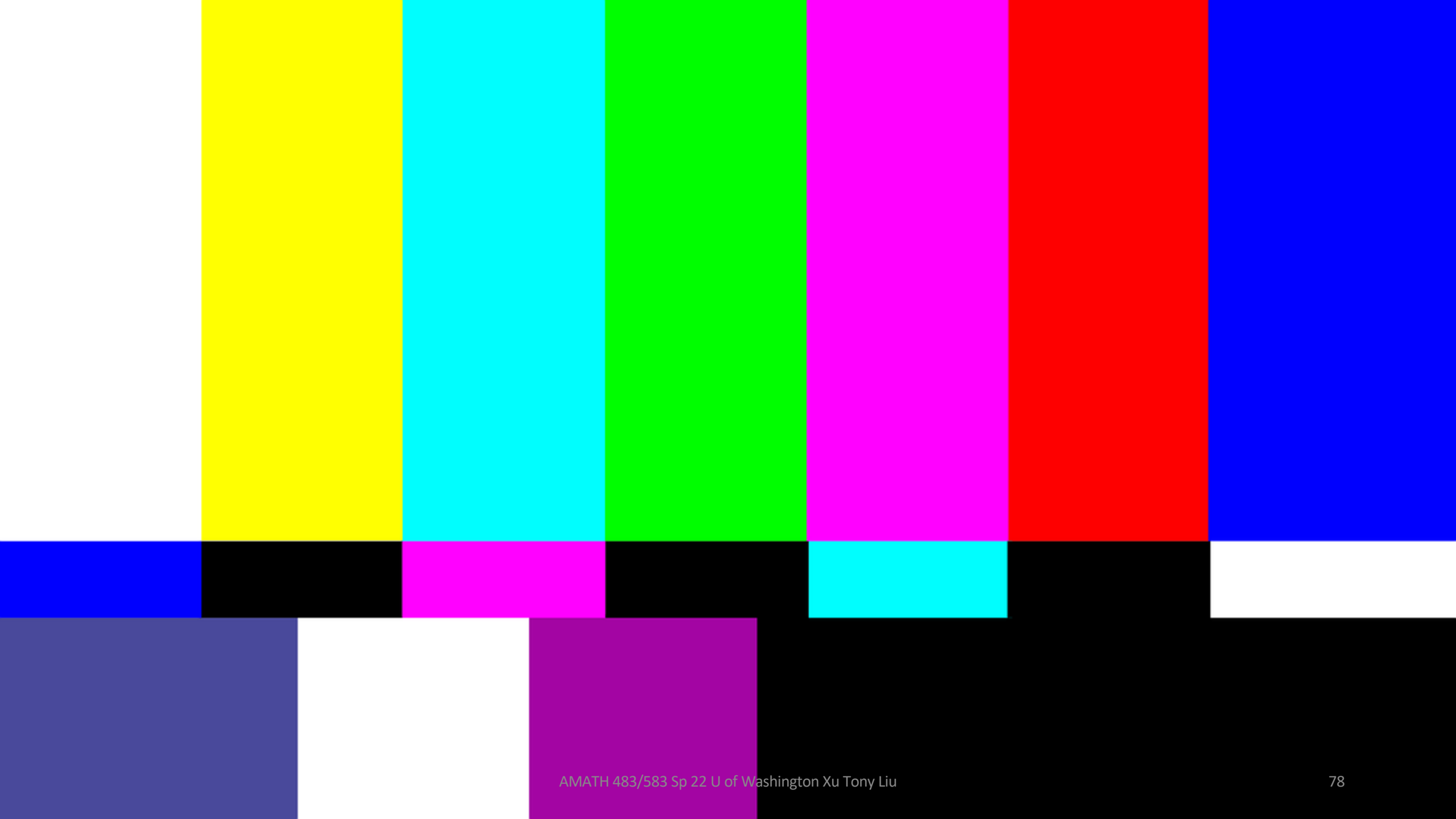
Every element is accessed N times

```
Matrix A(M,K), B(K,N), C(M,N);
...
for (int i = 0; i < N; ++i)
  for (int j = 0; j < N; ++j)
    for (int k = 0; k < N; ++k)
      C(i,j) += A(i,k) * B(k,j)
```

Maximize locality

Thank you!





Example: Matrix-Matrix Product

- For matrices $\mathbf{A} \in \mathbb{R}^{M \times K}$ and $\mathbf{B} \in \mathbb{R}^{K \times N}$, compute $\mathbf{C} \in \mathbb{R}^{M \times N}$

$$\mathbf{C} \leftarrow \mathbf{A} \times \mathbf{B} \qquad \text{Defined according to} \quad C_{ij} = \sum_k A_{ik} B_{kj}$$

- Workhorse computational kernel (underlying LINPACK, HPL)
- Compute-intensive: $O(N^3)$ work with $O(N^2)$ data
- Basic algorithm in C

```
double **A, double **B, double **C;
for (int i = 0; i < M; ++i)
  for (int j = 0; j < N; ++j)
    for (int k = 0; k < K; ++k)
      C[i][j] += A[i][k] * B[k][j];
```

Example: Matrix-Matrix Product

- For matrices $\mathbf{A} \in \mathbb{R}^{M \times K}$ and $\mathbf{B} \in \mathbb{R}^{K \times N}$, compute $\mathbf{C} \in \mathbb{R}^{M \times N}$

$$\mathbf{C} \leftarrow \mathbf{A} \times \mathbf{B} \quad \text{Defined according to} \quad C_{ij} = A_{ik} B_{kj}$$

- C does not have dynamic multidimensional arrays
- Array of pointers to pointers very bad for performance
- Implement mapping of 2D to 1D with "leading dimension" arithmetic

```
double *A, double *B, double *C;
int lda, ldb, ldc;
for (int i = 0; i < M; ++i)
  for (int j = 0; j < N; ++j)
    for (int k = 0; k < K; ++k)
      C[i*ldc+j] += A[i*lda+k] * B[k*ldb+j];
```

Example: Matrix-Matrix Product

- For matrices $\mathbf{A} \in \mathbb{R}^{M \times K}$ and $\mathbf{B} \in \mathbb{R}^{K \times N}$, compute $\mathbf{C} \in \mathbb{R}^{M \times N}$

$$\mathbf{C} \leftarrow \mathbf{A} \times \mathbf{B} \quad \text{Defined according to} \quad C_{ij} = A_{ik} B_{kj}$$

- For notational convenience:

Assume

```
#define A(i,j) A[(i)*lda+j]
#define B(i,j) B[(i)*ldb+j]
#define C(i,j) C[(i)*ldc+j]
double *A, double *B, double *C;
int lda, ldb, ldc;
for (int i = 0; i < M; ++i)
  for (int j = 0; j < N; ++j)
    for (int k = 0; k < K; ++k)
      C(i,j) += A(i,k) * B(k,j);
```

Example: Matrix-Matrix Product

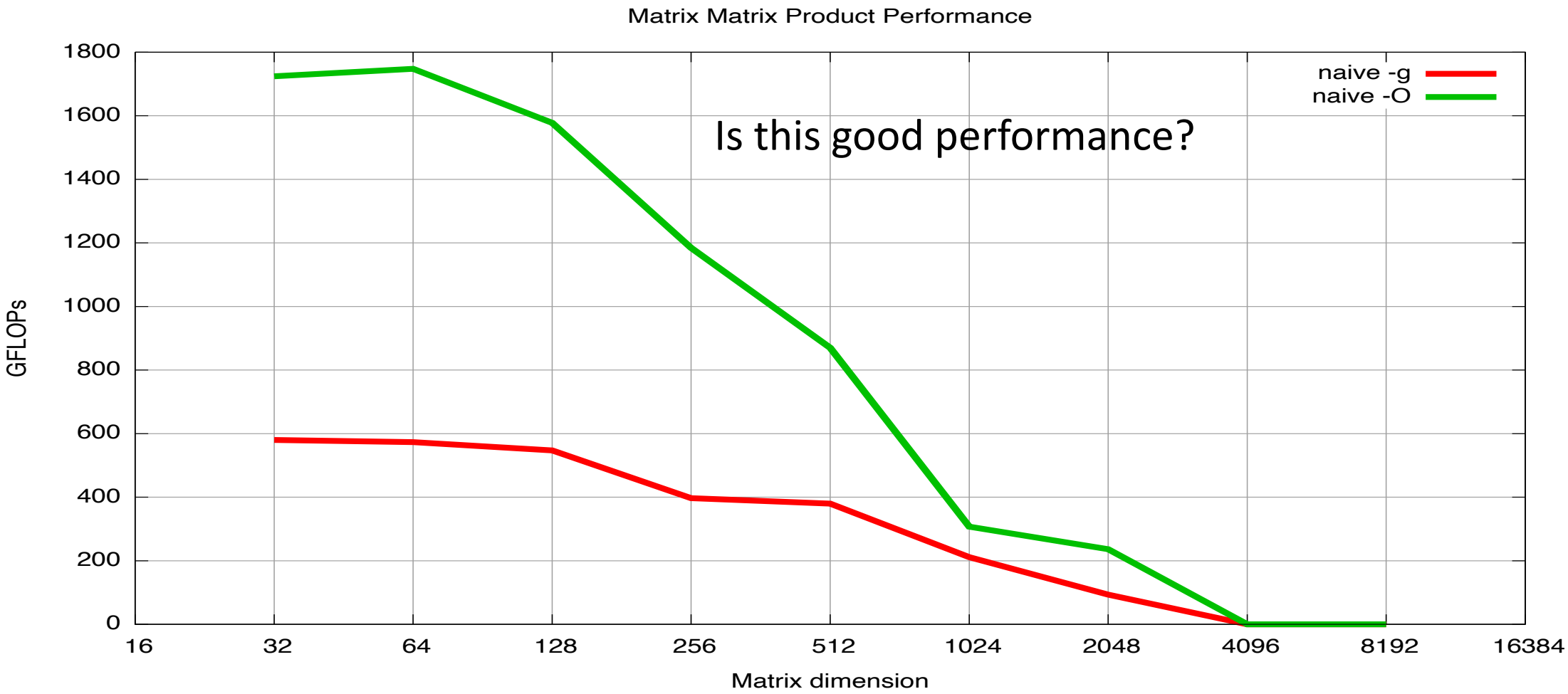
- For matrices $\mathbf{A} \in \mathbb{R}^{M \times K}$ and $\mathbf{B} \in \mathbb{R}^{K \times N}$, compute $\mathbf{C} \in \mathbb{R}^{M \times N}$

$$\mathbf{C} \leftarrow \mathbf{A} \times \mathbf{B}$$ Defined according to $$C_{ij} = A_{ik} B_{kj}$$

- For true notational convenience (assuming rest):

```
for (int i = 0; i < M; ++i)
  for (int j = 0; j < N; ++j)
    for (int k = 0; k < K; ++k)
      C(i,j) += A(i,k) * B(k,j);
```

Example: Base Case



Improving Locality

- Consider each step of inner loop

```
for (int i = 0; i < M; ++i)
  for (int j = 0; j < N; ++j)
    for (int k = 0; k < K; ++k)
      C(i,j) += A(i,k) * B(k,j);
```

- Load `C(i,j)` into register
- Load `A(i,k)` into register
- Load `B(k,j)` into register
- Multiply
- Add
- Store `C(i,j)`

- Four memory operations and two floating point operations per iteration
- 1/3 flop per cycle (if each operation is one cycle)

Improving Locality

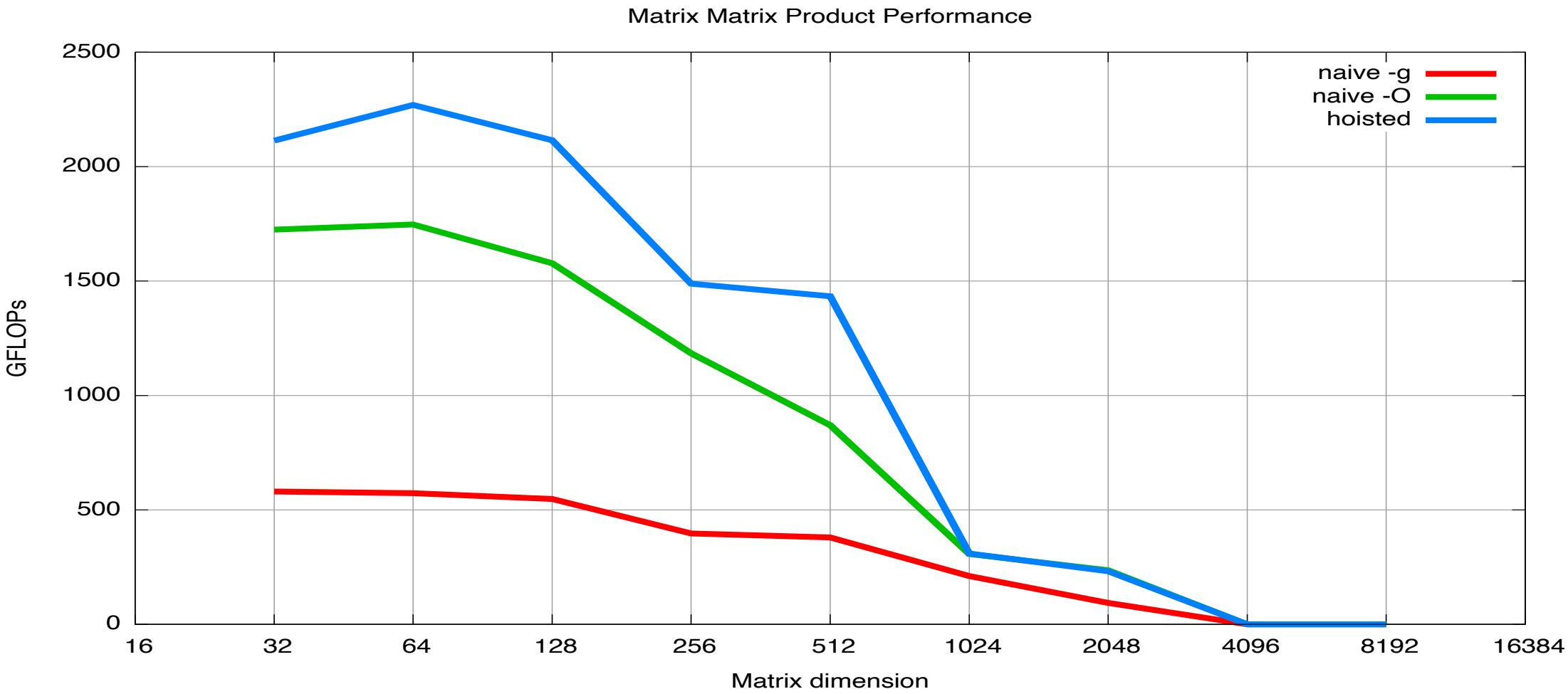
- Consider each step of inner loop

```
for (int i = 0; i < M; ++i)
  for (int j = 0; j < N; ++j) {
    double C00 = C(i,j);
    for (int k = 0; k < K; ++k)
      C00 += A(i,k) * B(k,j);
    C(i,j) = C00;
  }
```

- Load `A(i,k)` into register
- Load `B(k,j)` into register
- Multiply
- Add

- Two memory operations and two floating point operations per iteration
- 1/2 flop per cycle (if each operation is one cycle)

Example: Variable Hoisting



Improving Locality: Unroll and Jam

- Consider each step of inner loop

```
for (int i = 0; i < M; i += 2)
  for (int j = 0; j < N; j += 2) {
    double C00 = C(i,j),   C01 = C(i, j+1);
    double C10 = C(i+1,j), C11 = C(i+1, j+1);
    for (int k = 0; k < K; ++k)
      C00 += A(i,k)   * B(k,j); C01 += A(i,k)   * B(k,j+1);
      C10 += A(i+1,k) * B(k,j); C11 += A(i+1,k) * B(k,j+1);
    C(i,j)   = C00; C(i,j+1)   = C01;
    C(i+1,j) = C10; C(i+1,j+1) = C11;
  }
```

- Load `A(i,k)` and `A(i+1,k)` into registers – note reuse
- Load `B(k,j)` and `B(k,j+1)` into registers – note reuse
- Multiply (four times)
- Add (four times)
- Four memory operations and eight floating point operations per iteration
- 2/3 flop per cycle (if each operation is one cycle) – 2X the base case

Example: Register Locality