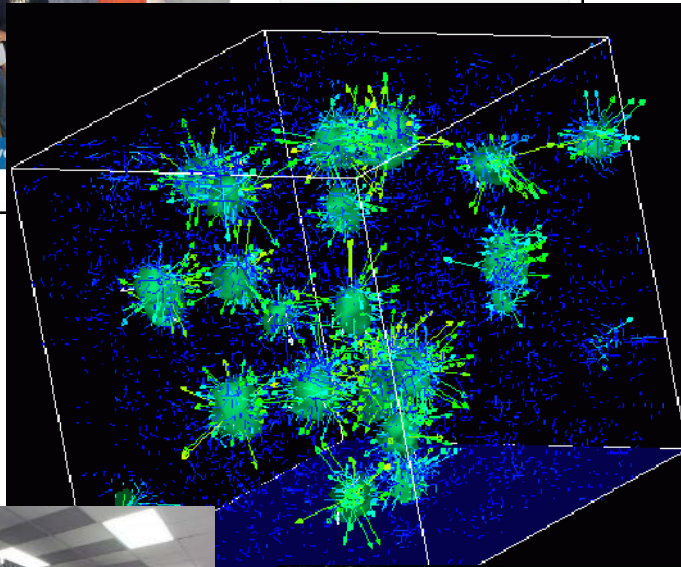




# Survey of Scientific Computing (SciComp 301)

Dave Biersach  
Brookhaven National  
Laboratory  
[dbiersach@bnl.gov](mailto:dbiersach@bnl.gov)



```
1 using System;
2 using System.Collections.Generic;
3 using System.ComponentModel;
4 using System.Data;
5 using System.Drawing;
6 using System.Linq;
7 using System.Text;
8 using System.Windows.Forms;
9
10 namespace SimpleEvents
11 {
12     public partial class Form1 : Form
13     {
14         Person person = new Person();
15
16         public Form1()
17         {
18             InitializeComponent();
19             person.FirstName = "Christian";
20             person.LastName = "Pano";
21         }
22
23         private void button1_Click(object sender, EventArgs e)
24         {
25             person.MainColor = textBox1.Text;
26         }
27     }
28 }
```

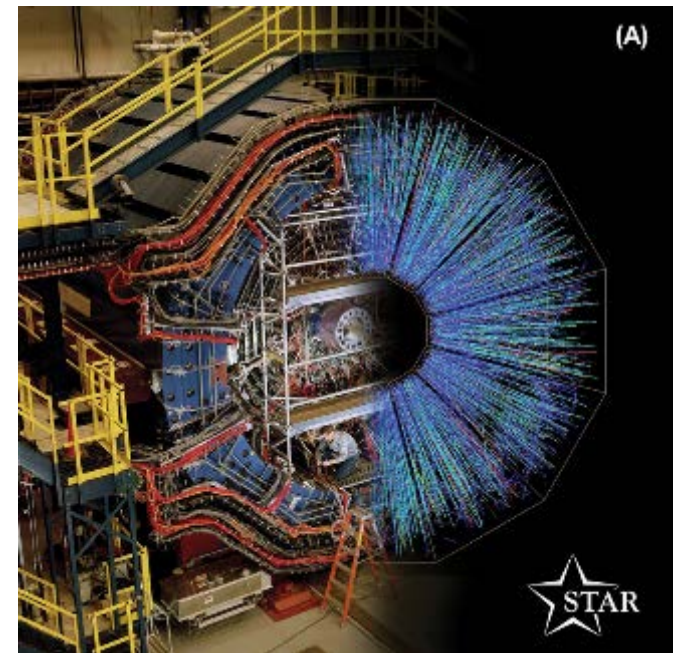
**Session 02**  
Code Structure, Variables

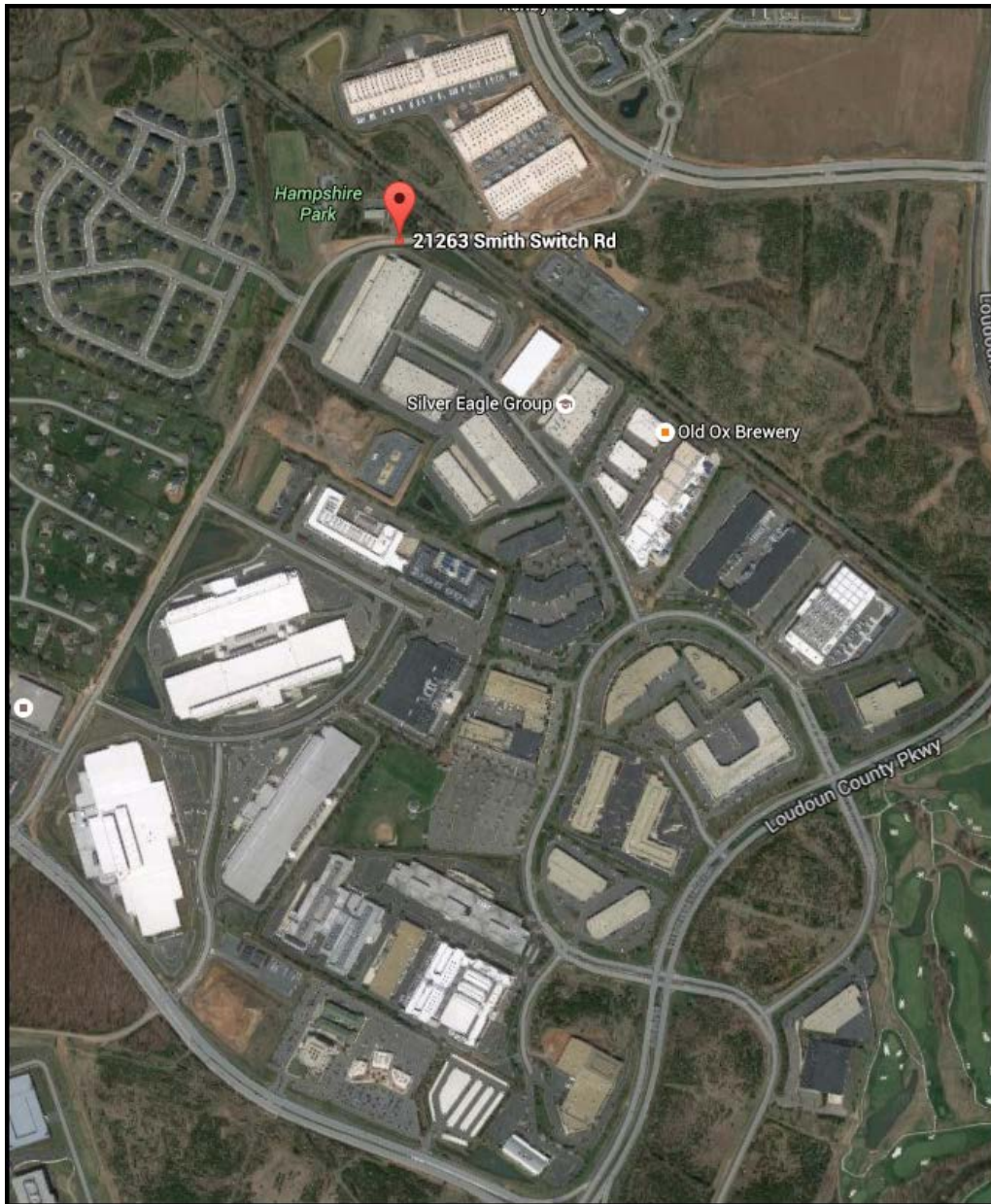
# Session Goals

- Access **your** remote PC in Amazon's cloud
- Review the rules for creating C++ **identifiers**
- Understand C++ **statements** and **scopes**
- Create C++ variables using built-in data **types**
- Display the values of variables on the console
- Create simple loops with the **for()** statement

# Scientific Computing in the Cloud

- The cloud is a great **equalizer**
- Allows participants to continue learning at home as on campus
- Cloud machines are fully isolated from school networks - eliminates local software installation restrictions & campus cybersecurity concerns
- Schools with low-end PC labs can still access the newest generation of hardware





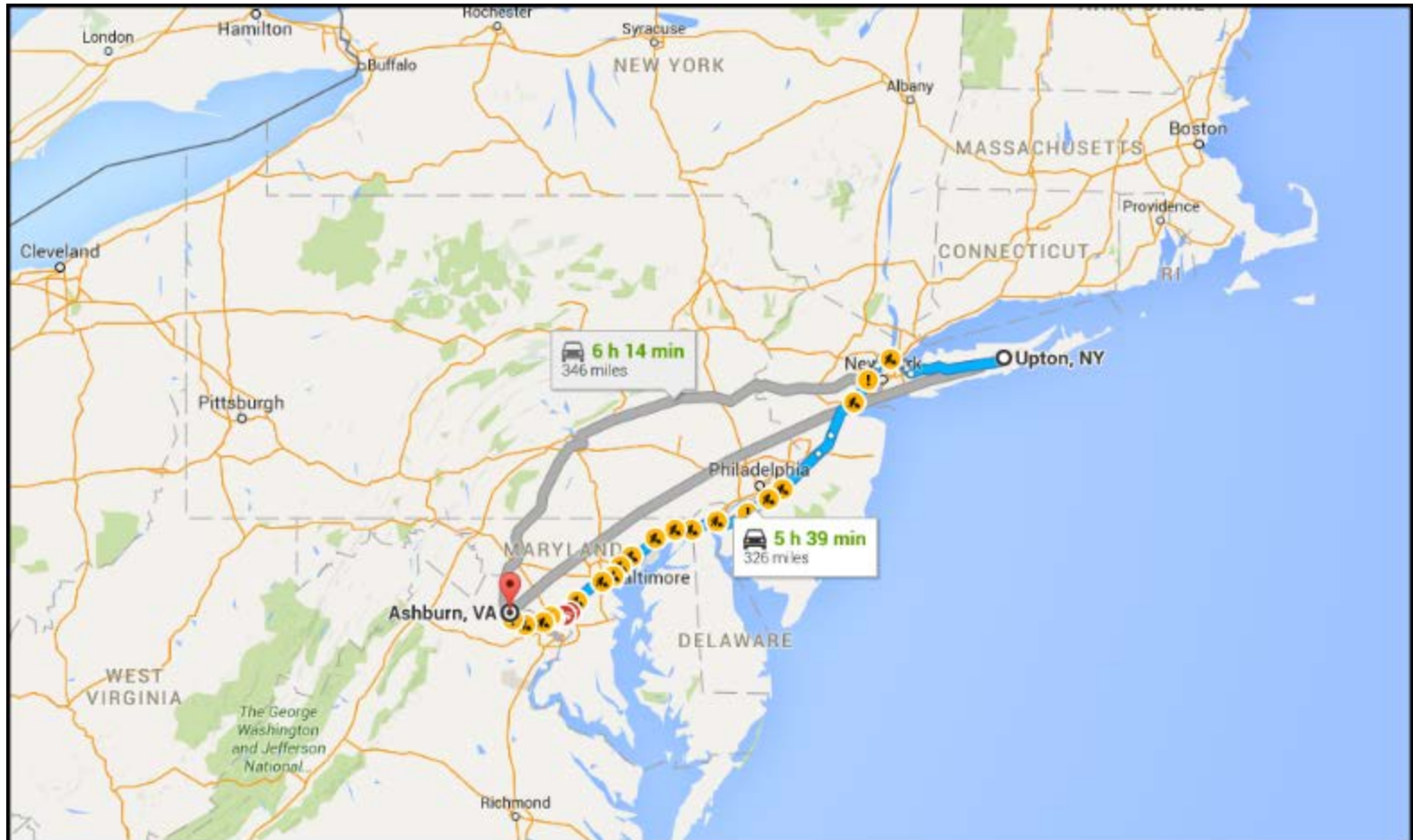
Amazon's  
23 data centers in  
Ashburn, Virginia



## Just two of Amazon's 23 cloud data centers in Ashburn, Virginia

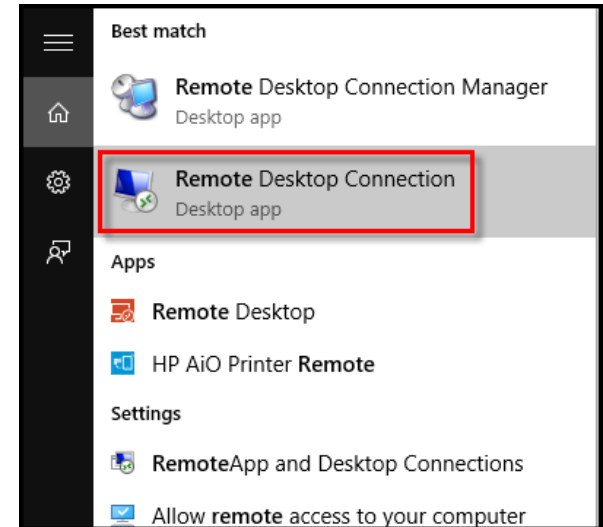


**BNL ↔ Ashburn**  
Roundtrip = 660 miles



# Accessing an Amazon Remote PC

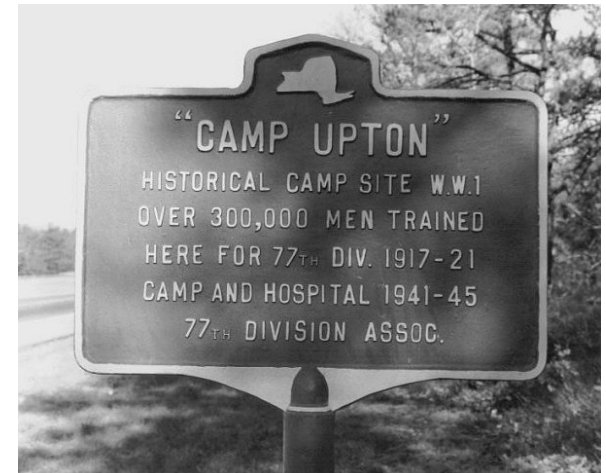
- Uses Microsoft's “**Remote Desktop Connection**” application
- Students have assigned credentials
  - The IP address (***computer name***) of their specific machine in Amazon's cloud
  - Their user name (case sensitive!)
  - Their password (case sensitive!)
- Students can access their Amazon machine **from their home**
- Educators can remotely monitor student progress **real-time** on the lab exercises



# Accessing an Amazon Remote PC

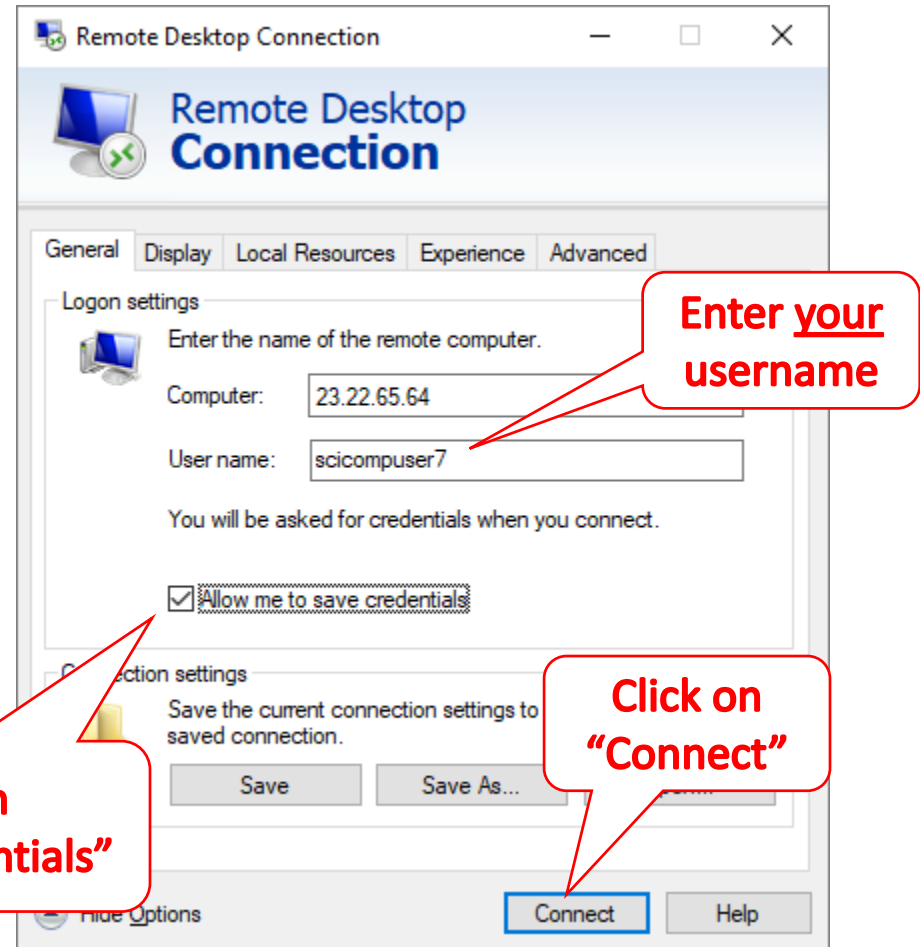
IP Address	Last Name	First Name
23.21.36.204		
23.22.65.64		
23.22.66.177		
23.22.77.143		
23.22.79.115		
23.23.69.92		
50.16.130.78		
50.16.135.127		
50.16.144.96		
50.16.147.112		
50.16.159.220		
50.16.160.201		
50.16.163.25		
50.16.163.117		
50.16.163.174		
50.16.165.70		
50.16.165.235		
50.16.170.168		
50.16.175.58		
50.16.175.233		

1. Write down your IP address, username, and password in your notebook
2. Take a picture of your login information to keep on your smart phone






# Accessing an Amazon Remote PC



# Accessing an Amazon Remote PC

Login to ip-172-31-68-103



Session


username

password

OK Cancel

**Drop down and select "Xvnc"**

Login to ip-172-31-68-103



Session

username

password

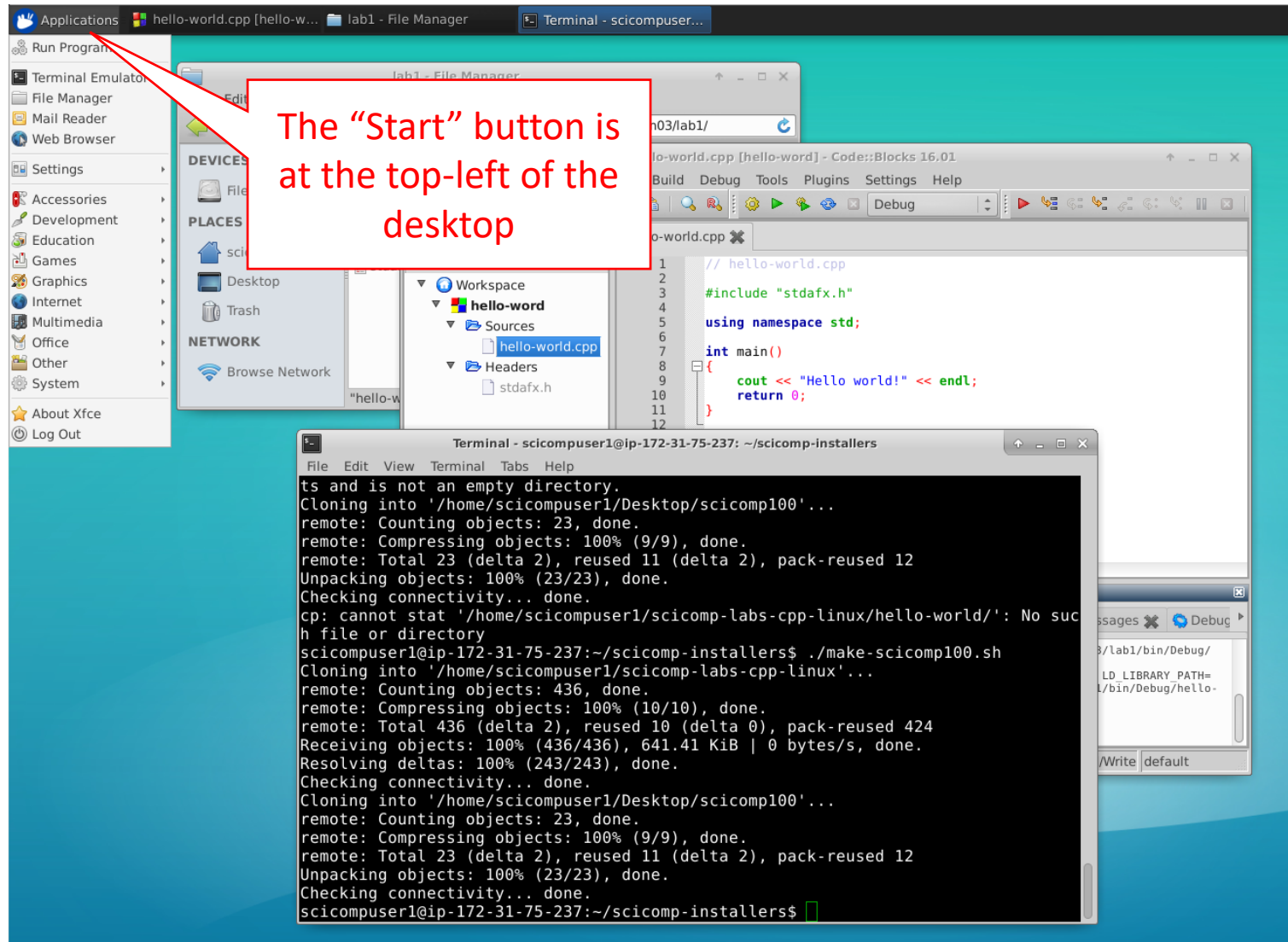
OK Cancel

**Enter your username**

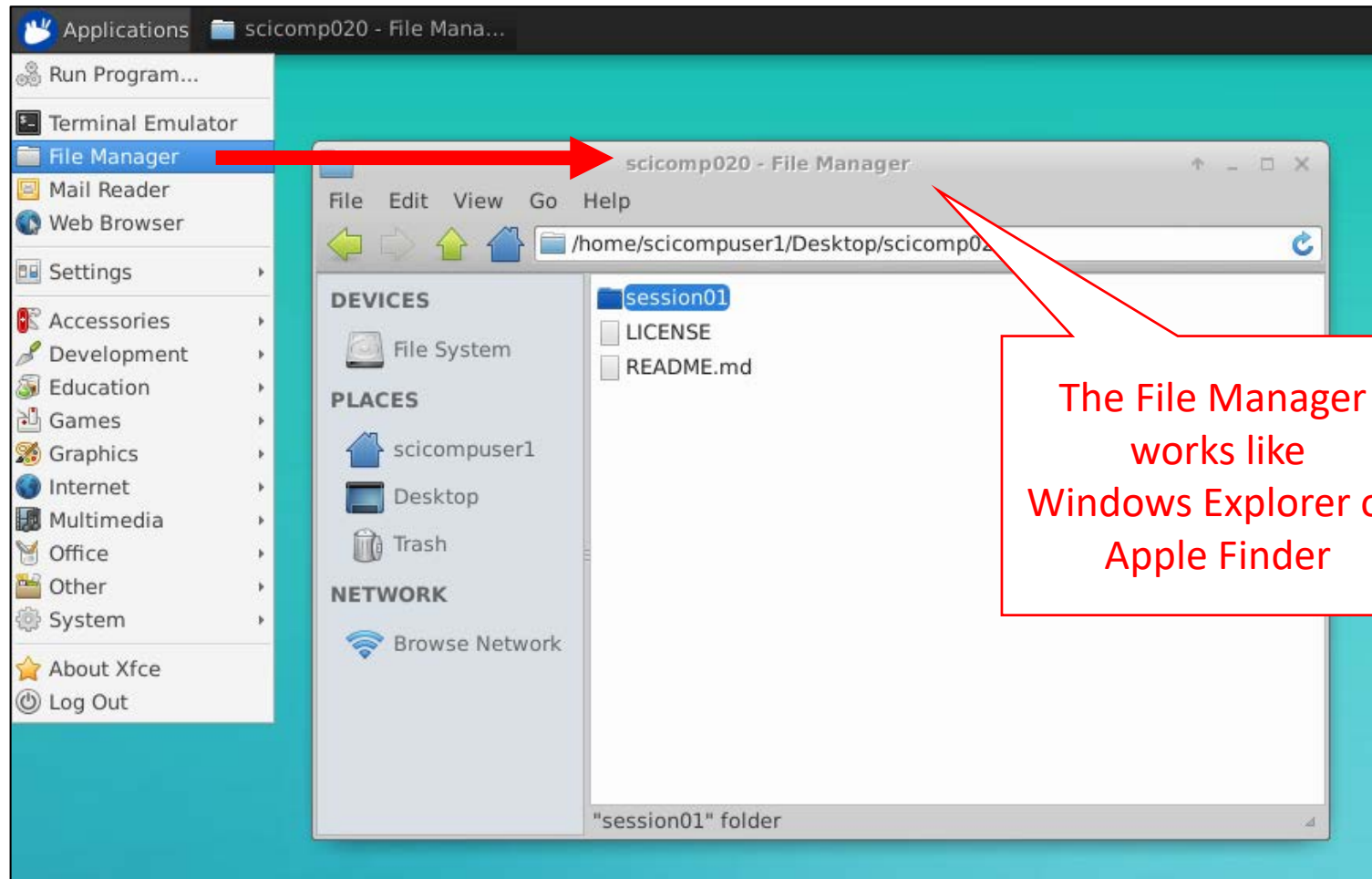
**Enter your password**

**Click "OK"**

# Ubuntu Linux with Xfce Desktop

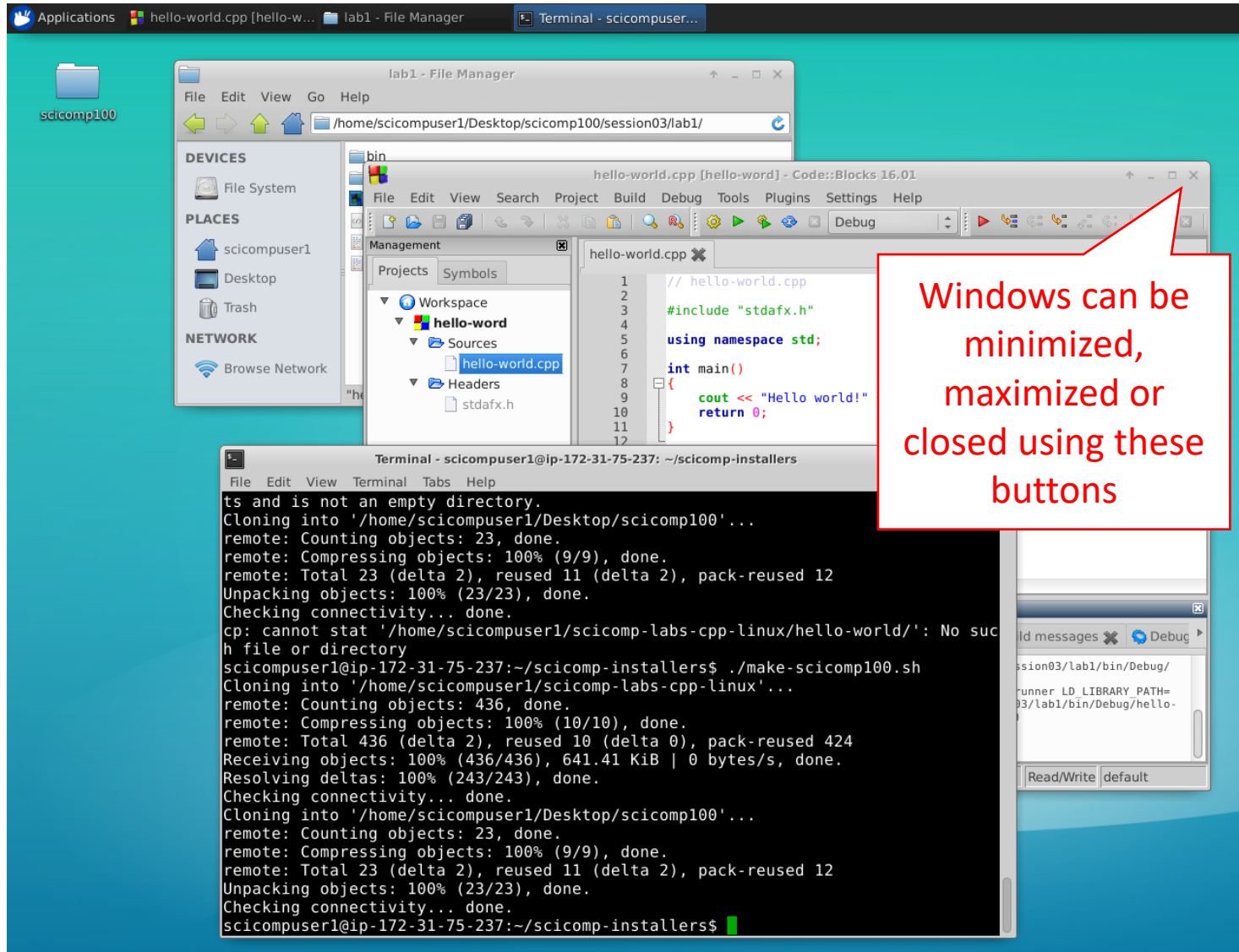


# Ubuntu Linux with Xfce Desktop

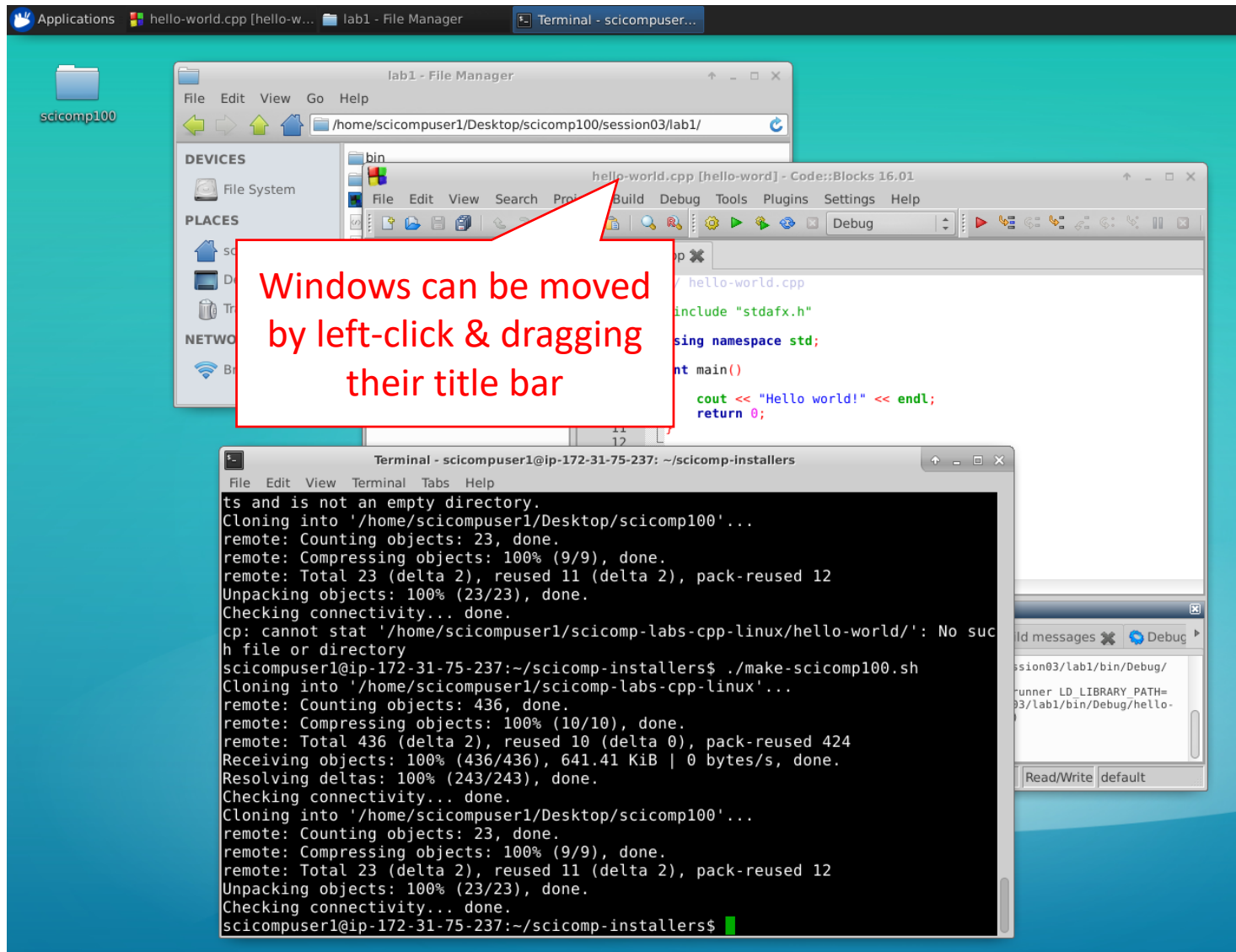




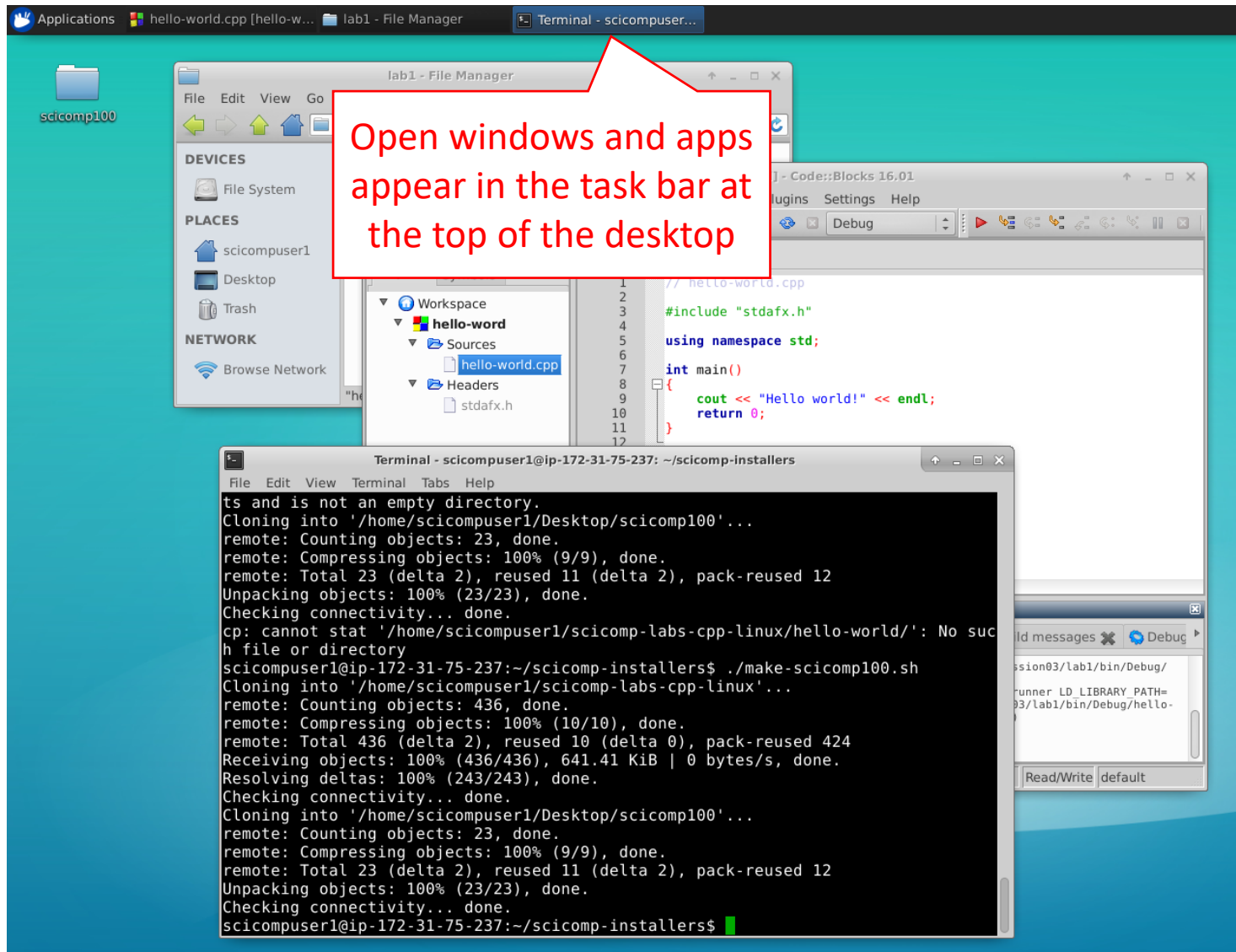
# Ubuntu Linux with Xfce Desktop



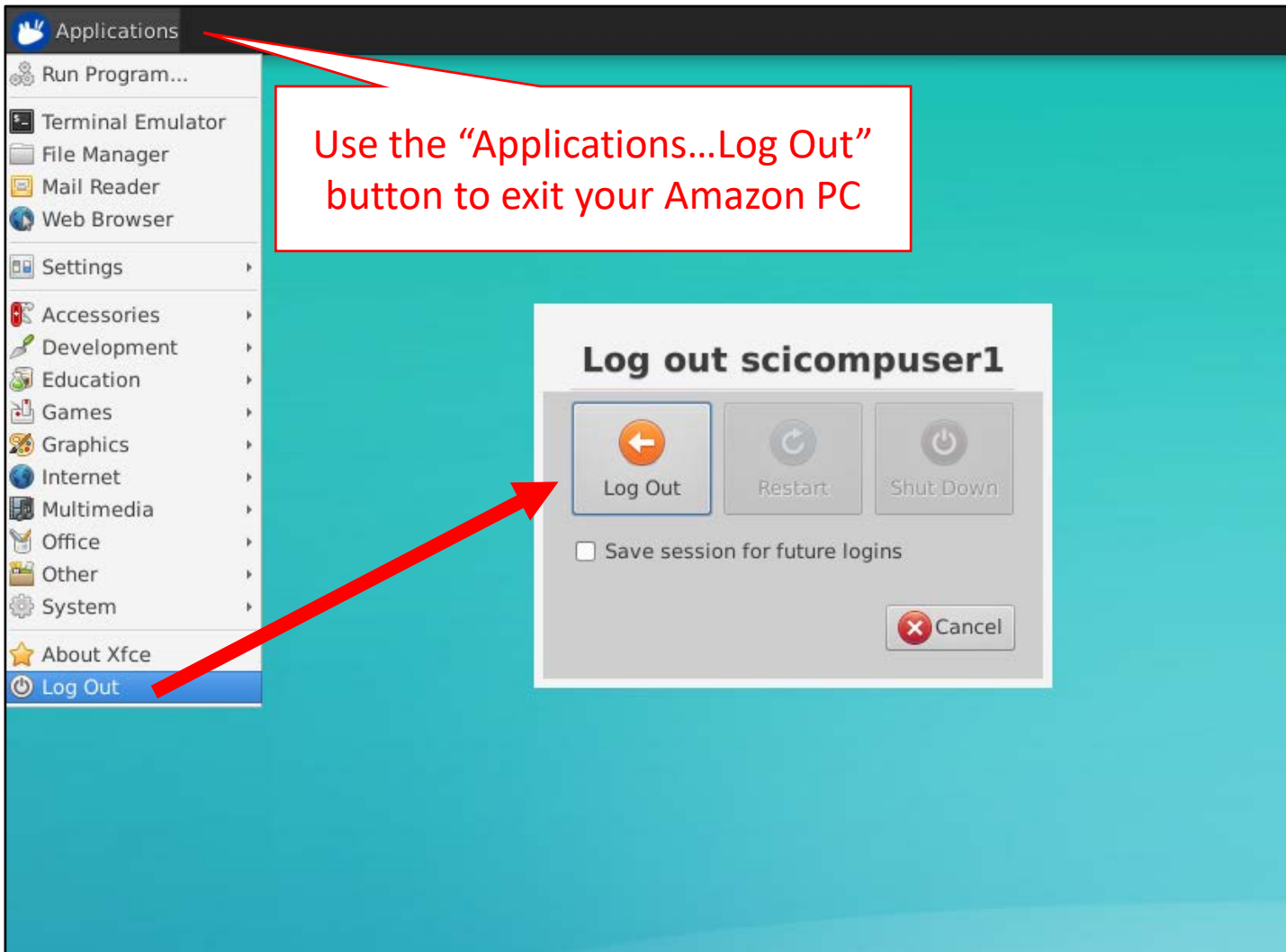
# Ubuntu Linux with Xfce Desktop



# Ubuntu Linux with Xfce Desktop

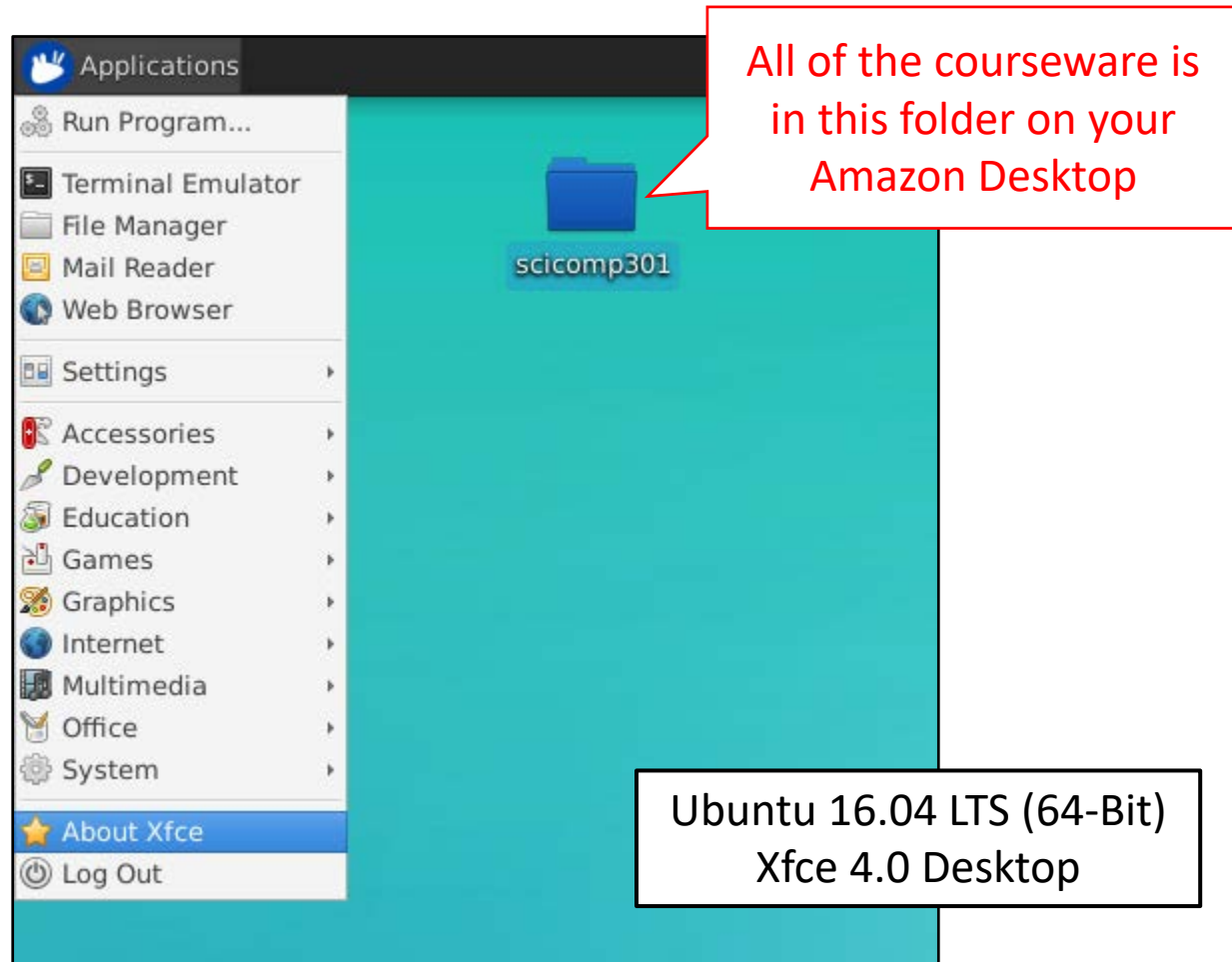


# Ubuntu Linux with Xfce Desktop

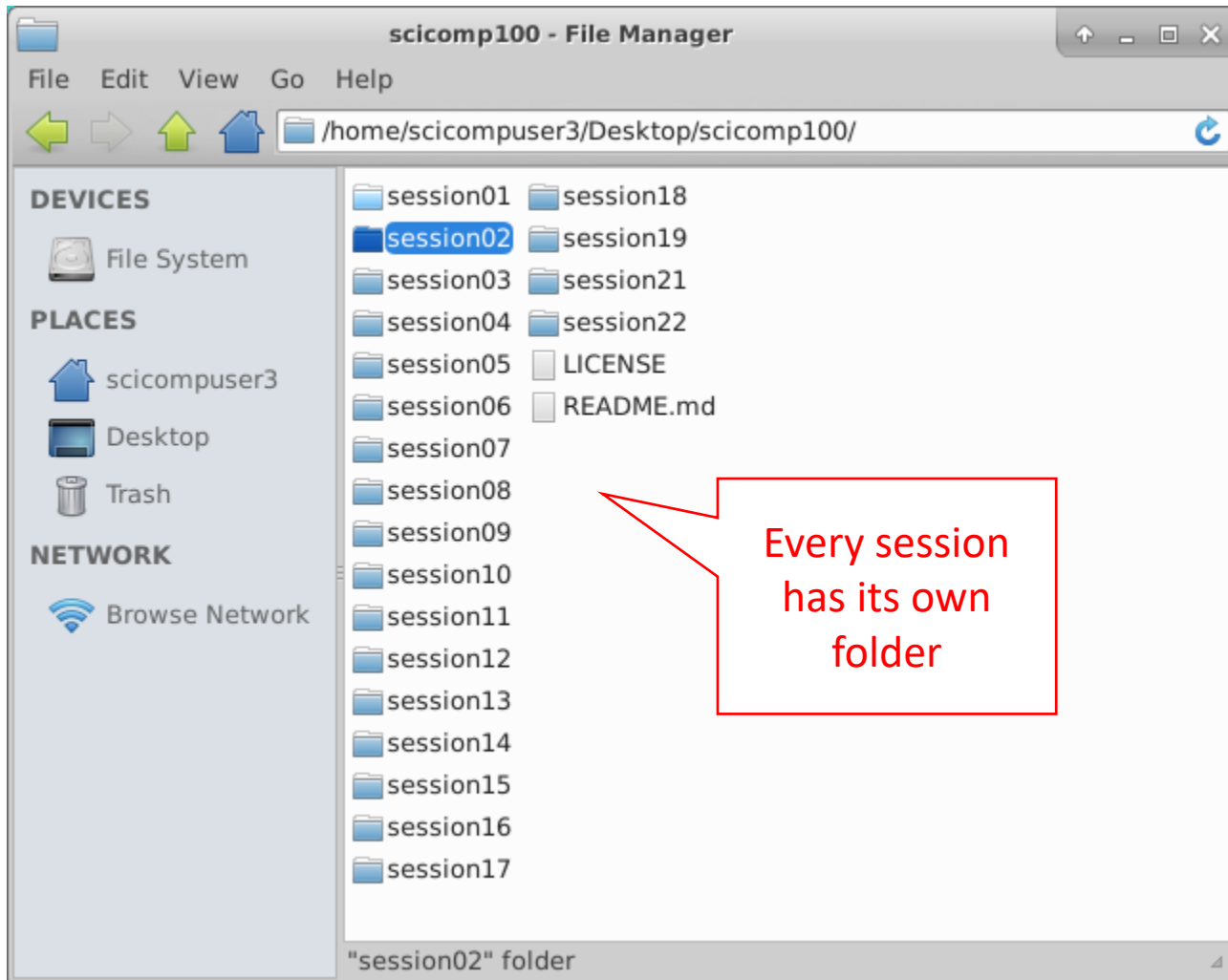




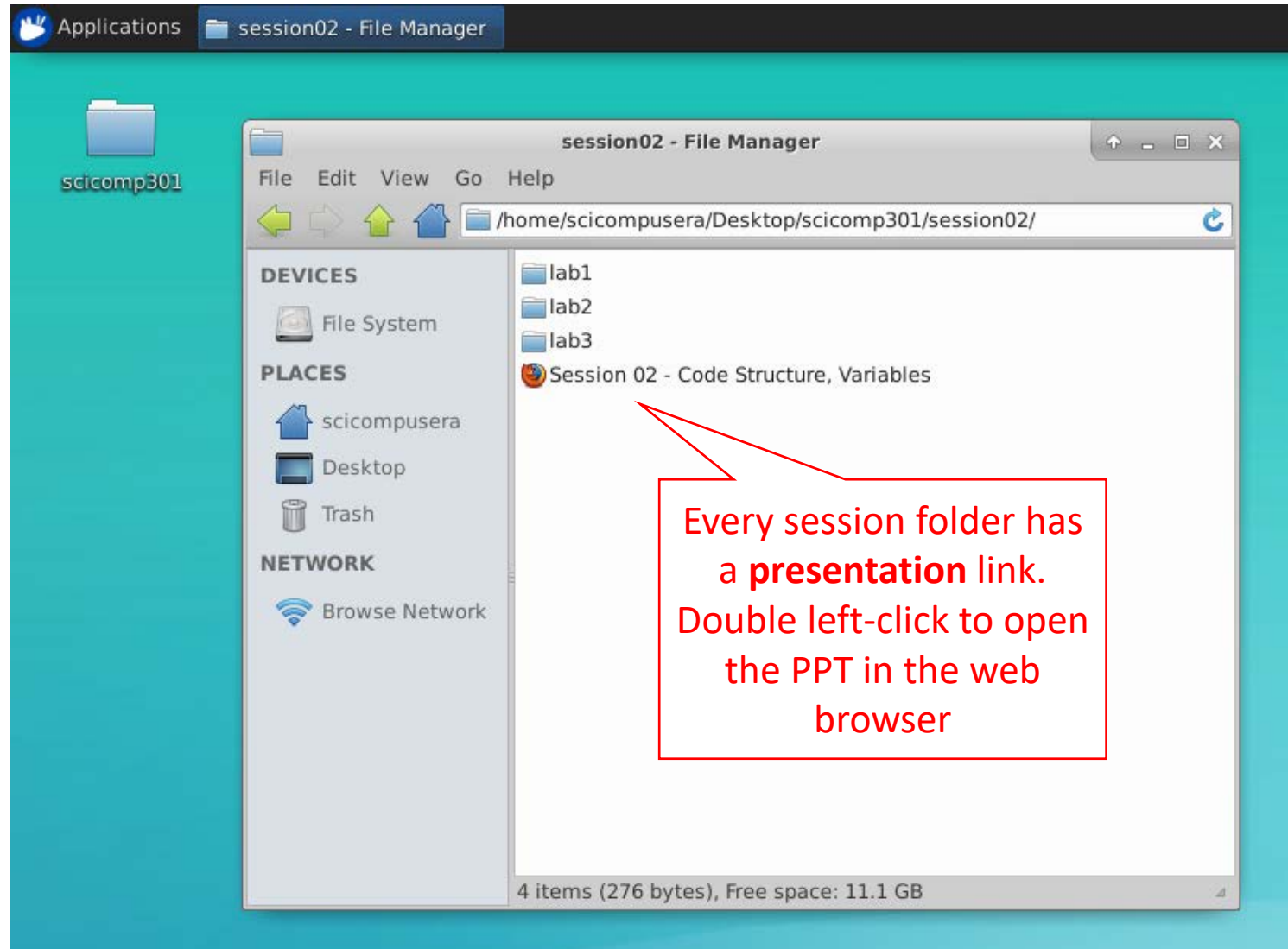
# SciComp Courseware Layout



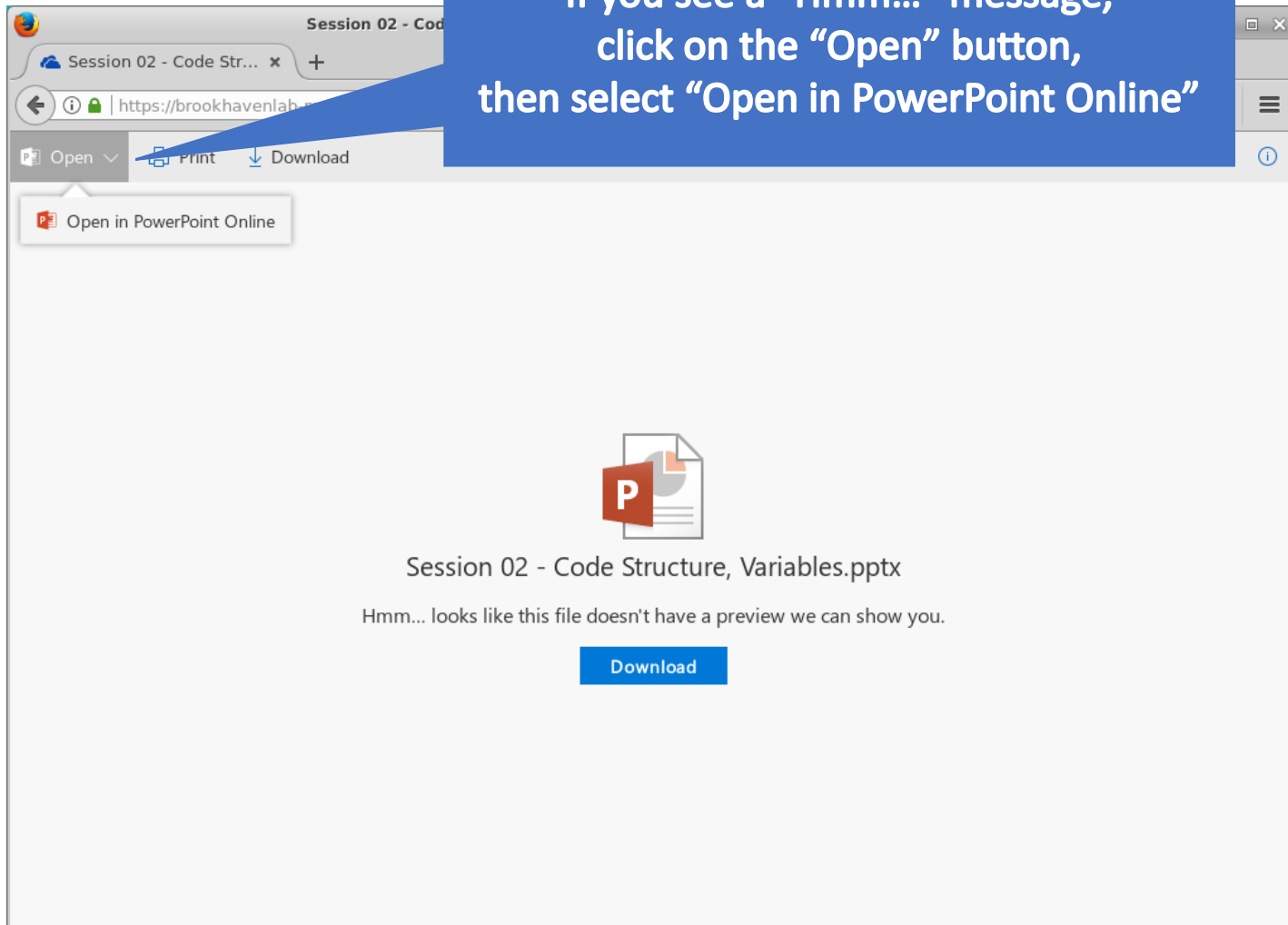
# SciComp Courseware Layout



# SciComp Courseware Layout



If you see a “Hmm...” message,  
click on the “Open” button,  
then select “Open in PowerPoint Online”





Session 02 - Code Structure, Variables.pptx - Mozilla Firefox

Session 02 - Code Str... x Session 02 - Code Str... x +

https://brookhavenlab-my.sharepoint.com/:p:/r/personal/dbiersach\_bn | Search

PowerPoint Online Guest Contributor


Download Start Slide Show Print to PDF Comments

## Survey of Scientific Computing (SciComp 301)

Dave Biersach  
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### Session 02 Code Structure, Variables

Left click on "Slide # of #" to jump to a specific slide



```
using System;
using System.Collections.Generic;
using System.Linq;
using System.Text;
using System.Threading.Tasks;
using System.Windows.Forms;

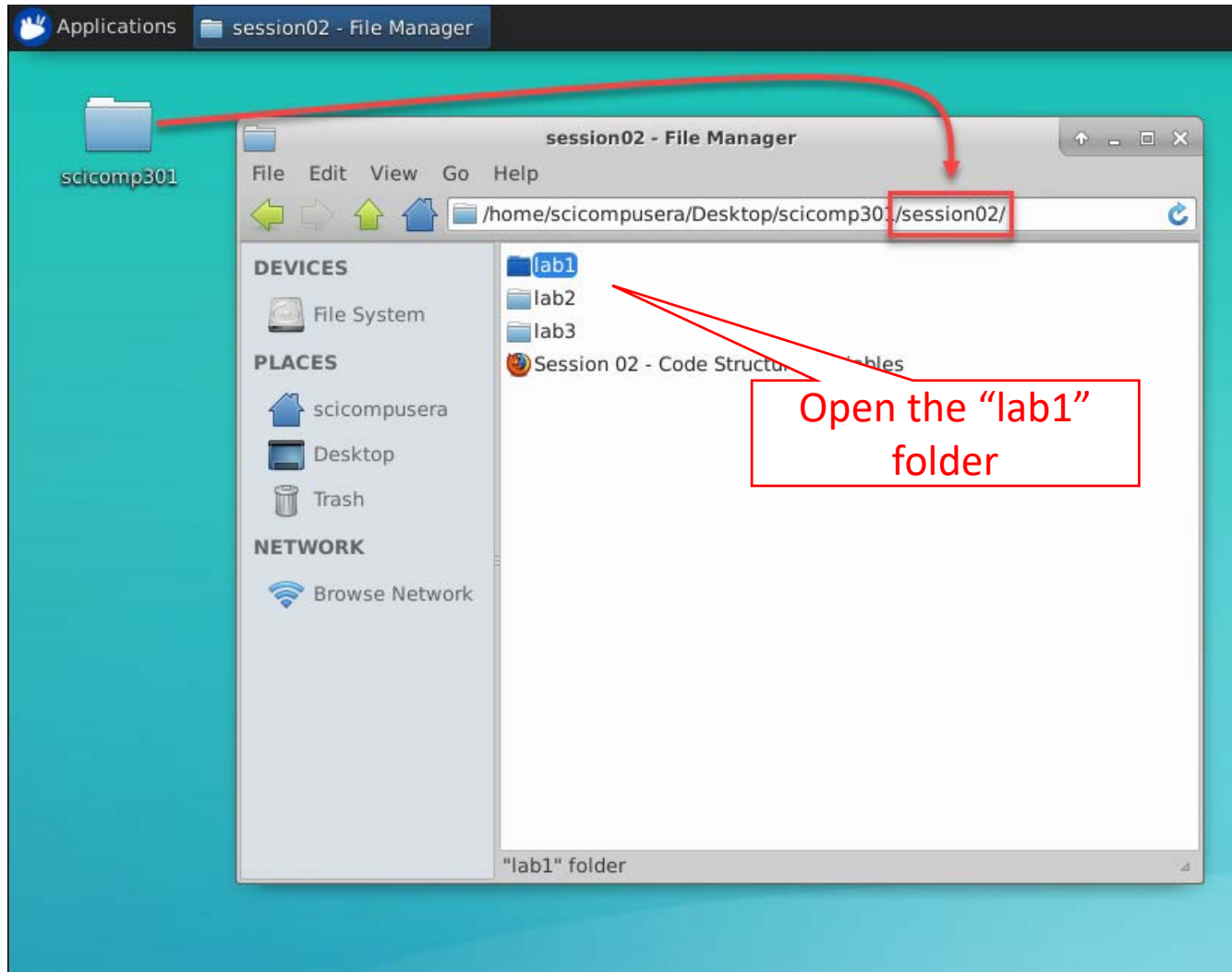
namespace SciComp301
{
    public partial class Form1 : Form
    {
        Person person = new Person();

        public Form1()
        {
            InitializeComponent();
            person.FirstName = "John";
            person.LastName = "Doe";

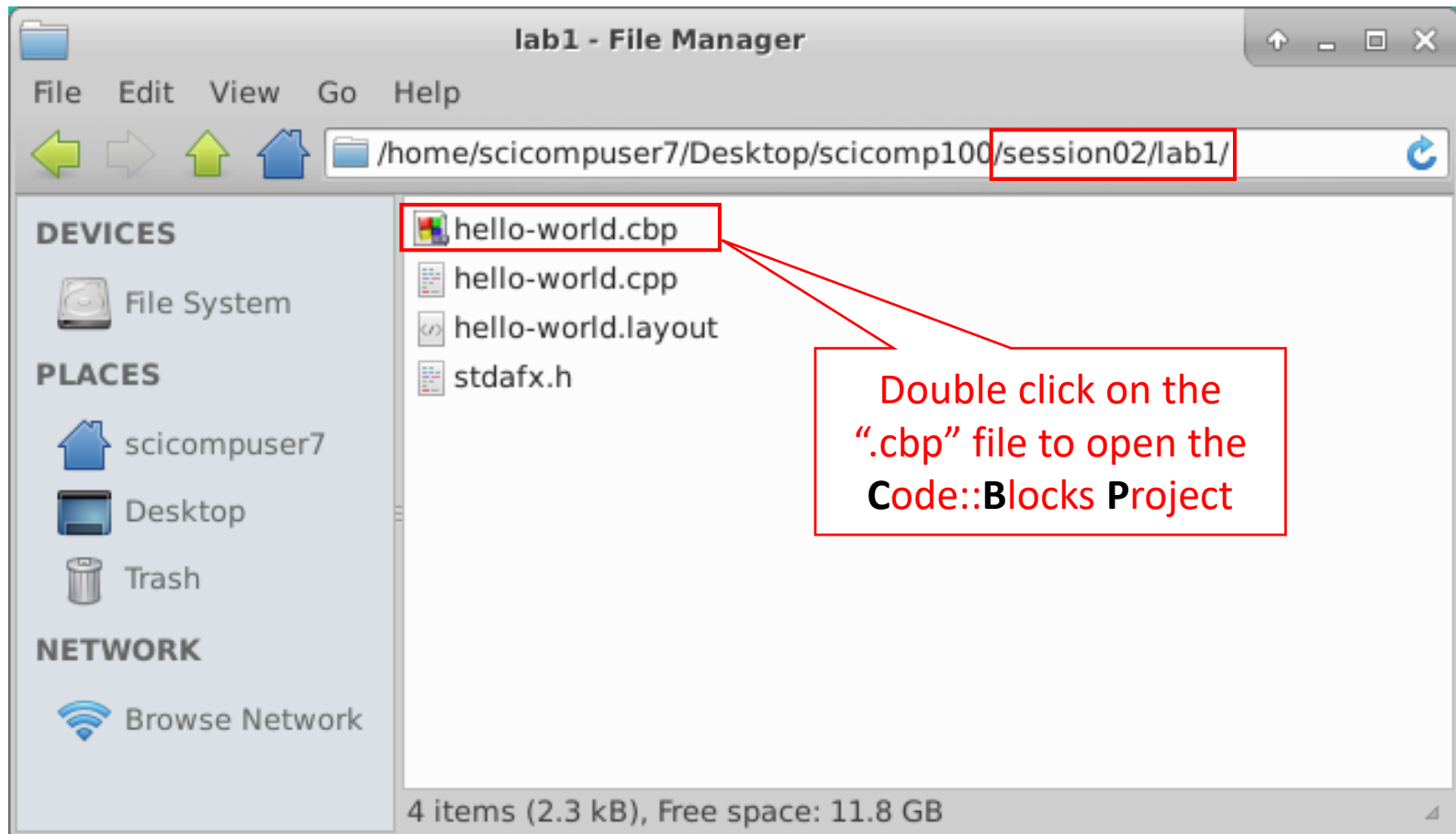
            Add_Click += button1_Click;
            person.FullName = FullName;
        }

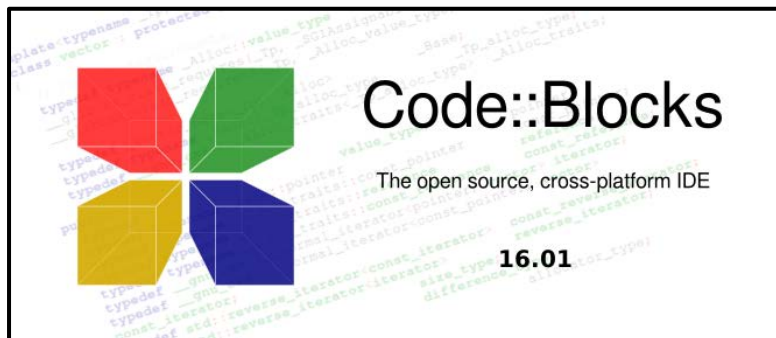
        private void button1_Click(object sender, EventArgs e)
        {
            person.FullName = FullName;
        }
    }
}
```

# Lab 1 – Hello World!



# Lab 1 – Hello World!





<http://www.codeblocks.org>

## Highlights:

- **Open Source!** GPLv3, no hidden costs.
- **Cross-platform.** Runs on Linux, Mac, Windows (uses wxWidgets).
- Written in C++. No interpreted languages or proprietary libs needed.
- Extensible through plugins

## Compiler:

- **Multiple compiler support:**
  - GCC (MingW / GNU GCC)
  - MSVC++
  - clang
  - Digital Mars
  - Borland C++ 5.5
  - Open Watcom
  - ...and more
- **Very fast** custom build system (no makefiles needed)
- Support for **parallel builds** (utilizing your CPU's extra cores)
- Multi-target projects
- Workspaces to combine multiple projects
- Inter-project dependencies inside workspace
- Imports MSVC projects and workspaces (NOTE: assembly code not supported yet)
- Imports Dev-C++ projects

## Debugger:

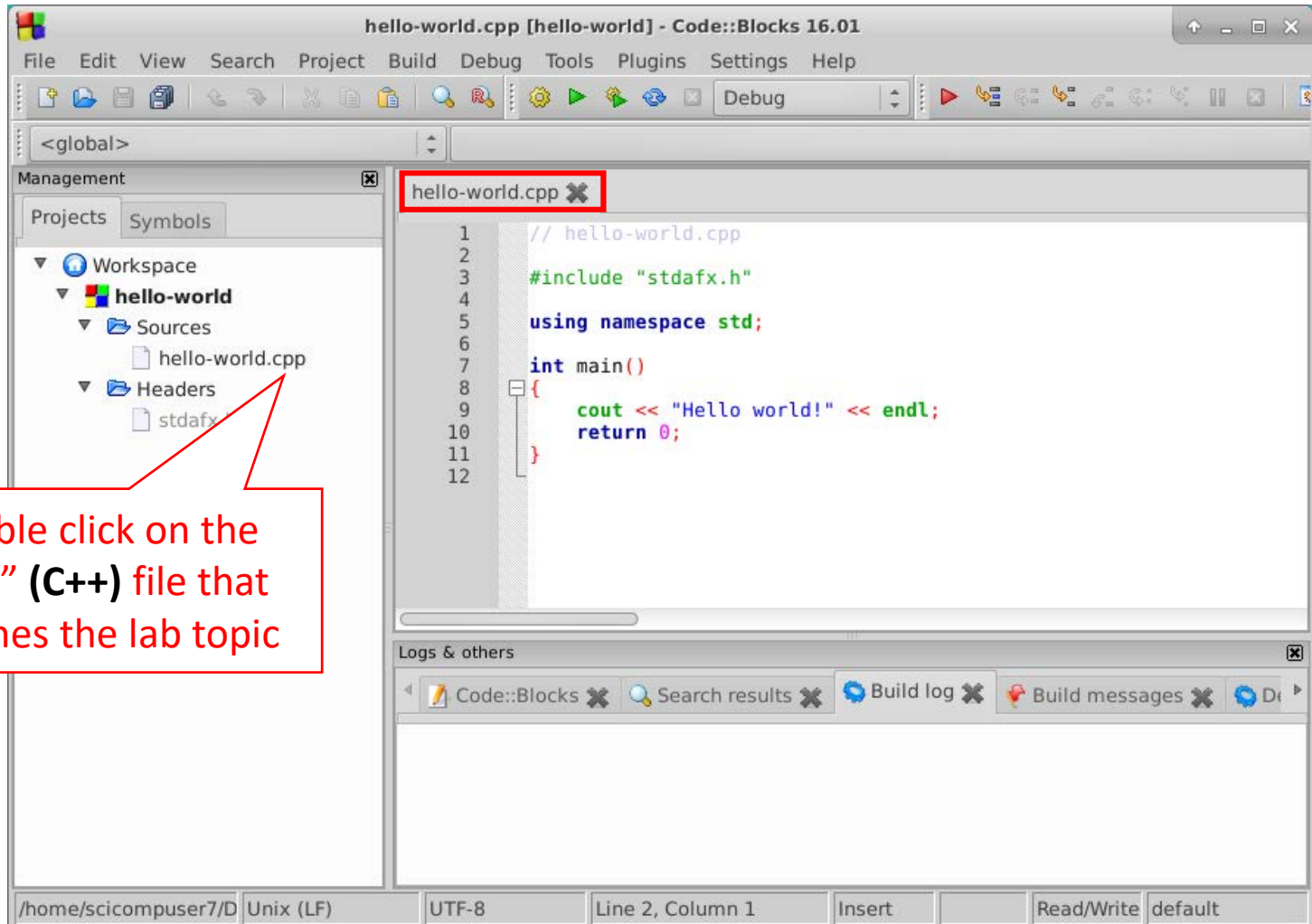
- Interfaces GNU GDB
- Also supports MS CDB (not fully featured)
- **Full breakpoints support:**
  - Code breakpoints
  - Data breakpoints (read, write and read/write)
  - Breakpoint conditions (break only when an expression is true)
  - Breakpoint ignore counts (break only after certain number of hits)
- Display local function symbols and arguments
- User-defined watches (support for watching user-defined types through scripting)
- Call stack
- Disassembly
- Custom memory dump
- Switch between threads
- View CPU registers

## Interface:

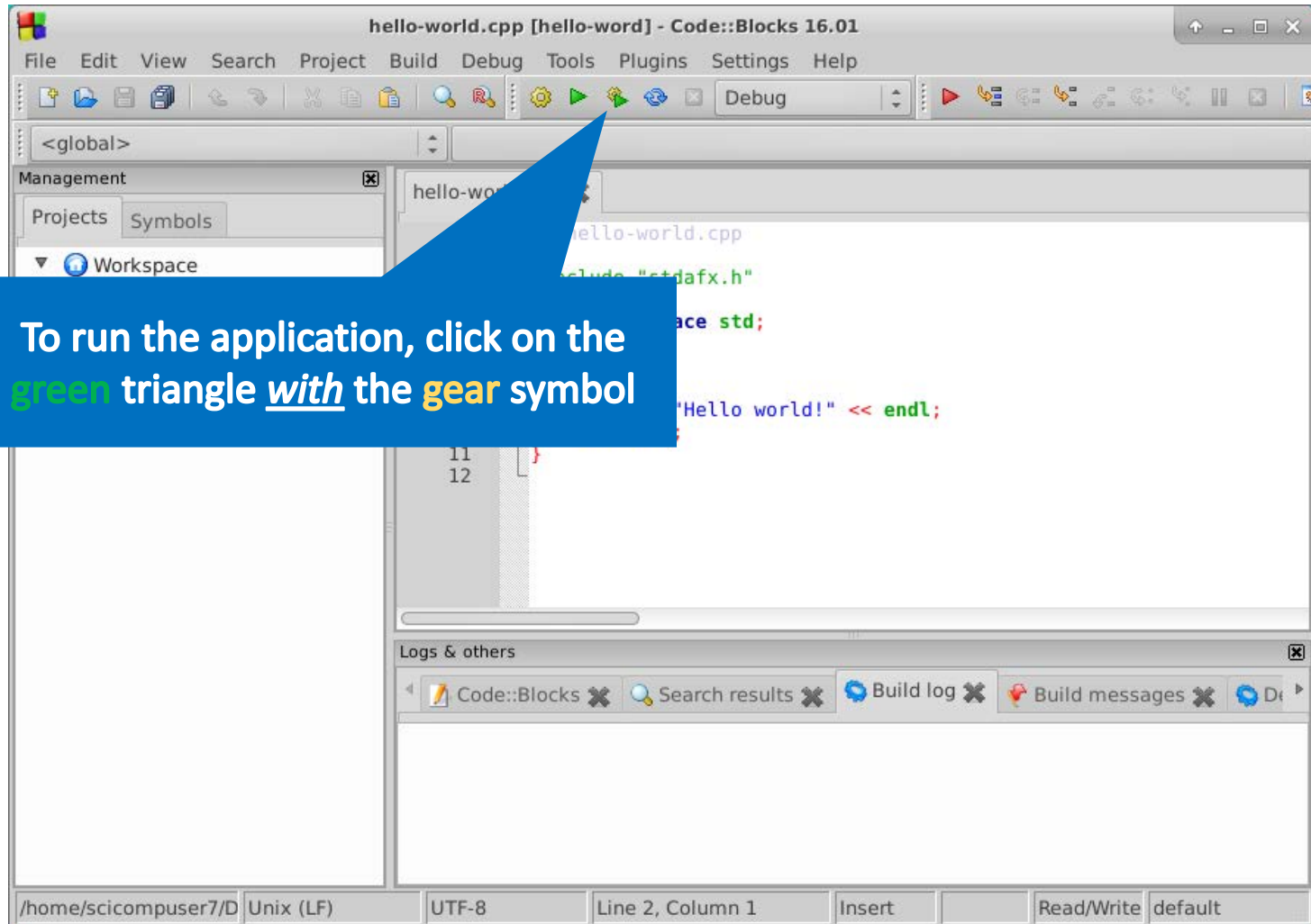
- Syntax highlighting, customizable and extensible
- Code folding for C, C++, Fortran, XML and many more files.
- Tabbed interface
- Code completion
- Class Browser
- Smart indent
- One-key swap between .h and .c/.cpp files
- Open files list for quick switching between files (optional)
- External customizable "Tools"
- To-do list management with different users



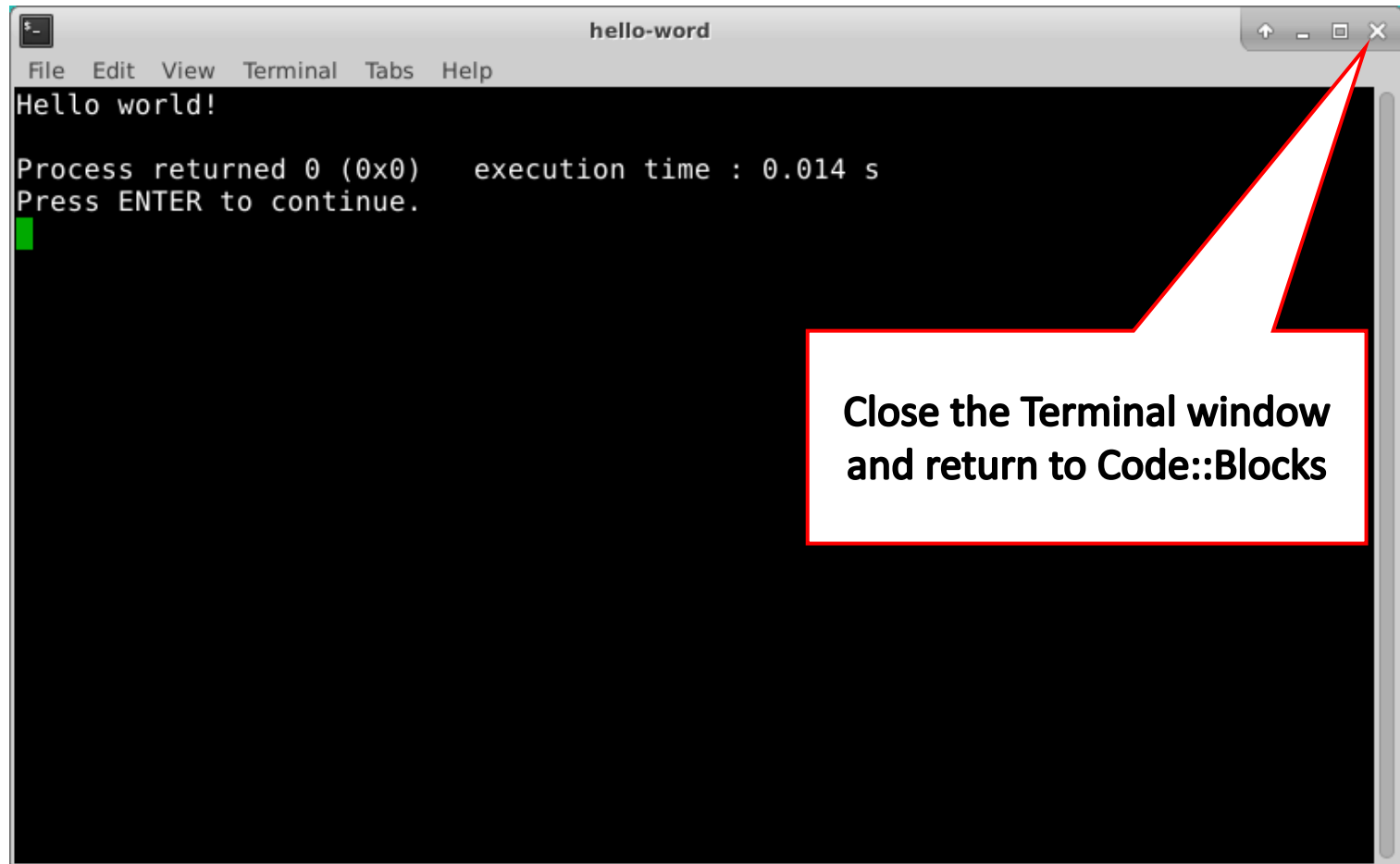
# Lab 1 – Hello World!



# Lab 1 – Hello World!



# Lab 1 – Hello World!



# Hints on Using Xfce & Code::Blocks

- Terminal = Shell = Console = Command Line
  - The shell is used to interact with character mode applications
  - Linux programmers mostly use the command line
  - Shell commands and file names are **case-sensitive**
  - Don't accumulate open **terminal windows** – close them!
- Only keep one (1) instance of **Code::Blocks** open
  - After each lab, close all open instances of Code::Blocks
  - To open a lab, be sure to double-click on the **.cbp** file (~~.cpp~~!)
- Your session will auto-logout after an hour of inactivity

# Identifiers

- Identifiers are just **names** – everything in code has a name!
  - Name must be < 64 chars in length, upper or lower case, numbers
  - Identifiers must start with a letter and cannot contain spaces!
- Three types of identifier “casing”
  1. CamelCaseEachWord (first letter is Capitalized)
  2. camelCaseEachWord (first letter is not capitalized)
  3. all lowercase (most common in C++)
- Identifiers in C++ are **case sensitive!!**
  - *n is not the same as N*
  - *Never* use ALLCAPS

# Identifiers

The diagram illustrates various identifiers in a C++ program. A central code block is surrounded by five callout boxes, each pointing to a specific identifier in the code:

- Variable Name:** Points to `ageInYears` in the line `double ageInYears = 49;`
- Function Name:** Points to `main` in the line `int main()`
- Object Name:** Points to `cout` in the line `cout.imbue(std::locale(""));`
- Method Name:** Points to `imbue` in the line `cout.imbue(std::locale(""));`
- C++ Keyword:** Points to `return` in the line `return 0;`

```
// AgeInSeconds.cpp

#include "stdafx.h"

using namespace std;

int main()
{
    double ageInYears = 49;

    double ageInSeconds =
        ageInYears * 60 * 60 * 24 * 365;

    cout.imbue(std::locale(""));
    cout << fixed << setprecision(2);

    cout << "Age (years) = "
        << ageInYears << endl;

    cout << "Age (secs) = "
        << ageInSeconds << endl;

    system("pause");
    return 0;
}
```



# Statements & Scopes

- A **statement** does something
  - A statement is either a declaration, a keyword, or a function
  - Statements are executed from top to bottom of the program
  - **Statements must be terminated with a semicolon!!**
- A **scope** contains one or more statements
  - A scope with **more than one statement** must be enclosed within open (left) and close (right) curly braces **}**
  - If you only want one statement in a scope, you don't need **}**
  - Scopes can be *nested* – each inner scope is further indented
  - Scope braces are like parenthesis – they must be balanced!
  - **You don't need a ; after a closing right brace }**

# Scopes

Opening of  
Scope

```
// AgeInSeconds.cpp

#include "stdafx.h"

using namespace std;

int main()
{
    double ageInYears = 49;

    double ageInSeconds =
        ageInYears * 60 * 60 * 24 * 365;

    cout.imbue(std::locale(""));
    cout << fixed << setprecision(2);

    cout << "Age (years) = "
        << ageInYears << endl;

    cout << "Age (secs) = "
        << ageInSeconds << endl;

    system("pause");
    return 0;
}
```

Statements are  
terminated with  
a semicolon ;

Closing of  
Scope

No semicolon needed  
after close of scope }

# Variable Types

- **Variables** store data in memory to be used later
  - Variables can be called whatever you want
  - Create variable names that mean something to a programmer
  - Use **camelCase #2** (first letter is lower case)
- Intrinsic (built-in) **types** for variables:
  - **int** = Stores integers (−2,147,483,648 to 2,147,483,647)
  - **double** = Stores real numbers with 15 digits of precision
  - **bool** = Stores “true” or “false” (Boolean data type)
  - **string** = Stores zero or more letters & numbers

# Creating a Variable

- You must **declare** and **define** a variable before you can use it
- **Declaring** a variable means to specify a type for an identifier
  - The data type always *precedes* the name of the variable
  - You can **declare** a variable **only once** per scope
- **Defining** a variable means to give it a specific value
  - The value type must match the variable type
  - You can **define** a variable **multiple times** per scope

```
int totalVotes = 123;  
double hourlyPay = 9.75;  
string firstName = "Dave";
```

# Operators

- C++ operators obey normal **PEMDAS** precedence
  - Expressions are evaluated left to right in your source code
  - Use **=** to assign a value to a variable
  - Use **\*** for multiplication and **/** for division operators
  - Use parenthesis to explicit specify the order of operations
  - “Greater than or equal to” operator is **>=**
  - “Less than or equal to” is operator **<=**

```
double degC = (degF - 32) * 5. / 9;
```

The period (decimal point) forces the numerator to be evaluated as a **double**

# Displaying Variables

- **cout** is used to display the value of variables
  - Represents “console output” (pronounced see-out, not coot)
  - The variables to display follow the stream **insertion operator** `<<`
  - Don’t forget the first and last quotation marks for literals!
- To specify the # of digits to show to **right** of decimal point:  

```
cout << fixed << setprecision(2);
```
- To **right justify** a column:  

```
cout << setw(7) << right;
```
- To adopt local language preference for digit separators:  

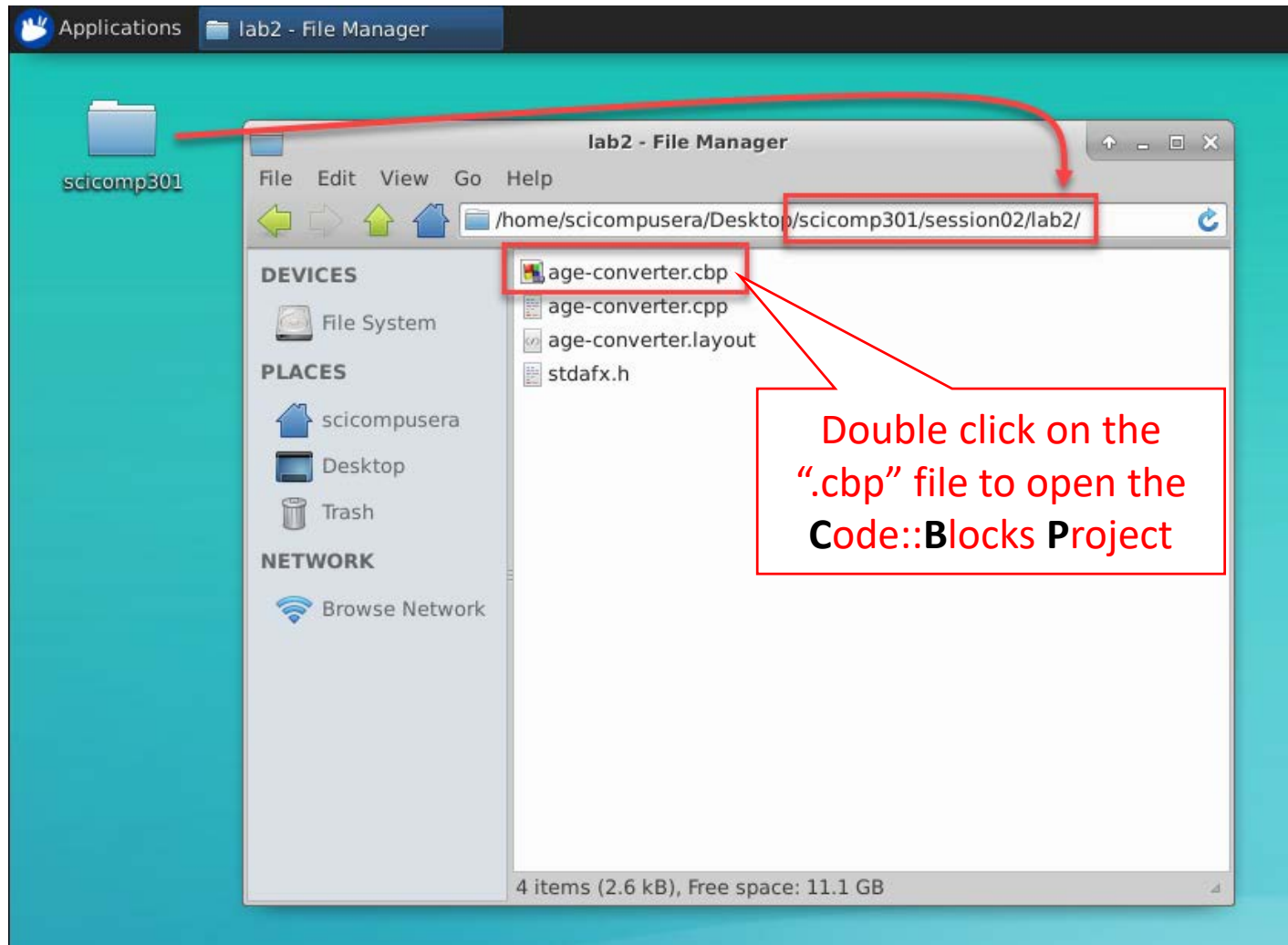
```
cout.imbue(std::locale(""));
```



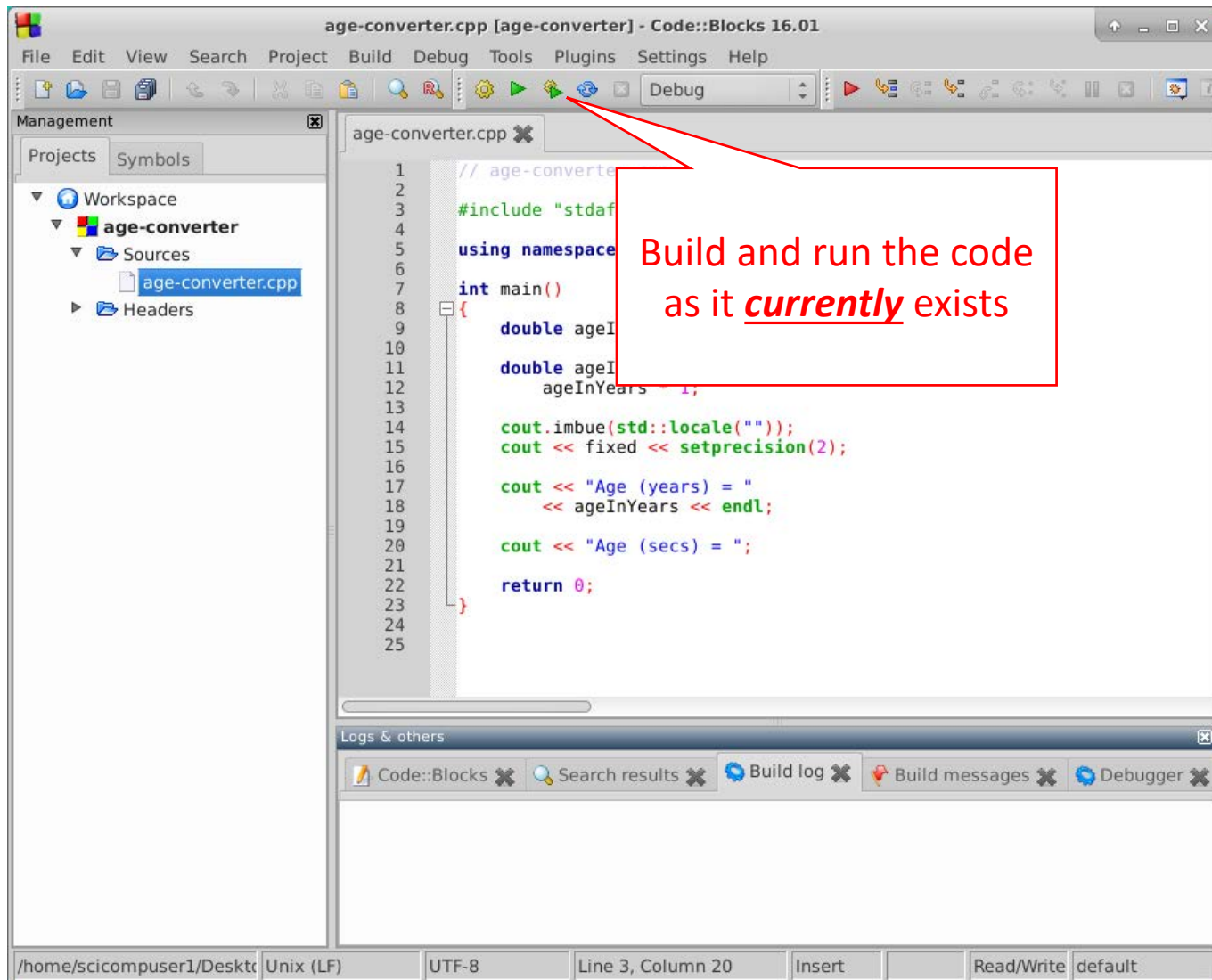
## Lab 2 – My Age In Seconds

- Your scientist has asked you to fix an existing buggy C++ console application using Code::Blocks
- Initialize a variable to hold your current age in years
- Develop and implement an equation that performs the correct **dimensional analysis** (factor label method) to convert years to seconds
- There is no need to accommodate **leap years** in the equation
- Display in the terminal window both your age in years *and* your age in seconds

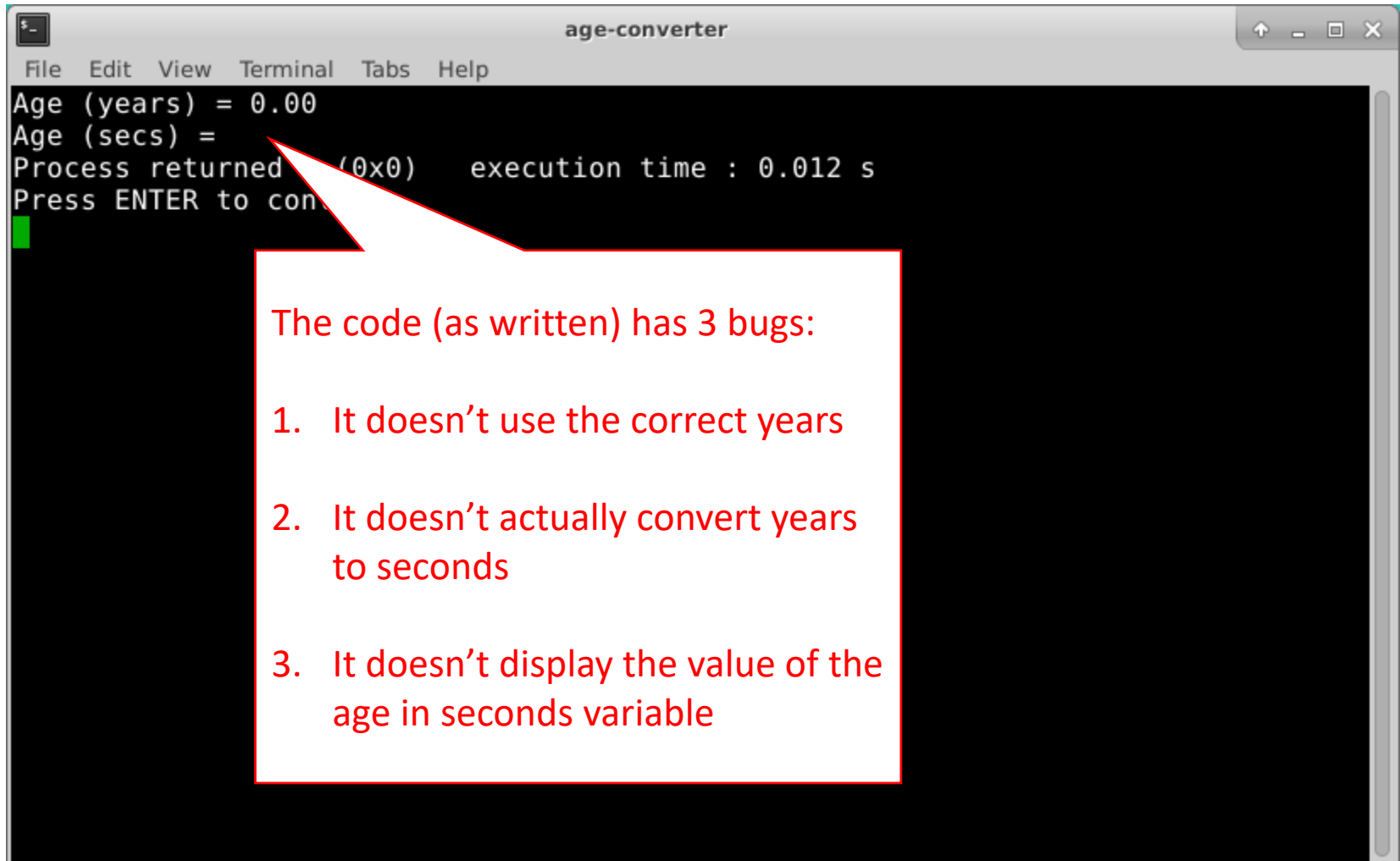
# Lab 2 – My Age In Seconds



# Lab 2 – My Age In Seconds



# Lab 2 – My Age In Seconds



The screenshot shows a terminal window with the title 'age-converter'. The output of the program is as follows:

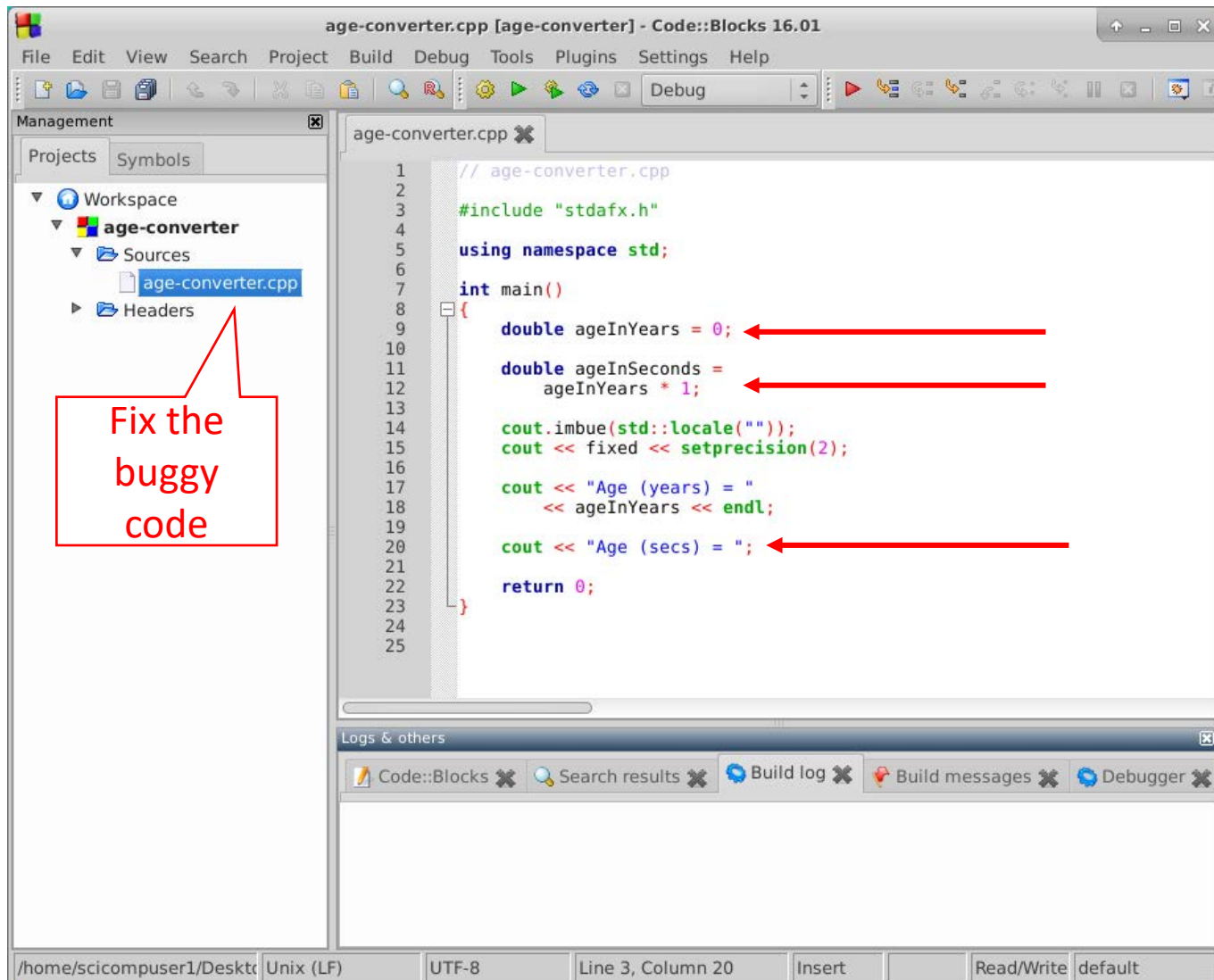
```
Age (years) = 0.00
Age (secs) =
Process returned (0x0)   execution time : 0.012 s
Press ENTER to con
```

A green cursor is visible on the line 'Press ENTER to con'. A red callout box points to the output and contains the following text:

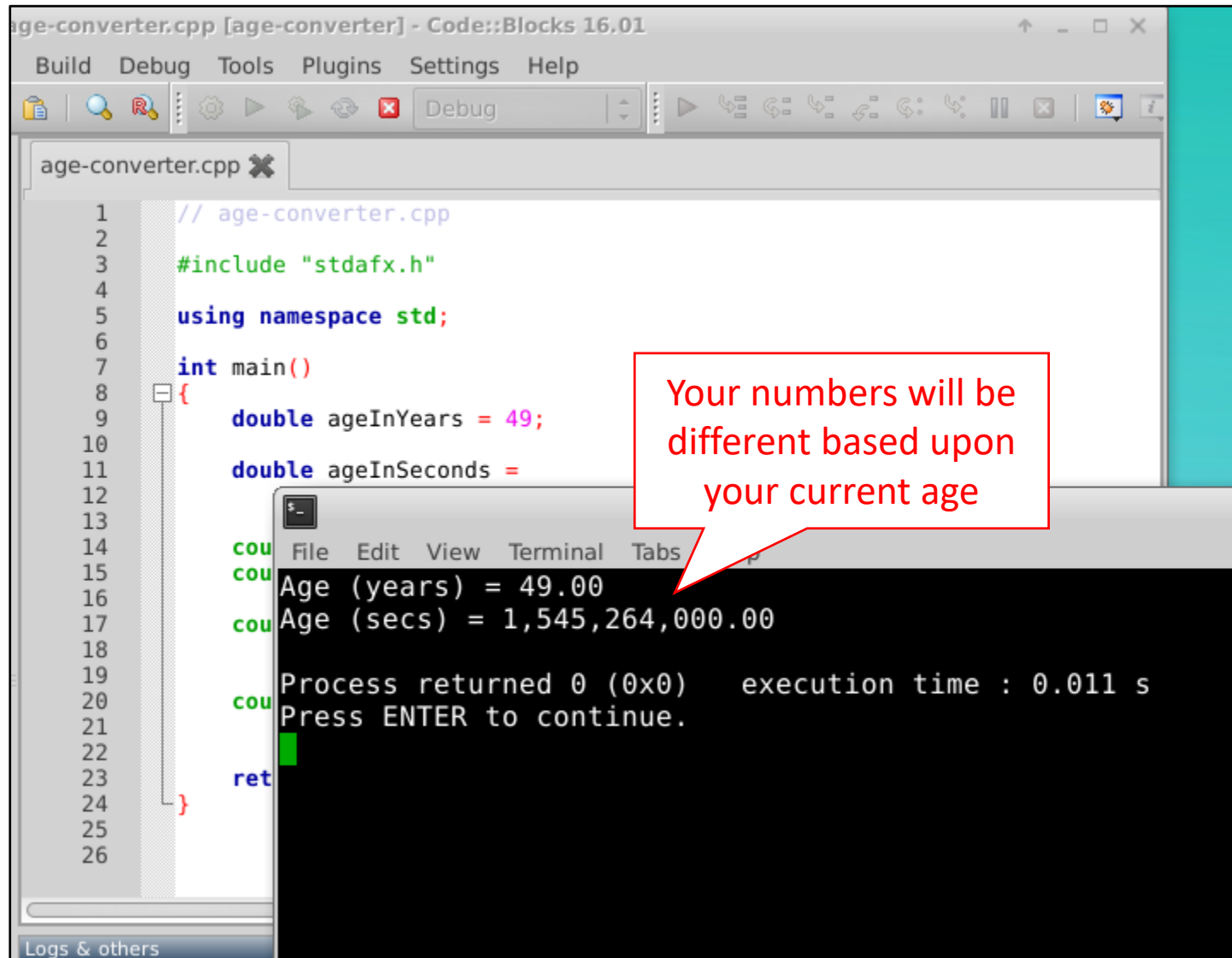
The code (as written) has 3 bugs:

1. It doesn't use the correct years
2. It doesn't actually convert years to seconds
3. It doesn't display the value of the age in seconds variable

# Lab 2 – My Age In Seconds



# Lab 2 – My Age In Seconds



The screenshot shows a C++ IDE with the file 'age-converter.cpp' open. The code is as follows:

```
1 // age-converter.cpp
2
3 #include "stdafx.h"
4
5 using namespace std;
6
7 int main()
8 {
9     double ageInYears = 49;
10
11     double ageInSeconds =
12
13
14     cout << "Age (years) = 49.00" << endl;
15     cout << "Age (secs) = 1,545,264,000.00" << endl;
16
17     Process returned 0 (0x0)    execution time : 0.011 s
18
19     Press ENTER to continue.
20
21
22
23     ret
24 }
25
26
```

The terminal output shows the program's execution results:

```
Age (years) = 49.00
Age (secs) = 1,545,264,000.00

Process returned 0 (0x0)    execution time : 0.011 s
Press ENTER to continue.
```

A red speech bubble points to the terminal output, stating: "Your numbers will be different based upon your current age".



# for() Loops

- **for()** loops execute all the statements within their scope as long as the 2<sup>nd</sup> part of the loop definition remains **true**

```
// Sum the numbers 1 to 10
double sum = 0;
for (double n = 1; n <= 10; n = n + 1)
{
    sum = sum + n;
}
```



The 3-part loop definition

- The three parts of the **for()** loop definition are:
  1. A statement to **declare the loop counter** variable
  2. A Boolean condition to define **how long** the loop should run
  3. An iterator statement to **adjust the loop counter** after each pass

## Lab 3 –Temperature Converter

- Fix the code to calculate the correct Celsius temperature for a given Fahrenheit temperature
- Display values between **-44°F** and **216°F** *inclusive*
- Your code should increment in steps of **4°F**
- The research question your scientists wants you to solve:

What is the **one temperate that is the same**  
in both Fahrenheit and Celsius?

# Lab 3 – Temperature Converter

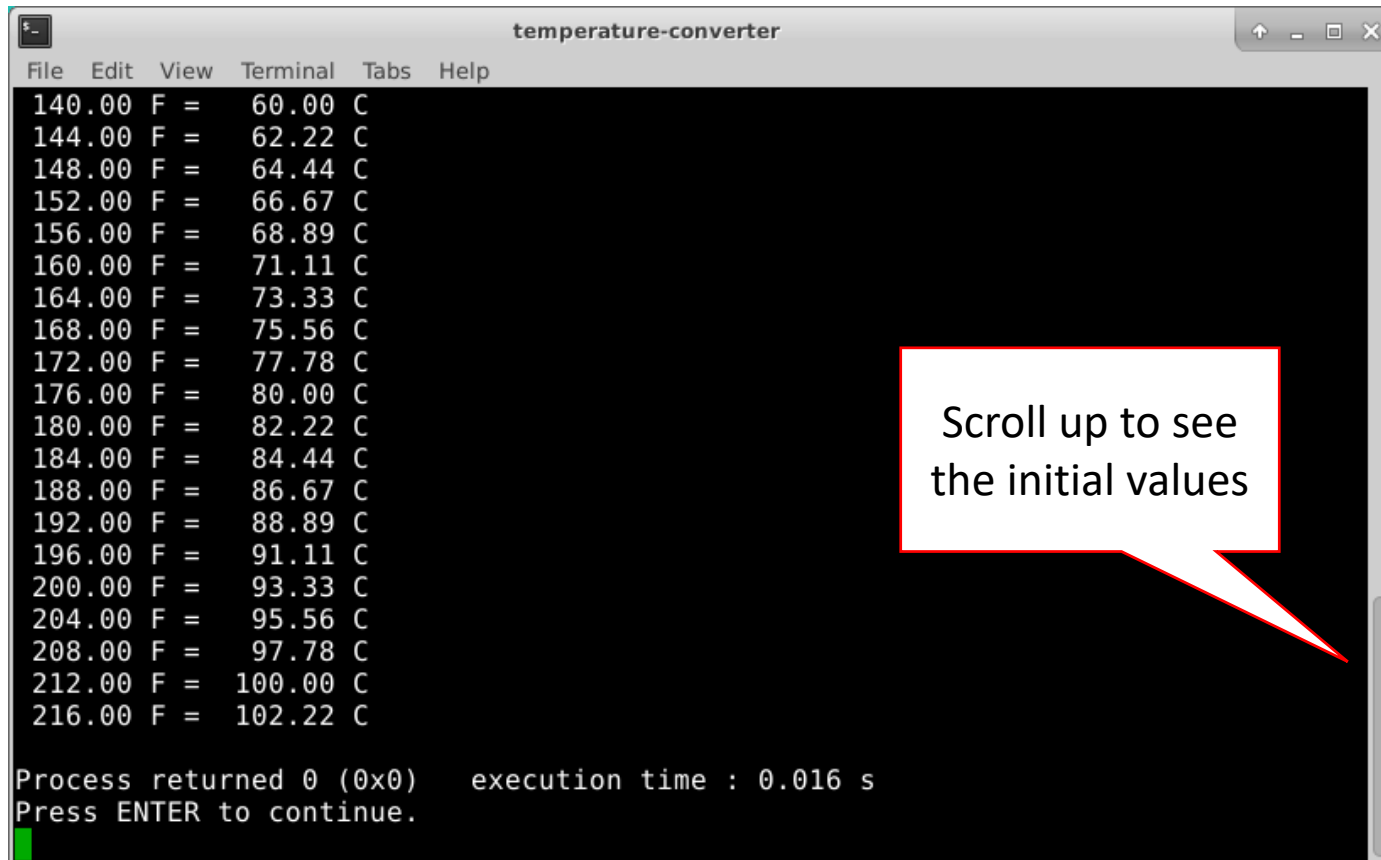
The screenshot shows a C++ code editor window titled "temperature-converter.cpp [temperature-converter] - Code::Blocks 16.01". The code is as follows:

```
1 // temperature-converter.cpp
2
3 #include "stdafx.h"
4
5 using namespace std;
6
7 int main()
8 {
9     cout.imbue(std::locale(""));
10    cout << fixed << setprecision(2);
11
12    for (double degF{ -44 }; degF <= 216; degF += 4) {
13
14        double degC = 0;
15
16        cout << setw(7) << right << degF << " F = "
17        << setw(7) << right << degC << " C"
18        << endl;
19    }
20    return 0;
21 }
```

Annotations in red boxes with arrows pointing to the code:

- Box 1: "Same as degF = 44" points to the initial value `-44` in the `for` loop.
- Box 2: "Same as degF = degF + 4" points to the increment `degF += 4` in the `for` loop.
- Box 3: "Set next column width" points to the `setw(7)` in the `cout` statement.
- Box 4: "Right justify next column" points to the `right` manipulator in the `cout` statement.

# Lab 3 – Temperature Converter



```
temperature-converter
File Edit View Terminal Tabs Help
140.00 F = 60.00 C
144.00 F = 62.22 C
148.00 F = 64.44 C
152.00 F = 66.67 C
156.00 F = 68.89 C
160.00 F = 71.11 C
164.00 F = 73.33 C
168.00 F = 75.56 C
172.00 F = 77.78 C
176.00 F = 80.00 C
180.00 F = 82.22 C
184.00 F = 84.44 C
188.00 F = 86.67 C
192.00 F = 88.89 C
196.00 F = 91.11 C
200.00 F = 93.33 C
204.00 F = 95.56 C
208.00 F = 97.78 C
212.00 F = 100.00 C
216.00 F = 102.22 C

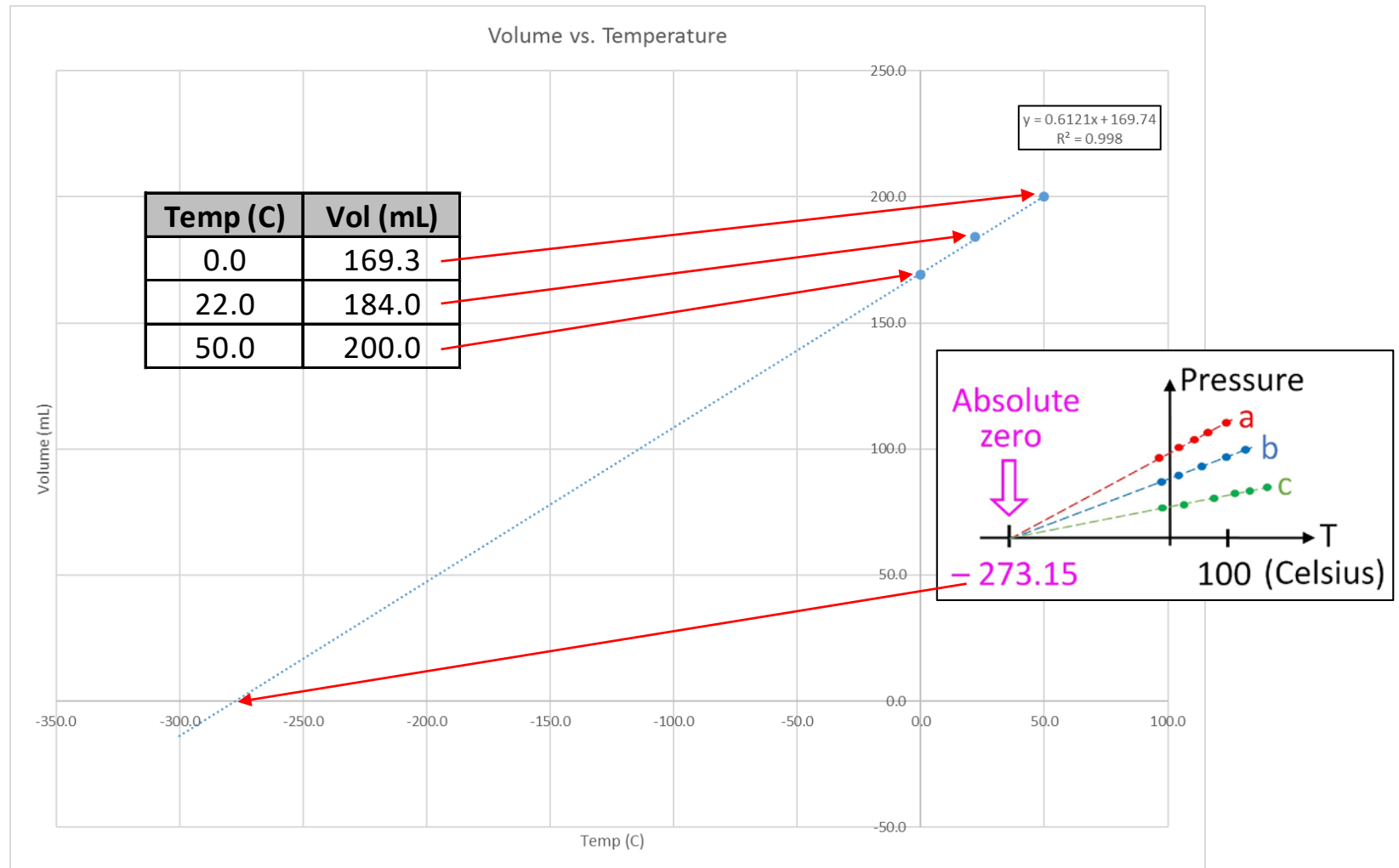
Process returned 0 (0x0)   execution time : 0.016 s
Press ENTER to continue.
```

Scroll up to see the initial values

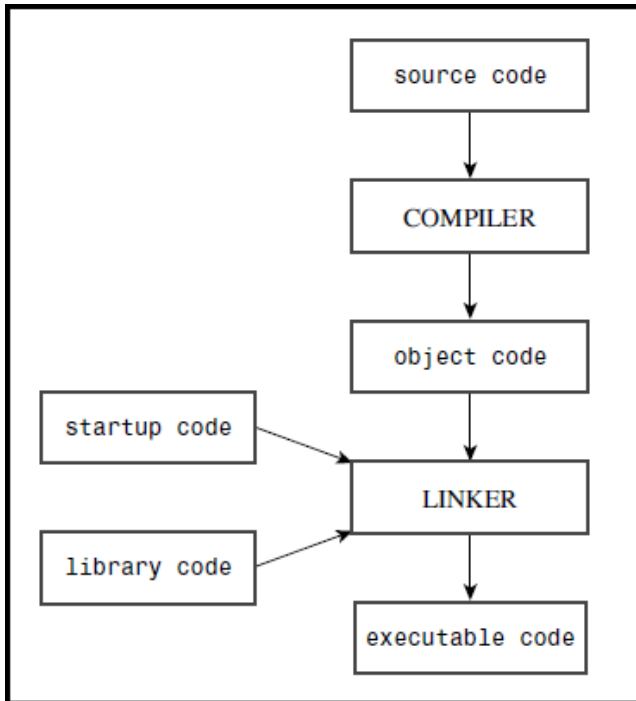
What is the **one temperate that is the same**  
in both Fahrenheit and Celsius?

# How did we calculate absolute zero in 1779?

( $PV = nRT$ )



# C++ Build Process



.h	header files - function declarations
.cpp	function definitions
.obj	output of compiler
.lib	output of linker - static library, embedded in final EXE
.dll	Windows shared object - dynamic link library
.exe	Windows executable - final output of linker

Header File Naming Conventions			
Kind of Header	Convention	Example	Comments
C++ old style	Ends in .h	iostream.h	Usable by C++ programs
C old style	Ends in .h	math.h	Usable by C and C++ programs
C++ new style	No extension	iostream	Usable by C++ programs, uses namespace std
Converted C	c prefix, no extension	cmath	Usable by C++ programs, might use non-C features, such as namespace std

A header between <> brackets (preferred) adds symbols to the compiler's **std** namespace, not the user's global namespace like "header.h" will



# Now you know...

- How to access your remote Amazon PC
- Linux with Xfce is quite similar to Microsoft Windows
- How to create and open a Code::Blocks project
- How to build & run a C++ console (shell) application
- The C++ build process is two phases: **compiling** then **linking**
- How to log out of your Linux (Ubuntu) desktop session

# Now you know...

- Rules for identifier casing
- C++ intrinsic **data types**
- Declaring and defining variables
- Statements and scopes **{}**
- Operators & Precedence
- Assignment Operator
- How to write messages and variables to the console window
- **for()** loops
- $-40^{\circ} \text{ F} = -40^{\circ} \text{ C}$
- Absolute Zero =  $-273.15^{\circ} \text{ C}$