ECE/ME/EMA/CS 759
High Performance Computing for Engineering Applications

Fall 2013

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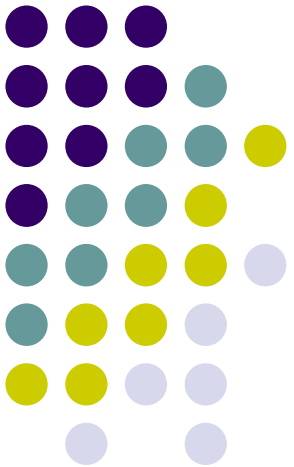
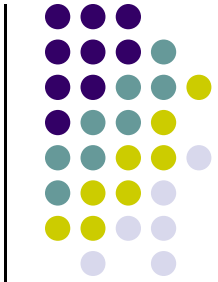
Department of Mechanical Engineering
University of Wisconsin, Madison

September 4, 2013



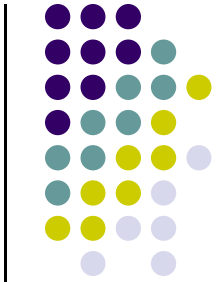
"I think there is a world market for maybe five computers."
T. J. Watson, chairman of IBM, 1943.



- Purpose of today's lecture
  - Get a 30,000 perspective on this class and understand whether this is a class worth taking

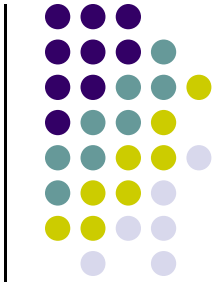
- What we will cover today
  - Course logistics
  - Brief overview of syllabus
  - Motivation and central themes of this class
  - Start quick overview of C programming language

Instructor: Dan Negrut



- Polytechnic Institute of Bucharest, Romania
  - B.S. – Aerospace Engineering (1992)
- University of Iowa
  - Ph.D. – Mechanical Engineering (1998)
- MSC.Software
  - Product Development Engineer 1998-2005
- University of Michigan
  - Adjunct Assistant Professor, Dept. of Mathematics (2004)
- Division of Mathematics and Computer Science, Argonne National Laboratory
  - Visiting Scientist 2004-2005, 2006, 2010
- University of Wisconsin-Madison, Joined in Nov. 2005
  - Research Focus: Computational Dynamics (Dynamics of Multi-body Systems)
  - Established the Simulation-Based Engineering Lab (http://sbel.wisc.edu)

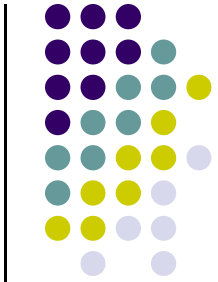
Acknowledgements



- Students helping with this class
  - Ang Li [grader]
  - Andrew Seidl [takes care of hardware and software]
  - Hammad Mazhar [help with CUDA & thrust]

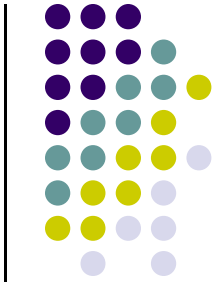
- NVIDIA, AMD & US Army ARO:
  - Financial support to build Euler, CPU/GPU cluster used in this class

Good to know…



- **Time** 8:00-9:15 AM Mo & Wd & Fr
- **Location** 2121ME
- **Office** 2035ME
- **Phone** 608 890-0914
- **E-Mail** negrut@engr.wisc.edu
- **Course Webpage** http://sbel.wisc.edu/Courses/ME964/2013/index.htm
- **Grades reported at:** learnuw.wisc.edu
- **ME759 Forum:** http://sbel.wisc.edu/Forum/viewforum.php?f=15

ME 759 Fall 2013

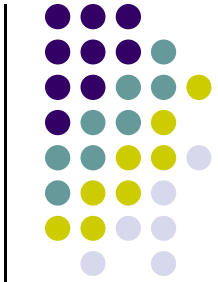


- Office Hours:
  - Monday 2 – 3:30 PM
  - Friday 2 – 3:30 PM

- Call or email to arrange for meetings outside office hours

- Walk-ins are fine as long as they are in the afternoon

References

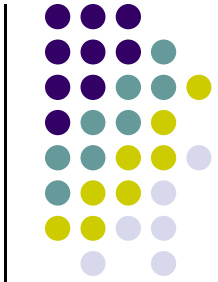


- No textbook is required, but there are some recommended ones:

- **Highly recommended**

  - NVIDIA CUDA C Programming Guide V5.5, 2013
  - R. Bryant and D. O'Hallaron, Computer Systems: A Programmer's Perspective, Prentice Hall, 2nd Edition, 2011
  - Jason Sanders and Edward Kandrot: CUDA by Example: An Introduction to General-Purpose GPU Programming, Addison-Wesley Professional, 2010 (on reserve, Wendt Lib.)
  - David B. Kirk and Wen-mei W. Hwu: Programming Massively Parallel Processors: A Hands-on Approach, Morgan Kaufmann, 2010 (on reserve, Wendt Lib.)
  - Peter Pacheco: An Introduction to Parallel Programming, Morgan Kaufmann, 2011
  - B. Kernighan and D. Ritchie, The C Programming Language
  - B. Stroustrup, The C++ Programming Language, Third Edition

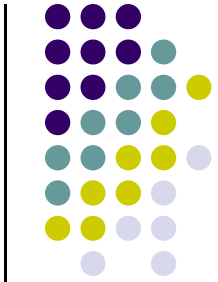
References [Cntd.]



- **Further reading**

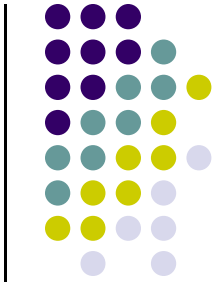
- D. Negrut, Primer: Elements of Processor Architecture. The Hardware/Software Interplay, available on class website
- Wen-mei W. Hwu (editor), GPU Gems 4, 2011, Addison Wesley
- Rob Farber: CUDA Application Design and Development, Morgan Kaufmann 2011
- H. Nguyen (editor), GPU Gems 3, Addison Wesley, 2007 (on reserve, Wendt Lib.)
- Peter Pacheco: Parallel Programming with MPI, Morgan Kaufmann, 1996
- T. Mattson, et al.: Patterns for Parallel Programming, Addison Wesley, 2005
- Michael J. Quinn: Parallel Programming in C with MPI and OpenMP, McGraw Hill, 2003
- A. Grama, A. Gupta, G. Karypis, V. Kumar: Introduction to Parallel Computing, Addison Wesley, 2003

Course Related Information



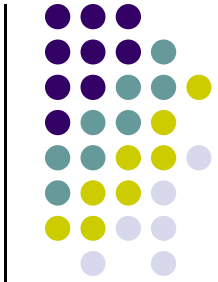
- This course is offered on an accelerated track
- Three lectures per week, each 75 minutes long
- Last lecture: November 8
  - 29 lectures total, just like a regular semester yet compressed in two months
- No class after November 8
  - I will still have office hours
  - Homework will continue to be assigned on a weekly schedule past Nov. 8
- Motivation:
  - It'll give us more than one month to work on a meaningful Final Project
    - More on this later

Course Related Information



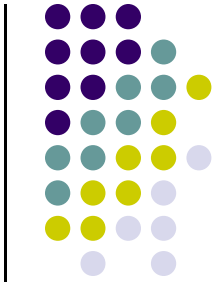
- Handouts will be printed out and provided before each lecture
- Lecture material (PDF and audio) will be made available online at class website
- Looking into retrieving videos of this class (Spring 2012 edition)
- Grades will be maintained online at Learn@UW
- Syllabus will be updated as we go
  - It will contain info about
    - Topics we cover
    - Homework assignments
  - Available at the course website
    - http://sbel.wisc.edu/Courses/ME964/2013/

The 964 Issue



- Class first taught in 2008
- Called ME964
- 900-level classes are experimental, need to change to 700 format
- Now cross-listed in ME, ECE, EMA, and CS as 759
- All old websites, links, forum, etc. – still reference the 964 number
- Apologies for any confusion this might cause

Grading

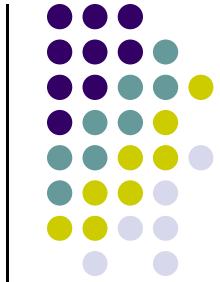


• Homework	40%
• Midterm Exam	15%
• Midterm Project	15%
• Final Project	25%
• Course Participation	5%
• Total	100%

NOTE:

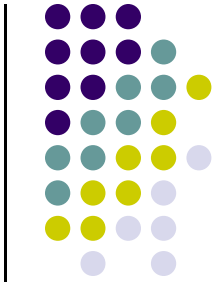
- Score related questions (homework/exam) must be raised prior to next class after the homework/exam is returned.

Homework Policies



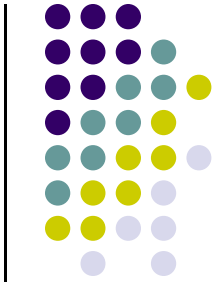
- There will be 12 HWs assigned
  - No late HW accepted
    - HW due at 11:59 PM on the due day
- The assignments with two lowest scores will be dropped when computing final score
- Homework and projects should be handed in using Learn@UW dropbox
  - There will be a window when you can submit your homework
- This class is hard because of the assignments. Very time consuming

Midterm Exam



- One midterm exam only, accounts for 15% of final grade
- Scheduled during regular class hours
- Tentatively scheduled on **November 8**
  - Review offered the day before, time/location TBA
- Doesn't require use of a computer (it's a pen and paper exam)
- It's a "closed books" exam
- Covers the entire material discussed in class up to that point

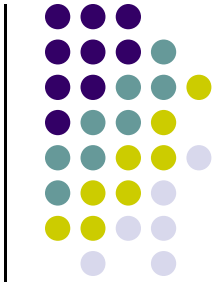
Midterm Project



- Has to do with implementation of a parallel solution for solving a large *dense* banded system of equations
  - Size: as high as you can go
  - Implemented in CUDA
  - Focus on banded matrices

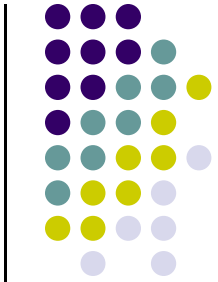
- Due on **November 15** at 11:59 PM
- Accounts for 15% of final grade
- Project is individual or produced by two-student teams
- Should contain a comparison of your parallel code with solvers that are available already in the Scientific Computing community
  - Intel MKL, LAPACK, Pardiso, etc,
- Should include profiling results and a weak scaling analysis

Final ~~Exam~~ Project



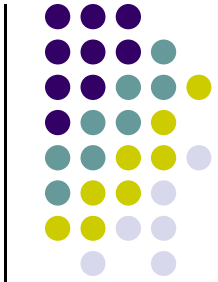
- There will be no final exam but rather a Final Project
- The Final Project is due on at 11:59 PM on the Monday of the finals week
- Each student/team will present the project in a 30 minute time slot
- Presentation time slots will be posted in doodle for you to choose a convenient one

~~Final Exam~~ Project



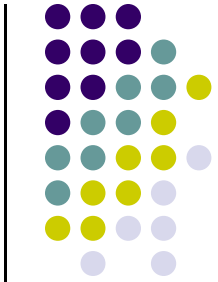
- Final Project (accounts for 25% of final grade):
  - It is an individual project or produced by a two-student team
  - You choose a problem that suites your research or interests
  - You are encouraged to tackle a meaningful problem
    - Attempt to solve a useful problem rather than a problem that you are confident that you can solve
    - Projects that are not successful are ok, provided you aim high enough and demonstrate good work
    - Continuing the Midterm Project topic is ok (shifting focus on sparse systems)
  - Work on Final Project starts on Nov. 15 after submitting project proposal

Class Participation



- Accounts for 5% of final grade. To earn the 5%, you must:
  - Contribute at least five meaningful posts on the class Forum
    - Forum is live at: http://sbel.wisc.edu/Forum/index.php?board=15.0
    - Forum meant to serve as a quick way to answer some of your questions by instructor and other 759 colleagues
    - You should get an email with login info shortly (today or tomorrow)

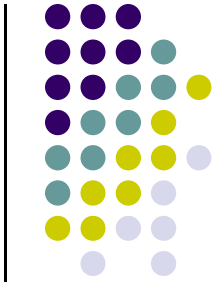
Scores and Grades



Score	Grade
92-100	A
86-91	AB
78-85	B
70-77	BC
60-69	C
50-59	D

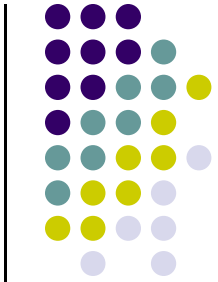
- Grading will not be done on a curve
- Final score will be rounded to the nearest integer prior to having a letter assigned
  - Example:
    - 85.59 becomes AB
    - 85.27 becomes B

Prerequisites



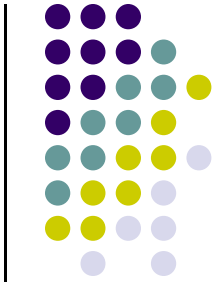
- This is a high-level graduate class in a very fluid topic
- Familiarity with C is needed
  - You can probably be fine if you are a friend of Java
- Decent programming skills are necessary
  - Understanding pointers
  - Being able to wrestle with a compile error on your own
  - Having used a debugger
  - Having used a profiler

Rules of Engagement



- You are encouraged to discuss assignments with other class students
  - Post and read posts on Forum
- Getting **verbal** advice and suggestions from anybody is fine
- copy/paste of non-trivial code is not acceptable
  - Non-trivial = more than a line or so
  - Includes reading someone else's code and then going off to write your own
- Use of third party libraries that directly implement the solution of a HW/Project is not acceptable unless explicitly asked to do so

A Word on Hardware…

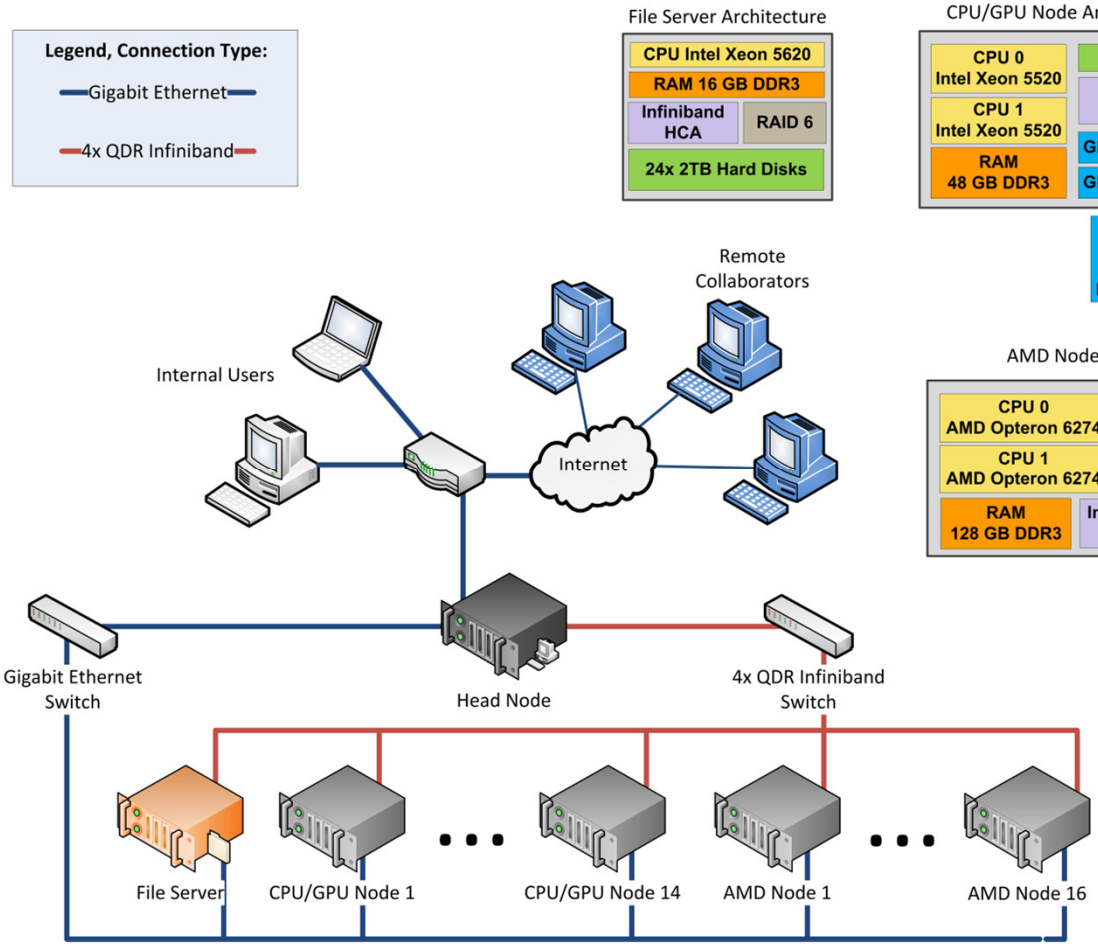


- The course designed to leverage a dedicated CPU/GPU cluster
  - Called Euler

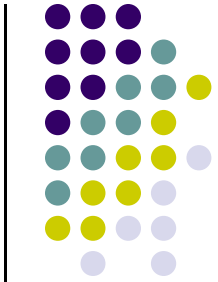
- Each student receives an individual account that will be used for
  - GPU computing
  - MPI-enabled parallel computing
  - OpenMP multi-core computing

- Advice: if possible, do all the programming on a local machine. Move to Euler for “production” runs

ME759
Heterogeneous Cluster

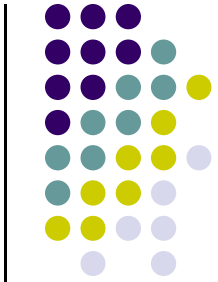


ME759
Heterogeneous Cluster



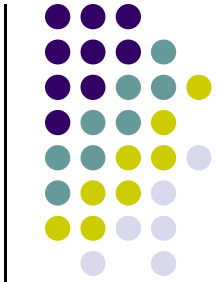
- More than 50,000 GPU scalar processors
- More than 1,200 CPU cores
- Fast Mellanox Infiniband Interconnect (QDR), 40Gb/sec
- About 2.7 TB of RAM
- More than 20 Tflops Double Precision

A Word on Software…



- We will use Linux as our operating system of choice
  - Euler runs Linux
- We'll use the following versions of libraries/releases:
  - CUDA: 5.0
  - MPI: 2.0
  - OpenMP: 3.0
- Reliance on makefiles generated with CMake, a build utility tool
  - Scripts will be available to you in order to facilitate compile/link/debug/profile process
- We will use a suite of debugging and profiling tools
  - gdb: debugger under Linux
  - cuda-gdb: debugger for CUDA applications running on the GPU
  - NVIDIA Profiler: Nsight
- Most of these tools are embedded in Eclipse
  - OK to work under Windows, yet make sure your code compiles/runs on Euler before submitting

Staying in Touch…

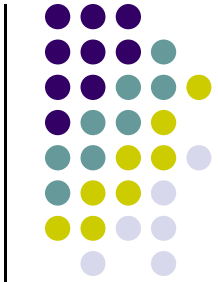


- Please do not email me unless you have a personal problem
  - Examples:
    - Good: Schedule a one-on-one meeting outside office hours
    - Bad: Asking me clarifications on Problem 2 of the current assignment (this needs to be on the Forum)
    - Bad: telling me that you can't compile your code (this should also go to the Forum)

- Any course-related question should be posted on the Forum
  - I continuously monitor the Forum
  - If you can answer a Forum post, please do so (counts towards your 5% class participation and helps me as well)
  - Keeps all of us on the same page

- The forum is *very* useful

Course Emphasis

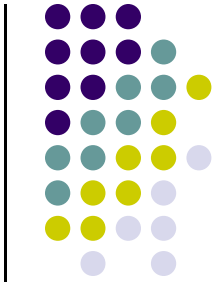


- There are multiple choices when it comes to implementing parallelism
  - PThreads, Intel's TBB, OpenMP, MPI, Ct, Cilk, CUDA, etc.

- Course focuses on parallelism enabled by
  - The Graphics Processing Unit (GPU), mostly aimed at fine grain level parallelism
  - OpenMP standard, aimed both at fine and coarse level parallelism
  - Message Passing Interface (MPI) standard, aimed at coarse grain parallelism

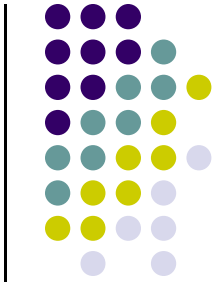
- This is not going to be a hard course but it'll be a very busy course
  - You'll easily understand all the material that we'll cover (no rocket science)
  - The assignments are going to be time consuming
    - Writing software is time consuming
    - Writing parallel computing software adds insult to injury

Course Objectives



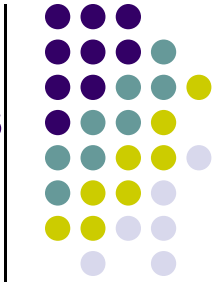
- Get familiar with today's High-Performance Computing (HPC) software and hardware
  - Usually "high-performance" implies execution on parallel architectures; i.e., architectures that have the potential to finish a run much faster than when the same application is executed sequentially
- Help you recognize applications/problems that can draw on HPC
- Help you gain basic skills that will help you map these applications onto a parallel computing hardware/software stack
  - Write code, build, link, run, debug, profile
- Introduce basic software design patterns for parallel computing

Course Objectives
[Cntd.]



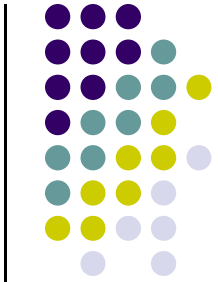
- What I'll try to accomplish
  - Provide enough information for you to start writing software that can leverage parallel computing to hopefully reduce the amount of time required by your simulations to complete
- What I will not attempt to do
  - Investigate how to design new parallel computing languages or language features, compilers, how new hardware should be designed, etc.
- To summarize,
  - I'm a Mechanical Engineer, a consumer of parallel computing
  - Focus is not on how to design parallel computing hardware or instruction architecture sets for parallel computing

Why This Title?



- Computer Science: ISA, Limits to Instruction Level Parallelism and Multithreading, Speculative Execution, Pipelining, Memory Hierarchy, Memory Models, Cache Coherence, etc.
  - Long story short: how should a processor be built?
- Electrical Engineering: how will we build the processor that the CS colleagues have in mind?
  - Lots of microarchitecture issues
- This class: how to use the system built by electrical engineers who implemented the architecture devised by the CS colleagues
  - At the end of the day, in our research in Science/Engineering we'll be dealing with one of the seven dwarfs…

Phillip Colella's "Seven Dwarfs"



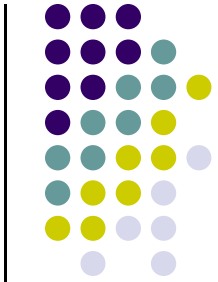
High-end simulation in the physical sciences = 7 numerical methods:

1. Structured Grids (including locally structured grids, e.g. Adaptive Mesh Refinement)
2. Unstructured Grids
3. Fast Fourier Transform
4. Dense Linear Algebra
5. Sparse Linear Algebra
6. Particles
7. Monte Carlo

- If add four more for embedded, covers all 41 EEMBC benchmarks
  8. Search/Sort
  9. Filter
  10. Combinational logic
  11. Finite State Machine

Slide from "Defining Software Requirements for Scientific Computing", Phillip Colella, 2004 .
Credit: D. Patterson
EEMBC: Embedded Microprocessor Benchmark Consortium

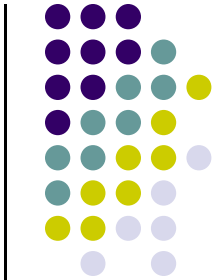
Profiling:
Who Will Be the Typical 759 Student?



- 37 students enrolled coming from four UW departments
  - Computer Science, Electrical Engineering, Engineering Mechanics, Mechanical Engineering

- "High Performance Computing for Engineering Applications"
  - There is no need to have a prior Engineering degree
  - The course assumes a level of programming experience of a typical Engineer

Auditing the Course



- Why auditing?
  - Augments your experience with this class
    - You get an account on the CPU/GPU cluster
    - You will be added to the email list
    - Can post questions on the forum

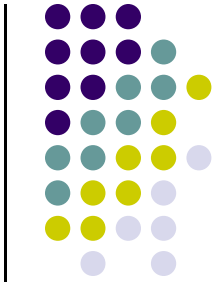
- How to register for auditing:
  - In order to audit a course, a student must first enroll in the course as usual. Then the student must request to audit the course online. (There is a tutorial available through the Office of the Registrar.) Finally, the student must save & print the form. Once they have obtained the necessary signatures, the form should be turned in to the Academic Dean in the Grad School at 217 Bascom. The Grad School offers more information on Auditing Courses in their Academic Policies and Procedures.

Tutorial website: http://www.registrar.wisc.edu/isis_helpdocs/enrollment_demos/V90CourseChangeRequest/V90CourseChangeRequest.htm

Auditing Courses: http://www.grad.wisc.edu/education/acadpolicy/guidelines.html#13

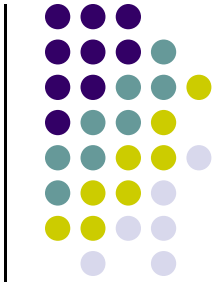
Overview of Material Covered

[Fall 2013]



- Quick C Intro
- General considerations in relation to trends in the chip industry
- Overview of parallel computation paradigms and supporting hardware/software
- GPU computing and the CUDA programming model
- GPU parallel computing using the thrust template library
- OpenMP programming
- MPI programming

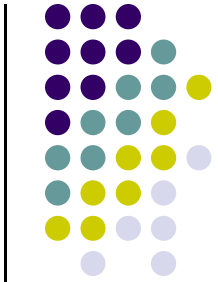
At the beginning of the road…



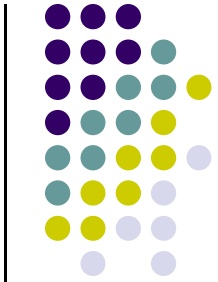
- Teaching the class for the fourth time
  - Rough edges remain
  - There might be questions that I don't have an answer for
    - I'll follow up on these and get back with you (on the Forum)

- Please ask questions (be curious)

My Advice to You [is simple]



- If you can, innovate, do something remarkable, amaze the rest of us…

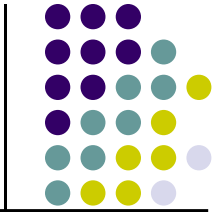


End ME759 Overview

Beginning: Quick Review of C

- Essential reading: Chapter 5 of “The C Programming Language” (Kernighan and Ritchie)
- Acknowledgement: Slides on this C Intro include material due to Donghui Zhang and Lewis Girod
- If these things look unfamiliar, please read the Primer document available on the class website

C Syntax and Hello World



#include inserts another file. ".h" files are called "header" files. They contain declarations/definitions needed to interface to libraries and code in other ".c" files.

What do the < > mean?

A comment, ignored by the compiler

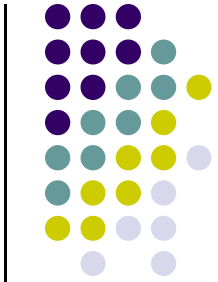
```
#include <stdio.h>
/* The simplest C Program */
int main(int argc, char **argv)
{
  printf("Hello World\n");
  return 0;
}
```

The main() function is always where your program starts running.

Blocks of code ("lexical scopes") are marked by { … }

Return '0' from this function

A Quick Digression About the Compiler



```
#include <stdio.h>
/* The simplest C Program */
int main(int argc, char **argv)
{
  printf("Hello World\n");
  return 0;
}
```

Preprocess

```
__extension__ typedef  unsigned long long int
__dev_t;
__extension__ typedef  unsigned int   __uid_t;
__extension__ typedef  unsigned int   __gid_t;
__extension__ typedef  unsigned long int
__ino_t;
__extension__ typedef  unsigned long long int
__ino64_t;
__extension__ typedef  unsigned int
__nlink_t;
__extension__ typedef  long int   __off_t;
__extension__ typedef  long long int
__off64_t;
extern void flockfile (FILE *__stream)  ;
extern int ftrylockfile (FILE *__stream)  ;
extern void funlockfile (FILE *__stream)  ;
int main(int argc, char **argv)
{
  printf("Hello World\n");
  return 0;
}
```

Compile

my_program

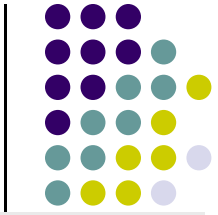
Compilation occurs in two steps: "Preprocessing" and "Compiling"

In Preprocessing, source code is "expanded" into a larger form that is simpler for the compiler to understand. Any line that starts with '#' is a line that is interpreted by the Preprocessor.

- Include files are "pasted in" (#include)
- Macros are "expanded" (#define)
- Comments are stripped out (/* */ , //)
- Continued lines are joined (\ )

The compiler then converts the resulting text (called translation unit) into binary code the CPU can execute.

Lexical Scoping



Every Variable is Defined within some scope. A Variable cannot be referenced by name (a.k.a. Symbol) from outside of that scope.

Lexical scopes are defined with curly braces { }.

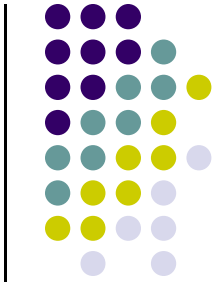
- The scope of Function Arguments is the complete body of that function.
- The scope of Variables defined inside a function starts at the definition and ends at the closing brace of the containing block
- The scope of Variables defined outside a function starts at the definition and ends at the end of the file. Called "Global" Vars.

```
void p(char x)
{
                /* p,x */
  char y;
                /* p,x,y */
  char z;
                /* p,x,y,z */
}
                /* p */
char z;
                /* p,z */

void q(char a)
{
  char b;
                /* p,z,q,a,b */

  {
    char c;
                /* p,z,q,a,b,c */
  }

  char d;
  /* p,z,q,a,b,d (not c) */
}

/* p,z,q */
```

char b?

legal?

Comparison and Mathematical Operators



```
== equal to
<  less than
<= less than or equal
>  greater than
>= greater than or equal
!= not equal
&& logical and
|| logical or
!  logical not
```

```
+  plus
-  minus
*  mult
/  divide
%  modulo
```

```
&  bitwise and
|  bitwise or
^  bitwise xor
~  bitwise not
<< shift left
>> shift right
```

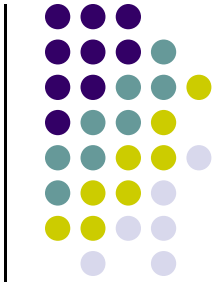
Beware division:

- 5 / 10 → 0 *whereas* 5 / 10.0 → 0.5
- Division by 0 will cause a FPE

Don't confuse & and &&..
1 & 2 → 0 *whereas* 1 && 2 → <true>

The rules of precedence are clearly defined but often difficult to remember or non-intuitive. When in doubt, add parentheses to make it explicit.

Assignment Operators



```
x = y    assign y to x
x++      post-increment x
++x      pre-increment x
x--      post-decrement x
--x      pre-decrement x
```

```
x += y   assign (x+y) to x
x -= y   assign (x-y) to x
x *= y   assign (x*y) to x
x /= y   assign (x/y) to x
x %= y   assign (x%y) to x
```

Note the difference between ++x and x++ (high vs low priority (precedence)):

```
int x=5;
int y;
y = ++x;
/* x == 6, y == 6 */
```

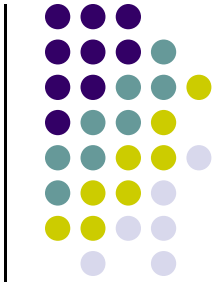
```
int x=5;
int y;
y = x++;
/* x == 6, y == 5 */
```

Don’t confuse “=“ and “==“!

```
int x=5;
if (x==6)   /* false */
{
  /* ... */
}
/* x is still 5 */
```

```
int x=5;
if (x=6)   /* always true */
{
  /* x is now 6 */
}
/* ... */
```

C Memory Pointers



- To discuss memory pointers, we need to talk first about the concept of memory

- We'll conclude by touching on a couple of other C elements:
  - arrays, typedef, and structs

The "memory"

Memory: similar to a big table of numbered slots where bytes of data are stored.

The number of a slot is its address.
A one byte value can be stored in each slot.

Some data values span more than one slot, like the character string "Hello\n"

A type provides a logical meaning to a span of memory. Some simple types are:

`char`	a single character (1 slot)
`char [10]`	an array of 10 characters
`int`	signed 4 byte integer
`float`	4 byte floating point
`int64_t`	signed 8 byte integer

Addr	Value
0	
1	
2	
3	
4	'H' (72)
5	'e' (101)
6	'l' (108)
7	'l' (108)
8	'o' (111)
9	'\n' (10)
10	'\0' (0)
11	
12	

What is a Variable?

A Variable names a place in memory where you store a Value of a certain Type.

You first Declare a variable by giving it a name and specifying its type and optionally an initial value

declare vs. define

```
char x;
char y='e';
```

Variable x declared but undefined

Initial value

Name

What names are legal?

Type is single character (char)

extern? static? const?

The compiler puts x and y somewhere in memory.

symbol table?

Symbol	Addr	Value
	0	
	1	
	2	
	3	
x	4	Some garbage
y	5	'e' (101)
	6	
	7	
	8	
	9	
	10	
	11	
	12	

Multi-byte Variables

Different types require different amounts of memory. Most architectures store data on "word boundaries", or even multiples of the size of a primitive data type (int, char)

```
char x;
char y='e';
int z = 0x01020304;
```

0x means the constant is written in hex

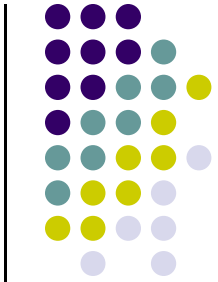
Symbol	Addr	Value
	0	
	1	
	2	
	3	
x	4	Some garbage
y	5	'e' (101)
	6	
	7	
z	8	4
	9	3
	10	2
	11	1
	12	

padding

An int requires 4 bytes

Architecture uses little-endian convention, since it stores the most significant byte first

One Quick Thing…



- I need one or two *volunteers* who can help my lab with expertise in MPI-enabled parallel computing
- Our needs in Computational Dynamics:
  - Some loose ends need to be taken care of (code not entirely finished)
  - Code is very slow (simulations run two weeks)
- To view where we use parallel computing in the lab, look here:
  - http://sbel.wisc.edu/Animations/
- What you get in return: conference/journal papers
- If interested, please email me your CV