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Fall 2010 Final Exam

CSC7700 Scientific Computing

December 6th 2010, 5.30pm to 7.30pm

### General Instructions

- This is a closed book exam.
- No calculators or electronic devices.
- Part I of the exam covers all the five course modules and is designed to take 80 minutes to complete. Part II of the exam is for the Networks and Data module and is designed to take 40 minutes to complete.
- Part I is worth 20% of the final grade. Each module includes 5 questions. All questions have equal weight. Answer all questions.
- Part II is worth 10% of your final grade. Answer only four out of five questions. If you answer all five, only the lowest graded four will be taken into consideration. Questions have two parts, you need to answer both parts of the four questions you select.

## Part I

Abby Zebang

## Module A: Basic Skills

1. Provide two reasons why the same text file can look different when viewed on different systems or within different tools.

- a) DOS & UNIX line ending conventions are different  
so a UNIX file opened in DOS mode may look like it is missing newlines (I believe DOS expects  $\text{newline} + \text{carriage return}$ . UNIX is just  $\text{newline}$ )
- b) Different character encoding ex) file written w/ UTF-8, read on system w/o Unicode support may result in missing characters or other weirdness

2. In the context of numerical simulations, explain what is meant by discretization and why it is used.

Discretization is taking a continuous function / phenomena & splitting into discrete parts

We need it because computers have limited resources, and must break what we are simulating down into discrete parts in order to be computationally feasible.

Example: ocean modelling, cannot simulate every atom in the ocean, so we make a 3D-grid where each grid location represents  $N$  volume of water <sup>can</sup> and calculate like that -

3. Briefly describe what a pseudo random-number generator is, and name three disadvantages over real random-number generators. Name two reasons why pseudo random-number generators are often used despite these disadvantages?

Pseudo random — Generates seemingly random numbers by applying mathematical formulas & Mersenne Twister

Positives

- 1) Easy to use - no external / specialized HW needed
- 2) Provides reproducible results. may be important for example in sharing code / output with other researchers

Negatives

- 1) Not truly random, will end up repeating at some point
- 2) Requires a seed value, if this is known by an attacker then we have no randomness / security may be affected
- 3) May be computationally intensive

4. Name one advantage and two potential disadvantages of the Newton-Raphson method over the bisection method for root-finding.

Advantage - Faster convergence!

Disadvantage - Requires that we know derivative of the function being studied

- There are "degenerating" cases where the algorithm will ping-pong back and forth and take a very long time to converge

5. Explain the difference between centralized and distributed version control systems, including one advantage and one disadvantage for each. Name one software implementation example for each kind of system.

Centralized - SUN

Advantage - Everything is located in one location

Disadvantage - Difficult to make local branches to commit often to separate from main branch

Distributed - Mercurial

Advantage - Can make local branches easily

Disadvantage - May be issues in pulling data down from remote server

## Module B: Networks and Data

1. List two TCP parameters used in `iperf` and briefly describe their influence on the performance of TCP.

`numstreams` - affects the number of simultaneous streams, may improve transfer bandwidth but is dangerous as it contracts TCP congestion controls

`Window size` - changes TCP window, i.e. time to receive acknowledgment before packet assumed lost. Increasing this can improve TCP speed by allowing it to ramp up higher before being ratcheted down by congestion controls.

2. Briefly describe what the server-side data processing plug-in included in the standard GridFTP installation does and what it can be used for (hint - you used it in your homework)

This allows us to tell the server to transfer data while our main job continues unimpeded & w/o the need for constant processing from our job

3. List two benefits that middleware provides to developers of distributed applications.

1) Abstracts some of the differences between machine hardware away such that multiple machines may be manipulated using the same interface

2) Hides low-level operations & book keeping that slows development time away from the end-user

4. Briefly outline two methods for accessing remote data in a distributed application.

RPC calls - lets us run functions on remote machines  
↳ get results back

CORBA - provides IDL, can be used to describe  
↳ access remote data types

5. Briefly outline two methods of doing remote visualization (based on distribution of the visualization pipeline)

Method 1: Batch-based

Submit a render request & dataset to remote machine,  
wait N minutes in queue, get pretty visualization back

Example - Complex Visit Scene,

Method 2 - Interactive.

Method 3 - Powerful graphics locally, large data storage remote  
Data streams to your machine, graphics rendered locally

Method 4 - Weak graphics locally, powerful network connection  
↳ Powerful remote graphics

Graphical requests sent over the network, visualizations  
are returned, in real time

## Module C: Simulations and Application Frameworks

1. What determines the accuracy of a simulation? List two ways in which accuracy can be improved.

Accuracy of a simulation depends upon appropriateness / power, of solving algorithms, coarseness/fidelity of simulation space (grid), input data which is fed to the simulation, and validity of assumptions made when programming the simulation

Improve accuracy by

- 1) Increasing grid/discretization level (needs more mem/CPU though)
- 2) Using better numerical methods to get better accuracy / CPU power

2. What is MPI, and what is it used for? Assume there are two processes, and process A needs to access an array element stored on process B. Schematically, how does this work?

MPI - "message passing interface", we use it to communicate between processes. can be used both on local node & across multiple nodes.

Schematically, Proc A makes a MPI-Recv call, which opens a buffer to receive the data. Proc B makes a MPI-Send call, which transmits the data to Proc A. The data can either be sent via local interconnects or over the network.

3. What is a software framework? Name one software framework, and provide three characteristic elements of a software framework.

A software framework consists of an API (application programming interface) defined datatypes which can be used to interact across software components, and a core capable of coordinating software components and requests.

Cactus  
is a software framework!

- 1) Modular
- 2) Extensible
- 3) Uses objects that can be passed between modules & operated on

4. What are CCL files in Cactus? List which CCL files exist, and what they define.

Cactus configuration files

schedule.ccl — determines when cactus functions will run, schedules  
interface.ccl — defines implementation name provided by them, <sup>grid storage</sup>  
provides inheritance, defines grid data to be stored.

param.ccl — describes theta parameters, acceptable values for each

configuration.ccl: defines shared Cactus functions & libraries provided/needed

5. Name and briefly describe five tools that support code development in large, distributed, international collaborations.

SVN — source management — allows multiple people to work on  
same code, manages conflicts, keeps code history

IRC — collaboration between developers in real-time, text based

Bug tracking (TRac, bugzilla) — keeps track of open  
bugs & feature requests

Skype — video chat, face-to-face voice communication

Email — one-on-one text & file transfer, not real-time  
so good for nonimportant things



## Module D. Scientific Visualization

1. Define and describe a "Visualization Pipeline"

A visualization pipeline describes the steps taken when producing graphical outputs. Example for Visk:

Load F5 file - tie to grid - tie to vector representation on grid - add transformation operation to resultant vector field

It is a sequential way of describing graphical/spatial operations.

2. What is the difference between the "push model" and the "pull model"?

The difference is in the push model, all of the data is pushed through the filters/transformations to get the final result.

In the pull model, data is "pulled" to appropriate modules as needed. Not all data may be used.

3. Describe the three atomic elements ("building blocks") in a visualization network.

fiber bundle - provides base unit of data

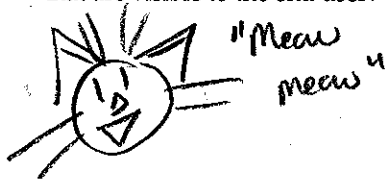
Data Transformations - converts data to spatial coordinates/geometry

Visual Transformations - represents spatial coordinates/geometry as polygons/colors/etc

4. Define and describe the purpose of a bi-vector.

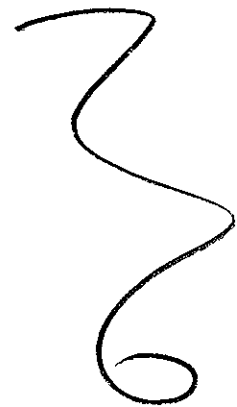
A bi-vector is two vectors stored together. You can use it to get the cross product. You can also use it + a scalar to make a vector to rotate objects with.

5. Which are the three property objects ("communication types") in the "F5" fiber bundle data model that are visible to the end user?



I wasn't sure so I asked my cat "meow"

Input - receives another object's input  
Output - forwards output to another object  
Attribute - data type being operated on



## Module E: Distributed Scientific Computing

1. We discussed five applications - Montage, Nektar, Climateprediction.net, SCOOP and Ensemble-based/Replica-Exchange simulations. For any THREE of these (you choose which three), answer any ONE of the following: Why they were distributed? How they were distributed? The Challenges &/or success in distributing them?

Distributed  
Because

Nektar  
Memory-bound,  
Needs 8TB+  
and no one  
machine can  
handle it

SCOOP  
Needs large computational  
power, but not very often  
(5% of year during hurricane  
season), distributed so  
we can request this high power  
only when needed

Climate prediction  
Needs a lot of  
CPU power & RAM  
a "petascale" before  
petascale computing ever  
reachable by traditional  
HPC

2. Estimate to within an order of magnitude the number of jobs that are executed in the Worldwide LHC Computing Grid (WLCG) per day. Estimate to within an order of magnitude the number of bytes of data generated (overall) by the WLCG. Estimate the cost of the LHC Experiment. Therefore what is the cost of generating a byte of data from the LHC experiment?

10,000 jobs/day

10 PB of data overall

LHC cost: \$100 billion

KB  $10^4$   
MB  $10^6$   
GB  $10^9$   
TB  $10^{12}$   
PB  $10^{15}$

million  $10^6$   
billion  $10^9$

$$\frac{\$10^{11}}{10^{21} \text{ bytes}} = .000000001 \$/\text{byte}$$

↑ probably off a bit.

3. Using your estimate (whatever it was) of number of jobs (on the WLCG) from the previous answer, given that there are approximately 250,000 cores as part of the WLCG, and that it has a typical utilization factor of 50%, estimate the average time each job takes. (assume: each job is a single-core job).

12.5 cores  
per job

125,000 cores used  
10,000 jobs/day

each job is single-core

125,000 jobs  
a day would be  
each job averages

Each job takes 12.5 CPU days on average  
with previous estimations, but we need to assume single-core only.

If we had 125,000 jobs per 11 day, that would be average of 1 day/job.

I think in class we said each job is ~4 hours. So, should be ~4.3 \* 250,000

jobs/day

NO TIME

4. List two factors – technological or non-technological, driving Cloud Computing. Provide a “real production” example of a Cloud offering. Is the Cloud offering an example of IaaS, PaaS or SaaS?

Tech - desire for large amounts CPU power w/o having

1) to build own cluster

2) Desire for large amount of storage space that is remotely managed.

Real “cloud offering - Amazon EC2

Not people as a service, but it is infrastructure as a service (CPUs, Hard drives, fast network, etc)

5. Provide one difference between predominantly HTC and HPC Grids. Provide a “real production” example of a HPC and HTC Grid.

HPC grids are primarily about maximum CPU performance / FLOPS,

HTC may have other priorities such as maximizing job throughput

Real HPC grid - Kraken

Real HTC grid - Climate prediction.org

## Part II

## Networks and Data

### Question 1

- A) How are layers used in network implementations?

Each layer builds upon the previous

- Layer 1 - point-to-point networking
- Layer 2 - Local addressing
- Layer 3 - Routing between different networks
- Layer 4 - distinguishing between sources on the same machine (ports)

It lets us form abstractions of what software should handle which duties

- B) What are the major differences between TCP and UDP?

### TCP

- In-order packet transmission
- Reliable - know if it failed or not
- Built-in congestion control

### UDP

- Packets may arrive out of order
- Unreliable, potentially packets may drop into the void w/o notification
- no congestion control!

## Question 2

- A) What data transmission protocol would you use for bulk data transmission and why? What protocol would you use for video or audio conference and why?

Bulk data - TCP, I want to make sure the data gets there in order & all of it is received!

Video - UDP - I want fast, low-latency video frames, who cares if 5% of them are lost I can still see Grandma Mamie & my cats @ home just fine! 😊

- B) Describe circuit network services and their advantage.

Circuit network services allow us to route large network paths on a switchable basis.

Example: Dr Allen is giving a seminar in Washington DC with people from China, India, and Poland. With a circuit network service we could request circuits from these be switched over at 1PM next Wednesday, reducing the number of hops & improving bandwidth over what we would normally have.

### Question 3

- A) Describe what a naming service is (in middleware implementations) and what is it used for.
- B) In your own words, describe the "end-to-end" argument.



#### Question 4

- A) List the usual sequence of operations for accessing data in a distributed file system.

- 1) Program generates request
- 2) Network transfers request
- 3) DFS server receives request
- 4) DFS accesses data (may access metadata first, then request data from server pointed to, etc)
- 5) Data sent across network
- 6) Program receives data

- B) Briefly describe the two possible (and sometimes conflicting) optimization goals of a scheduling system.

1) Optimize Throughput

- we want to optimize # of jobs that go through in a given amount of time!

2) Optimize (decrease) latency

- we want to minimize the amount of time a job sits in the queue!

### Question 5

- A) Describe use case scenarios where remote visualization is useful or needed.

1) We have a fat pipe to a GPU <sup>accelerated</sup> machine at another university. Instead of needing to buy a Nvidia Monstro card ourselves, we can run the viz remotely and see the results locally in real-time.

2) 20 world experts on black holes are located across the globe. With remote viz, everyone could see a copy of the same visualization, and interact/comment on it together.

- B) Describe some of the possible benefits of distributed visualization.

This allows datasets too large or complicated to be visualized by a single machine to be rendered by a cluster of them. This increases scale of problems we can handle.

We may also have many machines across the globe w/ large datasets on them. Instead of waiting to transfer all the data, we may instead want to render each piece remotely, transmit the images, & recombine elsewhere.