Introduction To Scientific Computing

CS 471/ Math 471

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Fosdick et al Quote

- “The computer has become at once the microscope and telescope of science”
- Modeling and simulation is used in place of building and testing
- From
  - models of nuclei, electrons, atoms, molecules
- To
  - models of global weather, the universe, ...

A History of Scientific Computing

- Involves the development of computers, communication, and software
- Computers
  - Babbage in the 1800s with his mechanical designs
  - Aiken, Stibitz in 1940s
    - numerical codes for shell trajectories, nuclear fission
    - non-numerical codes for code deciphering

Computing in the 1940s

- Speeds like one to a few hundreds per sec.
- Visions of early developers
  - study fundamental problems in mathematics and science
  - simulations of physical systems such as fluid flow and weather forecasting
  - concern for solving large systems using finite precision arithmetic -- accuracy, size, speed

Computer Development

- The visionaries were 50 years ahead of their time
  - 1940s
    - relay machines with a few operations per second
  - 1950s
    - electronic devices (vacuum tubes) with a few 100s to 1000s of operations per second

Computer Development Cont’d

- 1960s
  - transistor machines with a few 100s of thousands of operations per second
- 1970s
  - integrate circuits with millions of operations per second
  - late in decade, a few 100 millions of ops (Cray)
  - beginning of the micro/mini development

Computer Development Cont'd

- 1980s
  - by mid-80s, 500 million floating point ops
  - ever-increasing influence of commodity computers with the PC chip developments
  - multiprocessor machines commercially available (vector boards, parallel shared memory, distributed memory)
  - graphics and scientific vis. machines

Computing Machines Cont'd

- 1990s
  - from a billion to a few trillion flops
  - ever-increasing influence of commodity chips and components
  - PCs as powerful (more?) than workstations
  - visualization hardware available as commodity chips

Computing In The Future

- 1993 JPL report asks for
  - petaflop computing (10^15 flops)
  - petabyte storage
  - gigabytes of communication bandwidth
  - by 2010
- A pipe dream or reality?
  - 10K to 50K processors
  - fiber optic communication

Communication Developments

- 1960s and before
  - proprietary, special purpose (roll-your-own) buses, channels, "wires"
- 1970s
  - beginning of wide area networks
  - buses, backplanes beginning to be standardized
  - modems run at teletype speeds (10 char per sec)

Communication Developments

- 1980s
  - modems at a few 100 chars per sec.
  - long distant networks at few 100,000 bits/sec
  - prevalence of the TCP/IP protocol for communication
- 1990s
  - wide area networks, 1 Mbits initially

Communication 1990s

- Locally area networks now
  - 10 mbits for Ethernet
  - 100 mbits for FIDDI
  - 800 mbits for HIPPI
  - 622 mbits Myrinet to PCs
- Wide area networks now
  - T1 at 1.4 Mbits per second
  - T3 at 45 Mbits per second

1990s Communication

- Wide area networks now
  - backbone at 155 Mbits/sec
  - experiments at 622 Mbits/sec
- Next few years
  - gigabit Ethernet
  - gigabit WAN backbones
  - 6+ gigabit super-HIPPI

Scientific Computation-- Software

- 1940s-1950s
  - performed by individual researchers and organizations with the need
  - ad hoc development of software, very little sharing

Software -- 1960s

- Recognition of the need for organized reusable software
- Standardization recognized at important
  - Fortran Standardization, 1961-1966
  - development and distribution of software to be shared
    - libraries -- Wilkinson et al., Linear Algebra Handbk
    - applications -- COSMIC, SHARE

Applications Emphasized

- 1980s
  - recognition that to accomplish the goals of the early visionaries, emphasize had to be placed on
    - high performance computational machines
    - large “grand challenge” applications in science and engineering
    - involves physical systems

The Grand Challenges

- Areas of 1987 grand challenges
  - prediction of weather, climate, and global change
  - materials science
  - semi-conductor design
  - superconductivity
  - structural biology
  - design of drugs

Challenges Cont’d

- More grand challenges
  - human genome
  - quantum chromodynamics
  - astronomy
  - transportation
  - turbulence
  - combustion systems
  - enhanced oil and gas recovery

Challenges Cont'd

- More challenges
  - computational ocean sciences
  - speech
  - vision
- And more have been identified since
  - ASCI
  - DoD challenge problems
  - ...

For Fortran 90 Lectures

- Study the program hello.f90

```
program hello                    ! Header statement
  character(10)  t               ! Specification part
  intrinsic  date_and_time

  call  date_and_time( time=t )   ! Executable part
  print *, 'Hello world: the time is  ', t(1:2), ':',&
           t(3:4)

end program hello                ! End statement
```


My Square Root Program

- In the directory ~acpineda/CS471/LectureCode
  - a main program that approximates the square root of a number, read from standard input
  - study its structure -- named sqrteg.f90
  - it and a series of enhancements will be used to discuss the structure of Fortran 90 programs and survey of various features in the language that support scientific computation