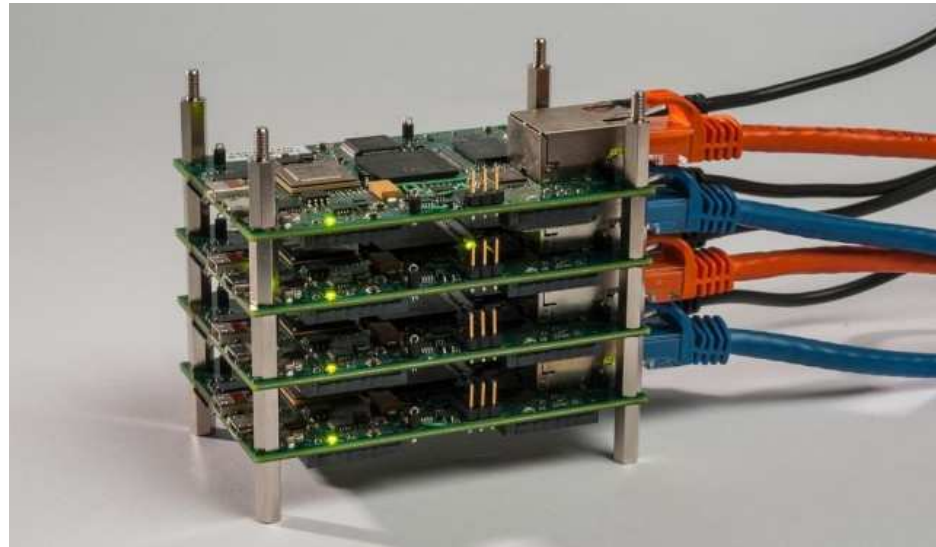


# Introduction to Programming and Computing for Scientists (2019 HT)

## Tutorial-4: Parallel (multi-cpu) Computing

# Outline

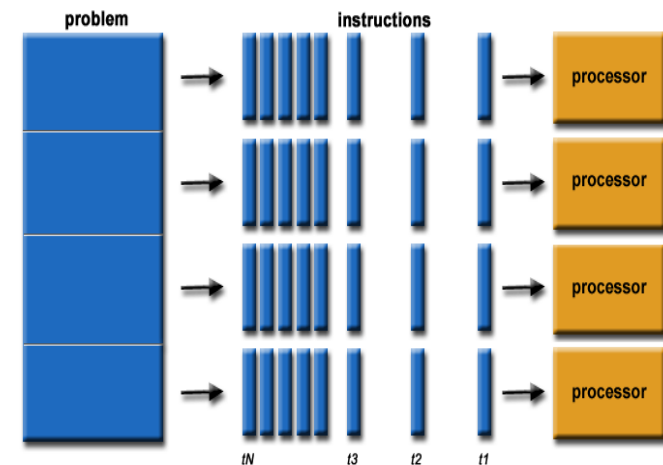
- Parallel computing in a nutshell:
  - motivation, terminology, solutions
- Howto ride on "big iron":
  - Login to remote computers
  - The practical basics of working with batch systems
- Multi-task jobs



<http://arstechnica.com/information-technology/2013/07/creating-a-99-parallel-computing-machine-is-just-as-hard-as-it-sounds>

# What is parallel computing?

- Traditional computing: serial execution of a single stream of instructions on a single processing element
- **Parallel computing**: simultaneous execution of stream(s) of instructions on multiple **processing elements**
  - **Non-sequential** execution of a computational task
  - (part of) the problem solved by **simultaneous** subtasks (processes)
  - Relies on the assumption that problems can be divided (decomposed) into smaller ideally independent ones that can be solved **parallel**



# What is parallel computing?

- **Parallelism levels** ("distance" among the processing elements):
  - Bit and Instruction level: inside the processors (e.g. 64 bits processor can execute 2 32 bits operations)
  - Multicore/multi cpu level: inside the same chip/computer. The processing elements share the memory, system bus and OS.
  - Network-connected computers: clusters, distributed computing. Each processing element has its own memory space, OS, application software and data
    - Huge difference depending on the interconnects: e.g. High Performance Computing (supercomputers) vs. High Throughput Computing (seti@home)

# Some classifications

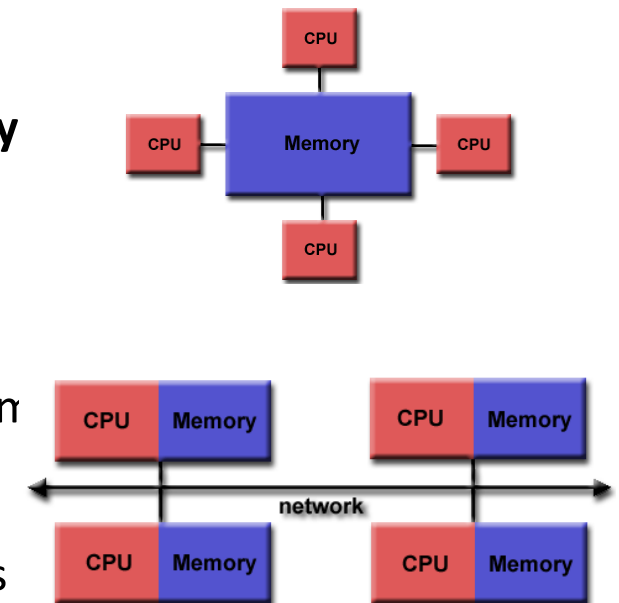
## Flynn's taxonomy:

	Single Instruction	Multiple Instruction
Single Data	SISD	MISD
Multiple Data	SIMD	MIMD

- SISD: sequential "normal" programs
- MIMD: most of the parallel programs
- SIMD: data chewing by the same algorithm
- *MISD: rarely exists*

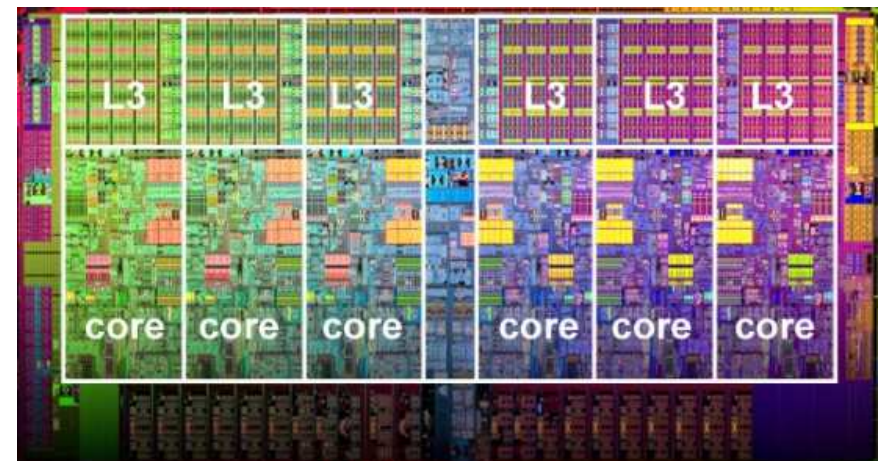
## SMP vs. MPP (or the shared memory vs. distributed memory debate):

- SMP: Symmetric Multi Processors system: shared memory approach
  - "single box" machines, OpenMP programming family
- MPP: Massively Parallel Processors system: distributed memory network-connected CPUs
  - "clusters", MPI programming family (message passing)
- SMPs are easier to program but scale worse than the MPPs



# Why parallel computing?

- It is cool
- Sometimes the problem does not fit into a single box: you need more resources than you can get from a single computer
- To obtain at least 10 times more power than is available on your desktop
- To get exceptional performance from computers
- To be couple of years ahead of what is possible by the current (hardware) technology
- The frequency scaling approach to increase performance does not work any longer (power consumption issues):
  - The new approach is to stuff more and more processing units into machines, introducing parallelism everywhere



# Measuring performance gain: the Speedup

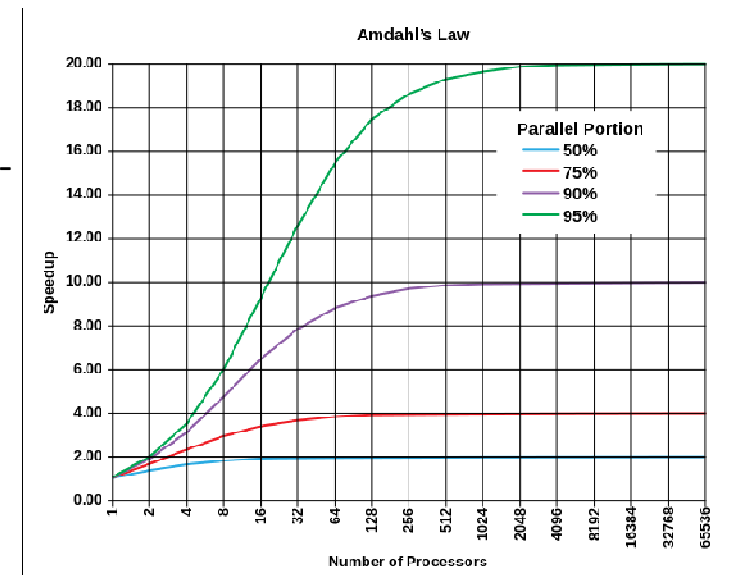
- In an ideal scenario a program running on **P processing elements** would execute **P times faster**..., giving us a linear speedup
- **Speedup  $S(n,P)$** : ratio of execution time of the program on a single processor ( $T_1$ ) and execution time of the parallel version of the program on P processors ( $T_p$ ):
  - In practice, the performance gain depends on the way the problem was divided among the processing elements and the system characteristics.
- **Amdahl's law**: gives an upper estimate for maximum **theoretical speedup** and states that it is limited by the non-parallelized part of the code:

$$S(n, P) \leq \frac{1}{\alpha + (1 - \alpha) / P} \leq \frac{1}{\alpha}$$

- alpha is the sequential fraction of the program
- e.g. if 10% of the code is non-parallizable, then the maximum speedup is limited by 10, independent of the number of used processors (!)

$$S(n, P) = \frac{T(n, 1)}{T(n, P)}$$

**n** denotes the problem size.  
**T** denotes the execution time.

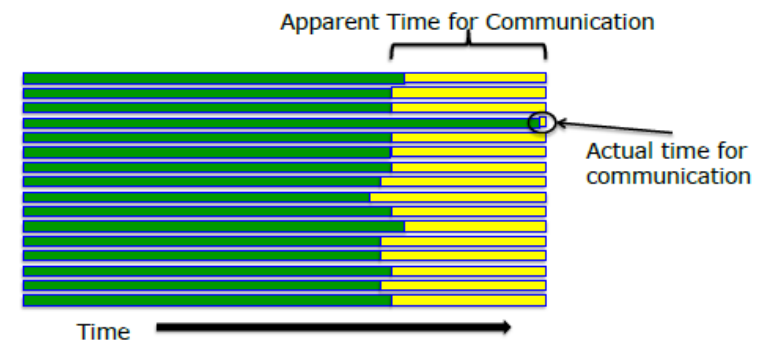


source: wikipedia

## The dark side ....

*"the bearing of a child takes nine months, no matter how many women are assigned"*

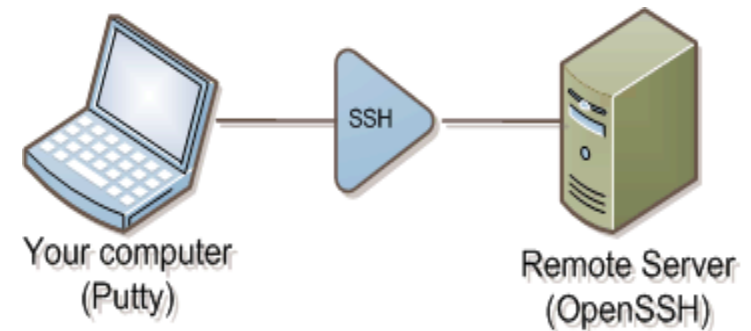
- Not everything is suitable for parallelization
- Complexity increases as more and more communication is involved:
  - embarrassingly parallel -> course-grained -> fine-grained problem domains
- Parallel computing opens up new set of problems:
  - Communication overheads
  - Concurrency problems
  - Synchronization delays
  - Race conditions and dead locks
- Nobody wants to debug a parallel code...
- Developing & deploying a parallel code usually consume more time than the expected speedup
- A practical advice for parallelization:
  - Unless you have an embarrassingly parallel problem, forget it
  - If you are stubborn, then at least use an available parallel (numerical) library and start with the profiling (understanding) of your program
  - Wait for the holy grail of computational science: automatic parallelization by compilers 😊





# Accessing remote computers

- **Secure Shell (SSH)** is a secure way of accessing remote computers, executing commands remotely or moving data between computers.
  - All network traffic is encrypted
  - The de-facto protocol for remote login & computer access
  - Available on non-linux platforms too (*putty and winscp on windows*)
  - SSH servers are listening to incoming connections on the standard TCP 22 port
  - Login is done with username/passwd or using keypairs (advanced topic)



**Exercise 1:** use the Linux **ssh** and **scp** commands:

- remote computer: **pptest-iridium.lunarc.lu.se**
- **ssh remote\_user@machine -X**
- **scp localfile user@machine:remote\_dir**

# Working on a remote computer: screen

IMAGINE that:

- You are being logged on a remote computer
- In the middle of a long task (e.g. compilation, download, etc
- Then, suddenly the network connection dies
- or you'd like to go home and continue the same work from your home desktop



*Is there a way to avoid losing all your work? How can one disconnect & reconnect to the same "session" without the need to restart everything from scratch?*

SOLUTION: use the **screen**! The utility that allows you to:

- Keep a session active even through network disruptions
- Disconnect and re-connect to a sessions from multiple locations (computers)
- Run a long remote running process without maintaining an active remote login session

# Working on a remote computer: screen

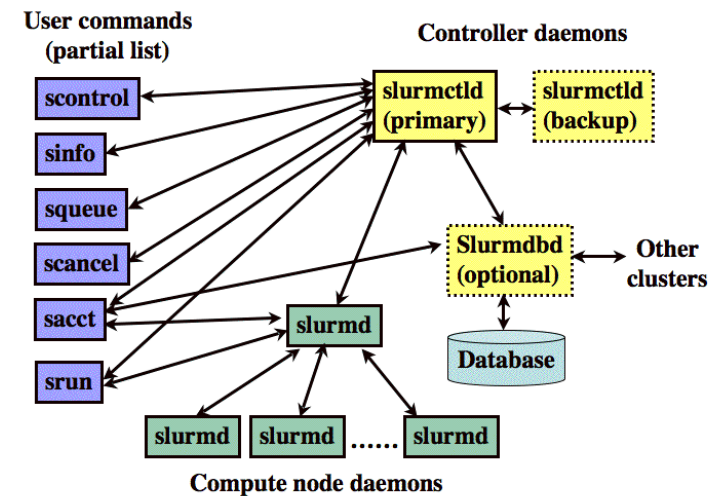
**Exercise 2:** use the Linux **screen** utility to manage remote screen sessions, connect, reconnect to active session, survive a network failure 😊

- Screen is started from the command line just like any other command
  - **[iridium ~]\$: screen**
  - You can create new “windows” inside screen, **ctr+a c** then rotate, switch between windows with **ctrl+a n**
- Listing your screens:
  - **[iridium ~]\$: screen -list**
- Disconnecting from your active session, screen (your task keeps running!):
  - **[iridium ~]\$: screen -d** or **ctrl+a d**
- Re-connecting to an active screen session (re-attach to screen):
  - **[iridium ~]\$: screen -r**
- Terminating, logging out of screen
  - type **exit** from inside all your active screen sessions
- Using screen to log your activity:
  - **[iridium ~]\$: screen -L** or **ctrl+a H** turns on/off logging during a screen session

# Working with a cluster

Goal: understand basic concepts of a cluster, Workload Management system, queue, jobs

- Cluster: *Iridium* cluster at LUNARC
- Frontend: **pptest-iridium.lunarc.lu.se**
- Batch system: **SLURM**



## Exercise 3:

- Look around on the front-end (e.g. inspect CPU and memory details):
  - `cat /proc/cpuinfo; cat /proc/meminfo; top`
  - `who, pwd`
- Check man pages for SLURM commands:
  - `sbatch, sinfo, squeue, scontrol, scancel`

# Working with a cluster

## Exercise 4: simple jobs with SLURM

- List SLURM queues (partitions)
  - > **sinfo**
- Create file **myscript** (use provided examples)
- Submit simple jobs and check their status:
  - > **sbatch myscript.simple**
  - > **cat slurm-<jobid>.out**
  - > **squeue**
  - > **scontrol show job <jobid>**
- Repeat with multi core/node jobs
  - **sbatch -N4 myscript.multinode**
  - **sbatch -n6 myscript.multinode**
  - In a multi-core advanced example, pay attention how jobs are distributed across nodes and cores

### Simple myscript:

```
#!/bin/sh
#SBATCH -J "simple job"
#SBATCH --time=1
echo "we are on the node"
hostname
who
sleep 2m
```

### Multicore/node myscript:

```
#!/bin/sh
#SBATCH -J "multi job"
#SBATCH --time=1
srun hostname |sort
sleep 5m
```

# Working with a cluster: task farming

## Exercise 5:

- With a help of a master script you are going to execute X number of subtasks on Y number of processing units
- The master script (*master.sh*) takes care of launching (new) subtasks as soon as a processing element becomes available
- The *worker.sh* script imitates a payload execution that corresponds to a subtask

## Steps:

1. Download, copy the scripts to a new directory on pp-test-iridium
2. Set the problem size (*NB\_of\_subtasks*) and the number of processing elements (*#SBATCH -n*) in the *master.sh*, the payload size (i.e. How long a subtask runs) in the *worker.sh*
3. Launch the taskfarm (*sbatch master.sh*), monitor the execution of the subtasks (*squeue -j <jobid> -s*) and finally check how much time the taskfarm processing required (check the output files of the subtasks and the slurm job)
4. Repeat the taskfarming with modified parameters, What is the speedup?

## Further reading

- Introduction Parallel computing (by Lawrence Livermore National Laboratory)
  - [https://computing.llnl.gov/tutorials/parallel\\_comp/](https://computing.llnl.gov/tutorials/parallel_comp/)
  - most of the images are taken from this tutorial
- SLURM:
  - <http://slurm.schedmd.com/quickstart.html>
- Lunarc Documentation
  - <http://lunarc-documentation.readthedocs.io/en/latest/>
- A very nice ssh environment for Windows platforms (instead of putty):
  - MobaXterm: <http://mobaxterm.mobatek.net/>

# Homework

- Submit HW-tutorial4 in Canvas