Parallel computing with Python

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Outline

Symmetric multiprocessing

- Multiprocessing: included in the standard library.
- Parallel Python.
- IPython.
- Others: POSH, pprocess, etc...

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Cluster computing

- Message Passing Interface (MPI): mpi4py, pyMPI, pypar, ...
- Parallel Virtual Machine (PVM): pypvm, pynpvm, ...
- IPython.
- Others: Pyro, ScientificPython, ...

Parallel GPU computing

- PyCUDA.
- PyOpenCL.
- Copperhead.
- Anaconda Accelerate.

Next ...

Parallel Python - PP

- PP is a python module.
- Parallel execution of python code on SMP and clusters.
- Easy to convert serial application in parallel.
- Automatic detection of the optimal configuration.
- Dynamic processors allocation (number of processes can be changed at runtime).
- Cross-platform portability and interoperability (Windows, Linux, Unix, Mac OS X).
- Cross-architecture portability and interoperability (x86, x86-64, etc.).
- Open source: `http://www.parallelpython.com/`.

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PP - module API

- Idea: Server provide you workers (processors).
- Workers do a job.
- class **Server** - Parallel Python SMP execution server class
  - **__init__**(self, ncpus='autodetect', ppservers=(), secret=None, restart=False, proto=2, socket_timeout=3600)
  - **submit**(self, func, args=(), depfuncs=(), modules=(), callback=None, callbackargs=(), group='default', globals=None)
  - Other: **get_ncpus**, **set_ncpus**, **print_stats**, ...
- class **Template**
  - **__init__**(self, job_server, func, depfuncs=(), modules=(), callback=None, callbackargs=(), group='default', globals=None)
  - **submit**(self, *args)

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PP - Examples

- First example: `pp_hello_world.py`
- More useful example: `pp_sum_primes_ntimes.py`
  - What happens if *n* is too different?
- A really useful example: `pp_sum_primes.py`
  - How long is the execution with different amount of workers?
- Template example: `pp_sum_primes_ntimes_Template.py`
- More involved examples: `pp_montecarlo_pi.py` and `pp_midpoint_integration.py`

Next ...

What is MPI?

- An interface specification: MPI = Message Passing Interface.
- MPI is a specification for the developers and users of message passing libraries.
- But, by itself, it is NOT a library (it is the specification of what such a library should be).
- MPI primarily follows the message-passing parallel programming model.
- The interface attempts to be: practical, portable, efficient and flexible.
- Provide virtual topology, synchronization, and communication functionality between a set of processes.
- Today, MPI implementations run on many hardware platforms: Distributed memory, Shared memory, Hybrid, ...

MPI concepts

- MPI processes.
- Communicator: connect groups of processes.
- Communication:
  - Point-to-point:
    - Synchronous: MPI_Send, MPI_Recv.
    - Asynchronous: MPI_ISend, MPI_Recv.
  - Collective: MPI_Bcast, MPI_Reduce, MPI_Gather, MPI_Scatter.
- Rank: within a communicator, every process has its own unique, integer identifier.

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mpi4py

- Python implementation of MPI.
- API based on the standard MPI-2 C++ bindings.
- Almost all MPI calls are supported.
- Code is easy to write, maintain and extend.
- Faster than other solutions (mixed Python and C codes).
- A *pythonic* API that runs at C speed.
- Open source: `http://mpi4py.scipy.org/`

mpi4py - Basic functions

- Python objects.
  - **send**(self, obj, int dest=0, int tag=0)
  - **recv**(self, obj, int source=0, int tag=0, Status status=None)
  - **bcast**(self, obj, int root=0)
  - **reduce**(self, sendobj, recvobj, op=SUM, int root=0)
  - **scatter**(self, sendobj, recvobj, int root=0)
  - **gather**(self, sendobj, recvobj, int root=0)
- C-like structures.
  - **Send**(self, buf, int dest=0, int tag=0)
  - **Recv**(self, buf, int source=0, int tag=0, Status status=None)
  - **Bcast**(self, buf, int root=0)
  - **Reduce**(self, sendbuf, recvbuf, Op op=SUM, int root=0)
  - **Scatter**(self, sendbuf, recvbuf, int root=0)
  - **Gather**(self, sendbuf, recvbuf, int root=0)

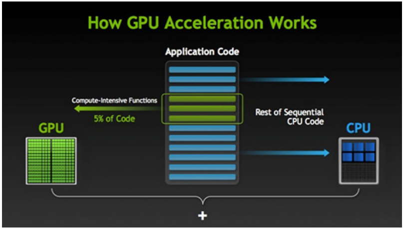
mpi4py - Examples

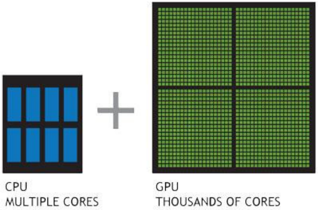
- First example: `mpi_hello_world.py`
- Message passing example: `mpi_simple.py`
- Point-to-point example: `mpi_buddy.py`
- Collective example: `mpi_matrix_mul.py`
- Reduce example: `mpi_midpoint_integration.py`

Next ...

What is GPU computing?

- GPU computing is the use of a graphics processing unit (GPU) together with a CPU to accelerate application.
- CPU consists of a few cores optimized for sequential serial processing.
- GPU has a massively parallel architecture consisting of thousands of smaller, more efficient cores designed for handling multiple tasks simultaneously.
- GPU can be seen as a co-processor of the CPU.





GPU computing

- Uses standard video cards by Nvidia or sometimes ATI.
- Uses a standard PC with Linux, MSW or MacOS.
- Programming model SIMD (Single Instruction, Multiple Data).
- Parallelisation inside card is done through *threads*.
- SIMT (Single Instruction, Multiple Threads).
- Dedicated software to access the card and start *kernels*.
- CUDA by Nvidia and OpenCL are the most popular solutions.

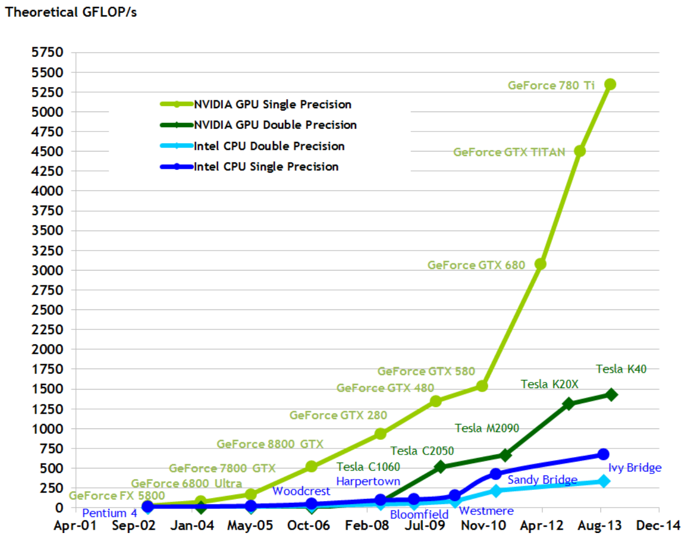
GPU computing - Advantages

- Hardware is cheap compared with workstations or supercomputers.
- Simple GPU already inside many desktops without extra investments.
- Capable of thousands of parallel threads on a single GPU card.
- Very fast for algorithms that can be efficiently parallelised.
- Better speedup than MPI for many threads due to shared memory.
- Several new high level libraries hiding complexity: BLAS, FFTW, SPARSE, ...
- In progress.

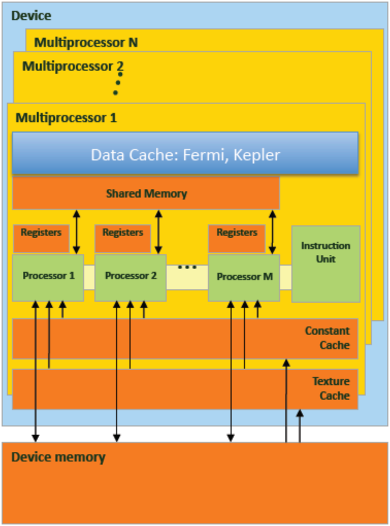
GPU computing - Disadvantages

- Limited amount of memory available (max. 2-24 GByte).
- Memory transfers between host and graphics card cost extra time.
- Fast double precision GPUs still quite expensive.
- Slow for algorithms without enough data parallellism.
- Debugging code on GPU can be complicated.
- Combining more GPUs to build a cluster is (was?) complex (often done with pthreads, MPI or OpenMP).
- In progress.

GPU computing



GPU hardware structure



Next ...

1. Python tools for parallel computing
2. Parallel Python
   - What is PP?
   - API
3. MPI for Python
   - MPI
   - mpi4py
4. GPU computing with Python
   - GPU computing
   - CUDA
   - PyCUDA
   - Anaconda Accelerate - Numbapro

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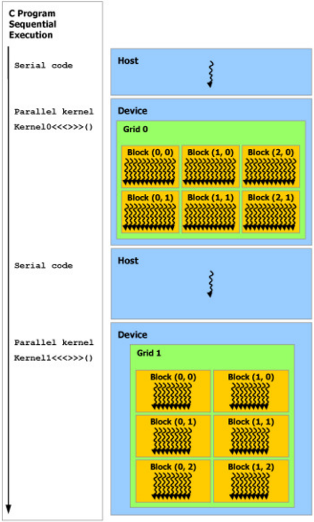
CUDA

- *Compute Unified Device Architecture* and is a software toolkit by Nvidia.
- Eases the use of Nvidia graphics cards for scientific programming.
- Special C compiler to build code both for CPU and GPU (nvcc).
- C Language extensions: distinguish CPU and GPU functions, access different types of memory on the GPU, specify how code should be parallelized on the GPU, ...
- Library routines for memory transfer between CPU and GPU.
- Extra BLAS, Sparse and FFT libraries for easy porting existing code.
- Mainly standard C on the GPU.

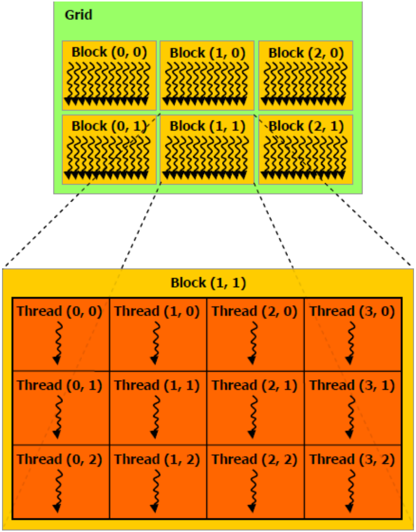
CUDA concepts

- Kernels: special functions executed in parallel on GPU.
- Memory transfer: copy the data between CPU and GPU memories.
- Host = CPU and Device = GPU.
- Thread: processes executed in parallel.
- Blocks: equal-size groups of threads.
- Grid: group of blocks. Execute the kernels.

CUDA programming model



CUDA programming model



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PyCUDA

- Wrapper of Nvidia CUDA for Python.
- Abstractions like pycuda.driver.SourceModule and pycuda.gpuarray.GPUArray make CUDA programming easier.
- PyCUDA puts the full power of CUDAs driver API at your disposal.
- Automatic Error Checking: All CUDA errors are automatically translated into Python exceptions.
- Speed: PyCUDA's base layer is written in C++.
- It is necessary to know C-like language.
- Open source: `http://mathema.tician.de/software/pycuda/`

PyCUDA - Examples

- First example: `pycuda_sumarrays.py`
- More involved example: `pycuda_montecarlo_pi.py`
- GPUArray example: `pycuda_montecarlo_pi_GPUArray.py`

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Anaconda Accelerate

- Allow developers to rapidly create optimized code that integrates well with NumPy.
- Offers developers the ability to code Python parallel implementations for multicore and GPU architectures.
- `http://docs.continuum.io/accelerate/index.html`
- But...it is not free....
- But...Anaconda Academic License.

Numbapro - Features

- Just-in-time compilation to target CPU, Multi CPU or GPU.
- Universal functions (*ufuncs*) and generalized universal functions (*gufuncs*).
- *ufuncs* and *gufuncs* are also compiled on the fly.
- Portable data-parallel programming.
- CUDA-based API is provided for writing CUDA code specifically in Python.
- Bindings to CUDA libraries: cuRAND, cuBLAS, cuFFT.
- `http://docs.continuum.io/numbapro/`

Numbapro - Examples

- *ufuncs* example: `numbapro_sumarrays.py`
- *Just-in-time* example: `numbapro_sumarrays_jit.py`
- *ufuncs* vs. *Just-in-time* example: `numbapro_saxpy.py`
- Target comparision example: `numbapro_discriminat.py`