

HPC Workshop

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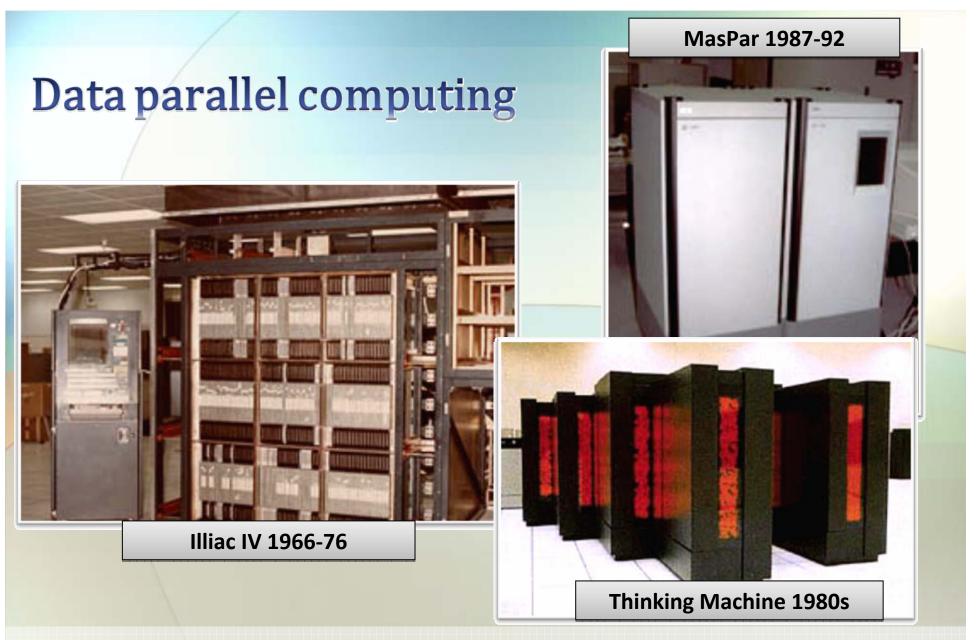
Faculty of Mathematics, Physics and Informatics

Paper and Tutorial

- Paper Focus: Performance considerations
- Tutorial focus: CUDA programming
- Paper and tutorial complement each other

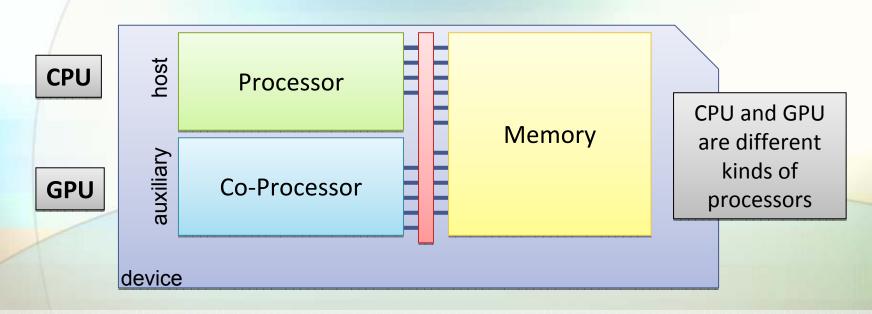
- Definition
 - Hybrid computing is binomial. It combines sequential processing and highly parallel processing, the SPMT kind.

SPMT ≠ SIMD



- All not successful. Limited to the SIMD parallelism.
- We needed the hybrid mode of computation.

Hybrid Co-processing



- CPU executes sequential components.
- Data parallel compute intensive functions are off-loaded to the GPU device.
- For example, body of C for-loops is prime candidate.
- Auxiliary Device = Accelerator

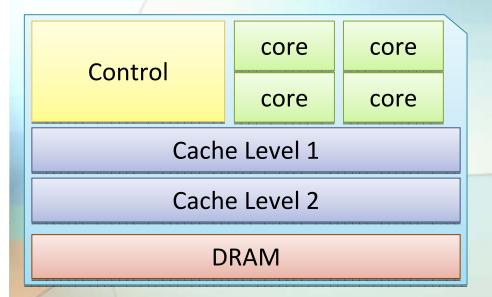
Hybrid Computing around the world. Are all paths leading to CPU+GPU?

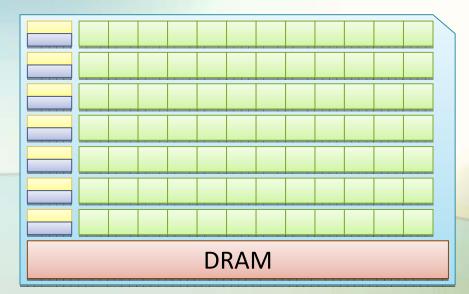
- Seattle based Cray announced a supercomputer CX1000 equipped with a TESLA GPU accelerator by NVIDIA.
- NVIDIA announced a new enhanced version of CUDA
 3.0 for FERMI GPUs.
- Jack Dongarra is working on a CUDA accelerated version of LAPAC! Essential for HPC.
- The new IBM server iDataPlex will be using NVIDIA M2050 or M2070 accelerators.

Continued

- TOP500 (June 2010)
 - #2 is a Chinese super powered by NVIDIA TESLA C2050 GPUs; Linpack speed 1.27 PFLOPs.
 - # 7 is also a Chinese hybrid CPU+GPU super with GPUs by AMD.
- Intel plans to design a super based on the MIC architecture (Many Integrated Cores). Unlike hybrid architectures the MIC architecture is based on the Intel standard processors.
- SGI plans a Petaflop hybrid supercomputer in one cabinet.
- AMD is developing CPU+GPU Fusion technology

Comparing CPU with GPU; Silicon use





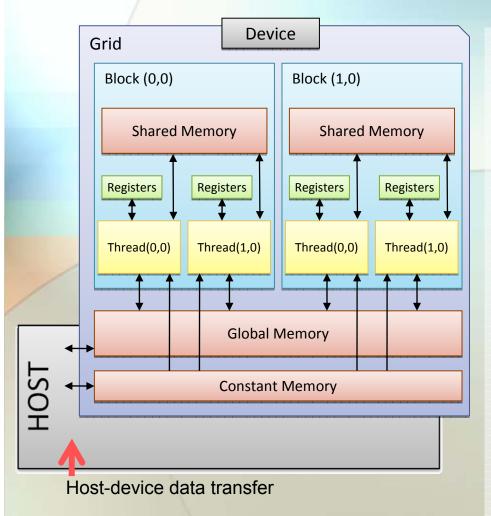
CPU

CPU increases speed
 of computation by multiple
 cores and by using cache
 to reduce memory access.

GPU

- GPU speeds up computation by much higher degree of parallelism.
- More transistors are used for processors.

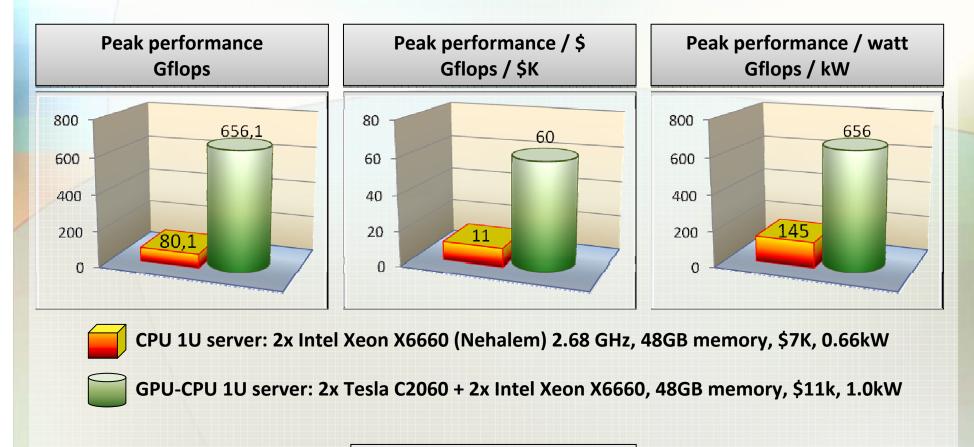
GPU Memory model



- Each thread has its individual register memory, fast.
- Threads within a block can communicate via shared memory, fast.
- Global memory is largest and slowest.
- Constant memory is read-only.
 Low latency.
- All the memories have independent disjoint address spaces.

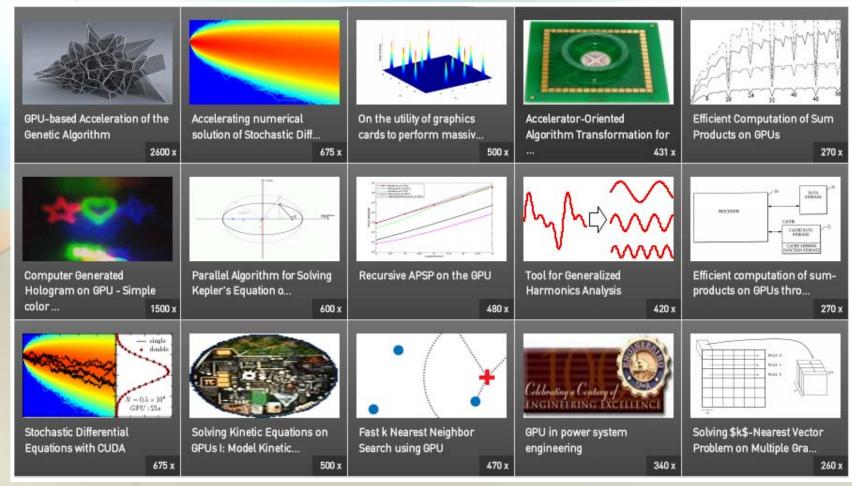
Performance comparison

Intel processor vs. Intel+TESLA C2060



Source: HPCwire May 2010

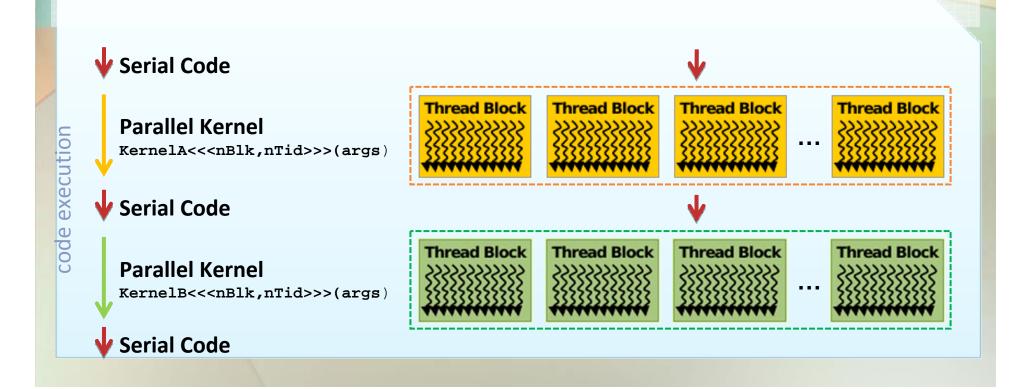
Scientific/engineering applications speedups



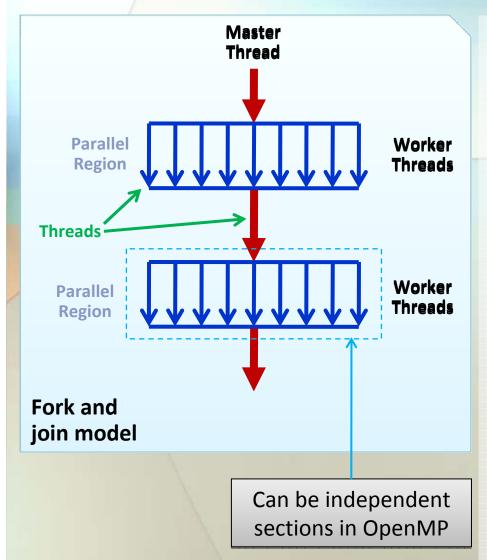
Source: NVIDIA

Hybrid algorithm execution

- CUDA = mixed serial code and parallel kernel, all in C
 - Serial C code executes in a CPU thread
 - Parallel kernel C code executes in thread blocks across multiple processing elements



CUDA similar to OpenMP



- CUDA is more scalable to massive parallelism
- CUDA is similar to OpenMP but less general
- CUDA is strictly limited to SPMT
- Single parallel function (kernel)
- Both allow incremental parallelization
- CUDA threads are very lightweight.
- How easy to program?
- Optimizing performance of CUDA programs is hard, for example Mark Harris' Optimizing Parallel Reduction in CUDA.

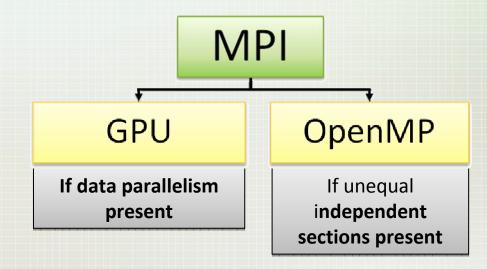
Speedup

Notation:

Speedup
$$\approx \frac{1}{\frac{f}{t} + (1-f)}$$

- f the parallel fraction
- t device speed/CPU speed
- max Speedup = 1 / (1-f)

 Multilevel Parallel processing



The hybrid computer at the University of Gdansk

Description
Tesla C1060 (NVIDIA grant)
240
1.3 GHz
4 GB (4294705152 bytes)
102 GB/sec (peak, dev to dev)
800 MHz
Intel Core i7 920C
2.8 GHz
12 GB PC-1200

Many HPC algorithms are hybrid

- Conjugate Gradient Method
- $x^{i+1} = x^i + \lambda^i p^i$

- The MRI problem requires solving large Ax=b where A is positive definite.
- The formation of A involves highly parallel matrix/matrix multiplication
 - Computational complexity: O(n³)
- In CGM The most compute intensive operation is the matrix/vector multiplication Ap
 - Computational complexity: O(n²)

CGM algorithm

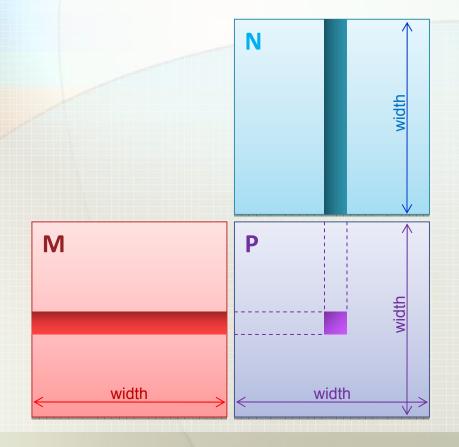
```
(x^{(0)} \in \Re^n \text{ given})
1. X := X^{(0)}
2. r := b - Ax
3. p := r
4. \alpha := ||\mathbf{r}||^2
5. while \alpha > \text{tol}^2:
   \lambda := \alpha / (p^T A p)
7. x := x + \lambda p
8. r := r - \lambda Ap
9. p := r + (||r||^2/\alpha)p
           \alpha := ||\mathbf{r}||^2
10.
11. end
Per iteration:
                        1 matrix-vector
multiplication
                         2 dot products
                         3 scalar-vector
```

multiplications

Storage: 4 vectors (x. r. n. An)

The Example

- A key mathematical computation in MRI
 - Square matrix/matrix multiplication

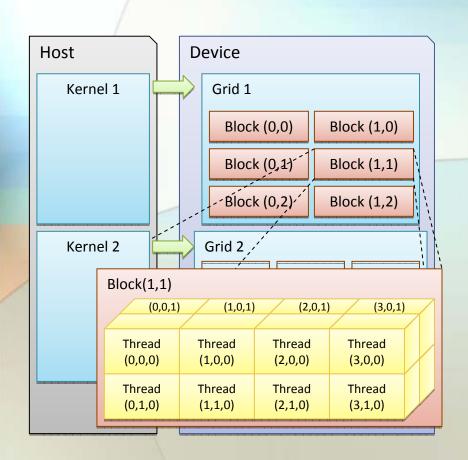


 $M \cdot N = P$

width*width independent dot products

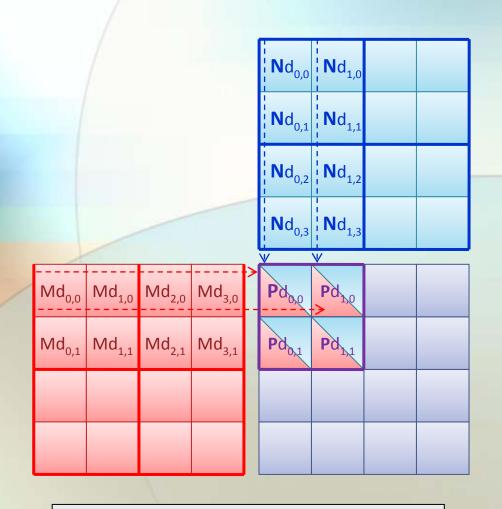
For width=1,000 we may have 1,000,000 parallel threads

Grouping of threads



- Grid contains blocks (1D or 2D).
- Blocks contain threads (1D, 2D or 3D).
- Limitation:
 - Up to 512 threads per one block.
 - If we use only one block and each element of P is calculated by one thread the largest matrix we can handle is 16x16 since 256 <512.</p>
 - For larger matrices we have to use multiple blocks.

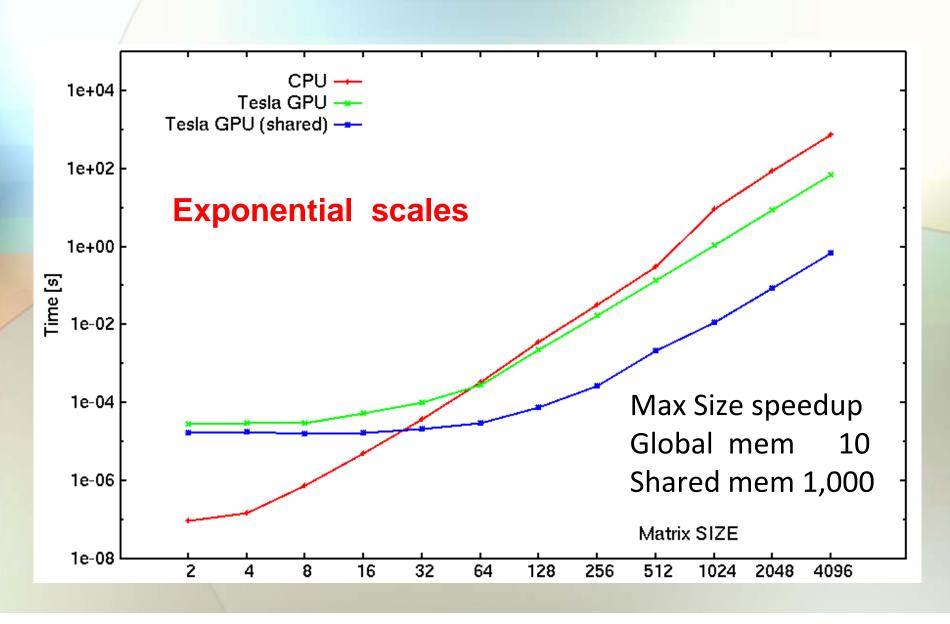
Tiling matrices to utilize shared memory



Multiplying efficiently large matrices requires Tiling

- The matrices are divided into multiple tiles and each tile of P is assigned to one block of threads.
- This way the number of threads per block does not exceed 512 and every element of P is calculated by one thread.
- The size of the tile is chosen so data can fit into the shared memory.

Relative Performance MatMult



Hybrid computer performance

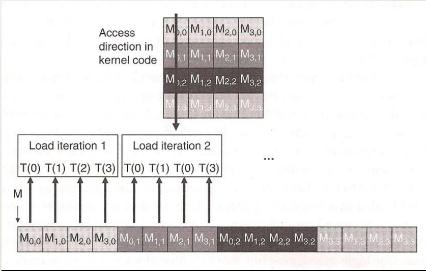
- From the performance perspective the major limitation of hybrid computation is the <u>GPU global memory bandwidth</u>.
- LOAD BALANCING
- SPMT but if-then-else instruction can split the execution path. This may cause a longer execution time and loss of performance.

Coalescing global memory access

- Small example of the memory pattern for coalescing global memory access that accelerates processing
- Information residing in shared memory does not need coalescing to achieve high speed data access.

 Global memory access coalescing takes place when the same instruction for all threads in a warp accesses consecutive global memory locations.

 In this case hardware combines (coalesces) all accesses into one consolidated and faster access.



Summary

- Hybrid computing is a paradigm discontinuity.
- IMAGINE A WORLD WHERE EVERYBODY HAS AN ACCESS TO PERSONAL SUPERCOMPUTING
 - Every researcher, information technology worker, every academic teacher has a Teraflop Computer on her desk.
 - This calls for resetting our research agenda
 - Create new programming methods for hybrid computing
 - Revisit parallel software packages (LAPACK; Jack D.) algorithms and related mathematics

Literature and References

- [1] Calvin Lin and Lawrence Snyder, *Principles of Parallel Programming*, Pearson International Edition, Addison Wesley 2009.
- [2] David B.Kirk and Wen-mei W.Hwu, *Programming Massively Parallel Processors*, Morgan Kaufmann, Elsevier 2010.
- [3] The CUDA Programming Guide, NVIDIA.
- [4] Mark Harris, Optimizing Parallel Reduction in CUDA, NVIDIA, 2007.
- [5] Liang Z.P. and Lauterbur P., *Principles of Magnetic Resonance Imaging*, A signal processing perspective, Wiley, New York, 1999.

THE END

THANK YOU

Timing data 1

SINGLE CPU Core i7 64bit 2.8GHz

SIZE	TIME	RUN COUNT
2	9.743286e-08	4096
4	1.494033e-07	2048
8	7.512598e-07	1024
16	5.197445e-06	512
32	3.879064e-05	256
64	3.382112e-04	126
128	3.561758e-03	64
256	3.198436e-02	32
512	3.056566e-01	16
1024	9.015563e+00	8
2048	8.564798e+01	4
4096	7.524644e+02	2

Times in seconds
Max time=752 sec

Timing Data 2

TESLA GPU 240 Cores 1.3GHz GLOBAL MEMORY

TIME	RUN COUNT
2.896618e-05	4096
2.955391e-05	2048
3.000104e-05	1024
5.449054e-05	512
1.006258e-04	256
2.920939e-04	126
2.319826e-03	64
1.673443e-02	32
1.333204e-01	16
1.062235e+00	8
8.486859e+00	4
6.796577e+01	2
	2.896618e-05 2.955391e-05 3.000104e-05 5.449054e-05 1.006258e-04 2.920939e-04 2.319826e-03 1.673443e-02 1.333204e-01 1.062235e+00 8.486859e+00

For the largest size matrix tested the speedup is

about 10.

Timing data 3

TESLA GPU 240 Cores 1.3GHz SHARED MEM

SIZE	TIME	RUN COUNT
2	1.689454e-05	4096
4	1.807400e-05	2048
8	1.638880e-05	1024
16	1.720564e-05	512
32	2.136294e-05	256
64	3.029413e-05	126
128	7.786980e-05	64
256	2.657310e-04	32
512	2.124511e-03	16
1024	1.163225e-02	8
2048	8.727042e-02	4
4096	6.912488e-01	2

For the largest size matrix tested the speedup is about 1,000

Workshop vs. conference

- Conference
 - We report what we have done
 - Indicate some future research plans
 - Few short discussions and panels

- Workshop
 - We discuss ideas to be explored
 - Mainly discussions and panels
 - Reports from small working groups