Rock' em Graphic Cards

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27.12.2013, 16:00

Layout

Layout

Big

Data

Big

Data

Buzz word for: “Pattern Recognition in large Datasets“

Pillar and Jets HH 901/902

NASA, ESA, and M. Livio and the Hubble 20th Anniversary Team (STScI) • Hubble Space Telescope WFC3/UVIS • STScI-PRC10-13e

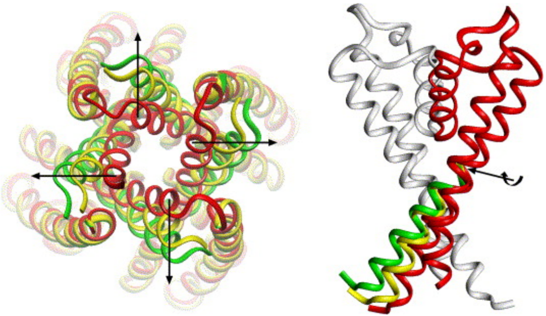

Figure: hERG - Possible Opening Movement[1]

[1] http://dx.doi.org/10.1016/j.bmcl.2005.01.008

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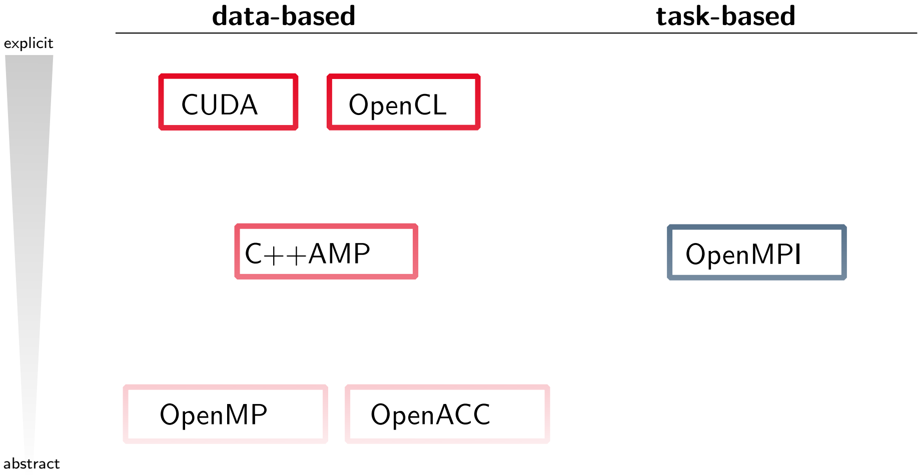
Layout

Parallelism



Parallelism

data-based	task-based

Types of Parallelism

Data-Parallelism

- Fry omelets for 8.000 people.

Task-Parallelism

- Cook a 5-course menu for one person.

Cook a menu for 8.000 people with an omelet as part of the dessert.

PP - Possible Problems

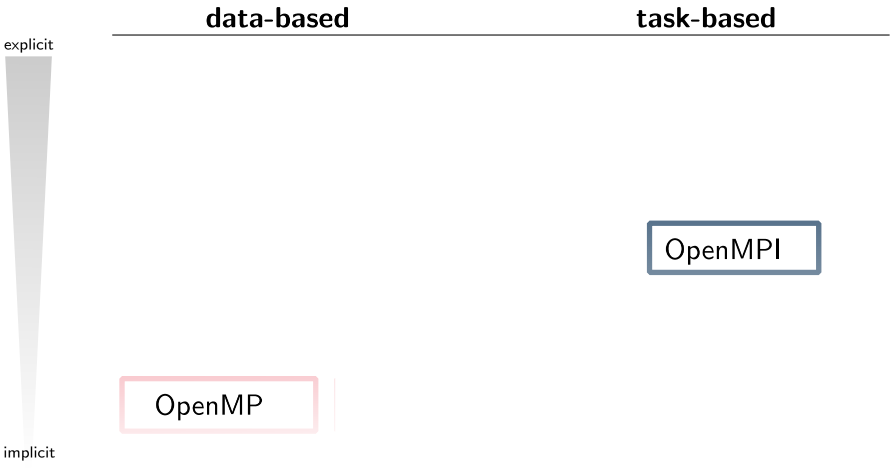
- Kitchen too small
- Only apprentices available
- Not enough frying pans
- Delivery paths too small (only one can access the fridge)
- Only one can write a new recipe into the book
- Transport 30 eggs in one go
- Serve the courses in the correct order

PP - Possible Problems

Kitchen too small	⇒	Global capacity limitation
Only apprentices available	⇒	Processor complexity limited
Not enough frying pans	⇒	Concurrent task number limited
Delivery paths too small (only one can access the fridge)	⇒	Band width limitation
Only one can write a new recipe into the book	⇒	Read-write access limitation
Transport 30 eggs in one go	⇒	coalescing memory access
Serve the courses in the correct order	⇒	Synchronization issues

Layout

Parallelism - Old Standards



OpenMPI - Installation Sprint

OpenMPI is one implementation of the standard MPI.

- Install openmpi and its devel packages
- Switch linker and compiler to mpicc
- Compile: `mpicc -I/usr/lib64/mpi/gcc/openmpi/include ...`
- Link: `mpicc -o "openmpi" ./src/openmpi.o -lmpi`
- Run code with: `mpirun -np 1 -hostfile hostfile ./openmpi`

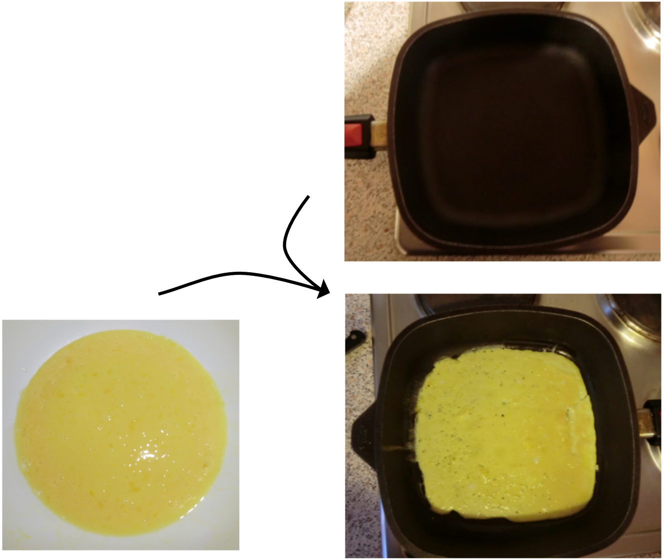
hostfile: a file with the names of usable hosts. "localhost" is fitting for testing purposes.
Dcoumentation: `http://www.open-mpi.org/`

OpenMPI - "Hello World"[2]

```c
#include <stdio.h>
#include <stdlib.h>
#include <mpi.h>

int main(int argc, char *argv[]) {
  int numprocs, rank, namelen;
  char processor_name[MPI_MAX_PROCESSOR_NAME];

  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  MPI_Get_processor_name(processor_name, &namelen);

  printf("Process %d on %s out of %d\n",
  rank, processor_name, numprocs);

  //cook one course per task ?

  MPI_Finalize();
}
```

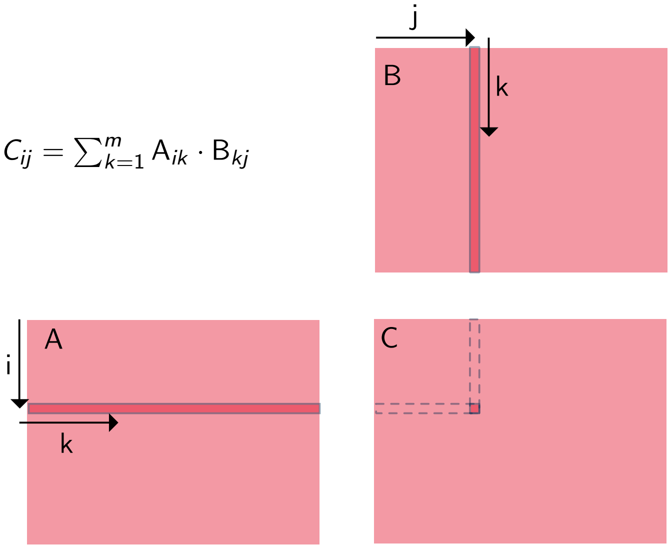
[2] http://www.linux-mag.com/id/5759/

Typical (Parallel) Task: Matrix-Multiplication



Matrix-Multiplication[3]

$$C_{ij} = \sum_{k=1}^{m} A_{ik} \cdot B_{kj}$$



[3] https://en.wikipedia.org/wiki/Matrix_multiplication

Matrix-Multiplication

```
const int NUM_ROWS_A  = 200;
const int NUM_COLS_A  = 300;
const int NUM_ROWS_B  = NUM_COLS_A;
const int NUM_COLS_B  = 400;

int *A = fillMatrix(NUM_ROWS_A, NUM_COLS_A);
int *B = fillMatrix(NUM_ROWS_B, NUM_COLS_B);
int *C =  (int*)malloc(sizeof(int)*NUM_ROWS_A  * NUM_COLS_B);

for (unsigned int i=0; i < NUM_ROWS_A; i++)
{
  for(unsigned int  j=0; j != NUM_COLS_B; ++j)
  {
    C[i*NUM_COLS_B +j] = 0;
    for(unsigned int  k=0; k != NUM_COLS_A; ++k)
    {
      C[i*NUM_COLS_B +j] += A[i*NUM_COLS_A +k ]
        * B[k*NUM_COLS_B +j ];
    }
  }
}
// Do what you need with C ...
free(A); free(B); free(C);
```

OpenMP - "Hello World"[4]

```c
#include <stdio.h>
#include <stdlib.h>
#include <omp.h>

int main(void) {
  //everything in the bracket is parallel!
  #pragma omp parallel
  {
  printf("Hello World !! This program has %d threads.. "
    "This line is printed by Thread: %d \n",
    omp_get_num_threads(),
    omp_get_thread_num());
  }
  return EXIT_SUCCESS;
}
```

[4] http://www.linux-mag.com/id/5759/

OpenMP - Matrix-Multiplication I

```
#include <stdio.h>
#include <stdlib.h>
#include <omp.h>

int * fillMatrix(const int num_rows, const int num_cols)
{
  int i;
  int *pointer = (int*)malloc(sizeof(int)*num_cols * num_rows);
  for(i = 0; i < num_cols * num_rows; i++) {
    pointer[i] = i;
  }
  return pointer;
}

int main(void) {
  const int NUM_ROWS_A = 2;
  const int NUM_COLS_A = 3;
  const int NUM_ROWS_B = NUM_COLS_A ;
  const int NUM_COLS_B = 4;

  int *A = fillMatrix(NUM_ROWS_A, NUM_COLS_A);
  int *B = fillMatrix(NUM_ROWS_B, NUM_COLS_B);
  int *C =  (int*)malloc(sizeof(int)*NUM_ROWS_A  * NUM_COLS_B);
```

OpenMP - Matrix-Multiplication II

```
//everything in the bracket is parallel!
#pragma omp parallel
{
  printf("Hello World! This program has %d threads.. "
      "This line is printed by Thread: %d \n",
      omp_get_num_threads(),
      omp_get_thread_num());
  for(unsigned int i = 0; i != NUM_ROWS_A; ++i)
  {
    for(unsigned int j=0; j != NUM_COLS_B; ++j)
    {
      C[i*NUM_COLS_B +j] = 0;
      for(unsigned int k=0; k != NUM_COLS_A; ++k)
      {
        C[i*NUM_COLS_B +j] += A[i*NUM_COLS_A +k ]
          * B[k*NUM_COLS_A +j ];
        printf( "C[%d, %d] is calculated by Thread: %d \n",
            i, j, omp_get_thread_num());
      }
    }
  }
} // end pragma
```

OpenMP - Matrix-Multiplication III

```
    for(unsigned int i = 0; i != NUM_ROWS_A; ++i)
    {
      for(unsigned int j=0; j != NUM_COLS_B; ++j)
      {
        printf( "Row: %d Column: %d Value: %d\n" , i,  j,
          C[i*NUM_COLS_B +j]);
      }
    }

    free(A);
    free(B);
    free(C);
    return EXIT_SUCCESS;
}
```

OpenMP MM- Output

```
  Hello World! This program has 4 threads..
    This line is printed by Thread: 2
C[0, 0] is calculated by Thread: 2
....
Hello World! This program has 4 threads..
    This line is printed by Thread: 3
C[0, 0] is calculated by Thread: 3
...
Hello World! This program has 4 threads..
    This line is printed by Thread: 0
Hello World! This program has 4 threads..
    This line is printed by Thread: 1
C[0, 0] is calculated by Thread: 1
...
```

OpenMP - Matrix-Multiplication IV

```
  int i, j, k, chunk;
...
  const int CHUNKSIZE = 4;
...
  chunk = CHUNKSIZE;

  #pragma omp parallel shared(A,B,C,chunk, i) private(j, k)
  {
    printf("Numer of launched threads: %d\n",
      omp_get_num_threads());
    #pragma omp for schedule(dynamic,chunk) nowait
    for (i=0; i < NUM_ROWS_A; i++)
    {
      for(j=0; j != NUM_COLS_B; ++j)
      {
        C[i*NUM_COLS_B +j] = 0;
        for(k=0; k != NUM_COLS_A; ++k)
        {
          C[i*NUM_COLS_B +j] += A[i*NUM_COLS_A +k ]
            * B[k*NUM_COLS_B +j ];
        }
      }
    } /* end of parallel for loop */
  }  /* end of parallel section */
```

OpenMP - Installation Sprint

- Install libgomp
- Compile: `gcc -fopenmp ...`
- Link: `gcc -o "openmp" ./src/openmp.o -lgomp`

Documentation: `http://www.openmp.org/mp-documents/OpenMP4.0.0.pdf`

Layout

Motivation

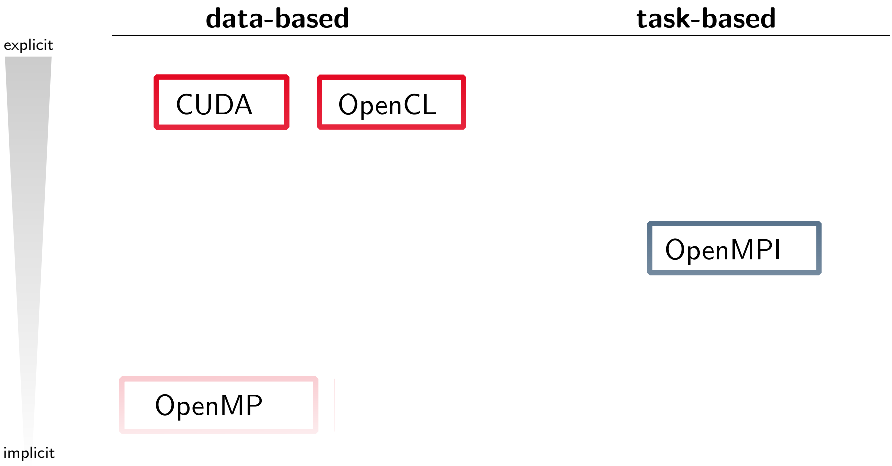
Parallelism

Old Standards
- OpenMPI
- OpenMP

Accelerator Cards
- CUDA
- OpenCL
- OpenACC
- Hardware
- C++AMP

The End

Parallelism



Accelerator Terminology

Some words:

- Host = master thread, often CPU
- Device = helper threads, often on accelerator cards
- Kernel = functions, running on the device

Some words:

- In order to run OpenCL- or CUDA-Code, please install the proprietary drivers for your graphic card!

CUDA- Matrix Multiplication I

```
#include <stdio.h>
#include <stdlib.h>

__global__ void matrixMultiply(int *A, int *B, int *C,
    int NUM_ROWS_A, int NUM_COLS_A,
    int NUM_ROWS_B, int NUM_COLS_B,
    int NUM_ROWS_C, int NUM_COLS_C) {
  int row = blockIdx.x * blockDim.x + threadIdx.y;
  int col = blockIdx.x * blockDim.x + threadIdx.x;

  if((row < NUM_ROWS_C) && (col < NUM_COLS_C))
  {
    int sum = 0;
    for (int k = 0; k < NUM_COLS_A; ++k)
    {
      sum += A[row*NUM_COLS_A + k] * B[k*NUM_COLS_B + col];
    }
    C[row*NUM_COLS_C+col] = sum;
  }

}

int main(void) {
```

CUDA - Matrix-Multiplication II

```
int *A = fillMatrix(NUM_ROWS_A, NUM_COLS_A);
int *B = fillMatrix(NUM_ROWS_B, NUM_COLS_B);
int *C =  (int*)malloc(sizeof(int)*NUM_ROWS_C  * NUM_COLS_C);
for(int i = 0; i != NUM_ROWS_C  * NUM_COLS_C; ++i)
{
  C[i] = -1;
}

cudaMalloc((void**) &dA, NUM_ROWS_A*NUM_COLS_A*sizeof(int));
cudaMalloc((void**) &dB, NUM_ROWS_B*NUM_COLS_B*sizeof(int));
cudaMalloc((void**) &dC, NUM_ROWS_C*NUM_COLS_C*sizeof(int));

cudaMemcpy(dA, A, NUM_ROWS_A*NUM_COLS_A*sizeof(int), cudaMemcpyHostToDevice);
cudaMemcpy(dB, B, NUM_ROWS_B*NUM_COLS_B*sizeof(int), cudaMemcpyHostToDevice);

// Initialize the grid and block dimensions here
dim3 dimGrid(1, 1,1);
dim3 dimBlock(NUM_COLS_C, NUM_ROWS_C, 1);

// Launch the GPU Kernel here
matrixMultiply<<<dimGrid, dimBlock>>>(dA, dB, dC, NUM_ROWS_A, NUM_COLS_A,
    NUM_ROWS_B, NUM_COLS_B, NUM_ROWS_C, NUM_COLS_C);
```

CUDA - Matrix-Multiplication III

```
    cudaThreadSynchronize();

    // Copy the GPU memory back to the CPU here
    cudaMemcpy(C, dC, NUM_ROWS_C*NUM_COLS_C*sizeof(int), cudaMemcpyDeviceToHost);

    cudaFree(dC);
    cudaFree(dB);
    cudaFree(dA);

    // Do what you need with C ...

    free(A);
    free(B);
    free(C);
    return EXIT_SUCCESS;
}
```

CUDA- Matrix Multiplication I

```
__global__ void matrixMultiply(int *A, int *B, int *C, int NUM_ROWS_A, int NUM_CO
    int NUM_ROWS_B, int NUM_COLS_B, int NUM_ROWS_C, int NUM_COLS_C) {
  int row = blockIdx.x * blockDim.x + threadIdx.y;
  int col = blockIdx.x * blockDim.x + threadIdx.x;

  if((row < NUM_ROWS_C) && (col < NUM_COLS_C))
  {
    int sum = 0;
    for (int k = 0; k < NUM_COLS_A; ++k)
    {
      sum += A[row*NUM_COLS_A + k] * B[k*NUM_COLS_B + col];
    }
    C[row*NUM_COLS_C+col] = sum;
  }
}

int main(void){

  dim3 dimGrid(1, 1,1);
  dim3 dimBlock(NUM_COLS_C, NUM_ROWS_C, 1);

  matrixMultiply<<<dimGrid, dimBlock>>>(dA, dB, dC, NUM_ROWS_A, NUM_COLS_A,
      NUM_ROWS_B, NUM_COLS_B, NUM_ROWS_C, NUM_COLS_C);
  cudaThreadSynchronize();
```

CUDA - Installation Sprint

- Install CUDA SDK and your os CUDA package (check compatibility of gcc!)
- Compile: `nvcc ... --compiler-bindir /path/to/special/gcc`
- Link: `gcc -L/usr/local/cuda/lib64 ... -lcudart`?

Documentation: `http://docs.nvidia.com/cuda/`

OpenCL - Vector Addition I[5]

```c
#include <stdio.h>
#include <stdlib.h>
#ifdef __APPLE__
#include <OpenCL/opencl.h>
#else
#include <CL/cl.h>
#endif

#define MAX_SOURCE_SIZE (0x100000)

int main(void) {
  // Create the two input vectors
  int i;
  const int LIST_SIZE = 1024;
  int *A = (int*)malloc(sizeof(int)*LIST_SIZE);
  int *B = (int*)malloc(sizeof(int)*LIST_SIZE);
  for(i = 0; i < LIST_SIZE; i++) {
    A[i] = i;
    B[i] = LIST_SIZE - i;
  }
```

[5] http://www.thebigblob.com/getting-started-with-opencl-and-gpu-computing/

OpenCL - Vector Addition II

```
// Load the kernel source code into the array source_str
FILE *fp;
char *source_str;
size_t source_size;
fp = fopen("src/vector_add_kernel.cl", "r");
if (!fp) {
  fprintf(stderr, "Failed to load kernel.\n");
  exit(1);
}
source_str = (char*)malloc(MAX_SOURCE_SIZE);
source_size = fread( source_str, 1, MAX_SOURCE_SIZE, fp);
fclose( fp );

// Get platform and device information
cl_platform_id platform_id = NULL;
cl_device_id device_id = NULL;
cl_uint ret_num_devices;
cl_uint ret_num_platforms;
cl_int ret = clGetPlatformIDs(1, &platform_id, &ret_num_platforms);
ret = clGetDeviceIDs( platform_id, CL_DEVICE_TYPE_GPU, 1,
    &device_id, &ret_num_devices);
```

OpenCL - Vector Addition III

```
// Create an OpenCL context
cl_context context = clCreateContext( NULL, 1, &device_id,
  NULL, NULL, &ret);
// Create a command queue
cl_command_queue command_queue = clCreateCommandQueue(
  context, device_id, 0, &ret);
// Create memory buffers on the device for each vector
cl_mem a_mem_obj = clCreateBuffer(context, CL_MEM_READ_ONLY,
  LIST_SIZE * sizeof(int), NULL, &ret);
cl_mem b_mem_obj = clCreateBuffer(context, CL_MEM_READ_ONLY,
  LIST_SIZE * sizeof(int), NULL, &ret);
cl_mem c_mem_obj = clCreateBuffer(context, CL_MEM_WRITE_ONLY,
  LIST_SIZE * sizeof(int), NULL, &ret);
// Copy the lists A and B to their respective memory buffers
ret = clEnqueueWriteBuffer(command_queue, a_mem_obj,
  CL_TRUE, 0, LIST_SIZE * sizeof(int), A, 0, NULL, NULL);
ret = clEnqueueWriteBuffer(command_queue, b_mem_obj,
  CL_TRUE, 0, LIST_SIZE * sizeof(int), B, 0, NULL, NULL);
// Create a program from the kernel source
cl_program program = clCreateProgramWithSource(context, 1,
  (const char **)&source_str, (const size_t *)&source_size,
  &ret);
```

OpenCL - Vector Addition IV

```
// Build the program
ret = clBuildProgram(program, 1, &device_id, NULL,
  NULL, NULL);

// Create the OpenCL kernel
cl_kernel kernel = clCreateKernel(program,
  "vector_add", &ret);

// Set the arguments of the kernel
ret = clSetKernelArg(kernel, 0, sizeof(cl_mem),
  (void *)&a_mem_obj);
ret = clSetKernelArg(kernel, 1, sizeof(cl_mem),
  (void *)&b_mem_obj);
ret = clSetKernelArg(kernel, 2, sizeof(cl_mem),
  (void *)&c_mem_obj);

// Execute the OpenCL kernel on the list
size_t global_item_size = LIST_SIZE; // Process the entire lists
size_t local_item_size = 64; // Process in groups of 64
ret = clEnqueueNDRangeKernel(command_queue, kernel, 1,
  NULL, &global_item_size, &local_item_size, 0, NULL, NULL);
```

OpenCL - Vector Addition V[6]

```
    // Read the memory buffer C on the device to the local variable C
   int *C = (int*)malloc(sizeof(int)*LIST_SIZE);
   ret = clEnqueueReadBuffer(command_queue, c_mem_obj,
     CL_TRUE, 0, LIST_SIZE * sizeof(int), C, 0, NULL, NULL);
   // Display the result to the screen
   for(i = 0; i < LIST_SIZE; i++)
     printf("%d + %d = %d\n", A[i], B[i], C[i]);
   // Clean up
   ret = clFlush(command_queue);
   ret = clFinish(command_queue);
   ret = clReleaseKernel(kernel);
   ret = clReleaseProgram(program);
   ret = clReleaseMemObject(a_mem_obj);
   ret = clReleaseMemObject(b_mem_obj);
   ret = clReleaseMemObject(c_mem_obj);
   ret = clReleaseCommandQueue(command_queue);
   ret = clReleaseContext(context);
   free(A);
   free(B);
   free(C);
   return 0;
 }
```

[6] http://www.thebigblob.com/getting-started-with-opencl-and-gpu-computing/

OpenCL - Vector Addition Summary

```
  // Get platform and device information
  cl_platform_id platform_id = NULL;
  cl_device_id device_id = NULL;
  cl_uint ret_num_devices;
  cl_uint ret_num_platforms;
  cl_int ret = clGetPlatformIDs(1, &platform_id, &ret_num_platforms);
  ret = clGetDeviceIDs( platform_id, CL_DEVICE_TYPE_GPU, 1,
      &device_id, &ret_num_devices);
...
  // Execute the OpenCL kernel on the list
  size_t global_item_size = LIST_SIZE; // Process the entire lists
  size_t local_item_size = 64; // Process in groups of 64
  ret = clEnqueueNDRangeKernel(command_queue, kernel, 1,
    NULL, &global_item_size, &local_item_size, 0, NULL, NULL);
...
   // Read the memory buffer C on the device to the local variable C
  int *C = (int*)malloc(sizeof(int)*LIST_SIZE);
  ret = clEnqueueReadBuffer(command_queue, c_mem_obj,
    CL_TRUE, 0, LIST_SIZE * sizeof(int), C, 0, NULL, NULL);
```

OpenCL - Installation Sprint

- Install Khronos OpenCL-Headers and if necessary SDK of AMD/NVIDIA
- Compile: `gcc ...`
- Link: `gcc ... -lOpenCL`

Documentation:

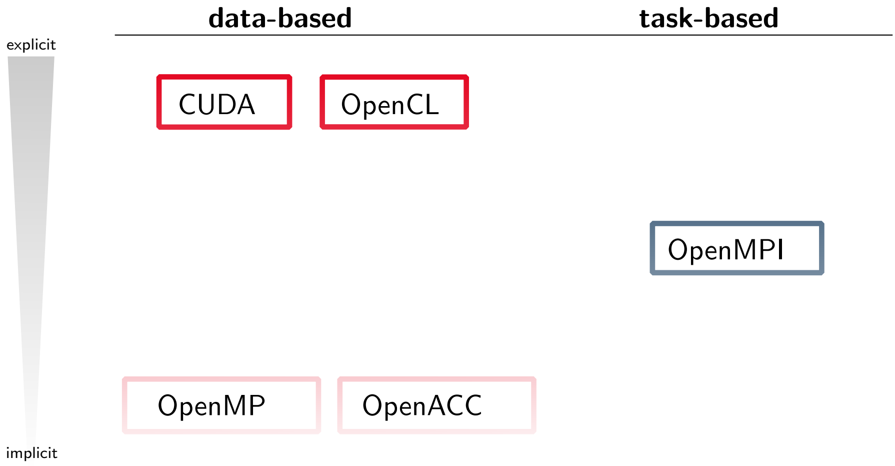
http://www.khronos.org/opencl/

http://www.khronos.org/files/opencl-1-2-quick-reference-card.pdf

General Code Structure

- Define accelerator device
- Initialize: memory on host and device
- Specify amount and dimensions of necessary kernel launches
- Launch Kernel
- Cleanup: Store result, free data

Parallelism



OpenMP - Matrix-Multiplication IV

```
#pragma omp parallel shared(A,B,C,chunk, i) private(j, k)
{
  printf("Numer of launched threads: %d\n",
    omp_get_num_threads());

  #pragma omp for schedule(dynamic,chunk) nowait
  for (i=0; i < NUM_ROWS_A; i++)
  {

    for(j=0; j != NUM_COLS_B; ++j)
    {
      C[i*NUM_COLS_B +j] = 0;
      for(k=0; k != NUM_COLS_A; ++k)
      {
        C[i*NUM_COLS_B +j] += A[i*NUM_COLS_A +k ]
          * B[k*NUM_COLS_B +j ];
      }
    }
  } /* end of parallel for loop */
}  /* end of parallel section */
```

OpenACC - Matrix-Multiplication

OpenMP:

```
    #pragma omp parallel shared(A,B,C,chunk, i) private(j, k)
    {
      #pragma omp for schedule(dynamic,chunk) nowait
      for (i=0; i < NUM_ROWS_A; i++)
      { ...
```

OpenACC:

```
    #pragma acc parallel
    {
      #pragma acc loop
      for (i=0; i < NUM_ROWS_A; i++)
      {

        for(j=0; j != NUM_COLS_B; ++j)
        {
          C[i*NUM_COLS_B +j] = 0;
          for(k=0; k != NUM_COLS_A; ++k) { ...
```

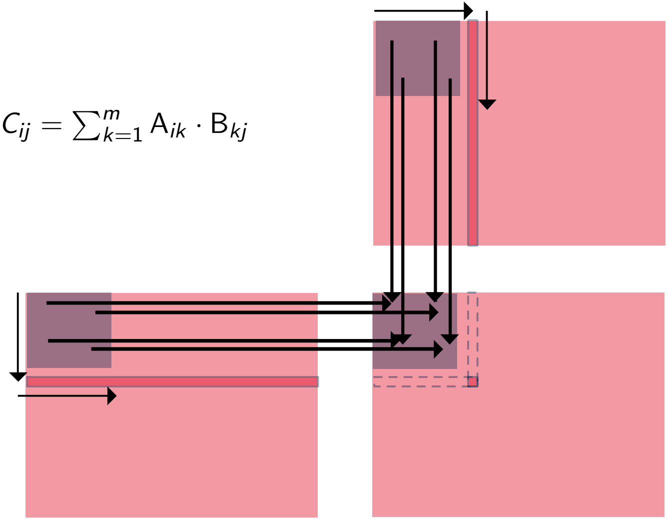
OpenACC - Installation Sprint?

Already available in cray, cups, pgi compilers.

Available in **gcc** in 2015?!

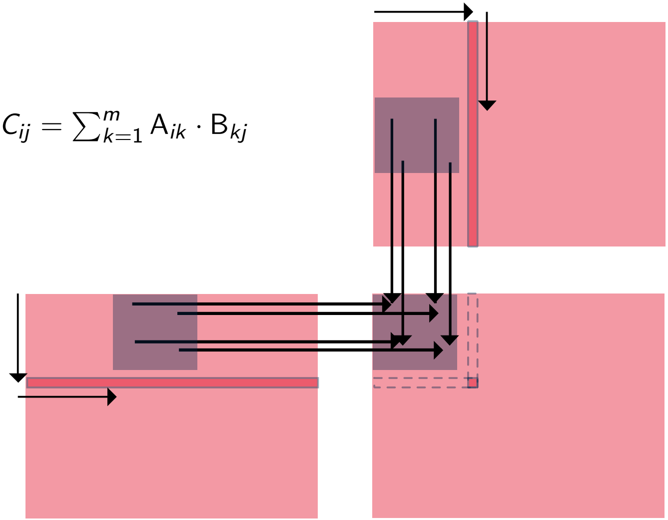
Tiled Matrix Multiplication I

$$C_{ij} = \sum_{k=1}^{m} A_{ik} \cdot B_{kj}$$



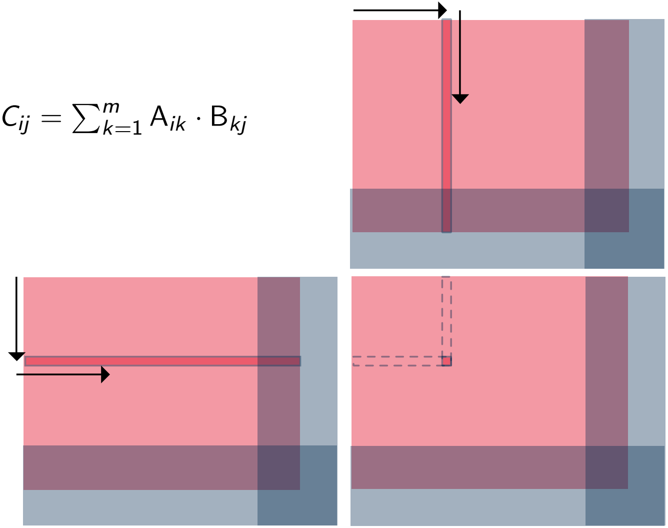
Tiled Matrix Multiplication II

$$C_{ij} = \sum_{k=1}^{m} A_{ik} \cdot B_{kj}$$

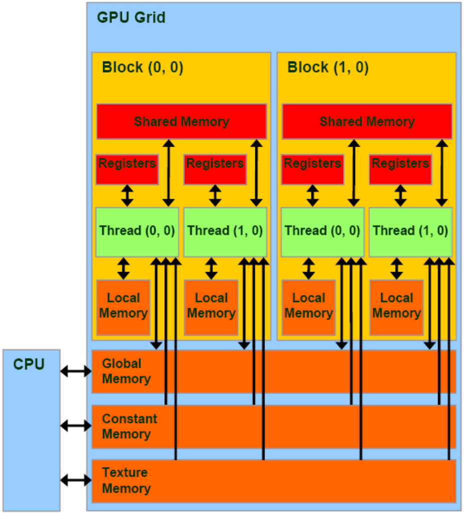


Tiled Matrix Multiplication - CUDA Warp Divergence

$$C_{ij} = \sum_{k=1}^{m} A_{ik} \cdot B_{kj}$$



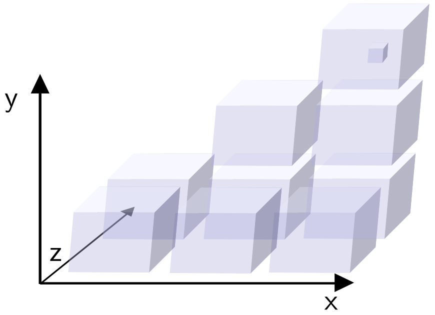
NVIDIA[7] - Simplified Architecture Scheme



[7] http://www.nvidia.com

Thread vs. Block vs. Grid Dimensions in CUDA

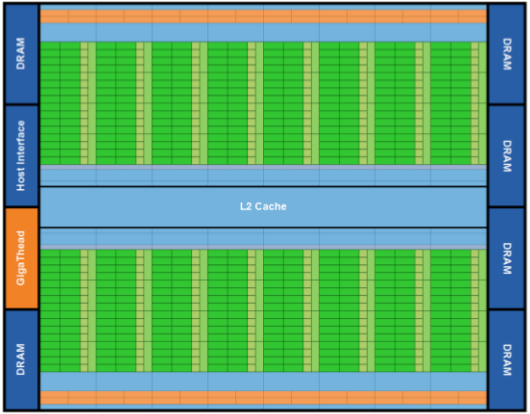
CUDA	OpenCL	OpenACC
thread	work-item	vector (worker)
block	work-group	worker / gang
grid		(gang)



Hardware

- Graphic Cards (AMD, NVIDIA)
- Xeon Phi (Intel)
- parallela (`http://parallela.org`
- FPGAs (field programmable gate arrays)

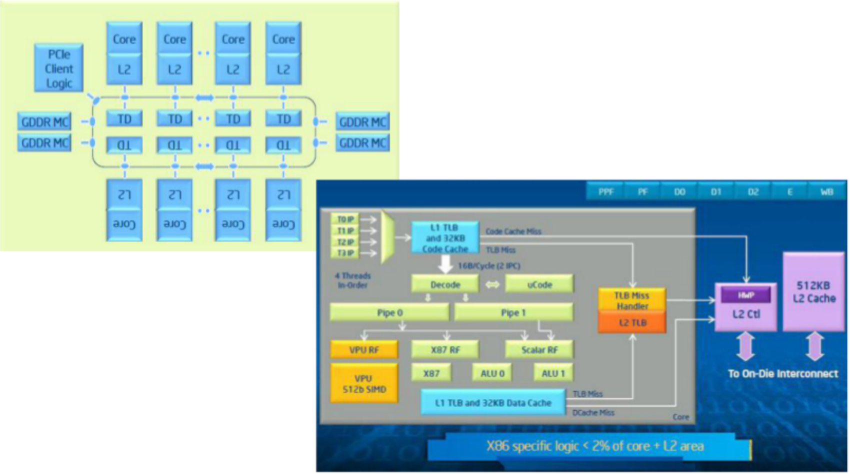
NVIDIA Tesla card[8] - 2000€



Fermi's 16 SM are positioned around a common L2 cache. Each SM is a vertical rectangular strip that contain an orange portion (scheduler and dispatch), a green portion (execution units), and light blue portions (register file and L1 cache).

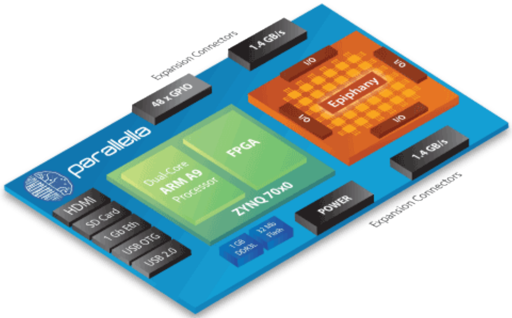
[8] http://www.nvidia.com/content/PDF/fermi_white_papers/NVIDIA_Fermi_Compute_Architecture_Whitepaper.pdf

Intel Xeon Phi[9] - 2000€



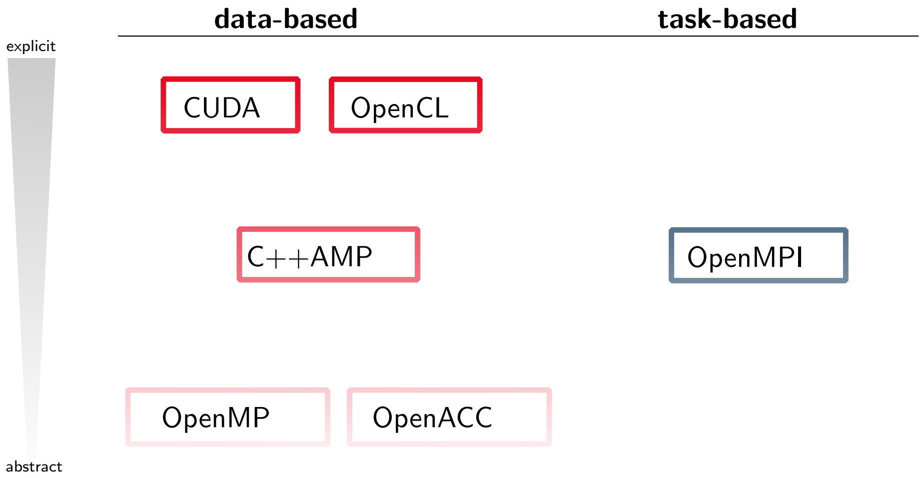
[9] http://software.intel.com/en-us/articles/intel-xeon-phi-coprocessor-codename-knights-corner

Parallela[10] - $99



10 `http://parallela.org`

Parallelism



Layout

I did not mention:

- POSIXThreads
- BOOST Threads
- Cilk (in C++: Cilk Plus)
- Intel Thread Building Blocks
- task-scheduling programs such as StarPU, oomps

... and languages such as Python with rudimentary multiprocessing abilities.

Parallelism