Scientific Computing WS 2019/2020

Lecture 28

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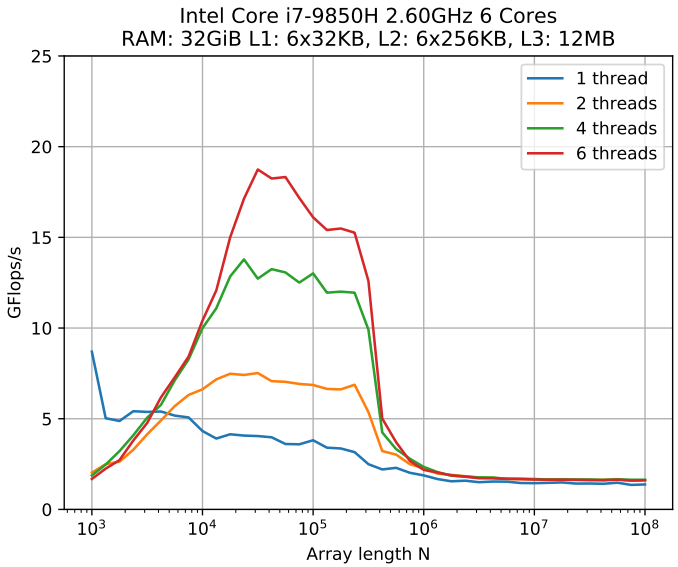
# Parallelization of vector operations

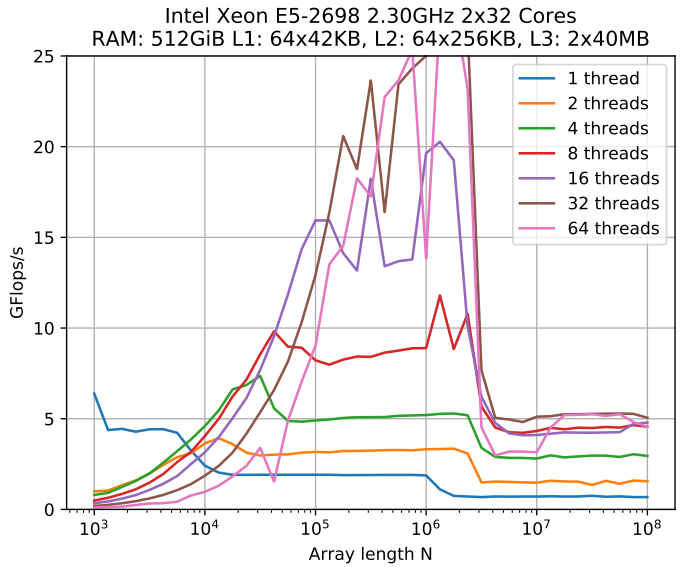
- For iterative methods it is important to parallelize vecotor operations:
  - Scalar product
  - Basic operationx
  - 'axpy' $\mathbf{x} = a\mathbf{x} + \mathbf{y}$
  - Sparse matrix $\times$ vector
- Few operations per memory access, relatively fine grained parallelism
- $\rightarrow$ benchmark this
  - STREAM benchmark
  - "Schönauer vector triad": $\mathbf{d} = \mathbf{a} + \mathbf{b} * \mathbf{c}$
    4 vectors, 2 Flops per index.

# Memory performance: vector triad I

## This laptop (gcc)




## WIAS compute server (gcc)

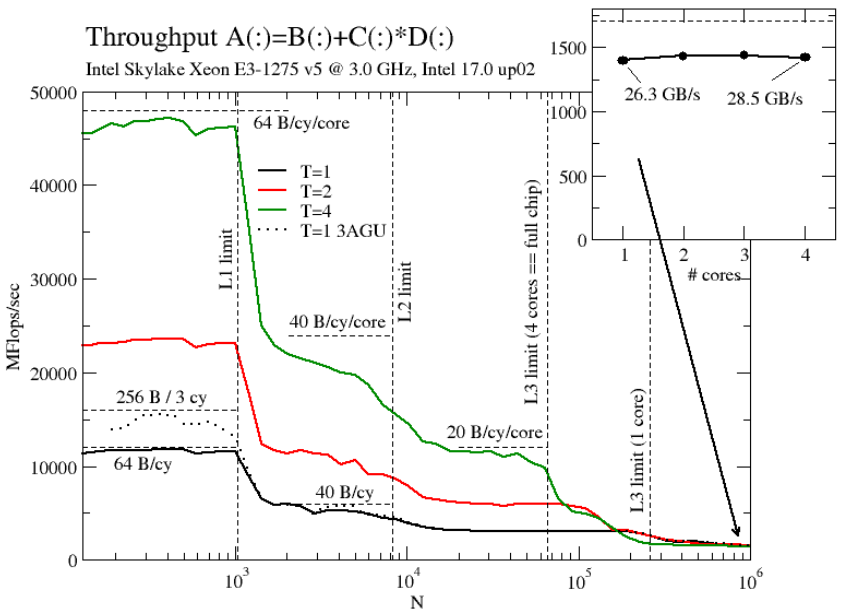



- Small problems: scalar is fastest due to scheduling overhead
- Medium problems: parallel is fast
- Large problems: no big difference due to memory bandwidth: all laptop cores access the memory through the same bottleneck
- "sweet spot" for parallel between $10^4$ and $5 \cdot 10^5 \ldots 5 \cdot 10^6$

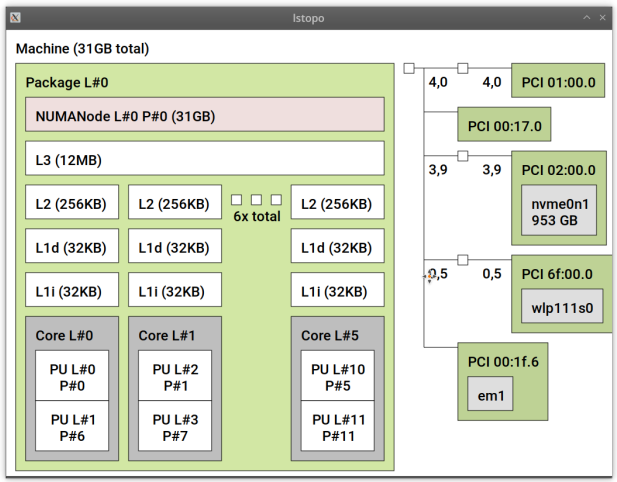
# Memory performance: vector triad II

## Benchmarking site of G. Hager

https://blogs.fau.de/hager/archives/tag/benchmarking




## lstopo for this laptop

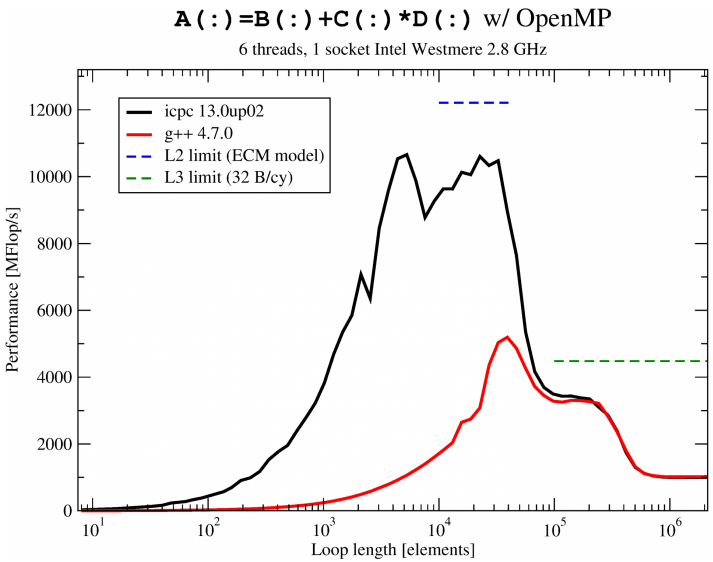



- Performance drops are correlated with cache sizes
- Most important: large L3 cache

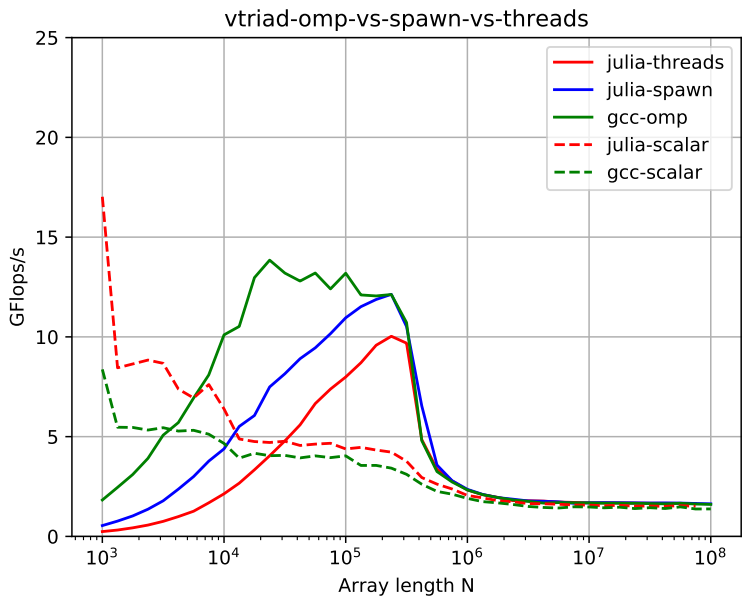
# Memory performance: vector triad III

gcc vs. icc (2013)

https://blogs.fau.de/hager/archives/tag/benchmarking




this laptop (4 threads)

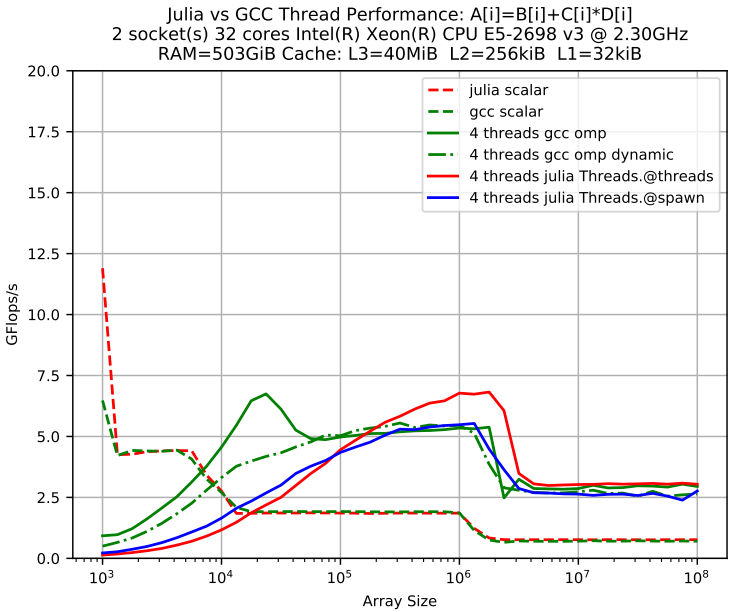



- Picture similar to early times of gnu compiler vs Intel
- Julia barrier implementation seems to need improvement
- "hand crafted" threading works better

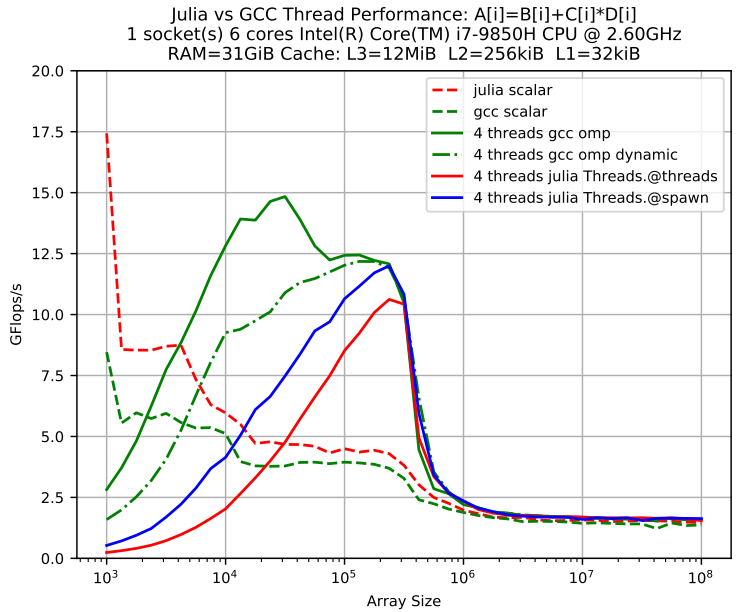
# Memory performance: vector triad IV

https://discourse.julialang.org/t/gcc-vs-threads-threads-vs-threads-spawn-for-large-loops/34273/9

## Julia vs gcc on Server




## Julia vs gcc on Laptop




- Laptop L3 cache too small for sustaining performance for large arrays
- Server has larger L3 cache and 2 sockets $\equiv$ 2 lanes to memory, $\Rightarrow$ still see paralllel speed-up for the largest case
- Julias 'Threads.@threads' performs quite well once the chunk size is large enough compared to the barrier implementation overhead

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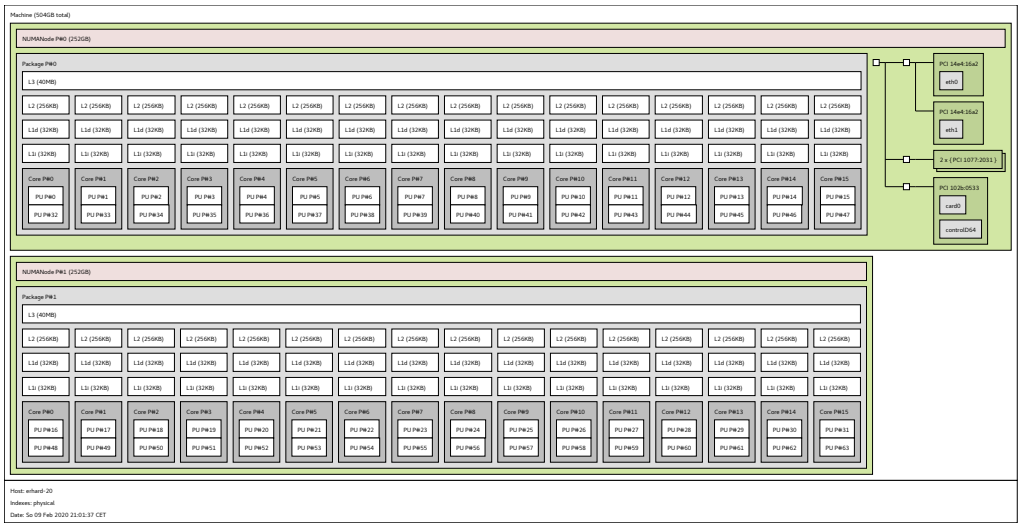
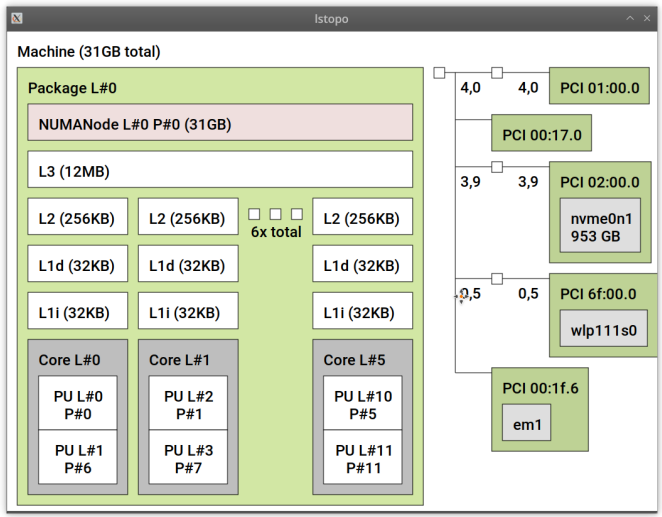
Server



Laptop

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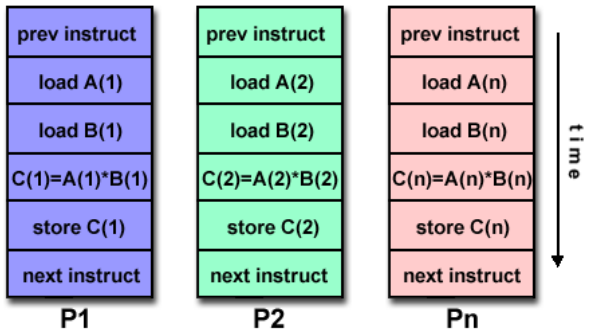
# SIMD Hardware: Graphics Processing Units ( GPU)

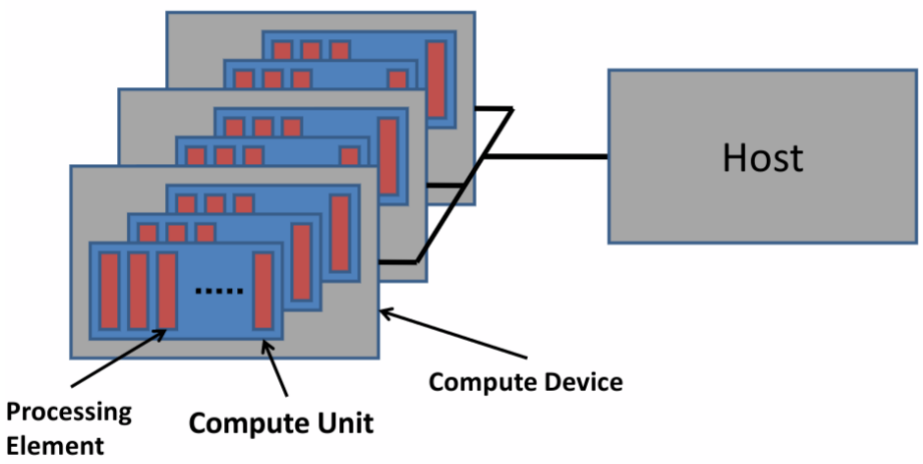


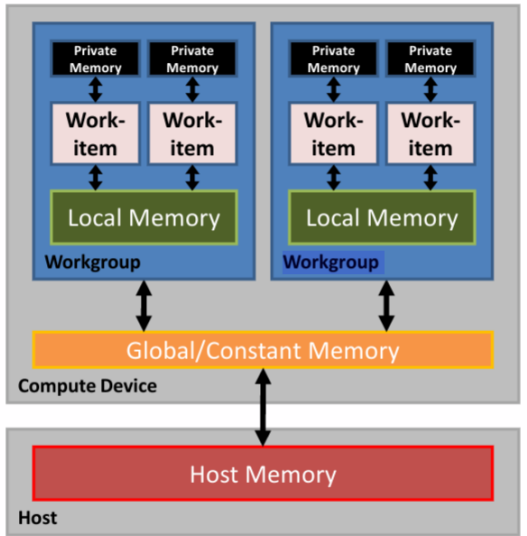

[Source: computing.llnl.gov/tutorials]

- Principle useful for highly structured data
- Example: textures, triangles for 3D graphis rendering
- During the 90's, *Graphics Processing Units* (GPUs) started to contain special purpose SIMD hardware for graphics rendering
- 3D Graphic APIs (DirectX, OpenGL) became transparent to programmers: rendering could be influenced by "shaders" which essentially are programs which are compiled on the host and run on the GPU

# General Purpose Graphics Processing Units (GPGPU)

- Graphics companies like NVIDIA saw an opportunity to market GPUs for computational purposes
- Emerging APIs which allow to describe general purpose computing tasks for GPUs: CUDA (Nvidia specific), OpenCL (ATI/AMD designed, general purpose), OpenACC based on compiler directives
- GPGPUs are *accelerator cards* added to a computer with own memory, many vector processing pipelines and special bus interconnect (NVidia Quadro GV100: 32GB +5120 units, NVLink; Tensor cores)
- CPU-GPU connection via mainbord bus / special link



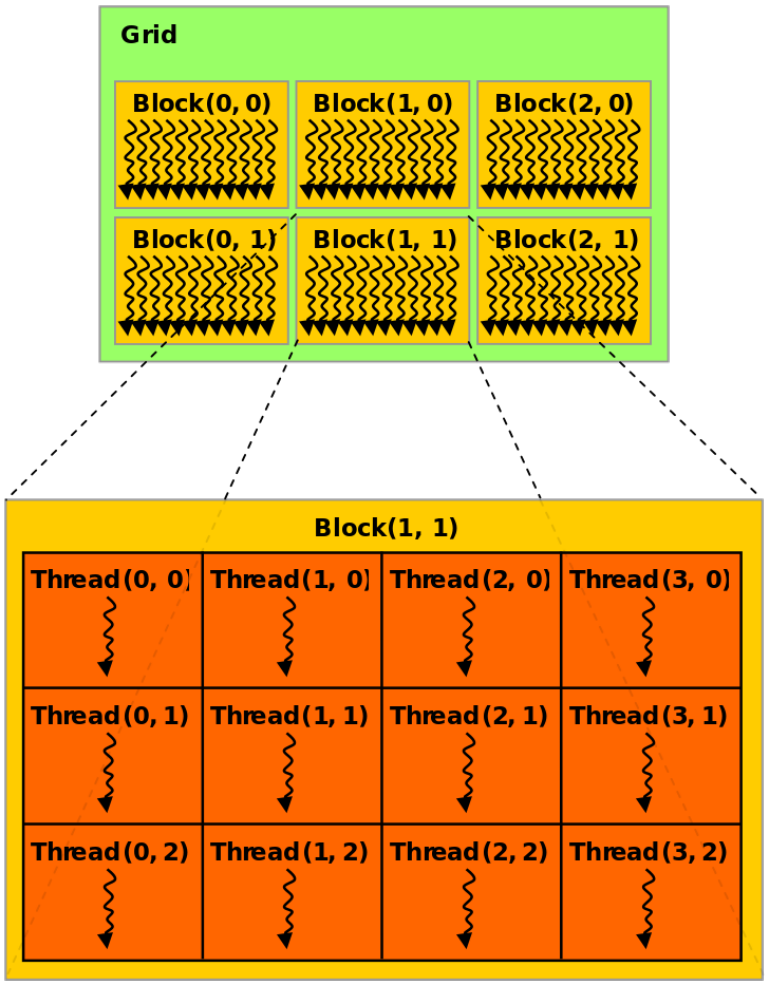
# GPU Programming paradigm

- CPU:
  - Sets up data
  - Triggers compilation of "kernels": the heavy duty loops to be executed on GPU
  - Sends compiled kernels ("shaders") to GPU
  - Sends data to GPU, initializes computation
  - Receives data back from GPU
- GPU:
  - Receive data from host CPU
  - Run the heavy duty loops in local memory
  - Send data back to host CPU
- For high performance one needs explicit management of these steps
- Bottleneck: Data transfer CPU $\leftrightarrow$ GPU
- High effiency only with good match between data structure and layout of GPU memory (2D rectangular grid)

# NVIDIA Cuda

- Established by NVIDIA GPU vendor
- Works only on NVIDIA cards
- Claimed to provide optimal performance

# CUDA Data organization




https://commons.wikimedia.org/wiki/File:Block-thread.svg

- *Threads* can be arranged in 1,2 or 3 dimensional *Blocks* and can execute a *kernel* within given 1/2/3D index range
- *Blocks* are arranged in a 2D *Grid*

# CUDA Kernel code

- The kernel code is the code to be executed on the GPU aka "Device"
- It needs to be compiled using special CUDA compiler

```
#include <cuda_runtime.h>

/*
 * CUDA Kernel Device code
 *
 * Computes the vector addition of A and B into C.
 * The 3 vectors have the same
 * number of elements numElements.
 */
__global__ void
vectorAdd(const float *A, const float *B, float *C, int numElements)
{
    int i = blockDim.x * blockIdx.x + threadIdx.x;

    if (i < numElements)
    {
        C[i] = A[i] + B[i];
    }
}
```

# CUDA Host code I

```
int main(void)
{   int numElements = 50000;
    size_t size = numElements * sizeof(float);

    // Allocate host vectors
    float *h_A = (float *)malloc(size);
    float *h_B = (float *)malloc(size);
    float *h_C = (float *)malloc(size);

    // Initialize the host input vectors
    for (int i = 0; i < numElements; ++i)
    {
        h_A[i] = rand()/(float)RAND_MAX;
        h_B[i] = rand()/(float)RAND_MAX;
    }
    // Allocate device vectors
    float *d_A = NULL;
    float *d_B = NULL;
    float *d_C = NULL;
    assert(cudaMalloc((void **)&d_A, size)==cudaSuccess);
    assert(cudaMalloc((void **)&d_B, size)==cudaSuccess);
    assert(cudaMalloc((void **)&d_C, size)==cudaSuccess);
    ...
```

# CUDA Host code II

```
...

cudaMemcpy(d_A, h_A, size, cudaMemcpyHostToDevice);
cudaMemcpy(d_B, h_B, size, cudaMemcpyHostToDevice);

// Launch the Vector Add CUDA Kernel
int threadsPerBlock = 256;
int blocksPerGrid =(numElements + threadsPerBlock - 1)
                   / threadsPerBlock;

vectorAdd<<<blocksPerGrid, threadsPerBlock>>>(d_A, d_B, d_C, numElements);

assert(cudaGetLastError()==cudaSuccess);
cudaMemcpy(h_C, d_C, size, cudaMemcpyDeviceToHost);

cudaFree(d_A);
cudaFree(d_B);
cudaFree(d_C);

free(h_A);
free(h_B);
free(h_C);
cudaDeviceReset();
```

# OpenCL

- "Open Computing Language"
- Vendor independent
- More cumbersome to code

# Example: OpenCL: computational kernel

```
__kernel void square(
    __global float* input, __global float* output)
{
    size_t i = get_global_id(0);
    output[i] = input[i] * input[i];
}
```

Declare functions with **__kernel** attribute

Defines an entry point or exported method in a program object

Use address space and usage qualifiers for memory

Address spaces and data usage must be specified for all memory objects

Built-in methods provide access to index within compute domain

Use **get_global_id** for unique work-item id, **get_group_id** for work-group, etc

[Source: http://sa10.idav.ucdavis.edu/docs/sa10-dg-opencl-overview.pdf]

# OpenCL: Resource build up, kernel creation

```
// Fill our data set with random float values
int count = 1024 * 1024;
for(i = 0; i < count; i++)
    data[i] = rand() / (float)RAND_MAX;

// Connect to a compute device, create a context and a command queue
cl_device_id device;
clGetDeviceIDs(CL_DEVICE_TYPE_GPU, 1, &device, NULL);
cl_context context = clCreateContext(0, 1, & device, NULL, NULL, NULL);
cl_command_queue queue = clCreateCommandQueue(context, device, 0, NULL);

// Create and build a program from our OpenCL-C source code
cl_program program = clCreateProgramWithSource(context, 1, (const char **) &src,
                                                NULL, NULL);
clBuildProgram(program, 0, NULL, NULL, NULL, NULL);

// Create a kernel from our program
cl_kernel kernel = clCreateKernel(program, "square", NULL);
```

[Source: http://sa10.idav.ucdavis.edu/docs/sa10-dg-opencl-overview.pdf]

# OpenCL: Data copy to GPU

```
// Allocate input and output buffers, and fill the input with data
cl_mem input = clCreateBuffer(context,  CL_MEM_READ_ONLY,  sizeof(float) * count,
                              NULL, NULL);

// Create an output memory buffer for our results
cl_mem output = clCreateBuffer(context, CL_MEM_WRITE_ONLY, sizeof(float) * count,
                               NULL, NULL);

// Copy our host buffer of random values to the input device buffer
clEnqueueWriteBuffer(queue, input, CL_TRUE, 0, sizeof(float) * count, data, 0,
                     NULL, NULL);

// Get the maximum number of work items supported for this kernel on this device
size_t global = count; size_t local = 0;
clGetKernelWorkGroupInfo(kernel, device, CL_KERNEL_WORK_GROUP_SIZE, sizeof(int),
                         &local, NULL);
```

[Source: http://sa10.idav.ucdavis.edu/docs/sa10-dg-opencl-overview.pdf]

# OpenCL: Kernel execution, result retrieval from GPU

```
// Set the arguments to our kernel, and enqueue it for execution
clSetKernelArg(kernel, 0, sizeof(cl_mem), &input);
clSetKernelArg(kernel, 1, sizeof(cl_mem), &output);
clSetKernelArg(kernel, 2, sizeof(unsigned int), &count);
clEnqueueNDRangeKernel(queue, kernel, 1, NULL, &global, &local, 0, NULL, NULL);

// Force the command queue to get processed, wait until all commands are complete
clFinish(queue);

// Read back the results
clEnqueueReadBuffer( queue, output, CL_TRUE, 0, sizeof(float) * count, results, 0,
                     NULL, NULL );

// Validate our results
int correct = 0;
for(i = 0; i < count; i++)
    correct += (results[i] == data[i] * data[i]) ? 1 : 0;

// Print a brief summary detailing the results
printf("Computed '%d/%d' correct values!\n", correct, count);
```

[Source: http://sa10.idav.ucdavis.edu/docs/sa10-dg-opencl-overview.pdf]

# OpenCL Summary

- Need good programming experience and system management skills in order to set up tool chains with properly matching versions, vendor libraries etc.
  - (I was not able to get this running on my laptop in finite time. . . )
- Very cumbersome programming, at least as explicit as MPI
- Data structure restrictions limit class of tasks which can run efficiently on GPUs.

# Compiler directive based GPU programming

- OpenMP
  - OpenMP4.0
  - Implentation in commercial compilers
  - GCC, Clang implementations under development
- OpenACC
  - Idea similar to OpenMP: use compiler directives
  - Future merge with OpenMP initially intended, now they seem to be competitors
  - Intended for different accelerator types (Nvidia GPU ...)
  - Commercial compiler vendors, e.g. PGI (with free academic license valid one year)
  - GCC, Clang implementations under development

# OpenACC code

- "Shader":

```
void vecaddgpu( float *restrict r, float *a, float *b, int n, int nrepeat)
{
  int irepeat;
  #pragma acc kernels loop present(r,a,b)
  for (irepeat=0;irepeat<nrepeat; irepeat++)
  for( int i = 0; i < n; ++i ) r[i] = a[i] + b[i] + irepeat;
}
```

- Invocation from CPU

```
a = (float*)malloc( n*sizeof(float) );
b = (float*)malloc( n*sizeof(float) );
r = (float*)malloc( n*sizeof(float) );
e = (float*)malloc( n*sizeof(float) );
#pragma acc data copyin(a[0:n],b[0:n]) copyout(r[0:n])
{
  vecaddgpu( r, a, b, n, nrepeat );
}
```

- Compile with PGI compiler (https://www.pgroup.com/)

```
pgcc -ta=tesla -fast -o add2 add2.c
```

# Other ways to program GPU

- Directly use graphics library
- Modern OpenGL with shaders
- WebGL: OpenGL in the browser. Uses html and javascript.
- Julia: CuArrays directly compile to kernel instructions

# WebGL Example

- Gray-Scott model for Reaction-Diffusion: two species.
  - $U$ is created with rate $f$ and decays with rate $f$
  - $U$ reacts wit $V$ to more $V$
  - $V$ deacays with rate $f + k$.
  - $U, V$ move by diffusion

$$1 \xrightarrow{f} U$$

$$U + 2V \xrightarrow{1} 3V$$

$$V \xrightarrow{f+k} 0$$

$$F \xrightarrow{f} 0$$

- Stable states:
  - No $V$
  - " Much of $V$, then it feeds on $U$ and re-creates itself
- Reaction-Diffusion equation from mass action law:

$$\partial_t u - D_u \Delta u + uv^2 - f(1-u) = 0$$

# Discretization

- ... GPUs are fast so we choose the explicit Euler method:

$$\frac{1}{\tau}(u_{n+1} - u_n) - D_u \Delta u_n + u_n v_n^2 - f(1 - u_n) = 0$$
$$\frac{1}{\tau}(v_{n+1} - u_v) - D_v \Delta v_n - u_n v_n^2 + (f + k)v_n = 0$$

- Finite difference/finite volume discretization on grid of size $h$

$$-\Delta u \approx \frac{1}{h^2}(4u_{ij} - u_{i-1,j} - u_{i+1,j} - u_{i,j-1} - u_{i,j+1})$$

# The shader

```
<script type="x-webgl/x-fragment-shader" id="timestep-shader">
precision mediump float;
uniform sampler2D u_image;
uniform vec2 u_size;
const float F = 0.05, K = 0.062, D_a = 0.2, D_b = 0.1;
const float TIMESTEP = 1.0;
void main() {
vec2 p = gl_FragCoord.xy,
     n = p + vec2(0.0, 1.0),
     e = p + vec2(1.0, 0.0),
     s = p + vec2(0.0, -1.0),
     w = p + vec2(-1.0, 0.0);

vec2 val = texture2D(u_image, p / u_size).xy,
     laplacian = texture2D(u_image, n / u_size).xy
    + texture2D(u_image, e / u_size).xy
    + texture2D(u_image, s / u_size).xy
    + texture2D(u_image, w / u_size).xy
    - 4.0 * val;

vec2 delta = vec2(D_a * laplacian.x - val.x*val.y*val.y + F * (1.0-val.x),
    D_b * laplacian.y + val.x*val.y*val.y - (K+F) * val.y);

gl_FragColor = vec4(val + delta * TIMESTEP, 0, 0);
```

# Why does this work so well here ?

- Data structure fits very well to topology of GPU
  - rectangular grid
  - 2 unknowns to be stored in x,y components of vec2
- No communication with CPU in the first place
- GPU speed allows to “break” time step limitation of explicit Euler
- Data stay within the graphics card: once we loaded the initial value, all computations, and rendering use data which are in the memory of the graphics card.
- Depending on the application, choose the best way to proceed
- e.g. deep learning (especially training speed)