An Introduction to OpenCL

John Stone
Theoretical and Computational Biophysics Group
Beckman Institute for Advanced Science and Technology
University of Illinois at Urbana-Champaign
http://www.ks.uiuc.edu/Research/gpu/

GPU Computing Brown Bag

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Aims of This Talk

- Give a rapid introduction to OpenCL for people that may already be somewhat familiar with GPUs and data-parallel programming concepts
- Rather than merely duplicating content found in existing OpenCL tutorials, I will delve more into details not (yet) covered in other online materials I've found
- Show a real (albeit simple) algorithm/kernel

Online OpenCL Materials

- Khronos OpenCL headers, specification, etc: http://www.khronos.org/registry/cl/
- Khronos OpenCL samples, tutorials, etc: http://www.khronos.org/developers/resources/opencl/
- AMD OpenCL Resources: http://developer.amd.com/gpu/ATIStreamSDK/pages/TutorialOpenCL.aspx
- NVIDIA OpenCL Resources: http://www.nvidia.com/object/cuda_opencl.html

What is OpenCL?

- Cross-platform parallel computing API and C-like language for heterogeneous computing devices
- Code is portable across various target devices:
  - Correctness is guaranteed
  - Performance of a given kernel is not guaranteed across differing target devices
- OpenCL implementations already exist for AMD and NVIDIA GPUs, x86 CPUs
- In principle, OpenCL could also target DSPs, Cell, and perhaps also FPGAs

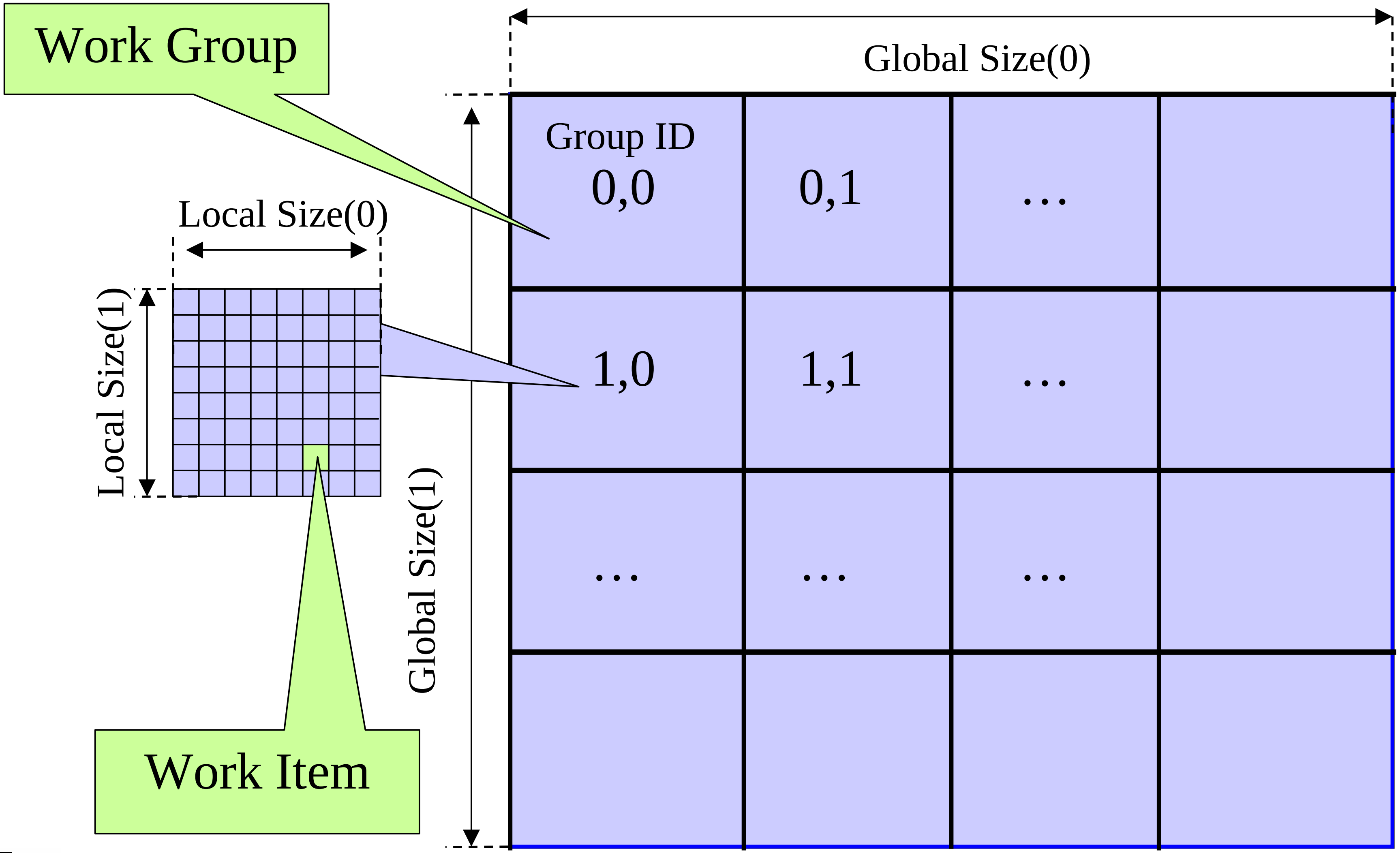
OpenCL Hardware Support

- Targets a broader range of CPU-like and GPU-like devices than CUDA
  - Targets devices produced by multiple vendors
  - Many features of OpenCL are optional and may not be supported on all devices
- OpenCL codes must be prepared to deal with much greater hardware diversity
- A single OpenCL kernel will likely not achieve peak performance on all device types

OpenCL Data Parallel Model

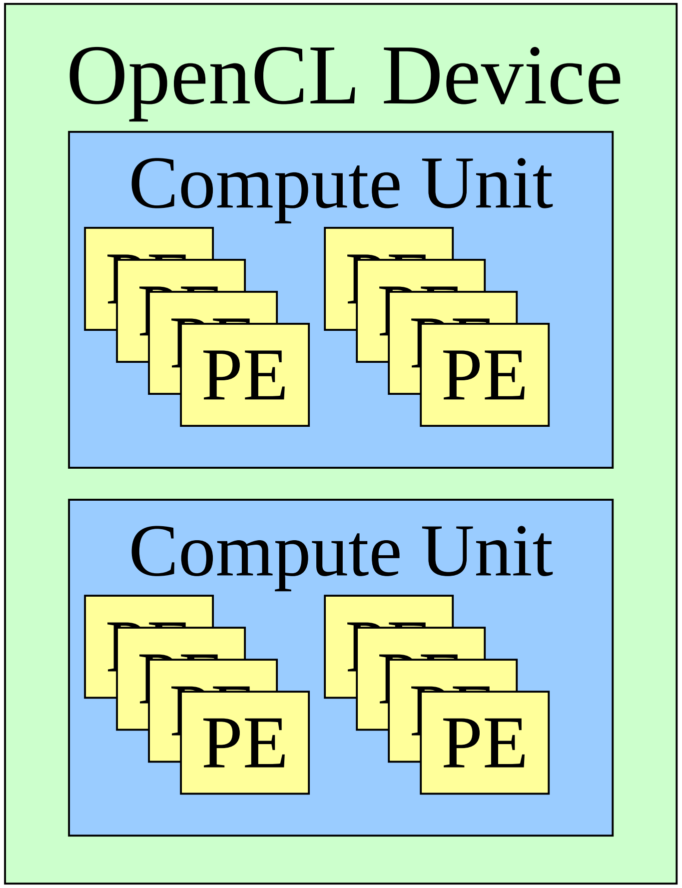
- Work is submitted to devices by launching kernels
- Kernels run over global dimension index ranges (NDRange), broken up into “work groups”, and “work items”
- Work items executing within the same work group can synchronize with each other with barriers or memory fences
- Work items in different work groups can’t sync with each other, except by launching a new kernel

OpenCL NDRange Configuration



OpenCL Hardware Abstraction

- OpenCL exposes CPUs, GPUs, and other Accelerators as “devices”
- Each “device” contains one or more “compute units”, i.e. cores, SMs, etc...
- Each “compute unit” contains one or more SIMD “processing elements”

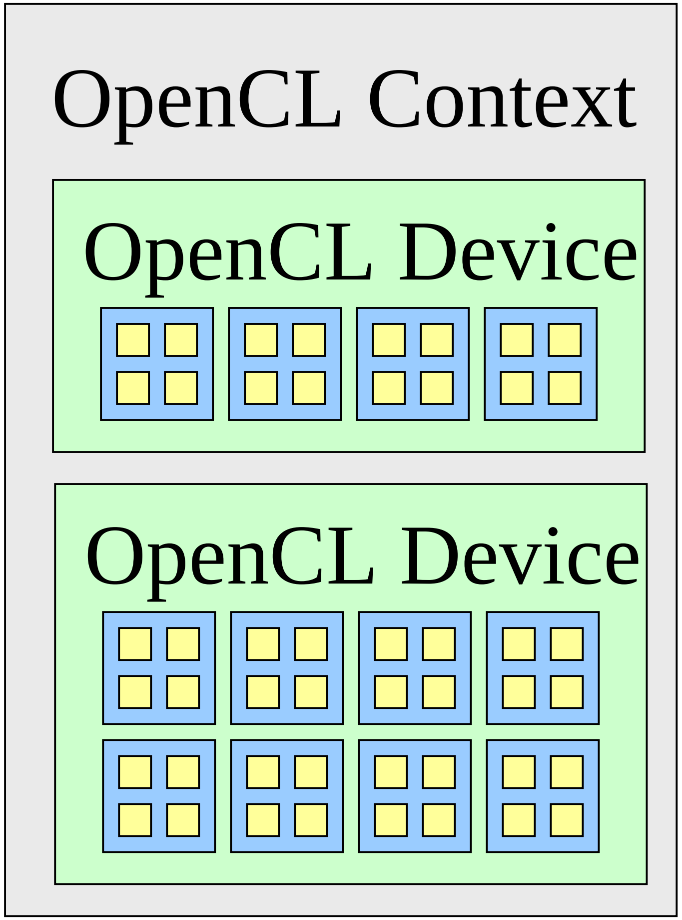


OpenCL Memory Systems

- __global – large, high latency
- __private – on-chip device registers
- __local – memory accessible from multiple PEs or work items. May be SRAM or DRAM, must query…
- __constant – read-only constant cache
- Device memory is managed explicitly by the programmer, as with CUDA
- Pinned memory buffer allocations are created using the CL_MEM_USE_HOST_PTR flag

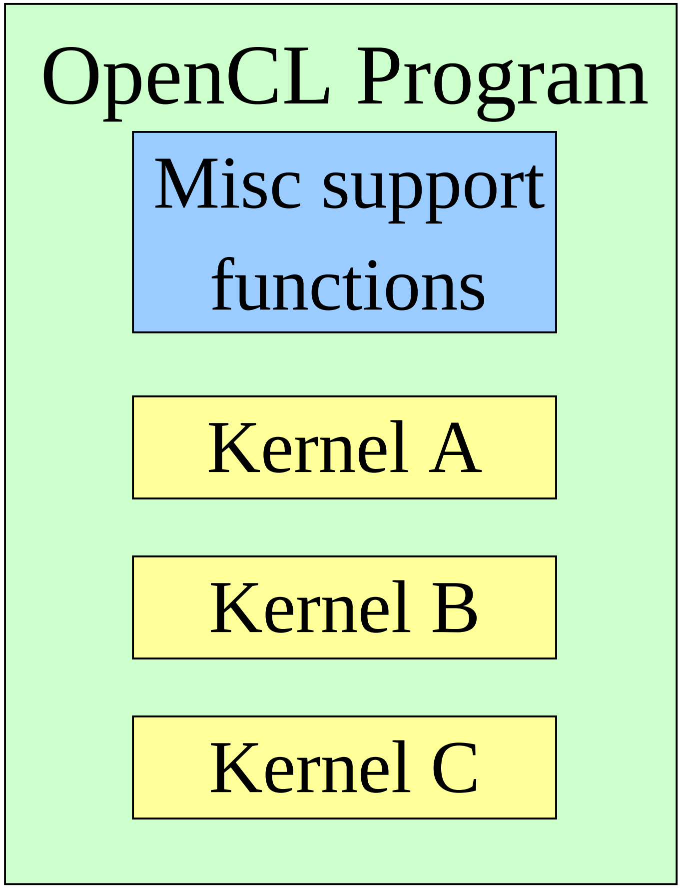
OpenCL Context

- Contains one or more devices
- OpenCL memory objects are associated with a context, not a specific device
- clCreateBuffer() emits error if an allocation is too large for any device in the context
- Each device needs its own work queue(s)
- Memory transfers are associated with a command queue (thus a specific device)



OpenCL Programs

- An OpenCL "program" contains one or more "kernels" and any supporting routines that run on a target device
- An OpenCL kernel is the basic unit of code that can be executed on a target device

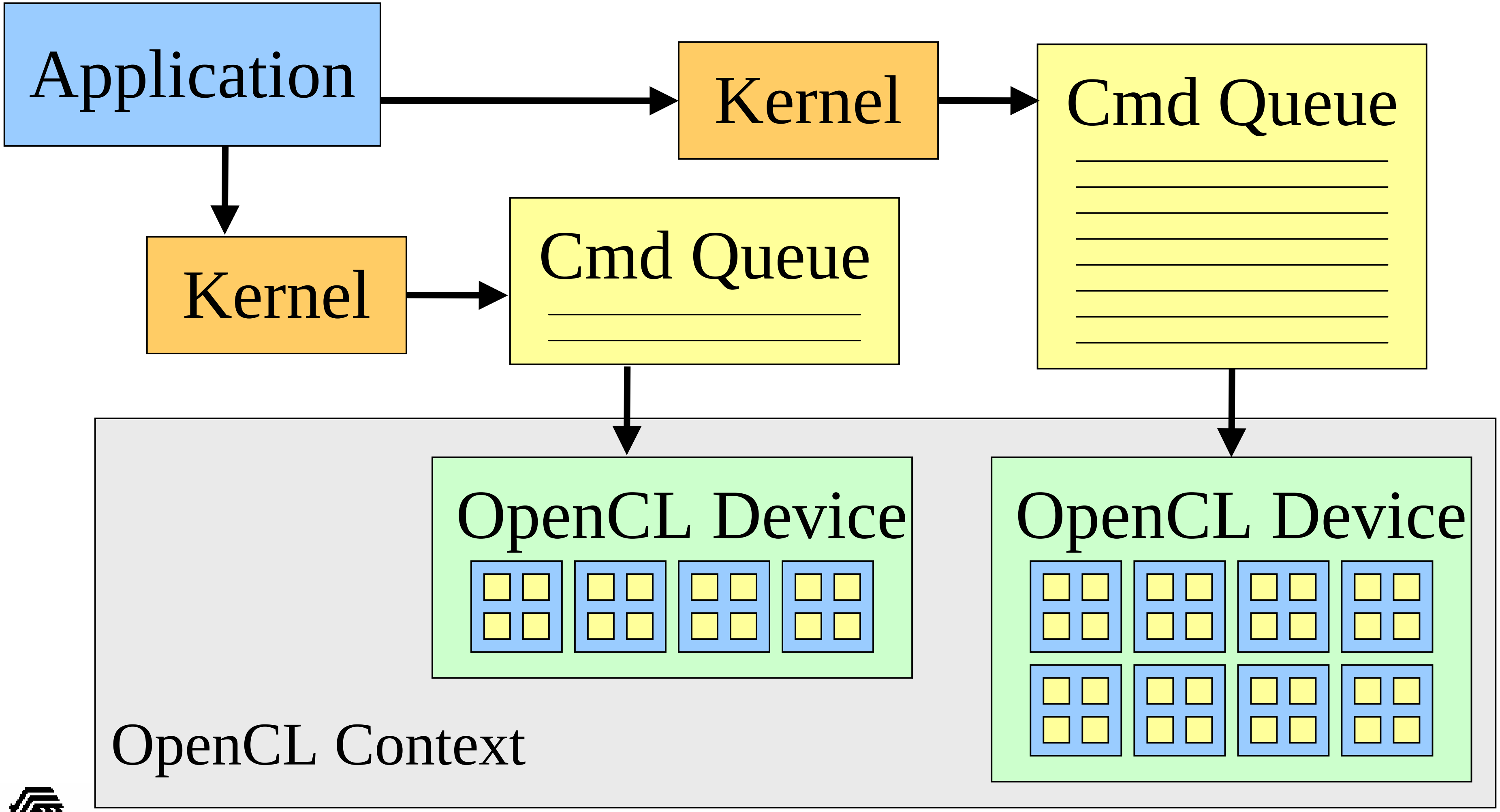


OpenCL Kernels

- Code that actually executes on target devices
- Analogous to CUDA kernels
- Kernel body is instantiated once for each work item
- Each OpenCL work item gets a unique index, like a CUDA thread does

```
__kernel void
vadd(__global const float *a,
        __global const float *b,
        __global float *result) {
  int id = get_global_id(0);
  result[id] = a[id] + b[id];
}
```

OpenCL Execution on Multiple Devices



OpenCL Application Example

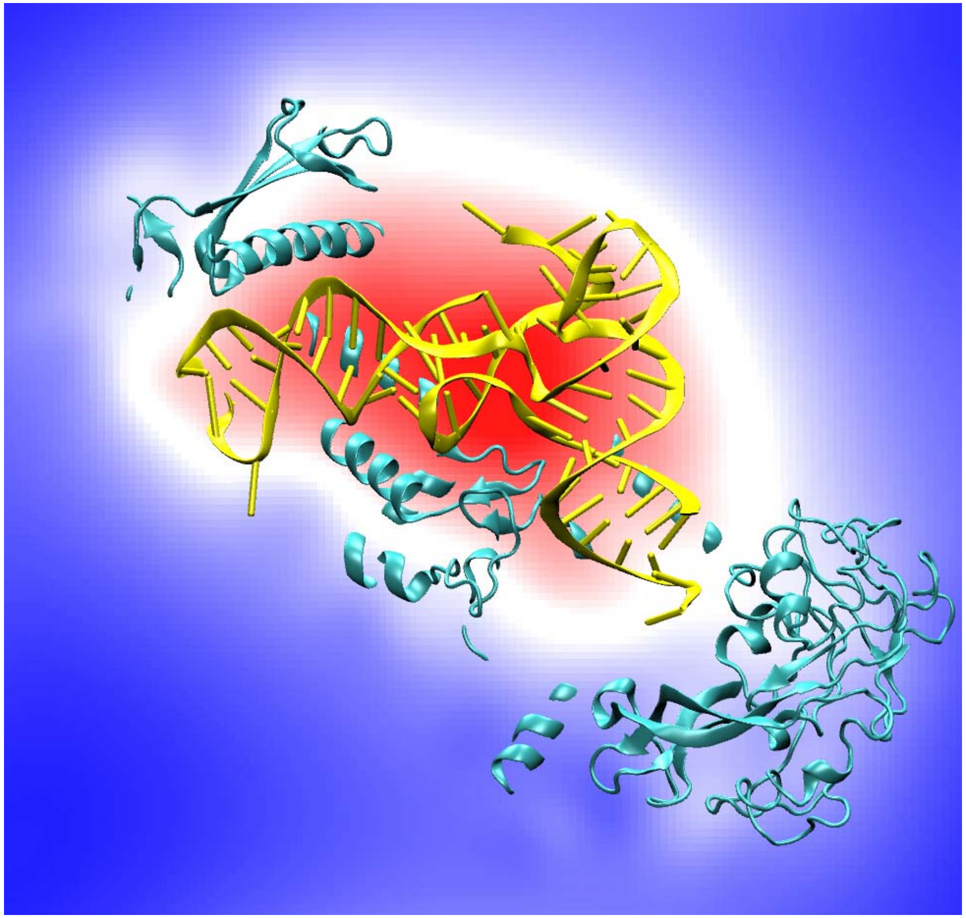
- The easiest way to really illustrate how OpenCL works is to explore a simple algorithm implemented using the OpenCL API
- Since many have been working with CUDA already, I’ll use the direct Coulomb summation kernel we originally wrote in CUDA
- I’ll show how CUDA and OpenCL have much in common, and also highlight some of the new issues one has to deal with in using OpenCL on multiple hardware platforms

Electrostatic Potential Maps

- Electrostatic potentials evaluated on 3-D lattice:

$$V_i = \sum_j \frac{q_j}{4\pi\epsilon_0 |\mathbf{r}_j - \mathbf{r}_i|}$$

- Applications include:
  - Ion placement for structure building
  - Time-averaged potentials for simulation
  - Visualization and analysis

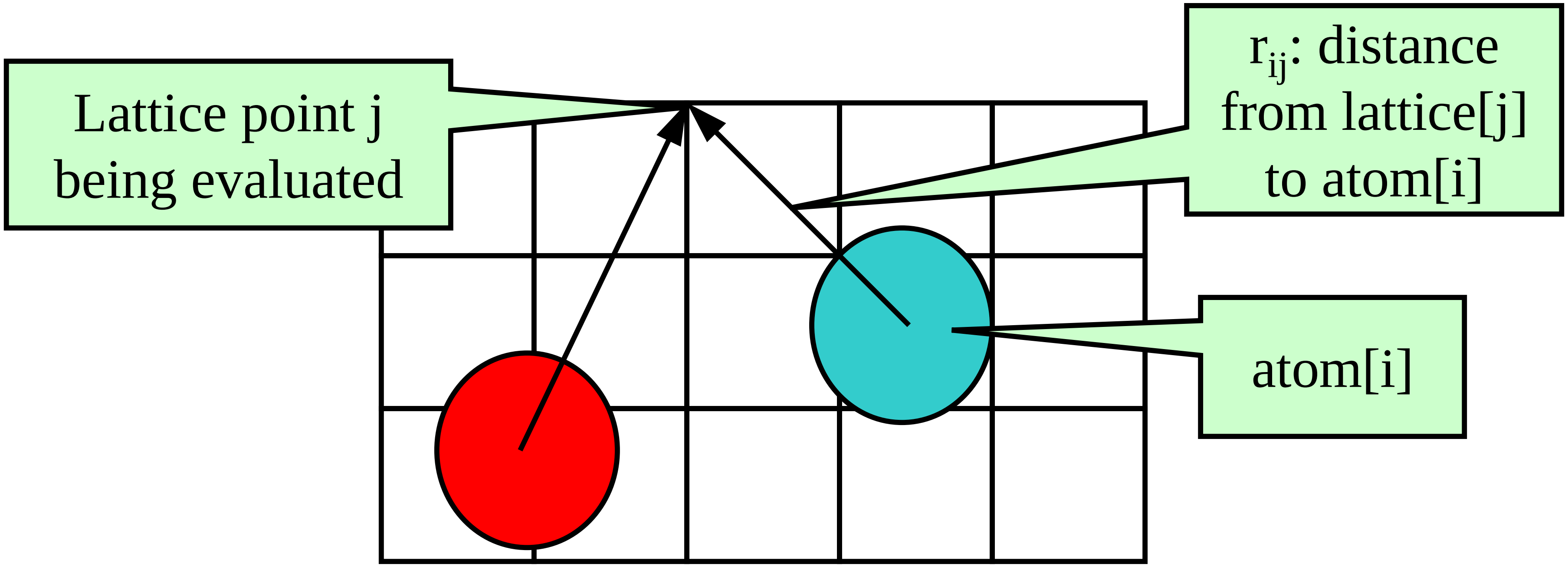


Isoleucine tRNA synthetase

Direct Coulomb Summation

- Each lattice point accumulates electrostatic potential contribution from all atoms:

  potential[j] += charge[i] / r_{ij}



Single Slice DCS: Simple (Slow) C Version

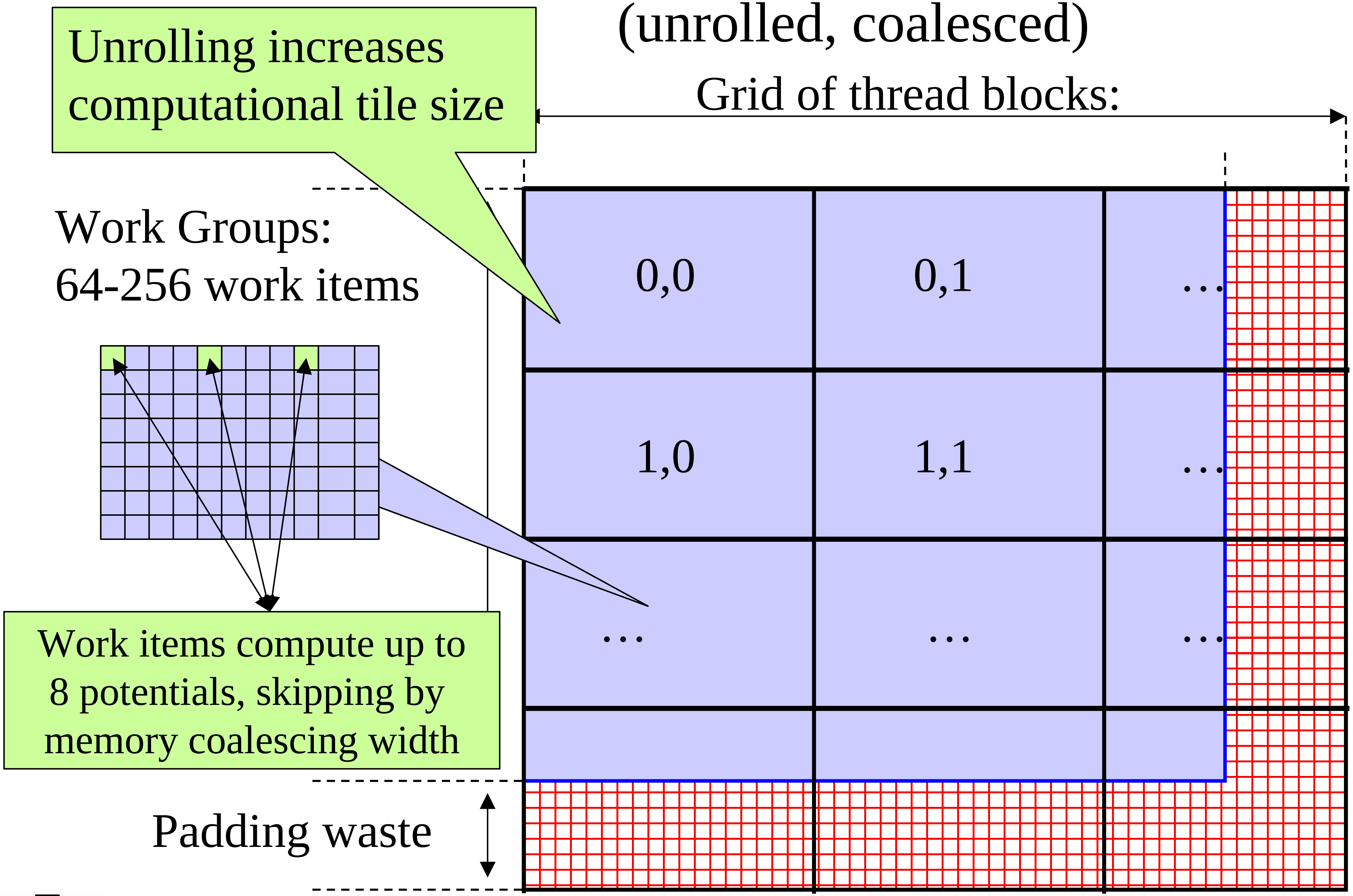
```
void cenergy(float *energygrid, dim3 grid, float gridspacing, float z, const float *atoms, int numatoms) {
  int i,j,n;
  int atomarrdim = numatoms * 4;
  for (j=0; j<grid.y; j++) {
    float y = gridspacing * (float) j;
    for (i=0; i<grid.x; i++) {
      float x = gridspacing * (float) i;
      float energy = 0.0f;
      for (n=0; n<atomarrdim; n+=4) {     // calculate potential contribution of each atom
        float dx = x - atoms[n    ];
        float dy = y - atoms[n+1];
        float dz = z - atoms[n+2];
        energy += atoms[n+3] / sqrtf(dx*dx + dy*dy + dz*dz);
      }
      energygrid[grid.x*grid.y*k + grid.x*j + i] = energy;
    }
```

Data Parallel Direct Coulomb Summation Algorithm

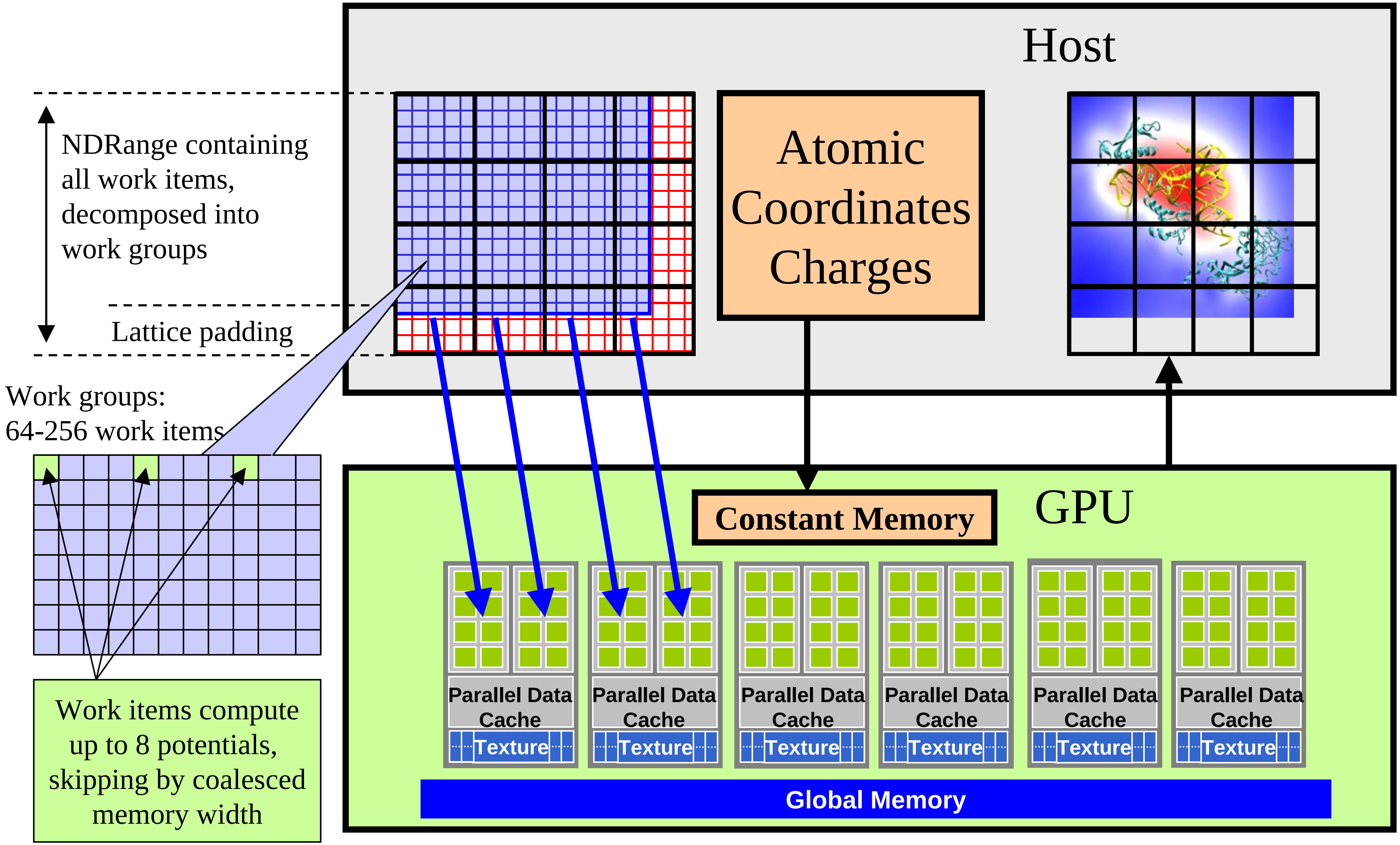
- Work is decomposed into tens of thousands of independent calculations
  - multiplexed onto all of the processing units on the target device (hundreds in the case of modern GPUs)
- Single-precision FP arithmetic is adequate for intended application
- Numerical accuracy can be improved by compensated summation, spatially ordered summation groupings, or accumulation of potential in double-precision
- Starting point for more sophisticated linear-time algorithms like multilevel summation

DCS Data Parallel Decomposition

(unrolled, coalesced)



Direct Coulomb Summation in OpenCL



Direct Coulomb Summation Kernel Setup

OpenCL:

```
__kernel void clenergy(…) {
  unsigned int xindex = (get_global_id(0) -
      get_local_id(0)) * UNROLLX +
      get_local_id(0);
  unsigned int yindex = get_global_id(1);
  unsigned int outaddr = get_global_size(0) *
      UNROLLX * yindex + xindex;
```

CUDA:

```
__global__ void cuenergy (…) {
  unsigned int xindex = blockIdx.x *
      blockDim.x * UNROLLX +
      threadIdx.x;
  unsigned int yindex = blockIdx.y *
      blockDim.y + threadIdx.y;
  unsigned int outaddr = gridDim.x *
      blockDim.x * UNROLLX * yindex
      + xindex;
```

DCS Inner Loop (CUDA)

```
…for (atomid=0; atomid<numatoms; atomid++) {
    float dy = coory - atominfo[atomid].y;
    float dyz2 = (dy * dy) + atominfo[atomid].z;
    float dx1 = coorx – atominfo[atomid].x;
    float dx2 = dx1 + gridspacing_coalesce;
    float dx3 = dx2 + gridspacing_coalesce;
    float dx4 = dx3 + gridspacing_coalesce;
    float charge = atominfo[atomid].w;
    energyvalx1 += charge * rsqrtf(dx1*dx1 + dyz2);
    energyvalx2 += charge * rsqrtf(dx2*dx2 + dyz2);
    energyvalx3 += charge * rsqrtf(dx3*dx3 + dyz2);
    energyvalx4 += charge * rsqrtf(dx4*dx4 + dyz2);
  }
```

DCS Inner Loop (OpenCL on NVIDIA GPU)

```
…for (atomid=0; atomid<numatoms; atomid++) {
    float dy = coory - atominfo[atomid].y;
    float dyz2 = (dy * dy) + atominfo[atomid].z;
    float dx1 = coorx – atominfo[atomid].x;
    float dx2 = dx1 + gridspacing_coalesce;
    float dx3 = dx2 + gridspacing_coalesce;
    float dx4 = dx3 + gridspacing_coalesce;
    float charge = atominfo[atomid].w;
    energyvalx1 += charge * native_rsqrt(dx1*dx1 + dyz2);
    energyvalx2 += charge * native_rsqrt(dx2*dx2 + dyz2);
    energyvalx3 += charge * native_rsqrt(dx3*dx3 + dyz2);
    energyvalx4 += charge * native_rsqrt(dx4*dx4 + dyz2);
  }
```

DCS Inner Loop (OpenCL on AMD CPU)

```
float4 gridspacing_u4 = { 0.f, 1.f, 2.f, 3.f };
gridspacing_u4 *= gridspacing_coalesce;
float4 energyvalx=0.0f;
…
for (atomid=0; atomid<numatoms; atomid++) {
    float dy = coory - atominfo[atomid].y;
    float dyz2 = (dy * dy) + atominfo[atomid].z;
    float4 dx = gridspacing_u4 + (coorx – atominfo[atomid].x);
    float charge = atominfo[atomid].w;
    energyvalx1 += charge * native_rsqrt(dx1*dx1 + dyz2);
}
```

Wait a Second, Why Two Different OpenCL Kernels???

- Existing OpenCL implementations don't necessarily autovectorize your code to the native hardware's SIMD vector width
- Although you can run the same code on very different devices and get the correct answer, performance will vary wildly…
- In many cases, getting peak performance on multiple device types or hardware from different vendors will presently require multiple OpenCL kernels

OpenCL Host Code

- Roughly analogous to CUDA driver API:
  - Memory allocations, memory copies, etc
  - Image objects (i.e. textures)
  - Create and manage device context(s) and associate work queue(s), etc…
  - OpenCL uses reference counting on all objects
- OpenCL programs are normally compiled entirely at runtime, which must be managed by host code

OpenCL Context Setup Code (simple)

```
cl_int clerr = CL_SUCCESS;
cl_context clctx = clCreateContextFromType(0, CL_DEVICE_TYPE_ALL, NULL,
    NULL, &clerr);

size_t parmsz;
clerr = clGetContextInfo(clctx, CL_CONTEXT_DEVICES, 0, NULL, &parmsz);

cl_device_id* cldevs = (cl_device_id *) malloc(parmsz);
clerr = clGetContextInfo(clctx, CL_CONTEXT_DEVICES, parmsz, cldevs, NULL);

cl_command_queue clcmdq = clCreateCommandQueue(clctx, cldevs[0], 0, &clerr);
```

OpenCL Kernel Compilation Example

OpenCL kernel source code as a big string

```
const char* clenergysrc =
  "__kernel __attribute__((reqd_work_group_size_hint(BLOCKSIZEX, BLOCKSIZEY, 1))) \n"
  "void clenergy(int numatoms, float gridspacing, __global float *energy, __constant float4 *atominfo) { \n“
     […etc and so forth…]
cl_program clpgm;
clpgm = clCreateProgramWithSource(clctx, 1, &clenergysrc, NULL, &clerr);
char clcompileflags[4096];
sprintf(clcompileflags, "-DUNROLLX=%d -cl-fast-relaxed-math -cl-single-precision-
     constant -cl-denorms-are-zero -cl-mad-enable", UNROLLX);
clerr = clBuildProgram(clpgm, 0, NULL, clcompileflags, NULL, NULL);
cl_kernel clkern = clCreateKernel(clpgm, "clenergy", &clerr);
```

Gives raw source code string(s) to OpenCL

Set compiler flags, compile source, and retreive a handle to the “clenergy” kernel

Getting PTX for OpenCL Kernel on NVIDIA GPU

```
cl_uint numdevs;
clerr = clGetProgramInfo(clpgm, CL_PROGRAM_NUM_DEVICES, sizeof(numdevs),
    &numdevs, NULL);
printf("number of devices: %d\n", numdevs);
char **ptxs = (char **) malloc(numdevs * sizeof(char *));
size_t *ptxlens = (size_t *) malloc(numdevs * sizeof(size_t));
clerr = clGetProgramInfo(clpgm, CL_PROGRAM_BINARY_SIZES, numdevs *
    sizeof(size_t *), ptxlens, NULL);
for (int i=0; i<numdevs; i++)
  ptxs[i] = (char *) malloc(ptxlens[i]+1);
clerr = clGetProgramInfo(clpgm, CL_PROGRAM_BINARIES, numdevs * sizeof(char *),
    ptxs, NULL);
if (ptxlens[0] > 1)
  printf("Resulting PTX compilation from build:\n’%s’\n“, ptxs[0]);
```

OpenCL Kernel Launch (abridged)

```
doutput = clCreateBuffer(clctx, CL_MEM_READ_WRITE, volmemsz, NULL, NULL);
datominfo = clCreateBuffer(clctx, CL_MEM_READ_ONLY, MAXATOMS * sizeof(cl_float4),
    NULL, NULL);
[…]
clerr = clSetKernelArg(clkern, 0, sizeof(int), &runatoms);
clerr = clSetKernelArg(clkern, 1, sizeof(float), &zplane);
clerr = clSetKernelArg(clkern, 2, sizeof(cl_mem), &doutput);
clerr = clSetKernelArg(clkern, 3, sizeof(cl_mem), &datominfo);
cl_event event;
clerr = clEnqueueNDRangeKernel(clcmdq, clkern, 2, NULL, Gsz, Bsz, 0, NULL, &event);
clerr = clWaitForEvents(1, &event);
clerr = clReleaseEvent(event);
[…]
clEnqueueReadBuffer(clcmdq, doutput, CL_TRUE, 0, volmemsz, energy, 0, NULL, NULL);
clReleaseMemObject(doutput);
clReleaseMemObject(datominfo);
```

Summary

- Incorporating OpenCL into an application requires adding far more “plumbing” in an application than for the CUDA runtime API
- Although OpenCL code is portable in terms of correctness, performance of any particular kernel is not guaranteed across different device types/vendors
- Apps have to check performance-related properties of target devices, e.g. whether __local memory is fast/slow (query CL_DEVICE_LOCAL_MEM_TYPE)
- It remains to be seen how OpenCL “platforms” will allow apps to concurrently use an AMD CPU runtime and NVIDIA GPU runtime (may already work on MacOS X?)

Acknowledgements

- Additional Information and References:
  - http://www.ks.uiuc.edu/Research/gpu/
- Questions, source code requests:
  - John Stone: johns@ks.uiuc.edu
- Acknowledgements:

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  - UIUC NVIDIA CUDA Center of Excellence
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Publications

http://www.ks.uiuc.edu/Research/gpu/

- Probing Biomolecular Machines with Graphics Processors. J. Phillips, J. Stone. *Communications of the ACM*, 52(10):34-41, 2009.
- GPU Clusters for High Performance Computing. V. Kindratenko, J. Enos, G. Shi, M. Showerman, G. Arnold, J. Stone, J. Phillips, W. Hwu. *Workshop on Parallel Programming on Accelerator Clusters (PPAC)*, IEEE Cluster 2009. In press.
- Long time-scale simulations of in vivo diffusion using GPU hardware. E. Roberts, J. Stone, L. Sepulveda, W. Hwu, Z. Luthey-Schulten. In *IPDPS'09: Proceedings of the 2009 IEEE International Symposium on Parallel & Distributed Computing*, pp. 1-8, 2009.
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- Multilevel summation of electrostatic potentials using graphics processing units. D. Hardy, J. Stone, K. Schulten. *J. Parallel Computing*, 35:164-177, 2009.

Publications (cont)

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- GPU acceleration of cutoff pair potentials for molecular modeling applications. C. Rodrigues, D. Hardy, J. Stone, K. Schulten, and W. Hwu. *Proceedings of the 2008 Conference On Computing Frontiers*, pp. 273-282, 2008.
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- Continuous fluorescence microphotolysis and correlation spectroscopy. A. Arkhipov, J. Hüve, M. Kahms, R. Peters, K. Schulten. *Biophysical Journal*, 93:4006-4017, 2007.