# An Introduction to OpenCL

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

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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 short sections of real OpenCL kernels used in scientific software

## 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:
  - Correctly-written OpenCL code will produce correct results across multiple types of OpenCL devices
  - Performance of a given kernel is **not guaranteed** across different target devices
- OpenCL implementations already exist for AMD and NVIDIA GPUs, x86 CPUs, IBM Cell
- OpenCL could in principle also support various DSP chips, FPGAs, and other hardware

# Supporting Diverse Accelerator Hardware in Production Codes….

- Development of HPC-oriented scientific software is already challenging
- Maintaining unique code paths for each accelerator type is costly and impractical beyond a certain point
- Diversity and rapid evolution of accelerators exacerbates these issues
- OpenCL ameliorates several key problems:
  - Targets CPUs, GPUs, and other accelerator devices
  - Common language for writing computational “kernels”
  - Common API for managing execution on target device

## Performance Variation of OpenCL Kernels

- 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

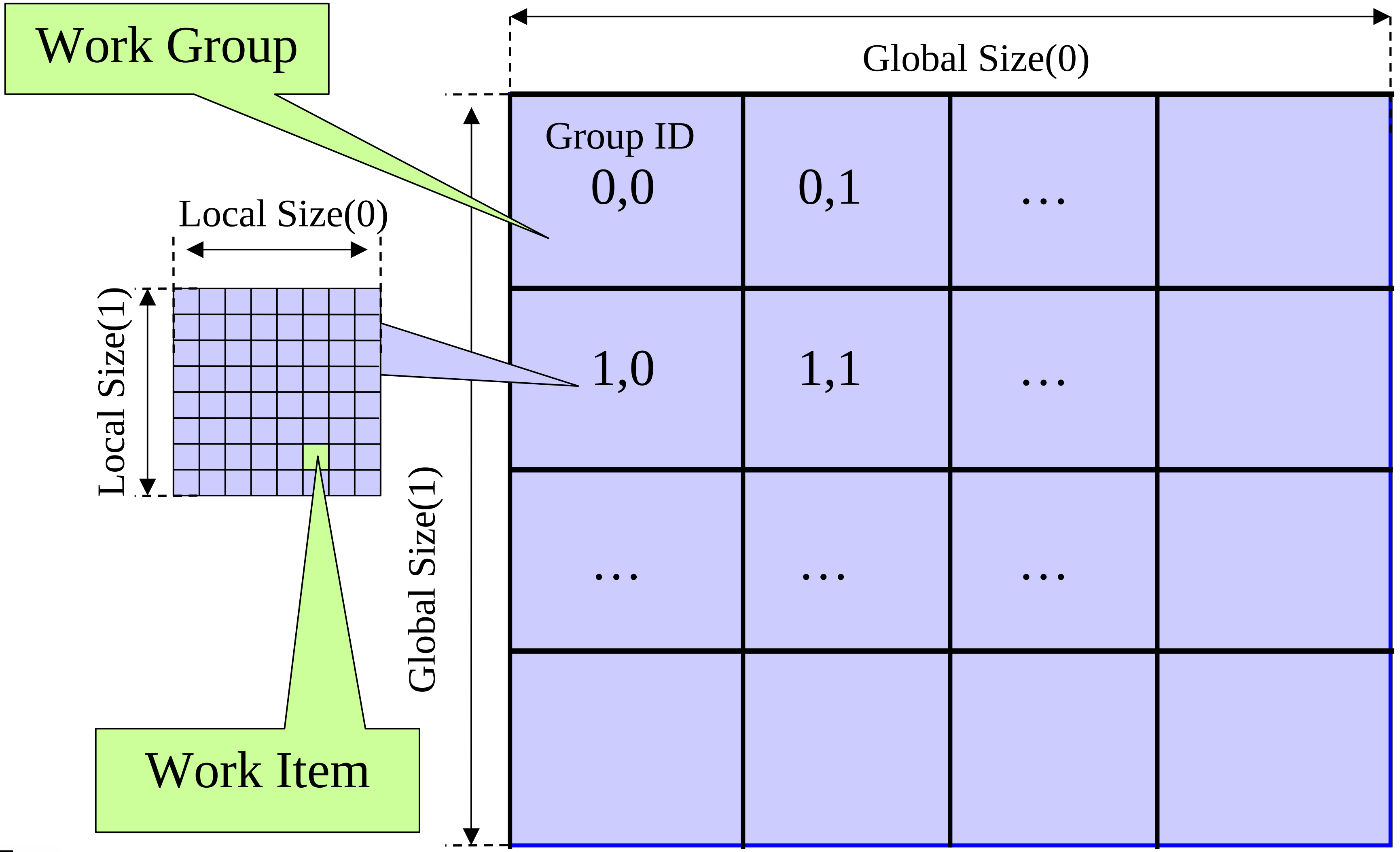
# Apparent Weaknesses of OpenCL 1.0

- OpenCL is a low-level API
  - Developers are responsible for a lot of plumbing, lots of objects/handles to keep track of
  - Even a basic OpenCL “hello world” is **much** more code to write than doing the same thing in the CUDA runtime API
- Developers are responsible for enforcing thread-safety
  - Some types of multi-accelerator codes are much more difficult to write than in the CUDA runtime API currently
- Great need for OpenCL middleware and/or libraries
  - Simplified device management, integration of large numbers of kernels into legacy apps, auto-selection of best kernels for device...
  - Tools to better support OpenCL apps in large HPC environments, e.g. clusters

# OpenCL Data Parallel Model

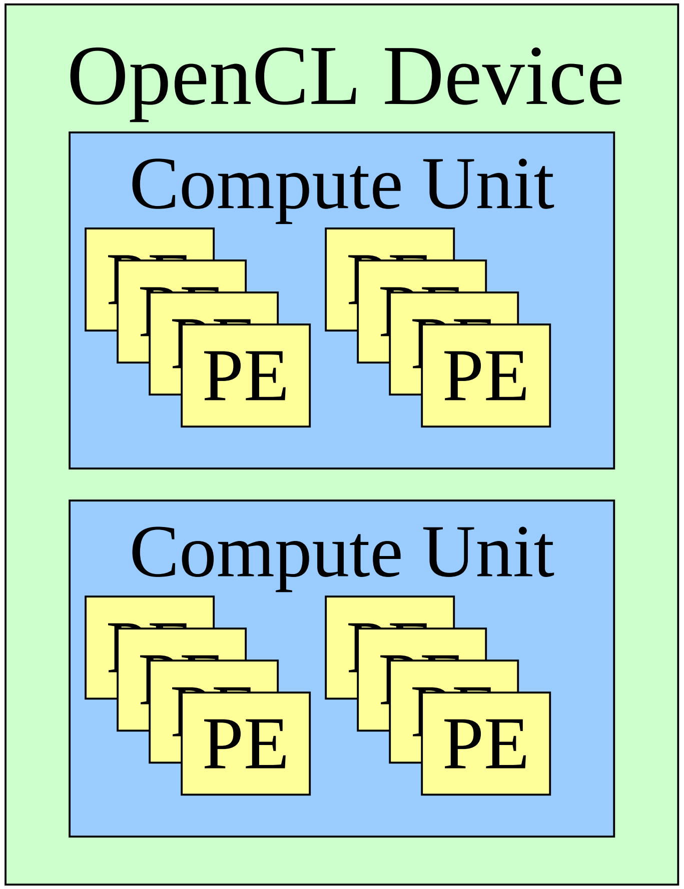
- Work is submitted to devices by launching kernels
- Kernels run over global dimension index ranges (NDRange), broken up into “work groups”, and “work items”
- Work items executing within the same work group can synchronize with each other with barriers or memory fences
- Work items in different work 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”

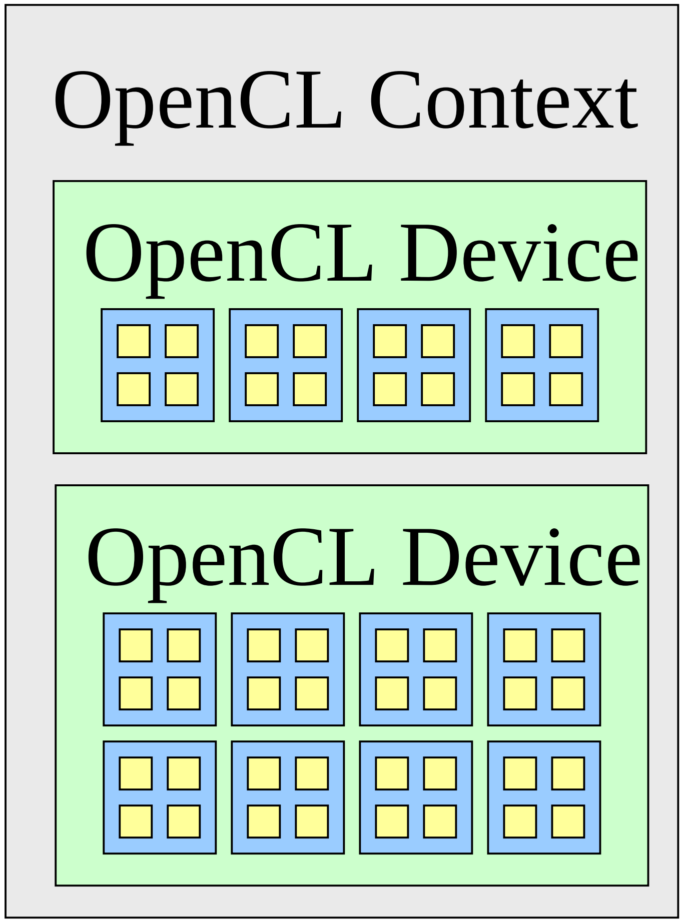


# OpenCL Memory Systems

- __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

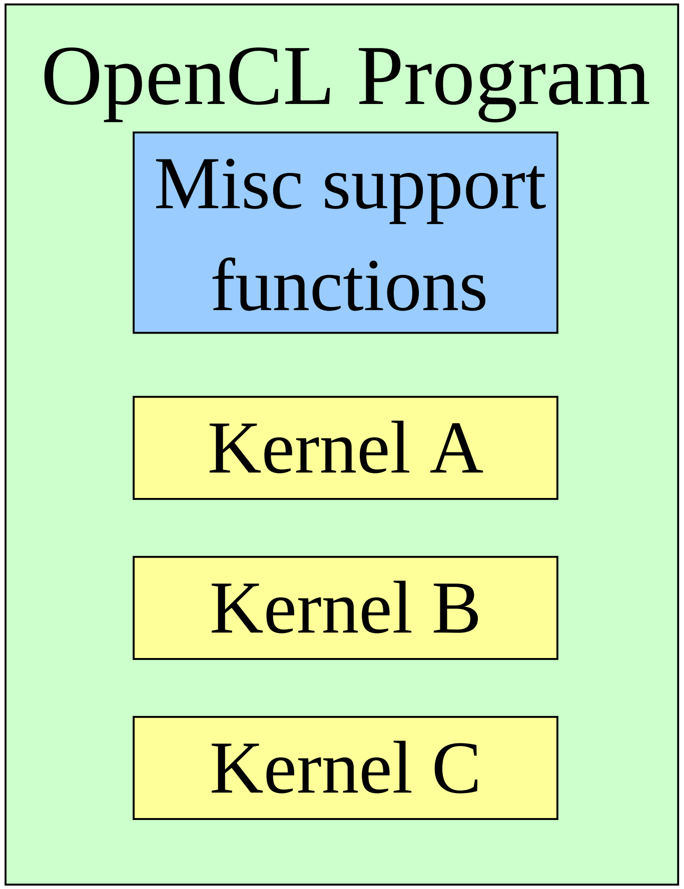
# OpenCL Context

- 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

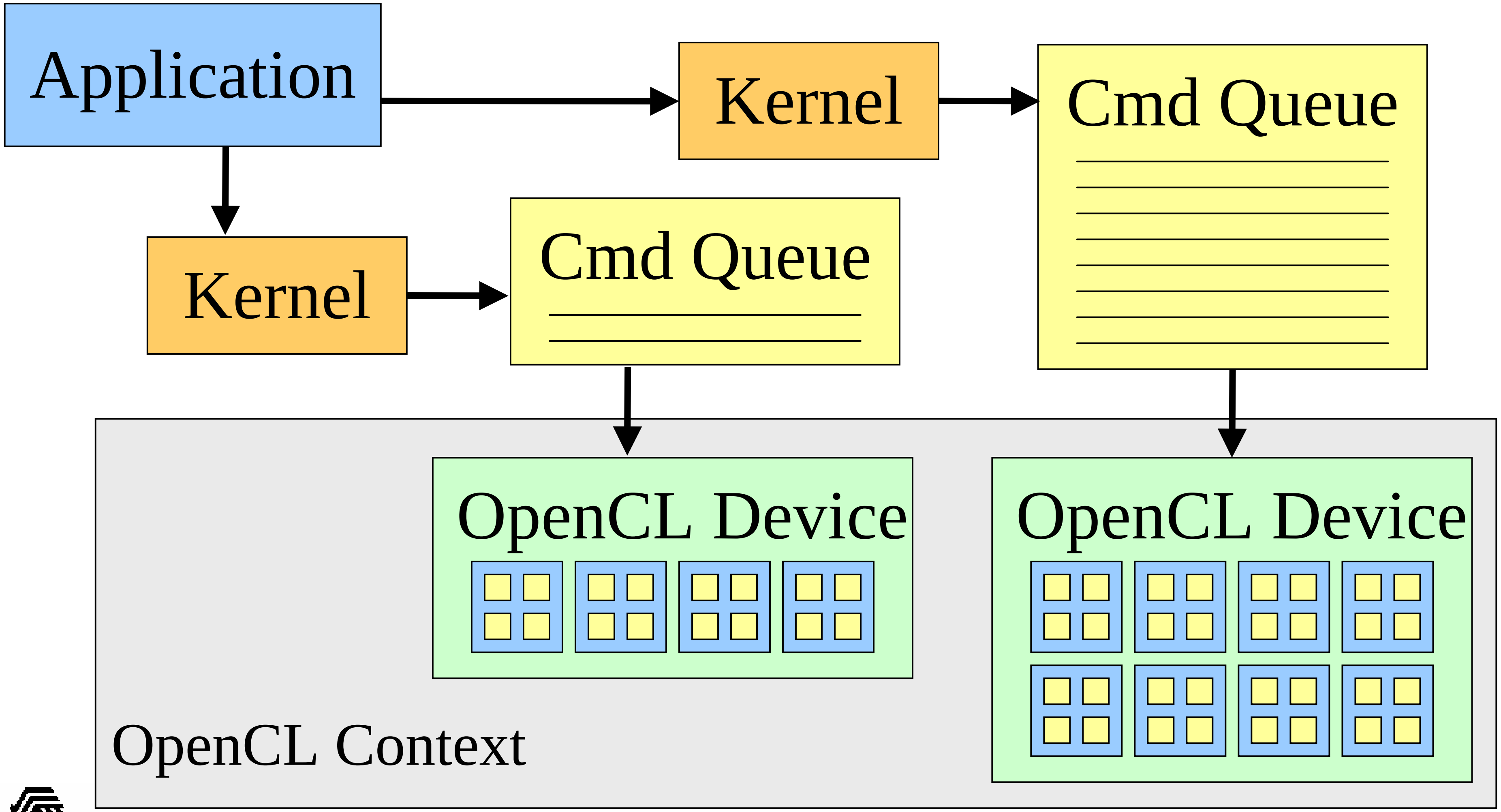


# OpenCL Kernels

- 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

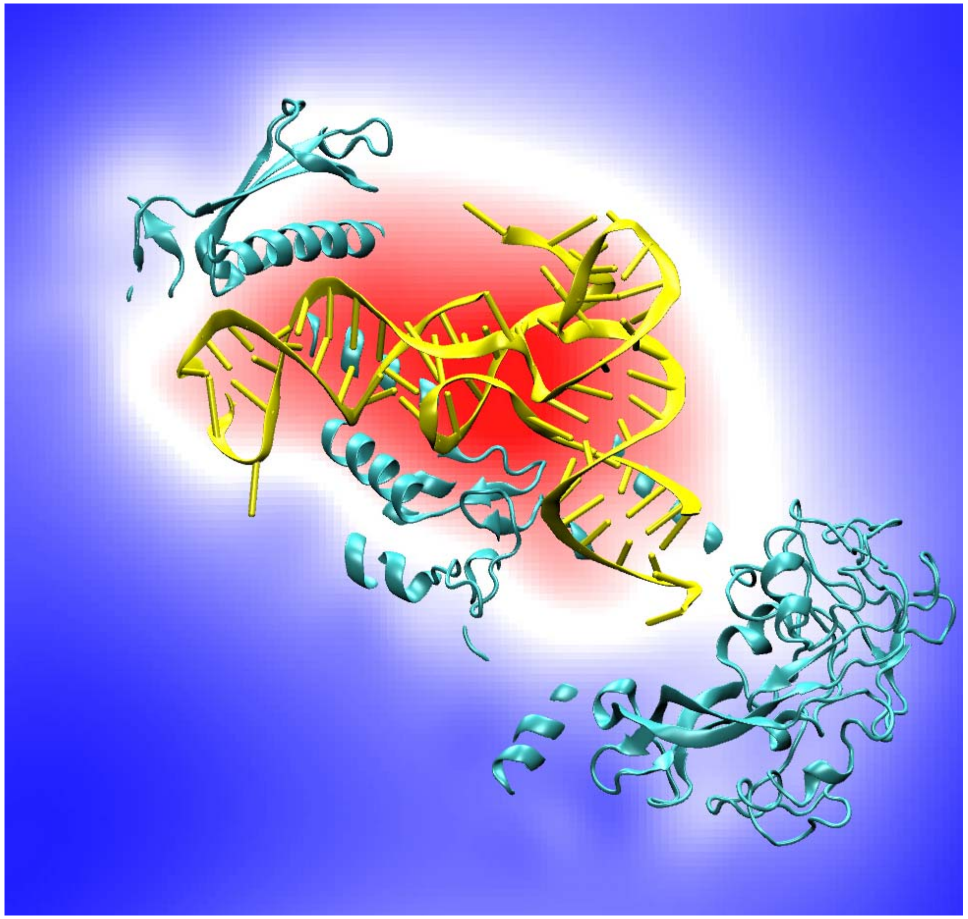
- The easiest way to really illustrate how OpenCL works is to explore a simple algorithm implemented using the OpenCL API
- Since many have been working with CUDA already, I’ll use the direct Coulomb summation kernel we originally wrote in CUDA
- I’ll show how CUDA and OpenCL have much in common, and 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:

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

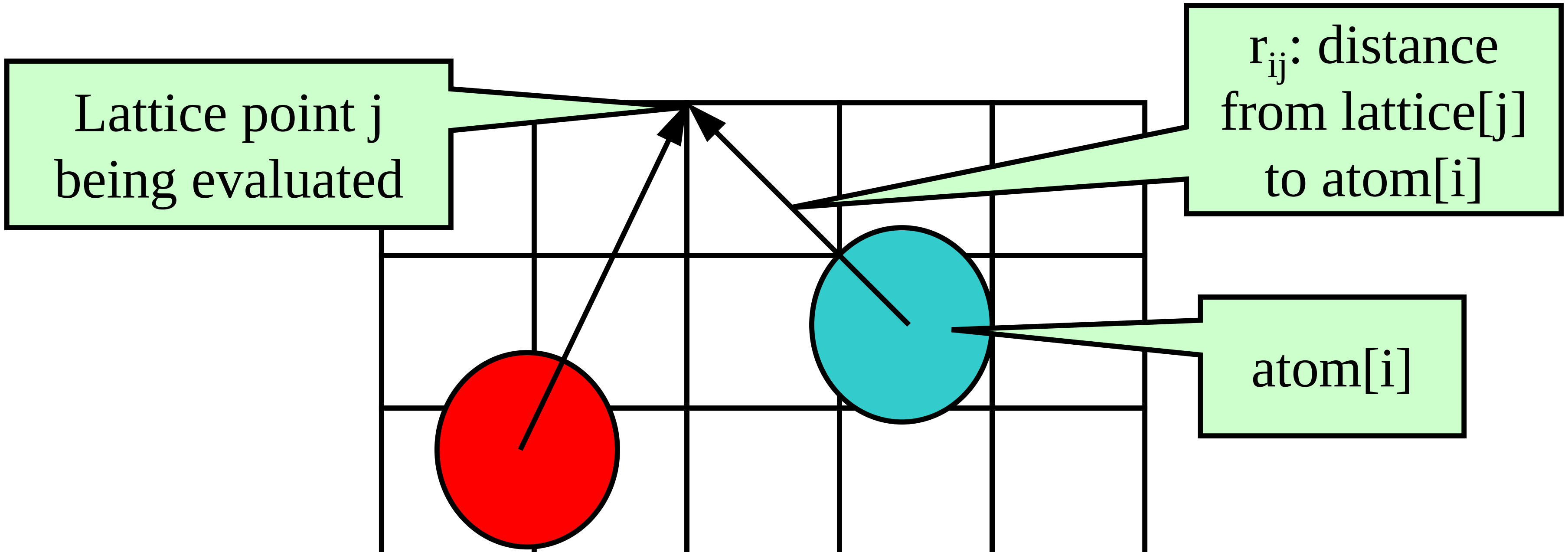
- Applications include:
  – Ion placement for structure building
  – Time-averaged potentials for simulation
  – Visualization and analysis


Isoleucine tRNA synthetase

# Direct Coulomb Summation

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

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


Lattice point j being evaluated
$r_{ij}$: distance from lattice[j] to atom[i]
atom[i]

## Single Slice DCS: Simple (Slow) C Version

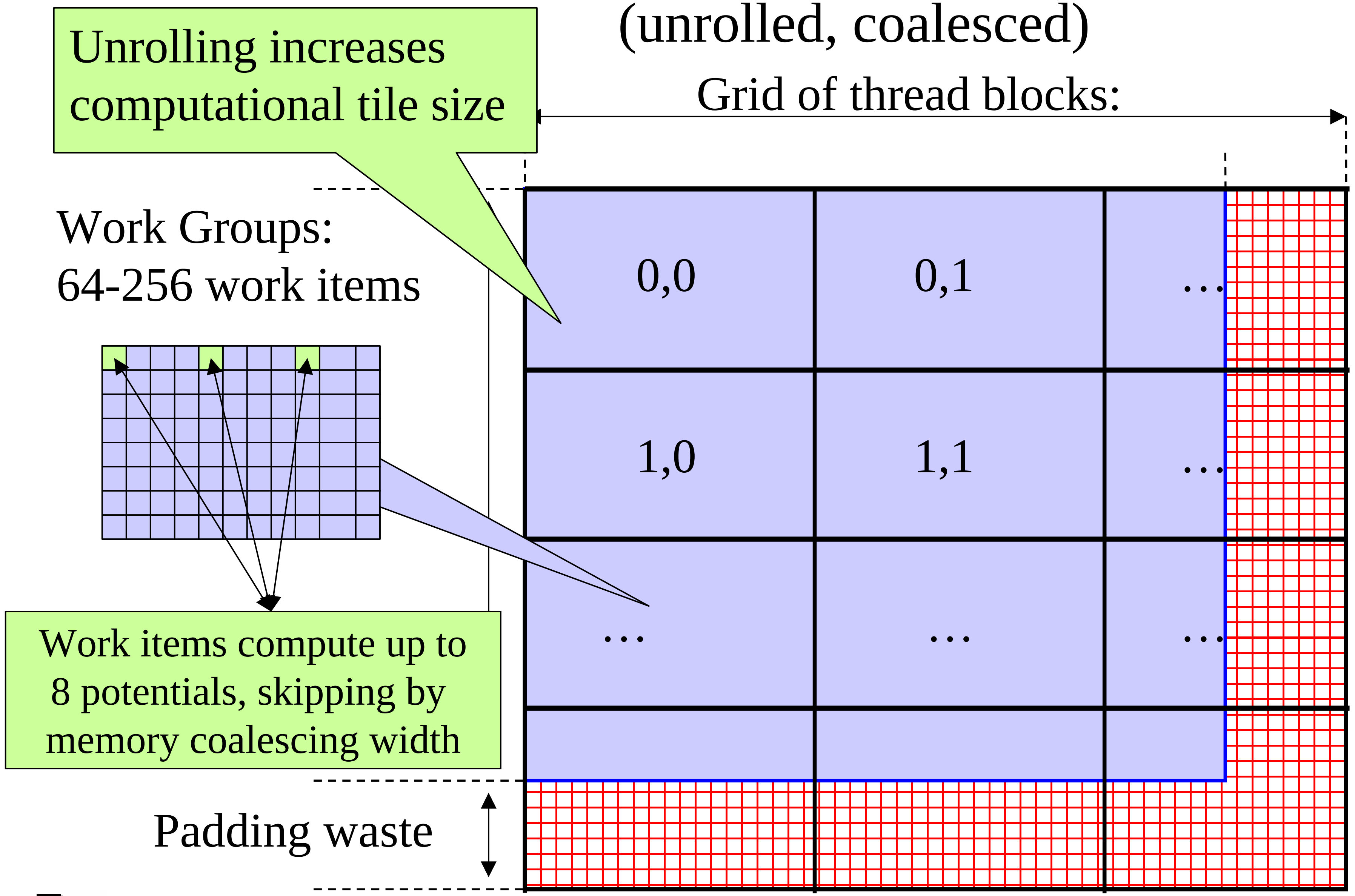
```
void cenergy(float *energygrid, dim3 grid, float gridspacing, float z, const float *atoms, int numatoms) {
  int i,j,n;
  int atomarrdim = numatoms * 4;
  for (j=0; j<grid.y; j++) {
    float y = gridspacing * (float) j;
    for (i=0; i<grid.x; i++) {
      float x = gridspacing * (float) i;
      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

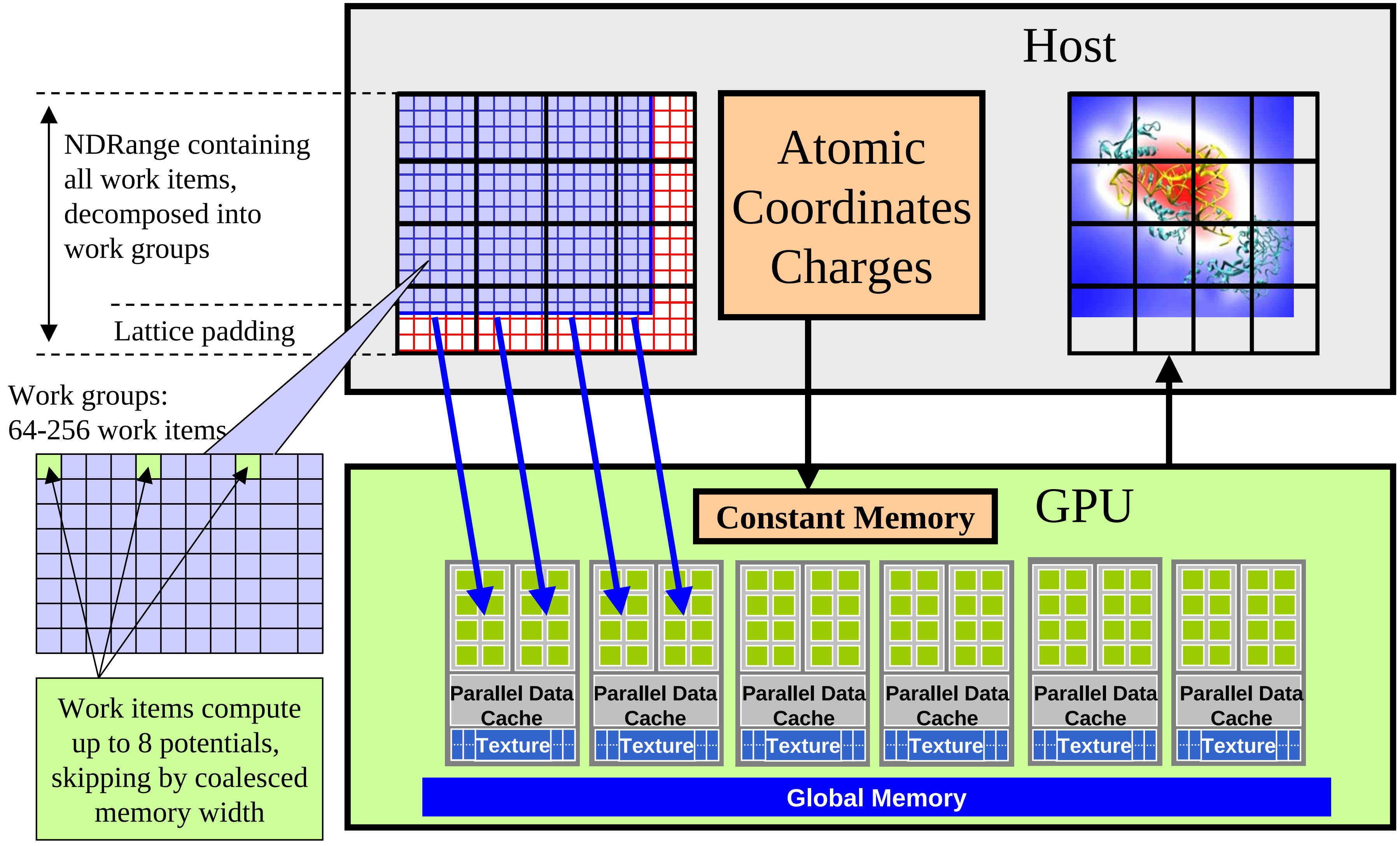
- Work is decomposed into tens of thousands of independent calculations
  - multiplexed onto all of the processing units on the target device (hundreds in the case of modern GPUs)
- Single-precision FP arithmetic is adequate for intended application
- Numerical accuracy can be improved by compensated 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)


Unrolling increases computational tile size
Grid of thread blocks:
Work Groups: 64-256 work items
0,0
0,1
…
1,0
1,1
…
…
…
…
Work items compute up to 8 potentials, skipping by memory coalescing width
Padding waste

# Direct Coulomb Summation in OpenCL


Host
NDRange containing all work items, decomposed into work groups
Lattice padding
Atomic Coordinates Charges
Work groups: 64-256 work items
GPU
Constant Memory
Parallel Data Cache
Texture
Global Memory
Work items compute up to 8 potentials, skipping by coalesced memory width

# 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, Scalar OpenCL

```
…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);
  }
```

Well-written CUDA code can often be easily ported to OpenCL if C++ features and pointer arithmetic aren't used in kernels.

# DCS Inner Loop, Vectorized OpenCL

```
 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);
 }
```

CPUs, AMD GPUs, and Cell often perform better with vectorized kernels.
Use of vector types may increase register pressure; sometimes a delicate balance…

## 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(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);
```

# Apples to Oranges Performance Results: OpenCL Direct Coulomb Summation Kernels

| OpenCL Target Device | OpenCL "cores" | Scalar Kernel: Ported from original CUDA kernel | 4-Vector Kernel: Replaced manually unrolled loop iterations with float4 vector ops |
|---|---|---|---|
| AMD 2.2GHz Opteron 148 CPU (a very old Linux test box) | 1 | 0.30 Bevals/sec, 2.19 GFLOPS | 0.49 Bevals/sec, 3.59 GFLOPS |
| Intel 2.2Ghz Core2 Duo, (Apple MacBook Pro) | 2 | 0.88 Bevals/sec, 6.55 GFLOPS | 2.38 Bevals/sec, 17.56 GFLOPS |
| IBM QS22 CellBE *** __constant not implemented yet | 16 | 2.33 Bevals/sec, 17.16 GFLOPS **** | 6.21 Bevals/sec, 45.81 GFLOPS **** |
| AMD Radeon 4870 GPU | 10 | 41.20 Bevals/sec, 303.93 GFLOPS | 31.49 Bevals/sec, 232.24 GFLOPS |
| NVIDIA GeForce GTX 285 GPU | 30 | 75.26 Bevals/sec, 555.10 GFLOPS | 73.37 Bevals/sec, 541.12 GFLOPS |

MADD, RSQRT = 2 FLOPS  All other FP instructions = 1 FLOP

# Getting More Performance: Adapting DCS Kernel to OpenCL on Cell

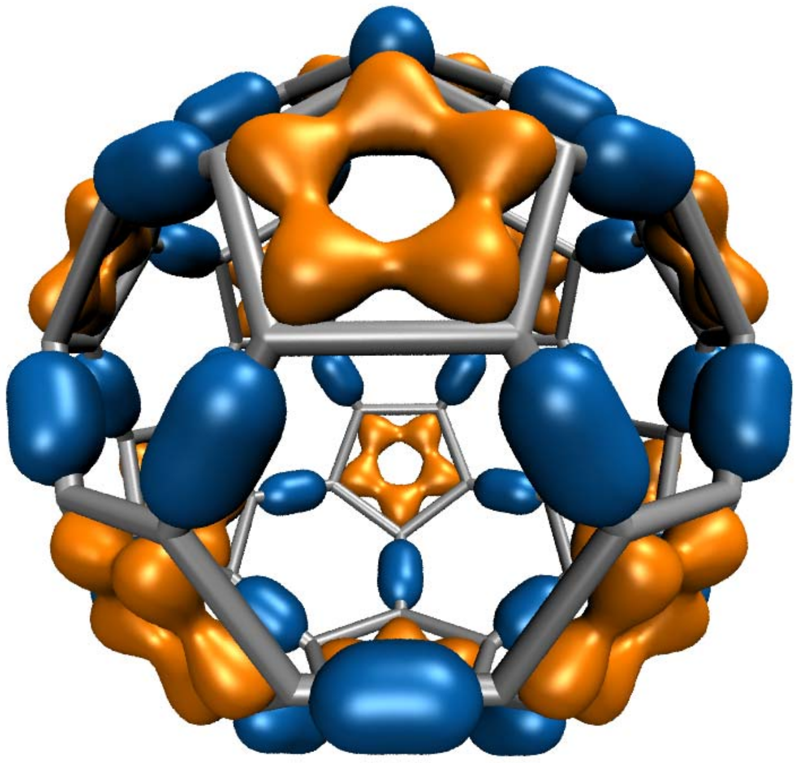
| OpenCL Target Device | Scalar Kernel: Ported directly from original CUDA kernel | 4-Vector Kernel: Replaced manually unrolled loop iterations with float4 vector ops | Async Copy Kernel: Replaced __constant accesses with use of async_work_group_copy(), use float16 vector ops |
|---|---|---|---|
| IBM QS22 CellBE *** __constant not implemented | 2.33 Bevals/sec, 17.16 GFLOPS **** | 6.21 Bevals/sec, 45.81 GFLOPS **** | 16.22 Bevals/sec, 119.65 GFLOPS |

Replacing the use of constant memory with loads of atom data to __local memory via async_work_group_copy() increases performance significantly since Cell doesn't implement __constant memory yet.

Tests show that the speed of native_rsqrt() is currently a performance limiter for Cell. Replacing native_rsqrt() with a multiply results in a ~3x increase in execution rate.

## Computing Molecular Orbitals

- Visualization of MOs aids in understanding the chemistry of molecular system
- MO spatial distribution is correlated with electron probability density
- Calculation of high resolution MO grids can require tens to hundreds of seconds on CPUs
- >100x speedup allows interactive animation of MOs @ 10 FPS

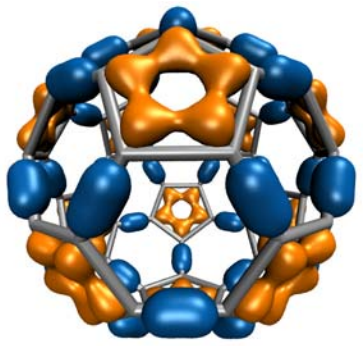


$C_{60}$

High Performance Computation and Interactive Display of Molecular Orbitals on GPUs and Multi-core CPUs. Stone et al., *GPGPU-2, ACM International Conference Proceeding Series*, volume 383, pp. 9-18, 2009

# Molecular Orbital Inner Loop, Hand-Coded SSE Hard to Read, Isn't It? (And this is the "pretty" version!)

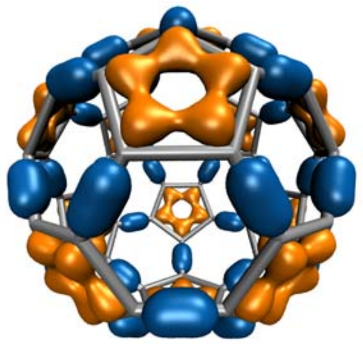
```
for (shell=0; shell < maxshell; shell++) {
  __m128 Cgto = _mm_setzero_ps();
  for (prim=0; prim<num_prim_per_shell[shell_counter]; prim++) {
    float exponent       = -basis_array[prim_counter    ];
    float contract_coeff =  basis_array[prim_counter + 1];
    __m128 expval = _mm_mul_ps(_mm_load_ps1(&exponent), dist2);
    __m128 ctmp = _mm_mul_ps(_mm_load_ps1(&contract_coeff), exp_ps(expval));
    Cgto = _mm_add_ps(contracted_gto, ctmp);
    prim_counter += 2;
  }
  __m128 tshell = _mm_setzero_ps();
  switch (shell_types[shell_counter]) {
    case S_SHELL:
      value = _mm_add_ps(value, _mm_mul_ps(_mm_load_ps1(&wave_f[ifunc++]), Cgto));    break;
    case P_SHELL:
      tshell = _mm_add_ps(tshell, _mm_mul_ps(_mm_load_ps1(&wave_f[ifunc++]), xdist));
      tshell = _mm_add_ps(tshell, _mm_mul_ps(_mm_load_ps1(&wave_f[ifunc++]), ydist));
      tshell = _mm_add_ps(tshell, _mm_mul_ps(_mm_load_ps1(&wave_f[ifunc++]), zdist));
      value = _mm_add_ps(value, _mm_mul_ps(tshell, Cgto));
      break;
```



Until now, writing SSE kernels for CPUs required assembly language, compiler intrinsics, various libraries, or a really smart autovectorizing compiler and lots of luck...

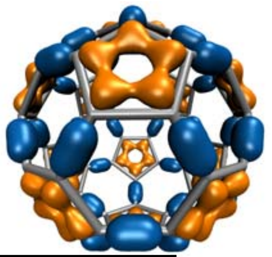
# Molecular Orbital Inner Loop, OpenCL Vec4 Ahhh, much easier to read!!!

```
for (shell=0; shell < maxshell; shell++) {
     float4 contracted_gto = 0.0f;
     for (prim=0; prim < const_num_prim_per_shell[shell_counter];  prim++) {
          float exponent          = const_basis_array[prim_counter     ];
          float contract_coeff = const_basis_array[prim_counter + 1];
          contracted_gto += contract_coeff * native_exp2(-exponent*dist2);
          prim_counter += 2;
     }
     float4 tmpshell=0.0f;
     switch (const_shell_symmetry[shell_counter]) {
          case S_SHELL:
               value += const_wave_f[ifunc++] * contracted_gto;      break;
          case P_SHELL:
               tmpshell += const_wave_f[ifunc++] * xdist;
               tmpshell += const_wave_f[ifunc++] * ydist;
               tmpshell += const_wave_f[ifunc++] * zdist;
               value += tmpshell * contracted_gto;
               break;
```



OpenCL's C-like kernel language is easy to read, even 4-way vectorized kernels can look similar to scalar CPU code.
All 4-way vectors shown in green.

# Apples to Oranges Performance Results: OpenCL Molecular Orbital Kernels



| Kernel | Cores | Runtime (s) | Speedup |
|---|---|---|---|
| Intel QX6700 CPU ICC-SSE (SSE intrinsics) | 1 | 46.580 | 1.00 |
| Intel Core2 Duo CPU OpenCL scalar | 2 | 43.342 | 1.07 |
| Intel QX6700 CPU ICC-SSE (SSE intrinsics) | 4 | 11.740 | 3.97 |
| Intel Core2 Duo CPU OpenCL vec4 | 2 | 8.499 | 5.36 |
| Cell OpenCL vec4*** no __constant | 16 | 6.075 | 7.67 |
| Radeon 4870 OpenCL scalar | 10 | 2.108 | 22.1 |
| Radeon 4870 OpenCL vec4 | 10 | 1.016 | 45.8 |
| GeForce GTX 285 OpenCL vec4 | 30 | 0.364 | 127.9 |
| GeForce GTX 285 CUDA 2.1 scalar | 30 | 0.361 | 129.0 |
| GeForce GTX 285 OpenCL scalar | 30 | 0.335 | 139.0 |
| GeForce GTX 285 CUDA 2.0 scalar | 30 | 0.327 | 142.4 |

Minor varations in compiler quality can have a strong effect on “tight” kernels. The two results shown for CUDA demonstrate performance variability with compiler revisions, and that with vendor effort, OpenCL has the potential to match the performance of other APIs.

# 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 Theoretical and Computational Biophysics Group,
      NIH Resource for Macromolecular Modeling and Bioinformatics
    - Prof. Wen-mei Hwu, Christopher Rodrigues, UIUC IMPACT Group
    - CUDA team at NVIDIA
    - 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.
- High Performance Computation and Interactive Display of Molecular Orbitals on GPUs and Multi-core CPUs. J. Stone, J. Saam, D. Hardy, K. Vandivort, W. Hwu, K. Schulten, *2nd Workshop on General-Purpose Computation on Graphics Pricessing Units (GPGPU-2), ACM International Conference Proceeding Series*, volume 383, pp. 9-18, 2009.
- Multilevel summation of electrostatic potentials using graphics processing units. D. Hardy, J. Stone, K. Schulten. *J. Parallel Computing*, 35:164-177, 2009.

# Publications (cont)

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

- Adapting a message-driven parallel application to GPU-accelerated clusters. J. Phillips, J. Stone, K. Schulten. *Proceedings of the 2008 ACM/IEEE Conference on Supercomputing*, IEEE Press, 2008.
- 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.
- GPU computing. J. Owens, M. Houston, D. Luebke, S. Green, J. Stone, J. Phillips. *Proceedings of the IEEE*, 96:879-899, 2008.
- Accelerating molecular modeling applications with graphics processors. J. Stone, J. Phillips, P. Freddolino, D. Hardy, L. Trabuco, K. Schulten. *J. Comp. Chem.*, 28:2618-2640, 2007.
- Continuous fluorescence microphotolysis and correlation spectroscopy. A. Arkhipov, J. Hüve, M. Kahms, R. Peters, K. Schulten. *Biophysical Journal*, 93:4006-4017, 2007.