An introduction to many-core parallel computing with OpenCL

Simon McIntosh-Smith

Twitter: @simonmcs

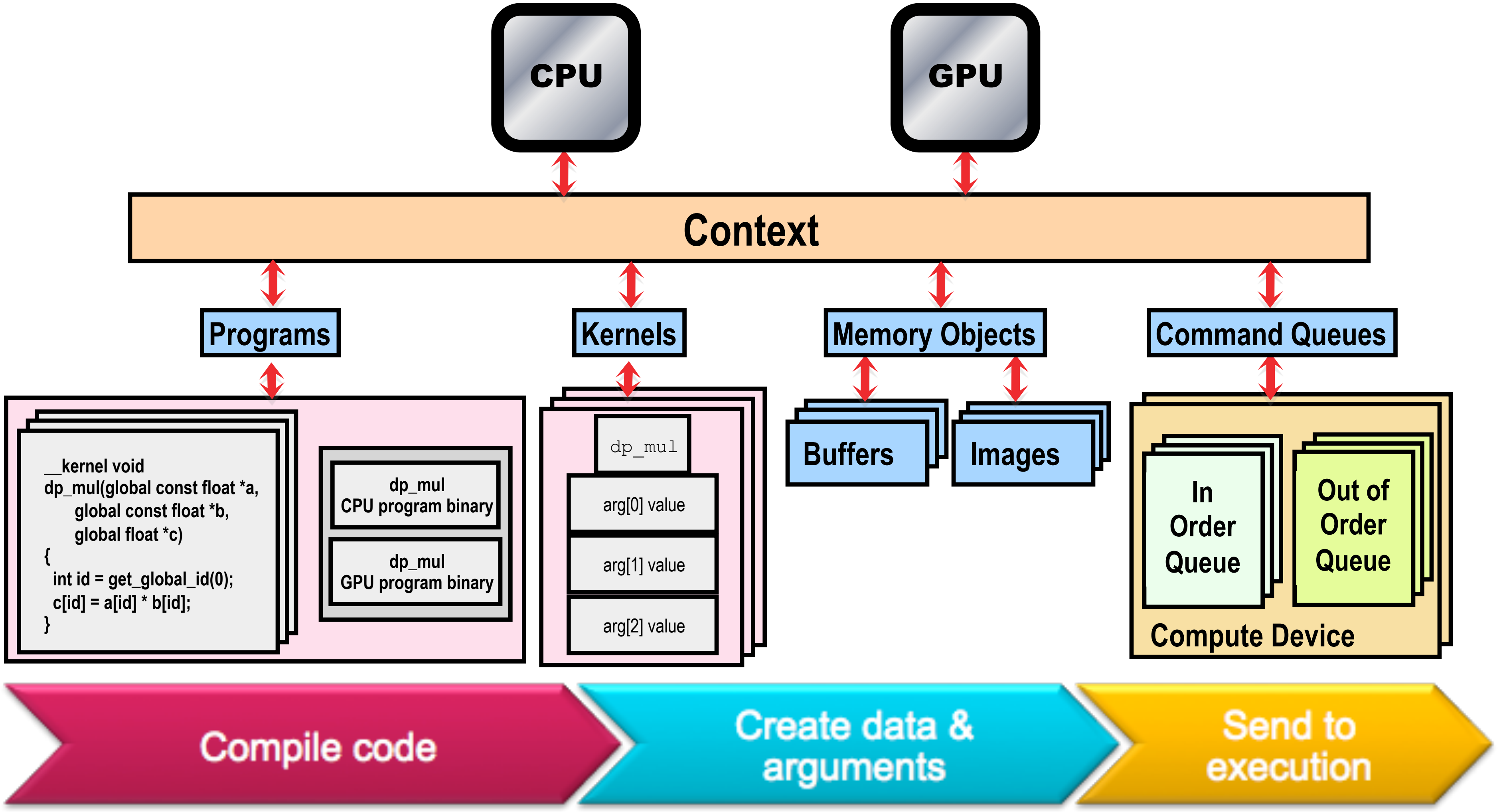
UPMARC summer school
Uppsala 28-29th 2014

Recap

5 simple steps in a basic OpenCL program:

1. Define the ***platform*** = devices + context + queues
2. Create and Build the ***program*** (dynamic library of kernels)
3. Setup ***memory*** objects
4. Define the ***kernels***
5. Submit ***commands*** … transfer memory objects and execute kernels

We have now covered the basic platform runtime APIs in OpenCL



```
__kernel void
dp_mul(global const float *a,
       global const float *b,
       global float *c)
{
  int id = get_global_id(0);
  c[id] = a[id] * b[id];
}
```

OPENCL KERNEL PROGRAMMING

OpenCL C kernel language

- Derived from **ISO C99**
  - A few ***restrictions***: no recursion, function pointers, functions in C99 standard headers (more later)
  - Preprocessing directives defined by C99 are supported (#include etc.)

- Built-in data types
  - Scalar and vector data types, pointers
  - Data-type conversion functions:
    - convert_type<_sat><_roundingmode>
  - Image types: image2d_t, image3d_t and sampler_t

OpenCL C Language Highlights

Function qualifiers

- **__kernel** qualifier declares a function as a kernel
  - I.e. makes it visible to host code
- Kernels can call other OpenCL functions
  - Not all OpenCL functions have to be marked as __kernels – they just won't be visible to the host

Address space qualifiers

- **__global, __local, __constant, __private**
- Pointer kernel arguments ***must*** be declared with an address space qualifier
- **__private** is default for variables declared inside a kernel

OpenCL C Language Highlights

Work-item functions ("n" indicates dimension – 0, 1, 2)

get_global_size(n)	number of work-items
get_local_size(n)	number of work-items in work-group
get_global_id(n)	global work-item ID
get_local_id(n)	work-item ID inside work-group
get_work_dim()	number of dimensions in use (1,2 or 3)
get_group_id(n)	ID of work-group

Synchronization functions

- **Barriers** - all work-items within a work-group must execute the barrier function before any work-item can continue
- **Memory fences** - provides ordering between memory operations

OpenCL C Language Restrictions

- Pointers to functions are ***not*** allowed
- Pointers to pointers allowed ***within*** a kernel, but not as an argument to a kernel invocation
- Bit-fields are not supported
- Variable length arrays and structures are not supported
- Recursion is not supported (yet!)
- Double types are optional in OpenCL v1.2, but the key word is reserved

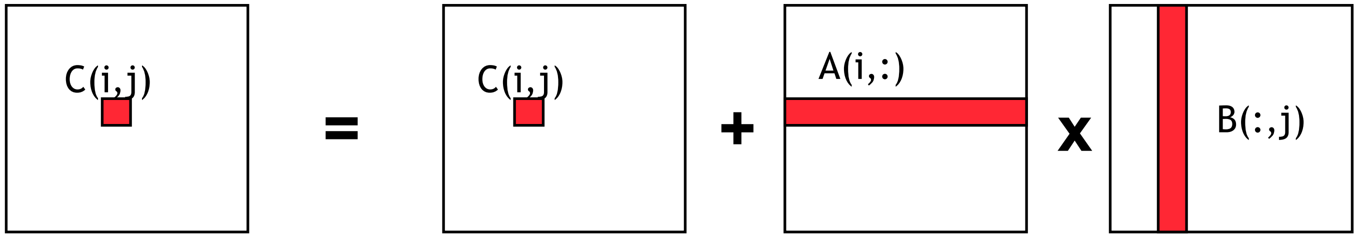
  (note: most implementations support double)

Matrix multiplication: sequential code

We calculate C=AB, all matrices square, of size "Order" on each side

```
void mat_mul(int Order, float *A, float *B, float *C)
{
  int i, j, k;
  for (i = 0; i < Order; i++) {
    for (j = 0; j < Order; j++) {
      for (k = 0; k < Order; k++) {
        // C(i, j) = sum(over k) A(i,k) * B(k,j)
        C[i*Order+j] += A[i*Order+k] * B[k*Order+j];
      }
    }
  }
}
```

Specialized to square matrices



Dot product of a row of A and a column of B for each element of C

Matrix multiplication performance

- Serial C code on CPU (single core).

Case	MFLOPS	
	CPU	GPU
Sequential C (not OpenCL)	887.2	N/A

Device is Intel® Xeon® CPU, E5649 @ 2.53GHz
using the gcc compiler.

These are not official benchmark results. You may observe completely different results should you run these tests on your own system.

Third party names are the property of their owners.

Matrix multiplication: sequential code

```
void mat_mul(int Order, float *A, float *B, float *C)
{
  int i, j, k;
  for (i = 0; i < Order; i++) {
    for (j = 0; j < Order; j++) {
      for (k = 0; k < Order; k++) {
        // C(i, j) = sum(over k) A(i,k) * B(k,j)
        C[i*Order+j] += A[i*Order+k] * B[k*Order+j];
      }
    }
  }
}
```

Matrix multiplication: OpenCL kernel (1/3)

```
__kernel void mat_mul(
 const int Order,
 __global float *A, __global float *B, __global float *C)
{
   int i, j, k;
   for (i = 0; i < Order; i++) {
     for (j = 0; j < Order; j++) {
       // C(i, j) = sum(over k) A(i,k) * B(k,j)
       for (k = 0; k < Order; k++) {
         C[i*Order+j] += A[i*Order+k] * B[k*Order+j];
       }
     }
   }
}
```

Mark as a kernel function and specify memory qualifiers

Matrix multiplication: OpenCL kernel (2/3)

```
__kernel void mat_mul(
  const int Order,
  __global float *A, __global float *B, __global float *C)
{
  int i, j, k;
  i = get_global_id(0);
  j = get_global_id(1);
      for (k = 0; k < Order; k++) {
        // C(i, j) = sum(over k) A(i,k) * B(k,j)
        C[i*Order+j] += A[i*Order+k] * B[k*Order+j];
      }

}
```

Remove outer loops and set work-item co-ordinates

Matrix multiplication: OpenCL kernel (3/3)

```
__kernel void mat_mul(
  __global float *A, __global float *B, __global float *C)
{
  int i, j, k;
  i = get_global_id(0);
  j = get_global_id(1);
  Order = get_global_id(0);
      for (k = 0; k < Order; k++) {
        // C(i, j) = sum(over k) A(i,k) * B(k,j)
        C[i*Order+j] += A[i*Order+k] * B[k*Order+j];

  }
}
```

Get "Order" from total number of work-items (global size)

Matrix multiplication: OpenCL kernel tweaked

Rearrange a bit and use a local scalar for intermediate C element values (a common optimization in Matrix Multiplication functions)

```
__kernel void mmul(
    __global float *A,
    __global float *B,
    __global float *C)
{
  int k;
  int i = get_global_id(0);
  int j = get_global_id(1);
  int Order = get_global_size(0);
  float tmp = 0.0f;
  for (k = 0; k < Order; k++)
   tmp += A[i*Order+k]*B[k*Order+j];

  C[i*Order+j] = tmp;
}
```

Matrix multiplication host program

```
#define DEVICE CL_DEVICE_TYPE_DEFAULT
int main(void)
{  // declarations (not shown)
    sz = N * N;
    std::vector<float> h_A(sz);
    std::vector<float> h_B(sz);
    std::vector<float> h_C(sz);

    cl::Buffer d_A, d_B, d_C;

// initialize matrices  and setup
// the problem (not shown)

   cl::Context context(DEVICE);
   cl::Program program(context,
       util::loadProgram("matmul1.cl“,
       true));
```

```
cl::CommandQueue queue(context);

auto mmul = cl::make_kernel
          <cl::Buffer, cl::Buffer, cl::Buffer>
                              (program, "mmul");

  d_A   = cl::Buffer(context, begin(h_A),
                                    end(h_A), true);
  d_B   = cl::Buffer(context, begin(h_B),
                                    end(h_B), true);
  d_C   = cl::Buffer(context,
                          CL_MEM_WRITE_ONLY,
                           sizeof(float) * sz);

  mmul(cl::EnqueueArgs( queue,
                          cl::NDRange(N,N)),
                          d_A,  d_B,  d_C);

  cl::copy(queue, d_C, begin(h_C),
                                    end(h_C));

  // Timing and check results (not shown)
}
```

Matrix multiplication performance

- Matrices are stored in global memory.

Case	**MFLOPS**	
	CPU	GPU
Sequential C (not OpenCL)	887.2	N/A
C(i,j) per work-item, all global	3,926.1	3,720.9

Device is Tesla® M2090 GPU from NVIDIA® with a max of 16 compute units, 512 PEs
Device is Intel® Xeon® CPU, E5649 @ 2.53GHz

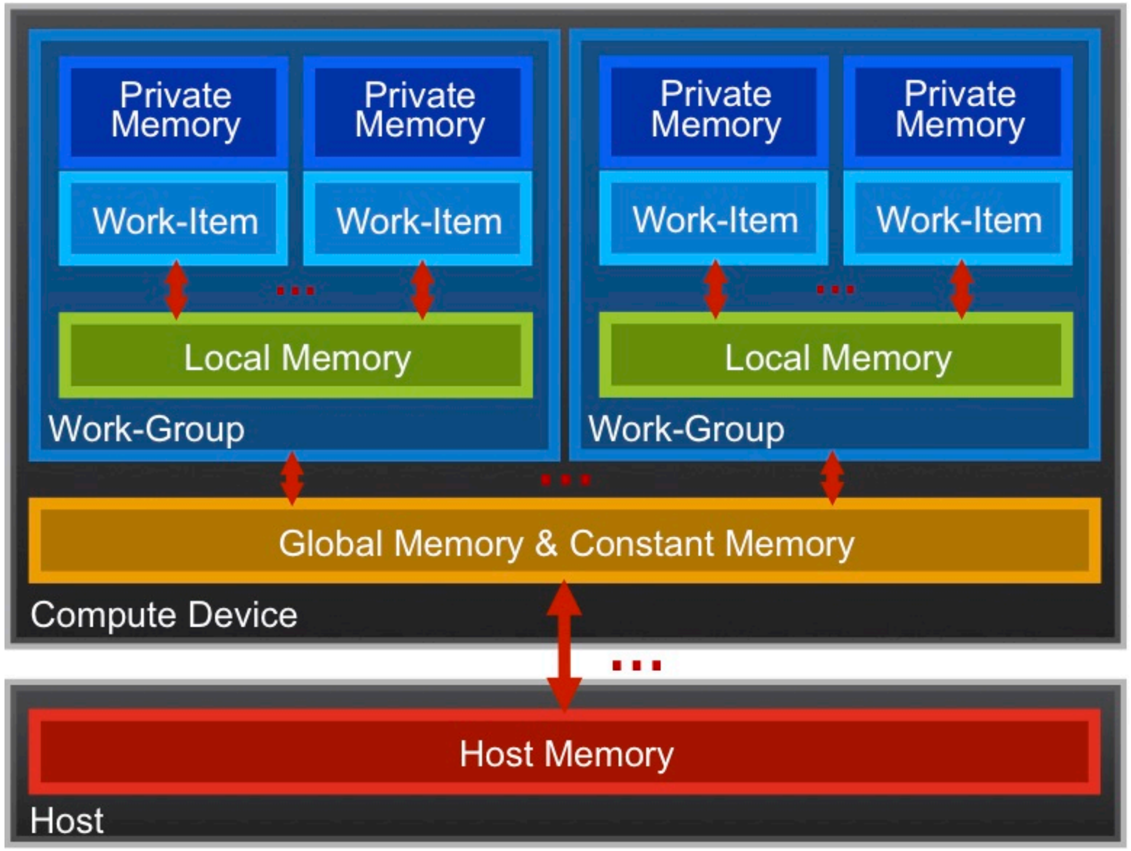
These are not official benchmark results. You may observe completely different results should you run these tests on your own system.

Third party names are the property of their owners.

EXPLOITING THE OPENCL MEMORY HIERARCHY

OpenCL Memory model

- Private Memory
  - Per work-item
- Local Memory
  - Shared within a work-group
- Global/Constant Memory
  - Visible to all work-groups
- Host memory
  - On the CPU

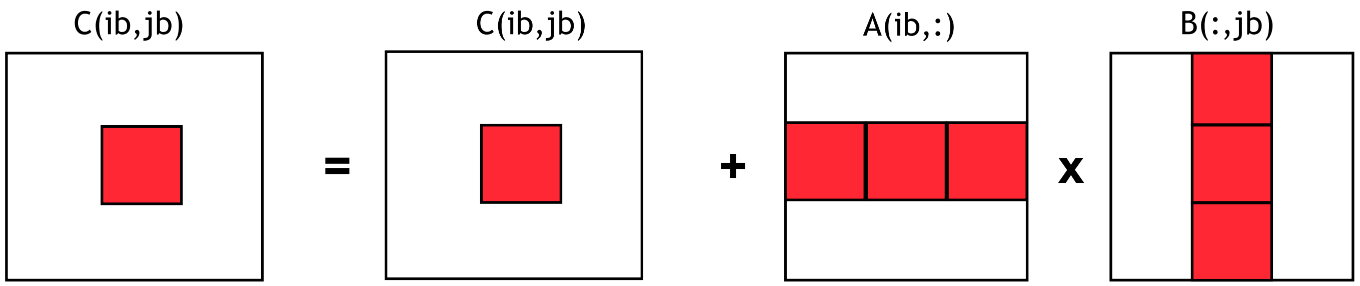


Memory management is **explicit**:
You are responsible for moving data from
host → global → local *and* back

Optimizing matrix multiplication

- Matrix multiply often benefits from reusing data as much as possible.

- So let's have each work-item compute a **sub block** of C



- We'll need to do something new:
  - Cache the sub blocks of A and B in local memory
  - Have to ensure local memory consistency (using barriers)

Memory Consistency

- OpenCL uses a **relaxed consistency** memory model; i.e.
  – The state of memory visible to a work-item is not guaranteed to be consistent across the collection of work-items at all times.
- Within a work-item:
  – Memory has load/store consistency to the work-item's own view of memory, i.e. it sees its own reads and writes correctly
- Within a work-group:
  – Local memory is consistent between work-items at a barrier.
- Global memory is consistent within a work-group at a barrier, **but *not* guaranteed across different work-groups!!**
  – This is a common source of bugs!
- Consistency of memory shared between **commands** (e.g. kernel invocations) is enforced by **synchronization** (barriers, events, in-order queue)

Work-Item Synchronization

Ensure correct order of memory operations to local or global memory (with flushes or queuing a memory fence)

- Within one work-group
  `void barrier()`
  - Takes optional flags
    CLK_LOCAL_MEM_FENCE and/or CLK_GLOBAL_MEM_FENCE
  - A work-item that encounters a barrier() will wait until ALL work-items in its work-group reach the barrier()
  - Corollary: If a barrier() is inside a branch, then the branch must be taken by either:
    - ALL work-items in the work-group, OR
    - NO work-item in the work-group

- Between different work-groups
  - No guarantees as to where and when a particular work-group will be executed relative to another work-group
  - **Cannot exchange data, or have barrier-like synchronization between two different work-groups! (Critical issue!)**
  - **Only solution: finish the kernel and start another**

Blocked matrix multiply: **kernel**

```
#define blksz 16
__kernel void mmul(
                const unsigned int N,
                __global float* A,
                __global float* B,
                __global float* C,
                __local  float* Awrk,
                __local  float* Bwrk)
{
   int kloc, Kblk;
   float Ctmp=0.0f;

   //  compute element C(i,j)
   int i = get_global_id(0);
   int j = get_global_id(1);

   // Element C(i,j) is in block C(Iblk,Jblk)
   int Iblk = get_group_id(0);
   int Jblk = get_group_id(1);

   // C(i,j) is element C(iloc, jloc)
   //  of block C(Iblk, Jblk)
   int iloc = get_local_id(0);
   int jloc = get_local_id(1);
   int Num_BLK = N/blksz;

 // calc. upper-left-corner and inc. for A and B
 int Abase = Iblk*N*blksz;        int Ainc  = blksz;
 int Bbase = Jblk*blksz;          int Binc  = blksz*N;

// C(Iblk,Jblk) = (sum over Kblk) A(Iblk,Kblk)*B(Kblk,Jblk)
 for (Kblk = 0;  Kblk<Num_BLK;  Kblk++)
 {
    //Load A(Iblk,Kblk) and B(Kblk,Jblk).
    //Each work-item loads a single element of the two
    //blocks which are shared with the entire work-group

    Awrk[jloc*blksz+iloc] = A[Abase+jloc*N+iloc];
    Bwrk[jloc*blksz+iloc] = B[Bbase+jloc*N+iloc];

    barrier(CLK_LOCAL_MEM_FENCE);

    #pragma unroll
    for(kloc=0; kloc<blksz; kloc++)
       Ctmp+=Awrk[jloc*blksz+kloc]*Bwrk[kloc*blksz+iloc];

    barrier(CLK_LOCAL_MEM_FENCE);
    Abase += Ainc;      Bbase += Binc;
 }
 C[j*N+i] = Ctmp;
}
```

Blocked matrix multiply: **kernel**

It's getting the indices right that makes this hard

```
#define blksz 16
__kernel void mmul(
                const unsigned int N,
                __global float* A,
                __global float* B,
                __global float* C,
                __local  float* Awrk,
                __local  float* Bwrk)
{
   int kloc, Kblk;
   float Ctmp=0.0f;

   //  compute element C(i,j)
   int i = get_global_id(0);
   int j = get_global_id(1);

   // Element C(i,j) is in block C(Iblk,Jblk)
   int Iblk = get_group_id(0);
   int Jblk = get_group_id(1);

   // C(i,j) is element C(iloc, jloc)
   //  of block C(Iblk, Jblk)
   int iloc = get_local_id(0);
   int jloc = get_local_id(1);
   int Num_BLK = N/blksz;
```

Load A and B blocks, wait for all work-items to finish

```
 // calc. upper-left-corner and inc. for A and B
 int Abase = Iblk*N*blksz;       int Ainc  = blksz;
 int Bbase = Jblk*blksz;         int Binc  = blksz*N;

// C(Iblk,Jblk) = (sum over Kblk) A(Iblk,Kblk)*B(Kblk,Jblk)
 for (Kblk = 0;  Kblk<Num_BLK;  Kblk++)
 {
    //Load A(Iblk,Kblk) and B(Kblk,Jblk).
    //Each work-item loads a single element of the two
    //blocks which are shared with the entire work-group

    Awrk[jloc*blksz+iloc] = A[Abase+jloc*N+iloc];
    Bwrk[jloc*blksz+iloc] = B[Bbase+jloc*N+iloc];

    barrier(CLK_LOCAL_MEM_FENCE);

    #pragma unroll
    for(kloc=0; kloc<blksz; kloc++)
       Ctmp+=Awrk[jloc*blksz+kloc]*Bwrk[kloc*blksz+iloc];

    barrier(CLK_LOCAL_MEM_FENCE);
    Abase += Ainc;       Bbase += Binc;
 }
 C[j*N+i] = Ctmp;
}
```

Wait for everyone to finish before going to next iteration of Kblk loop.

Blocked matrix multiply: **Host**

```
#define DEVICE CL_DEVICE_TYPE_DEFAULT
int main(void)
{  // declarations (not shown)
  sz = N * N;
  std::vector<float> h_A(sz);
  std::vector<float> h_B(sz);
  std::vector<float> h_C(sz);

 cl::Buffer d_A, d_B, d_C;

// initialize matrices  and setup
// the problem (not shown)

 cl::Context context(DEVICE);
 cl::Program program(context,
    util::loadProgram("mmulblock.cl“,
        true));

cl::CommandQueue queue(context);

auto mmul = cl::make_kernel
        <int, cl::Buffer, cl::Buffer, cl::Buffer,
            cl::LocalSpaceArg,  cl::LocalSpaceArg >
                                    (program, "mmul");

  d_A   = cl::Buffer(context, begin(h_A), end(h_A),true);
  d_B   = cl::Buffer(context, begin(h_B), end(h_B),true);
  d_C   = cl::Buffer(context,
            CL_MEM_WRITE_ONLY, sizeof(float) * sz);

  cl::LocalSpaceArg Awrk =
                cl::Local(sizeof(float) * N);
  cl::LocalSpaceArg Bwrk =
                cl::Local(sizeof(float) * N);
  mmul(cl::EnqueueArgs( queue,
              cl::NDRange(N,N),  cl::NDRange(16,16)),
              N, d_A,  d_B,  d_C, Awrk, Bwrk);

  cl::copy(queue, d_C, begin(h_C), end(h_C));

   // Timing and check results (not shown)
}
```

Blocked matrix multiply: **Host**

```
#define DEVICE CL_DEVICE_TYPE_DEFAULT
int main(void)
{  // declarations (not shown)
  sz = N * N;
  std::vector<float> h_A(sz);
  std::vector<float> h_B(sz);
  std::vector<float> h_C(sz);

 cl::Buffer d_A, d_B, d_C;

// initialize
// the prob

 cl::Context context(DEVICE);
 cl::Program program(context,
    util::loadProgram("mmulblock.cl“,
        true));

cl::CommandQueue queue(context);
```

Setup local memory with blocks of A and B (16 by 16) that should fit in local memory.

```
auto mmul = cl::make_kernel
        <int, cl::Buffer, cl::Buffer, cl::Buffer,
              cl::LocalSpaceArg,  cl::LocalSpaceArg >
                               (program, "mmul");

  d_A   = cl::Buffer(context, begin(h_A), end(h_A),true);
  d_B   = cl::Buffer(context, begin(h_B), end(h_B),true);
  d_C   = cl::Buffer(context,
             CL_MEM_WRITE_ONLY, sizeof(float) * sz);

  cl::LocalSpaceArg Awrk =
                  cl::Local(sizeof(float) * 16*16);
  cl::LocalSpaceArg Bwrk =
                  cl::Local(sizeof(float) * 16*16);
  mmul(cl::EnqueueArgs( queue,
           cl::NDRange(N,N),  cl::NDRange(16,16)),
           N, d_A,  d_B,  d_C, Awrk, Bwrk);

  cl::copy(queue, d_C, begin(h_C), end(h_C));

   // Timing and check results (not shown)
}
```

One work-item per element of the C matrix organized into 16 by 16 blocks.

Matrix multiplication performance

- Matrices are stored in global memory.

Case	**MFLOPS**	
	CPU	GPU
Sequential C (not OpenCL)	887	N/A
C(i,j) per work-item, all global	3,926	3,721
Block oriented approach using local mem		119,305

Device is Tesla® M2090 GPU from NVIDIA® with a max of 16 compute units, 512 PEs
Device is Intel® Xeon® CPU, E5649 @ 2.53GHz

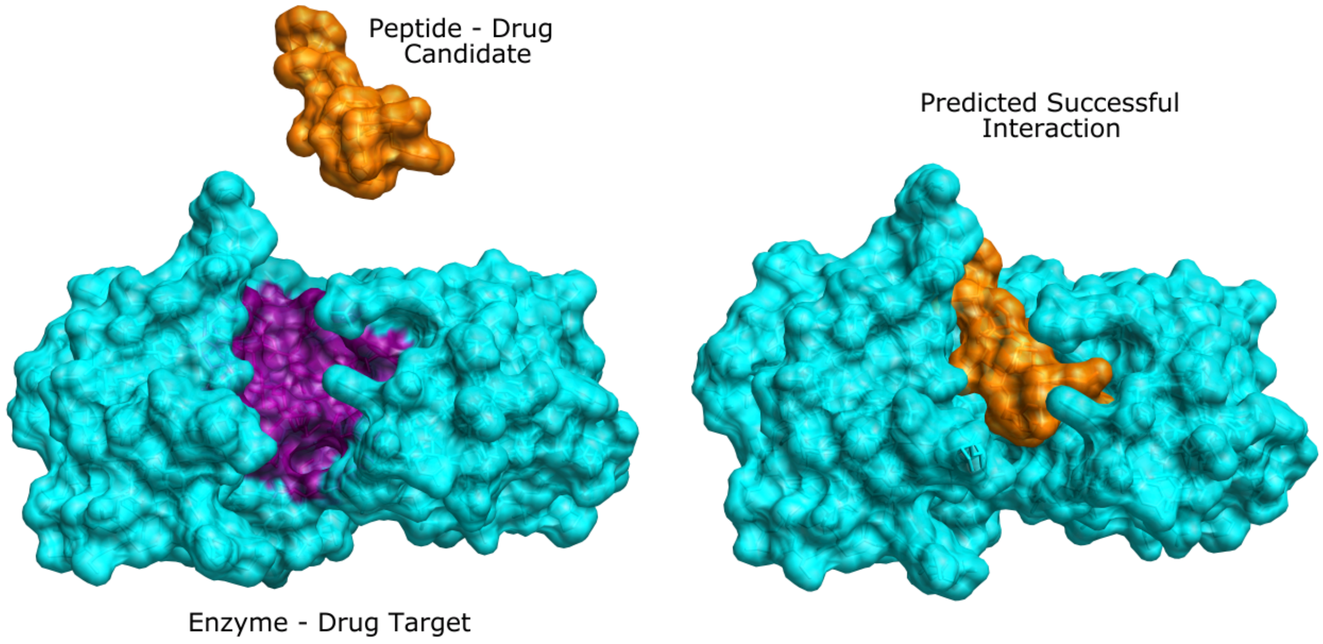
The CuBLAS SGEMM provides an effective measure of peak achievable performance on the GPU. CuBLAS performance = 283,366 MFLOPS

Third party names are the property of their owners.

These are not official benchmark results. You may observe completely different results should you run these tests on your own system.

USING OPENCL FOR REAL RESEARCH

Molecular Docking in Bristol



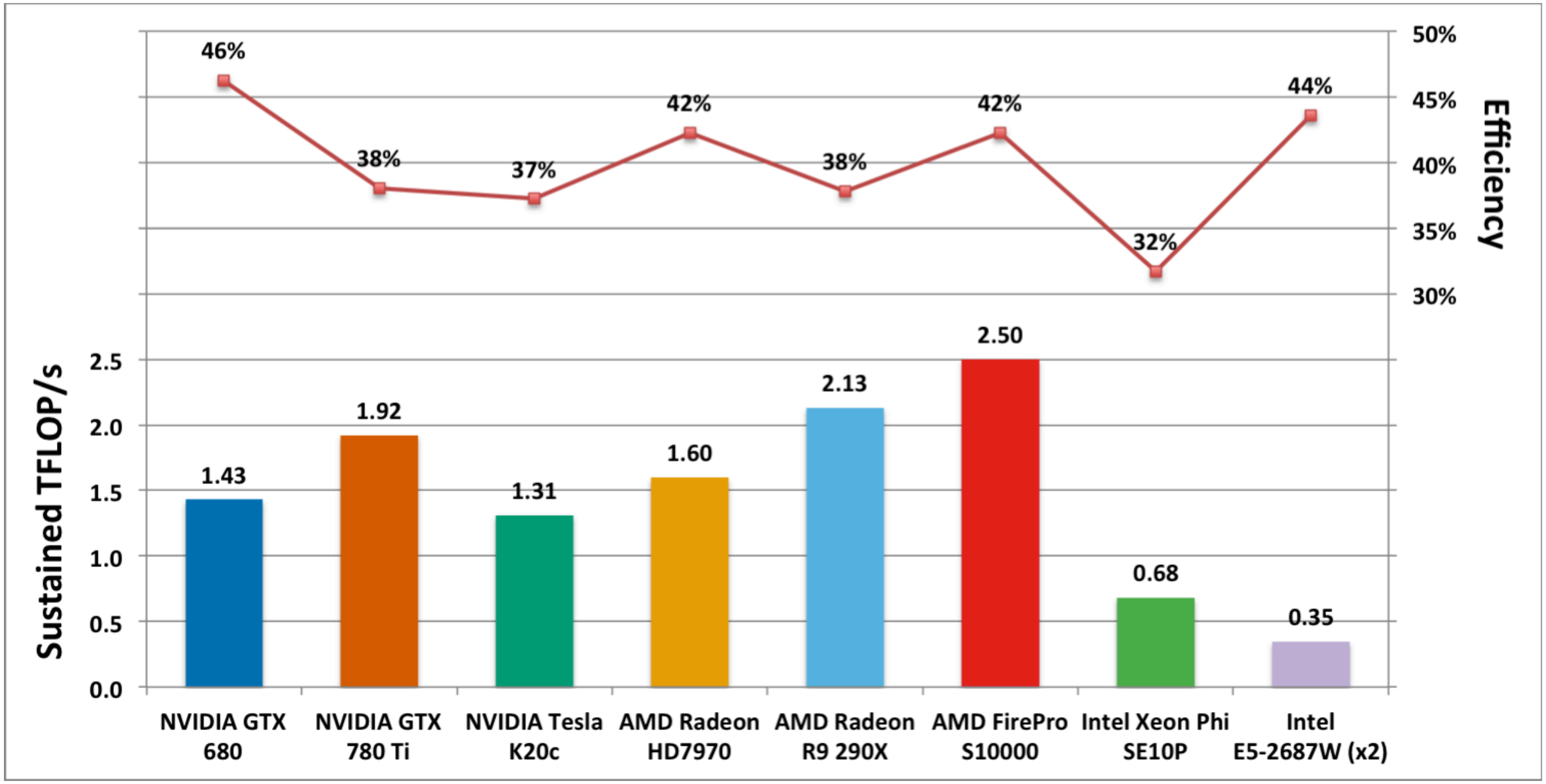
BUDE (Bristol University Docking Engine) is one of the fastest and most accurate molecular docking codes in the world.

BUDE is being used to find new drug targets for influenza, malaria, Alzheimer's, Emphysema, Insulin signalling and more

"High Performance *in silico* Virtual Drug Screening on Many-Core Processors", S. McIntosh-Smith, J. Price, R.B. Sessions, A.A. Ibarra, IJHPCA 2014. DOI: 10.1177/1094342014528252

Molecular Docking in Bristol

Performance portable molecular docking with BUDE.

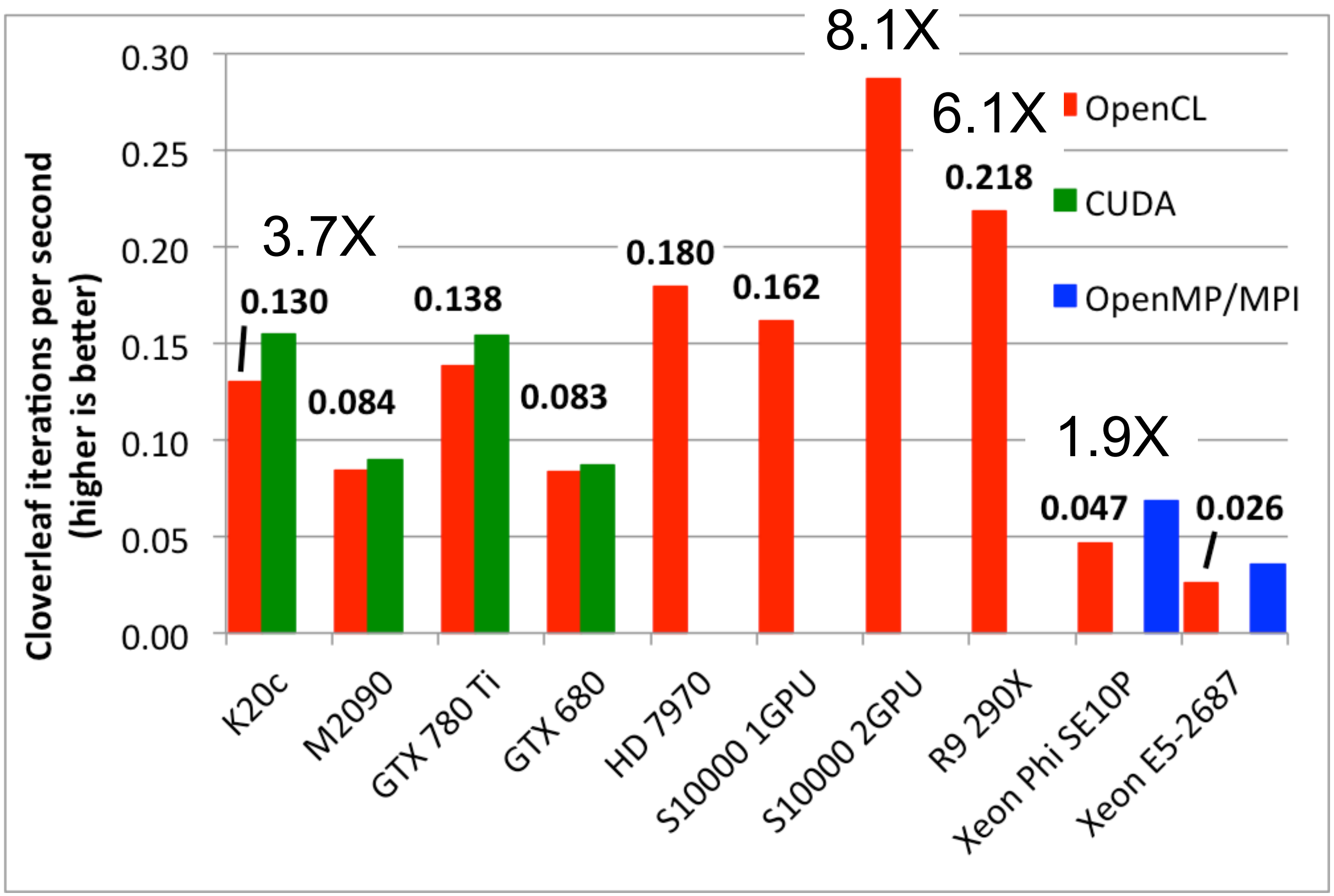


"High Performance *in silico* Virtual Drug Screening on Many-Core Processors", S. McIntosh-Smith, J. Price, R.B. Sessions, A.A. Ibarra, IJHPCA 2014.
DOI: 10.1177/1094342014528252

CloverLeaf: Peta→Exascale hydrodynamics mini-app

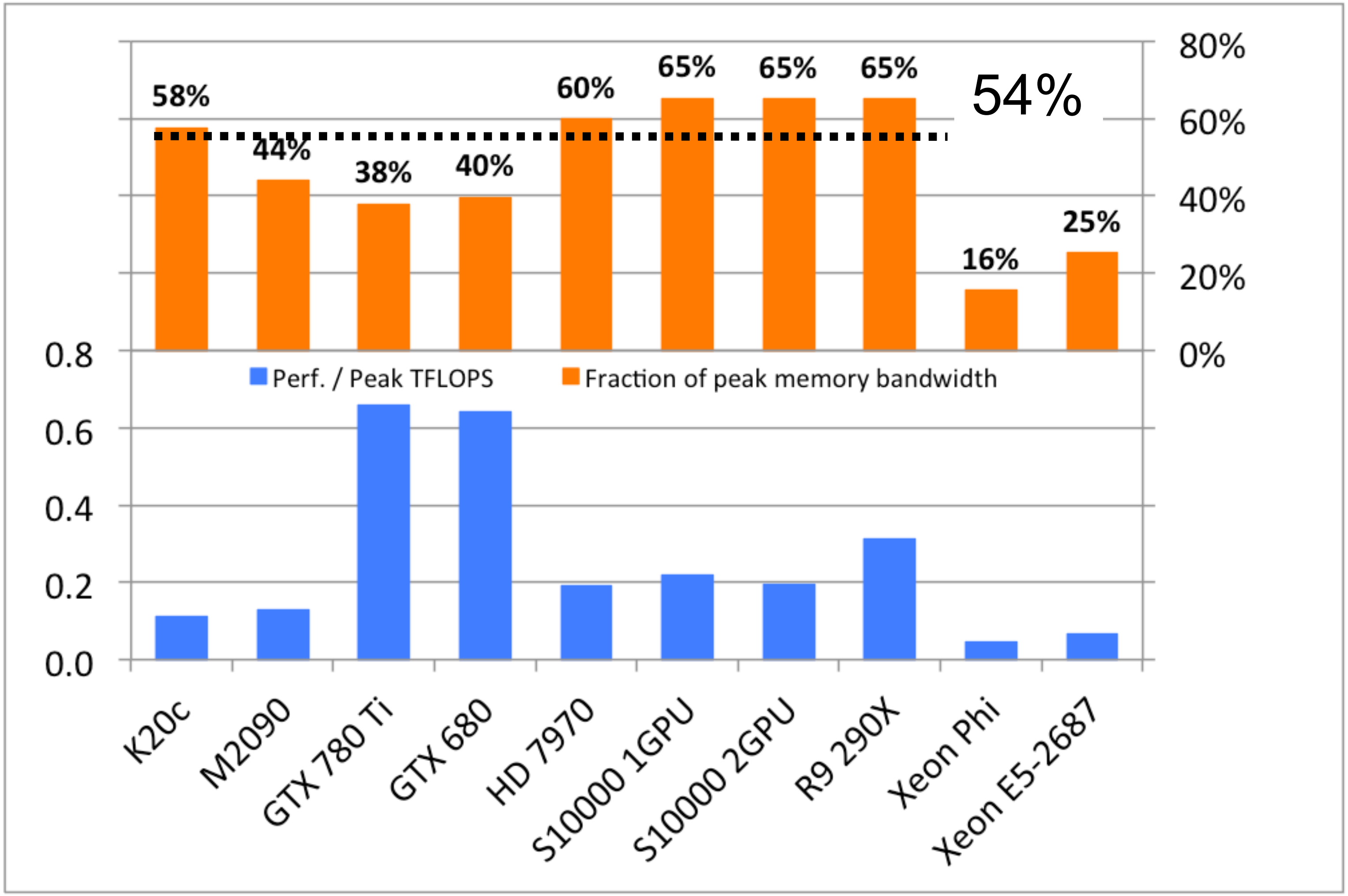
- CloverLeaf is a bandwidth-limited, structured grid code
- Solves the compressible Euler equations, which describe the conservation of energy, mass and momentum in a system
- Optimised parallel versions exist in OpenMP, MPI, OpenCL, OpenACC, CUDA and Co-Array Fortran

Results – performance



"On the performance portability of structured grid codes on many-core computer architectures", S.N. McIntosh-Smith, M. Boulton, D. Curran and J.R. Price, ISC, Leipzig, June 2014. DOI: 10.1007/978-3-319-07518-1_4

CloverLeaf sustained bandwidth



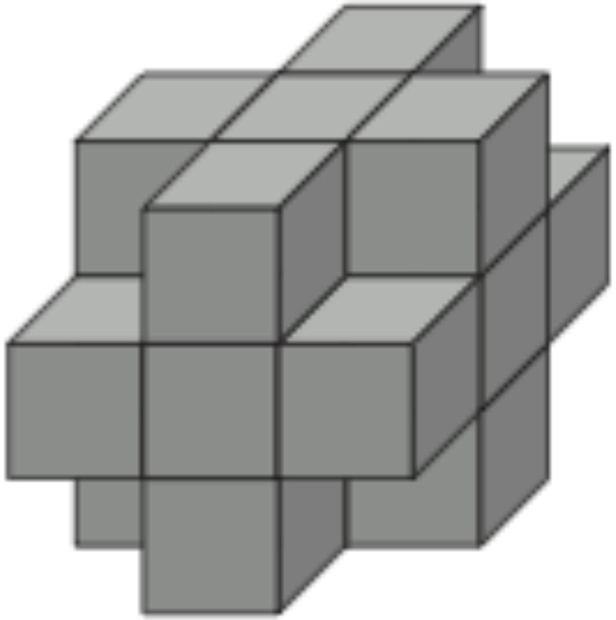
"On the performance portability of structured grid codes on many-core computer architectures", S.N. McIntosh-Smith, M. Boulton, D. Curran and J.R. Price, ISC, Leipzig, June 2014. DOI: 10.1007/978-3-319-07518-1_4

Lattice Boltzmann (LBM)

- A versatile approach for solving incompressible flows based on a simplified gas-kinetic description of the Boltzmann equation (used for CFD etc)
- Ports well to most parallel architectures
- We targeted one of the most widely used variants, **D3Q19-BGK**

"Evaluation of a performance portable lattice Boltzmann code using OpenCL", S.N. McIntosh-Smith and D. Curran, IWOCL, May 12-13, 2014 Bristol, UK. To appear in ACM ICPS, ISBN 978-1-4503-3007-7

D3Q19-BGK LBM



- To update a cell, need to access 19 of the 27 surrounding cell values in the 3D grid

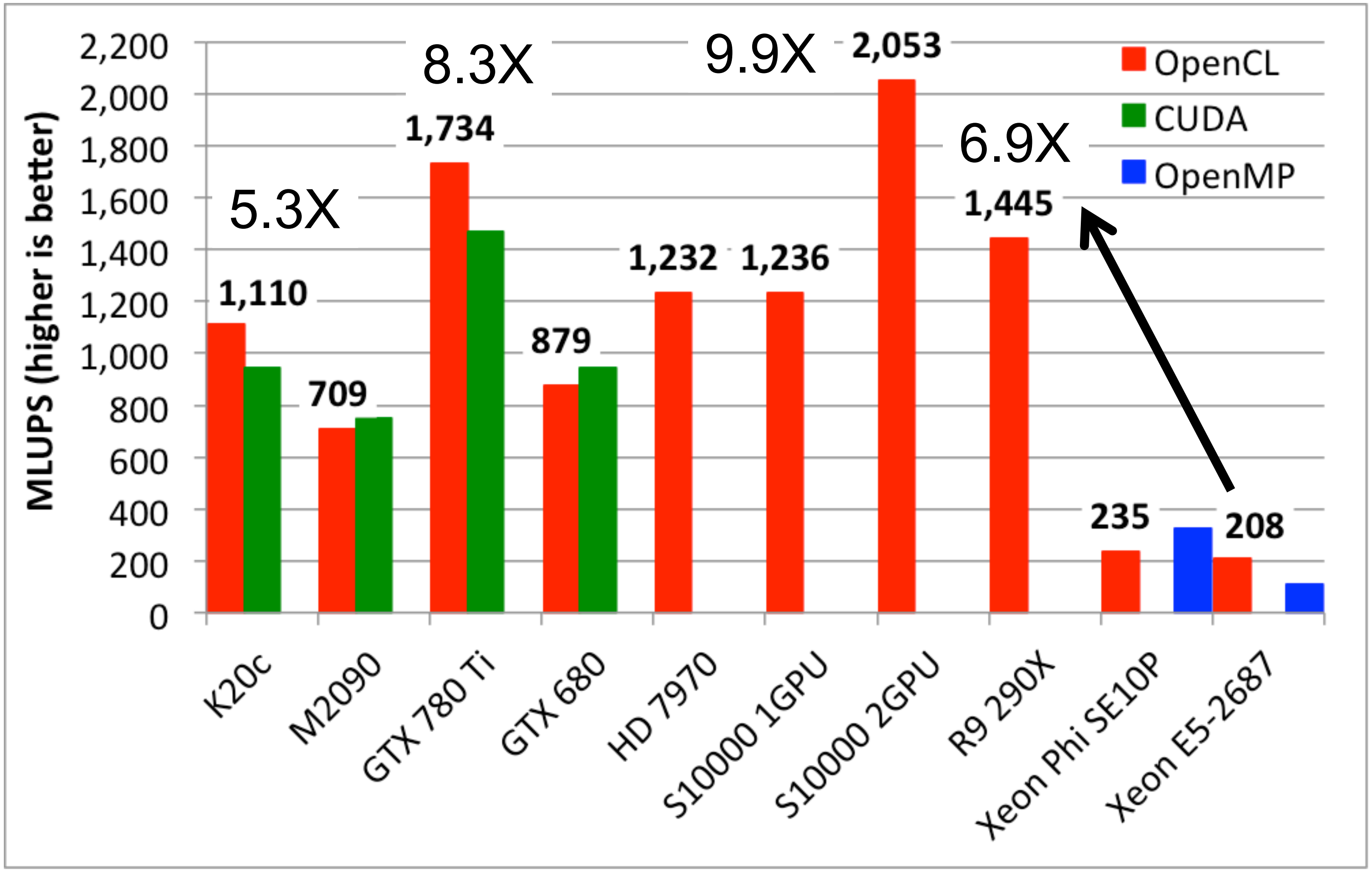
“Evaluation of a performance portable lattice Boltzmann code using OpenCL”, S.N. McIntosh-Smith and D. Curran, IWOCL, May 12-13, 2014 Bristol, UK. To appear in ACM ICPS, ISBN 978-1-4503-3007-7

Methodology

- Developed a code that was efficient but not over complicated
- "Identical" versions in OpenCL and CUDA
  - Single precision grid 128^3 (~2m grid points, 304 MBytes)
  - The OpenCL three dimensional work-group size was fixed at (128,1,1) for ***all*** OpenCL runs on ***all*** devices
  - Same arrangement for CUDA version
- The OpenMP code was as close as possible to the OpenCL/ CUDA versions
- Ensured the OpenMP code was being vectorised by the compiler (latest Intel icc)

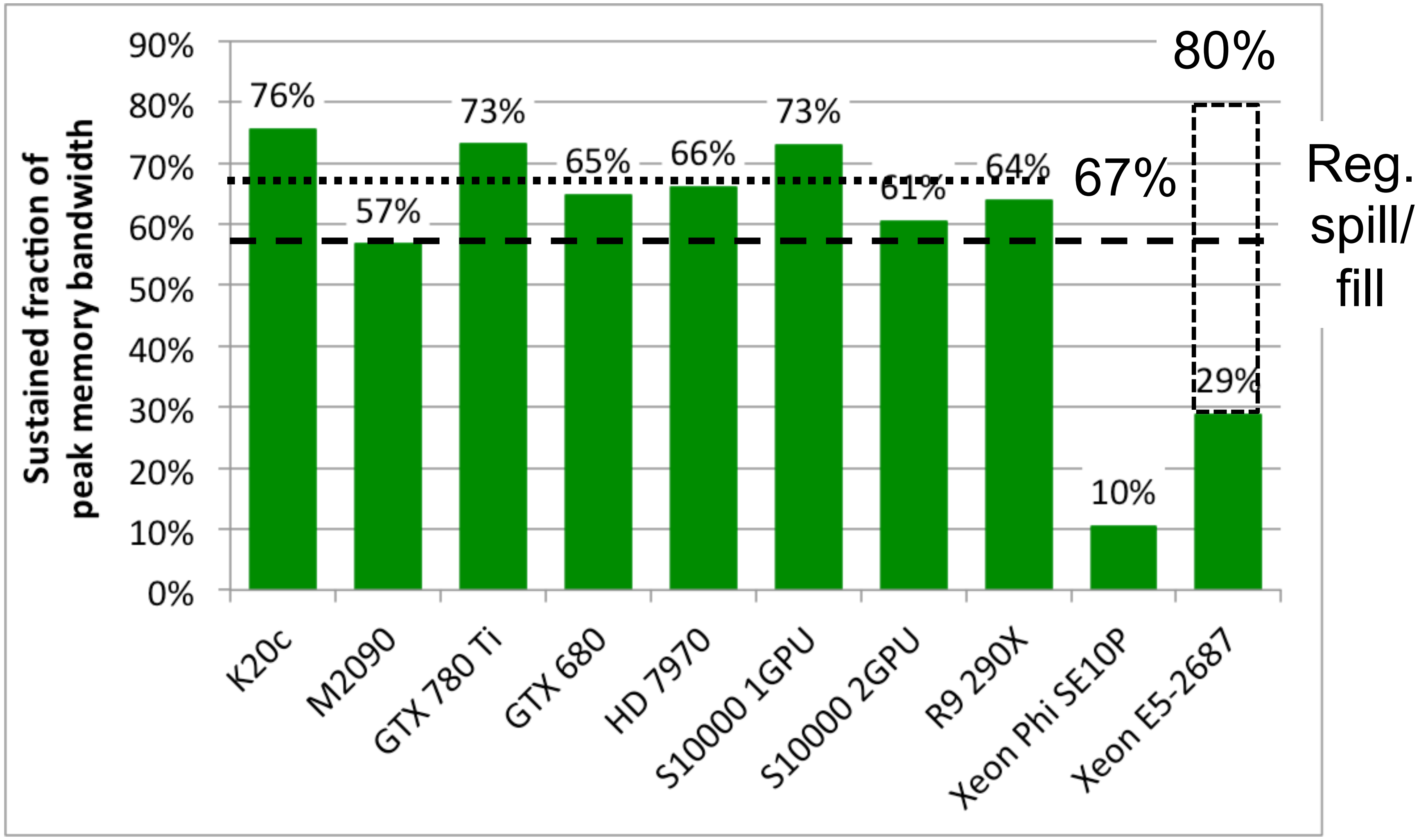
"Evaluation of a performance portable lattice Boltzmann code using OpenCL", S.N. McIntosh-Smith and D. Curran, IWOCL, May 12-13, 2014 Bristol, UK. To appear in ACM ICPS, ISBN 978-1-4503-3007-7

Performance results for 128^3



Single precision results

Performance results for 128^3



OpenCL single precision results

So perf. portable, but is it fast?

- On an Nvidia K20, our best 128^3 D3Q19-BGK LBM single precision performance in OpenCL was **1,110** MLUPS
- In the literature, the fastest quoted results are ~**1,000** MLUPS (Januszewski and Kostur's *Sailfish* program) and **982** MLUPS (Mawson and Revell)
- Our results are a **13%** improvement over Mawson-Revell and a **10%** improvement over Januszewski-Kostur

"Evaluation of a performance portable lattice Boltzmann code using OpenCL", S.N. McIntosh-Smith and D. Curran, IWOCL, May 12-13, 2014 Bristol, UK. To appear in ACM ICPS, ISBN 978-1-4503-3007-7

SOME CONCLUDING REMARKS

Conclusions

- OpenCL has ***widespread*** industrial support
- OpenCL defines a platform-API/framework for ***heterogeneous computing***, not just GPGPU or CPU-offload programming
- OpenCL has the potential to deliver ***portably performant code***; but it has to be used correctly
- The latest ***C++ and Python APIs*** makes developing OpenCL programs much simpler than before
- OpenCL is the ***only*** parallel programming standard that enables mixing task parallel and data parallel code in a single program and load balancing across **a wide variety of parallel hardware.** ***It's fun to use too!!!***

OpenCL-related things

- OpenCL's Standard Portable Intermediate Representation (SPIR)
  - Based on LLVM's Intermediate Representation (IR)
  - Makes interchangeable front- and back-ends straightforward

- OpenCL 2.0
  - Released Nov 2013, only partial implementations so far
  - Lots of other improvements

- SYCL
  - Single source C++ higher level parallel programming in OpenCL
  - http://www.khronos.org/opencl/sycl/

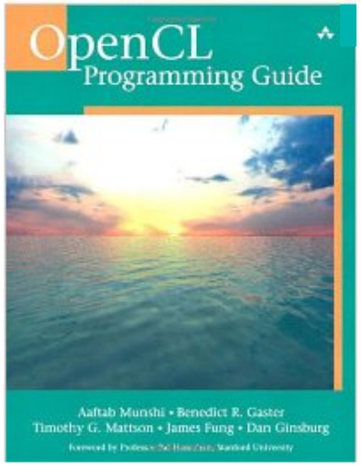
- For the latest news on SPIR and new OpenCL versions see:
  - http://www.khronos.org/opencl/

Third party names are the property of their owners.

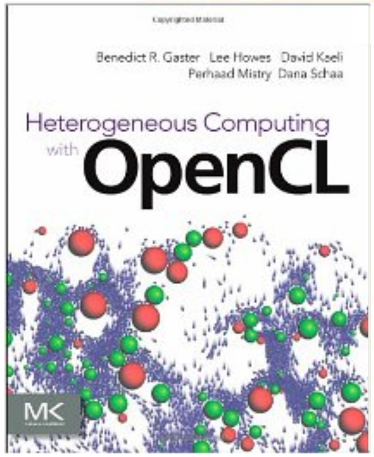
OpenCL resources

- Khronos website
  - https://www.khronos.org/opencl/
- Annual OpenCL workshop, **IWOCL**
  - http://iwocl.org
  - In May each year (in Boston for 2015)
- **HandsOnOpenCL** training course online
  - http://handsonopencl.github.io
  - Dozens of exercises and solutions in C, C++ and Python
  - Includes CUDA to OpenCL tutorial

OpenCL books


OpenCL
Programming Guide
Aaftab Munshi • Benedict R. Gaster
Timothy G. Mattson • James Fung • Dan Ginsburg

OpenCL Programming Guide:
Aaftab Munshi, Benedict Gaster, Timothy G. Mattson and James Fung, 2011


Benedict R. Gaster Lee Howes David Kaeli
Perhaad Mistry Dana Schaa
Heterogeneous Computing
with
OpenCL
MK

Heterogeneous Computing with OpenCL
Benedict Gaster, Lee Howes, David R. Kaeli, Perhaad Mistry and Dana Schaa, 2011

I'm hiring!

- Looking for a postdoc for a 3 year post on the prestigious FP7 Mont Blanc project
  – Can we build an Exascale supercomputer form European technologies, such as ARM-based CPUs and GPUs?
  – Post to look at software fault tolerance techniques for Exascale computing
- Also looking for PhD students
- Email me at simonm at cs.bris.ac.uk