OpenACC and C++: An Application Perspective

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Big thanks to PGI for all the hard work
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Brent Leback
Michael Wolfe
Douglas Miles

SAND2015-2057 C
What is it about?

**Goal**
- add (a few) pragmas and run on GPUs
- portable
- pretty good performance

**Reality end of 2013**
- big performance issues since data is transferred very often
- issues with unstructured code (i.e. complex code path)
- C++!! almost didn’t work
- non trivial amount of pragma decoration
“Solved” by OpenACC 2.0: Data Management Issues

Common use-case with occasional resize of data
=> cannot use simple data region around timestep loop

```c
void foo(int* x, int m, int& length) {
    if(m>length) {
        delete [] x;
        x = new int[m];
        length = m;
    }
    for(int i=0;i<m;i++) {
        ...
    }
}

void run(int* x, int& length, int nsteps) {
    for(int t = 0; t<nsteps; t++) {
        int m = bla(x,length);
        foo(x,m,length);
    }
}
```
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Want a data region for x here, but can’t because foo might reallocate
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    }
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```

Want a data region for x here, but can’t because *foo* might reallocate

Workaround: use ‘deviceptr’ with ‘acc_malloc’ and ‘acc_free’
Compiler C++ issue: Class Members

- Root issue: OpenACC didn’t know what to do with ‘this->’

```cpp
struct FooOpenACC {
    double a; int N;
    void scale(double* x) {
        #pragma acc parallel loop copy(x[0:N])
        for(int i=0; i<N; i++)
            update_val(x[i]);
    }
    void update_val(double& x) {
        x*=a;
    }
};
```
Compiler C++ issue: Class Members

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  }
};
```

Didn’t know what to do because it has implicit ‘this-&gt;’ in front.

Workaround: make local copies of everything
Standard C++ Issue: deep copy

When using classes it is not clear how to copy internal allocations

```c++
struct DataStructure {
    double* data;
    int* idx;
    int N;

    double access(int i) {
        return data[idx[i]];
    }
};

void update(DataStructure a, DataStructure b) {
    #pragma acc parallel loop
    for(int i=0; i<a.N; i++) {
        a.access(i) += b.access(i);
    }
}
```
Standard C++ Issue: deep copy

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    int* idx;
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}

void update(DataStructure a, DataStructure b) {
    #pragma acc parallel loop
    for(int i=0; i<a.N; i++) {
        a.access(i)+=b.access(i);
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```

How to convey that ‘idx’ and ‘data’ of ‘a’ and ‘b’ have to be copied or already exist on device. How to get correct device pointers into copies of a and b.
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    int N;

    double access(int i) {
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    }
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How to convey that `idx` and `data` of `a` and `b` have to be copied or already exist on device. How to get correct device pointers into copies of `a` and `b`.
void ForceLJ::compute_fullneigh(Atom &atom, Neighbor &neighbor, int me) {

    const int nlocal = atom.nlocal;
    const int nall = atom.nlocal + atom.ghost;
    const MMD_float* const restrict x = atom.d_x;
    MMD_float* const restrict f = atom.d_f;
    const int* const restrict neighbors = neighbor.d_neighbors;
    const int* const restrict numneigh = neighbor.d_numneigh;
    const int nmax = neighbor.nmax;
    const int maxneighs = neighbor.maxneighs;
    const MMD_float sigma6_ = sigma6;
    const MMD_float epsilon_ = epsilon;
    const MMD_float cutforcesq_ = cutforcesq;

    #pragma acc data deviceptr(x,neighbors,numneigh,f) {
        #pragma acc kernels
        for(int i = 0; i < nlocal; i++) {
            f[i * PAD + 0] = 0.0;
        }

        #pragma acc kernels
        for(int i = 0; i < nlocal; i++) {
            ...
        }
    }
}
How that added up in miniMD 1.2

```c
void ForceLJ::compute_fullneigh(Atom &atom, Neighbor &neighbor, int me)
{
    const int nlocal = atom.nlocal;
    const int nall = atom.nlocal + atom.ghost;
    const MMD_float* const restrict x = atom.d_x;
    MMD_float* const restrict f = atom.d_f;
    const int* const restrict neighbors = neighbor.d_neighbors;
    const int* const restrict numneigh = neighbor.d_numneigh;
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    for(int i = 0; i < nlocal; i++) {
        ...
    }
}
```

Extract members of other classes

Make local copies of members of ‘this’ class
void ForceLJ::compute_fullneigh(Atom &atom, Neighbor &neighbor, int me) {
    const int nlocal = atom.nlocal;
    const int nall = atom.nlocal + atom.nghost;
    const MMD_float* const restrict x = atom.d_x;
    MMD_float* const restrict f = atom.d_f;
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    Extract members of other classes
    Make local copies of members of 'this' class
    Use explicit device allocations (manage data movement with host and device pointers)
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void ForceLJ::compute_fullneigh(Atom &atom, Neighbor &neighbor, int me) {
    const int nlocal = atom.nlocal;
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```

- Extract members of other classes
- Make local copies of members of ‘this’ class
- Use explicit device allocations (manage data movement with host and device pointers)
- Manually inline function calls to ‘neighbor’
void ForceLJ::compute_fullneigh(Atom &atom, Neighbor &neighbor, int me) {
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        for(int i = 0; i < nlocal; i++) {
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        }
    }

    #pragma acc kernels
    for(int i = 0; i < nlocal; i++) {
        ... 
    }
}
Working with PGI on solutions for C++

- Some of the solutions came as part of OpenACC 2.0
  - unstructured data regions, function calls
  - But: C++ still didn’t work

- (i) Sandia provided stripped down examples for C++ features
- (ii) Discussed possible solutions and acceptable restrictions
- (iii) PGI fixed compiler
- (iv) Sandia tested
- (v) rinse and repeat for last 15 months
Data Management: using UVM

- Auto replace “new” allocations with UVM allocations
  - total allocations limited to device space
  - can be slower than unstructured data regions due to page size granularity
  - but effectively zero data management!!

```c
int size = 10000000;
int nsteps = 100;
double* x = new double[size];

for(int k = 0; k < nsteps; k++) {
    if( k%20 != 0) {
        #pragma acc parallel loop copy(x[0:size])
        for(int i = 0; i < size; i++)
            x[i]*=a;
    } else {
        for(int i = 0; i < size; i++)
            x[i]*=a;
    }
}
```

![Chart showing comparison between Copy and UVM methods in terms of time in seconds.]
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  } else {
    for(int i = 0; i < size; i++)
      x[i]*=a;
  }
}
```

![Bar chart showing comparison between Copy and UVM time in seconds]

Not Needed
Data Management: Unstructured data regions
(And why that’s sometimes better than UVM)

int size = 10000000;
int nsteps = 100;
double* x = new double[size];

#pragma acc enter data copyin(x[0:size])
for(int k=0;k<loop;k++) {
    if(k%20!=0) {
        #pragma acc parallel loop
        for(int i=0; i<size; i++)
            x[i]*=a;
    } else {
        #pragma acc update self(x[0:size])
        for(int i=0; i<size; i++)
            x[i]*=a;
            #pragma acc update device(x[0:size])
    }
}
#pragma acc exit data delete(x)

UVM will copy page by page: due to PCIe latency effective Bandwidth ~500MB/s
But couldn’t you use structured regions?

In the previous example structured regions possible, but not with classes

class FooOpenACC {
    double a; double* x; int N;
public:
    FooOpenACC(double a_, double* x_, int N_):
        a(a_), x(x_), N(N_){
            #pragma acc enter data pcreate(this)
            #pragma acc update device(this)
            #pragma acc enter data create(x[0:N])
        }
    void scale() {
        #pragma acc parallel loop
        for(int i=0; i<N; i++)
            x[i]*=a;
    }
    void host_scale() {
        update_host();
        for(int i=0; i<N; i++)
            x[i]*=a;
        update_device();
    }
    void update_host() {
        #pragma acc update self(x[0:N])
    }
    void update_device() {
        #pragma acc update device(x[0:N])
    }
};

FooOpenACC f(a,x,size);

for(int k=0;k<loop;k++) {
    if(k%20!=0) {
        f.scale();
    } else {
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```

The outer loop doesn’t know what FooOpenACC is doing.
Combination: C++ Classes now work for MiniMD

Unstructured data regions for device copies of class instances

```cpp
Integrate::Integrate() {
    sort_every=20;
    #pragma acc enter data pcreate(this)
}

Integrate::~Integrate() {
    #pragma acc exit data delete(this)
}
```

Update device copy if it was potentially changed

```cpp
void Integrate::initialIntegrate() {
    #pragma acc update device(this)
    #pragma acc parallel loop
    for(MMD_int i = 0; i < nlocal; i++) {
        v[i * PAD + 0] += dtforce * f[i * PAD + 0];
        x[i * PAD + 0] += dt * v[i * PAD + 0];
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Refers to device copy (e.g. device-this->…)
Relies on UVM for x and v
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Refers to device copy (e.g. device-this->…) Relies on UVM for x and v
miniMD-OpenACC-UVM 2.0

- based on miniMD-OpenMP-Scalable => no algorithm changes
- use UVM to manage data transfers => minimal data clauses
- biggest change: atomic counters need to be allocated

![Graph showing LOC and Time improvements](image-url)
miniMD-OpenACC-UVM 2.0

- based on miniMD-OpenMP-Scalable => no algorithm changes
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150 lines are atomic counters
60 #pragma acc

LOC

<table>
<thead>
<tr>
<th></th>
<th>OpenMP</th>
<th>OpenACC-UVM</th>
<th>OpenACC-1.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Changed</td>
<td></td>
<td>260</td>
<td>630</td>
</tr>
<tr>
<td>Unchanged</td>
<td>630</td>
<td>260</td>
<td></td>
</tr>
</tbody>
</table>

Time

3x

Changed

Unchanged
miniMD-OpenACC-UVM 2.0

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![Graph showing LOC and Time comparison between OpenMP, OpenACC-UVM, and OpenACC-1.0]
Open Issues

- Still many bugs in the compiler: please try out and report (turnaround and responsiveness is pretty good)
- Compiler vendor specific solutions: what about generic concept of UVM, implicit routine generation?
- Sometimes tricky to get the order right (class creation / attach) and to know when routine is needed and when not
- Performance issues compared with Cuda
  - classes are copied into global memory, much slower than constant cache
  - it's hard to get the settings right to get __ldg loads
  - __ldg loads are slower than texfetch1D in some cases

*Not yet ready for prime time, but it is getting there.*
Questions and further discussion: crtrott@sandia.gov