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Multicore/GPGPU Portable Computational Kernels via Multidimensional Arrays

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Performance-Portable Thread-Level Parallelism

- **Portability with Performance is a Challenge**
  - CPU-Multicore and GPGPU-Manycore (e.g., NVIDIA)
  - Language constraints (e.g., CUDA)
  - Performance concerns: memory access patterns dominate
- **Data Parallel Computational Kernels**
  - Defer task parallelism, pipeline parallelism, ...
  - parallel_for and parallel_reduce semantics
- **“Natural” Data Structures**
  - For scientific & engineering computations
  - Multidimensional array (a la FORTRAN)

Trilinos' Kokkos-Array *Library*

- **An API and Library; Not a Compiler**
  - **Computational kernels written in subset of C++ (CUDA v3.x)**
  - **Computing on multidimensional arrays**
  - **Running on a compute device**
    - ***CPU Multicore, NVIDIA GPGPU, Intel Knights Ferry***

- **Simple API**
  - **Very simple C++ class API for multidimensional arrays**
  - **Very simple "functor" pattern for computational kernels**
  - **In the *spirit* of Intel's Threaded Building Blocks (TBB) or Thrust**

Abstractions

- **Manycore Compute Device**
  - Provides many threads of execution
  - Owns memory space accessible to and shared by those threads
  - At most one device per process (MPI rank)
    - *Choice:* for hybrid parallel programming *simplicity*
    - Two levels: global (MPI) and local (data parallel)
- **Multidimensional Array**
  - and multivector – a special case not covered in this presentation
- **Partitioning and Mapping of Arrays onto a Device**
- **Data Parallel Computational Kernels**

Abstraction: Multidimensional Array

- **Homogeneous Collection of Data Members**
  - Mathematical, plain-old-data type (for now)
  - Members reside in the memory space of a compute device
  - Members referenced by a multi-index in a multi-index space
- **Multi-index (i0 , i1 , i2 , …)**
  - Ordered list of indices of a simple integer type
  - Rank – the number of indices
- **Multi-index Space**
  - Cartesian product of integer ranges
    - Kokkos array: [0 .. N0) x [0 .. N1) x [0 .. N2) x …
    - Abbreviated as: (N0 , N1 , N2 , …)
  - Cardinality = N0 * N1 * N2 * …

Abstraction: Mapping

- **Multidimensional Array's Map**
  - Bijective map : multi-index space ↔ array data members
  - [0 .. N0) x [0 .. N1) x [0 .. N2) x … ↔ array data members
- **Two Well-Known Examples**
  - Base location + offset into contiguous block of memory
  - FORTRAN : (i0 – 1) + N0 * ((i1 – 1) + N1 * ((i2 – 1) + N2 * (…)))
  - C : (…((((i0) * N1 + i1) * N2 + i2) * N3 + i3) * …)
- **Key Concept: Choose the Optimal Map for a Device**
  - Multiple valid maps; your favorite map is not the only valid map
  - Different devices may have different optimal maps

Abstraction: Parallel Partitioning

- **Partition Data for Parallel Work**
  - Partition into NP atomic units of parallel work
  - Multidimensional array (and multivector) index space has one parallel work dimension: (<u>NP</u> , N1 , N2 , …)
  - Matrices and Grids have multiple parallel work dimensions
    - These are related but different abstractions

- **Parallel Work via Computational Kernel**
  - Atomic unit of parallel work identified by index : ip $\in$ [0 .. NP)
  - Computational kernel must
    - Update only those array members with index (ip , * , * , …)
    - Not query data being updated by different unit of work

Abstraction: Data Parallel Computational Kernels

- **"Parallel For" Kernel** $f:(\{\alpha\},\{X\})\rightarrow\{Y\}$
  - **$\{\alpha\}$ are shared parameters**
  - **{X} and {Y} are sets of partitioned multidimensional arrays**
  - **f can be independently applied to each atomic unit of work**

- **"Parallel Reduce" Kernel** $f:(\{\alpha\},\{X\})\rightarrow(\{\beta\},\{Y\})$
  - **$\{\beta\}$ are reduction parameters**
  - **Each atomic unit of work contributes to parameters**

    $$f:(\{\alpha\},\{X(ip,\cdots)\}\rightarrow\{\beta[ip]\},\{Y(ip,\cdots)\})$$

  - **Contributions are reduced by a *mathematically* commutative and associative function**

    $$f_R:(\{\beta[ip]\}\forall ip)\rightarrow\{\beta\}$$

Kokkos::MDArrayView API
Multi-index Space and Data Access

```
namespace Kokkos {
template< typename ValueType ,
          class DeviceType , class MapOption = ... >
class MDArrayView {
public:
  // Query rank and dimensions of multi-index space
  size_type rank() const ;
  size_type dimension( irank ) const ;

  // Access data member on the device via its multi-index
  KOKKOS_MACRO_DEVICE_FUNCTION
  ValueType & operator()( iP , i1 , i2 , ... ) const ;
};
}
```

- Index space known on the host and on the device
- Data members reside only on the device
  - Data members only accessible on the device

Kokkos::MDArrayView API
Copy Array Member Data

```
namespace Kokkos {
template< typename ValueType ,
          class DeviceDest ,
          class MapDest ,
          class DeviceSource ,
          class MapSource >
void deep_copy(
  const MDArrayView<ValueType,DeviceDest,  MapDest>   & dest ,
  const MDArrayView<ValueType,DeviceSource,MapSource> & source );
}
```

- **“Deep Copy” – Copy Member Data**
  - **Between arrays on the same device or different devices**
  - **Between arrays with the same map or different maps**

Kokkos::MDArrayView API
Shared Ownership View Semantics

```
namespace Kokkos {
template< typename ValueType , class DeviceType , class MapOption >
class MDArrayView {
public:
  MDArrayView(); // NULL view

  // New view of same data viewed by RHS (a "shallow copy")
  MDArrayView( const MDArrayView & RHS );

  // Clear this view: if the last view then deallocate member data
  ~MDArrayView();

  // Clear this view and then assign to be a new view of RHS data
  MDArrayView & operator = ( const MDArrayView & RHS );
};
// Allocate a multidimensional array
template< typename ValueType , class DeviceType , class MapOption >
MDArrayView< ValueType , DeviceType , MapOption >
  create_mdarray( NP , N1 , N2 , ... );
}
```

API Requirements: Users' Functors

- Functor: work function + work data
  - Work function is called thread-parallel
    - Called NP times on up to NP different threads
  - Work data reside on the compute device
  - Work data are accessed through Views
- Functors are Passed by Value to the Compute Device
  - Functor members are copied
  - Copying a view is 'shallow' – the view is copied not the data
- Functors are Compiled for the Compute Device
  - Work function is restricted: CUDA 3.x – a subset of C++
  - NO memory management on the compute device
  - Thread safety – only access 'ip' data members

API Requirements For Users' Parallel-For Functor

```
namespace MyNamespace {
template< class DeviceType >
class MyFunctor {
public:
  typedef DeviceType device_type ; // Required to identify device

  KOKKOS_MACRO_DEVICE_FUNCTION
  void operator()( int ip ) const ; // Required work operator

  // Input and output arrays for the operation:
  typedef MDArrayView< myValueType , device_type > myArrayType ;
  const myArrayType myInputA , myInputB , ... ;
  const myArrayType myOutputX , myOutputY , ... ;

  // Constructor copies views ("shallow copy") of input and output
  MyFunctor( const myArrayType & A , ... )
    : myInputA( A ), ... {}
};
}
```

API Requirements For Users' Parallel-Reduce Functor

```
namespace MyNamespace {
template< class DeviceType > class MyFunctor {
public:
  typedef DeviceType device_type ;
  typedef ... value_type ; // Parameter type, could be a "struct"

  // Operator contributes to the update value
  KOKKOS_MACRO_DEVICE_FUNCTION
  void operator()( int ip , value_type & update ) const ;

  // update = reduce_operation( update , input );
  KOKKOS_MACRO_DEVICE_FUNCTION
  static void join( volatile       value_type & update ,
                    volatile const value_type & input );

  // Initialize to the "identity" value for the reduce_operation
  KOKKOS_MACRO_DEVICE_FUNCTION
  static void init( value_type & output );
};
}
```

Calling Functors on the Device

- Copy Functor to the device and run it
- Call parallel_for Functor NP times:
  - Work function is called thread-parallel

```
Kokkos::parallel_for( NP , MyFunctor( ... ) );
```

- Call parallel_reduce Functor NP times:
  - Return single-value parameter result:

```
value = Kokkos::parallel_reduce( NP , MyFunctor( ... ) );
```

  - Output multiple-value parameter ‘struct’ result:

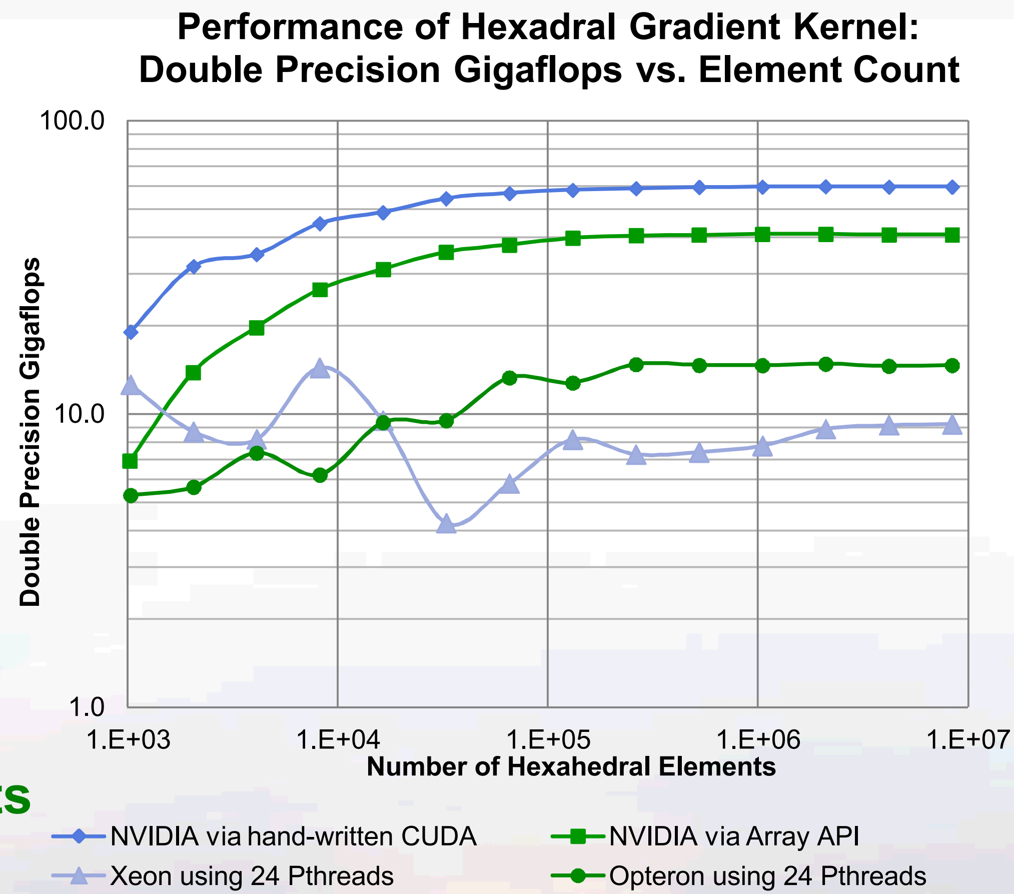
```
Kokkos::parallel_reduce( NP , MyFunctor( ... ) , value );
```

  - Store the result on the device (single or multiple value):

```
Kokkos::ValueView<value_type,device_type> result ;
Kokkos::parallel_reduce( NP , MyFunctor( ... ) , result );
```

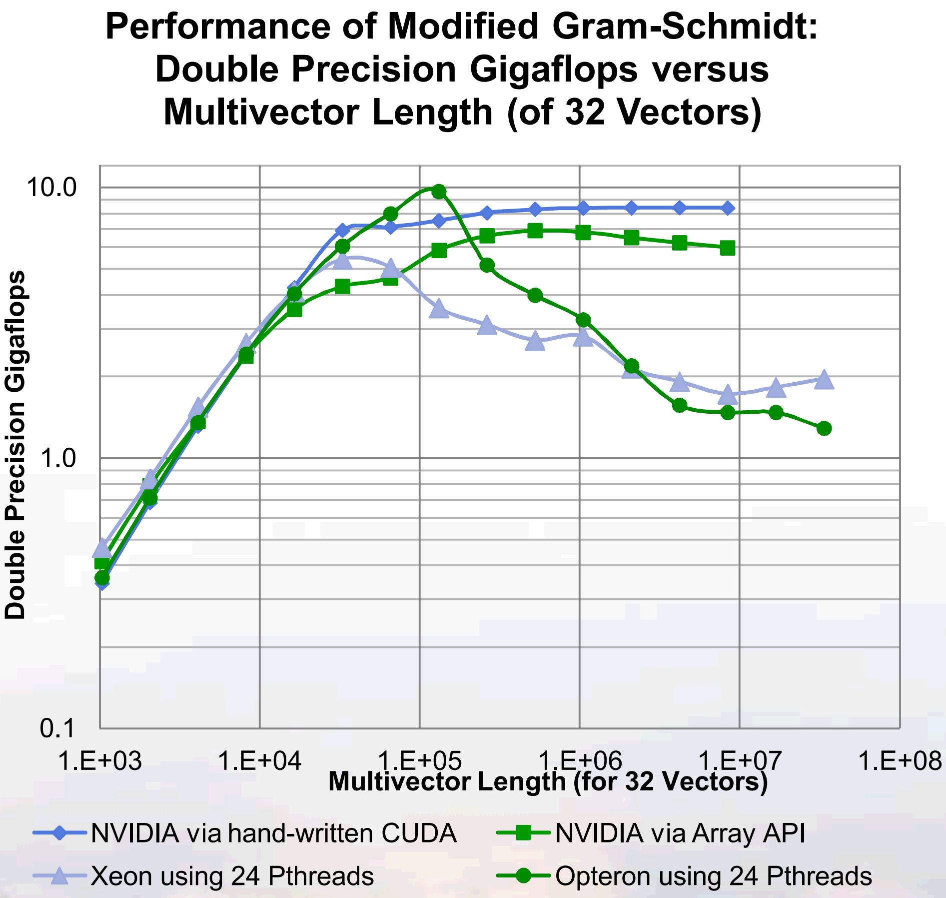
Performance Test Case #1: Parallel_For on Hexahedral Basis Gradient

- **Finite Element Kernel**
  - Input coordinates (NP,3,8)
  - Output gradients (NP,3,8)
  - Double precision
  - 6.6 flops per value access
  - Xeon: 2 x 6core x 2 HT
  - Opteron: 2 x 12core
  - NVIDIA C2070 (448 cores)
- **vs. Hand-written CUDA**
  - No in-code index-map
  - Hard-coded memory offsets
  - Within 20% performance



Performance Test Case #2: Gram-Schmidt Orthogonalization

- Classical Algorithm
  - sequence of parallel_for and parallel_reduce operations
  - Double precision
  - 2 * N * M^2 flops (M=32)
  - Xeon: 2 x 6core x 2 HT
  - Opteron: 2 x 12core
  - NVIDIA C2070 (448 cores)
- Minimize data exchange
  - Launch sequence of functors on the device
  - Leave and use reduction values on the device



Conclusion & Plans

- **Performance-portable multidimensional array programming model**
  - Demonstrated on Xeon, Opteron, and NVIDIA
  - "Classical" multidimensional array data access interface
  - C++ templated on the device and the multi-index map
    - Choose map which is optimal for the device
  - Shared-ownership view semantics
- **Plans**
  - Other devices; e.g., Intel Knights Ferry
  - Evaluate with more complex kernels & mini-applications
  - Expand to multi-parallel-index arrays: grids, matrices
- **Available: http://trilinos.sandia.gov**