Portable and Productive Performance on Hybrid Systems with libsci_acc

Luiz DeRose

Sr. Principal Engineer

Programming Environments Director

Cray Inc.

What is Cray Libsci_acc?

- **Provide basic scientific libraries optimized for hybrid systems**
  - Incorporate the existing GPU libraries into Cray libsci
- **Independent to, but fully compatible with OpenACC**
- **Multiple use case support**
  - Get the base use of accelerators with no code change
  - Get extreme performance of GPU with or without code change
- **Provide additional performance and usability**
- **Two interfaces**
  - Simple interface
    - **Auto-adaptation**
    - Base performance of GPU with minimal (or no) code change
    - Target for anybody: non-GPU users and non-GPU expert
  - Expert interface
    - Advanced performance of the GPU with controls for data movement
    - Target for CUDA, OpenACC, and GPU experts
      - **Does not imply that the expert interfaces are always needed to get great performance**

Why libsci_acc ?

- **Code modification is required to use existing GPU libraries!**

- **Several scientific library packages already exist**
  - CUBLAS, CUFFT, CUSPARSE (NVIDIA), MAGMA (U Tennessee), CULA (EM Photonics)

- **No Compatibility to Legacy APIs**
  - cublasDgemm(….)
  - magma_dgetrf(…)
  - culaDgetrf(…)
  - Why not dgemm(), dgetrf()?

- **Not focused on Fortran API (C/C++)**
  - Require CUDA data types, primitives and functions in order to call them

- **Performance**

Auto-tuning

- **Cray Autotuning framework has been built to tune BLAS for accelerators**
  - GPU kernel codes are built using code generator
  - Enormous offline auto-tuning is used to build a map of performance to input
  - An adaptive library is built from the results of the auto-tuning
  - At run-time, your code is mapped to training set of input
  - Best kernel for your problem is used

Simple Interface

- **Supports the standard API in the original form**
- **Will perform all GPU dirty-work for you**
  - Initialize data structures on GPU
  - Split your problem into a CPU portion and GPU portion
  - Copy data to the GPU memory from CPU memory
  - Perform GPU and CPU operations
  - Copy data back to CPU memory
- **Library-heavy codes can use GPUs with no code change**
- **Is not only a tool for simple usage**
  - **If you don't need the data on the GPU afterwards, use the simple interface**
- **Simple API has automatic adaptation**

Adaptation in the Simple Interface

- You can pass either host pointers or device pointers with the simple interface

- A is in host memory

```
dgetrf(M, N, A, lda, ipiv, &info)
```

  - Performs hybrid operation on GPU
  - if problem is too small, performs host operation

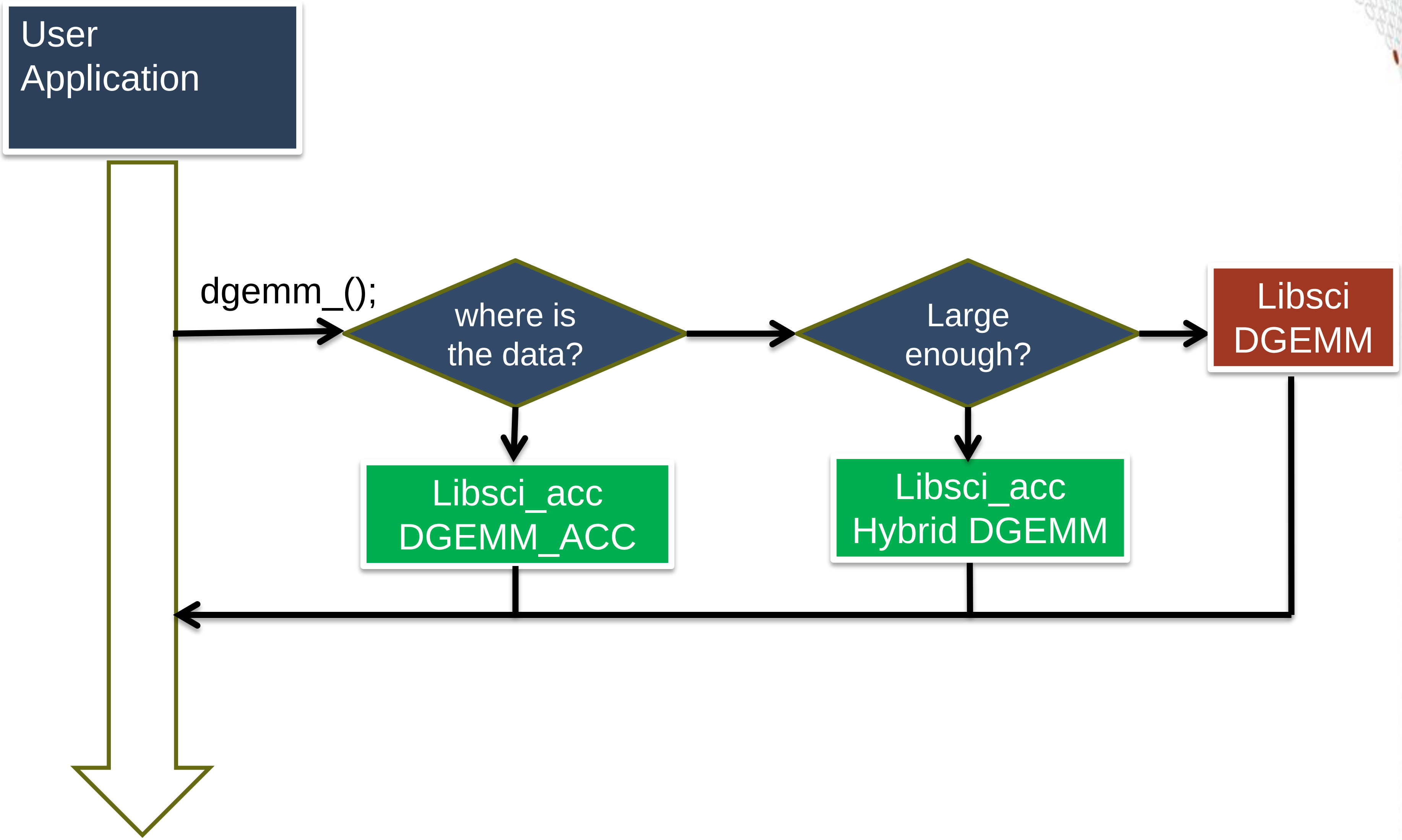
- Pass Device memory

```
dgetrf(M, N, d_A, lda, ipiv, &info)
```

  - Performs hybrid operation on GPU

- **BLAS 1 and 2 performs computation local to the data location**
  - CPU-GPU data transfer is too expensive to exploit hybrid execution

Libsci_acc: Simple Interface for BLAS3 and LAPACK



Expert Device & CPU Interface

- **Device interface gives higher degrees of control**

- **Allow users to explicitly specify the execution**
  - Every routine in libsci has a version with _acc and _cpu suffix
    - e.g. dgetrf_acc, dgetrf_cpu

  - Simple API for device memory and _acc API are the same

Usage - Basics

- **Supports Cray and GNU compilers.**

- **Fortran and C interfaces (column-major assumed)**
  - Load the module craype-accel-nvidia35.
  - Compile as normal (dynamic libraries used)

- **To enable threading in the CPU library, set OMP_NUM_THREADS**
  - E.g. export OMP_NUM_THREADS=16

- **Assign 1 single MPI process per node**
  - Multiple processes cannot share the single GPU

- **Execute your code as normal**

Libsci_acc with OpenACC

- If the code uses OpenACC, it’s possible to use the library with directives
- All data management performed by OpenACC
- Calls the device version of dgemm
- All data is in CPU memory before and after data region

```
!$acc data copy(a,b,c)

!$acc parallel
!Do Something
!$acc end parallel

!$acc host_data use_device(a,b,c)

call dgemm_acc('n','n',m,n,k,&
               alpha,a,lda,&
               b,ldb,beta,c,ldc)

!$acc end host_data
!$acc end data
```

Libsci_acc with OpenACC

- Libsci_acc is a bit smarter that this
- Since ‘a,’ ‘b’, and ‘c’ are device arrays, the library knows it should run on the device
- So just dgemm is sufficient

```
!$acc data copy(a,b,c)

!$acc parallel
!Do Something
!$acc end parallel

!$acc host_data use_device(a,b,c)

call dgemm    ('n','n',m,n,k,&
               alpha,a,lda,&
               b,ldb,beta,c,ldc)

!$acc end host_data
!$acc end data
```

libsci_acc BLAS Routines Available

- **BLAS 3 - Full HYBRID Implementations**
  - [s,d,c,z]GEMM
  - [s,d,c,z]GEMM
  - [s,d,c,z]TRSM
  - [z,c]HEMM
  - [s,d,c,z]SYMM
  - [s,d,c,z]SYRK
  - [z,d]HERK
  - [s,d,c,z]SYR2K
  - [s,d,c,z]TRMM
- **The following are supported without HYBRID implementations because there is no performance advantage**
  - All BLAS 2 Routines
  - All BLAS 1 Routines

libsci_acc LAPACK Routines Available

- **Full HYBRID Implementations:**
  - [d,z]GETRF (LU Factorization)
  - [d,z]POTRF (Cholesky Factorization)
  - [d,z]GETRS (System Solver)
  - [d,z]POTRS (System Solver)
  - [d,z]GESDD* (Generalized Singular Values)
  - [d,z]GEBRD (Generalized Bidiagonalization)
  - [d,z]GEQRF* (QR Factorization)
  - [d,z]GELQF (LQ Factorization
  - [d,z]GEEV (Non-symmetric Eigenvalues)
  - DSYEVR* / ZHEEVR* (Hermitian/Symmetric Eigenvalues)
  - DSYEV / DSYEVD (Hermitian/Symmetric Eigenvalues)
  - ZHEEV / ZHEEVD (Hermitian/Symmetric Eigenvalues)
  - DSYGVD / ZHEGVD (Hermitian/Symmetric Eigenvalue System Solver)

* Include Cray Proprietary Optimizations

Summary

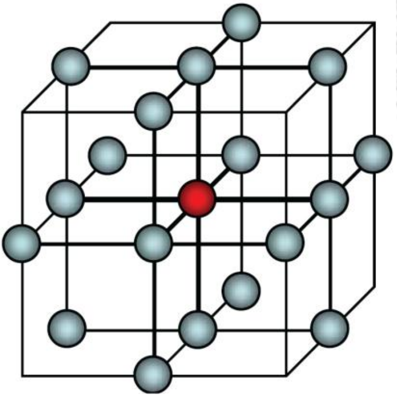
- **Access to libsci_acc routines is simple**
  - No need to explicitly link - Programming Environment drivers (cc, ftn, CC) do this for you
  - Just target the GPU by loading module

- **Can automatically take advantage of threading on CPU**
  - Just set OMP_NUM_THREADS and run

- **Simple interface available to enable hybrid, CPU or GPU execution of a routine depending on where memory pointers reside and problem size**

- **Interface for advanced control is also available**

Case Study: the Himeno Benchmark



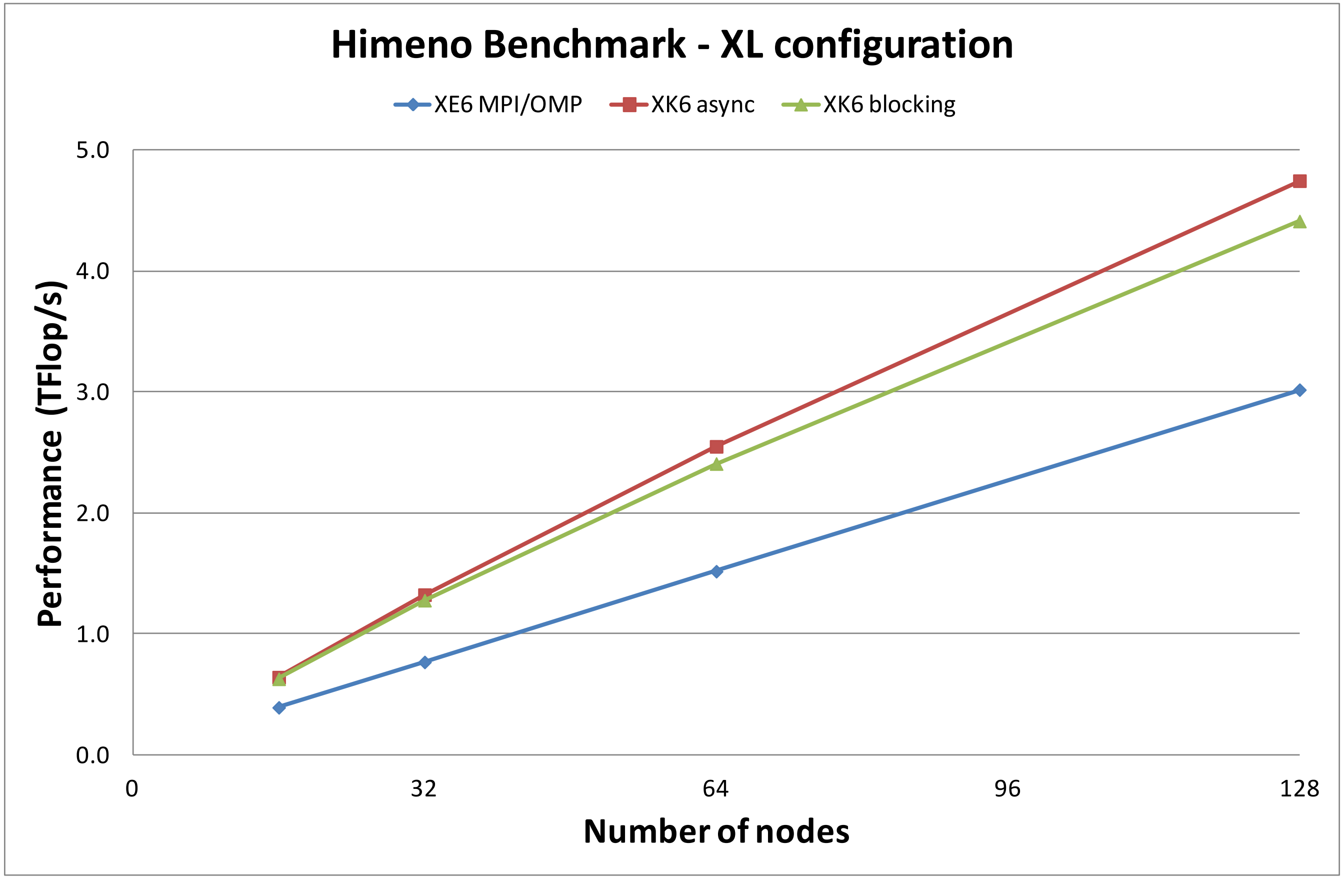
- Parallel 3D Poisson equation solver
  - Iterative loop evaluating 19-point stencil
  - Memory intensive, memory bandwidth bound
- Fortran, C, MPI and OpenMP implementations available from http://accc.riken.jp/HPC_e/himenobmt_e.html
- Strong scaling benchmark
  - XL configuration: 1024 x 512 x 512 global volume
  - Expect halo exchanges to become significant
  - Use asynchronous GPU data transfers and kernel launches to help avoid this

Porting Himeno to the Cray XK6

- **Several versions tested, with communication implemented in MPI and Fortran coarrays**
- **GPU version using OpenACC accelerator directives**
  - Total number of accelerator directives: **27**
    - plus **18** "end" directives
- **Arrays reside permanently on the GPU memory**
- **Data transfers between host and GPU are:**
  - Communication buffers for the halo exchange
  - Control value
- **Cray XK6 timings compared to best Cray XE6 results (hybrid MPI/OpenMP)**

Himeno performance

- XK6 GPU is about 1.6x faster than XE6
- OpenACC async implementation is ~ 8% faster than OpenACC blocking



CloverLeaf

- **2D hydro code, with several stencil-type operations**

- **Developed by AWE**
  - Using to explore programming models
  - to be released as Open Source to the Mantevo project hosted by Sandia (miniapps)

- **Current performance for 87 steps**

Mesh	CUDA	OpenACC
960x960	2.44	2.03
3840x3840	37.42	31.77

GAMESS

- **Computational chemistry package suite developed and maintained by the Gordon Group at Iowa State University**
  - http://www.msg.ameslab.gov/gamess/

- **ijk-tuples kernel - Source changes**
  - CUDA - **1800 lines of hand-coded** CUDA
  - OpenACC – approximately **75 directives added** to the original source

- **Performance of ijk-tuples on 16 XK6 Nodes with Fermi**
  - CPU Only (16 ranks per node) 311 Seconds
  - CUDA – 134 seconds
  - OpenACC – 138 seconds
  - **CUDA was only ~3% faster than OpenACC**

- **Performance of ijk-tuples on 16 XK6 Nodes with Kepler**
  - CPU Only (16 ranks per node) 311 Seconds
  - CUDA – 76.6 seconds
  - OpenACC – 68.1 seconds
  - **OpenACC was ~12.5% faster than CUDA !!**

Summary

- **Cray provides a high level programming environment for acceletate Computing**
  - Fortran, C, and C++ compilers
    - **OpenACC directives to drive compiler optimization**
    - Compiler optimizations to take advantage of accelerator and multi-core X86 hardware appropriately

  - Cray **Reveal**
    - **Scoping analysis** tool to assist user in understanding their code and taking full advantage of SW and HW system

  - **Cray Performance Measurement and Analysis toolkit**
    - Single tool for GPU and CPU performance analysis with statistics for the whole application
  - **Parallel Debugger support** with allinea www.allinea.com DDT
  - Auto-tuned Scientific Libraries support
    - Getting performance from the system … **no assembly required**