rocFFT An open-source GPU FFT Library for Exascale Systems Malcolm Roberts, Fei Zheng, and Bragadeesh Natarajan malcolm.roberts@amd.com 2020-02-14

Outline

- ► ROCm: Radeon Open Compute Platform
- ► The HIP programming language
- ▶ rocFFT
 - Design
 - Features
 - Usage
- Sample applications

2/12 AMDA

ROCm: Radeon Open Compute

https://rocm.github.io/

- Open source drivers and libraries
 - Community engagement encouraged!
- ► HPC and machine learning applications
- ► Focus on multi-gpu computation
- Some libraries of interest to the HPC community:
 - ► rocBLAS
 - rocSPARSE: sparse BLAS
 - rocALUTION: sparse solvers
 - ▶ rocFFT
- Written in the HIP programming language



HIP: Heterogeneous-Computing Interface for Portability

HIP is a C++ dialect for GPU programming.

Sample differences between HIP, CUDA, and OpenCL:

Term	HIP	CUDA	OpenCL
Device kernel	global	global	kernel
Thread index	threadIdx.x	${\tt threadIdx.x}$	get_local_id(0)
Kernel launch	${\tt hipLaunchKernelGGL}$	<<< >>>	${\tt clEnqueueNDRangeKernel}$

The hipify tool converts CUDA code to HIP code.

OpenCL continues to be supported.

Compiler is a branch of clang, and will be upstreamed.

rocFFT: An open-source GPU FFT Library for Exascale Systems

github.com/ROCmSoftwarePlatform/rocFFT

- Open source:
- ▶ Written in C++ and HIP
- can also be compiled with nvcc
- ► rocfft interface provides flexibility
- ▶ Alternative hipfft interface: usage similar to cufft

rocFFT: design

rocfft.h provides a C interface.

Based on the input parameters, we create a tree structure:

- ▶ Input and output buffers, strides, etc are assigned recursively.
- Leaf nodes contain device kernels.
- A plan is executed by traversing the leaf nodes sequentially.

Most kernels are generated.

Kernel types:

- Stockham
- Transpose
- Bluestein
- ► Real/complex stages.

The host code is stored in librocfft.so; device kernels are in librocfft-device.so.

rocFFT: features

- ▶ 1D, 2D, and 3D, transforms.
- Batched transforms.
- Single and double precision.
- ► In-place and out-of-place transforms.
- ► Input and output strides.
- ► Complex data format: interleaved or planar (aka "split").
- Extensive testing on several Linux distributions.

rocFFT: usage

The rocfft interface is defined in rocfft.h.

- 1. rocfft_setup()
- 2. Optional: create a rocfft_plan_description for advanced stride and other format choices.
- 3. Create a rocfft_plan, possibly using the description above.
- 4. Create a rocfft_execution_info
 - 4.1 Get the scratch memory requirements of the rocfft_plan
 - 4.2 Allocate the work buffer and associate it to the rocfft_execution_info
- 5. Allocate the input and output buffers and set up the input data.
- 6. Execute the plan with rocfft_execute.
- 7. Free the buffers, destroy the rocFFT structures, and rocfft_cleanup().

rocFFT: rocfft interface example

```
// create the plan:
rocfft_plan_create(&plan,
                  rocfft_placement_inplace,
                   rocfft_transform_type_complex_forward,
                   rocfft_precision_double,
                  1, // dimension
                  &length, // transform lengths (column-major)
                  1. // batch size
                  NULL); // optional description
// allocate the work memory and associate it to the execution info:
rocfft_execution_info_create(&planinfo);
rocfft_plan_get_work_buffer_size(gpu_plan, &wsize);
hipMalloc(&wbuffer, wsize);
rocfft_execution_info_set_work_buffer(planinfo, wbuffer, wsize);
// execute the plan:
rocfft_execute(gpu_plan, gpu_in, planinfo);
```

rocFFT: hipfft interface example

```
// Create the plan:
hipfftPlan1d(&plan, // plan handle
            Nx, // transform lengths
            HIPFFT_Z2Z, // transform type (HIPFFT_C2C for float)
            1): // number of transforms
// Can also call hipfftPlanMany (row-major)
// Work memory is automatically created and associated with the plan.
// Execute the plan:
hipfftExecZ2Z(plan, x, x, direction);
```

Frontier CAAR Projects

Some CAAR (Center for Accelerated Application Readiness) applications which target Frontier and which use FFTs (www.olcf.ornl.gov/caar/frontier-caar):

- ► GESTS (GPUs for Extreme-Scale Turbulence Simulations) High-resolution pseudospectral code: 35 trillion grid points.
- NAMD (Nanoscale Molecular Dynamics)
 Molecular simulator; can use rocFFT as the backend.
- ▶ PIConGPU (Particle-in-cell on Graphics Processing Units) Plasma simulator: PIC methods often use FFTs to resolve the underlying Maxwell equations.

Conclusion

rocFFT is:

- ► An open-source GPU FFT library from AMD
- ▶ Part of ROCm: the Radeon Open Compute Platform
- ► Uses the HIP programming language
- ▶ Will be used by a number of applications for exascale computing.

Available at: github.com/ROCmSoftwarePlatform/rocFFT