KokkACC: Enhancing Kokkos with OpenACC

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kokkos https://kokkos.org

OpenACC https://www.openacc.org

Kokkos Programing Model & KokkACC Implementation

MOTIVATION

Improve programming productivity:

- OpenACC codes are simpler to implement and maintain than other codes, such as CUDA, HIP, OpenCL, etc.
- Both (Kokkos and OpenACC) aim to be architecture agnostic, which make both models very similar and facilitate the implementation of the Kokkos features using OpenACC.
- Portable back-end. OpenACC model can target different architectures.
- Use OpenACC features to complement Kokkos features to improve performance on existing applications.
- Simplify the porting of OpenACC applications to Kokkos.

ATOMIC OPERATIONS & MEMORY

```
#pragma acc routine seq
inline unsigned int atomic_fetch_add( volatile
↪  unsigned int *const dest, const unsigned int
↪  &val ) {
  unsigned int retval;
  unsigned int *ptr = const_cast<unsigned int
   ↪  *>(dest);
  #pragma acc atomic capture {
    retval = ptr[0];
    ptr[0] += val;
  }
  return retval;
}
```

OpenACC

Kokkos atomic operations can be implemented by using OpenACC annotations.

- Kokkos::malloc (acc_malloc),
- Kokkos::free (acc_free) and
- Kokkos::view are used to represent user data.
- Kokkos::deep_copy (acc_memcpy_[to/from]_device) is used for memory transfers.

Single Range

```
auto X  = static_cast<double*>(Kokkos::kokkos_malloc<>(N * sizeof(double)));
auto Y  = static_cast<double*>(Kokkos::kokkos_malloc<>(N * sizeof(double)));

Kokkos::parallel_for( "axpy_init", N, KOKKOS_LAMBDA ( int n )
{
 X[n] = InitValue;
 Y[n] = InitValue;
});

Kokkos::parallel_for( "axpy_computation", N, KOKKOS_LAMBDA ( int n )
{
  double alpha = ALPHA;
  Y[n] += alpha * X[n];
});
```

kokkos

```
template <class TagType> inline void execute_impl() const
{
  OpenACCExec::verify_is_process("Kokkos::Experimental::OpenACC parallel_for");
  OpenACCExec::verify_initialized("Kokkos::Experimental::OpenACC parallel_for");

  const auto begin = m_policy.begin();
  const auto end   = m_policy.end();
  if (end <= begin) return;
  const FunctorType a_functor(m_functor);

  #pragma acc parallel loop gang vector copyin(a_functor)
  for (auto i = begin; i < end; i++)
    a_functor(i);
}
```

OpenACC

Multi-Dimensional

```
SIZE = M * N * sizeof(double);
Kokkos::View <double**> X("X", M , N);
Kokkos::View <double**> Y("Y", M , N);

typedef Kokkos::MDRangePolicy< Kokkos::Rank<2> >mdrange_policy;

Kokkos::parallel_for( "axpy_init", mdrange_policy( {0, 0}, {M, N} ), KOKKOS_LAMBDA ( int m, int n  )
{
  X(m, n) = InitValue;
  Y(m, n) = InitValue;
} );

Kokkos::parallel_for( "axpy_computation", mdrange_policy( {0, 0}, {M, N} ), KOKKOS_LAMBDA ( int m, int n )
{
  double alpha = ALPHA;
  Y(m, n) += alpha * X(m, n);
} );
```

kokkos

```
template <class TagType, int Rank> inline typename std::enable_if<Rank == 2>::type execute_functor( const
↪  FunctorType& functor, const Policy& policy ) const
{
  const FunctorType a_functor(functor);
  int begin1 = policy.m_lower[0];
  int end1 = policy.m_upper[0];
  int begin2 = policy.m_lower[1];
  int end2 = policy.m_upper[1];

  #pragma acc parallel loop gang vector collapse(2) copyin(a_functor)
  for (auto i0 = begin1; i0 < end1; i0++) {
    for (auto i1 = begin2; i1 < end2; i1++) {
      a_functor(i0, i1);
    }
  }
```

OpenACC

DESCRIPTIVE (OPENACC) VS PRESCRIPTIVE (CUDA)

OpenACC faster than CUDA?

Next, we highlight why it is possible to provide competitive or even better performance using a high-level and high programming productivity descriptive (pragma-based) model (OpenACC) than using a low-level prescriptive (device-specific) model (CUDA) for C++ Metaprogramming solutions (Kokkos).

- C++ Metaprogramming solutions, like Kokkos, rely on C++ lambdas. C++ lambdas are defined by application programmers and can express any operation.
- Device-specific solutions like CUDA weren't designed to work at lambda level originally. CUDA Kokkos back-end relies on CUDA developers, who don't know which operations will be computed by GPU kernels, but they must take decisions about size of CUDA blocks, memory usage, synchronization, etc. This makes the optimization of these solutions extremely difficult or even impossible.
- OpenACC backend relies on compiler, which can take better decisions depending on the operations defined by C++ lambdas and application developers.

Hierarchical Parallelism

```
SIZE = M * N * sizeof(double);
auto X  = static_cast<double*>(Kokkos::kokkos_malloc<>(SIZE));
auto Y  = static_cast<double*>(Kokkos::kokkos_malloc<>(SIZE));

typedef Kokkos::TeamPolicy<>               team_policy;
typedef Kokkos::TeamPolicy<>::member_type  member_type;

Kokkos::parallel_for( "axpy_init", team_policy( M, Kokkos::AUTO ), KOKKOS_LAMBDA ( const member_type
↪  &teamMember )
{
  const int i = teamMember.league_rank();
  Kokkos::parallel_for( Kokkos::TeamThreadRange( teamMember, N ), [&] ( const int j )
  {
    X[i * N + j] = InitValue;
    Y[i * N + j] = InitValue;
  } );
} );

Kokkos::parallel_for( "axpy_computation", team_policy( M, Kokkos::AUTO ), KOKKOS_LAMBDA ( const
↪  member_type &teamMember )
{
  const int i = teamMember.league_rank();
  Kokkos::parallel_for( Kokkos::TeamThreadRange( teamMember, N ), [&] ( const int j )
  {
    double alpha = ALPHA;
    Y[i * N + j] += alpha * X[i * N + j];
  } );
} );
```

kokkos

```
template <class TagType> inline void execute_impl() const {
 OpenACCExec::verify_is_process( "Kokkos::Experimental::OpenACC parallel_for");
 OpenACCExec::verify_initialized("Kokkos::Experimental::OpenACC parallel_for");
 auto league_size   = m_policy.league_size();
 auto team_size     = m_policy.team_size();
 auto vector_length = m_policy.impl_vector_length();
 const FunctorType a_functor(m_functor);

 #pragma acc parallel loop gang copyin(a_functor)
 for ( int i = 0; i < league_size; i++ ) {
   int league_id = i;
   typename Policy::member_type team( league_id, league_size, team_size, vector_length );
   a_functor(team);
 }
}
#pragma acc routine worker
template <typename iType, class Lambda>
KOKKOS_INLINE_FUNCTION void parallel_for( const Impl::TeamThreadRangeBoundariesStruct<iType,
↪  Impl::OpenACCExecTeamMember>& loop_boundaries, const Lambda& lambda ) {
  #pragma acc loop worker
  for (iType j = loop_boundaries.start; j < loop_boundaries.end; j++) {
    lambda(j);
  }
}
```

OpenACC

CONCLUSIONS & FUTURE EFFORTS

OpenACC vs CUDA:

- Competitive performance for Single Range.
- Better performance for Multi-Dimensional.
- Competitive performance for Hierarchical Parallelism parallel_for and worse performance for parallel_reduce.
- Competitive (lulesh) and better performance (miniFE) on mini-apps.

OpenACC vs OpenMP Target:

- Better performance in most of the cases tested.

KOKKACC is aligned with other important efforts:

- Analysis, codesign and development of the OpenACC capacity for C++.
- Enhancing C++ [for HPC] using the capacity of OpenACC.
- Design of new OpenACC capabilities.

Future Efforts:

- Implement future/current Kokkos features in OpenACC back end parallel_scan, tasking, etc.
- Explore novel optimizations

REPOSITORY & CONTACTS

https://github.com/ORNL/kokkos-ornl/tree/openacc

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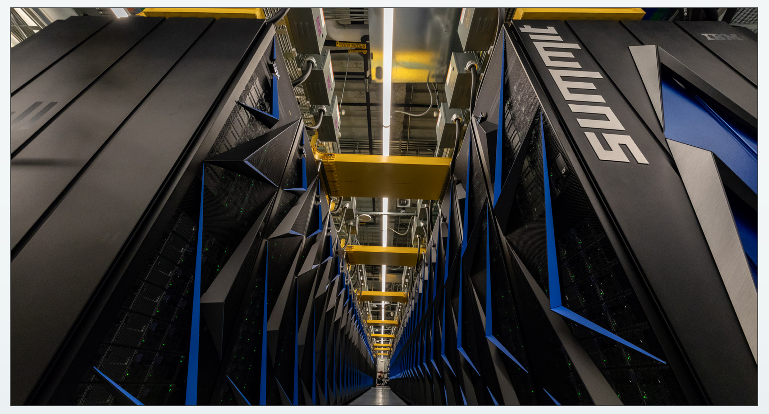
Performance Analysis

PLATFORM

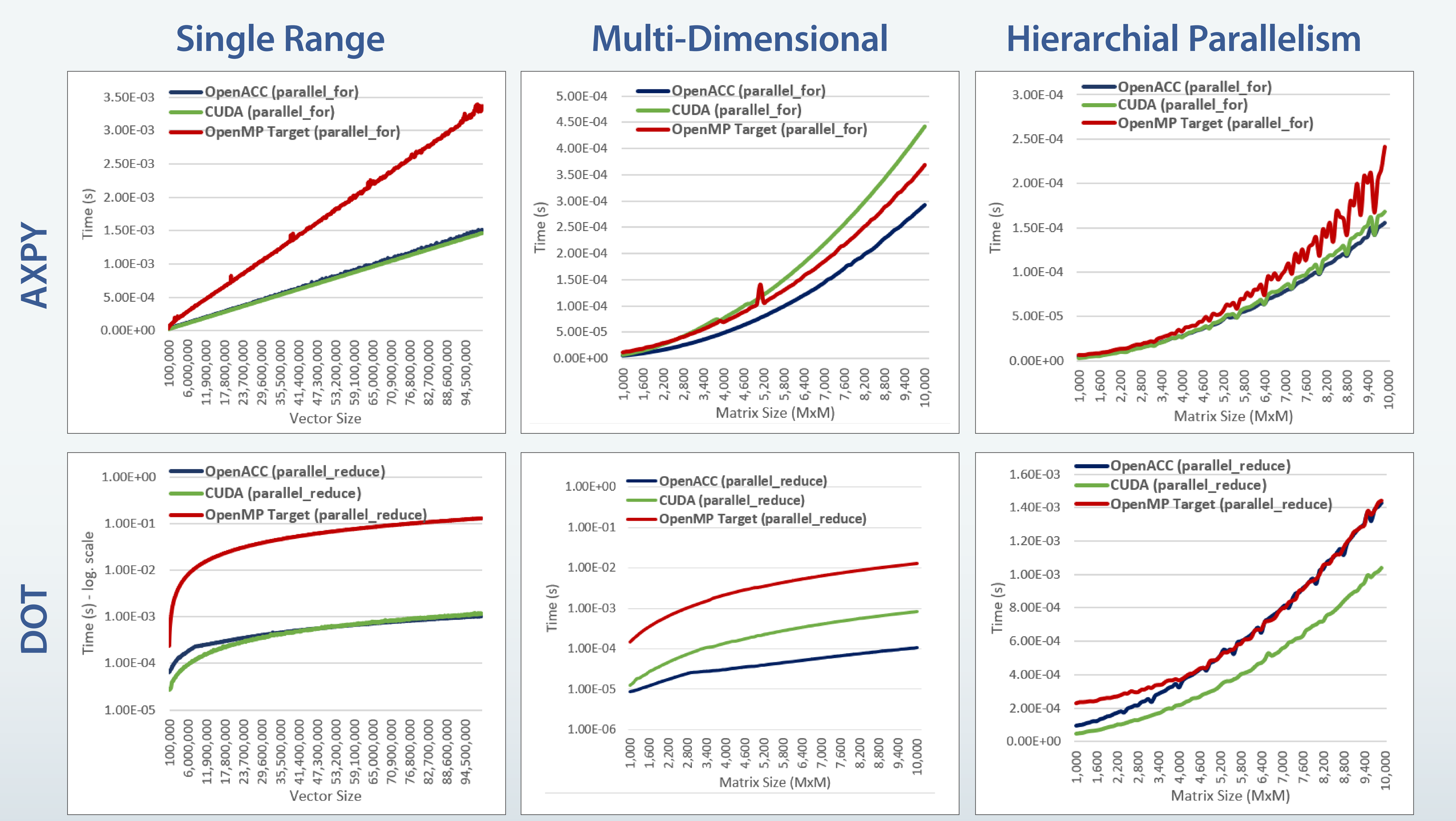
ORNL SUMMIT

- 1x NVIDIA Volta V100 GPU (16 GB)
- CUDA back-end (CUDA 11.0.3)
- OpenMP Target back-end (LLVM 15.0.0 git)
- OpenACC back-end (NVHPC 21.3)



ECP EXASCALE COMPUTING PROJECT — kokkos — OpenACC

MINI-BENCHMARKS



ECP MINI-APPS