Modern C++ for Parallelism in Scientific Computing

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Scientific computing parallelism

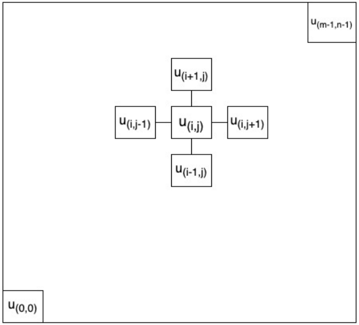
- Large amounts of data:
  often cartesian multi-dimensional arrays, sometimes unstructured data
- Large amounts of parallelism:
  each element of output array independent.
- No explicit threading
  parallelism created by some runtime
- Range algorithm notion:
  do some operation on each element of a dataset

Power method

```
Let $A$ a matrix of interest
Let $x$ be a random vector
For iterations until convergence
    compute the product $y \leftarrow Ax$
    compute the norm $\gamma = \|y\|$
    normalize $x \leftarrow y/\gamma$
```

- Method for computing largest eigenvalue of a matrix
- Also Google Pagerank
- Stands for many scientific codes: Krylov methods, eigenvalues

Stencil operations



·	-1	·
-1	4	-1
·	-1	·

- This rectangular $m \times n$ thing is the vector
- The $4, -1, \ldots$ stencil is / stands for the matrix.
- Goes by: difference stencil, convolution, Toeplitz matrix

Array parallelism

Traditional C implementation:

```
for ( idxint i=0; i<m; i++ )
  for ( idxint j=0; j<n; j++ )
    out[ IINDEX(i,j,m,n,b) ] = in[ IINDEX(i,j,m,n,b) ] * factor;
```

```
// seq.cpp
#define IINDEX( i,j,m,n,b ) ((i)+b)*(n+2*b) + (j)+b
```

- Two / three-dimensional loop
- all dimensions large
- every output element independent

Reductions

ℓ_2 reduction:

```
for ( idxint i=0; i<m; i++ )
  for ( idxint j=0; j<n; j++ ) {
    auto v = out[ IINDEX(i,j,m,n,b) ];
    sum_of_squares += v*v;
  }
return std::sqrt(sum_of_squares);
```

- Parallel except for the accumulation
- Obviously should not be done through atomic operation

Stencil computation

```
for ( idxint i=0; i<m; i++ ) {
  for ( idxint j=0; j<n; j++ ) {
    out[ IINDEX(i,j,m,n,b) ] = 4*in[ IINDEX(i,j,m,n,b) ]
      - in[ IINDEX(i-1,j,m,n,b) ] - in[ IINDEX(i+1,j,m,n,b) ]
      - in[ IINDEX(i,j-1,m,n,b) ] - in[ IINDEX(i,j+1,m,n,b) ];
  }
}
```

- Differential operator / image convolution
- Structure can be more complicated in scientific codes

Tools: mdspan and cartesian_product

```
private:
  real *_data{nullptr};
  md::mdspan<
    real,
    md::dextents<idxint,2>
          > cartesian_data;
```

```
//! pointer to the data as 2D array
auto& data2d() {
  return cartesian_data; };
const auto& data2d() const {
  return cartesian_data; };
```

mdspan and cartesian_product

```
const auto& s = data2d();
int b = this->border();
idxint
  lo_m = static_cast<idxint>(b),
  hi_m = static_cast<idxint>(s.extent(0)-b),
  lo_n = static_cast<idxint>(b),
  hi_n = static_cast<idxint>(s.extent(1)-b);
range2d = rng::views::cartesian_product
  ( rng::views::iota(lo_m,hi_m),rng::views::iota(lo_n,hi_n) );
```

- Vector allocated with size $(m+2b)\times(n+2b)$ to include border
- for handling of boundary conditions / halo regions in PDEs.

Implementation 1: OpenMP parallelism

Annotate loops as parallel and/or reduction:

```
    #pragma omp parallel for reduction(+:sum_of_squares)
    for ( idxint i=0; i<m; i++ )
      for ( idxint j=0; j<n; j++ ) {
        auto v = out[ IINDEX(i,j,m,n,b) ];
        sum_of_squares += v*v;
      }
    return std::sqrt(sum_of_squares);
  };
```

- Static assigment of iterations to threads by default
- Highly controlled affinity
- ‘`oned`’ as above, ‘`clps`’ for both loops collapsed
- Can be formulated as range algorithm.

Implementation 2: range over indices

```
auto array = this->data2d();
#pragma omp parallel for reduction(+:sum_of_squares)
for ( auto ij : this->inner() ) {
  auto [i,j] = ij;
  auto v = array[i,j];
  sum_of_squares += v*v;
}
return std::sqrt(sum_of_squares);
```

- Range over indices, not over data
- Indices are a subset of the full data!

Stencil operation

```
// span.cpp
auto out = this->data2d();
const auto in = other.data2d();
#pragma omp parallel for
for ( auto ij : this->inner() ) {
  auto [i,j] = ij;
  out[ i,j ] = 4*in[ i,j ]
    - in[ i-1,j ] - in[ i+1,j ] - in[ i,j-1 ] - in[ i,j+1 ];
}
```

- Hard to formulate as range algorithm
- Performance not necessarily determined by floating point operations.

Implementation 3: Sycl

Open standard, but mostly pushed by Intel

```
q.submit([&] (handler &h) {
  accessor D_a(Buf_a,h,write_only);
  h.parallel_for
    (range<2>(msize-2,nsize-2),
     [=](auto index){
       auto row = index.get_id(0) + 1;
       auto col = index.get_id(1) + 1;
       D_a[row][col] = 1.;
     });
}).wait();
```

- Heterogeneous CPU/GPU code, transparent data movement
- Range algorithm-like syntax, but explicit task queue

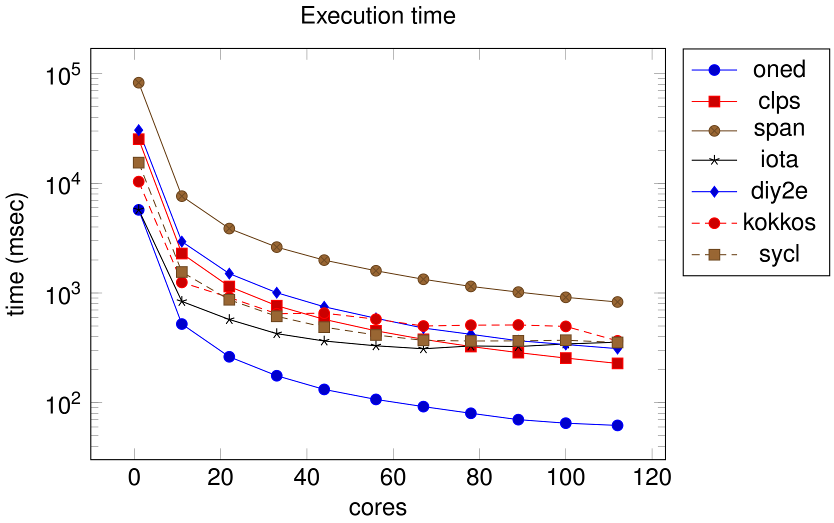
Implementation 4: Kokkos

Open Source heterogeneous execution layer

```
Kokkos::parallel_for
  ("Update x",
   Kokkos::MDRangePolicy<Kokkos::Rank<2>>
       ({1, 1}, {msize-1, nsize-1}),
   KOKKOS_LAMBDA(int i, int j) {
    x(i, j) = Ax(i, j) / norm;
  });
```

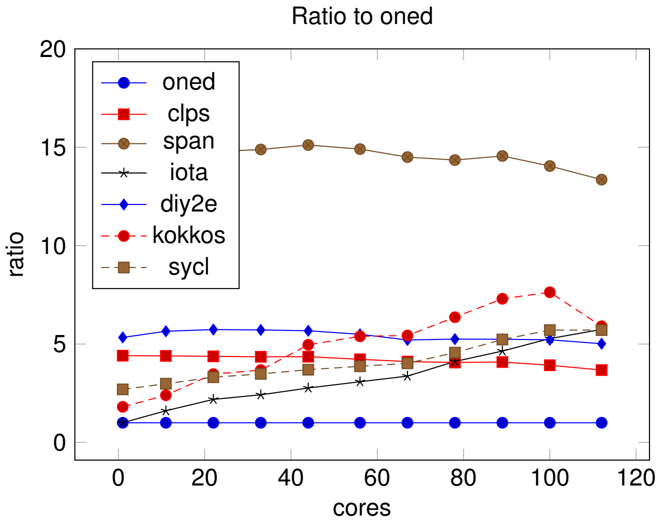
- Same code for CPU and GPU
- Implicit task queue
- Two-dimensional indexing
- Range algorithm-like philosophy

Comparing models (Intel)

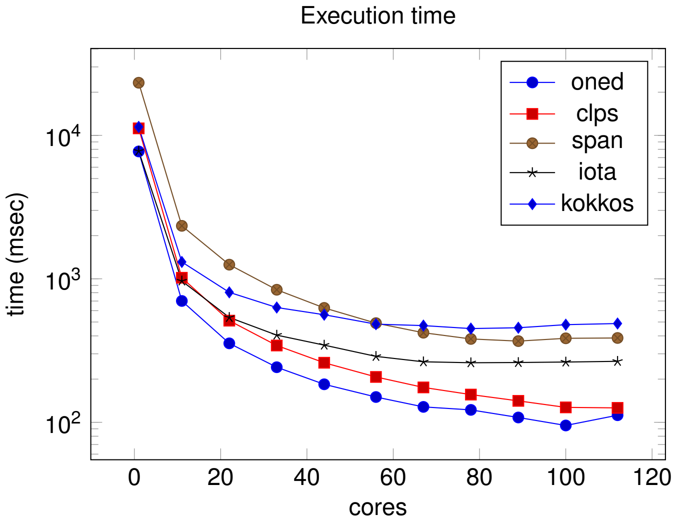


Intel compiler. C-style variant fastest.

Ratio to fastest (Intel)

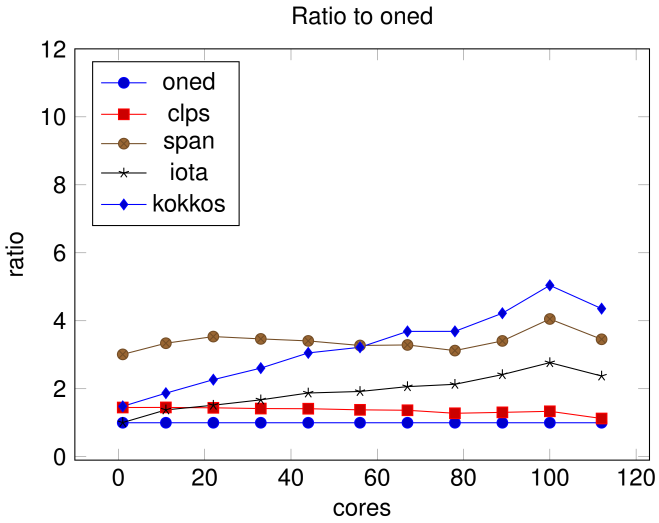


Comparing models (Gcc)



Gcc compiler. less variance between variants

Ratio to fastest (Gcc)



Where do we lose performance?

Hint: `perf` output on the ‘span’ variant:

```
      55.60%  [.]
       ↪std::ranges::cartesian_product_view<std::ranges::iota_view<long,
       ↪long>, std::ranges::iota_view<long, long>
       ↪>::_Iterator<true>::operator+=
      18.73%  [.] __divti3
      11.33%  [.]
       ↪linalg::bordered_array_span<float>::central_difference_from
       5.37%  [.]
       ↪linalg::bordered_array_span<float>::scale_interior
       5.01%  [.] linalg::bordered_array_span<float>::l2norm
       2.69%  [.] __divti3@plt
```

Index calculations take lots of time.

Conclusion and Acknowledgement

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