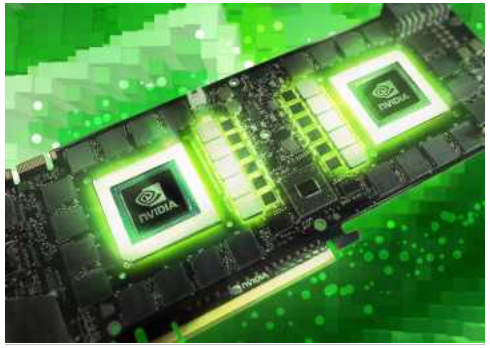
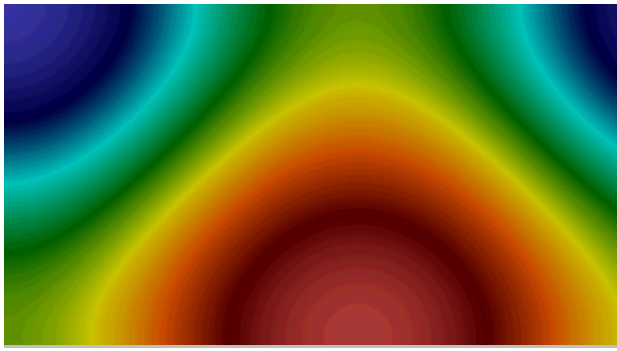
SAND2018-1534C



ACS Technical Exchange: Threaded Assembly in Aria Expressions

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TF Team, STK Team

U.S. DEPARTMENT OF ENERGY | NNSA National Nuclear Security Administration

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Motivation

Trinity (ATS-I) Phase I
"Haswell" CPUs
2 socket x 16 core x 2 ht
4 wide vector instructions

Trinity Phase II
"Knight's Landing"
1 socket x 68 cores x 4 ht
8 wide vector instructions

Sierra (ATS-II)
Power9 CPUs
NVIDIA Volta GPUs
120-150 PetaFlops

Technologies

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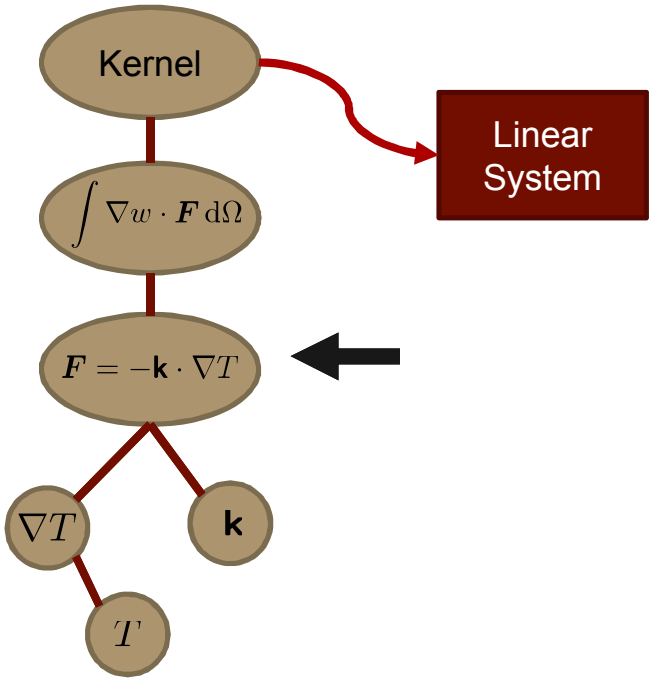
- Technologies
  - Threading
  - Vectorization
- Software Abstractions
  - Kokkos
  - stk::simd
- Prototype work in Ariamini

Expression Subsystem



$$\boldsymbol{F} = -\mathbf{k} \cdot \nabla T$$

public:
Expression()
…
void compute_values()
void compute_sensitivities()

private:
Expression_Handle gradT
Expression_Handle k
values
sensitivities //wrt each dof

Expression Subsystem

$$\boldsymbol{F} = -\mathbf{k} \cdot \nabla T$$

public:
Expression()
…
void compute_values()
void compute_sensitivities()

private:
Expression_Handle gradT
Expression_Handle k
values
sens

compute_values()

for each element:
  for each integration point:
    for each dim:
      values(elm, pt, dim)
        = -k(elm,pt)*gradT(elm, pt, dim)

compute_sensitivities()

for each element:
  for each integration point:
    for each dim:
      for each dof:
      sens(elm, pt, dim, dof)
        += -k.sens(…, dof)*gradT(…)
         - k(elem, pt)*gradT.sens(…, dof)

Threading

```
for(bucket : element_buckets) {
  for(workset : bucket) {
    set_mesh_object_couriers(workset_elems);
    evaluate_expressions();
    evaluate_kernels(rhs, lhs);
    sum_into_linear_system(rhs, lhs);
  }
}

//-------------------------
void evaluate_expressions() {
  for(expr : ordered_expressions) {
    expr.prepare_to_recompute(); //resizes and zeros storage if needed
    expr.compute_values();
    expr.compute_sensitivities();
  }
}
```

Threading

```
resize_expression_storage(num_concurrent_worksets);
Kokkos::parallel_for(bucket : element_buckets) {
  for(workset : bucket) {
    start = workset_index * workset_size;
    num_elems = workset_size;
    ElementRange scratch_range(
       start, start + num_elems);
    set_mesh_object_couriers(scratch_range, workset_elems);
    evaluate_expressions(scratch_range);
    evaluate_kernels(scratch_range, rhs, lhs);
    atomic_sum_into_linear_system(rhs, lhs);
  }
}

//------------------------
void evaluate_expressions(ElementRange elem_range) {
  for(expr : ordered_expressions) {
    expr.prepare_to_recompute(elem_range); //resizes and zeros storage if needed
    expr.compute_values(elem_range);
    expr.compute_sensitivities(elem_range);
  }
}
```

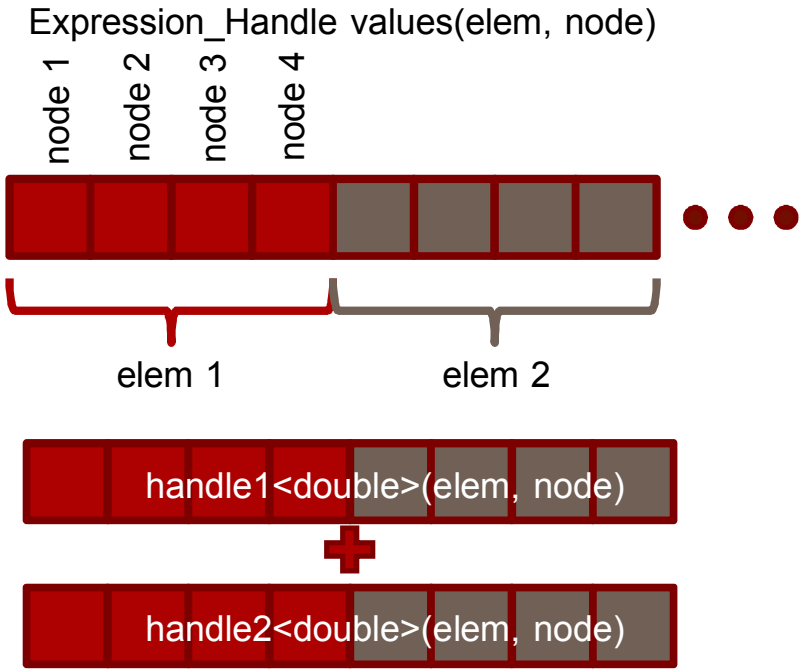
Threading

```
void Scalar_Vector_Product_Expression::compute_values() {
  for(int elem = 0; elem < nelem; ++elem) {
    for(int ip = 0; ip < nip; ++ip) {
      for(int dim = 0; dim < ndim; ++dim) {
        values(elem, ip, dim) =
          scalar(elem, ip) * vector(elem, ip, dim);
      }
    }
  }
}
//------
void Scalar_Vector_Product_Expression::compute_sensitivities()
{
  //...
}
```

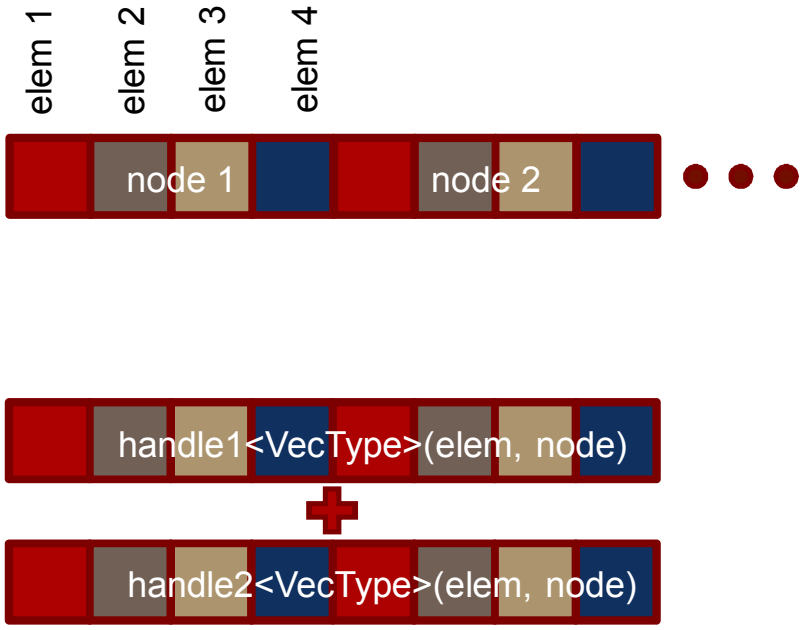
Threading

```
void Scalar_Vector_Product_Expression::compute_values(ElemRange elem_range) {
  for(auto elem : elem_range) {
    for(auto ip : my_sizes.get_points()) {
      for(auto dim : my_sizes.get_dims()) {
        values(elem, ip, dim) =
          scalar(elem, ip) * vector(elem, ip, dim);
      }
    }
  }
}
//------
void Scalar_Vector_Product_Expression::compute_sensitivities(ElemRange elem_range)
{
  //...
}
```

Vectorization



4 elem x 4 node = 16 scalar additions



4-wide intrinsic: 4 elem x 4 node = 4 vector additions

Vectorization

```
resize_expression_storage(num_concurrent_worksets);
Kokkos::parallel_for(bucket : element_buckets) {
  for(workset : bucket) {
    start = workset_index * workset_size;
    num_elems = workset_size;
    ElementRange scratch_range(
       start, start + num_elems);
    set_mesh_object_couriers(scratch_range, workset_elems);
    evaluate_expressions(scratch_range);
    evaluate_kernels(scratch_range, rhs, lhs);
    atomic_sum_into_linear_system(rhs, lhs);
  }
}

//------------------------
void evaluate_expressions(ElementRange elem_range) {
//...
```

Vectorization

```
resize_expression_storage(num_concurrent_worksets);
Kokkos::parallel_for(bucket : element_buckets) {
  for(workset : bucket) {
    start = workset_index * workset_size / VecLength;
    remainder = worset_size % VecLength;
    num_simd_elems = workset_size / VecLength;
    if (remainder) num_simd_elems++; //Pad if remainder
    ElementRange scratch_range(
       start, start + num_simd_elems);
    set_mesh_object_couriers(scratch_range, workset_elems);
    evaluate_expressions(scratch_range);
    evaluate_kernels(scratch_range, rhs, lhs);
    atomic_sum_into_linear_system(rhs, lhs);
  }
}

//------------------------
void evaluate_expressions(ElementRange elem_range) {
//...
```

Intrusiveness

- Vectorization
  - Most expressions remained unchanged
  - Gather from stk fields
  - Scatter into linear system
  - Interface with TPLs
- Threading
  - Expressions receive ElementRange chunk of elements
  - Expression_Handles now wrap Kokkos::Views

Code Changes for GPU

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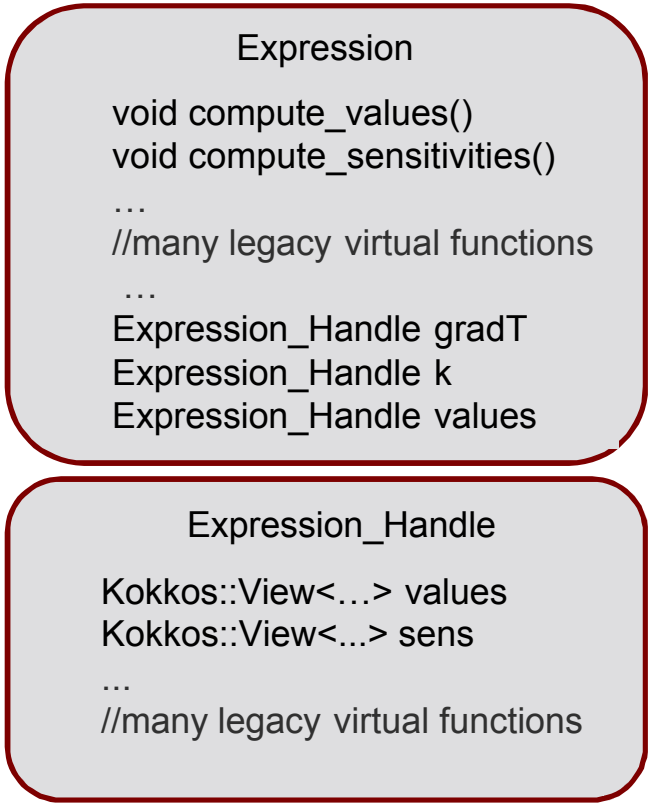
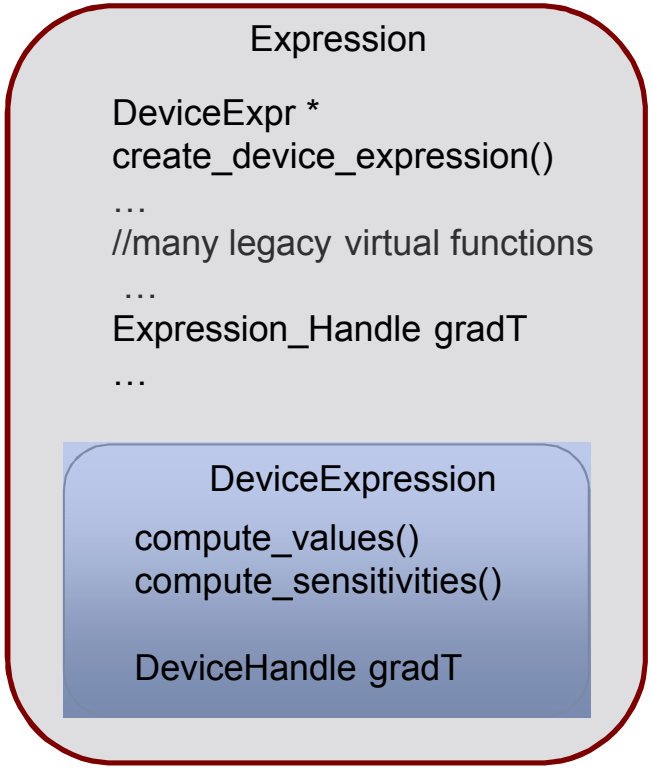


- Nested parallelism
- Virtual dispatch requires objects allocated on device
- Device classes must be copyable (relocatable-device code)
- Caching of member variables to local (places in register)
- Nested classes providing device-specific version of class

Code Changes for GPU



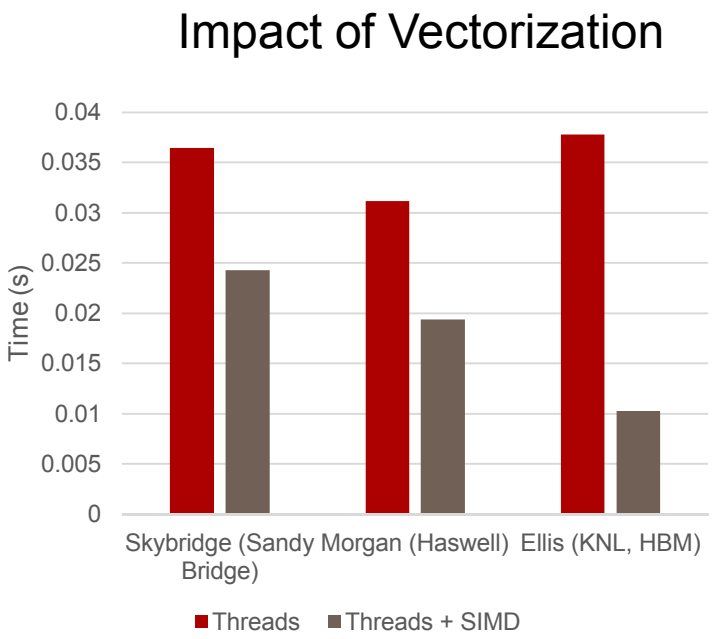
DeviceExpression Allocation

```
ExprType * p
  = static_cast<ExprType *>
    (Kokkos::kokkos_malloc<>(sizeof(ExprType)));
Kokkos::parallel_for(
    Kokkos::RangePolicy<>(0, 1),[=] DEVICE(const int i)
{
  new (p) ExprType(rhs);
});
Kokkos::fence();
```

constructor for DeviceExpression sets up DeviceHandles
DeviceHandles and DeviceExpression UVM accessible

Ariamini

- **prototype iterations**
- **vectorization crucial**
- **threading less clear on KNL**
- **GPU**
- SAND2017-9807PE



Aria Performance

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Milestone problems (from NGP performance test suite)

8M element conduction
- conduction only
- one block
- volume and surface assembly
- Dirichlet BCs

AFF performance test
- 3.5M elements
- 318 blocks
- conduction and radiation
- volume and surface assembly
- Dirichlet BCs

Aria vs. Ariamini

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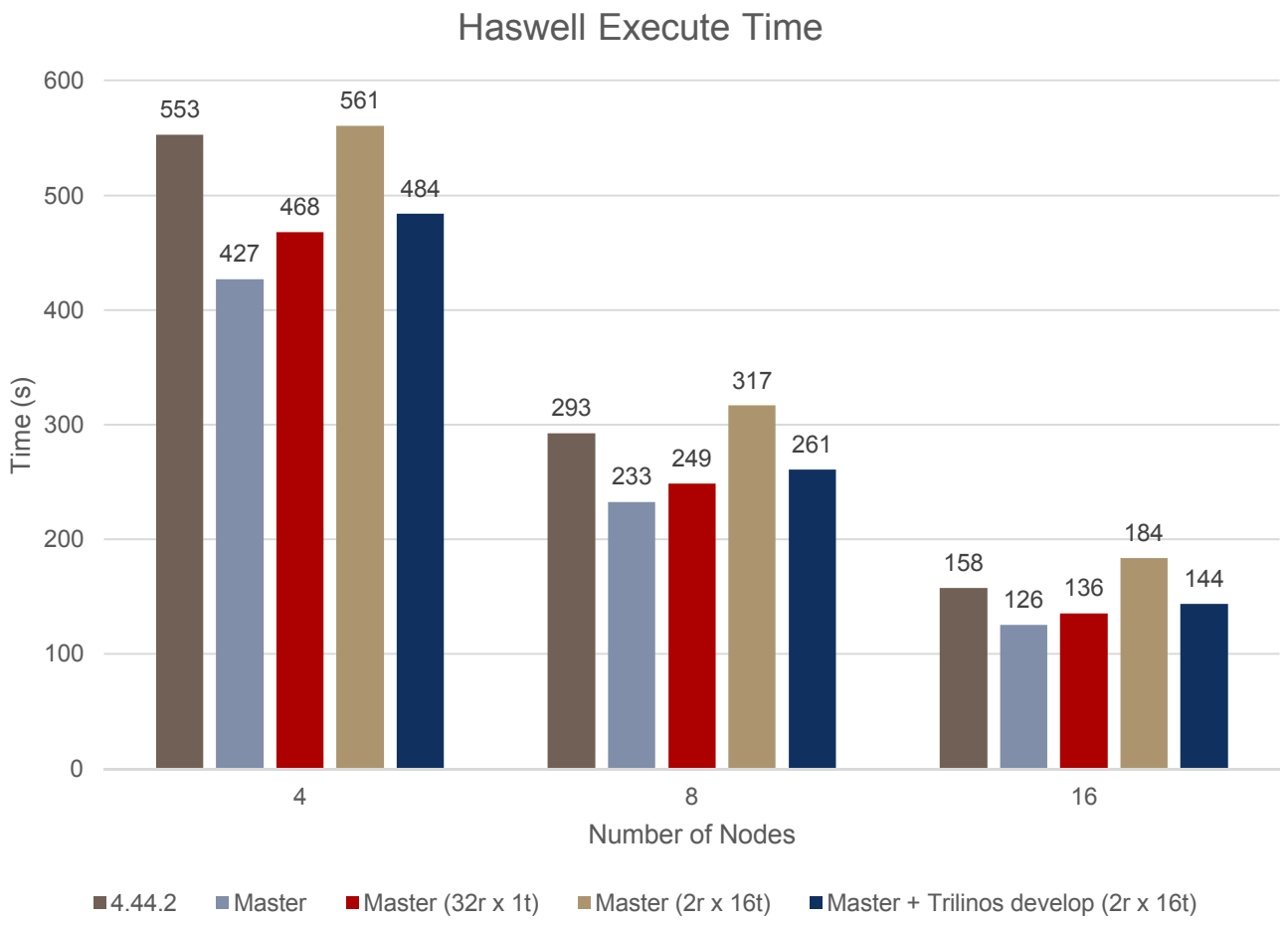
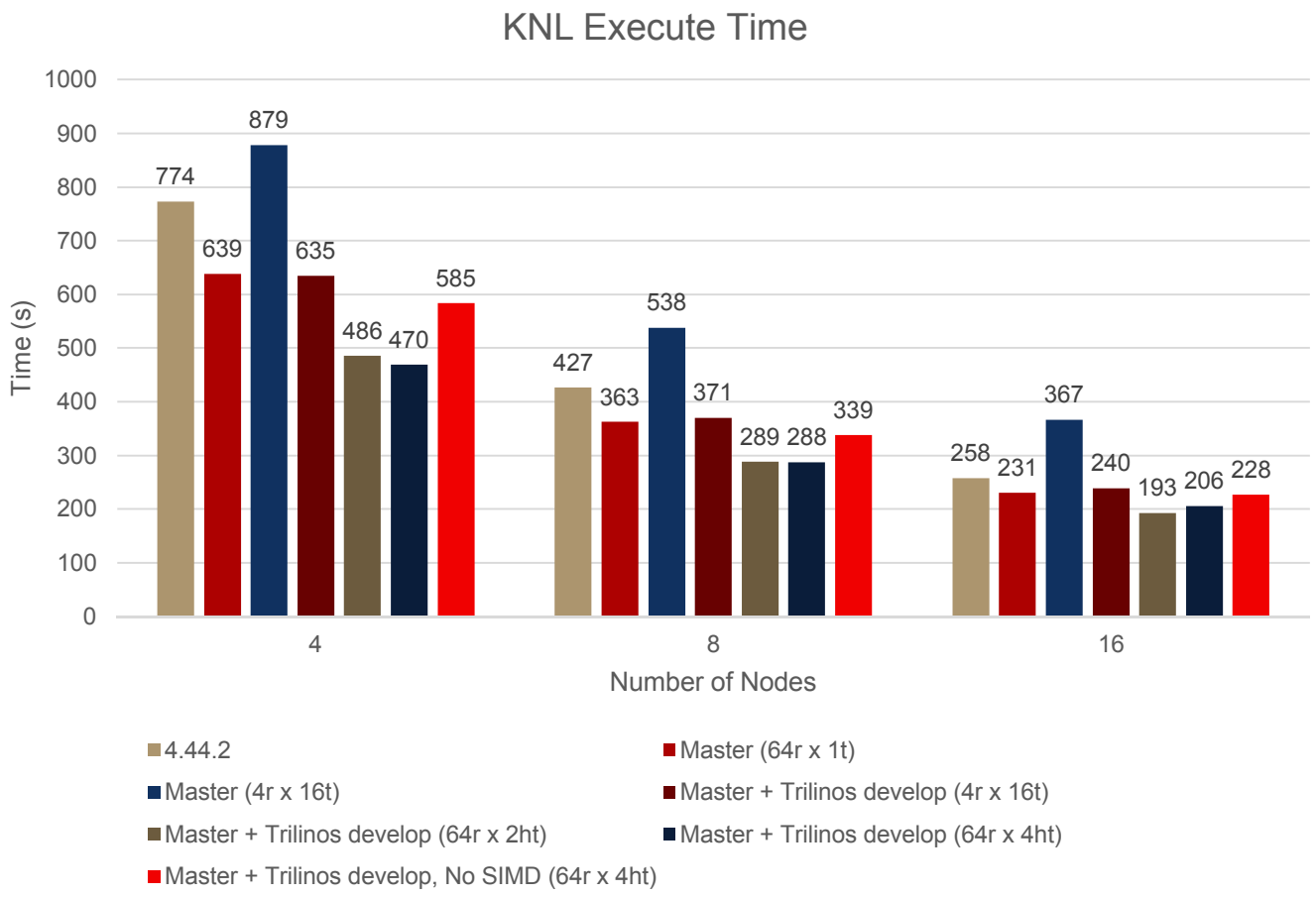
- optimization not included in Aria
  - master element
  - compile-time sizes everywhere
- application code much more complex
- ”real” problems and load balancing
  - volume algorithm now threads over all blocks
- load complete
- Dirichlet BCs

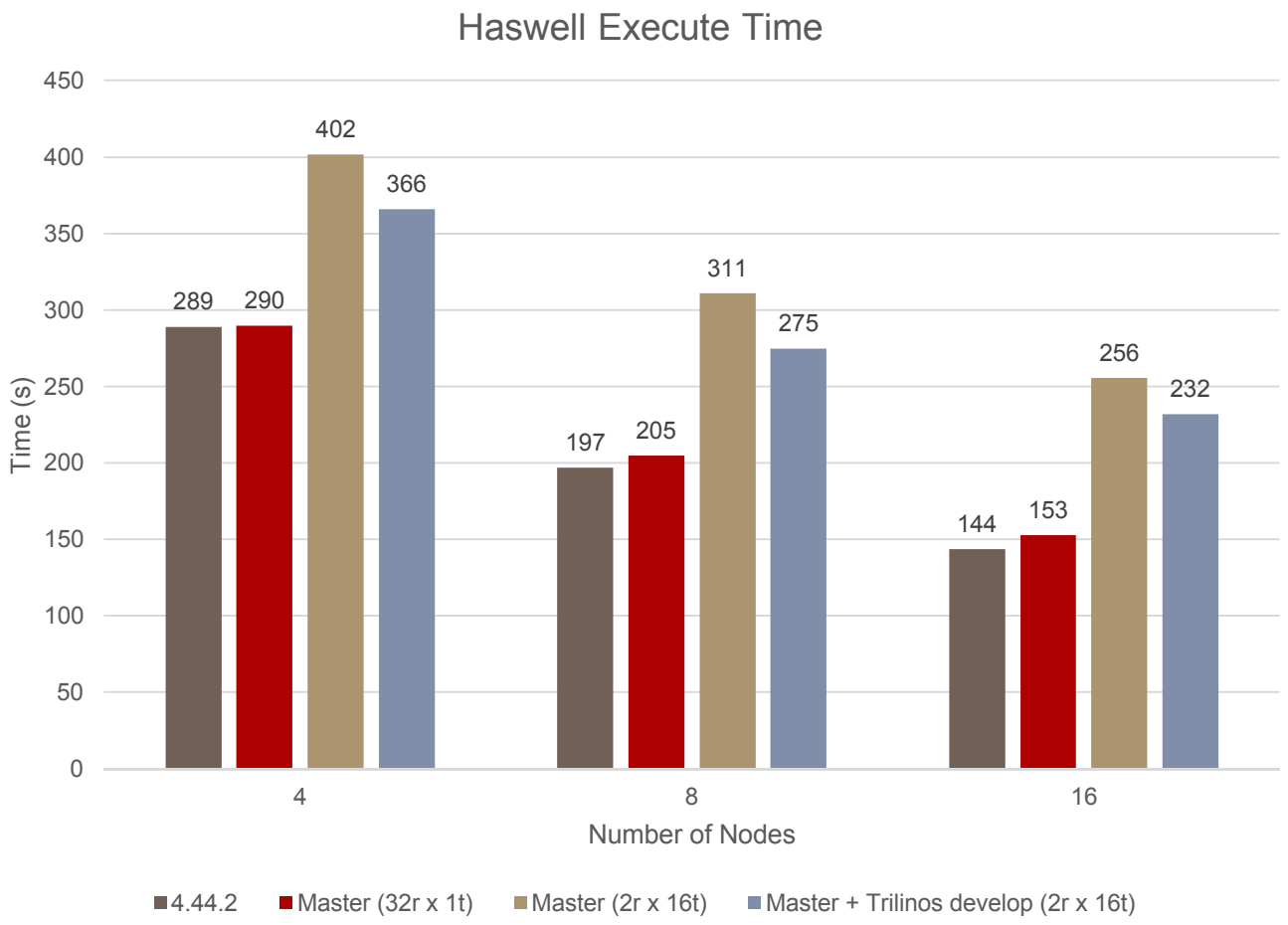
8M Element Conduction



8M Element Conduction

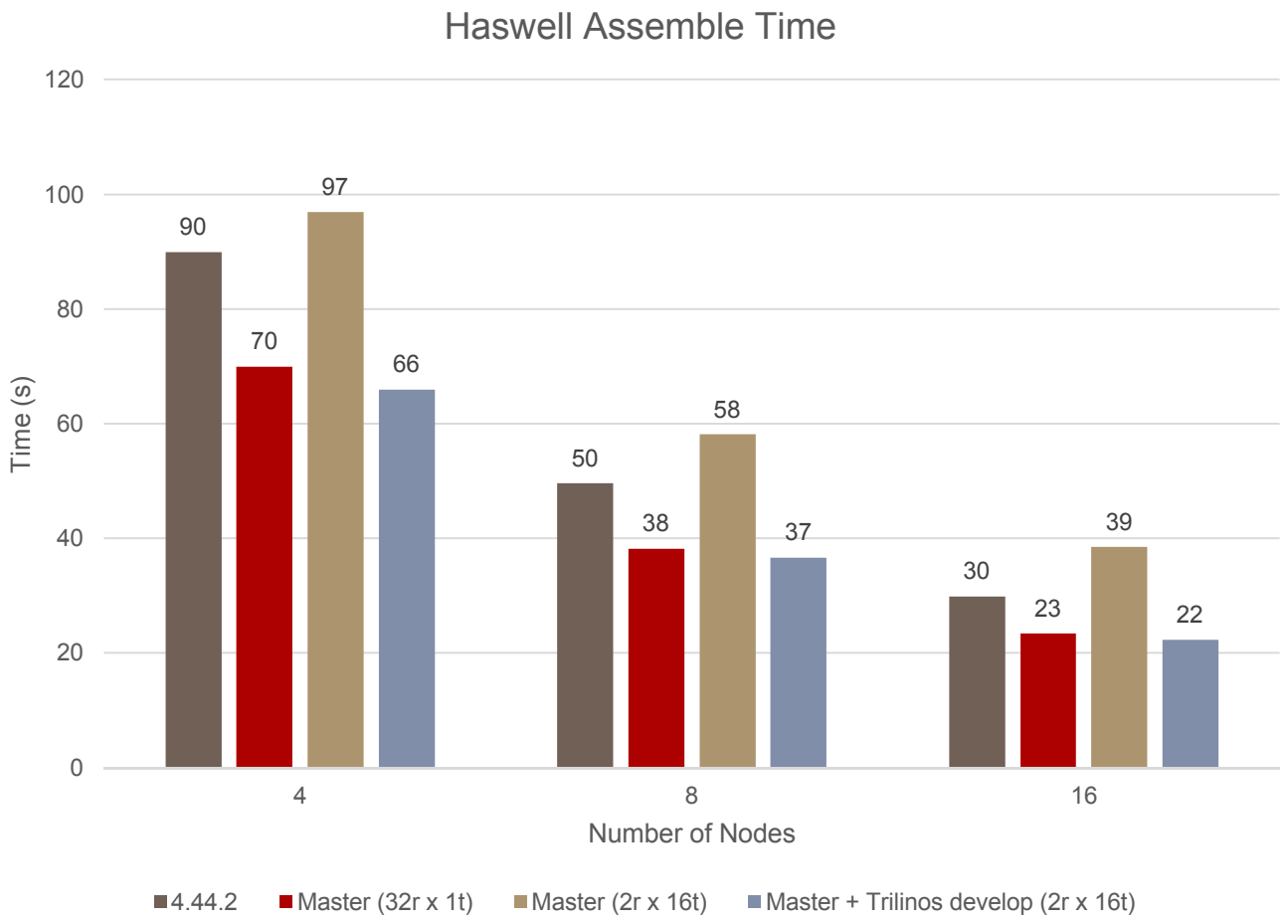


AFF Test Case



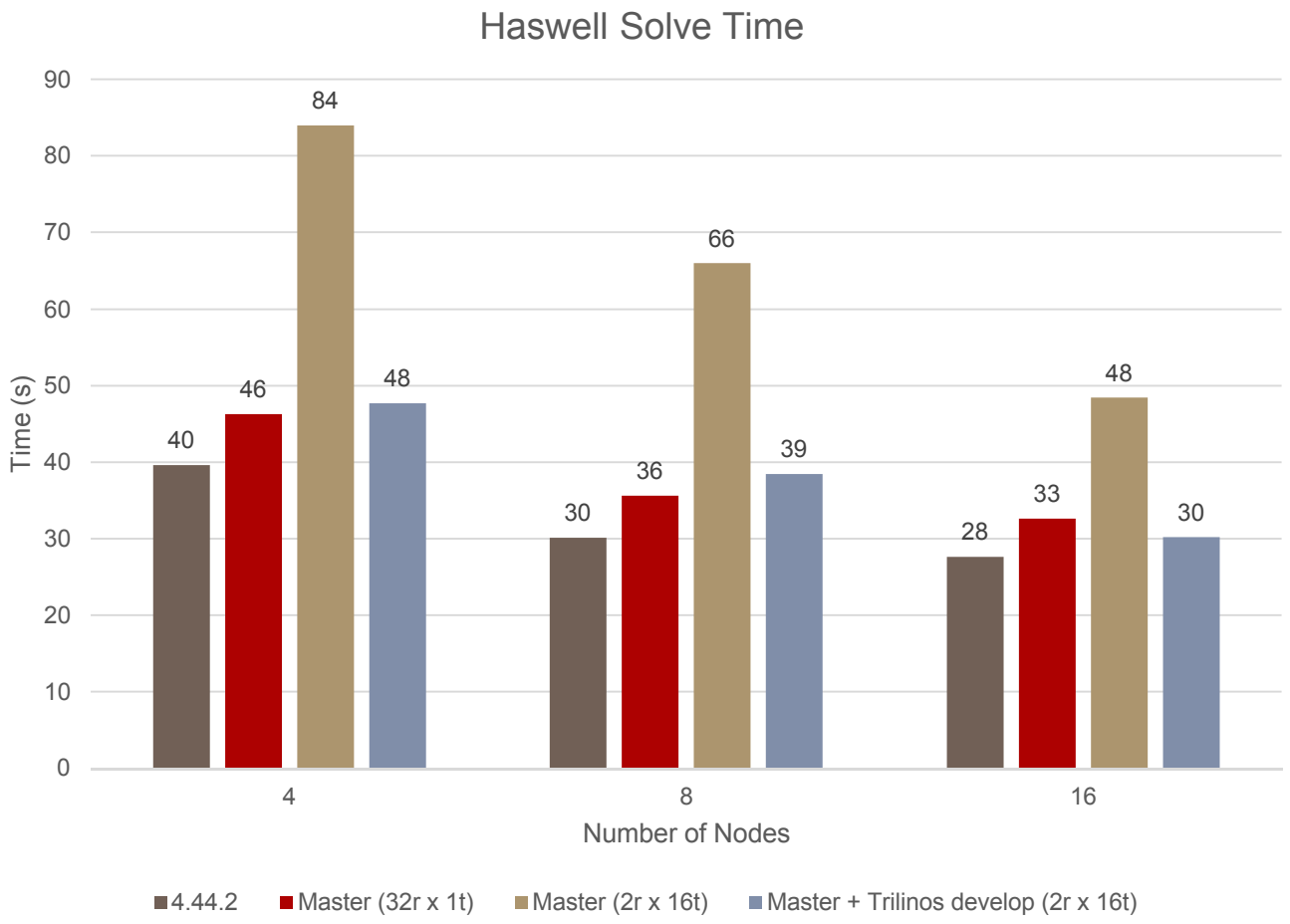
Includes non-threaded enclosure radiation

AFF Test Case



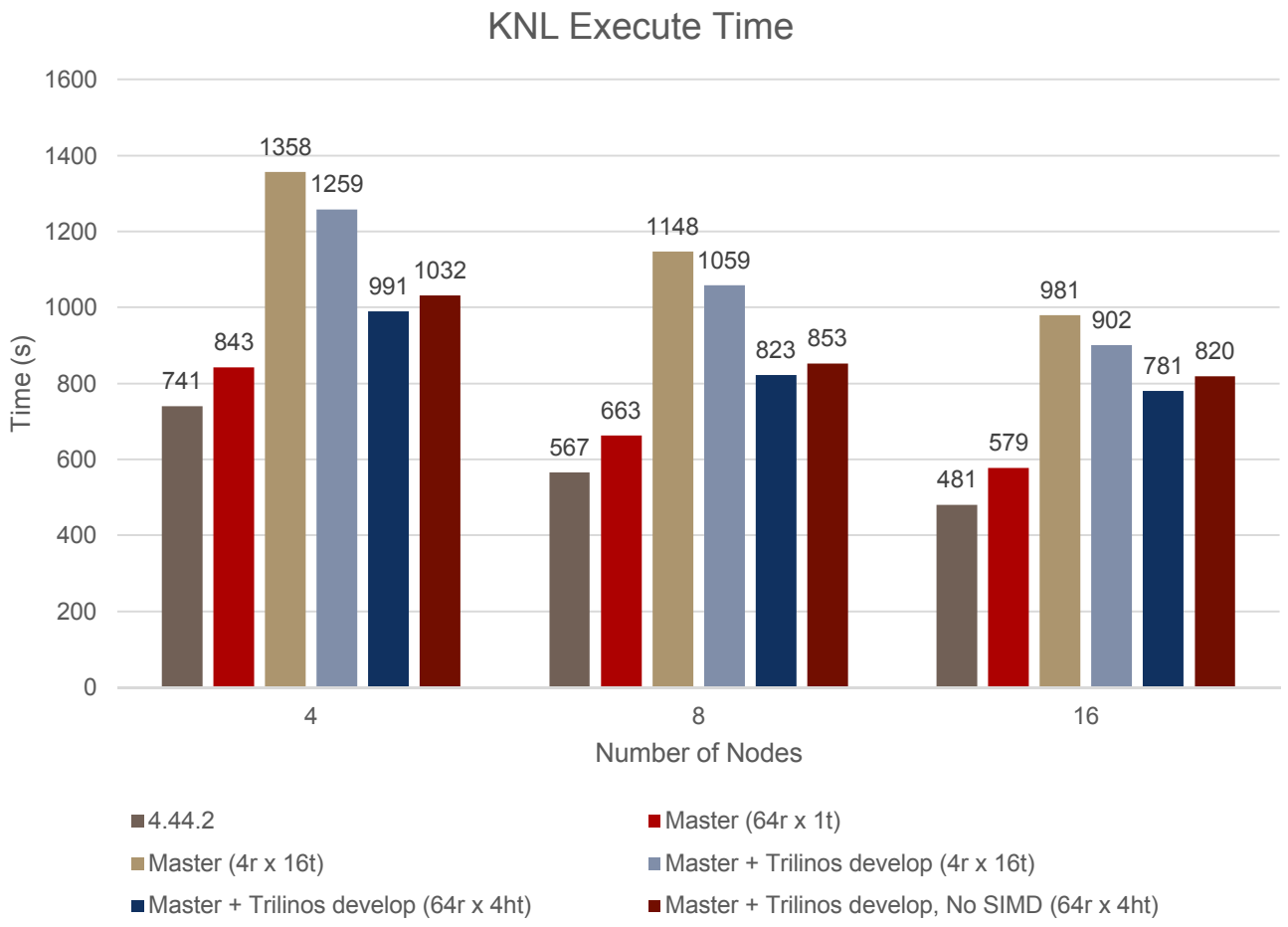
Includes non-threaded enclosure radiation

AFF Test Case



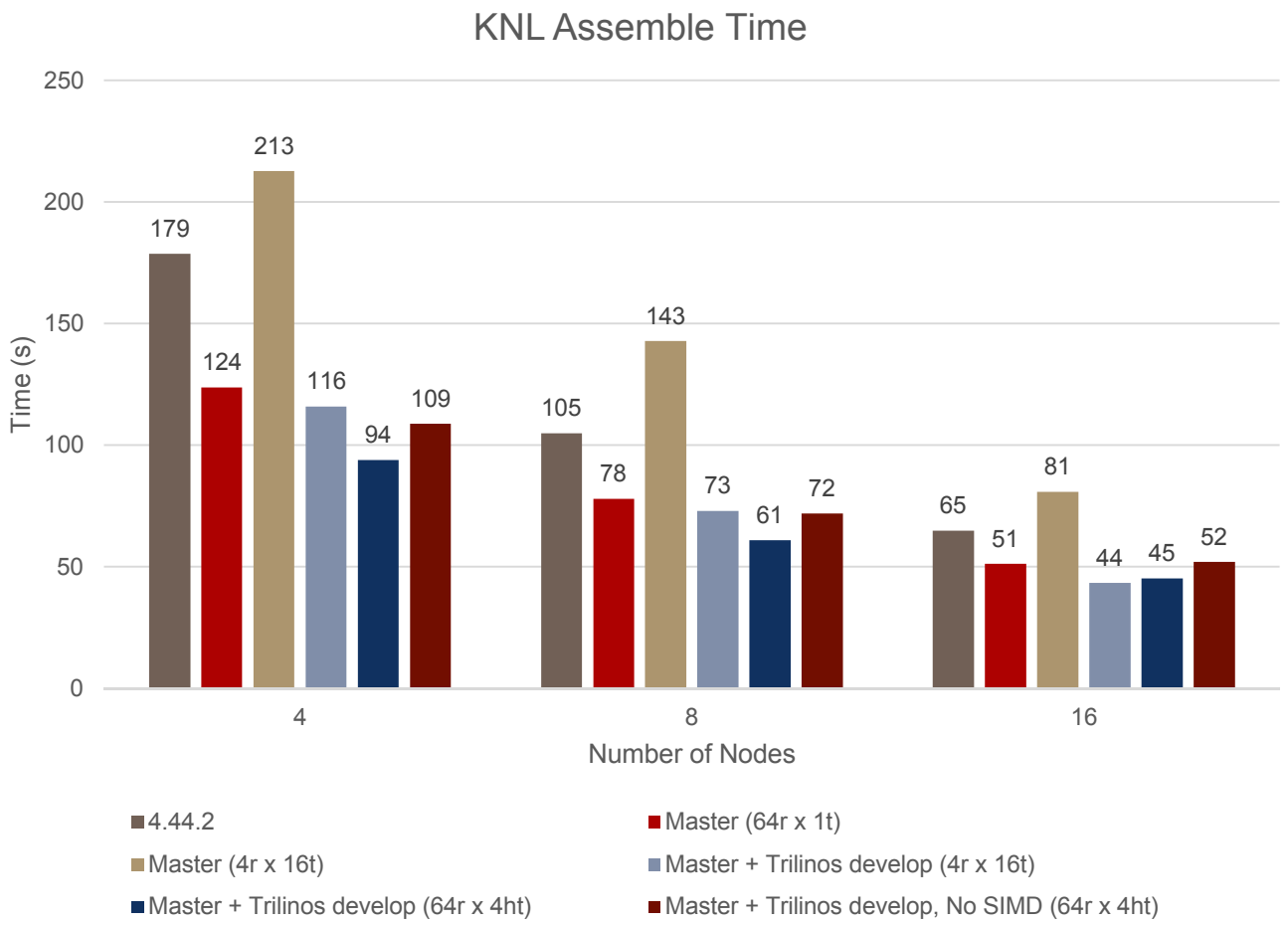
Includes non-threaded enclosure radiation

AFF Test Case



Includes non-threaded enclosure radiation

AFF Test Case



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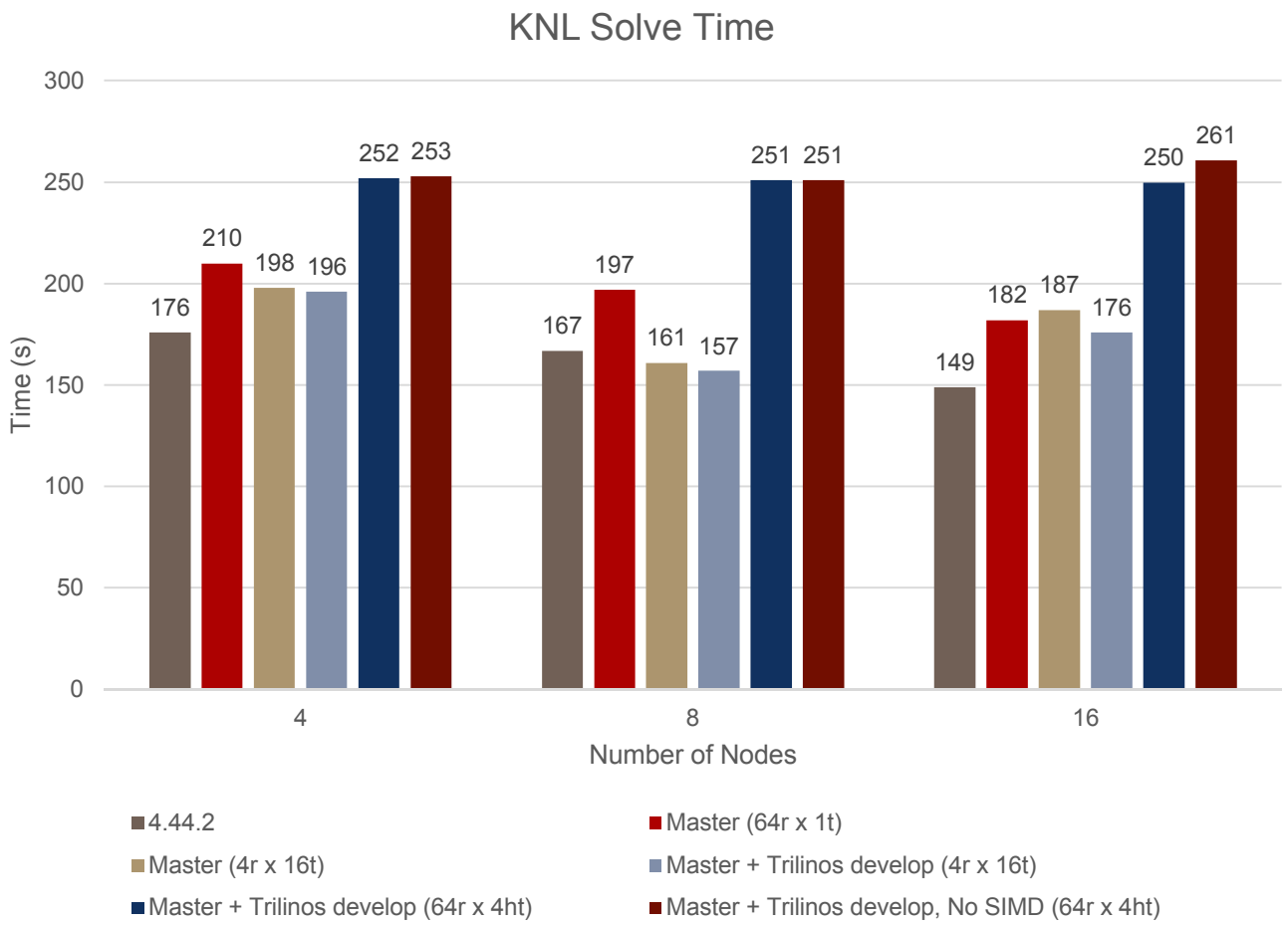
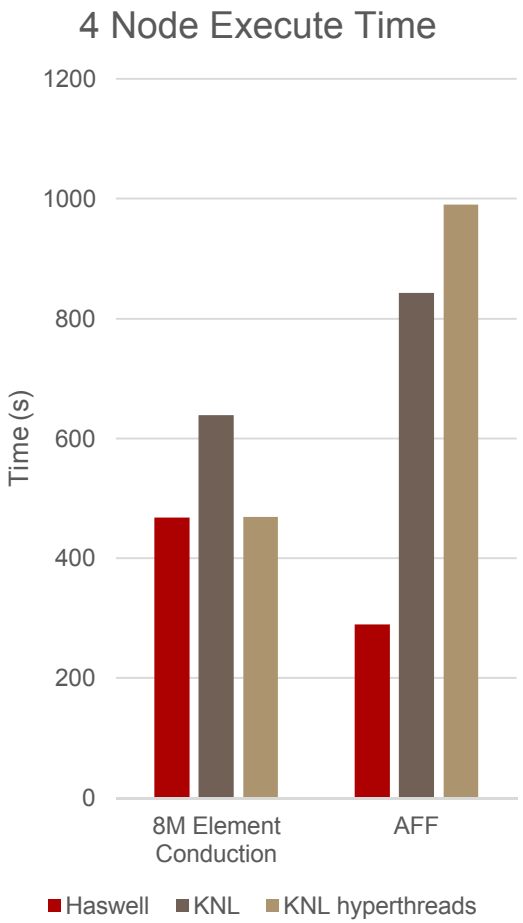
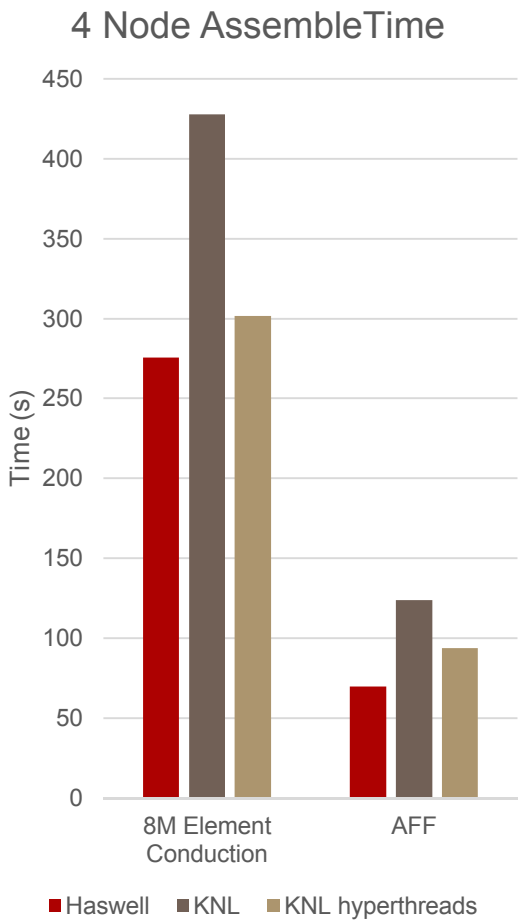
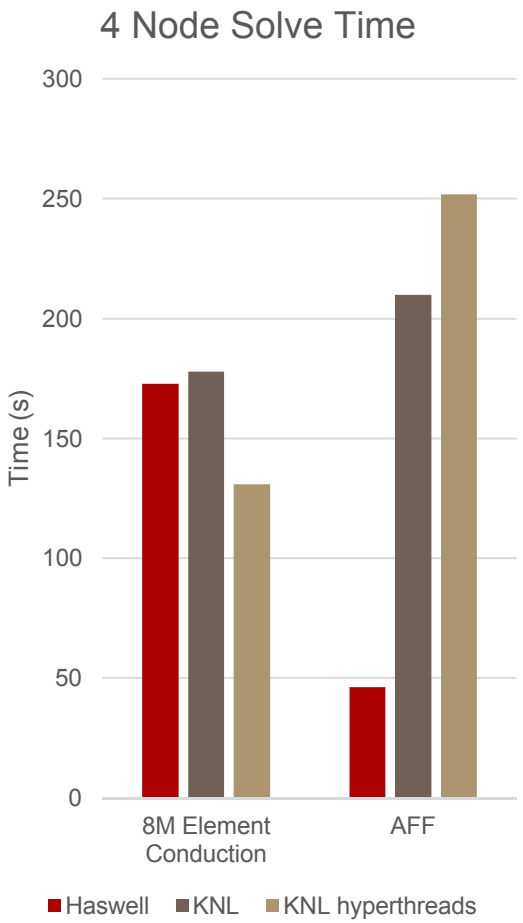


Haswell vs KNL comparisons







Haswell: 32r x 1t; KNL: 64r x 1t; KNL hyperthreads: 64r x 4ht

Conclusions

- Ariamini
- Aria transition
- Speedup vs 4.44
- Vectorization
- Threading
  - Haswell
  - KNL

For more information: SAND2017-9807PE

Questions?

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Questions?

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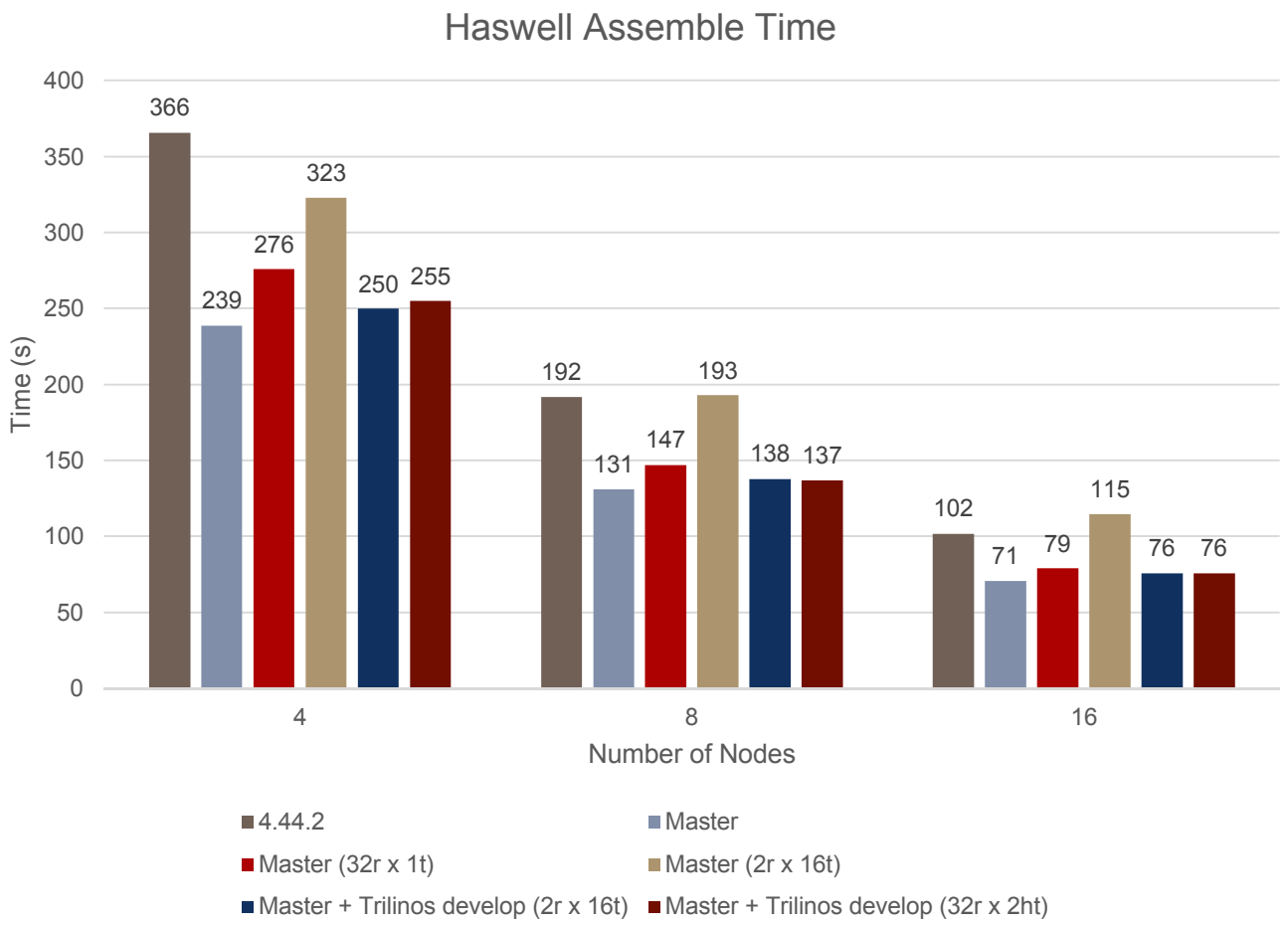
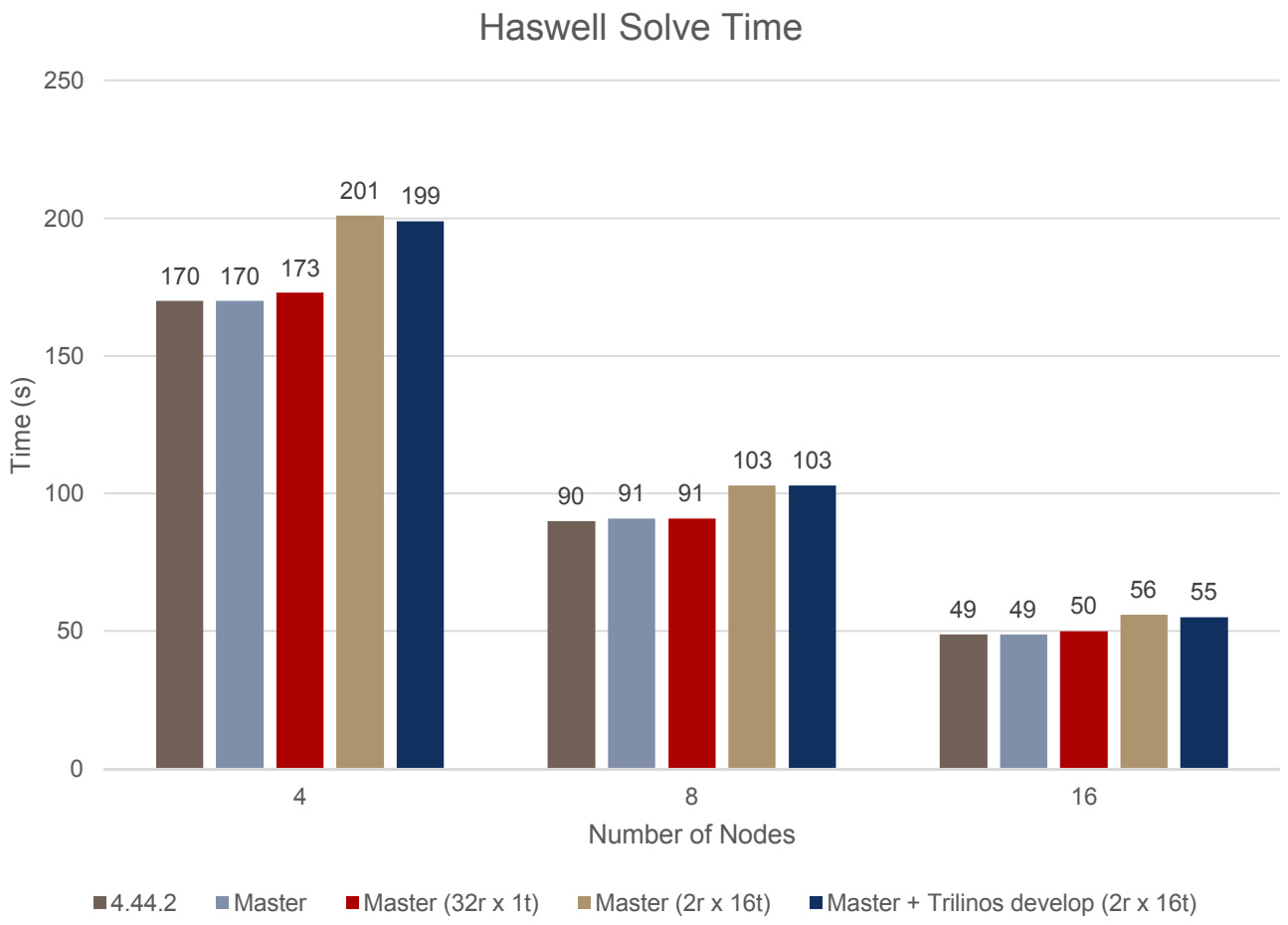
Backup Slides

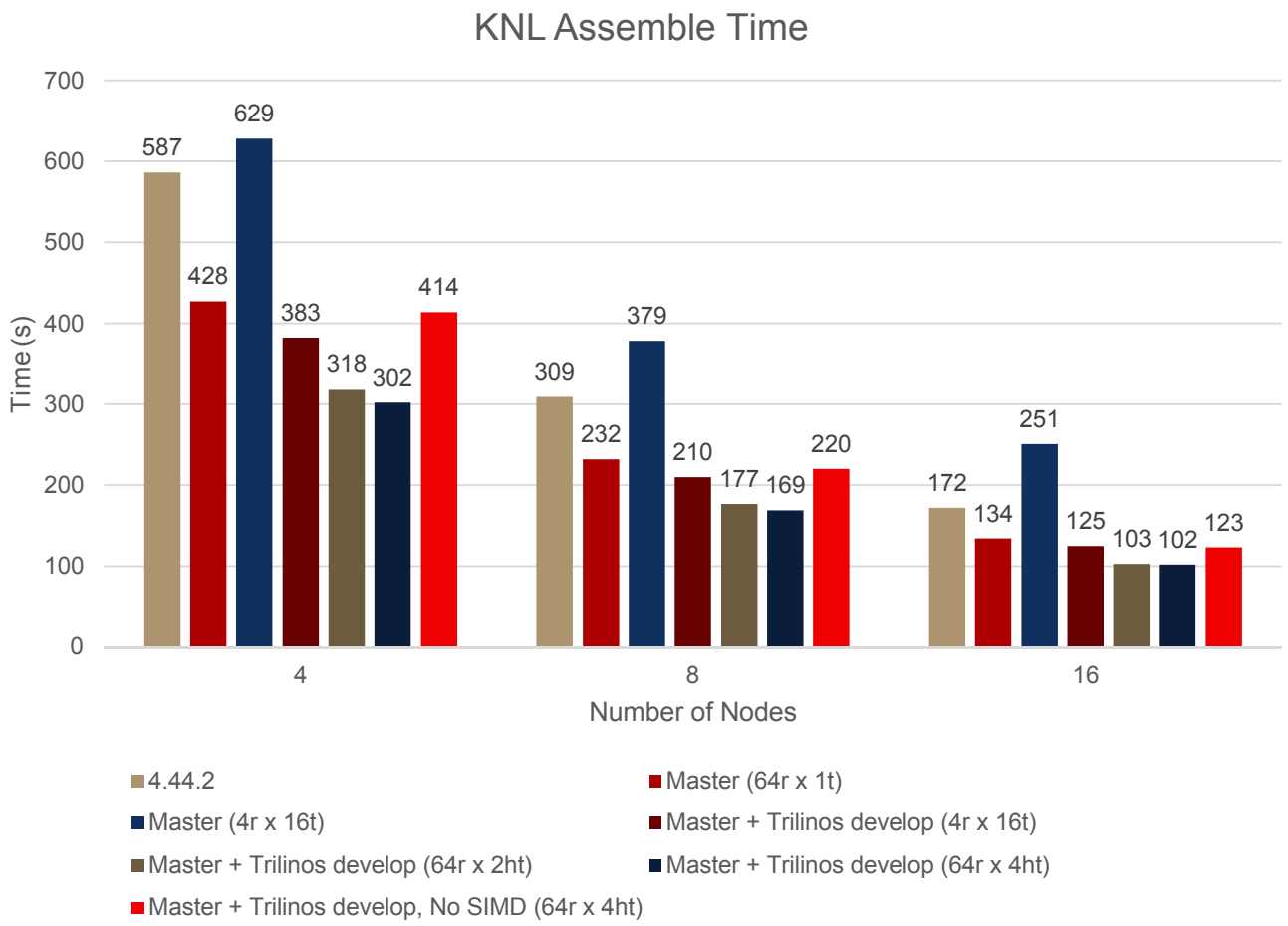
8M Element Conduction



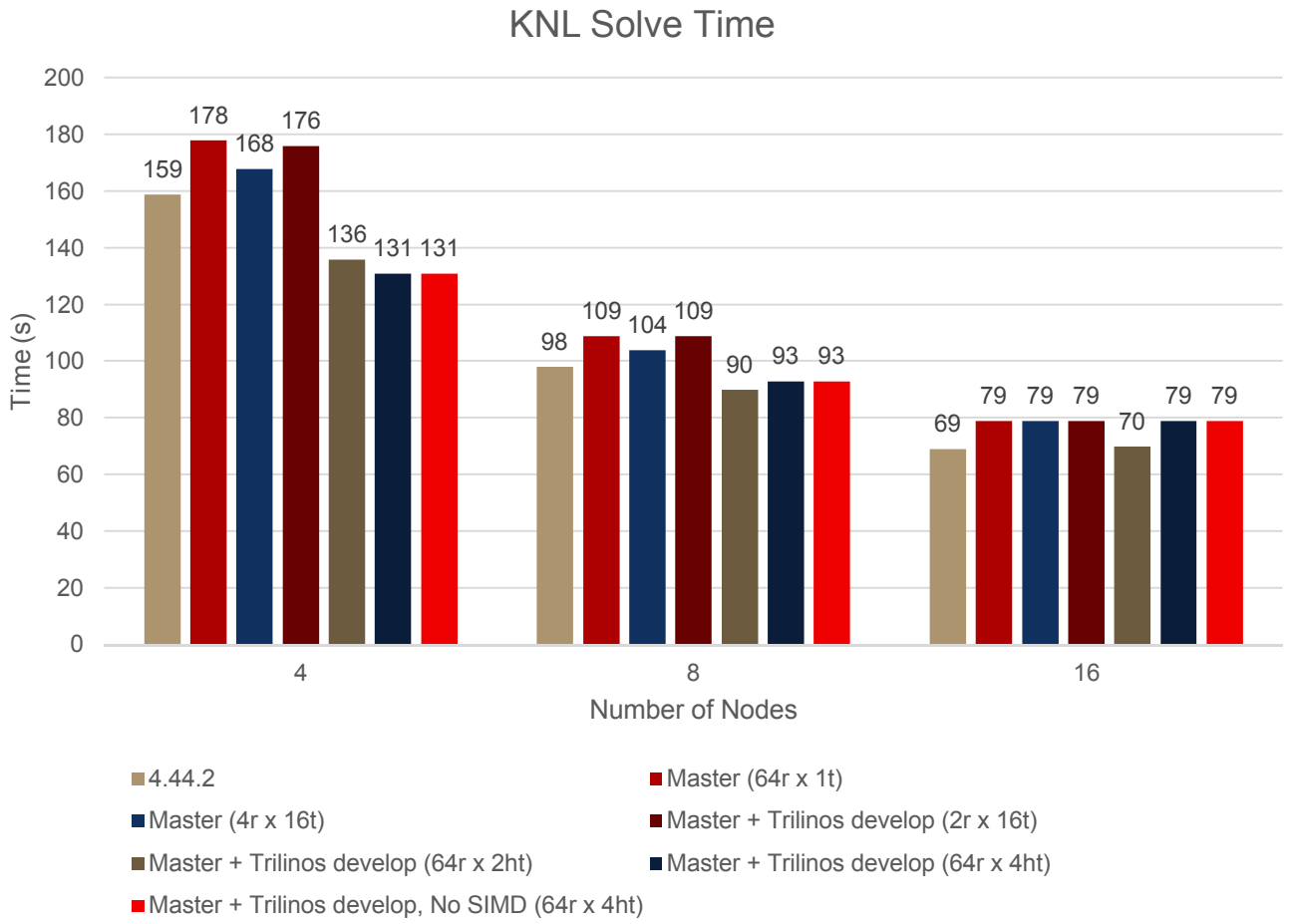
8M Element Conduction



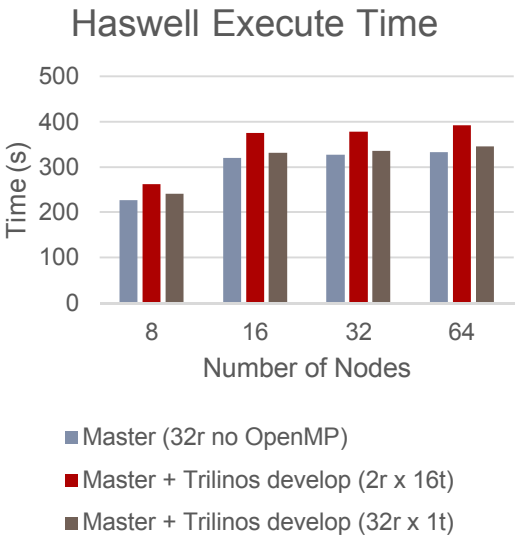
8M Element Conduction

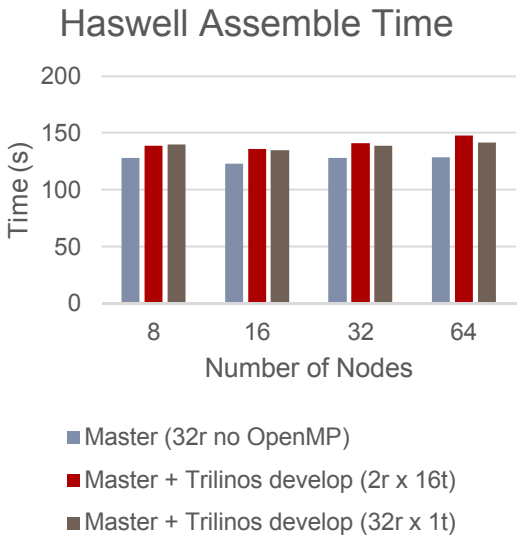


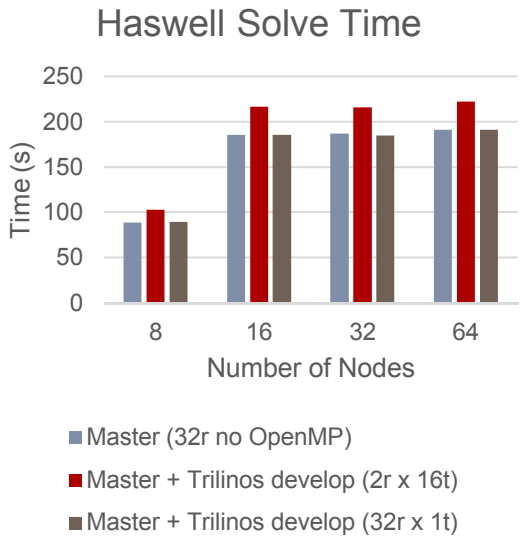
8M Element Conduction

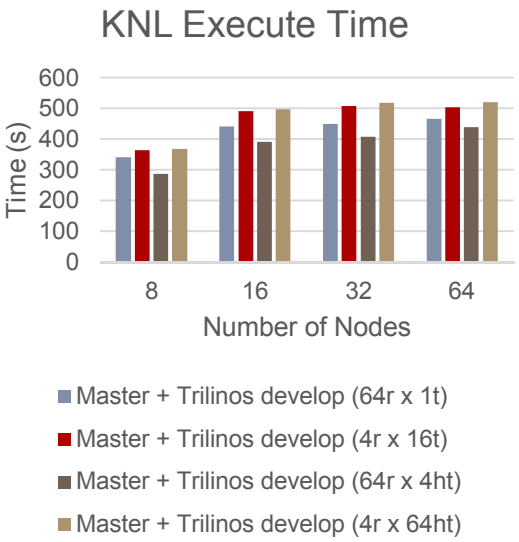


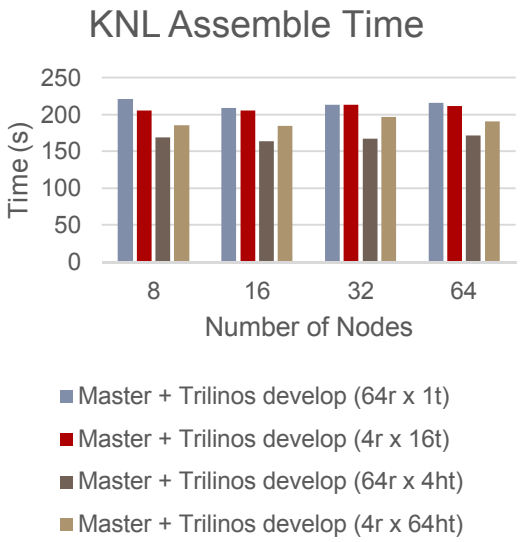
Weak Scaling

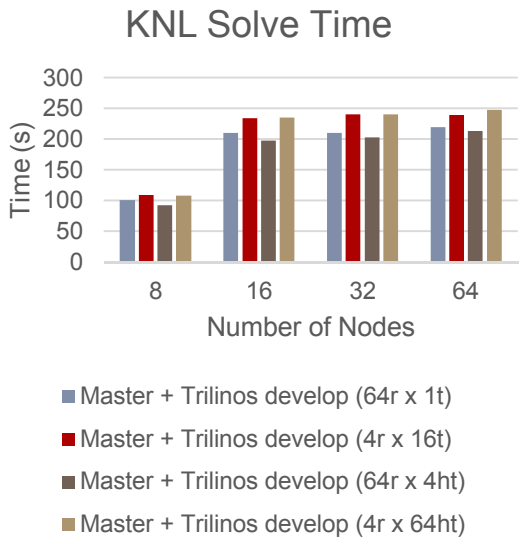












Efficiency

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$$\text{eff} = \frac{t_{mpi}}{t_{threads}}$$