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Title: Porting Eulerian Multiphysics Solver xRAGE to GPU-Capable C++

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Porting Eulerian Multiphysics Solver xRAGE to GPU-Capable C++

Student Talk

Dylan Lyon

Kokkos Usergroup Meeting
December 12-14, 2023

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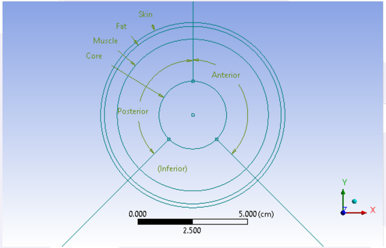
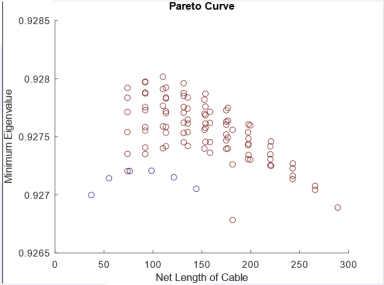
Introduction

- B.S. Aerospace Engineering, University of Central Florida
  - Barnes-Hut n-body code, C++ w/ OpenMPI & OpenMP
  - Human body model, 1D "tree" FDM code, Matlab & C++
  - Architecture solids FEM code, Matlab & Julia w/ multithreading
- M.S. Mechanical Engineering, University of Michigan
  - Learned Kokkos at Masters level
- LANL Post-Masters Research Assistant
  - Eulerian Applications Group



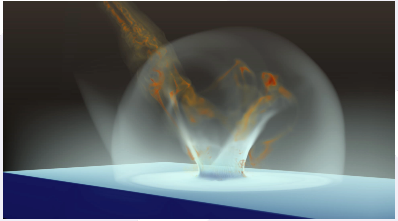
Fiala model of human arm

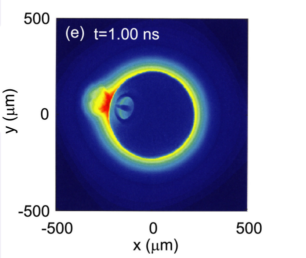


Predicted minimum sway eigenvalue with increasing cable stay lengths

xRAGE
Program Overview

- Finite volume multiphysics code
- Written in Fortran 90
- Used on many different architectures and clusters w/w/o GPUs


xRAGE simulation of Chicxulub asteroid [1]



xRAGE simulation of asymmetric ICF implosion shot [2]

xRAGE
Porting to C++

- New GPU clusters (Venado, Sierra)
- New Accelerated Computing Unit "APU" clusters (El Capitan)
  - Prototype rzVernal already operational

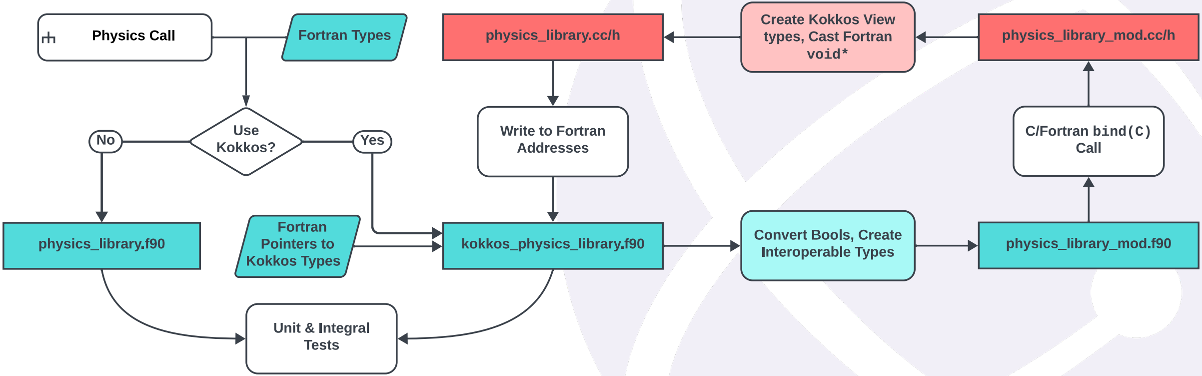
Takeaway:

- Want to take advantage of GPUs
- Avoid machine-specific xRAGE implementations

→ Use Kokkos

xRAGE
Porting Overview

Moving to C++ with Kokkos, one physics package at a time



xRAGE - Conduction
Overview

- Heat transfer by particle collisions
- Conduction always performs local conduction solve:

Equation 1 - Local Heat Conduction

$$\rho C_v \frac{\delta T}{\delta t} = \vec{\nabla} \cdot \left[\kappa \left(\rho, T \right) \vec{\nabla} T \right] \quad (1)$$

xRAGE - Conduction
Multigroup & Nonlocal

Local conduction diffs when simulating fast electrons in hot plasma

- Mean free path λ and therefore κ increase with electron energy

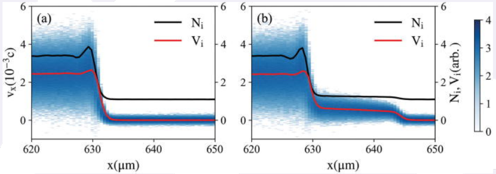
$\rightarrow$ **Multigroup**: Must solve conduction per electron energy group

- Mean free path λ is on the order of temperature scale length $\frac{T}{\nabla \cdot T}$

$\rightarrow$ **Nonlocal**: Must consider nonzero gradient lengths (Preheat)

Equation 2 - Electron Mean Free Path [3]

$$\lambda_g = \frac{2}{\sqrt{1 + \langle Z \rangle}} \frac{(k_B \mathcal{E}_g)^2}{4\pi n_e e^4 \ln(\Lambda)} \quad (2)$$



Preheat in C^{6+} [4]

xRAGE - Conduction
Conduction Layout

Local conduction solve to get particle currents at faces
$\longrightarrow$ Use currents as input to nonlocal multigroup model [5]

Three layers of iteration:

- N Time substeps OR energy conservation residual iterations
  - M Nonlocal flow convergence iterations
    - K Electron energy groups, $\mathcal{O}(10)$

Leaving $N+1$ local matrix constructions and $(N+1)\times(M+1)\times K$ nonlocal matrix constructions per xRAGE timestep

Takeaway:

Speed Up Matrix Construction

xRAGE - Conduction
Matrix Construction

Current implementation:

- Uses temporaries extensively
- Analog of the Fortran implementation

Current work:

- Reuse temporaries of same sizes

Future (potential) work:

- Use and reuse `Kokkos::Experimental::ScatterViews`
- Use memory pools to minimize malloc calls

Scatter Views

Scatter Views
Usage

Common patterns in Finite Volume codes:

- Cell-to-Face-to-Cell
  1. Interpolate cell-centered values to faces
  2. Perform operation at faces
  3. Use face values to get cell-centered value

  Examples: Opacity across cells, advections

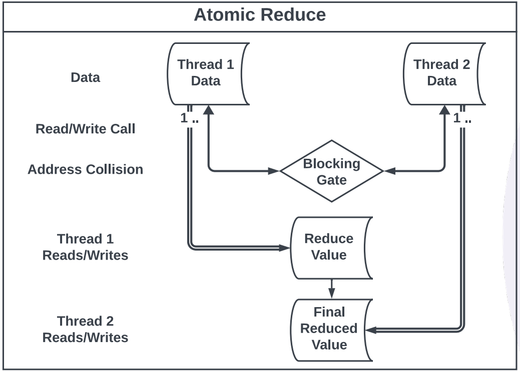
- Cell-to-Partition
  1. Reduce all cell values to one per-node value

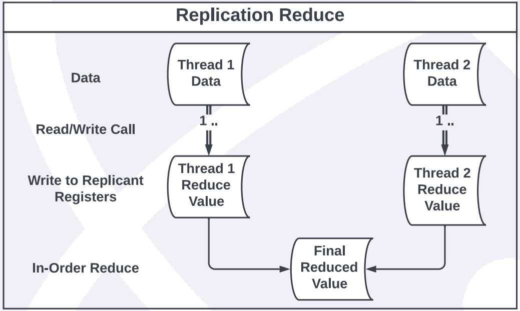
  Examples: Global energy conservation

Takeaway:

1. Both have data races
2. Widely varying concurrency
3. Thread read/write collisions depend on thread counts

Scatter Views
Reduce Approaches





Scatter Views
Overview

`Kokkos::Experimental::ScatterView`

- Automatic switching between `Kokkos::Atomic` and data replication approaches
- Thread scalable at high thread counts
- No need to manually write data replication approach where high concurrency is *possible* [6]

Scatter Views
Example

Face Flow Reduce

```
// Original View to reduce
Kokkos::View<double*> dflxeng( "dflxeng", numcells );

// Reusable ScatterView
Kokkos::Experimental::ScatterView<ReductionExecSpace, double*> dflxeng_sv = ...
                    Kokkos::Experimental::create_scatter_view( dflxeng );

// Scatter pattern kernel
Kokkos::parallel_for( "scatter_pattern_kernel",
                      Kokkos::RangePolicy<ReductionExecSpace> ( 0, numcells ),
                      KOKKOS_LAMBDA ( const size_t idx ) {
    // Create "accessor" View.
    //      For atomic approach, will be atomic single address
    //      For replication approach, will be replicant View
    auto dflxeng_access = dflxeng_sv.access();

    // Perform operation without data race
    dflxeng_access(idx) += max(face_flow(face_idx(idx)), 0.0);
}

// If using replication approach, perform the in-order reduction.
Kokkos::Experimental::contribute(dflxeng, dflxeng_sv);
```

Conclusion

- Porting strategy for xRAGE
- Approaches for accelerating Conduction matrix construction
- ScatterView, a Kokkos feature for fast scatter over any hardware

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