From PeleC to PeleACC, to PeleC++

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The Pele Project

Solves reacting Navier-Stokes on structured grid using AMR and embedded boundaries based on AMReX library

PeleC

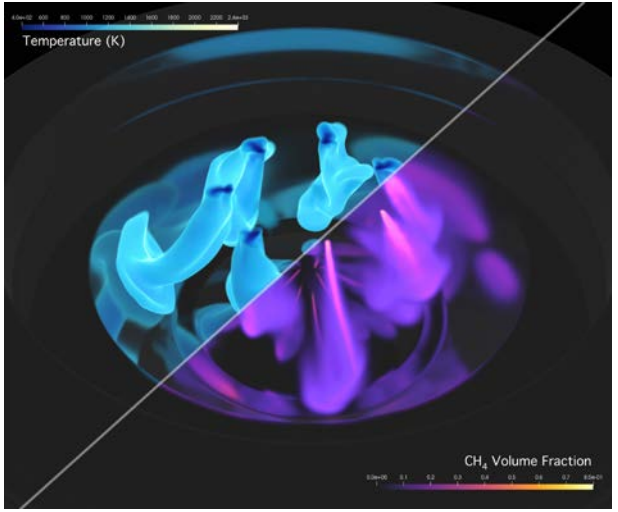
- Compressible combustion simulations
- Explicit time stepping

PeleLM

- Low-mach combustion simulations
- Implicit, requiring linear solver

PelePhysics

- Shared code for chemistry/reactions

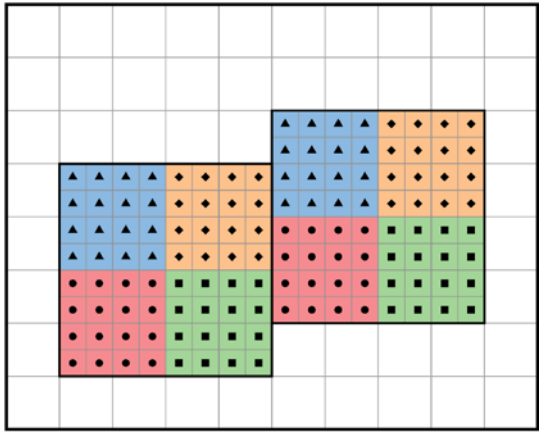


PeleC Overview

- 50k LOC
- 11373 lines of C++
- 38905 lines of Fortran (including duplicate dimension-specific code)
- High level C++ orchestration with Fortran kernels
- Source code generator used for chemistry to unroll code
- C++ -> Fortran -> C
  - Mixed languages pose many issues

Original PeleC Programming Model

- MPI + OpenMP
- Ranks operate in bulk-synchronous data-parallel fashion
- Threads operate on independent tiles
- Originally focused on KNL and vectorization (lowered loops)



AMReX FAB data structures[1].

```
#pragma omp parallel
for (MFIter mfi(F,true); mfi.isValid(); ++mfi) {
    const Box& box = mfi.tilebox();
    Array4<Real const> const& u = U.const_array(mfi);
    Array4<Real      > const& f = F.array(mfi);
    f2(box, u, f); // Call Fortran kernel
}
```

PeleC on GPUs

- Xeon Phi discontinued; GPUs become focus for birth of Exascale
- Quickest way to utilizing GPUs
  - Offload kernels to device
- OpenACC most mature Fortran GPU programming model at the time
- Tied to PGI compiler
- Introduced in 2011
  - Used in production since ~2014
- OpenMP 4 introduced for accelerators in 2013
  - Jeff Larkin (NVIDIA) - GTC **March 2018** – OpenMP on GPUs, **First Experiences** and Best Practices
- OpenACC pragmas have a straightforward mapping to OpenMP pragmas
- Minimize the need to modify current PeleC code
- Don’t need to remove current OpenMP pragmas

PeleC OpenACC Programming Model

- Memory management originally done explicitly
- Later used AMReX's GPU memory management
  - Use `default(present)`
- Just need to make sure every routine under kernel is decorated as `seq` device routine
- Run with MPS, 7 ranks per Summit GPU to obtain asynchronous kernels

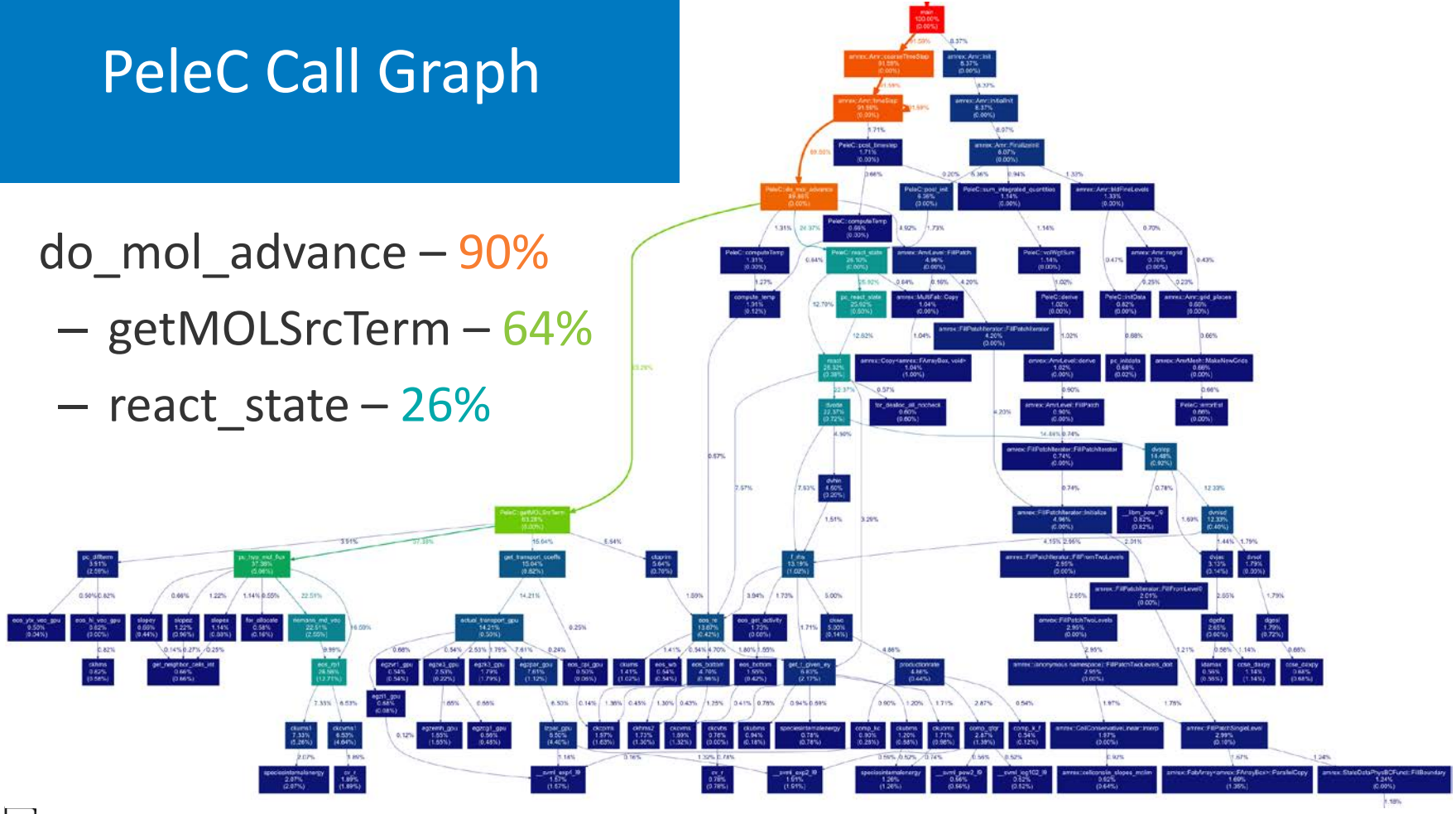
```
for (MFIter mfi(mf, TilingIfNotGPU()); mfi.isValid(); ++mfi)
{
    const Box& bx = mfi.tilebox();
    FArrayBox& fab = mf[mfi];
    plusone_acc(BL_TO_FORTRAN_BOX(tbx),
                BL_TO_FORTRAN_ANYD(fab));
}
```

```
subroutine plusone_acc()
!$acc parallel loop gang vector collapse(3) default(present)
do k = lo3, hi3
   do j = lo2, hi2
      do i = lo1, hi1
         data(i,j,k) = data(i,j,k) + 1.0_amrex_real
         call deep_nest_of_functions()
      end do
   end do
end do
!$acc end parallel loop
end subroutine plusone_acc
```

Figure 2: OpenACC approach to launching a kernel on the GPU.

PeleC Call Graph

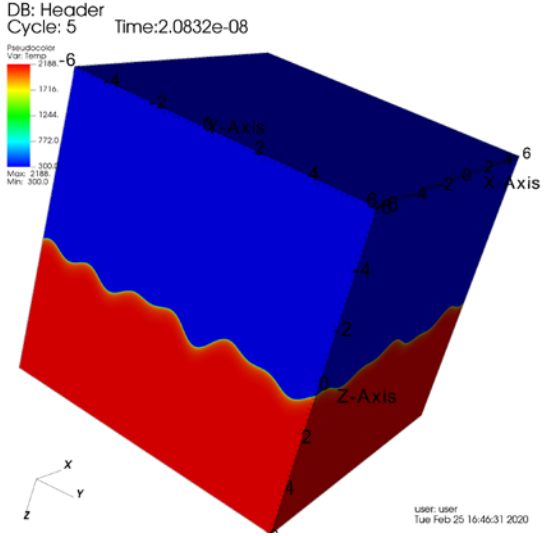
- do_mol_advance – 90%
  - getMOLSrcTerm – 64%
  - react_state – 26%

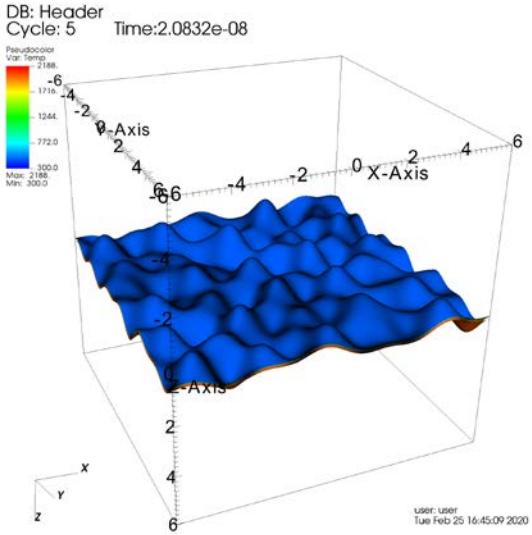


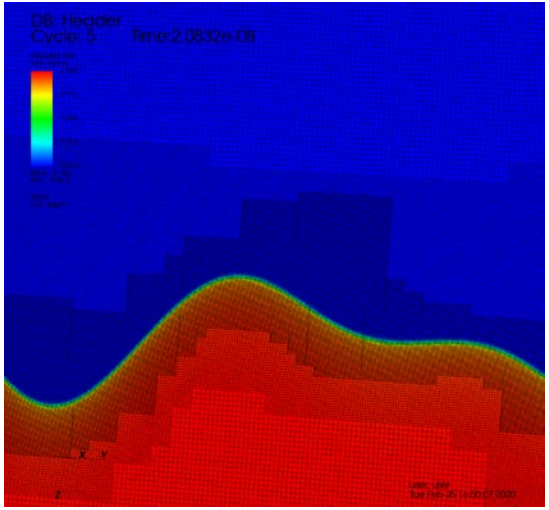
OpenACC Effort

- 90% of runtime under one routine
- Around 5 kernel routines under `getMOLSrcTerm` to parallelize on GPU
  - Around 50 routines to label as `seq`
- react_state is implicit ODE solver with thousands of if conditions
  - Implement a simpler explicit solver instead
  - Explicit solver written in C and CUDA
  - Explicit solver 6x slower on CPU
    - Completely dominates runtime (`react_state` now around 90%)

Test Case – Pre-mixed Flame

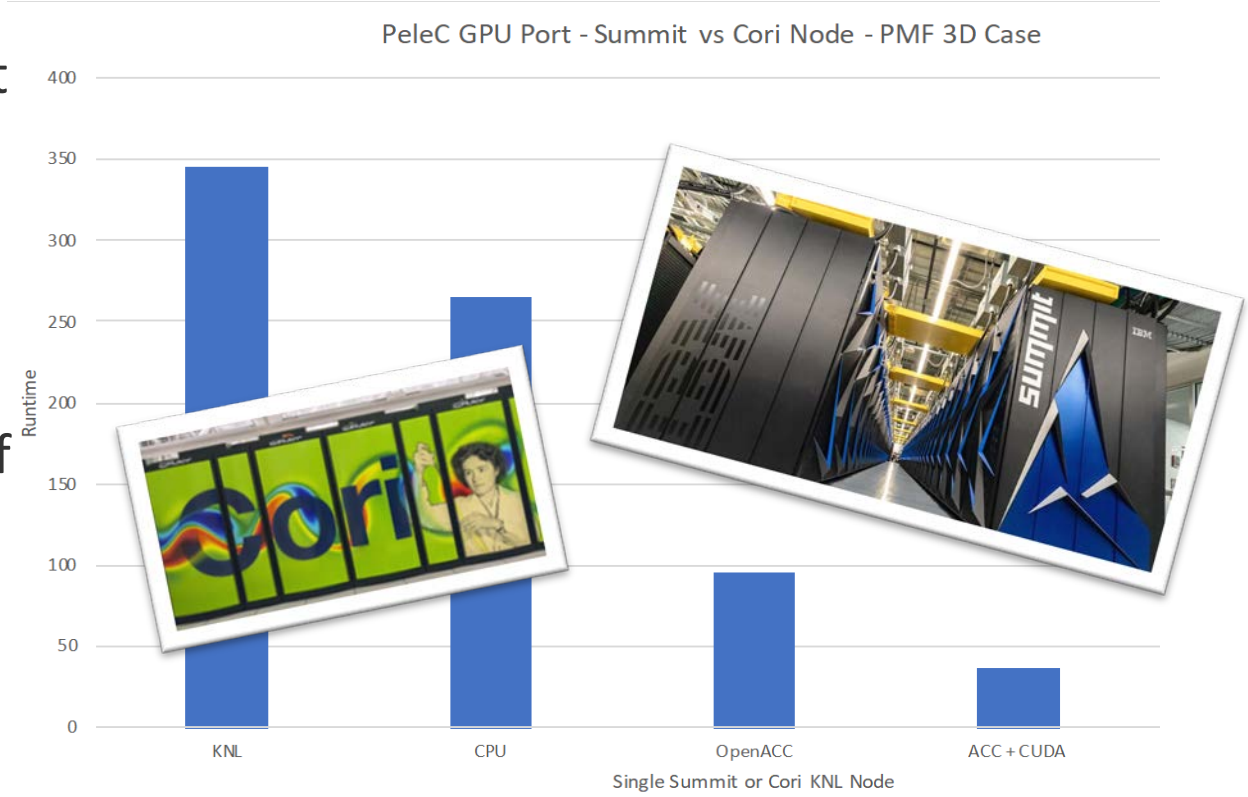






OpenACC Results

- Initial OpenACC port over 3x faster than Cori KNL
- 8x faster with CUDA `react_state()`
- 2 people, 3 weeks of development time
- 1 major bug found and reported to PGI



C++ Effort

- AMReX GPU strategy was emerging alongside our OpenACC effort
  - Much like Kokkos using C++ lambdas, but need not be as general
- Steven Reeves, graduate student at LBL prototyped PeleC on the GPU over 6 months by porting every necessary routine to C++
  - Performance much better than OpenACC prototype
- However, once AMReX's memory management was used in OpenACC, performance over OpenACC seemed to be a toss-up (mostly due to sharing of `react_state` routine)
- Performance in general was 16-18x faster than KNL

OpenACC vs C++ Prototype

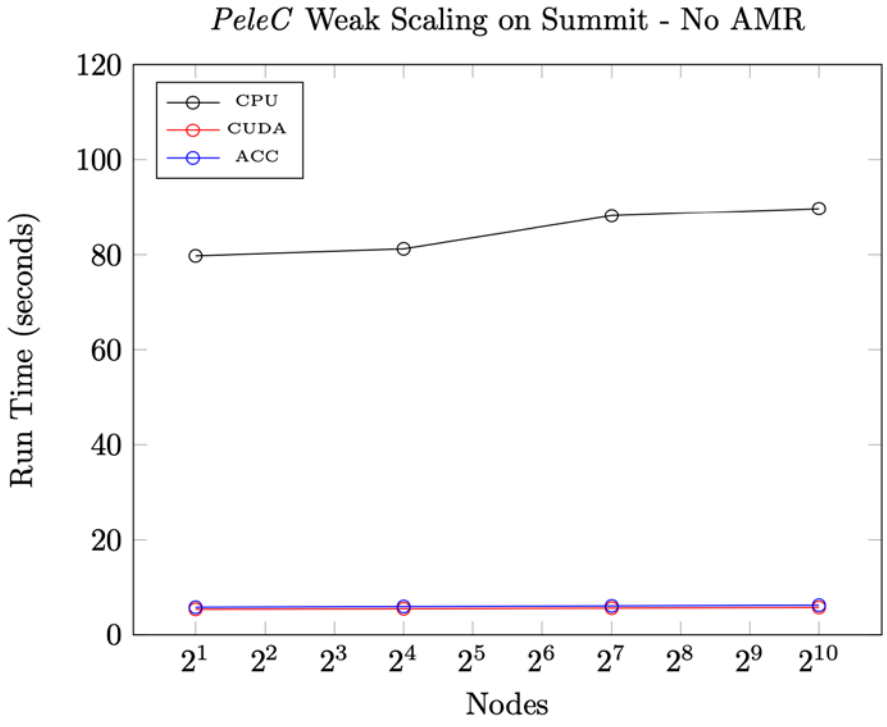
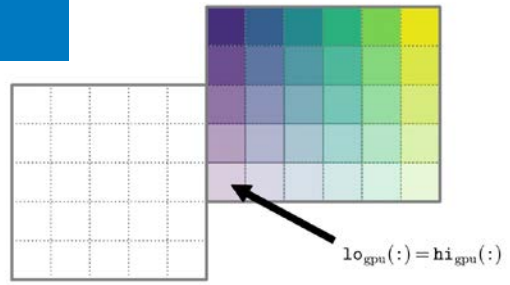


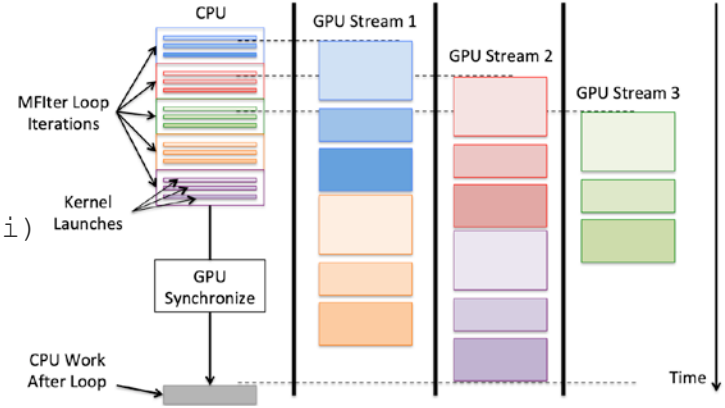
Figure 3: Weak scaling of PMF problem with 2^{23} cells per node and no AMR.

C++ Effort

- MPI+CUDA for GPUs
- Essentially one thread per cell
- Focus on maximum parallelism in kernel (hoisted loops)
- 1 rank per GPU with CUDA streams for asynchronous behavior




```
#pragma omp parallel if (amrex::Gpu::notInLaunchRegion())
for (MFIter mfi(mf,TilingIfNotGPU()); mfi.isValid(); ++mfi)
{
    const Box& bx = mfi.tilebox();
    Array4<Real> const& fab = mf.array(mfi);
    amrex::ParallelFor(bx, ncomp,
    [=] AMREX_GPU_DEVICE (int i, int j, int k, int n)
    {
        fab(i,j,k,n) += 1.;
```



AMReX GPU strategy[2].

C++ Results

- 2x faster on CPU
- 18x faster than fastest CPU case using Intel compiler
- 56x faster than GCC CPU on Summit
- 124x faster than original Fortran on Summit CPUs

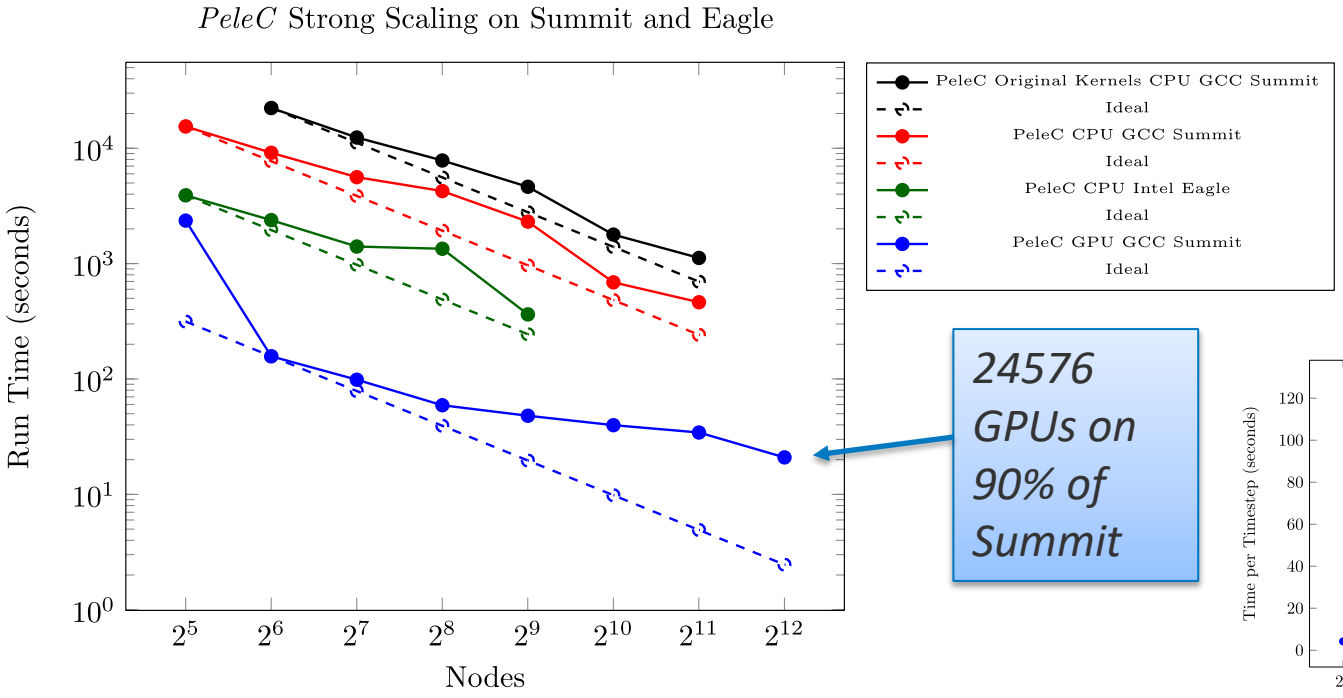


Figure 1: Strong scaling of PMF case with drm19 chemistry on Summit and Eagle machines. 360M cells with 2 levels of AMR.

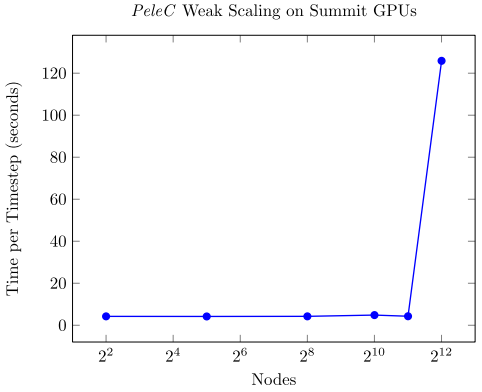


Figure 1: Weak scaling of PMF case with drm19 chemistry with no AMR. 2^{22} cells per node.

Conclusions

- OpenACC allowed us to prototype PeleC on GPU very quickly
- Performance can be similar to CUDA
- Code quickly became displeasing
- Mixed languages cause problems for readability, debugging, profiling, and compiler optimizations

- PeleC now 19363 lines of C++
- Fortran appears to be not beneficial to PeleC in any way
- Even 2x faster on the CPU
- Easier to debug and profile
- Kernels easier to write and to read
- Much less duplicate code necessary for dimensions
- Ability to use many compilers
- Good performance portability

References

1. https://amrex-codes.github.io/amrex/docs_html/Basics.html#mfiter-and-tiling
2. https://amrex-codes.github.io/amrex/docs_html/GPU.html#overview-of-amrex-gpu-strategy

Q&A

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