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)

```c
#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
}
```

AMReX FAB data structures\(^1\).
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 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`
  – Wrote Fortran version of Fuego code generator for these routines
• `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%)
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

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

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

**Figure 2:** OpenACC approach to launching a kernel on the GPU.
Test Case – Pre-mixed Flame
OpenACC Results

- Initial OpenACC port over 3x faster than Cori KNL
- 8x faster with CUDA react_state()
- 2 people, 5 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 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**

*PeleC* Weak Scaling on Summit - No AMR

**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 perfectly nested loops)
- 1 rank per GPU with CUDA streams for asynchronous behavior

```cpp
#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.;
    });
}
```
C++ Results

**PeleC Strong Scaling on Summit and Eagle**

- **Run Time (seconds)**
  - PeleC Original Kernels CPU GCC Summit Ideal
  - PeleC CPU GCC Summit Ideal
  - PeleC CPU Intel Eagle Ideal
  - PeleC GPU GCC Summit Ideal

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

- **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**

**PeleC Weak Scaling on Summit GPUs**

- **24576 GPUs on 90% of Summit**

**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
• Non-ubiquitous programming models lack support, robustness, and flexibility
• Fortran was holding us back

• 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
• 1 graduate student 6 months + 2 staff 12 weeks to completely move to C++
References

Q&A

www.nrel.gov

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