Lattice Simulations using OpenACC compilers

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OpenACC is a programming standard for parallel computing developed by Cray, CAPS, Nvidia and PGI. The standard is designed to simplify parallel programming of heterogeneous CPU/GPU systems.

from Wikipedia

The OpenACC Application Program Interface describes a collection of compiler directives to specify loops and regions of code in standard C, C++ and Fortran to be offloaded from a host CPU to an attached accelerator, providing portability across operating systems, host CPUs and accelerators.

from openacc.org

The directives and programming model defined in this document allow programmers to create high-level host+accelerator programs without the need to explicitly initialize the accelerator, manage data or program transfers between the host and accelerator, or initiate accelerator startup and shutdown.

from openacc.org

Programs I have had some experience with :

1. Staggered fermions with wilson gauge action on
   (a) single GPU – in some detail
   (b) multi GPU – preliminary

2. Wilson fermions with Wilson gauge action on
   single GPU – preliminary

Main bottlenecks is slow data movement between CPU & GPU.
Speed is about 5 GB/s.

Impossible to avoid CPU completely as I/O , if-then clause is evaluated on CPU.
BLAS functions are launched from CPU and MPI calls (at least for Fermi GPUs) are launched from CPUs.

Single GPU code

```
subroutine congrad(nitcg)
... All kinds of definitions and declarations ...
!$ACC  data copy(nitcg,alpha,betad,betan)
!$ACC+ copyin(nx,iup,idn,u,r)
!$ACC+ copyout(x,y)
!$ACC+ create(ud,ap,atap,p)
*
      call linkc_acc
!!$OMP parallel do default(shared)
!$ACC  parallel loop collapse(2) reduction(+:betan) present(p,r,x)
      do l = 1, mvd2
      do ic=1,nc
         p(l,ic) = r(l,ic) ; x(l,ic) = (0.,0.)
         betan=betan+conjg(r(l,ic))*r(l,ic)
      end do
      end do
```

```
!       betan=real(zdotc(mv3d2,r,1,r,1))
!$ACC   update host(betan)
       if (betan.lt.delit) go to 30
!$ACC   parallel present(beta,betan,betad,alphan)
        beta=betan/betad ; betad=betan ; alphan=betan
!$ACC   end parallel
        do nx = 1, nitrc  Main loop of conjugate gradient begins
        nitcg ← nitcg+1    ;    ap = 0

        call fmv(0,mvd2,ap,p)    →(Matrix-vector multiplication)

        alphad=⟨ap,ap⟩ + ⟨p,p⟩    ;   alpha=alphan/alphad
        atap ← p    ;    x ← x + alpha * p
```

```
        call fmtv(atap,ap)    →(Matrix-vector multiplication)

        r ← r - alpha * atap
        betan=⟨r, r⟩
!$ACC   update host(betan)          Exit condition evaluated on CPU
        if (betan .lt. delit) go to 30
        beta=betan/betad ; betad=betan ; alphan=betan
        p ← r + beta * p
        end do          Main loop of conjugate gradient ends
30      continue
*
        y = 0           Solution on the second half lattice
        call fmv(mvd2,mv,y,x)    →(Matrix-vector multiplication)
*
!$ACC   end data
        return
```

Matrix-vector multiplication routine

```
      subroutine fmv(noff,nsz,v,w)
```

... *All kinds of definitions and declarations* ...

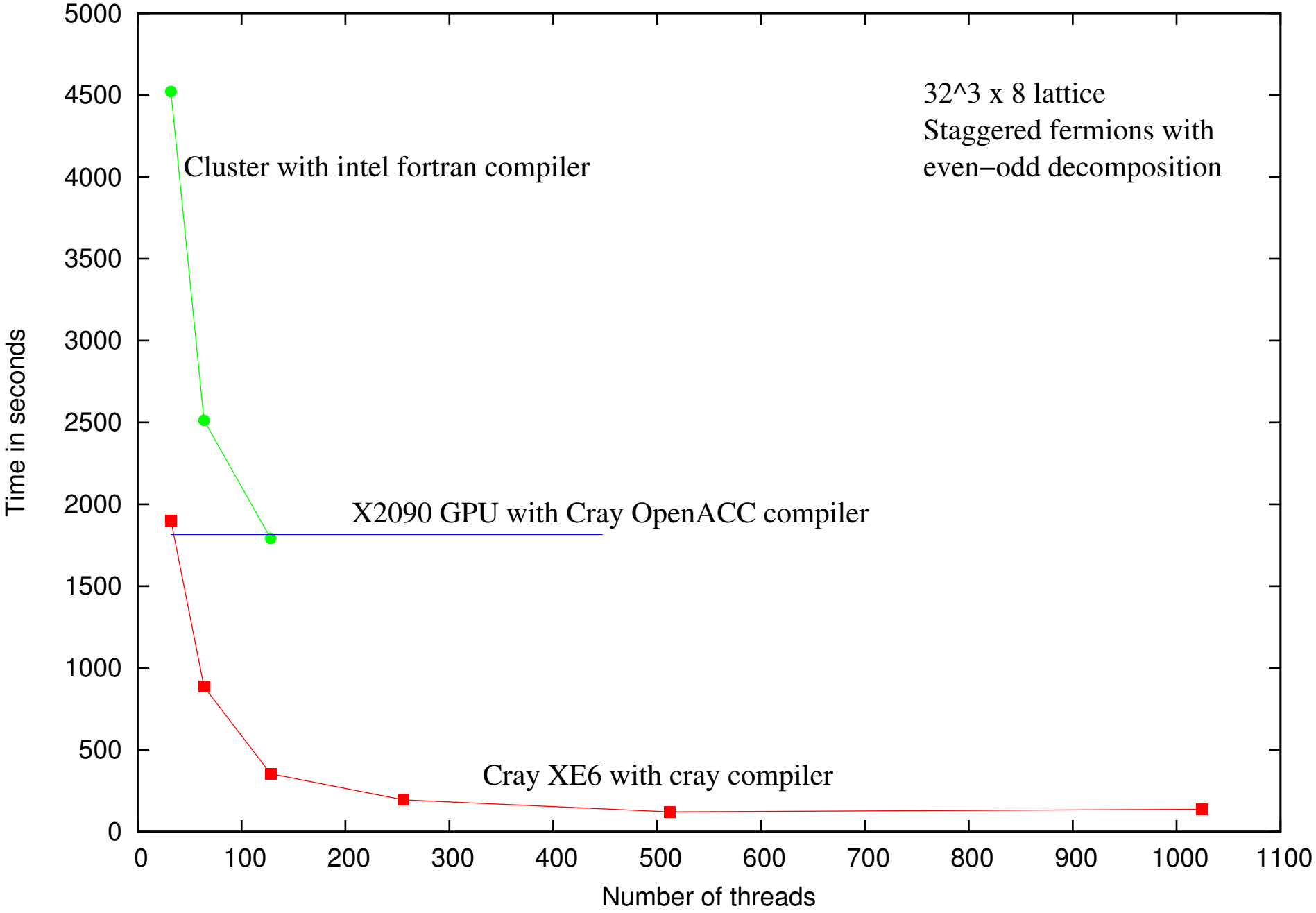
```
!!$OMP parallel do default(shared)
!!$OMP+      private(nnu,px1,px2,px3,px4,px5,px6)
!!$OMP^ private(v1,v2,v3)
!$ACC  parallel loop present(u,ud,v,w,iup,idn)
!$ACC+ private(nnu,px1,px2,px3,px4,px5,px6,v1,v2,v3)
!$ACC+ vector_length(32)
      do  l = noff+1, noff+mvd2
```

⋮

Routine identical to CPU version

⋮

```
      enddo
      return
```


32^3 x 8 lattice
Staggered fermions with
even−odd decomposition
Cluster with intel fortran compiler
X2090 GPU with Cray OpenACC compiler
Cray XE6 with cray compiler
Time in seconds
Number of threads
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
0
100
200
300
400
500
600
700
800
900
1000
1100

Multi-GPU code

```
        ⋮
         ap_loc ← 0
!$ACC  parallel loop present(u,ud,ap_loc,p,iup,idn)
      do  l = base+1, base+nvd2
        v1 = ap_loc(1,l-base)
        ⋮
```

Lines identical to scalar version

```
        ⋮
        ap_loc(3,l-base) = v3
      enddo
!$ACC update host(ap_loc)
      call MPI_ALLGATHER(ap_loc,3*nvd2,MPI_DOUBLE_COMPLEX,
     +           ap,3*nvd2,MPI_DOUBLE_COMPLEX,MPI_COMM_WORLD,ierr)
!$ACC  update device (ap)
```

Worry about async compiler options.

Summary

- Coding effort is only marginally higher than OpenMP. Almost each OpenMP directive can be replaced with a OpenACC directive. Only additional directive is the creation of a data region with a list of variables (scalars + arrays) so that the compiler knows which variables to copy to the GPU and back again.
  One data structure I haven't explored is `deviceptr`.

- Performance of single GPU staggered fermion code is roughly equivalent to 128 cores of cluster with QDR infiniband interconnect.

- Performance of single GPU Wilson fermion code is roughly equivalent to 96 cores. About 30% difference in performance between hand coded CUDA and OpenACC code.

- GPU with 6GB memory fits in a 32^4 Wilson fermion lattice or a 10×40^3 staggered fermion lattice.

- Real gain comes only when the whole conjugate gradient routine is on the GPU.

- Extremely useful if one does not have access to conventional supercomputers.

- For Multi-GPU programs MPI calls on the Fermi GPUs can only be made from the CPU so every MPI call involves a data transfer from the GPU to CPU and back. Each such copy adds a significant ($\sim$ 15%) overhead to the runtime. For

Kepler GPUs the construct host_data use_device cuts this down to a certain extent.

- Further performance gains can be obtained by using mixed-precision routines and improved storage schemes.

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