May 3, 2013

BLUE WATERS

SUSTAINED PETASCALE COMPUTING

OpenACC compiling and performance tips

GREAT LAKES CONSORTIUM FOR PETASCALE COMPUTATION

OpenACC compiler support

Cray

Module load PrgEnv-cray craype-accel-nvidia35

- Fortran
  - -h acc, noomp # openmp is enabled by default, be careful mixing
  - -fpic -dynamic
  - -rm # include a .lst listing file to show the loop markup
  - -G2 # -g has been observed to break Cray OpenACC code
- C
  - -h pragma=acc -h nopragma=omp
  - -fpic -dynamic
  - -h msgs # show loop markup in stdout/stderr
  - -Gp # bonus points to the person who synchronizes Cray compiler flags between fortran and c...

Cray -rm # loop mark

```
arnoldg@h2ologin2:~/Mori/pic2.0-acc-f> ftn -h acc -rm -c push2.f

!$acc parallel num_gangs(1) vector_length(3072)
ftn-7271 crayftn: WARNING GPUSH2L, File = push2.f, Line = 145
  Unsupported OpenACC vector_length expression: Converting 3072 to 1024.

arnoldg@h2ologin2:~/Mori/pic2.0-acc-f> grep --after-context=5 '!$acc parallel num_gangs(1)
vector_length(3072)' push2.lst
  145.  + G----------< !$acc parallel num_gangs(1) vector_length(3072)
ftn-7271 ftn: WARNING File = push2.f, Line = 145
  Unsupported OpenACC vector_length expression: Converting 3072 to 1024.

  146.    G            !!$acc kernels
  147.    G            !!data copy(part),copyin(fxy),create(nn,mm,dxp,dyp,np,mp,dx,dy,vx,vy)
arnoldg@h2ologin2:~/Mori/pic2.0-acc-f> grep 'line 145 ' push2.lst
  A region starting at line 145 and ending at line 240 was placed on the accelerator.

arnoldg@h2ologin2:~/Mori/pic2.0-acc-f>
```

OpenACC compiler support

PGI

Module load PrgEnv-pgi cudatoolkit

- Cudatoolkit is required, PGI is creating CUDA code as intermediate
  - -ta=nvidia,keepgpu,keepptx
- Fortran , C # nice
  - -acc -ta=nvidia
  - -mcmodel=medium
  - -Minfo=accel

GNU

- Don't touch that dial!

PGI -Minfo=accel

```
arnoldg@h2ologin2:~/Mori/pic2.0-acc-f> ftn -acc -ta=nvidia -Minfo=accel -c push2.f
gpush2l:
    145, Accelerator kernel generated
        145, CC 1.3 : 18 registers; 112 shared, 32 constant, 0 local memory bytes
             CC 2.0 : 26 registers; 0 shared, 132 constant, 0 local memory bytes
        148, !$acc loop vector(3072) ! blockidx%x threadidx%x
        169, Sum reduction generated for sum1
    145, Generating present_or_copy(part(:4,:nop))
         Generating present_or_copyin(fxy(:,:,:))
         Generating compute capability 1.3 binary
         Generating compute capability 2.0 binary
    148, Loop is parallelizable
```

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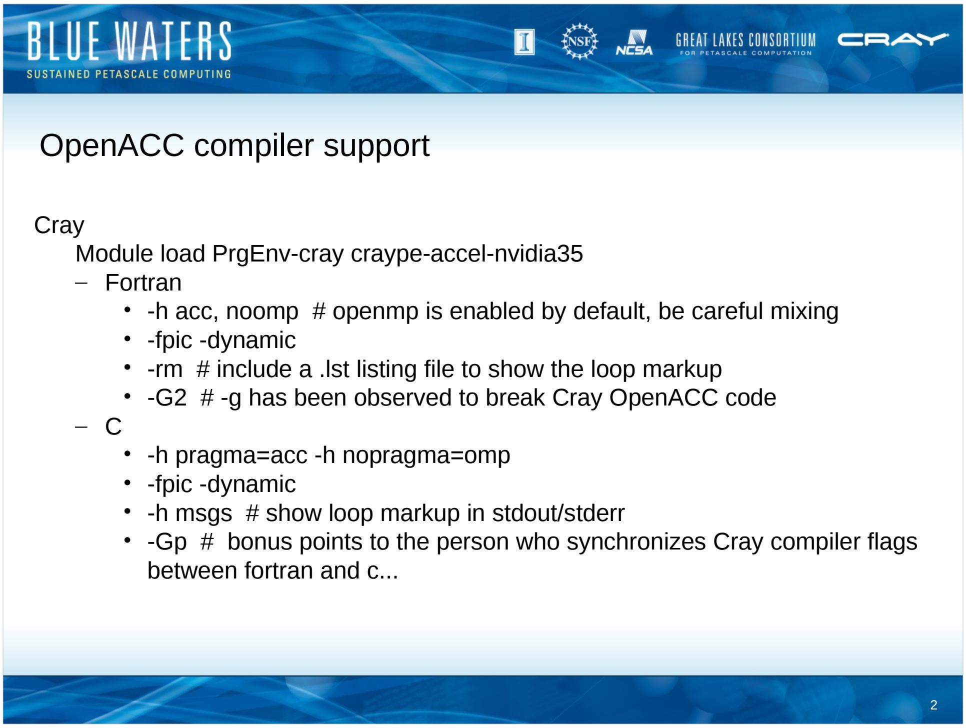

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  - -Gp # bonus points to the person who synchronizes Cray compiler flags between fortran and c...

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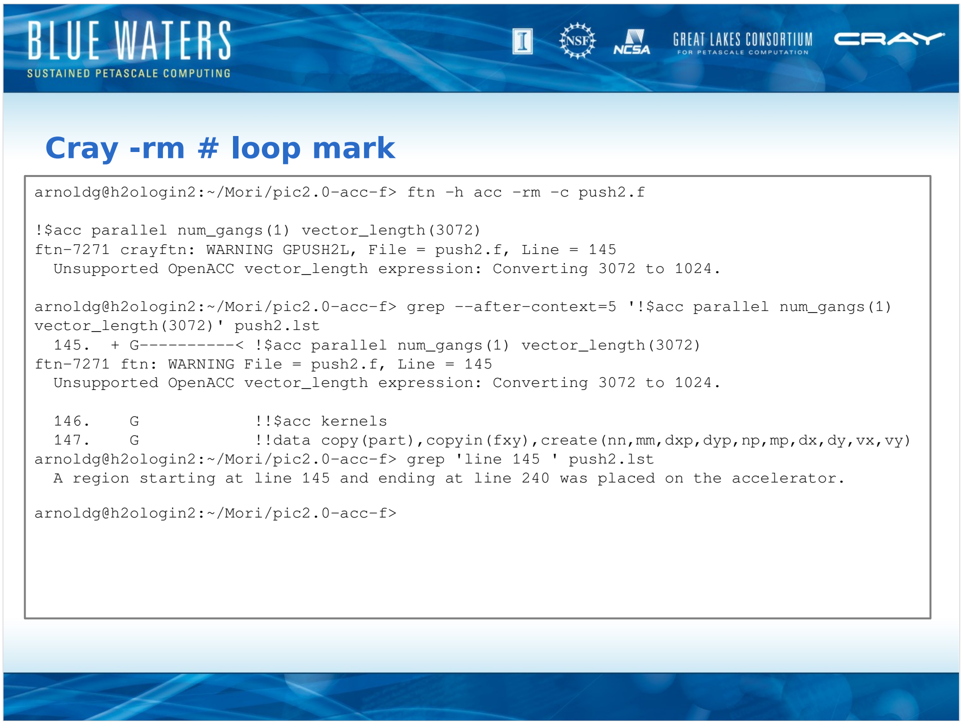
Watch out for the differences in flags when using the Cray compiler environment.

Omitting craype-accel-nvidia35 can result in silent failure mode:

```
  ftn -h acc -c myfile.c
  ...
  ldd a.out
          not a dynamic executable
```

...you've made an executable that will not use the accelerator at runtime, but the code will probably run .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Cray -rm # loop mark

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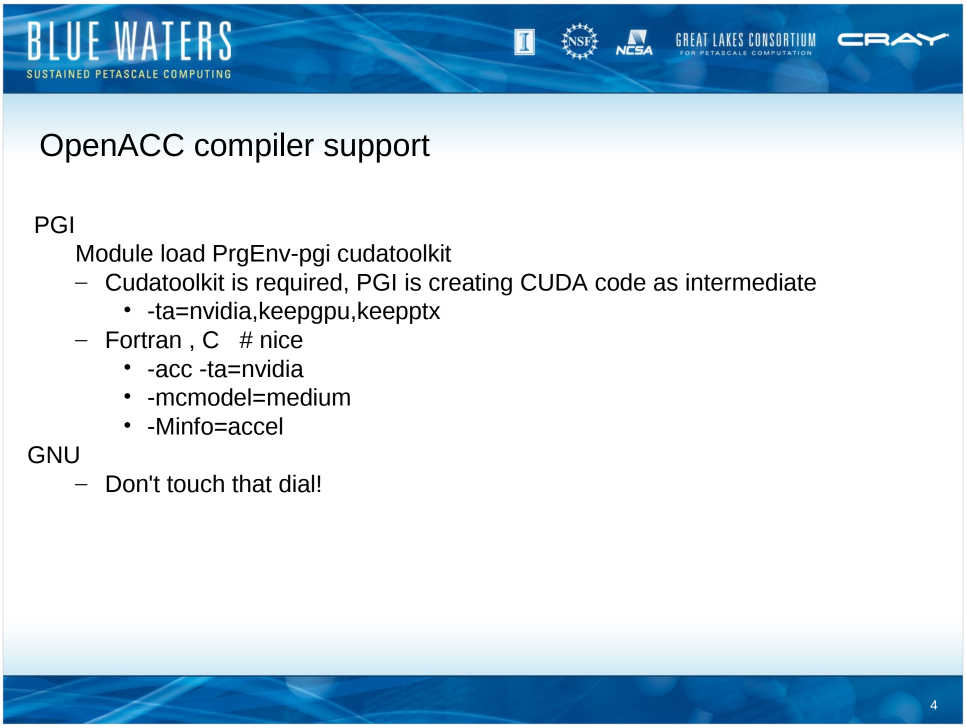
arnoldg@h2ologin2:~/Mori/pic2.0-acc-f>
```

Cray loop mark .lst listings are a good source of information about how the compiler optimized (or could not optimize) your code. Along with basic profiling info, this is a good starting point for code optimization.



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- Fortran , C   # nice
  - -acc -ta=nvidia
  - -mcmodel=medium
  - -Minfo=accel

GNU

- Don't touch that dial!

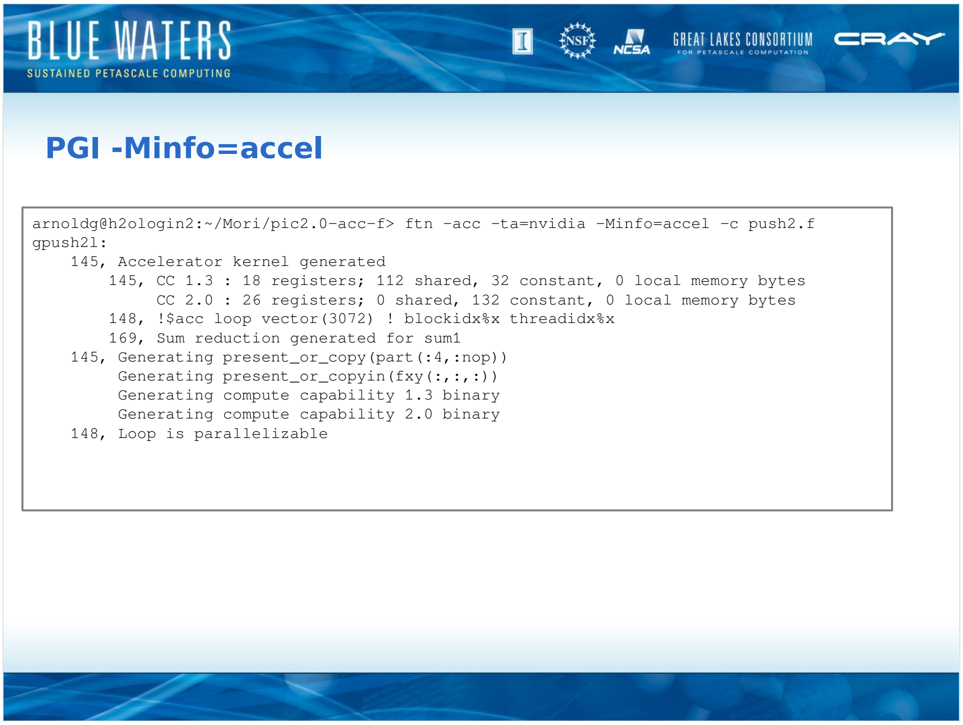
Omitting the cudatoolkit module will result in silent failure mode (program compiles and links with possibly just a warning):

```
/opt/pgi/12.10.0/linux86-64/12.10/lib/libacc1mp.a(nvinitx.o): In function `__pgi_cu_init_y':
/usr/pgrel/extract/x86/2012/rte/accel/hammer/lib-linux86-64mp/../src-nv/nvinitx.c:238: warning: Using 'dlopen' in statically linked applications requires at runtime the shared libraries from the glibc version used for linking
```

Keepgpu and keepptx will preserve the intermediate cuda and/or Nvidia ptx assembly files. This is in contrast to the Cray compiler that compiles directly to ptx assembly and creates no intermediate cuda source.

mcmodel=medium allows for larger static memory (> 2 GB)

GNU may pickup OpenACC support once it becomes part of a future OpenMP standard.



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PGI -Minfo=accel

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         Generating compute capability 1.3 binary
         Generating compute capability 2.0 binary
    148, Loop is parallelizable
```

Similar to the Cray loopmark report, PGI compilers can emit detailed information about optimizations. -Minfo=accel will add comments for each OpenACC directive found and what was done (or not done) with that code region.