

Course Objective:

Enable you to scale your applications on multiple GPUs and optimize with profiler tools

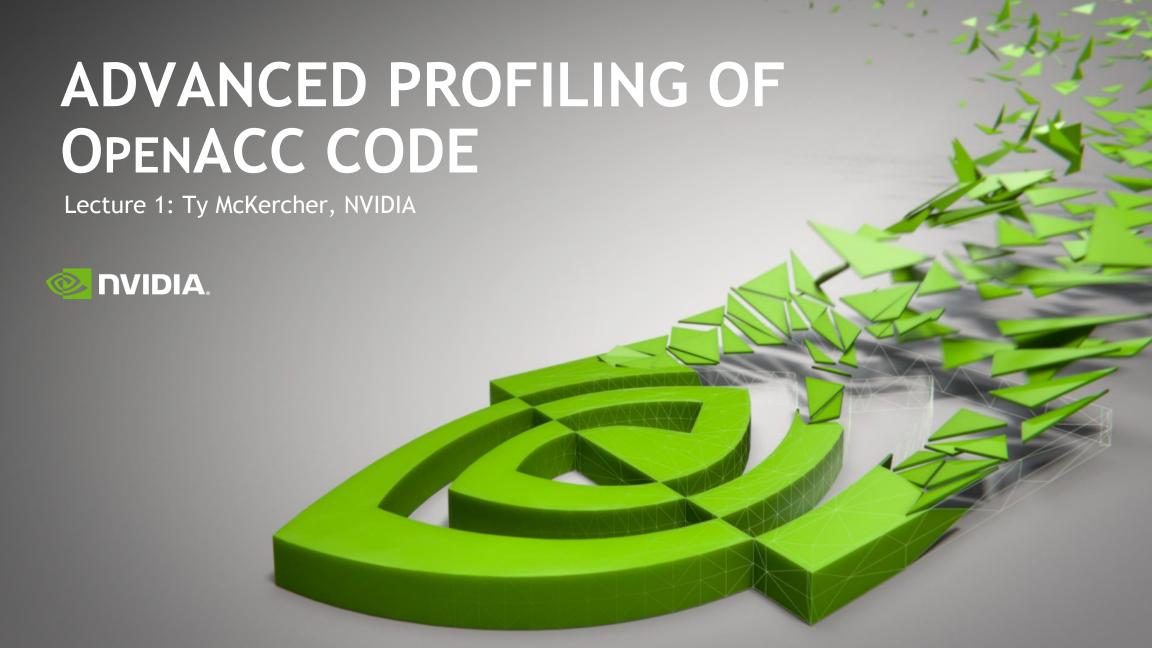
Course Syllabus

May 19: Advanced Profiling of OpenACC Code

May 26: Office Hours

June 2: Advanced multi-GPU Programming with MPI and OpenACC

June 9: Office Hours



3 WAYS TO ACCELERATE APPLICATIONS

Applications

Libraries

OpenACC Directives

Programming Languages

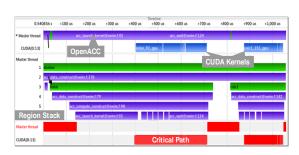
"Drop-in"
Acceleration

Easily Accelerate Applications

Maximum Flexibility

OPENACC PROFILING TOOLS

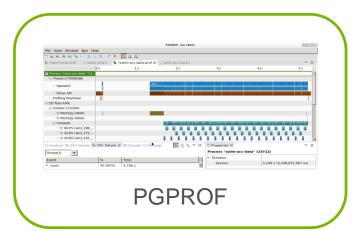


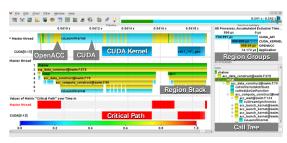


Score-P



TAU





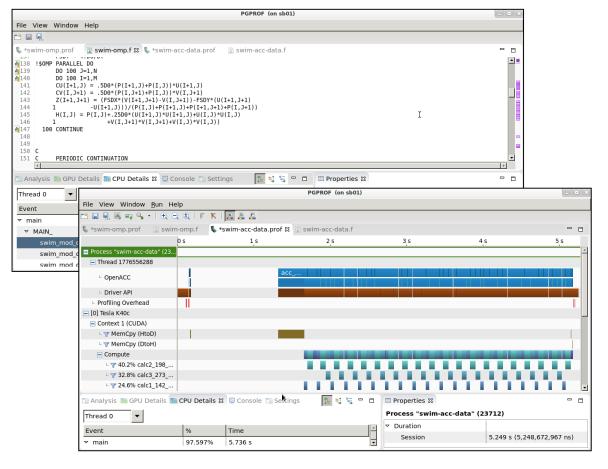
Vampir

The OpenACC profiling interface lets us easily measure and investigate implicit operations introduced by the compiler or runtime. Implementation was straightforward and basically worked out of the box.

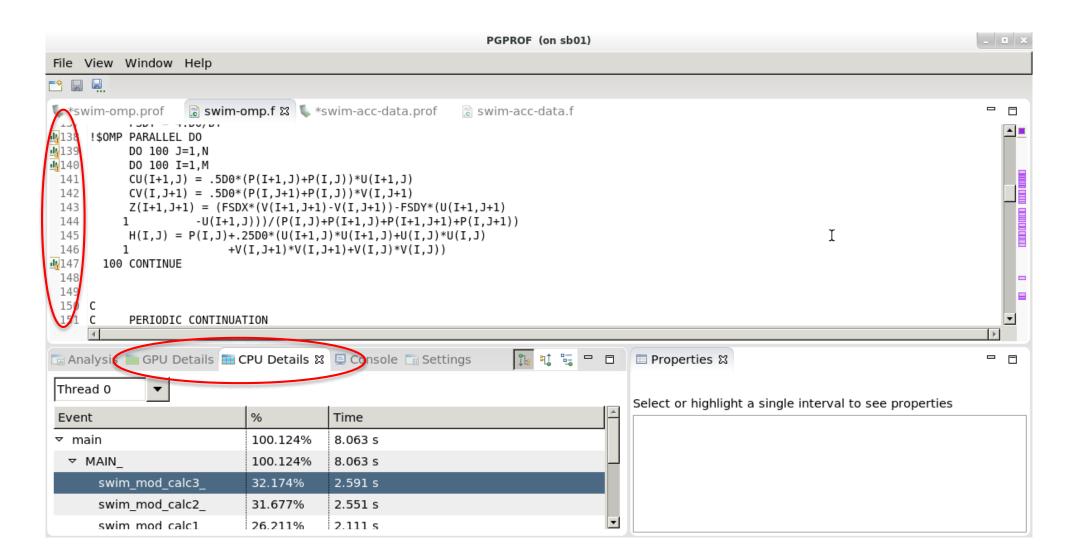
Dipl.-Ing. Robert Dietrich, T-U Dresden

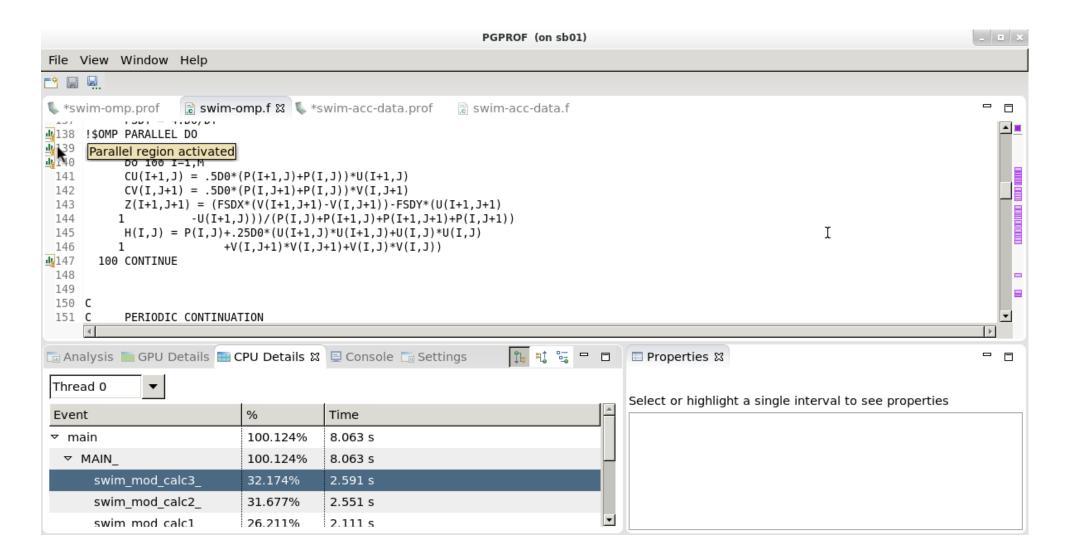
PGPROF: OPENACC CPU AND GPU PROFILER

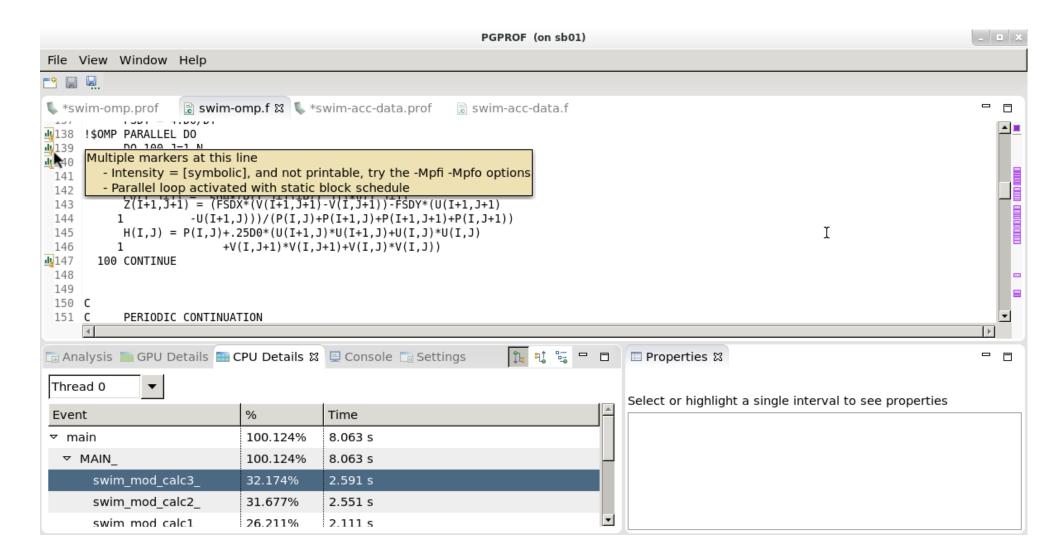
Available with the latest OpenACC Toolkit

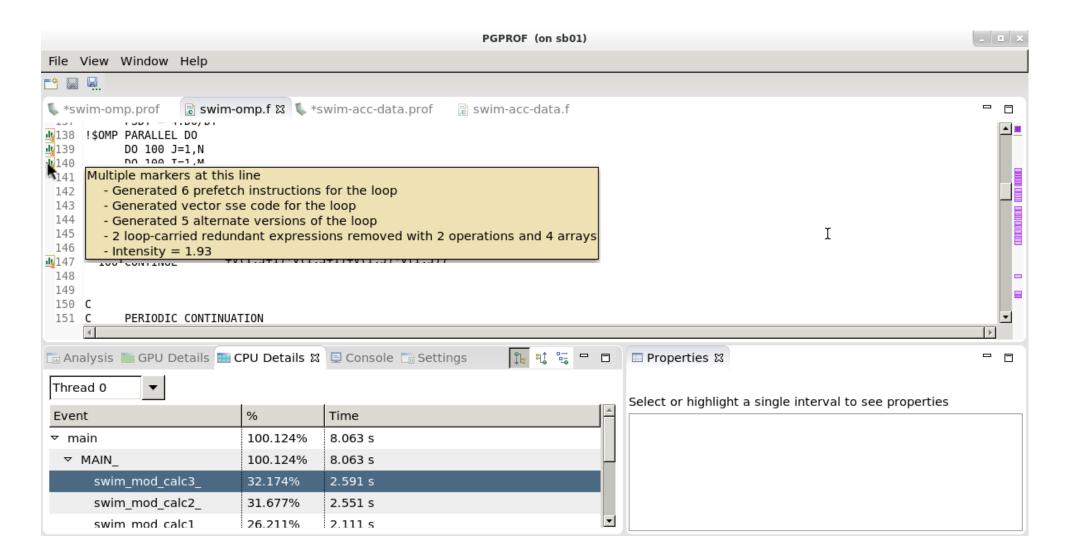


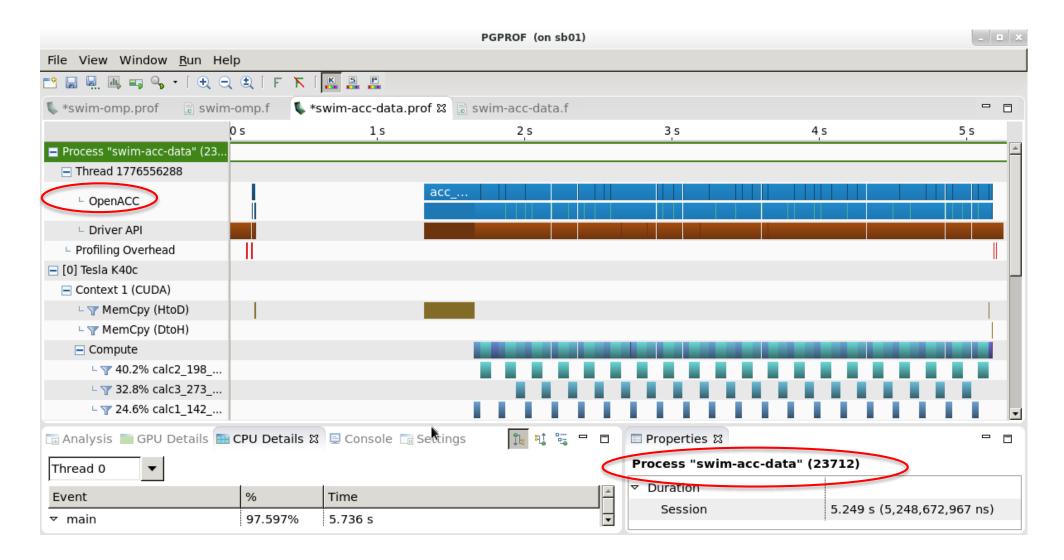
- For 64-bit multicore processor-based systems with or without accelerators
- Supports thread-level OpenMP profiling
- Supports profiling OpenACC and CUDA Fortran codes on NVIDIA CUDA-enabled GPU accelerators
- Graphical and command-line user interfaces
- Function level (routine) and source code line level profiling
- Comprehensive built-in help facilities











More on Visual Profiler Office Hour on May 26th

PGPROF Quick Start Guide: http://www.pgroup.com/resources/pgprof-quickstart.htm

PGPROF User's Guide*: http://www.pgroup.com/doc/pgprofug.pdf

Agenda

Profiling application - Getting Started

Acceleration with Managed Memory

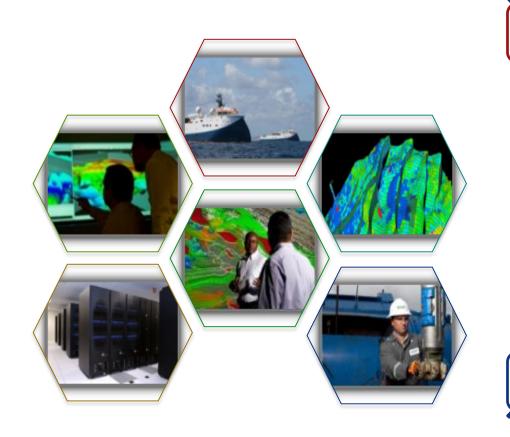
Optimization with Data Directives

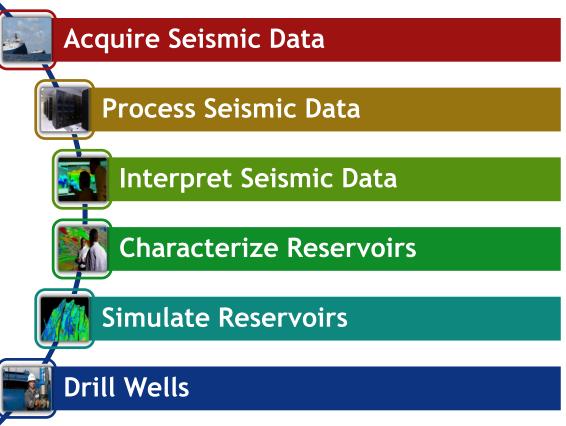
Multicore comparison

Seismic Unix Configuration

Profiling Application - Getting Started

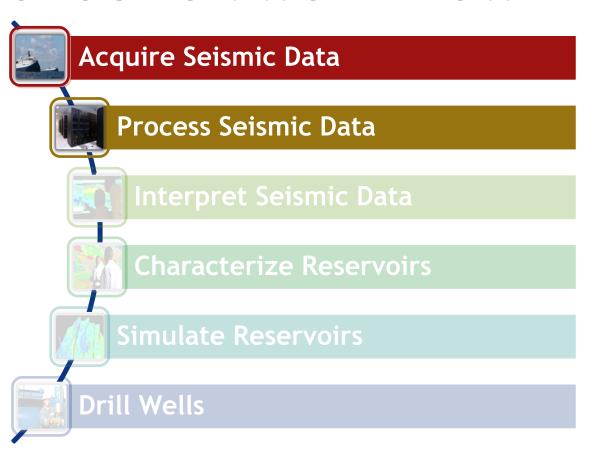
EXPLORATION & PRODUCTION WORKFLOW



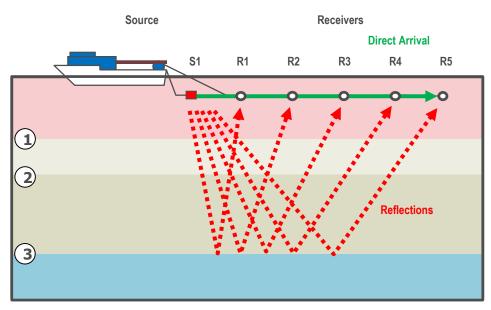


EXPLORATION & PRODUCTION WORKFLOW



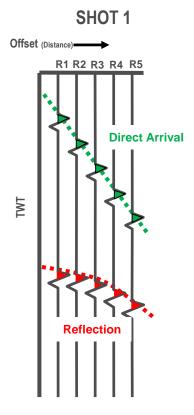


ACQUIRE SEISMIC DATA



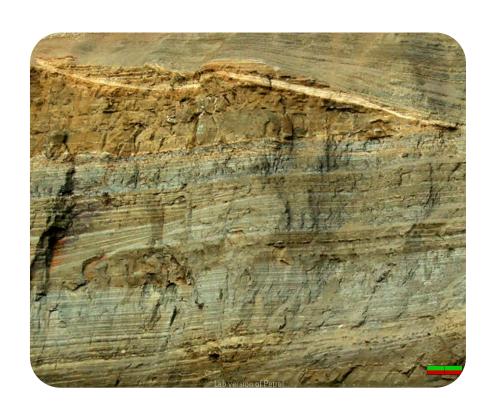
For each shot, reflections are recorded in 5 receivers

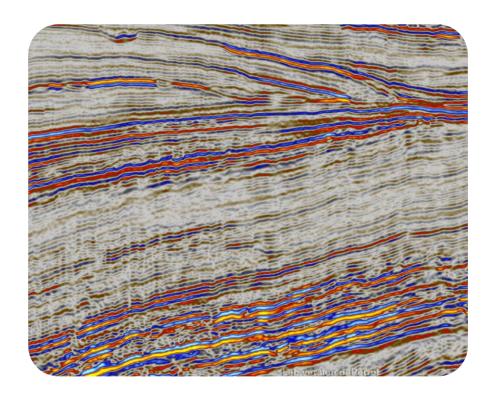
There are 5 'bounce' points along interface 3



REAL ROCK VS SEISMIC REFLECTION

Imaging, signal processing, filtering, ray tracing

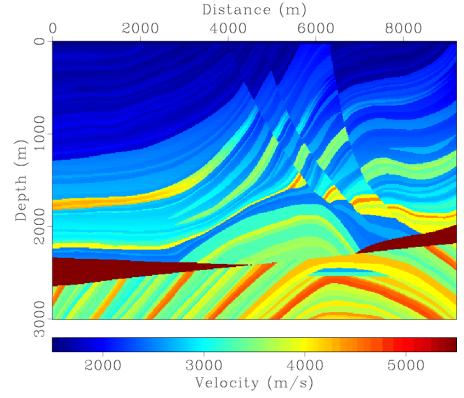




USE KNOWN MODEL

Verify accuracy of imaging algorithms

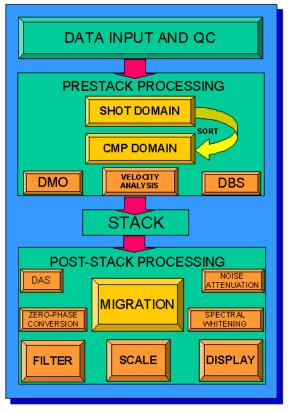
- Industry standard dataset
- Compare against known truth
- Refine seismic algorithms
- Improve confidence in drilling decisions



PROCESS SEISMIC DATA

Open Source Seismic*Unix Package

Typical Seismic Processing Flow



- Iterative process
 - Can take several months
- Migration most time consuming
 - Collapse diffractions
 - Correctly position dip events
- Trusted tool: Kirchhoff Migration

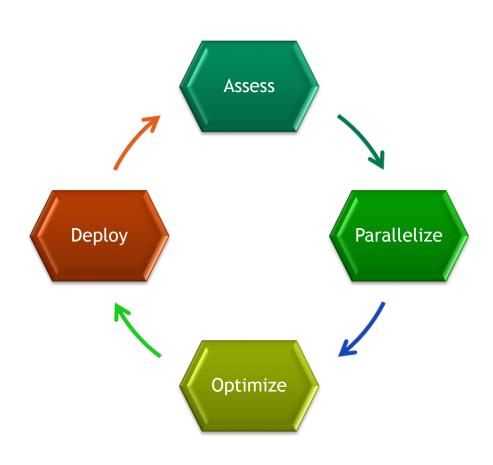
PSEUDO-CODE FOR KIRCHHOFF MIGRATION

sukdmig2d

- Update residual travel times
- Loop over traces
 - Combine travel times (sum2)
 - Migrate trace (mig2d)
 - Low-pass filter trace
 - Compute amplitudes
 - Interpolate along lateral
 - Interpolate along depth
- Write output

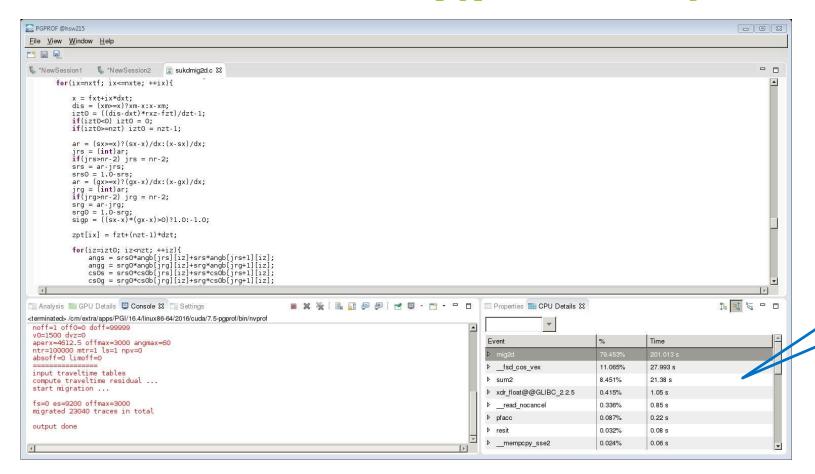
```
main() {
  resit();
  do {
    sum2(...,ttab, tt);
    sum2(...,tsum, tsum);
    mig2d(..., mig, ..., mig1, ...);
  } while (fget(tr) && jtr<ntr);</pre>
  fput(tr);
```

HOW YOU ACCELERATE CODE WITH GPUS



ASSESS BASELINE CPU PROFILE

Use pgprof sukdmig2d



Function	Percent Runtime
mig2d	79 %
sum2	8.5 %
resit	< 1%

RESULTS

SUKDMIG2D	Configuration	Model Size	Cores	Elapsed Time (s)	Speed up
CPU Only (Baseline)	2x E5-2698 v3 2.30GHz	2301 x 751	1	218	1.00



PARALLELIZE

Parallel Directives

#pragma
Parallelize for loops

Vectorize

Compiler vectorizes inner loops

PARALLELIZE

Parallel Directives

restrict on pointers!
limits aliasing
www.wikipedia.org/wiki/Restrict

#pragma

Parallelize outer for loops

Compiler parallelizes inner loop

```
void sum2(int nx, int nz,float a1,float a2,
  float ** restrict t1, float ** restrict t2, float **
restrict t)
{
  int ix,iz;

  #pragma acc parallel for
  for(ix=0; ix < nx; ++ix)
  {
    for(iz=0; iz < nz; ++iz)
       t[ix][iz] = a1*t1[ix][iz]+a2*t2[ix][iz];
  }
}</pre>
```

PARALLELIZE

Resolve Errors!

Parallel Directives

#pragma
Parallelize for outer loop

Parallelize inner loops

Resolve loop carried depend

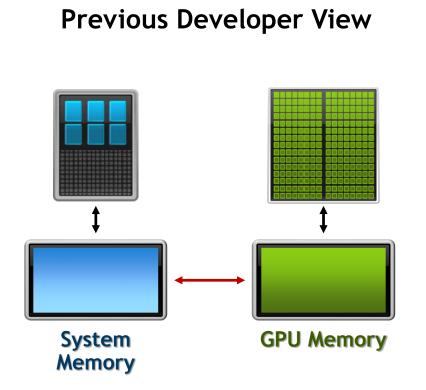
Add acc loop directive

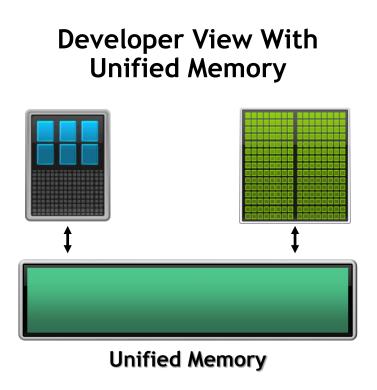
```
Resit (managed):

537, Accelerator kernel generated
Generating Tesla code
538, #pragma acc loop gang /* blockIdx.x */
553, #pragma acc loop vector(128) /* threadIdx.x */

540, Loop carried dependence of t->-> prevents parallelization
Loop carried backward dependence of t->-> prevents vector
```

UNIFIED MEMORY IMPROVES PRODUCTIVITY





OPENACC AND UNIFIED MEMORY

All heap allocations are in managed memory (Unified Memory Heap)

Pointers can be used on GPU and CPU

Enabled with compiler switch -ta=tesla:managed,...

More Info at "OpenACC and CUDA Unified Memory", by Michael Wolfe, PGI Compiler Engineer: https://www.pgroup.com/lit/articles/insider/v6n2a4.htm



OPENACC AND UNIFIED MEMORY

Advantages

No need for any data clauses

No need to fully understand application data flow and allocation logic

Incremental profiler-driven acceleration possible

Outlook to GPU programming on Pascal

RESULTS

SUKDMIG2D	Configuration	Model Size	Cores	Elapsed Time (s)	Speed up
CPU Only (Baseline)	2x E5-2698 v3 2.30GHz	2301 x 751	1	218	1.00
OpenACC (Managed)	1x K40 GPU	2301 x 751	2880	46	4.70

RESULTS

SUKDMIG2D	Configuration	Model Size	Cores	Elapsed Time (s)	Speed up
CPU Only (Baseline)	2x E5-2698 v3 2.30GHz	2301 x 751	1	218	1.00
OpenACC (Managed)	1x K40 GPU	2301 x 751	2880	46	4.70

Now optimize using the Verbose output from compiler!



OPTIMIZATION

Compile

```
pgcc -acc \
  -ta=tesla:managed
```

Profile!

pgprof <managed binary>

```
==55246== Profiling result:
            Time
                     Calls
                                Avg
                                          Min
Time (%)
                                                    Max Name
                       23040
 42.82%
         4.03645s
                              175.19us
                                        121.12us
                                                   196.38us
                                                             mig2d 787 gpu
 28.79%
         2.71389s
                       23040
                              117.79us
                                        80.800us
                                                  135.68us
                                                             mig2d 726 gpu
                              37.291us
         2.57762s
                                       33.248us
                                                  42.240us
                                                             sum2 571 gpu
 1.00%
        93.936ms
                                    3.2000us 12.992us
                                                        [CUDA memcpy HtoD]
 0.04% 3.4627ms
                           3.4627ms
                                     3.4627ms
                                              3.4627ms
                                                         resit 537 gpu
 0.00%
       126.14us
                         1 126.14us 126.14us 126.14us
                                                         timeb 592 gpu
==55246== API calls:
Time(%)
            Time
                     Calls
                                 Ava
                                          Min
                                                    Max Name
 30.16%
         11.5982s
                     230423
                             50.334us
                                            118ns
                                                   3.9101ms
                                                              cuMemFree
 29.21% 11.2327s
                     230429
                             48.746us
                                        10.132us
                                                  12.821ms
                                                             cuMemAllocManaged
 27.15%
         10.4430s
                     253444
                             41.204us
                                        1.0420us
                                                   3.4680ms
                                                             cuStreamSynchronize
 10.42%
         4.00751s
                     115202
                                        5.4290us
                              34.786118
                                                   99.805ms
                                                              cuLaunchKernel
         433.50ms
                                 303ns
                                                  429.42118
  1.13%
                     1428513
                                            141ns
                                                              cuPointerGetAttrib
  0.81%
         310.55ms
                              310.55 \text{ms}
                                        310.55 \text{ms}
                                                  310.55ms
                                                             cuDevicePrimary...
         273.10ms
                       23040 11.853us
                                        7.3210us
                                                   409.13us
                                                              cuMemcpyHtoDAsync
         125.36ms
                           1 125.36ms
                                        125.36ms
  0.33%
                                                  125.36ms
                                                             cuDevicePrimary...
  0.06%
         24.165ms
                              24.165ms
                                        24.165ms
                                                  24.165ms
                                                             cuMemHostAlloc...
  0.02%
         9.5668ms
                                        9.5668ms
                                                  9.5668ms
                           1 9.5668ms
                                                              cuMemFreeHost.
  0.00%
         534.34us
                           1 534.34us
                                        534.34us
                                                   534.34us
                                                              cuMemAllocHost
  0.00%
         461.71us
                              461.71118
                                        461.71118
                                                  461.71118
                                                             cuModuleLoad..
  0.00%
         363.83us
                             181.91us
                                        180.02us
                                                  183.81us
                                                             cuMemAlloc
```

Managed Compile

Verbose output Guided enhancements Targeted changes

Common Optimizations

Data Movement Copy, copyin, copyout Create, delete Update

Loop Collapse

```
main:
 453, Generating update host(mig[:noff][:nxo][:nzo])
 455, Generating update host(mig1[:noff][:1][:1])
 459, Generating update host(mig1[:noff][:nxo][:nzo])
resit:
 539, Generating copyin(ttab[:ns],tb[:][:nz])
sum2:
 571, Generating copyin(t2[:nx][:nz],t1[:nx][:nz])
      Generating copyout(t[:nx][:nz])
mig2d:
 721, Generating copy(ampt1[nxtf:nxte-nxtf+1][:])
     Generating copyin(cssum[nxtf:nxte-nxtf+1][:],tvsum[nxtf:nxte-nxtf+1][
     Generating copy(tmt[nxtf:nxte-nxtf+1][:],ampti[nxtf:nxte-nxtf+1][:])
     Generating copyin(pb[:][:])
     Generating copy(ampt[nxtf:nxte-nxtf+1][:])
     Generating copyin(cs0b[:][:],angb[:][:])
     Generating copy(zpt[nxtf:nxte-nxtf+1])
 782, Generating copy(mig1[nxf:nxe-nxf+1][:])
     Generating copyin(ampt1[:][:], tb[:][:], tsum[:][:], ampt[:][:], ...
     Generating copy(mig[nxf:nxe-nxf+1][:])
     Generating copyin(zpt[:])
```

Data Movement

Analyze data flow in application Explicitly use data directives

Move data directive to main

Create only when possible

Copyin move data to GPU

Update to move data to host

```
main:
#pragma acc enter data create(tb,pb,cs0b,ang0)
#pragma acc enter data create(tt,tsum)
#pragma acc enter data copyin(mig, ttab)

#pragma acc enter data create(tvsum,csum )
#pragma acc enter data copyin(cs, tv)
#pragma acc enter data copyin(mig1)

After processing:

#pragma acc update host(mig)
#pragma acc update host(mig1)
```

Data Movement

Explicitly use present for data already on GPU!

Collapse

Increase the threads nx*nz

Present

Data is already on the GPU Prevent data movement

```
sum2: (managed)
571, Generating copyin(t2[:nx][:nz],t1[:nx][:nz])
    Generating copyout(t[:nx][:nz])
```

```
void sum2(int nx, int nz,float a1,float a2,
  float ** restrict t1, float ** restrict t2, float **
restrict t)
{
  int ix,iz;

  #pragma acc parallel for collapse(2) present(t1,t2,t)
  for(ix=0; ix < nx; ++ix)
  {
    for(iz=0; iz < nz; ++iz)
       t[ix][iz] = a1*t1[ix][iz]+a2*t2[ix][iz];
  }
}</pre>
```

Data Movement

Move large data transfers to main i.e. mig, mig1

Minimize Copyin, Copyout

Maximize Create, Present Prevents data transfers

Use Copyin, Copyout, Copy only when data changes!

Delete happens when leaving scope

```
mig2d:
721, Generating copy(ampt1[nxtf:nxte-nxtf+1][:])
    Generating copyin(cssum[nxtf:nxte-nxtf+1][:],tvsum[...
    Generating copy(tmt[nxtf:nxte-nxtf+1][:],ampti[...
    Generating copyin(pb[:][:])
    Generating copy(ampt[nxtf:nxte-nxtf+1][:])
    Generating copyin(cs0b[:][:],angb[:][:])
    Generating copy(zpt[nxtf:nxte-nxtf+1])
782, Generating copy(mig1[nxf:nxe-nxf+1][:])
    Generating copyin(ampt1[:][:], tb[:][:], tsum[:][:], ...
    Generating copy(mig[nxf:nxe-nxf+1][:])
```

```
void mig2d(float * restrict trace, int nt, float ft,...)
{
...
#pragma acc data
  copyin(trace[0:nz],trf[0:nt+2*mtmax]) \
  present(mig, mig1, tb,tsum,tvsum,cssum,pb,... \
  create(tmt[0:nxt][0:nzt], ampt[0:nxt][0:nzt],...
  {
```

Data Movement

Use present for data already on GPU!

Collapse

Increase the threads nx*ns

Present

Data is already on the GPU Prevent data movement

```
Resit: (managed)
539, Generating copyin(ttab[:ns],tb[:][:nz])
```

Data Movement

mig, mig1 data large

Move to main

Copyin at start

Mark as present

Copyout for snapshots

Minimize Copyin, Copyout

Use create Prevents copy in/out

Delete happens when leaving scope

```
void mig2d(float * restrict trace, int nt, float
ft,...)
#pragma acc data
  copyin(trace[0:nz],trf[0:nt+2*mtmax]) \
  present(mig, mig1, tb,tsum,tvsum,cssum,pb,... \
  create(tmt[0:nxt][0:nzt], ampt[0:nxt][0:nzt],...
   #pragma acc parallel for
   for (ix=nxtf; ix <= nxte; ++ix) {</pre>
      #pragma acc loop
      for (iz=izt0; iz < nzt; ++iz) {</pre>
```

Compile

pgcc -acc -ta=tesla

Profile

pgprof <tesla binary>

mig2d and sum2 about the same.

- cuAllocManged (11s) removed.
- cuMemFree (11.5s) reduced to milliseconds.

```
==2242== Profiling result:
Time(%)
             Time
                      Calls
                                             Min
                                                       Max
                                                            Name
                                   Avq
 41.54% 3.95071s
                                      118.88us
                                                 192.61us
                                                            mig2d 787 gpu
                             171.47us
                      23040
 27.91% 2.65415s
                                       78.241us
                                                  133.09us
                                                            mig2d 726 gpu
                             115.20us
 26.27%
        2.49826s
                             36.143us
                                       32.768us
                                                  40.416us
                                                            sum2 569 gpu
                                                             pgi uacc cuda fill 32 gpu
  2.88%
         274.19ms
                              3.9660us
                                       3.5520us
                                                  13.120us
        128.68ms
                             2.7920us
                                       2.4960us
                                                  1.6815ms
                                                            [CUDA memcpy HtoD]
                                                            resit 535 qpu
  0.04%
        3.4187ms
                             3.4187ms
                                       3.4187ms
                                                  3.4187ms
         226.15us
                                                  223.68us
                                                             [CUDA memcpy DtoH]
 0.00%
                             113.07us
                                       2.4640us
  0.00% 123.43us
                             123.43us 123.43us
                                                 123.43us
                                                            timeb 592 gpu
==2242== API calls:
Time (%)
             Time
                      Calls
                                             Min
                                                       Max
                                                            Name
                                   Ava
         9.71880s
                                       1.8870us
                                                  3.4228ms
                                                            cuStreamSynchronize
 85.89%
                             70.300us
        869.62ms
  7.69%
                                                  452.72us
                                                            cuLaunchKernel
                              4.7170us
                                       3.4420us
                                                            cuDevicePrimaryCtxRetain
  2.94%
         333.00ms
                             333.00ms
                                       333.00ms
                                                  333.00ms
                             4.2870us
                                       2.8370us
                                                  426.78us
        197.59ms
                                                            cuMemcpyHtoDAsync
        130.58ms
                             130.58ms
                                       130.58ms
                                                  130.58 \text{ms}
                                                            cuDevicePrimaryCtxRelease
         28.337ms
                             28.337ms
                                       28.337ms
                                                  28.337ms
                                                            cuMemHostAlloc
        23.059ms
                                 500ns
                                           260ns
                                                 11.292118
                                                            cuPointerGetAttributes
  0.20%
                      46084
                                      10.027ms
  0.09%
        10.027ms
                             10.027 \text{ms}
                                                 10.027ms
                                                            cuMemFreeHost.
 0.03% 2.9512ms
                             95.199us
                                      2.9220us
                                                  300.63us
                                                            cuMemAlloc
 0.01% 806.38us
                                      188.55us
                             403.19us
                                                  617.83us
                                                            cuModuleLoadData
```

RESULTS

SUKDMIG2D	Configuration	Model Size	Cores	Elapsed Time (s)	Speed up
CPU Only (Baseline)	2x E5-2698 v3 2.30GHz	2301 x 751	1	218	1.00
OpenACC (GPU Managed)	1x K40 GPU	2301 x 751	2880	46	4.70
OpenACC (GPU Native)	1x K40 GPU	2301 x 751	2880	12	15.60

Multicore Comparison

How about Multi-Core / OMP / pthread?

Done!

Re-Compile

```
pgcc -acc -ta=multicore
```

Profile!

```
pgprof
  --cpu-profiling on \
  --cpu-profiling-scope function \
  --cpu-profiling-mode top-down \
  <app> <args>
```

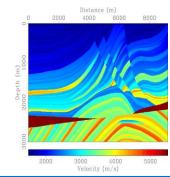
```
====== CPU profiling result (top down):
72.91% main
 69.84% mig2d
   43.19% pgi acc barrier
    | 43.19% mp barrier tw
       0.02% mp pcpu_get_team_lcpu
         0.02% mp pcpu struct
            0.01% tls get addr
    0.12% malloc@@GLIBC 2.2.5
   2.79% pgi acc barrier
    | 2.79% mp barrier tw
    0.00% .ACCENTER
     0.00% mp barrierr
  0.10% fsd cos vex
  0.05% pgi acc pexit
    0.05% mp cpexit
      0.05% mp barrierw
22.18% mp slave
 22.18% mp cslave
    22.18% mp barrier_tw
     0.02% mp pcpu yield
       0.02% sched vield
4.77% fsd cos vex
0.09% <u>Filt</u>
-- more --
```

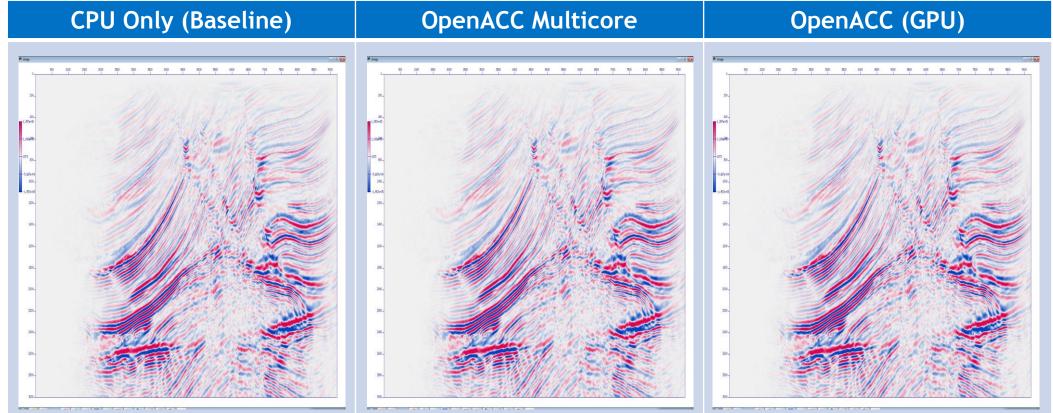
RESULTS

SUKDMIG2D	Configuration	Model Size	Cores	Elapsed Time (s)	Speed up
CPU Only (Baseline)	2x E5-2698 v3 2.30GHz	2301 x 751	1	218	1.00
OpenACC CPU (Multicore)	2x E5-2698 v3 2.30GHz	2301 x 751	16	29	7.50
OpenACC GPU (Managed)	1x K40 GPU	2301 x 751	2880	46	4.70
OpenACC GPU (Native)	1x K40 GPU	2301 x 751	2880	12	15.60

DEPLOY

How do the results compare?





Homework

QWIKLABS: GETTING ACCESS

- 1. Go to https://developer.nvidia.com/qwiklabs-signup
- 2. Register with OpenACC promo code to get free access
- 3. Receive a confirmation email with access instructions

Questions?

Email to openacc@nvidia.com

ACCESS TO HOMEWORK

Qwiklab:

Profile-driven approach to accelerate Seismic application with OpenACC

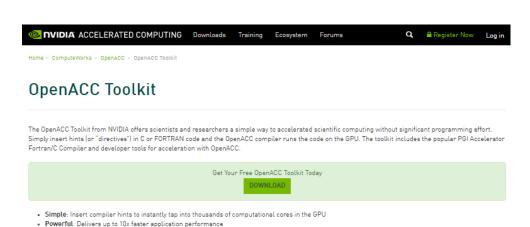
Link: http://bit.ly/oaccnvlab6

Requirements: OpenACC Compiler and CUDA-aware MPI

Link to the source code on github thorough the qwiklab if you want to try it on your machine

INSTALL THE OPENACC TOOLKIT (OPTIONAL)

- Go to developer.nvidia.com/openacctoolkit
- Register for the OpenACC Toolkit
- Install on your personal machine (Linux Only)
- Free workstation license for academia/90 day free trial for the rest



OpenACC Toolkit Features

The toolkit includes a complete set of developer tools designed to provide significant application acceleration with a minimum amount of coding. It features the PGI Accelerator Fortran/C Workstation Compiler Suite for Linux, which supports OpenACC 2.0. The compiler is available at no cost for academia. Non-academic developers will receive a free 90-day trial.

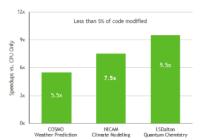
. Free: The OpenACC Toolkit with compiler included is available at no charge for academia*

Other tools include:

- GPU Wizard to identify if GPU-accelerated libraries can accelerate portions of code without any additional programming
- PGProf Profiler to easily find where to add OpenACC directives to further increase performance
- OpenACC Code Samples to get started with simple and real-world examples
- Documentation including OpenACC Best Practices Guide for maximizing application performance

Every registered toolkit user also receives two free 90-minute, on-demand training sessions to quickly learn and master OpenACC techniques.

Application Acceleration



LS-DALTON: Benchmark on Oak Ridge Titan Supercomputer, AMD CPU vs Tesla K20X GPU. Test input: Alanine-3 on CCSDIT module.

OSSIO: additional information here.

COSMO: additional information here. NICAM: Benchmark on TiTech TSUBAME 2.5, Westmere CPU vs. K20X, additional information here

* A Free University Developer license is a special single-user node-locked license to the 64-bit Linux version of PGI Accelerator Fortran/C/C++ WorkstationTM



SETUP SEISMIC UNIX

Center for Wave Phenomena

Download Seismic Unix

ftp://ftp.cwp.mines.edu/pub/cwpcodes/cwp_su_all_43R8.tgz

Unpack to ~/cwp

Set environment variables

CWPROOT=~/cwp

PATH=~/cwp/bin:\$PATH

Edit Makefile.config, build

Use PGI compilers (CC=pgcc, FC=pgfortran)

OPTC=-g, FFLAGS=\$(FOPTS)

SETUP SEISMIC UNIX

Marmousi Datasets

Download Marmousi data, velocity, and density files

http://www.trip.caam.rice.edu/downloads/ieee.tar.gz

Convert SEGY format to SU format

```
#!/bin/bash
segyread tape=data.segy conv=0 endian=0 > data.su
segyread tape=velocity.segy conv=0 endian=0 > velocity.su
suflip flip=0 < velocity.su > velocity1.su
sustrip < velocity1.su > velocity.h@ ftn=0
suwind < data.su > data1.su tmax=2.9
```

SETUP SEISMIC UNIX

Smooth, build ray trace model, migrate

```
#!/bin/bash
nz = 751
nx = 2301
dz = 4
dx = 4
nt = 750
ntr=96
dt = 4000
ifile = data1.su
ofile = datamiq.su
tfile = tfile
vfile = velocity.h@
```

#smoothing

time smooth2 < \$vfile n1=\$nz n2=\$nx r1=20 r2=20 >smoothvel

#raytrace

time rayt2d < smoothvel dt=0.004 nt=751 dz=\$dz nz=\$nz dx=\$dx nx=\$nx fxo=0 dxo=25 nxo=369 fxs=0 dxs=100 nxs=93 >\$tfile

#migrate (Example)

sukdmig2d infile=\$ifile datain=\$ifile outfile=\$ofile
dataout=\$ofile ttfile=\$tfile fzt=0 dzt=4 nzt=751 fxt=0
dxt=25 nxt=369 fs=0 ns=93 ds=100 nzo=751 dzo=4 dxm=25
mtr=1

WHERE TO FIND HELP

- OpenACC Course Recordings https://developer.nvidia.com/openacc-courses
- PGI Website http://www.pgroup.com/resources
- OpenACC on StackOverflow http://stackoverflow.com/questions/tagged/openacc
- OpenACC Toolkit http://developer.nvidia.com/openacc-toolkit
- Parallel Forall Blog http://devblogs.nvidia.com/parallelforall/
- GPU Technology Conference http://www.gputechconf.com/
- OpenACC Website http://openacc.org/

Course Syllabus

May 19: Advanced Profiling of OpenACC Code

May 26: Office Hours <- Visual Profiler

June 2: Advanced multi-GPU Programming with MPI and OpenACC

June 9: Office Hours