OPENACC TUTORIAL

ESM SYMPOSIUM JSC 2019

28 May 2019 | Andreas Herten | Forschungszentrum Jülich

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Outline

Now: Download and install
PGI Community Edition

Jump to Task 0

The GPU Platform

CPU vs. GPU

A matter of specialties

Transcripting one

Transporting many

Graphics: Lee [2] and Bob Adams [3]

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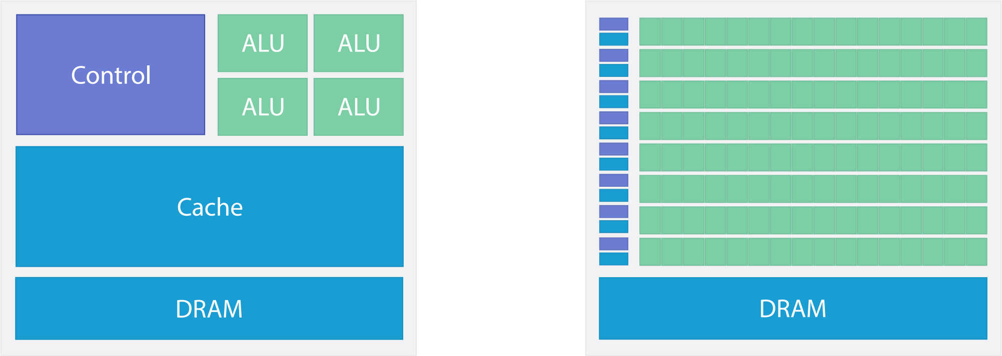
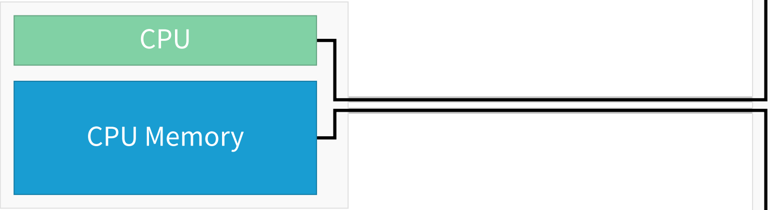
CPU vs. GPU

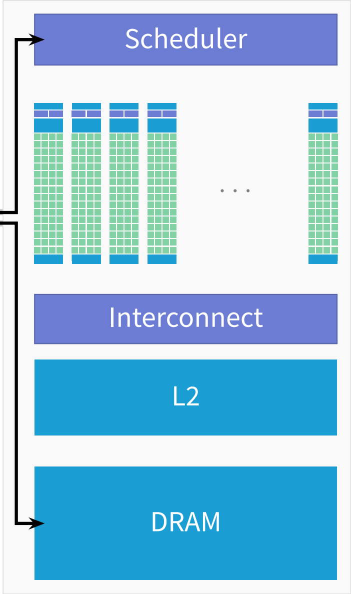
Chip



Processing Flow

CPU → GPU → CPU

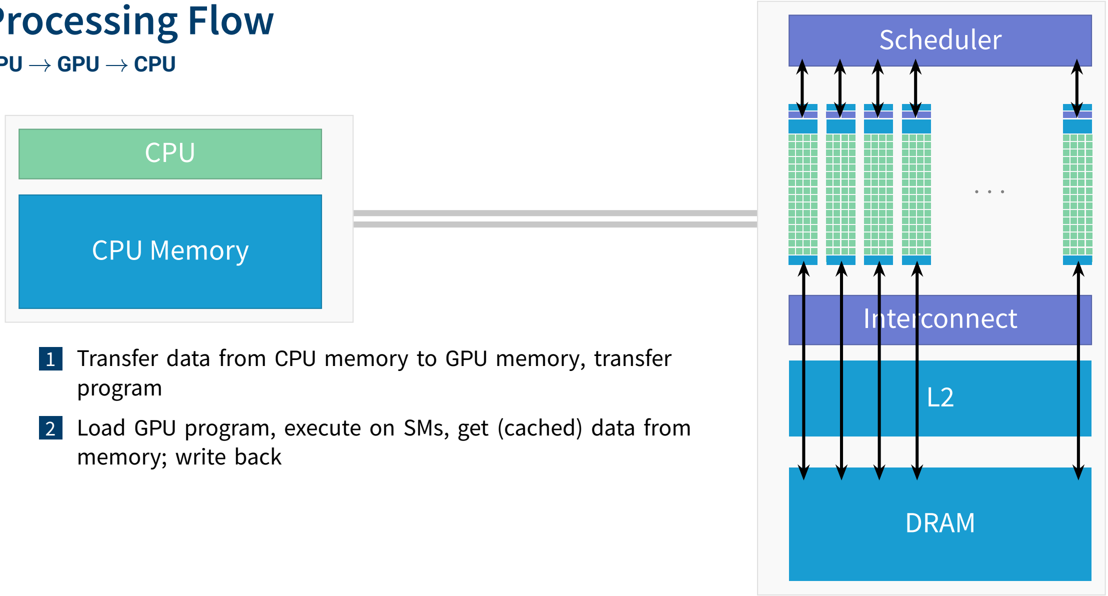




1. Transfer data from CPU memory to GPU memory, transfer program
2. Load GPU program, execute on SMs, get (cached) data from memory; write back

Processing Flow

CPU → GPU → CPU



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Processing Flow

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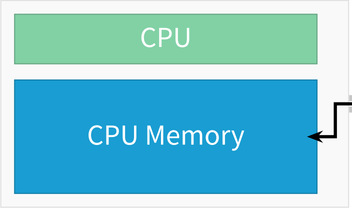
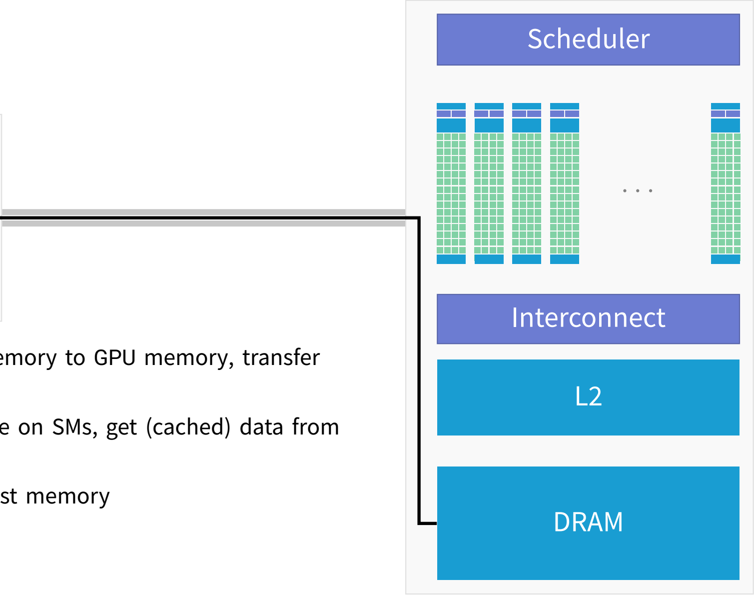
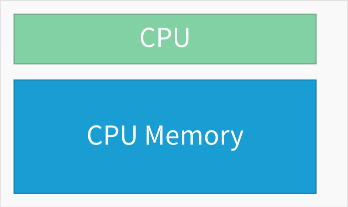


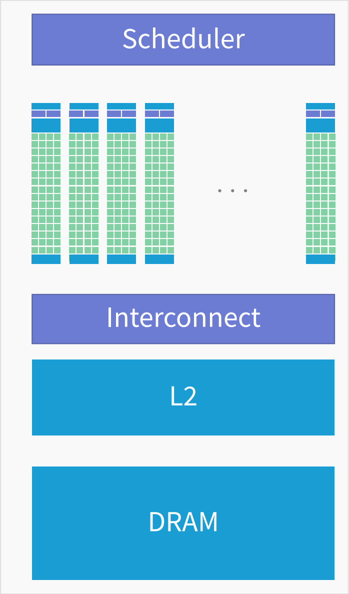


1. Transfer data from CPU memory to GPU memory, transfer program
2. Load GPU program, execute on SMs, get (cached) data from memory; write back
3. Transfer results back to host memory

Processing Flow

CPU → GPU → CPU





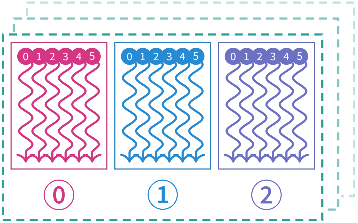
1. Transfer data from CPU memory to GPU memory, transfer program
2. Load GPU program, execute on SMs, get (cached) data from memory; write back
3. Transfer results back to host memory

- *Old:* Manual data transfer invocations – UVA
- *New:* Driver automatically transfers data – UM

CUDA Threading Model

Warp the kernel, it’s a thread!

- Methods to exploit parallelism:
  - Thread → Block
  - Block → Grid
  - Threads & blocks in 3D



- Execution entity: **threads**
  - Lightweight → fast switchting!
  - 1000s threads execute simultaneously → order non-deterministic!
- Parallel function: **kernel**

Getting GPU-Acquainted

Preparations

Done?

→ bit.ly/esm-acc

Task 0*: Setup

- Login to JUWELS

  `ssh name1@juwels.fz-juelich.de`
- Source our environment

  `source $PROJECT_training1916/env.sh` (→ `man esm-tutorial`)
- Copy material to your home directory (call `esm_sync_material`)
- Directory of tasks: `$HOME/GPU/Tasks/Tasks/`
- Solutions are always given, you decide when to look (`$HOME/GPU/Tasks/Solutions/`)

Getting GPU-Acquainted

Some Applications

TASK 0

GEMM

N-Body

Task 0: Getting Started

- Change to `GPU/Tasks/Task0/` directory
- Read `Instructions.rst`

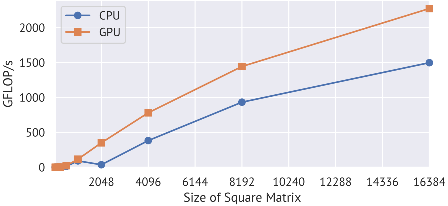
Mandelbrot

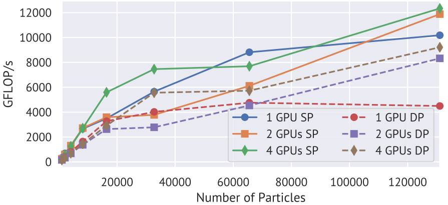
Dot Product

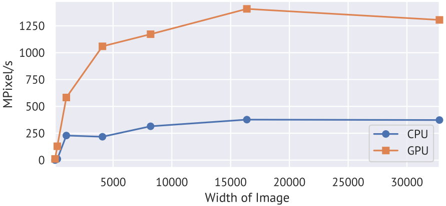
Getting GPU-Acquainted

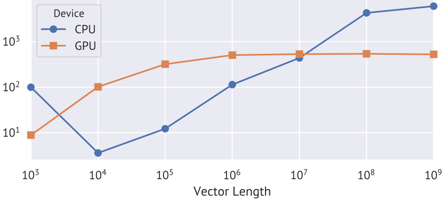
TASK 0

Some Applications









Primer on Parallel Scaling

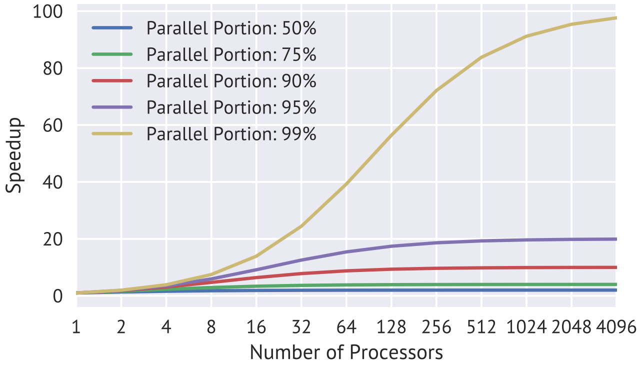
Amdahl's Law

Possible maximum speedup for N parallel processors

Total Time $t = t_{\textbf{serial}} + t_{\textbf{parallel}}$

N Processors $t(N) = t_s + t_p / N$

Speedup $s(N) = t / t(N) = \frac{t_s + t_p}{t_s + t_p / N}$



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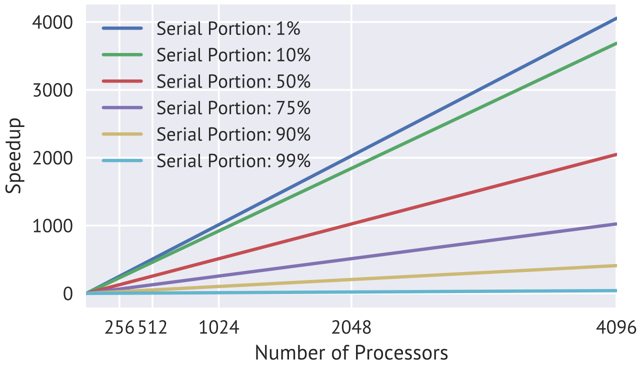
Primer on Parallel Scaling II

Gustafson-Barsis's Law

[...] speedup should be measured by scaling the problem to the number of processors, not fixing problem size.

– John Gustafson



Parallelism

Parallel programming is not easy!

Things to consider:

- Is my application **computationally intensive** *enough*?
- What are the levels of **parallelism**?
- How much **data** needs to be **transferred**?
- Is the **gain** worth the pain?

Possibilities

Different levels of *closeness* to GPU when GPU-programming, which **can** ease the *pain*…

- OpenACC
- OpenMP
- Thrust
- PyCUDA
- CUDA Fortran
- CUDA
- OpenCL

Primer on GPU Computing

Drop-in Acceleration

Easy Acceleration

Flexible Acceleration

About OpenACC

History

2011 OpenACC 1.0 specification is released
NVIDIA, Cray, PGI, CAPS

2013 OpenACC 2.0: More functionality, portability

2015 OpenACC 2.5: Enhancements, clarifications

2017 OpenACC 2.6: Deep copy, …

2018 OpenACC 2.7: Clarifications, more host, …

→ `https://www.openacc.org/` (*see also: Best practice guide*)

Support

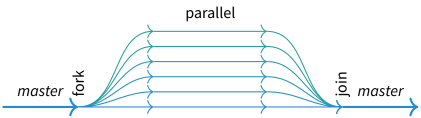
- Compiler: PGI, GCC, Clang, *Sunway*
- Languages: C/C++, Fortran

Open{MP↔ACC}

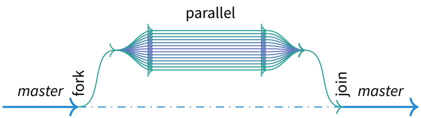
Everything's connected

- OpenACC modeled after OpenMP …
- … but specific for accelerators
- Might eventually be absorbed into OpenMP
- OpenACC more descriptive, OpenMP more prescriptive
- Basic principle same: Fork/join model

  Master thread launches parallel child threads; merge after execution



OpenMP



OpenACC

Modus Operandi

Three-step program

1. Annotate code with directives, indicating parallelism
2. OpenACC-capable compiler generates accelerator-specific code
3. $uccess

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1 Directives

pragmatic

- Compiler directives state intent to compiler

C/C++

```c
#pragma acc kernels
for (int i = 0; i < 23; i++)
// ...
```

Fortran

```fortran
!$acc kernels
do i = 1, 24
! ...
!$acc end kernels
```

- Ignored by compiler which does not understand OpenACC
- High level programming model for many-core machines, especially accelerators
- OpenACC: Compiler directives, library routines, environment variables
- Portable across host systems and accelerator architectures

2 Compiler

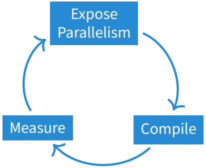
Simple and abstracted

- Compiler support
  - PGI *Best performance, great support, free*
  - GCC *Actively performance-improved, OSS*
  - Clang *First alpha version*
- Trust compiler to generate intended parallelism; always check status output!
- No need to know ins'n'outs of accelerator; leave it to expert compiler engineers*
- One code can target different accelerators: GPUs, or even multi-core CPUs → **Portability**

**: Eventually you want to tune for device; but that's possible*

3 $uccess

Iteration is key



- Serial to parallel: fast
- Serial to fast parallel: more time needed
- Start simple → refine

⇒ **Productivity**

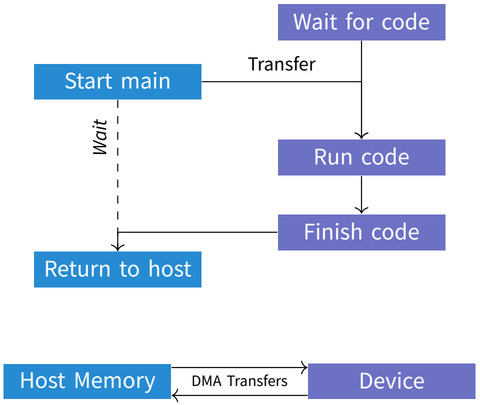
- Because of *generalness*: Sometimes not last bit of hardware performance accessible
- But: Use OpenACC together with other accelerator-targeting techniques (CUDA, libraries, …)

OpenACC Accelerator Model

For computation and memory spaces

- Main program executes on host
- Device code is transferred to accelerator
- Execution on accelerator is started
- Host waits until return (except: async)

- Two separate memory spaces; data transfers back and forth
  - Transfers hidden from programmer
  - Memories not coherent!
  - Compiler helps; GPU runtime helps



OpenACC Programming Model

A binary perspective

- OpenACC interpretation needs to be activated as compile flag

  PGI `pgcc -acc [-ta=tesla|-ta=multicore]`

  GCC `gcc -fopenacc`

  → Ignored by non-OpenACC compiler!

- Additional flags possible to improve/modify compilation

  `-ta=tesla:cc70` Use compute capability 7.0

  `-ta=tesla:lineinfo` Add source code correlation into binary

  `-ta=tesla:managed` Use unified memory

  `-fopenacc-dim=geom` Use *geom* configuration for threads

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A Glimpse of OpenACC

```
#pragma acc data copy(x[0:N],y[0:N])
#pragma acc parallel loop
{
    for (int i=0; i<N; i++) {
        x[i] = 1.0;
        y[i] = 2.0;
    }
    for (int i=0; i<N; i++) {
        y[i] = i*x[i]+y[i];
    }
}
```

- Compiler directives, ignored by incapable compilers
- Syntax **Fortran**

```
!$acc directive [clause, [, clause] ...]
!$acc end directive
```


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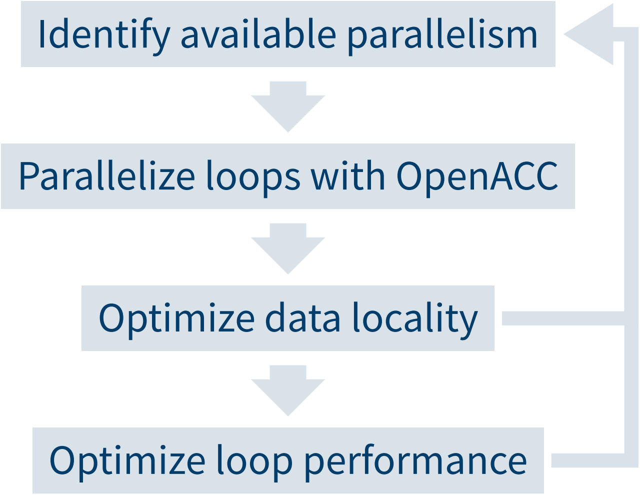
OpenACC by Example

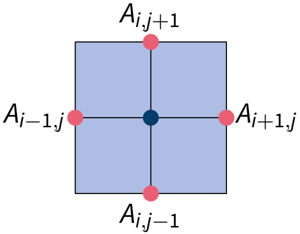
Parallelization Workflow

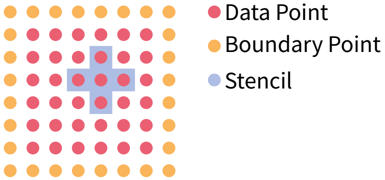


Jacobi Solver

Algorithmic description

- Example for acceleration: **Jacobi solver**
- Iterative solver, converges to correct value
- Each iteration step: compute average of neighboring points
- Example: 2D Poisson equation: $\nabla^2 A(x,y) = B(x,y)$





$$A_{k+1}(i,j) = -\frac{1}{4}\left(B(i,j) - \left(A_k(i-1,j) + A_k(i,j+1), + A_k(i+1,j) + A_k(i,j-1)\right)\right)$$

Jacobi Solver

Source code

```
while ( error > tol && iter < iter_max ) {
    error = 0.0;
    for (int ix = ix_start; ix < ix_end; ix++) {
        for (int iy = iy_start; iy < iy_end; iy++) {
            Anew[iy*nx+ix] = -0.25 * (rhs[iy*nx+ix] -
                (   A[iy*nx+ix+1] + A[iy*nx+ix-1]
               + A[(iy-1)*nx+ix] + A[(iy+1)*nx+ix]));
            error = fmaxr(error, fabsr(Anew[iy*nx+ix]-A[iy*nx+ix]));
    }}
    for (int iy = iy_start; iy < iy_end; iy++) {
        for( int ix = ix_start; ix < ix_end; ix++ ) {
            A[iy*nx+ix] = Anew[iy*nx+ix];
    }}
    for (int ix = ix_start; ix < ix_end; ix++) {
            A[0*nx+ix]       = A[(ny-2)*nx+ix];
            A[(ny-1)*nx+ix] = A[1*nx+ix];
    }
    // same for iy
    iter++;
}
```

Iterate until converged

Iterate across matrix elements

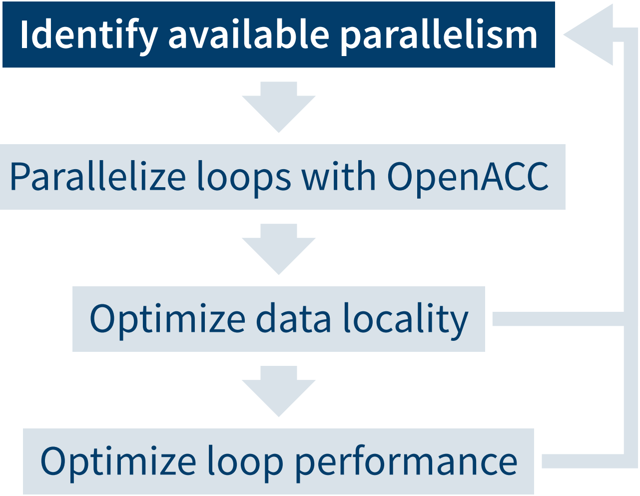
Calculate new value from neighbors

Accumulate error

Swap input/output

Set boundary conditions

Parallelization Workflow



Profiling

Profile

[…] premature optimization is the root of all evil.
Yet we should not pass up our [optimization] opportunities […]

– Donald Knuth [6]

- Investigate hot spots of your program!

→ Profile!

- Many tools, many levels: perf, PAPI, Score-P, Intel Advisor, NVIDIA Visual Profiler, …
- Here: Examples from PGI

Identify Parallelism

TASK 1

Generate Profile

- Use `pgprof` to analyze unaccelerated version of Jacobi solver
- Investigate!

Task 1: Analyze Application

- Change to `Task1/` directory
- Reset to original environment: `module purge && module load PGI`
- Compile: `make task1`
  Usually, compile just with `make` (but this exercise is special)
- Submit *profiling run* to the batch system: `make task1_profile`
  Study `srun` call and `pgprof` call; try to understand

??? Where is hotspot? Which parts should be accelerated?

Profile of Application

Info during compilation

```
$ pgcc -DUSE_DOUBLE -Minfo=all,intensity -fast -Minfo=ccff -Mprof=ccff
poisson2d_reference.o poisson2d.c -o poisson2d
poisson2d.c:
main:
     68, Generated vector simd code for the loop
         FMA (fused multiply-add) instruction(s) generated
     98, FMA (fused multiply-add) instruction(s) generated
    105, Loop not vectorized: data dependency
    123, Loop not fused: different loop trip count
         Loop not vectorized: data dependency
         Loop unrolled 8 times
```

- Automated optimization of compiler, due to `-fast`
- Vectorization, FMA, unrolling

Profile of Application

Info during run

```
$ pgprof --cpu-profiling on [...] ./poisson2d
======== CPU profiling result (flat):
Time(%)      Time  Name
 59.24%     930ms  main (poisson2d.c:128 0x372)
 12.10%     190ms  main (poisson2d.c:128 0x38c)
  4.46%      70ms  main (poisson2d.c:128 0x37e)
  3.18%      50ms  main (poisson2d.c:128 0x394)
  2.55%      40ms  main (poisson2d.c:128 0x378)
  1.91%      30ms  __fsd_exp_fma3 (0x8ea210c4)
  1.91%      30ms  __c_mcopy8_sky (0x8e60f197)
======== Data collected at 100Hz frequency
```

- $\approx$ 70 % in `main()`
- Since everything is in `main` – limited helpfulness
- Let's look into `main`!

Code Independency Analysis

Independence is key

```
while ( error > tol && iter < iter_max ) {
    error = 0.0;
    for (int ix = ix_start; ix < ix_end; ix++) {
        for (int iy = iy_start; iy < iy_end; iy++) {
            Anew[iy*nx+ix] = -0.25 * (rhs[iy*nx+ix] -
                (  A[iy*nx+ix+1] + A[iy*nx+ix-1]
               + A[(iy-1)*nx+ix] + A[(iy+1)*nx+ix]));
            error = fmaxr(error, fabsr(Anew[iy*nx+ix]-A[iy*nx+ix]));
    }}
    for (int iy = iy_start; iy < iy_end; iy++) {
        for( int ix = ix_start; ix < ix_end; ix++ ) {
            A[iy*nx+ix] = Anew[iy*nx+ix];
    }}
    for (int ix = ix_start; ix < ix_end; ix++) {
            A[0*nx+ix]      = A[(ny-2)*nx+ix];
            A[(ny-1)*nx+ix] = A[1*nx+ix];
    }
    // same for iy
    iter++;
}
```

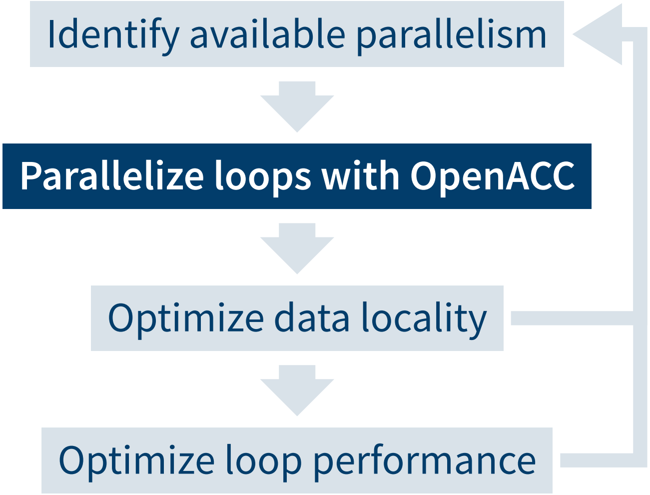
Data dependency between iterations

Independent loop iterations

Independent loop iterations

Independent loop iterations

Parallelization Workflow



Parallel Loops: Parallel

Maybe the second most important directive

- Programmer identifies block containing parallelism
  $\rightarrow$ compiler generates parallel code (*kernel*)
- Program launch creates *gangs* of parallel threads on parallel device
- Implicit barrier at end of parallel region
- Each gang executes same code sequentially

OpenACC: `parallel`

```
#pragma acc parallel [clause, [, clause] ...] newline
{structured block}
```

Parallel Loops: Parallel

Clauses

Diverse clauses to augment the parallel region

`private(var)`	A copy of variables `var` is made for each gang
`firstprivate(var)`	Same as `private`, except `var` will initialized with value from host
`if(cond)`	Parallel region will execute on accelerator only if `cond` is true
`reduction(op:var)`	Reduction is performed on variable `var` with operation op; supported: `+ * max min …`
`async[(int)]`	No implicit barrier at end of parallel region

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Parallel Loops: Loops

Maybe the third most important directive

- Programmer identifies loop eligible for parallelization
- Directive must be directly before loop
- Optional: Describe type of parallelism

OpenACC: `loop`

```
#pragma acc loop [clause, [, clause] ...] newline
{structured block}
```

Parallel Loops: Loops

Clauses

`independent`	Iterations of loop are data-independent (implied if in `parallel` region (and no `seq` or `auto`))
`collapse(int)`	Collapse `int` tightly-nested loops
`seq`	This loop is to be executed sequentially (not parallel)
`tile(int[,int])`	Split loops into loops over tiles of the full size
`auto`	Compiler decides what to do

Parallel Loops: Parallel Loops

Maybe the most important directive

- Combined directive: shortcut
  Because its used so often
- Any clause that is allowed on `parallel` or `loop` allowed
- Restriction: May not appear in body of another parallel region

OpenACC: `parallel loop`

```
#pragma acc parallel loop [clause, [, clause] ...]
```

Parallel Loops Example

```
double sum = 0.0;
#pragma acc parallel loop
for (int i=0; i<N; i++) {
    x[i] = 1.0;
    y[i] = 2.0;
}
#pragma acc parallel loop reduction(+:sum)
{
for (int i=0; i<N; i++) {
    y[i] = i*x[i]+y[i];
    sum+=y[i];
}
}
```

Kernel 1

Kernel 2

Parallel Jacobi

TASK 2

Add parallelism

- Add OpenACC parallelism to main double loop in Jacobi solver source code
- Profile code

→ Congratulations, you are a GPU developer!

Task 2: A First Parallel Loop

- Change to `Task2/` directory
- Compile: `make`
- Submit parallel run to the batch system: `make run`
  Adapt the `srun` call and run with other number of iterations, matrix sizes
- Profile: `make profile`
  `pgprof` or `nvprof` is prefix to call to `poisson2d`

Parallel Jacobi

Source Code

```c
#pragma acc parallel loop reduction(max:error)
for (int ix = ix_start; ix < ix_end; ix++)
{
  for (int iy = iy_start; iy < iy_end; iy++)
    {
      Anew[iy*nx+ix] = -0.25 * (rhs[iy*nx+ix] - ( A[iy*nx+ix+1] + A[iy*nx+ix-1]
                                                 + A[(iy-1)*nx+ix] +
                                                   A[(iy+1)*nx+ix] ));
        error = fmaxr( error, fabsr(Anew[iy*nx+ix]-A[iy*nx+ix]));
    }
}
```

Parallel Jacobi

Compilation result

```
$ make
pgcc -DUSE_DOUBLE -Minfo=accel -fast -acc -ta=tesla:cc70,managed poisson2d.c
 poisson2d_reference.o -o poisson2d
poisson2d.c:
main:
    109, Accelerator kernel generated
         Generating Tesla code
        109, Generating reduction(max:error)
        110, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
        112, #pragma acc loop seq
    109, Generating implicit copyin(A[:],rhs[:])
         Generating implicit copyout(Anew[:])
    112, Complex loop carried dependence of Anew-> prevents parallelization
         Loop carried dependence of Anew-> prevents parallelization
         Loop carried backward dependence of Anew-> prevents vectorization
```

Parallel Jacobi

Run result

```
$ make run
PGI_ACC_POOL_ALLOC=0 srun --gres=gpu:4 --pty ./poisson2d
Jacobi relaxation calculation: max 500 iterations on 2048 x 2048 mesh
Calculate reference solution and time with serial CPU execution.
    0, 0.249999
  100, 0.249760
  200, 0...
Calculate current execution.
    0, 0.249999
  100, 0.249760
  200, 0...
2048x2048: Ref:  61.7959 s, This:  18.4224 s, speedup:     3.35
```

`pgprof` / `nvprof`

NVIDIA's command line profiler

- Profiles applications, mainly for NVIDIA GPUs, but also CPU code
- GPU: CUDA kernels, API calls, OpenACC
- `pgprof` vs `nvprof`: Twins with other configurations
- Generate concise performance reports, full timelines; measure events and metrics (hardware counters)

⇒ Powerful tool for GPU application analysis

→ `http://docs.nvidia.com/cuda/profiler-users-guide/`

Profile of Jacobi

With pgprof

```
$ make profile
==116606== PGPROF is profiling process 116606, command: ./poisson2d 10
==116606== Profiling application: ./poisson2d 10
Jacobi relaxation calculation: max 10 iterations on 2048 x 2048 mesh
Calculate reference solution and time with serial CPU execution.
2048x2048: Ref:   0.8378 s, This:   0.2716 s, speedup:     3.08
==116606== Profiling result:
GPU activities:   99.97%  227.22ms        10  22.722ms  20.956ms  35.399ms  main_109_gpu
                   0.01%  25.472us        10  2.5470us  2.3680us  3.1680us  [CUDA memcpy DtoH]
                   0.01%  22.112us        10  2.2110us  1.9840us  2.9440us  main_109_gpu__red
                   0.01%  19.360us        10  1.9360us  1.7600us  2.3040us  [CUDA memset]

==116606== Unified Memory profiling result:
Device "Tesla V100-SXM2-16GB (0)"
   Count  Avg Size  Min Size  Max Size  Total Size  Total Time  Name
    5895  117.69KB  4.0000KB  0.9961MB  677.5000MB  76.01850ms  Host To Device
    3930  168.06KB  4.0000KB  0.9961MB  645.0000MB  56.85597ms  Device To Host
    2032         -         -         -           -  222.6040ms  Gpu page fault groups
Total CPU Page faults: 2361
```

Profile of Jacobi

With pgprof

```
$ make profile
==116606== PGPROF is profiling process 116606, command: ./poisson2d 10
==116606== Profiling application: ./poisson2d 10
Jacobi relaxation calculation: max 10 iterations on 2048 x 2048 mesh
Calculate reference solution and time with serial CPU execution
2048x2048: Ref:   0.8378 s, This:
==116606== Profiling
GPU activities:   99.
                   0.0
                   0.0
                   0.0

==116606== Unified Mem
Device "Tesla V100-SXM2-16GB (0)"
   Count  Avg Size  Min Size  Max Size  Total Size  Total Time  Name
    5895  117.69KB  4.0000KB  0.9961MB  677.5000MB  76.01850ms  Host To Device
    3930  168.06KB  4.0000KB  0.9961MB  645.0000MB  56.85597ms  Device To Host
    2032         -         -         -           -  222.6040ms  Gpu page fault groups
Total CPU Page faults: 2361
```

Only one function is parallelized!
Let's do the rest!

More Parallelism: Kernels

More freedom for compiler

- Kernels directive: second way to expose parallelism
- Region may contain parallelism
- Compiler determines parallelization opportunities

→ More freedom for compiler

- Rest: Same as for `parallel`

OpenACC: `kernels`

```
#pragma acc kernels [clause, [, clause] ...]
```

Kernels Example

```
double sum = 0.0;
#pragma acc kernels
{
for (int i=0; i<N; i++) {
    x[i] = 1.0;
    y[i] = 2.0;
}
for (int i=0; i<N; i++) {
    y[i] = i*x[i]+y[i];
    sum+=y[i];
}
}
```

Kernels created here

`kernels` vs. `parallel`

- Both approaches equally valid; can perform equally well
- `kernels`
  - Compiler performs parallel analysis
  - Can cover large area of code with single directive
  - Gives compiler additional leeway
- `parallel`
  - Requires parallel analysis by programmer
  - Will also parallelize what compiler may miss
  - More explicit
  - Similar to OpenMP
- Both regions may not contain other `kernels`/`parallel` regions
- No braunching into or out
- Program must not depend on order of evaluation of clauses
- At most: One `if` clause

Parallel Jacobi II

Add more parallelism

- Add OpenACC parallelism to other loops of `while` (L:123 – L:141)
- Use either `kernels` or `parallel`
- Do they perform equally well?

Task 3: More Parallel Loops

- Change to `Task3/` directory
- Compile: `make`
  Study the compiler output!
- Submit parallel run to the batch system: `make run`

? What's your speed-up?

Parallel Jacobi

Source Code

```
while ( error > tol && iter < iter_max ) {
    error = 0.0;
    #pragma acc parallel loop reduction(max:error)
    for (int ix = ix_start; ix < ix_end; ix++) {
        for (int iy = iy_start; iy < iy_end; iy++) {
            Anew[iy*nx+ix] = -0.25 * (rhs[iy*nx+ix] -
                (  A[iy*nx+ix+1] + A[iy*nx+ix-1]
               + A[(iy-1)*nx+ix] + A[(iy+1)*nx+ix]));
            error = fmaxr(error, fabsr(Anew[iy*nx+ix]-A[iy*nx+ix]));
    }}
    #pragma acc parallel loop
    for (int iy = iy_start; iy < iy_end; iy++) {
        for( int ix = ix_start; ix < ix_end; ix++ ) {
            A[iy*nx+ix] = Anew[iy*nx+ix];
    }}
    #pragma acc parallel loop
    for (int ix = ix_start; ix < ix_end; ix++) {
            A[0*nx+ix]      = A[(ny-2)*nx+ix];
            A[(ny-1)*nx+ix] = A[1*nx+ix];
    }
    // same for iy
    iter++;
}
```

Parallel Jacobi II

Compilation result

```
$ make
pgcc -c -DUSE_DOUBLE -Minfo=accel -fast -acc -ta=tesla:cc70,managed
 poisson2d_reference.c -o poisson2d_reference.o
poisson2d.c:
main:
    109, Accelerator kernel generated
         Generating Tesla code
        109, Generating reduction(max:error)
        110, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
        112, #pragma acc loop seq
    109, ...
    121, Accelerator kernel generated
         Generating Tesla code
        124, #pragma acc loop gang /* blockIdx.x */
        126, #pragma acc loop vector(128) /* threadIdx.x */
    121, Generating implicit copyin(Anew[:])
         Generating implicit copyout(A[:])
    126, Loop is parallelizable
    133, Accelerator kernel genera...
```

Parallel Jacobi II

Run result

```
$ make run
PGI_ACC_POOL_ALLOC=0 srun --gres=gpu:4 --pty ./poisson2d
Jacobi relaxation calculation: max 500 iterations on 2048 x 2048 mesh
Calculate reference solution and time with serial CPU execution.
    0, 0.249999
  100, 0.249760
  200, 0...
Calculate current execution.
    0, 0.249999
  100, 0.249760
  200, 0...
2048x2048: Ref:  61.6953 s, This:   0.4035 s, speedup:   152.90
```


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Parallel Jacobi II

Run result

```
$ make run
PGI_ACC_POOL_ALLOC=0 srun --gres=gpu:4 --pty ./poisson2d
Jacobi relaxation calculation: max 500 iterations on 2048 x 2048 mesh
Calculate reference solution and time with serial CPU execution.
    0, 0.249999
  100, 0.249760
  200, 0...
Calculate current execution.
    0, 0.249999
  100, 0.249760
  200, 0...
2048x2048: Ref:  61.6953 s, This:   0.4035 s, speedup:   152.90
```

Done?!

OpenACC by Example

Data Transfers

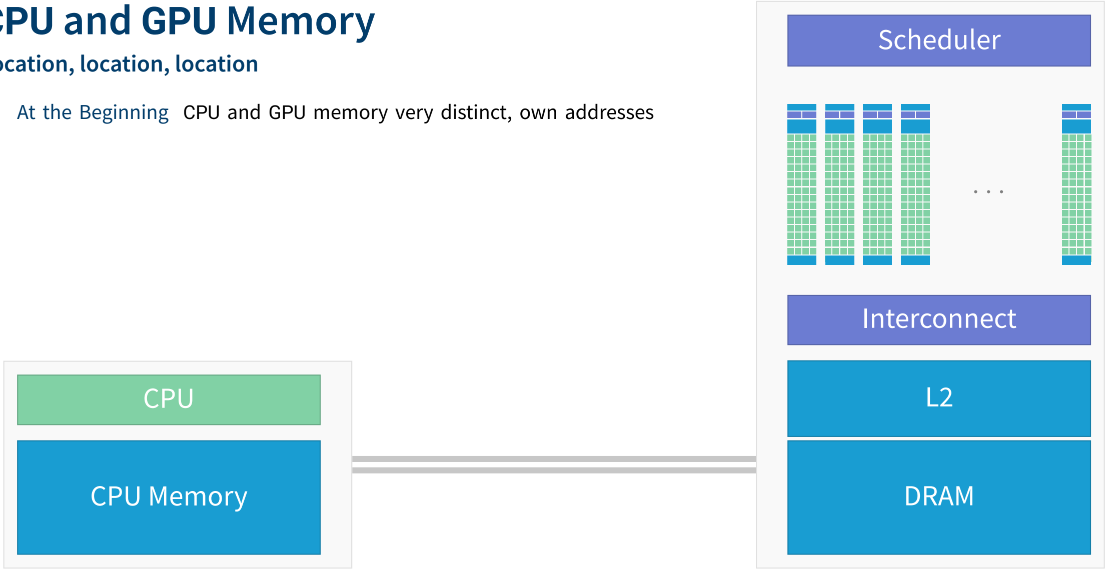
Automatic Data Transfers

- Up to now: We did not care about **data transfers**
- Compiler and runtime care
- Magic keyword: `-ta=tesla:managed`
- Only feature of (recent) NVIDIA GPUs!

CPU and GPU Memory

Location, location, location

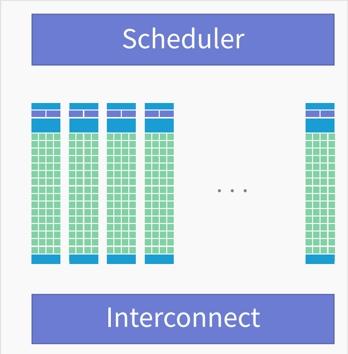
At the Beginning CPU and GPU memory very distinct, own addresses

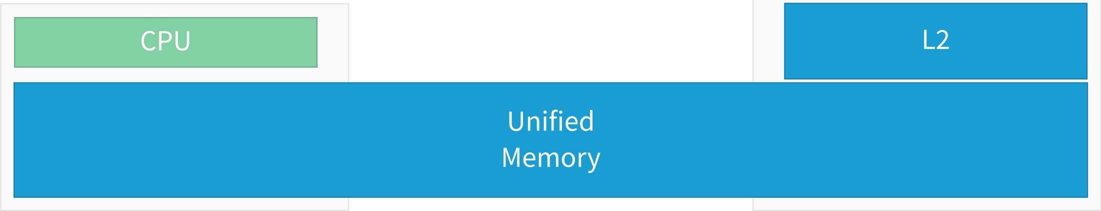


CPU and GPU Memory

Location, location, location

- At the Beginning: CPU and GPU memory very distinct, own addresses
- CUDA 4.0: Unified Virtual Addressing: pointer from same address pool, but data copy manual
- CUDA 6.0: Unified Memory*: Data copy by driver, but whole data at once
- CUDA 8.0: Unified Memory (truly): Data copy by driver, page faults on-demand initiate data migrations (Pascal)
- Future*: Address Translation Service: Omit page faults





Portability

- Managed memory: Only NVIDIA GPU feature
- Great OpenACC features: Portability

→ Code should also be fast without `-ta=tesla:managed`!

- Let's remove it from compile flags!

```
$ make
pgcc -c -DUSE_DOUBLE -Minfo=accel -fast -acc -ta=tesla:cc70
poisson2d_reference.c -o poisson2d_reference.o
poisson2d.c:
PGC-S-0155-Compiler failed to translate accelerator region (see -Minfo messages): Could not
 find allocated-variable index for symbol - rhs (poisson2d.c: 109)
...
PGC/x86-64 Linux 19.3-0: compilation aborted
```

Copy Statements

- Compiler implicitly created `copy` clauses to copy data to device

```
134, Generating implicit copyin(A[:])
     Generating implicit copyout(A[nx*(ny-1)+1:nx-2])
```

- It couldn't determine length of copied data …
- …but before: no problem – Unified Memory!
- Now: Problem! We need to give that information! (see also later)

OpenACC: `copy`

```
#pragma acc parallel copy(A[start:end])
```

Also: `copyin(B[s:e])` `copyout(C[s:e])` `present(D[s:e])` `create(E[s:e])`

Data Copies

TASK 4

Get that data!

- Add `copy` clause to parallel regions
- Check correctness with Visual Profiler

Task 4: Data Copies

- Change to `Task4/` directory
- Work on TODOs
- Compile: `make`
- Submit parallel run to the batch system: `make run`
- Generate profile with `make profile_tofile`

? What's your speed-up?

Data Copies

Compiler Output

```
$ make
pgcc -DUSE_DOUBLE -Minfo=accel -fast -acc -ta=tesla:cc70 poisson2d.c poisson2d_reference.o -o poisson2d
poisson2d.c:
main:
    109, Generating copy(A[:ny*nx],Anew[:ny*nx],rhs[:ny*nx])
         ...
    121, Generating copy(Anew[:ny*nx],A[:ny*nx])
         ...
    131, Generating copy(A[:ny*nx])
         Accelerator kernel generated
         Generating Tesla code
        132, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
    137, Generating copy(A[:ny*nx])
         Accelerator kernel generated
         Generating Tesla code
        138, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
```

Data Copies

Run Result

```
$ make run
srun --gres=gpu:4 --pty ./poisson2d
Jacobi relaxation calculation: max 500 iteratio ... 48 x 2048 mesh
Calculate reference solution and time ... xecution.
    0, 0.249999
  100, 0.249760
  200, 0...
Calculate current execution.
    0, 0.249999
  100, 0.249760
  200, 0...
2048x2048: Ref:  68.8658 s, This:  48.7855 s, speedup:     1.41
```

Slower?! Why?

PGI/NVIDIA Visual Profiler

- GUI tool accompanying `pgprof` / `nvprof`

  PGI: Start `pgprof` without parameters

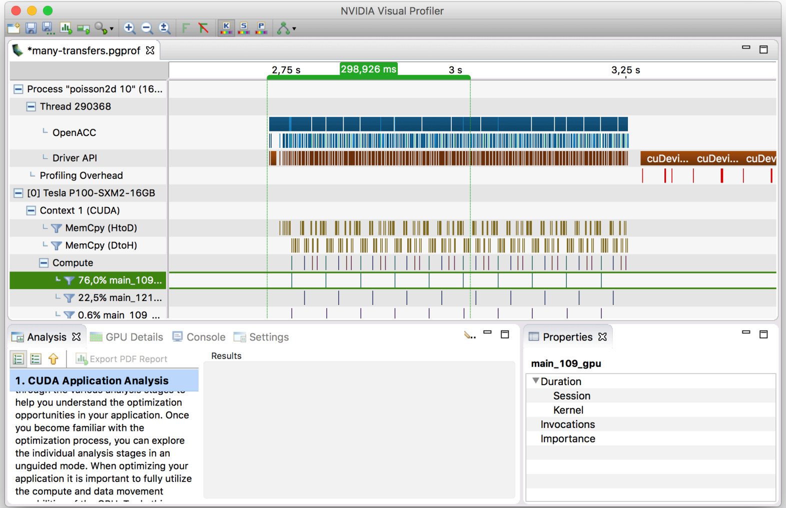
  NVIDIA: Start `nvvp`
- Timeline view of all things GPU

  → Study stages and interplay of application
- Interactive or with input from command line profilers
- View launch and run configurations
- Guided and unguided analysis

→ `https://developer.nvidia.com/nvidia-visual-profiler`

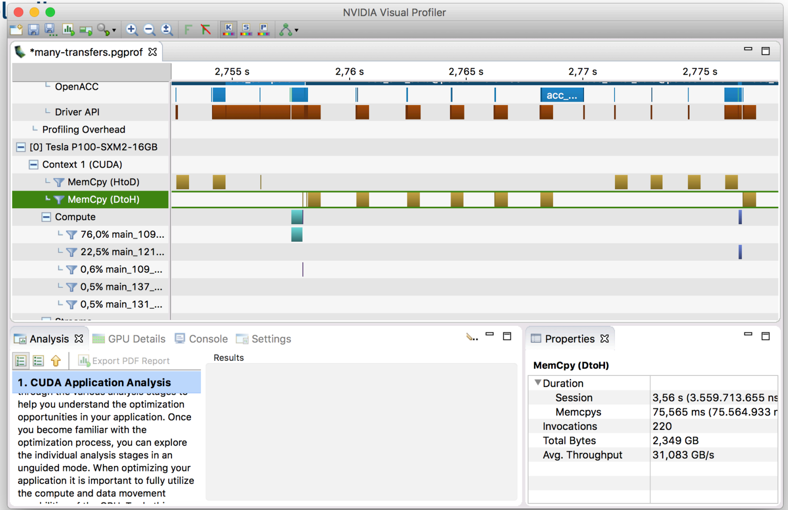
PGI/NVIDIA Visual Profiler

Overview

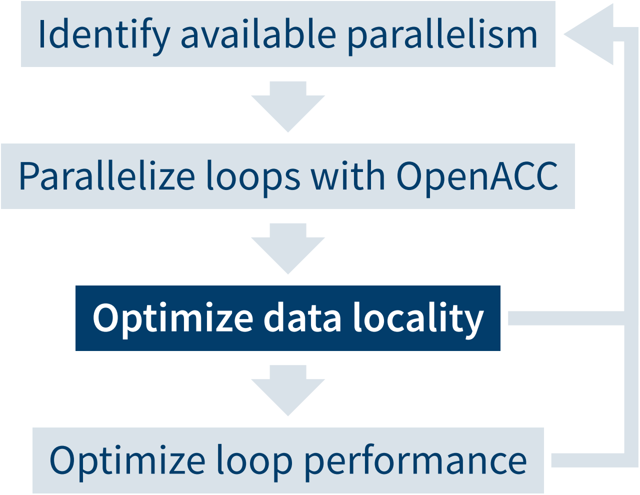


PGI/NVIDIA Visual Profiler

Zoom in to kernel calls



Parallelization Workflow



Analyze Jacobi Data Flow

In code

```
while (error > tol && iter < iter_max) {
    error = 0.0;
```

A, Anew resident on host

copy

```
#pragma acc parallel loop
```

Copies are done in **each** iteration!

```
for (int ix = ix_start; ix < ix_end; ix++) {
    for (int iy = iy_start; iy < iy_end; iy++) {
    // ...
}}
```

A, Anew resident on **device**

A, Anew resident on **host**

```
    iter++
}
```

Analyze Jacobi Data Flow

In code

```
while (error > tol && iter < iter_max) {
    error = 0.0;
```

A, Anew resident on **host**

copy

```
#pragma acc parallel loop
```

A, Anew resident on **device**

```
for (int ix = ix_start; ix < ix_end; ix++) {
    for (int iy = iy_start; iy < iy_end; iy++) {
    // ...
}}
```

Copies are done in **each** iteration!

A, Anew resident on **device**

A, Anew resident on **host**

```
    iter++
}
```

Analyze Jacobi Data Flow

Summary

- By now, whole algorithm is using GPU
- At beginning of `while` loop, data copied to device; at end of loop, coped by to host
- Depending on type of parallel regions in `while` loop: Data copied in between regions as well
- **Slow! Data copies are expensive!**

Data Regions

To manually specify data locations

- Defines region of code in which data remains on device
- Data is shared among all kernels in region
- Explicit data transfers

OpenACC: `data`

```
#pragma acc data [clause, [, clause] ...]
```

Data Regions

Clauses

Clauses to augment the data regions

- `copy(var)` Allocates memory of `var` on GPU, copies data to GPU at beginning of region, copies data to host at end of region
  Specifies size of `var`: `var[`*`lowerBound:size`*`]`
- `copyin(var)` Allocates memory of `var` on GPU, copies data to GPU at beginning of region
- `copyout(var)` Allocates memory of `var` on GPU, copies data to host at end of region
- `create(var)` Allocates memory of `var` on GPU
- `present(var)` Data of `var` is not copies automatically to GPU but considered present

Data Region Example

```
#pragma acc data copyout(y[0:N]) create(x[0:N])
{
    double sum = 0.0;
    #pragma acc parallel loop
    for (int i=0; i<N; i++) {
        x[i] = 1.0;
        y[i] = 2.0;
    }
    #pragma acc parallel loop
    for (int i=0; i<N; i++) {
        y[i] = i*x[i]+y[i];
    }
}
```

Data Regions II

Looser regions: `enter data` directive

- Define data regions, but not for structured block
- Closest to `cudaMemcpy()`
- Still, explicit data transfers

OpenACC: `enter data`

```
#pragma acc enter data [clause, [, clause] ...]
#pragma acc exit data [clause, [, clause] ...]
```

Data Region

TASK 5

More parallelism, Data locality

- Add `data` regions such that all data resides on device during iterations
- Optional: See your success in Visual Profiler

Task 5: Data Region

- Change to `Task5/` directory
- Work on TODOs
- Compile: `make`
- Submit parallel run to the batch system: `make run`

? What's your speed-up?

- Generate profile with `make profile_tofile`

Parallel Jacobi II

Source Code

```
#pragma acc data copy(A[0:nx*ny]) copyin(rhs[0:nx*ny]) create(Anew[0:nx*ny])
while ( error > tol && iter < iter_max )
{
    error = 0.0;

    // Jacobi kernel
    #pragma acc parallel loop reduction(max:error)
    for (int ix = ix_start; ix < ix_end; ix++)
    {
        for (int iy = iy_start; iy < iy_end; iy++)
        {
            Anew[iy*nx+ix] = -0.25 * (rhs[iy*nx+ix] - ( A[iy*nx+ix+1] + A[iy*nx+ix-1]
                                                 + A[(iy-1)*nx+ix] + A[(iy+1)*nx+ix] ));
            error = fmaxr( error, fabsr(Anew[iy*nx+ix]-A[iy*nx+ix]));
        }
    }

    // A <-> Anew
    #pragma acc parallel loop
    for (int iy = iy_start; iy < iy_end; iy++)
    // …
}
```

Data Region

Compiler Output

```
$ make
pgcc -DUSE_DOUBLE -Minfo=accel -fast -acc -ta=tesla:cc70 poisson2d.c
poisson2d_reference.o -o poisson2d
poisson2d.c:
main:
    104, Generating copyin(rhs[:ny*nx])
         Generating create(Anew[:ny*nx])
         Generating copy(A[:ny*nx])
    110, Accelerator kernel generated
         Generating Tesla code
        110, Generating reduction(max:error)
        111, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
        113, #pragma acc loop seq
        ...
```

Data Region

Run Result

```
$ make run
Jacobi relaxation calculation: max 500 iterations on 2048 x 2048 mesh
Calculate reference solution and time with
    0, 0.249999
  100, 0.249760
  200, 0...
Calculate current exec
    0, 0.249999
  100, 0.249760
  200, 0...
2048x2048: Ref:  69.0761 s, This:   0.4004 s, speedup:   172.53
```

Wow!

But can we be even better?

OpenACC by Example

Optimize Loop Performance

Parallelization Workflow

Identify available parallelism

Parallelize loops with OpenACC

Optimize data locality

Optimize loop performance

Understanding Compiler Output

```
110, Accelerator kernel generated
     Generating Tesla code
    110, Generating reduction(max:error)
    111, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
    114, #pragma acc loop seq
    114, Complex loop carried dependence of Anew-> prevents parallelization
```

```
110 #pragma acc parallel loop reduction(max:error)
111 for (int ix = ix_start; ix < ix_end; ix++)
112 {
113     // Inner loop
114     for (int iy = iy_start; iy < iy_end; iy++)
115     {
116         Anew[iy*nx+ix] = -0.25 * (rhs[iy*nx+ix] - ( A[iy*nx+ix+1] +  A[iy*nx+ix-1] +
            ↪  A[(iy-1)*nx+ix] + A[(iy+1)*nx+ix] ));
117         error = fmaxr( error, fabsr(Anew[iy*nx+ix]-A[iy*nx+ix]));
118     }
119 }
```

Understanding Compiler Output

```
110, Accelerator kernel generated
     Generating Tesla code
    110, Generating reduction(max:error)
    111, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
    114, #pragma acc loop seq
    114, Complex loop carried dependence of Anew-> prevents parallelization
```

- Outer loop: Parallelism with gang and `vector`
- Inner loop: Sequentially per thread (`#pragma acc loop seq`)
- Inner loop was never parallelized!
- **Rule of thumb: Expose as much parallelism as possible**

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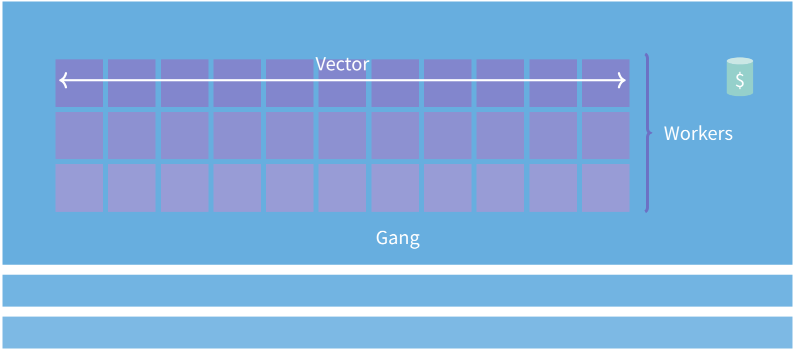
OpenACC Parallelism

3 Levels of Parallelism



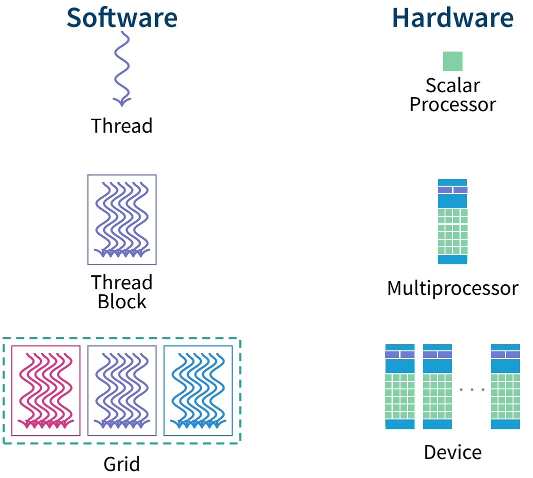
Vector
Vector threads work in lockstep (SIMD/SIMT parallelism)

Worker
Has 1 or more vector; workers share common resource (*cache*)

Gang
Has 1 or more workers; multiple gangs work independently from each other

CUDA Parallelism

CUDA Execution Model



- **Threads** executed by scalar processors (*CUDA cores*)

- Thread **blocks**: Executed on multiprocessors (*SM*)
- Do not migrate
- Several concurrent thread blocks can reside on multiprocessor
  Limit: Multiprocessor resources (register file; shared memory)

- Kernel launched as **grid** of thread blocks
- Blocks, grids: Multiple dimensions

From OpenACC to CUDA

$\texttt{map}(||_{\text{acc}}, ||_{\texttt{<<<>>>}})$

- In general: Compiler free to do what it thinks is best
- Usually

gang	Mapped to blocks *(coarse grain)*
worker	Mapped to threads *(fine grain)*
vector	Mapped to threads *(fine SIMD/SIMT)*
seq	*No parallelism; sequential*

- Exact mapping compiler dependent
- Performance tips
  - Use vector size divisible by 32
  - Block size: `num_workers` × `vector_length`

Declaration of Parallelism

Specify configuration of threads

- Three **clauses** of parallel region (`parallel`, `kernels`) for changing distribution/configuration of group of threads
- Presence of keyword: Distribute using this level
- Optional size: Control size of parallel entity

OpenACC: `gang worker vector`

```
#pragma acc parallel loop gang vector
```

Also: `worker`

Size: `num_gangs(n)`, `num_workers(n)`, `vector_length(n)`

Understanding Compiler Output II

```
110, Accelerator kernel generated
     Generating Tesla code
    110, Generating reduction(max:error)
    111, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
    114, #pragma acc loop seq
    114, Complex loop carried dependence of Anew-> prevents parallelization
```

- Compiler reports configuration of parallel entities
  - **Gang** mapped to `blockIdx.x`
  - **Vector** mapped to `threadIdx.x`
  - **Worker** not used
- Here: 128 threads per block; as many blocks as needed
  128 seems to be default for Tesla/NVIDIA

More Parallelism

Task 6

Unsequentialize inner loop

- Add `vector` clause to inner loop
- Study result with profiler

Task 6: More Parallelism

- Change to `Task6/` directory
- Work on TODOs
- Compile: `make`
- Submit to the batch system: `make run`
- Generate profile with `make profile_tofile`

? What's your speed-up?

More Parallelism

Compiler Output

```
$ make
pgcc -DUSE_DOUBLE -Minfo=accel -fast -acc -ta=tesla:cc70 poisson2d.c poisson2d_reference.o
 -o poisson2d
poisson2d.c:
main:
    104, Generating create(Anew[:ny*nx])
         Generating copyin(rhs[:ny*nx])
         Generating copy(A[:ny*nx])
    110, Accelerator kernel generated
         Generating Tesla code
        110, Generating reduction(max:error)
        111, #pragma acc loop gang /* blockIdx.x */
        114, #pragma acc loop vector(128) /* threadIdx.x */
        ...
```

Data Region

Run Result

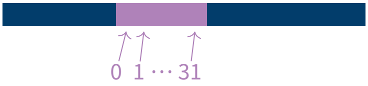
```
$ make run
Jacobi relaxation calculation: max 500 iterations on 2048 x 2048 mesh
Calculate reference solution and time ... on.
     0, 0.249999
   100, 0.249760
   200, 0...
Calculate current execution.
     0, 0.249999
   100, 0.249760
   200, 0...
2048x2048: Ref:  69.3831 s, This:   0.9627 s, speedup:    72.07
```

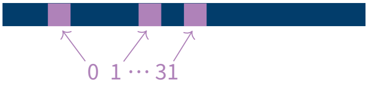
Actually slower!
Why?

Memory Coalescing

Memory in batch

- Coalesced access *good*
  - Threads of warp (group of 32 contiguous threads) access adjacent words
  - Few transactions, high utilization
- Uncoalesced access *bad*
  - Threads of warp access scattered words
  - Many transactions, low utilization
- Best **performance**: `threadIdx.x` should access contiguously





Jacobi Access Pattern

A coalescion of data

Improve memory access pattern: Loop order in main loop

```
#pragma acc parallel loop reduction(max:error)
for (int ix = ix_start; ix < ix_end; ix++) {
    #pragma acc loop vector
    for (int iy = iy_start; iy < iy_end; iy++) {
        Anew[ iy*nx + ix ] = -0.25 *
        ↪  (rhs[iy*nx+ix] -
           (  A[iy*nx+ix+1] + A[iy*nx+ix-1]
          + A[(iy-1)*nx+ix] + A[(iy+1)*nx+ix]));
        //...
```

- `ix` Outer run index; accesses consecutive memory locations
- `iy` Inner run index; accesses offset memory locations

→ Change order to optimize pattern!

Jacobi Access Pattern

A coalescion of data

Improve memory access pattern: Loop order in main loop

```
#pragma acc parallel loop reduction(max:error)
for (int iy = iy_start; iy < iy_end; iy++) {
    #pragma acc loop vector
    for (int ix = ix_start; ix < ix_end; ix++) {
        Anew[ iy*nx + ix ] = -0.25 *
        ↪  (rhs[iy*nx+ix] -
            (  A[iy*nx+ix+1] + A[iy*nx+ix-1]
           + A[(iy-1)*nx+ix] + A[(iy+1)*nx+ix]));
        //...
```

- ix Outer run index; accesses consecutive memory locations
- iy Inner run index; accesses offset memory locations

→ Change order to optimize pattern!

Fixing Access Pattern

Task 7

Loop change

- Interchange loop order for Jacobi loops
- Also: Compare to loop-fixed CPU reference version

Task 7: Loop Ordering

- Change to `Task7/` directory
- Work on TODOs
- Compile: `make`
- Submit to the batch system: `make run`

? What's your speed-up?

Fixing Access Pattern

Compiler output (unchanged)

```
$ make
pgcc -DUSE_DOUBLE -Minfo=accel -fast -acc -ta=tesla:cc70 poisson2d.c
poisson2d_reference.o -o poisson2d
poisson2d.c:
main:
    104, Generating create(Anew[:ny*nx])
         Generating copyin(rhs[:ny*nx])
         Generating copy(A[:ny*nx])
    110, Accelerator kernel generated
         Generating Tesla code
        110, Generating reduction(max:error)
        111, #pragma acc loop gang /* blockIdx.x */
        114, #pragma acc loop vector(128) /* threadIdx.x */
        ...
```

Fixing Access Pattern

Run Result

```
$ make run
Jacobi relaxation calculation: max 500 iterations on 2048 x 2048 mesh
Calculate reference solution and time with
    0, 0.249
  100, 0.249
  200, 0...
Calculate cu
    0, 0.249
  100, 0.249
  200, 0...
2048x2048: Ref:  72.1309 s, This:   0.2365 s, speedup:   304.95
```

Again with proper CPU version!

Memory access pattern is also very important on CPU!

Fixing Access Pattern

Run Result II

```
$ make run
Jacobi relaxation calculation: max 500 iterations on 2048 x 2048 mesh
Calculate reference solution and time with serial CPU execution.
    0, 0.249999
  100, 0.249760
  200, 0...
Calculate current execution.
    0, 0.249999
  100, 0.249760
  200, 0...
2048x2048: Ref:   6.6684 s, This:   0.2361 s, speedup:    28.24
```

28 × is great!

Page-Locked Memory

Pageability

- Host memory allocated with `malloc()` is pageable
  - Memory pages of memory can be moved by kernel, e.g. swapped to disk
  - Additional indirection
- NVIDIA GPUs can allocate **page-locked memory** (*pinned* memory)
  - \+ Faster (safety guards are skipped)
  - \+ Interleaving of execution and copy (asynchronous)
  - \+ Directly map into GPU memory*
  - – Scarce resource; OS performance could degrade
- OpenACC: Very easy to use pinned memory
  `-ta=tesla:pinned`

Page-Locked Memory

Loop change

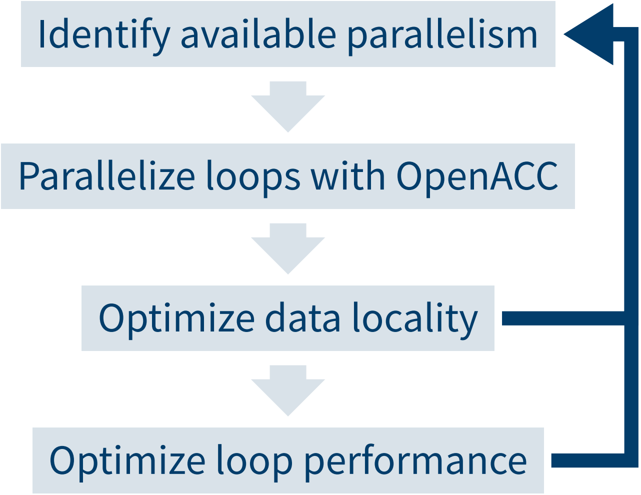
TASK 7'

- Compare performance with and without pinned memory
- Also test unified memory again

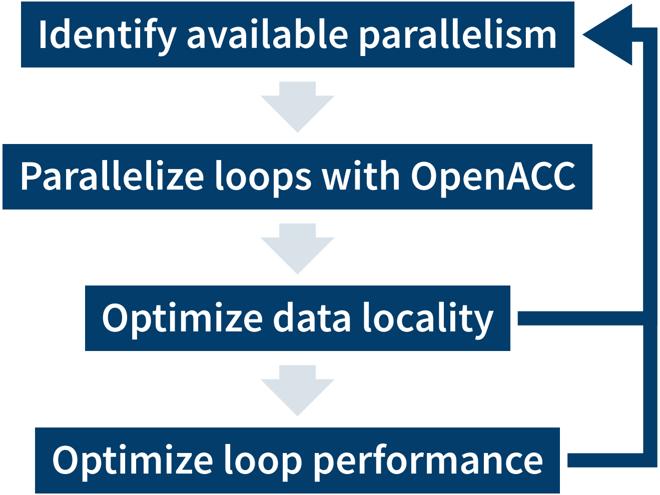
Task 7': Pinned Memory

- Like in Task 7, but change compilation to include `pinned` or `managed`
- Submit to the batch system: `make run`

Parallelization Workflow



Parallelization Workflow



Interoperability

Interoperability

- OpenACC can operate together with
  - Applications
  - Libraries
  - CUDA
- Both directions possible: Call OpenACC from others, call others from OpenACC

The Keyword

OpenACC's Rosetta Stone

`host_data use_device`

- Background
  - GPU and CPU are different devices, have different memory
  - → Distinct address spaces
- OpenACC hides handling of addresses from user
  - For every chunk of accelerated data, **two** addresses exist
  - One for CPU data, one for GPU data
  - OpenACC uses appropriate address in accelerated kernel
- **But:** Automatic handling not working when out of OpenACC (OpenACC will default to host address)

→ `host_data use_device` uses the address of the GPU device data for scope

The host_data Construct

Example

- Usage:

```
double* foo = new double[N];            // foo on Host
#pragma acc data copyin(foo[0:N])  // foo on Device
{
  ...
  #pragma acc host_data use_device(foo)
  some_lfunc(foo);                    // Device: OK!
  ...
}
```

- Directive can be used for structured block as well

The Inverse: deviceptr

When CUDA is involved

- For the inverse case:
  - Data has been copied by CUDA or a CUDA-using library
  - Pointer to data residing on devices is returned

  → Use this data in OpenACC context
- `deviceptr` clause declares data to be on device
- Usage:

```
float * n;
int n = 4223;
cudaMalloc((void**)&x,(size_t)n*sizeof(float));
// ...
#pragma acc kernels deviceptr(x)
for (int i = 0; i < n; i++) {
    x[i] = i;
}
```

Interoperability

Tasks

cuBLAS

Task 1

Introduction to BLAS

- Use case: Anything linear algebra
- **BLAS**: Basic Linear Algebra Subprograms
  - Vector-vector, vector-matrix, matrix-matrix operations
  - Specification of routines
  - Examples: *SAXPY*, *DGEMV*, *ZGEMM*

  → `http://www.netlib.org/blas/`
- **cuBLAS**: NVIDIA's linear algebra routines with BLAS interface, readily accelerated

  → `http://docs.nvidia.com/cuda/cublas/`
- **Task 1**: Use cuBLAS for vector addition, everything else with OpenACC

Task 8-1

cuBLAS OpenACC Interaction

- cuBLAS routine used:

```
cublasDaxpy(cublasHandle_t handle, int n,
            const double          *alpha,
            const double          *x, int incx,
            double                *y, int incy)
```

- `handle` capsules GPU auxiliary data, needs to be created and destroyed with `cublasCreate` and `cublasDestroy`
- `x` and `y` point to addresses on **device**!
- cuBLAS library needs to be linked with `-lcublas`

Task 8-1

TASK 8-1

Vector Addition with cuBLAS

- Use cuBLAS for vector addition

Task 8-1: OpenACC+cuBLAS

- Change to `Task8-1/` directory
- Work on TODOs in `vecAddRed.c`
  - Use `host_data use_device` to provide correct pointer
  - Check cuBLAS documentation for details on `cublasDaxpy()`
- Compile: `make`
- Submit to the batch system: `make run`

CUDA

Task 8-2

CUDA Need-to-Know

- Use case:
  - Working on legacy code
  - Need the *raw* power (/flexibility) of CUDA
- CUDA need-to-knows:
  - Thread → Block → Grid
    Total number of threads should map to your problem; threads are alway given per block
  - A kernel is called from every thread on GPU device
    Number of kernel threads: *triple chevron syntax*
    `kernel<<<nBlocks, nThreads>>>(arg1, arg2, ...)`
  - Kernel: Function with `__global__` prefix
    Aware of its index by global variables, e.g. `threadIdx.x`

→ `http://docs.nvidia.com/cuda/`

Task 8-2

TASK 8-2

Vector Addition with CUDA Kernel

- CUDA kernel for vector addition, rest OpenACC
- Marrying CUDA **C** and OpenACC:
  - All direct CUDA interaction wrapped in wrapper file `cudaWrapper.cu`, compiled with `nvcc` to object file (`-c`)
  - `vecAddRed.c` calls external function from `cudaWrapper.cu` (**`extern`**)

Task 8-2: OpenACC+CUDA

- Change to `Task8-2/` directory
- Work on TODOs in `vecAddRed.c` and `cublasWrapper.cu`
  - Use `host_data use_device` to provide correct pointer
  - Implement computation in kernel, implement call of kernel
- Compile: `make`; Submit to the batch system: `make run`

Thrust

Thrust

Iterators! Iterators everywhere! 🚀

- $\frac{\text{Thrust}}{\text{CUDA}} = \frac{\text{STL}}{\text{C++}}$
- Template library
- Based on iterators, but also works with plain C
- Data-parallel primitives (`scan()`, `sort()`, `reduce()`, ...); algorithms

→ http://thrust.github.io/
http://docs.nvidia.com/cuda/thrust/

Thrust

Code example

```
int a = 42;
int n = 10;
thrust::host_vector<float> x(n), y(n);
// fill x, y

thrust::device_vector d_x = x, d_y = y;

using namespace thrust::placeholders;
thrust::transform(d_x.begin(), d_x.end(), d_y.begin(), d_y.begin(), a * _1 + _2);

x = d_x;
```

Task 8-3

Vector Addition with Thrust

- Use Thrust for reduction, everything else of vector addition with OpenACC

Task 8-3: OpenACC+Thrust

- Change to `Task8-3/` directory
- Work on TODOs in `vecAddRed.c` and `thrustWrapper.cu`
  - Use `host_data use_device` to provide correct pointer
  - Implement call to `thrust::reduce` using `c_ptr`
- Compile: `make`
- Submit to the batch system: `make run`

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cuFFT

Task 8-4

Stating the Problem

- We want to solve the Poisson equation

$$\Delta\Phi(x,y) = -\rho(x,y)$$

  with periodic boundary conditions in x and y
- Needed, e.g., for finding electrostatic potential Φ for a given charge distribution ρ
- Model problem

$$\begin{aligned} \rho(x,y) &= \cos(4\pi x)\sin(2\pi y) \\ (x,y) &\in [0,1)^2 \end{aligned}$$

- Analytically known: $\Phi(x,y) = \Phi_0 \cos(4\pi x)\sin(2\pi y)$
- Let's solve the Poisson equation with a Fourier Transform!

Task 8-4

Introduction to Fourier Transforms

- Discrete Fourier Transform and Re-Transform:

$$\hat{f}_k = \sum_{j=0}^{N-1} f_j e^{-\frac{2\pi i k}{N} j} \quad \Leftrightarrow \quad f_j = \sum_{k=0}^{N-1} \hat{f}_k e^{\frac{2\pi i j}{N} k}$$

- Time for all $\hat{f}_k$: $\mathcal{O}(N^2)$
- Fast Fourier Transform: Recursively splitting $\rightarrow \mathcal{O}(N \log(N))$
- Find derivatives in Fourier space:

$$f_j' = \sum_{k=0}^{N-1} i k \hat{f}_k e^{\frac{2\pi i j}{N} k}$$

It's just multiplying by ik!

Task 8-4

Plan for FFT Poisson Solution

Start with charge density ρ

1. Fourier-transform ρ
   $\hat{\rho} \leftarrow \mathcal{F}(\rho)$
2. *Integrate* ρ in Fourier space twice
   $\hat{\phi} \leftarrow -\hat{\rho} / \left(k_x^2 + k_y^2\right)$
3. Inverse Fourier-transform $\hat{\phi}$
   $\phi \leftarrow \mathcal{F}^{-1}(\hat{\phi})$

cuFFT

OpenACC

cuFFT

Task 8-4

cuFFT

- cuFFT: NVIDIA's (Fast) Fourier Transform library
  - 1D, 2D, 3D transforms; complex and real data types
  - Asynchronous execution
  - Modeled after FFTW library (API)
  - Part of CUDA Toolkit

  → https://developer.nvidia.com/cufft

```
cufftDoubleComplex *src, *tgt;                 // Device data!
cufftHandle plan;
// Setup 2d complex-complex trafo w/ dimensions (Nx, Ny)
cufftCreatePlan(plan, Nx, Ny, CUFFT_Z2Z);
cufftExecZ2Z(plan, src, tgt, CUFFT_FORWARD); // FFT
cufftExecZ2Z(plan, tgt, tgt, CUFFT_INVERSE); // iFFT
// Inplace trafo  ^----^
cufftDestroy(plan);                            // Clean-up
```

Task 8-4

Synchronizing cuFFT

- CUDA Streams enable interleaving of computational tasks
- cuFFT uses streams for asynchronous execution
- cuFFT runs in default CUDA stream;
  OpenACC not $\rightarrow$ trouble

$\Rightarrow$ Force cuFFT on OpenACC stream

```
#include <openacc.h>
// Obtain the OpenACC default stream id
cudaStream_t accStream = (cudaStream_t) acc_get_cuda_stream(acc_async_sync);
// Execute all cufft calls on this stream
cufftSetStream(accStream);
```

Task 8-4

TASK 8-4

OpenACC and cuFFT

- Use case: Fourier transforms
- Use cuFFT and OpenACC to solve Poisson's Equation

Task 8-4: OpenACC+cuFFT

- Change to `Task8-4/` directory
- Work on TODOs in `poisson.c`

  `solveRSpace` Force cuFFT on correct stream; implement data handling with `host_data use_device`

  `solveKSpace` Implement data handling and parallelism
- Compile: `make`
- Submit to the batch system: `make run`

Conclusions

Conclusions

- OpenACC directives and clauses
  `#pragma acc parallel loop copyin(A[0:N]) reduction(max:err) vector`
- Start easy, optimize from there
- PGI / NVIDIA Visual Profiler help to find bottlenecks
- OpenACC is interoperable to other GPU programming models
- Don’t forget the CPU version!

Thank you for your attention!

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List of Tasks

Task 0*: Setup
Task 2: A First Parallel Loop
Task 3: More Parallel Loops
Task 4: Data Copies
Task 5: Data Region
Task 6: More Parallelism
Task 7: Loop Ordering
Task 7': Pinned Memory
Task 8-1: OpenACC+cuBLAS
Task 8-2: OpenACC+CUDA
Task 8-3: OpenACC+Thrust
Task 8-4: OpenACC+cuFFT

Glossary I

API A programmatic interface to software by well-defined functions. Short for application programming interface. 49

CUDA Computing platform for GPUs from NVIDIA. Provides, among others, CUDA C/C++. 10, 17, 24, 49, 62, 63, 90, 108, 111, 117, 118, 119, 128, 129, 134, 136

GCC The GNU Compiler Collection, the collection of open source compilers, among others for C and Fortran. 23, 26

NVIDIA US technology company creating GPUs. 19, 49, 61, 64, 69, 70, 71, 103, 114, 128, 132, 135, 136, 137

Glossary II

OpenACC Directive-based programming, primarily for many-core machines. 2, 17, 18, 19, 20, 21, 22, 24, 25, 26, 27, 28, 29, 32, 38, 39, 41, 43, 45, 49, 52, 55, 60, 64, 65, 72, 76, 79, 84, 85, 88, 90, 91, 103, 105, 106, 108, 109, 111, 114, 115, 116, 119, 123, 127, 129, 130, 132, 134

OpenCL The *Open Computing Language*. Framework for writing code for heterogeneous architectures (CPU, GPU, DSP, FPGA). The alternative to CUDA. 17

OpenMP Directive-based programming, primarily for multi-threaded machines. 2, 17, 20, 54

PAPI The Performance API, a C/C++ API for querying performance counters. 33

Pascal GPU architecture from NVIDIA (announced 2016). 62, 63

Glossary III

perf Part of the Linux kernel which facilitates access to performance counters; comes with command line utilities. 33

PGI Compiler creators. Formerly *The Portland Group, Inc.*; since 2013 part of NVIDIA. 2, 23, 26, 33

Thrust A parallel algorithms library for (among others) GPUs. See `https://thrust.github.io/`. 17, 120, 121, 122, 123, 134

CPU Central Processing Unit. 4, 5, 6, 7, 8, 9, 23, 49, 62, 63, 99, 101, 109, 132, 136

GPU Graphics Processing Unit. 2, 3, 4, 5, 6, 7, 8, 9, 11, 12, 13, 17, 18, 23, 25, 45, 49, 61, 62, 63, 64, 69, 75, 77, 103, 109, 115, 118, 132, 135, 136, 137

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