Intermediate OpenMP for Perl Programmers

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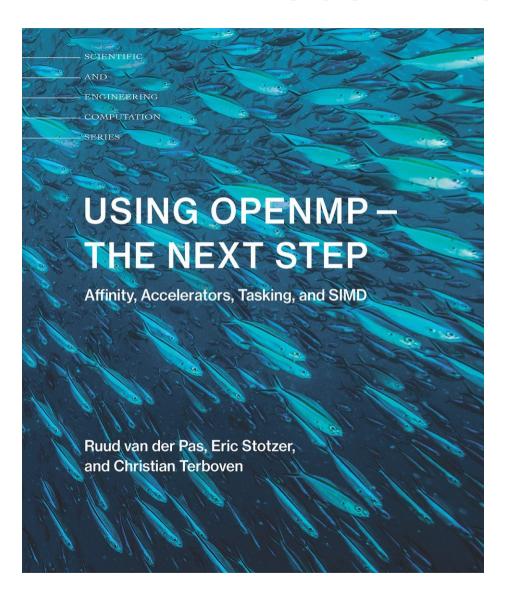
GCC – GOMP

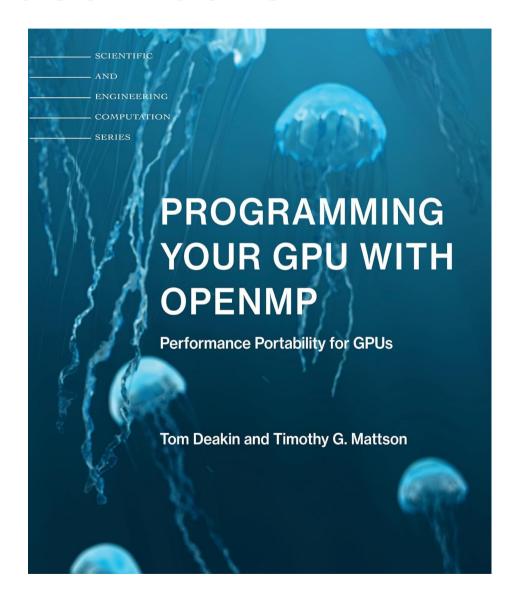
GNU Offloading and Multi Processing Runtime Library https://gcc.gnu.org/wiki/openmp

- GCC 4.2 supports OpenMP spec 2.5
- GCC 4.4 supports OpenMP spec 3.0
- GCC 4.7 supports OpenMP spec 3.1
- OpenMP spec 4.1 support:
 - C/C++ support in GCC 4.9
 - Fortran support in GCC 4.9.1
- GCC 5 supports offloading (e.g., to GPU)
- GCC 6 supports OpenMP spec 4.5 for C/C++
- GCC 7 mostly supports OpenMP spec 4.5 for Fortran (fully in GCC 11)
- GCC 9 partially supports OpenMP spec 5.0 for C/C++
- GCC 10 adds OpenMP spec 5.0 support and initial Fortran support



Recommended Books







Talk Assumptions

- Discussing only C examples (so C++ or Fortran)
- Information based on OpenMP spec 4.5
- Any GCC >= 5

Note: regarding wider compiler support:

- OpenMP is supported by many commercial compilers
- Inline::C uses the compiler used to create perl
- We assume 99+% perl's are compiled with GCC



Current State of Perl Options

OpenMP is best accessed from Perl via Inline::C. We assume GCC (see previous slide). Examples in this talk will use the following Perl modules:

- Alien::OpenMP
 - Works "with" Inline::C
- OpenMP::Simple
 - Alien::OpenMP + helper C functions & macros
- OpenMP::Environment
 - Perlish way to interact with %ENV OpenMP cares about
- No compiler support beyond GCC is planned (is there a demand?)



Example Perl Program

```
use strict;
use warnings;
use OpenMP::Simple;
use OpenMP::Environment;
use Test::More tests => 8;
use Inline (
   C = > 'DATA',
   with => qw/OpenMP::Simple/,
);
my $env = OpenMP::Environment->new;
note qq{Testing macro provided by OpenMP::Simple, 'PerlOMP UPDATE WITH ENV NUM THREADS'};
for my $num threads (1 .. 8) {
   my $current value = $env->omp num threads($num threads);
   is get num threads(), $num threads,
       sprintf qq{The number of threads (%0d) spawned in the OpenMP runtime via OMP NUM THREADS, as expected},
       $num threads;
 DATA
int get num threads() {
 PerlOMP UPDATE WITH ENV NUM THREADS
 int ret = 0;
 #pragma omp parallel
    #pragma omp single
   ret = omp get num threads();
 return ret;
 END
```





General Use Case Addressed

- An HPC developer familiar with OpenMP and Perl wants to use Perl as "host" language as the driver for OpenMP based Inline::C calls
- The perl process is not threaded, subroutines are
- Perl variables are fairly regular (e.g., 1D or 2D arrays, list of strings, etc)
- Nearly all data accesses to Perl variable is read-only



Example, OpenMP + C + GCC

```
#include <stdio.h>
#include <omp.h>
int main() {
                                     ./first-example.x
                                   running with 48 threads
 int ret = 0:
 #pragma omp parallel
  #pragma omp single
   ret = omp_get_num_threads();
 printf("running with %d threads\n", ret);
 return ret;
```



Example, OpenMP + Perl

```
use strict;
                                                                  ok 1 - The number of threads (1) spawned in the OpenMP
use warnings;
                                                                         runtime via OMP NUM THREADS, as expected
                                                                  ok 2 - The number of threads (2) spawned in the OpenMP
                                                                         runtime via OMP NUM THREADS, as expected
use OpenMP::Simple;
                                                                  ok 3 - The number of threads (3) spawned in the OpenMP
use OpenMP::Environment;
                                                                         runtime via OMP NUM THREADS, as expected
Use Test::More tests => 8;
                                                                  ok 4 - The number of threads (4) spawned in the OpenMP
                                                                         runtime via OMP NUM THREADS, as expected
use Inline (
                                                                  ok 5 - The number of threads (5) spawned in the OpenMP
           => 'DATA',
                                                                         runtime via OMP NUM THREADS, as expected
     with => qw/OpenMP::Simple/,
                                                                  ok 6 - The number of threads (6) spawned in the OpenMP
                                                                         runtime via OMP NUM THREADS, as expected
);
                                                                  ok 7 - The number of threads (7) spawned in the OpenMP
                                                                         runtime via OMP NUM THREADS, as expected
my $env = OpenMP::Environment->new;
                                                                  ok 8 - The number of threads (8) spawned in the OpenMP
                                                                         runtime via OMP NUM THREADS, as expected
for my $num threads (1 .. 8) {
     my $current value = $env->omp num threads($num threads);
     is _get_num_threads(), $num_threads,
        sprintf gg{The number of threads (%0d) spawned in the OpenMP
               runtime via OMP NUM THREADS, as expected}, $num threads;
  DATA
int _get_num_threads() {
  PerlOMP UPDATE WITH ENV NUM THREADS
  int ret = 0;
  #pragma omp parallel
     #pragma omp single // first thread to reach here runs it, no others
     ret = omp get num threads();
  return ret;
```

pen**MP**

Recap

 Following slides recap the last few talks on OpenMP

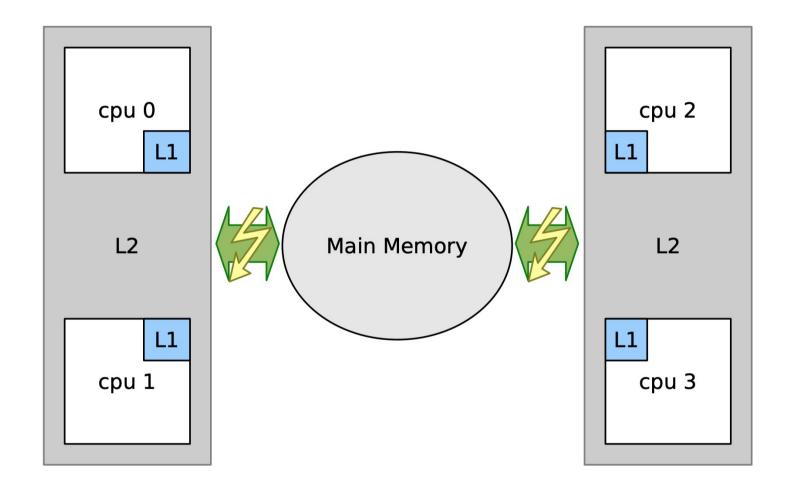
 Please find and watch my other TPRC talks on OpenMP for Perl programmers

And here we go...





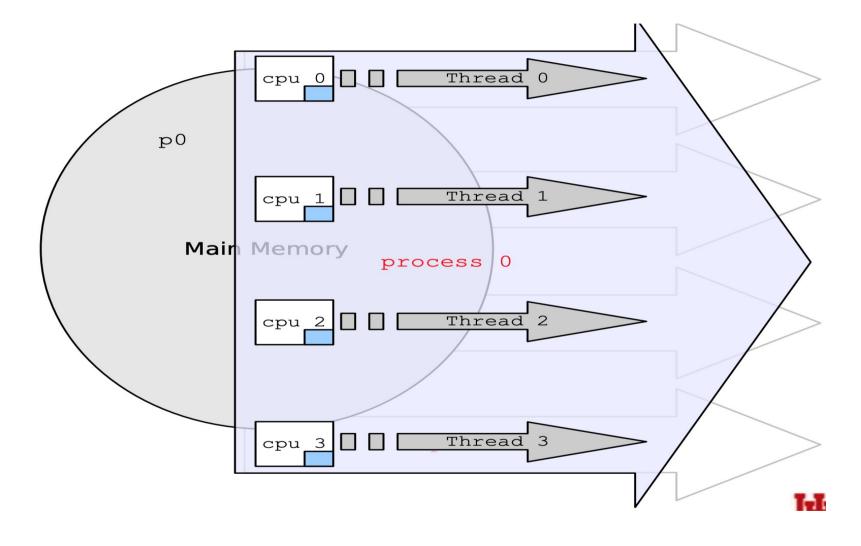
OpenMP Memory Models







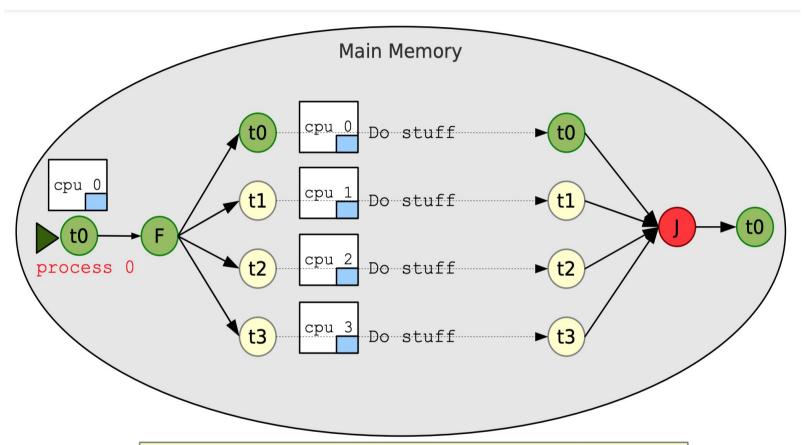
OpenMP Memory Models







OpenMP Execution Model



Here, thread 0 is on CPU 0; at the fork, 3 new threads are created and are distributed to the remaining 3 CPUs.





Variables

- Variables can shared among threads
- Or can be private to a thread
- Variable initializations can be specified





Worksharing

Parallelizing loops across threads

```
#include <stdio.h>
#include <omp.h>
int main() {
    int matrix[10][15];
    int i, j;
    // Initialize matrix
   for (i = 0; i < 10; ++i) {
        for (j = 0; j < 15; ++j) {
            matrix[i][j] = i * M + j;
    // Parallel region with shared clause
    #pragma omp parallel shared(matrix) private(i, j)
        #pragma omp for
        for (i = 0; i < 10; ++i) {
            printf("Thread %d handles row %d\n", omp_get_thread_num(), i);
            for (j = 0; j < 15; ++j) {
                matrix[i][j] *= 2; // Modify matrix element
   return 0;
```





Atomicity

- Memory can be set aside and updated safely, using, #pragma omp atomic
- #pragma omp critical is also an option





```
#include <stdio.h>
#include <omp.h>
int main() {
   #pragma omp parallel
     #pragma omp single
                           // Only 1 thread is running
                           // Task #1
        #pragma omp task
          printf("Perl ");
                                                     qcc -fopenmp ./basic-task.c
                                                     OMP NUM THREADS=4 ./a.out
        #pragma omp task
                           // Task #2
                                                   Perl rocks!
          printf("rocks! ");
                                                   $ OMP NUM THREADS=4 ./a.out
                                                   rocks! Perl
        // <~ other threads begin executing
           tasks at the end of the 'single'
           block
   return 0;
```

- Tasking was introduced in 2008 in OpenMP 3.0 (GCC 4.4)
- Generated tasks are atomically assigned to an available (real) CPU thread
- 2 different execution orderings are possible (<u>see output</u>)

- Any thread can generate a task
- #pragma omp single when starting out so that you can think about your code more easily
- All threads in the parallel region are available to pick up a task
- #pragma omp taskwait is a synchronization barrier – when no more new tasks are available, all threads wait until all theads are idle to proceed



```
private (list)
firstprivate (list)
default (shared none)
if ([task:] scalar-logical-expression)
final (scalar-logical-expression)
mergeable
depend (dependency-type: list)
priority (priority-value)
untied
Affected by:
OMP_MAX_TASK PRIORITY
                        (supported by OpenMP::Environment)
```



Synchronizing Tasks

```
#include <stdio.h>
#include <omp.h>
int main() {
   #pragma omp parallel
     #pragma omp single
                         // Only 1 thread is running
                           // Task #1
        #pragma omp task
          printf("Perl ");
                                                  $ qcc -fopenmp ./basic-task.c
                                                  $ OMP NUM THREADS=4 ./a.out
        #pragma omp taskwait
                                                  Perl rocks!
        #pragma omp task
                           // Task #2
                                                  $ OMP NUM THREADS=4 ./a.out
          printf("rocks! ");
                                                  Perl rocks!
                                                  $ OMP_NUM_THREADS=4 ./a.out
                                                  Perl rocks!
   return 0;
}:w
```

- Tasking was introduced in 2008 in OpenMP 3.0 (GCC 4.4)
- Generated tasks are atomically assigned to an available (real) CPU thread
- 2 different execution orderings are possible (<u>see output</u>)

OpenMP Tasking + Perl

```
use strict;
use warnings;
                                                                on 1 threads!
                                                                rocks Perl on 2 threads!
use OpenMP::Simple;
                                                                rocks Perl Perl rocks on 3 threads!
use OpenMP::Environment;
                                                                Perl rocks on 4 threads!
                                                                Perl rocks on 5 threads!
use Inline (
                                                                Perl rocks on 6 threads!
         => 'DATA',
                                                                Perl rocks on 7 threads!
    with => qw/OpenMP::Simple/.
                                                                Perl rocks on 8 threads!
) ;
                                                                Perl rocks on 9 threads!
                                                                Perl rocks on 10 threads!
my Senv = OpenMP::Environment->new;
                                                                Perl rocks on 11 threads!
                                                                Perl rocks on 12 threads!
                                                                Perl rocks on 13 threads!
for my $num_threads ( 1 .. 16 ) {
                                                                Perl rocks on 14 threads!
    my $current value = $env->omp num threads($num threads);
                                                                Perl rocks on 15 threads!
    my $qot threads = run tasks();
                                                                Perl rocks on 16 threads!
 DATA
int run_tasks() {
    int got num threads = 0;
    PerlOMP UPDATE WITH ENV NUM THREADS
    #pragma omp parallel
        got num threads = omp get num threads();
        #pragma omp single // Ensure only one thread creates the initial task
          #pragma omp task
                               // Task #1
          {printf("Perl ");}
          #pragma omp task
          {printf("rocks ");} // Task #2
          #pragma omp task
          {printf("on %d threads!\n", got_num_threads);} // Task #3
          #pragma omp taskwait
    return got_num_threads;
```



Thread Affinity

- Setting thread affinity (OMP_PROC_BIND) helps optimize performance by improving cache and memory access patterns on NUMA architectures.
- OMP_PROC_BIND has 4 possible values:
 - true or close (as in near)
 - master
 - spread
 - false (or unset)



Thread Affinity

- OMP_PROC_BIND=true Or OMP_PROC_BIND=close:
 - Threads are bound close to where the master thread is running. It is useful for ensuring threads operate near each other to minimize cross-socket memory access.
- OMP_PROC_BIND=spread:
 - Threads are spread out across the available sockets (NUMA nodes). This setting aims to balance the workload across all available CPU sockets.
- OMP_PROC_BIND=master:
 - Threads are bound to the same CPU core as the master thread. This can be useful in scenarios where thread locality with respect to the master thread is critical.
- OMP_PROC_BIND=false or unset:
 - OpenMP runtime system decides the thread binding strategy based on the system default or runtime decisions. This may vary between different OpenMP implementations and system configurations.



Thread Affinity

```
use strict;
use warnings;
use OpenMP::Simple;
use OpenMP::Environment;
use Inline (
   C = > 'DATA',
    with => qw/OpenMP::Simple/,
);
my $env = OpenMP::Environment->new;
foreach my $policy (qw/true close spread master false/) {
  for my $num_threads ( 1 .. 16 ) {
    my $current value = $env->omp num threads($num threads);
   my $current_policy = $env->omp_proc_bind($policy);
                                                                            OpenMP runtime
    my $got threads = runit();
___DATA
int runit() {
    PerlOMP_UPDATE_WITH_ENV__NUM_THREADS
    // Start a parallel region
    #pragma omp parallel
        int thread_id = omp_get_thread_num();
       printf("Thread %d is running on CPU %d\n", thread_id, sched_getcpu());
    return 0;
  END
```



SIMD

Single Instruction Multiple Data

- SIMD and Performance: <u>SIMD OpenMP directives are essential for achieving high performance on modern processors by exploiting parallelism at the instruction level.</u> Proper usage of SIMD can significantly accelerate computational tasks that operate on large arrays or matrices.
- Limitations: Not all loops can be effectively vectorized using SIMD directives. Loop-carried dependencies, complex control flow, or irregular memory access patterns may hinder vectorization.
- Evolution: OpenMP continues to evolve with newer versions (5.0 and beyond), introducing enhancements and new features for SIMD support, such as SIMD-awareness in array sections (simd clause with aligned, linear, etc.).
- The simd construct has been introduced, but no new environmental variables or runtime functions have been introduced to support it.



SIMD Example

```
#include <stdio.h>
#include <omp.h>
int main() {
    int matrix[100][50];
    int result[100][50];
    int i, j, k; // Declare loop indices outside of the loops
    // Initialize matrix
    for (i = 0; i < 100; ++i) {
        for (i = 0; j < 50; ++j)
            matrix[i][j] = i * 50 + j;
    // Parallel region with nested loop vectorization
    #pragma omp parallel for collapse(2) private(i, j, k)
    for (i = 0; i < 100; ++i) {
        for (j = 0; j < 50; ++j) {
            #pragma omp simd
            for (k = 0; k < 4; ++k)  // Assume vector length is 4
                result[i][j] += matrix[i][j] * k;
    return 0;
```



SIMD Support in CPUs

- x86 (Intel and AMD):
 - SSE (Streaming SIMD Extensions): Introduced with Pentium III processors, SSE provides SIMD support for operations on floating-point and integer data types. SSE has evolved through multiple versions (SSE2, SSE3, SSE4) with increased capabilities for parallel processing.
 - AVX (Advanced Vector Extensions): AVX builds upon SSE and offers wider SIMD registers (256-bit and 512-bit), enabling higher throughput for vectorized operations.
 AVX2 and AVX-512 further enhance vectorization performance.
- ARM (Various Manufacturers):
 - NEON: NEON is ARM's SIMD architecture extension, providing similar functionality to SSE on x86 processors. It supports vector operations on integers and floating-point data types, enhancing performance for multimedia and signal processing applications.
- Compiler vendors such as GCC, Intel ICC, Clang, and others implement SIMD support for various architectures. They provide tools and flags (-fopenmp, -mavx, -mfpu=neon, etc.) to enable and control SIMD vectorization, ensuring compatibility with OpenMP directives for parallel programming.





Heterogeneous Architectures

(e.g., GPUs)

```
#include <stdio.h>
#include <omp.h>
int main() {
  int a = 10, b = 20, c;
  #pragma omp target map(from:c)
     c = a + b;
  printf("Result: %d\n", c);
  return 0;
```



Compiling for GPUs

Requires use of target OpenMP directive

 Requires compiler support that link to external libraries (e.g., CUDA, etc)

Enabled in gcc via -fopenmp



GCC Offloading & nvptx-none

Offloading Support:

GCC introduced support for offloading computations to accelerators such as GPUs starting from version 4.9. This allows parallel sections of code annotated with OpenMP directives (target, parallel, etc.) to be executed on devices like NVIDIA GPUs.

Target Architecture:

-foffload=nvptx-none specifies that the offloaded code should target NVIDIA GPUs using the NVIDIA Parallel Thread Execution (PTX) intermediate representation (nvptx). PTX is a portable assembly-like language that NVIDIA GPUs can execute.

Compilation Process:

When you compile a program with **-foffload=nvptx-none**, GCC generates PTX code (nvptx) instead of native GPU machine code. PTX is architecture-independent and serves as an intermediate representation.

The generated PTX code can then be further compiled and optimized by NVIDIA's CUDA toolchain (nvptx-as, nvptx-nvcc) into executable machine code (cubin) that runs on NVIDIA GPUs.



GCC Offloading & nvptx-none

Command Usage:

Example command to compile a program (program.c) with OpenMP offloading to NVIDIA GPUs:

```
gcc -o program -fopenmp -foffload=nvptx-none program.c
```

- -fopenmp: Enables OpenMP support in GCC.
- -foffload=nvptx-none: Specifies that the offloaded code should target NVIDIA GPUs using PTX.

CUDA Toolkit Requirement:

To execute programs compiled with <code>-foffload=nvptx-none</code>, you need to have the NVIDIA CUDA toolkit installed on your system. The CUDA toolkit provides necessary libraries and tools (nvptx-as, nvptx-nvcc) to compile PTX code into executable GPU machine code.

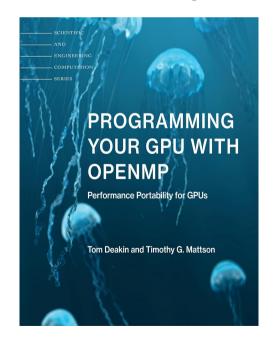
Hardware and Driver Support:

Ensure that your system has compatible NVIDIA GPU hardware ad drivers installed. The CUDA toolkit supports a wide range of NVIDIA GPUs, and performance can vary based on GPU architecture and capabilities.



More OpenMP, GPUs, Offloading

- https://gcc.gnu.org/projects/gomp/
- https://gcc.gnu.org/wiki/Offloading
- Many online tutorials and examples
- Books exist, such as:





Present & Future Direction

- All Perl modules presented here are geared towards running and controlling Inline:: C with OpenMP
- Current work is easy getting Perl variables into and out of Inline::C'd functions
- Near future: more options from OpenMP::Simple for OpenMP first programmers (variable IN,OUT; internal transforms)
- Ultimate goal: provide thread-safe (OpenMP) RW of variables directly via Perl API (or similar type of library via OpenMP::Simple)



Perl+OpenMP for Fortran?

- Very possible with gfortran and highly desirable, but ..
- I'd need a suitable Inline module for Fortran 90
- I am open to doing this pro bono if we had a working Inline::Fortran module



OpenACC

- a programming standard for parallel computing developed by Cray, CAPS, Nvidia and PGI
- Same directives/runtime based approach as OpenMP
- Also supported by GCC (9.1 offers "nearly complete OpenACC spec 2.5 support)
- Perl+OpenMP project has no intention to support it
- But the opportunity is there
- I am open to being sponsored for the work



Perl+OpenMP

Where it happens!

- https://github.com/Perl-OpenMP
- May become part of Perl Community's HPC Perl Committee (details still being worked out)





Thank You













