Codee Training Series

April 26-27, 2022

NERSC

codee

Shift Left Performance

Automated Code inspection for Performance

Walkthrough Exercise: Calculating π on the GPU with OpenMP/OpenACC

Goals

- Produce OpenACC version for GPU
- Produce OpenMP version for GPU
- Build & run an OpenMP code on the GPU (for problem size N=900000000)
- Build & run an OpenACC code on the GPU (for problem size N=900000000)

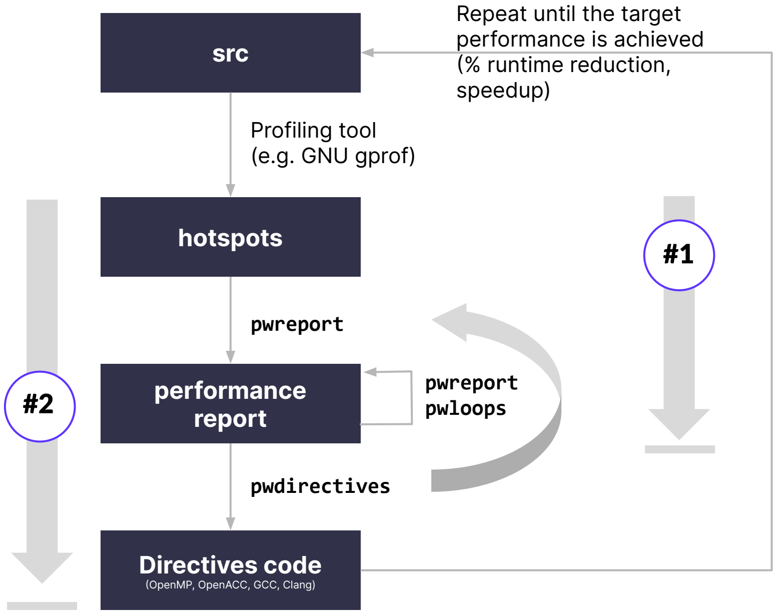
The GPU programming challenges: Example code PI

		Challenges of GPU acceleration addressed in introductory course			Other GPU programming challenges to be addressed in next advanced course			
		Find opportunities for offloading	Optimize memory layout for data transfers	Identify defects in data transfers	Exploit massive parallelism through loop nest collapsing	Minimize data transfers across consecutive loop nests	Minimize data transfers through convergence loops	Identify auxiliary functions to be offloaded
Example codes used in this introductory course	PI	x	-	-	-	-	-	-
	MATMUL	x	x	x	x	x	-	-
	LULESHmk	x	x	x	x	x	x	x
	HEAT	x	-	-	-	x	x	-
	Your code!	Probably all of these challenges apply, and even more!						

The source code of PI

```
int main(int argc, char *argv[]) {
    if (argc != 2) {
        printf("Usage: %s <steps>\n", argv[0]);
        printf("  <steps> controls the precision of the approximation.\n");
        return 0;
    }

    // Reads the test parameters from the command line
    unsigned long N = atol(argv[1]);
    printf("- Input parameters\n");
    printf("steps\t= %lu\n", N);

    printf("- Executing test...\n");
    double time_start = getClock();
    // ================================================

    double out_result;

    double sum = 0.0;
    for (int i = 0; i < N; i++) {
        double x = (i + 0.5) / N;
        sum += sqrt(1 - x * x);
    }

    out_result = 4.0 / N * sum;

    // ================================================
    double time_finish = getClock();

    // Prints an execution report
    printf("time (s)= %.6f\n", time_finish - time_start);
    printf("result\t= %.8f\n", out_result);
    const double realPiValue = 3.141592653589793238;
    printf("error\t= %.1e\n", fabs(out_result - realPiValue));

    return 0;
}
```

Inspecting the code and optimizing its performance with Codee



- **#1** **Get the performance optimization report for the whole code base**
- **#2** **Create performance-optimized code for the hotspot automatically**

1: Produce the entry-level report for default #actions (`pwreport --evaluation`)

```
$ pwreport --evaluation pi.c
Target Lines of code Analyzed lines Analysis time # actions Effort Cost   Profiling
------ ------------- -------------- ------------- --------- ------ ------ ---------
pi.c   43            4              33 ms         2         16 h   523€   n/a

ACTIONS PER OPTIMIZATION TYPE
Target Serial scalar Serial control Serial memory Vectorization Multithreading Offloading
------ ------------- -------------- ------------- ------------- -------------- ----------
pi.c   0             0              0             2             n/a            n/a

Target : analyzed directory or source code file
Lines of code : total lines of code found in the target (computed the same way as the sloccount tool)
Analyzed lines : relevant lines of code successfully analyzed
Analysis time : time required to analyze the target
# actions : total actionable items (opportunities, recommendations, defects and remarks) detected
Effort : estimated number of hours it would take to carry out all actions (serial scalar, serial control, serial memory, vectorization,
multithreading and offloading with 1, 2, 4, 8, 12 and 16 hours respectively)
Cost : estimated cost in euros to carry out all the actions, paying the average salary of 56,286€/year for a professional C/C++ developer
working 1720 hours per year
Profiling : estimation of overall execution time required by this target

SUGGESTIONS
  You can specify multiple inputs which will be displayed as multiple rows (ie. targets) in the table, eg:
        pwreport --evaluation some/other/dir pi.c

  Use --actions to find out details about the detected actions:
        pwreport --actions pi.c

  Multithreading and offloading actions are filtered by default. Use --include-tags to enable them:
        pwreport --include-tags all pi.c

  You can focus on a specific optimization type by filtering by its tag (serial-scalar, serial-control, serial-memory, vectorization,
multithreading, offloading), eg.:
        pwreport --actions --include-tags serial-scalar pi.c

1 file successfully analyzed and 0 failures in 33 ms
```

By default multithreading and offloading are disabled in Codee.

Rationale: Codee forces the user to explicitly enable multithreading and offloading capabilities to avoid common errors resulting from a misconfigured software environment (eg. lack of an OpenMP compiler with offload)

2: Produce the entry-level report for ALL #actions (pwreport --evaluation --include-tags all)

```
$ pwreport --evaluation --include-tags all pi.c
Target Lines of code Analyzed lines Analysis time # actions Effort Cost    Profiling
------ ------------- -------------- ------------- --------- ------ ------- ---------
pi.c   43            4              34 ms         4         44 h   1439€   n/a

ACTIONS PER OPTIMIZATION TYPE
Target Serial scalar Serial control Serial memory Vectorization Multithreading Offloading
------ ------------- -------------- ------------- ------------- -------------- ----------
pi.c   0             0              0             2             1              1

Target : analyzed directory or source code file
Lines of code : total lines of code found in the target (computed the same way as the sloccount tool)
Analyzed lines : relevant lines of code successfully analyzed
Analysis time : time required to analyze the target
# actions : total actionable items (opportunities, recommendations, defects and remarks) detected
Effort : estimated number of hours it would take to carry out all actions (serial scalar, serial control, serial memory, vectorization,
multithreading and offloading with 1, 2, 4, 8, 12 and 16 hours respectively)
Cost : estimated cost in euros to carry out all the actions, paying the average salary of 56,286€/year for a professional C/C++ developer
working 1720 hours per year
Profiling : estimation of overall execution time required by this target

SUGGESTIONS
  You can specify multiple inputs which will be displayed as multiple rows (ie. targets) in the table, eg:
        pwreport --evaluation some/other/dir --include-tags all pi.c

  Use --actions to find out details about the detected actions:
        pwreport --actions --include-tags all pi.c

  You can focus on a specific optimization type by filtering by its tag (serial-scalar, serial-control, serial-memory, vectorization,
multithreading, offloading), eg.:
        pwreport --actions --include-tags serial-scalar pi.c

1 file successfully analyzed and 0 failures in 34 ms
```

By enabling ALL actions in the report now identifies 1 offload opportunity

3: Produce the report of ALL #actions per type of loops (pwreport --evaluation --include-tags all --level 2)

```
$ pwreport --evaluation --level 2 --include-tags all pi.c
Target Lines of code Analyzed lines Analysis time # actions Effort Cost    Profiling
------ ------------- -------------- ------------- --------- ------ ------- ---------
pi.c   43            4              33 ms         4         44 h   1439€   n/a

ACTIONS PER OPTIMIZATION TYPE
Target Serial scalar Serial control Serial memory Vectorization Multithreading Offloading
------ ------------- -------------- ------------- ------------- -------------- ----------
pi.c   0             0              0             2             1              1

ACTIONS PER LOOP TYPE PER OPTIMIZATION TYPE
Loop Type No. Loops Serial scalar Serial control Serial memory Vectorization Multithreading Offloading
--------- --------- ------------- -------------- ------------- ------------- -------------- ----------
Low       1         0             0              0             2             1              1
Medium    0         0             0              0             0             0              0
High      0         0             0              0             0             0              0

Target : analyzed directory or source code file
Lines of code : total lines of code found in the target (computed the same way as the sloccount tool)
Analyzed lines : relevant lines of code successfully analyzed
Analysis time : time required to analyze the target
# actions : total actionable items (opportunities, recommendations, defects and remarks) detected
Effort : estimated number of hours it would take to carry out all actions (serial scalar, serial control, serial memory, vectorization,
multithreading and offloading with 1, 2, 4, 8, 12 and 16 hours respectively)
Cost : estimated cost in euros to carry out all the actions, paying the average salary of 56,286€/year for a professional C/C++ developer
working 1720 hours per year
Profiling : estimation of overall execution time required by this target

SUGGESTIONS
  You can specify multiple inputs which will be displayed as multiple rows (ie. targets) in the table, eg:
        pwreport --evaluation some/other/dir --include-tags all pi.c

  Use --actions to find out details about the detected actions:
        pwreport --actions --include-tags all pi.c

  You can focus on a specific optimization type by filtering by its tag (serial-scalar, serial-control, serial-memory, vectorization,
multithreading, offloading), eg.:
        pwreport --actions --include-tags serial-scalar pi.c

1 file successfully analyzed and 0 failures in 33 ms
```

By increasing the details of the report, the tool reports that ALL the actions are identified in the scope of loops that have LOW difficulty from the performance optimization viewpoint

4: Produce the Codee Actions Report for the target function (pwreport --actions)

```
$ pwreport --actions --include-tags all pi.c:main
ACTIONS REPORT

  FUNCTION BEGIN at pi.c:main:12:1
    12: int main(int argc, char *argv[]) {

    LOOP BEGIN at pi.c:main:31:5
      31:     for (int i = 0; i < N; i++) {

      [RMK011] pi.c:31:5 the vectorization cost model states the loop might benefit from explicit vectorization

      [OPP001] pi.c:31:5 is a multi-threading opportunity
      [OPP002] pi.c:31:5 is a SIMD opportunity
      [OPP003] pi.c:31:5 is an offload opportunity
    LOOP END
  FUNCTION END


CODE COVERAGE
  Analyzable files:            1 / 1     (100.00 %)
  Analyzable functions:        1 / 1     (100.00 %)
  Analyzable loops:            1 / 1     (100.00 %)
  Parallelized SLOCs:          0 / 25    (  0.00 %)

METRICS SUMMARY
  Total recommendations:        0
  Total opportunities:          3
  Total defects:                0
  Total remarks:                1

SUGGESTIONS

  Use --level 0|1|2 to get more details, e.g:
        pwreport --level 2 --actions --include-tags all pi.c:main

  3 opportunities for parallelization were found in your code, get more information with pwloops:
        pwloops pi.c:main

  More details on the defects, recommendations and more in the Knowledge Base:

        https://www.appentra.com/knowledge/
1 file successfully analyzed and 0 failures in 34 ms
```

Each action is reported in the scope of the corresponding loop:
- vectorization (loop:31 OPP002 related to RMK011)
- multithreading (loop:31 OPP001)
- offloading (loop:31 OPP003)

5: Produce the detailed actions for the target function (`pwreport --actions --level 2`)

```
$ pwreport --actions --level 2 --include-tags all pi.c:main
ACTIONS REPORT

  FUNCTION BEGIN at pi.c:main:12:1
    8: int main(int argc, char *argv[]) {

    LOOP BEGIN at pi.c:main:31:5
      31:     for (int i = 0; i < N; i++) {
      32:         double x = (i + 0.5) / N;
      33:         sum += sqrt(1 - x * x);
      34:     }

      [OPP003] pi.c:31:5 is an offload opportunity
        Compute patterns:
          - 'scalar' over the variable 'sum'

        SUGGESTION: use pwloops to get more details or pwdirectives to generate directives:
          pwloops pi.c:main:31:5
          pwdirectives --omp offload pi.c:main:31:5 --in-place
          pwdirectives --acc pi.c:main:31:5 --in-place

        More information on: https://www.appentra.com/knowledge/opportunities

    LOOP END
  FUNCTION END
. . .
```

By enabling the detailed report for OPP003 (offload opportunity) you obtain suggestions to invoke pwdirectives for automatic annotation of the source code with OpenMP and OpenACC offload directives
(note: source code edited "in-place" by default")

6a: Annotate the code for GPU + OpenMP (pwdirectives --omp offload)

```
$ pwdirectives --omp offload pi.c:main:31:5 -o pi_ompOff.c
Results for file 'pi.c':
  Successfully parallelized loop at 'pi.c:main:31:5' [using offloading]:
      [INFO] pi.c:31:5 Parallel scalar reduction pattern identified for variable 'sum' with associative, commutative operator '+'
      [INFO] pi.c:31:5 Available parallelization strategies for variable 'sum'
      [INFO] pi.c:31:5   #1 OpenMP scalar reduction (* implemented)
      [INFO] pi.c:31:5   #2 OpenMP atomic access
      [INFO] pi.c:31:5   #3 OpenMP explicit privatization
      [INFO] pi.c:31:5 Loop parallelized with teams using OpenMP directive 'target teams distribute parallel for'
Successfully created pi_ompOff.c


Minimum software stack requirements: OpenMP version 4.0 with offloading capabilities


$ cat pi_ompOff.c
…
   // ===============================================

    double out_result;

    double sum = 0.0;
    #pragma omp target teams distribute parallel for shared(N) map(to: N) reduction(+: sum) map(tofrom: sum) schedule(static)
    for (int i = 0; i < N; i++) {
        double x = (i + 0.5) / N;
        sum += sqrt(1 - x * x);
    }

    out_result = 4.0 / N * sum;

    // ===============================================

…
```

Just copy & paste the suggested invocation of pwdirectives, which will rewrite the code for you adding OpenMP directives

(note: source code edited "in-place" by default" and in this example we are using “-o” to write a separate source code file)

By default the OpenMP generated code:
- offloads the computation with "target teams"
- manages data transfers with “map”
- splits workload with “schedule(static)”

6b: Annotate the code for GPU + OpenACC (`pwdirectives --acc`)

```
$ pwdirectives --acc pi.c:main:31:5 -o pi_acc.c
Results for file 'pi.c':
  Successfully parallelized loop at 'pi.c:main:31:5' [using offloading without teams]:
          [INFO] pi.c:31:5 Parallel scalar reduction pattern identified for variable 'sum' with associative, commutative operator '+'
          [INFO] pi.c:31:5 Available parallelization strategies for variable 'sum'
          [INFO] pi.c:31:5   #1 OpenACC scalar reduction (* implemented)
          [INFO] pi.c:31:5   #2 OpenACC atomic access
          [INFO] pi.c:31:5 Parallel region defined by OpenACC directive 'parallel'
          [INFO] pi.c:31:5 Loop parallelized with OpenACC directive 'loop'
          [INFO] pi.c:31:5 Data region for host-device data transfers defined by OpenACC directive 'data'
Successfully created pi_acc.c

Minimum software stack requirements: OpenACC version 2.0 with offloading capabilities


$ cat pi_acc.c
...
   // ================================================

    double out_result;

    double sum = 0.0;
    #pragma acc data copyin(N) copy(sum)
    {
    #pragma acc parallel
    {
    #pragma acc loop reduction(+: sum)
    for (int i = 0; i < N; i++) {
        double x = (i + 0.5) / N;
        sum += sqrt(1 - x * x);
    }
    } // end parallel
    } // end data

    out_result = 4.0 / N * sum;

    // ================================================
...
```

In a similar manner, for OpenACC just copy & paste the suggested invocation of pwdirectives, which will rewrite the code for you adding OpenACC directives (note: source code edited "in-place" by default" and in this example we are using "-o" to write a separate source code file)

By default the OpenACC generated code:
- offloads the computation with "parallel"
- manages data transfers with "data copy"

(note: OpenACC provides a more elegant solution to manage data transfers for double** data types)

7: Benchmarking on Perlmutter @NERSC (using Nvidia toolchain)

Launch script “launch.sh”

```
#!/bin/bash
#SBATCH -A ntrain2_g
#SBATCH --reservation=codee_day1
#SBATCH -C gpu
#SBATCH -q regular
#SBATCH -t 0:10:00
#SBATCH -N 1
#SBATCH --ntasks-per-node=1
#SBATCH -c 128
#SBATCH --gpus-per-task=1

export SLURM_CPU_BIND="cores"
srun PI.sh
```

PI execution script “PI.sh”

```
#!/bin/bash

rm pi pi_ompOff pi_acc

nvc pi.c -lm -fast -o pi
./pi 900000000

nvc -mp=gpu -fast -gpu=cc80 -lm pi_ompOff.c -o pi_ompOff
./pi_ompOff 900000000

nvc -acc -fast -gpu=cc80 -lm pi_acc.c -o pi_acc
./pi_acc 900000000
```

```
$ nvc pi.c -lm -fast -o pi
$ ./pi 900000000
- Input parameters
steps     = 900000000
- Executing test...
time (s)= 0.873033
result     = 3.14159265
error     = 8.0e-15
```

By default, the recommendation for Perlmutter @NERSC is to use the Nvidia Programming Environment

```
$ nvc -mp=gpu -fast -gpu=cc80 -lm pi_ompOff.c -o pi_ompOff
$ ./pi_ompOff 900000000
- Input parameters
steps     = 900000000
- Executing test...
time (s)= 0.172202
result     = 3.14159265
error     = 8.9e-14
```

PI code runs correctly on the GPU @perlmutter and 5.1x faster using OpenMP offload

```
$ nvc -acc -fast -gpu=cc80 -lm pi_acc.c -o pi_acc
$ ./pi_acc 900000000
- Input parameters
steps     = 900000000
- Executing test...
time (s)= 0.119455
result     = 3.14159265
error     = 1.3e-14
```

PI code runs correctly on the GPU @perlmutter and 7.3x faster using OpenACC offload

Final remarks about using Codee at NERSC

- First, remember to load the Codee module
  `$ module load codee`
- The flag --help lists all the options available in the Codee command-line tools
  ```
  $ pwreport --help
  $ pwloops --help
  $ pwdirectives --help
  ```
- You can run Codee command-line tools on the login nodes (no need to run them on the compute nodes)
- Build and run the example codes on the compute nodes using the batch scripts
  - Scripts tuned to use the appropriate reservations: *codee_day1*, *codee_day2*
- Remember to check the open catalog of rules for performance optimization:

https://www.codee.com/knowledge/

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