Heterogeneous Computing for Scientific Applications

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Outline

- Analysis, parallelism characterization of NAS-MZ suite of benchmarks
- NPB-MZ Hybrid Design and Implementation
- Work distribution schemes for hybrid executions
- Evaluation Results

NPB-MZ Parallel Benchmarks

- Data Structures and Input Size
- Computation Structure
- Sources of Parallelism

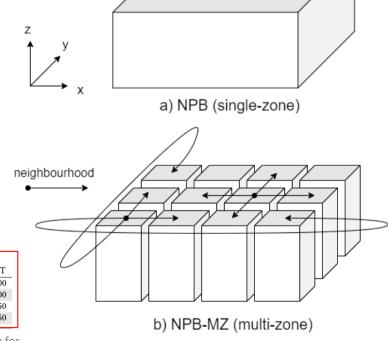
Data Structures and Input Size

- Data Structures
 - 3D mesh organized in "zones"
 - A zone is a set of multidimensional matrices
- Input Size

size increases

- Different classes: A, B, C, D, E
- Number of zones: from 16 to 4096
- Iterative solvers
 - From 250 to 500 iterations

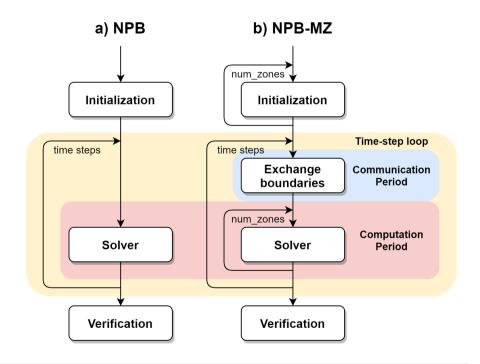
Input	3D volume	Memory	Num. zones (x × y)			Zone size (points per zone)			Time steps		ps
Class	$x \times y \times z$ (points)	(GB)	LU	SP & BT		LU	SP	BT	LU	SP	BT
В	$304 \times 208 \times 17$	≈ 0.2	4×4	8 × 8	1	67 184	16 786	from 2 992 to 59 976	250	400	200
С	$480 \times 320 \times 28$	≈ 0.8	4×4	16 × 16	ĺ	268 800	16 800	from 2 912 to 60 648	250	400	200
D	$1632 \times 1216 \times 34$	≈ 13	4×4	32×32		4 217 088	65 892	from 11 968 to 243 236	300	500	250
E	$4\ 224 \times 3\ 456 \times 92$	≈ 250	4×4	64×64		83 939 328	327 888	from 59 248 to 1 203 452	300	500	250



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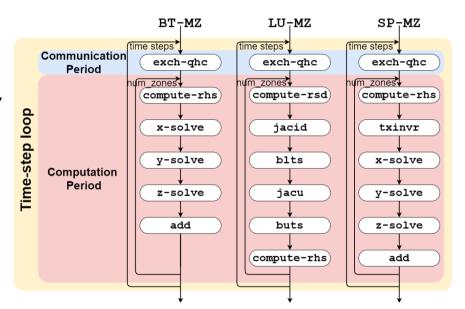
Computational Periods

- For all benchmarks:
 - Initialization
 - Several stages
 - Computation Period
 - Solver composed of several stages
 - Applied to each zone
 - Communication Period
 - Exchange of border values between zones
 - One single stage
 - Verification



Stages within the Compute Period and Communication Period

- Three benchmarks:
 - BT-M7
 - "Many zones with small, medium and large sizes"
 - SP-MZ
 - "Many zones with small sizes and all of them equal"
 - LU-MZ
 - "Few zones and with very large size"
 - Computation Period
 - Composed of different stages per each benchmark
 - Communication Period
 - Single stage and common to each benchmark



Computation Period(I): Inter-Zone Parallelism

- Traversal of zones
 - Single loop that runs over the set of zones
 - Zones are identified
 - Number from 0 up to the NUM-ZONES-1
 - Several stages applied per each zone
 - Different in BT-MZ, SP-MZ and LU-MZ

Example with SP-MZ:

```
for (t=0; t<ITERS; t++) {
    exch-qbc();

    for (zone = 0; zone < NUM-ZONES; zone++)

        compute-rhs(zone, ...); Inter-zone parallelism
        txinvr(zone, ...);
        x-zolve(zone, ...);
        y-solve(zone, ...);
        z-solve(zone, ...);
        add(zone, ...);
    }
}</pre>
```

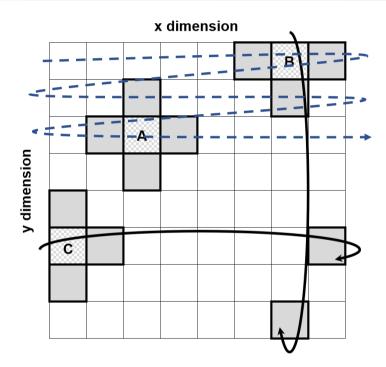
Computation Period(II): Intra-Zone Parallelism

- Processing of one stage on one zone
 - Sequence of several loop nests
 - For CPU execution
 - Loop nest is parallelized (e.g.: OpenMP)
 - For GPU execution
 - Loop nest is transformed to CUDA kernel

• Example: BT-MZ, x-solve stage

Communication Period: Zone Adjacency

- Adjacent zones
 - 4 neighbors
 - north
 - south
 - east
 - west
- Exchange border values between adjacent zones



Communication Period: Intra-Zone Parallelism

• Processing of zone borders

```
for (zone=0; zone<NUM-ZONES; zone++) {
  east-zone = adjacency-east[zone]
  north-zone = adjacency-north[zone];

  copy-face(tmpEast, mesh[east-zone]);
  copy-face(tmpNorth, mesh[north-zone]);

  compute-border(mesh[zone], tmpEast, tmpNorth);
  copy-face(mesh[east-zone], tmpEast);
  copy-face(mesh[north-zone], tmpNorth);
}</pre>
```

```
void compute-border(...) {

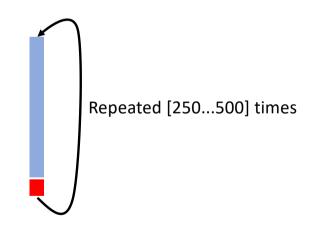
for (k=0; k<z-dim; k++)
  for (j=0; j<y-dim; j++)
    for (i=0; i<x-dim; i++)
    /* Some matrix-based
        computations */</pre>
```

```
void copy-face(...) {

for (k=0; k<z-dim; k++)
  for (j=0; j<y-dim; j++)
    /* Some matrix-based
    computations */</pre>
```

Summary: Computation and Communication Periods, Sources of Parallelism

- Two levels of parallelism:
 - Coarse grain parallelism: INTER-ZONE parallelism
 - Fine grain parallelism : INTRA-ZONE parallelism
- Parallelism is repeated many times
 - Computation Period
 - INTER-ZONE: mapped to CPUs and GPUs
 - INTRA-ZONE: mapped to CPUs or GPUs
 - Communication Period
 - INTRA-ZONE: mapped to CPUs or GPUs



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NPB-MZ Hybrid Design and Implementation

- Hybrid Execution Model: OpenMP+CUDA
 - Computing Unit Abstraction
 - libCU-rtl
 - Address Space Abstraction
 - libAS-rtl
 - Work Distribution Schemes
 - libSCHEDULING-rtl
- NPB-MZ Hybrid Parallelization

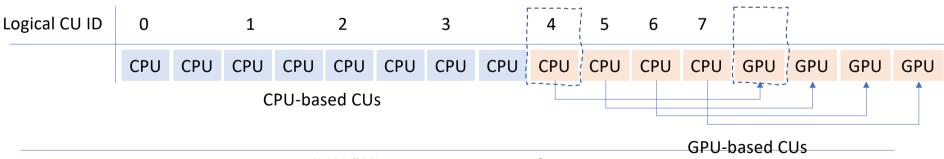
Computing Units (I)

- Computing Units (CUs)
 - Logical view of all available CPUs and GPUs
 - A CU can be of type CPU or GPU
 - If CU type is of CPU
 - CU maps onto <u>one or more</u> physical <CPU>
 - If CU type is of GPU
 - CU maps to <u>one pair</u> of physical <CPU, GPU>
 - The CPU controls the GPU

- Computing Units (CUs)
 - NCU = number of available CUs
 - CUs are numbered from 0 up to the NCU-1
 - NCPU = Number of CPU-based CUs
 - NGPU = Number of GPU-based CUs
 - [0 .. NCPU-1] correspond to CPU-based CUs
 - [NCPU .. NCU-1] correspond to GPU-based CUs
- CUs and Threads
 - We run as many threads as the number of NCU

Computing Units (II)

- Example:
 - Execution with 8 CUs = 4 x CPU-based CUs + 4 GPU-based CUs
 - CPU-based CU = 2 x CPUs
 - GPU-based CU = CPU + GPU
 - => 12 physical CPUS + 4 physical GPUS
 - 12 threads mapped onto 12 physical CPUs



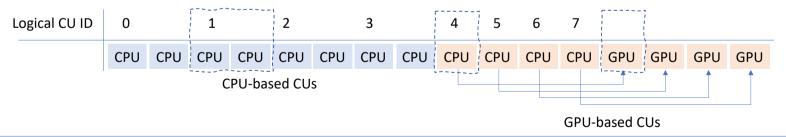
Hybrid Execution Model: OpenMP + CUDA

- How do we introduce the abstraction of a CU in OpenMP+CUDA?
 - Implement runtime support to bridge the two execution models
 - libCU-rtl
- Parallelism for CUs is created through omp parallel construct
 - 1 CPU-based CU: 1 OpenMP thread
 - 1 GPU-based CU: 1 OpenMP thread that controls a device
- CUs are formed through OMP PLACES
- Name spaces for CU, OpenMP threads and CUDA devices
 - Logical CU id ⇔ OpenMP Thread id
 - OpenMP Thread id = CU id
 - Logical CU id ⇔ CUDA Device id
 - CUDA Device id = CU id NCPU

CUs definition and OpenMP thread places

Example

- OMP_PLACES = "{0, 1}, {2, 3}, {4, 5}, {6, 7}, {8}, {9}, {10}, {11}"
- OMP PROC BIND=TRUE
- NCPU = 4 with 2 inner CPUs
- NGPU = 4
- Logical CU ids match OpenMP logical thread ids



Runtime Support for CUs

 Small set of runtime primitives 	Number of GPU-based CUs and					
RUNTIME::gpus	CPU-based CUs					
RUNTIME::cpus	Over if CH is marred onto CDH on CDH					
RUNTIME::isGPU()	Query if CU is mapped onto CPU or GPU					
RUNTIME::isCPU()	Get a CPU/GPU id in OpenMP/CUDA					
RUNTIME::GPU()						
RUNTIME::CPU()	Get a number of inner threads for a CPU-based CU					
RUNTIME::innerCPUs()	TOT a Cro-pased Co					
RUNTIME::getTask()	Get a task mapped to the current CU					
RUNTIME::getCU()	Get/set the CU logical ID					
RUNTIME::setCU()	dee, see the co logical ib					
RUNTIME::commitTask()	Start/end of the execution					
RUNTIME::executeTask()	of an assigned task					
RUNTIME::synchronize()	Synchronize with corresponding device					
	if CU is mapped to a GPU					

Code Transformation for CU support

CU parallelism

```
OMP_PROC_BIND=TRUE

OMP_PLACES = "{0, 1},{2, 3},{4, 5},{6, 7},

{8}, {9}, {10}, {11}"
```

CU computations

```
unsigned int CU = RUNTIME::getCU();
if (RUNTIME::isCPU(CU)) {
   NT = RUNTIME::innerCPUs();
#pragma parallel num_threads(NT) proc_bind(master)
{
   /* COMPUTATIONS */
} // parallel

}
else if (RUNTIME::isGPU(CU)) {
   cudaSetDevice(RUNTIME::GPU(CU));
   some-GPU-kernel-1<<<<gri>grid, block, shared>>>(...);
}
```

Distributed Address Space: OpenMP + CUDA

- How do we introduce the abstraction of a AS in OpenMP+CUDA?
 - Implement runtime support to bridge the two execution models
 - libAS-rtl
- Several Address Spaces (AS)
 - Host
 - Devices
- Name space for AS
 - [0...NCPU-1] => **HOST**
 - [NCPU...NGPU-1] => **DEVICES**
- Monitor data placement
 - Maintain a map of data structures and AS

Runtime Support for Data Placement

• Small set of runtime primitives

```
PLACEMENT::getAS()
PLACEMENT::alloc()
PLACEMENT::migrate()
PLACEMENT::copy()
PLACEMENT::isGPU()
PLACEMENT::isCPU()
PLACEMENT::isCPU()
Query if memory (e.g.: a zone) is mapped onto CPU or GPU
```

Work Distribution: OpenMP + CUDA

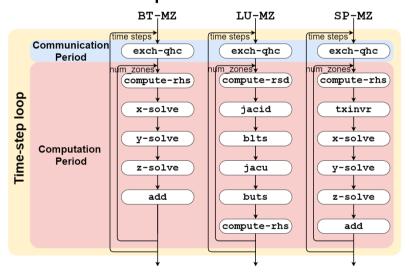
- OpenMP work distribution schemes are not suitable
 - TASKS: you do not have control over which thread will execute a task
 - LOOPs: available loop schedulers are not suitable, not designed for heterogeneity
 - STATIC, DYNAMIC, GUIDED
- Implement a runtime support to bridge the two execution models at the application level
 - libSCHEDULING-rtl

Runtime Support for Scheduling

- Assume tasks are numbered from [0...N_{tasks}-1]
 - Inputs for schedulings
 - N_{tasks}
 - NCPU
 - NGPU
- SCHEDULING-rtl
 - SCHEDULING::Static()
 - SCHEDULING::Dynamic()
 - SCHEDULING::pcf-Static()
 - SCHEDULING::pcf-Guided()
 - SCHEDULING::ClusteredGuided()

Computation Period: Code Transformation

INTER-ZONE parallelism



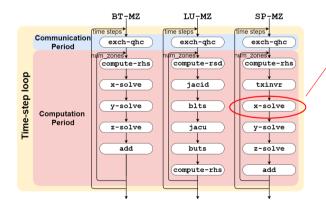
• Example: SP-MZ

```
SCHEDULE::Static(NUM ZONES, RUNTIME::cpus, RUNTIME::gpus);
#pragma omp parallel \
           num threads(RUNTIME::cpus+RUNTIME::gpus)
                                        OMP PROC BIND=TRUE
 unsigned int task;
  task = RUNTIME::getTask();
  while (task!=NO TASK) {
   unsigned int zone = task;
   unsigned int CU = RUNTIME::getCU();
   if (PLACEMENT::qetAS(mesh[zone])!=CU) PLACEMENT::migrate(mesh[zone], CU);
   RUNTIME::executeTask();
   compute-rhs(zone, ...);
   txinvr(zone, ...);
   x-zolve(zone, ...);
   v-solve(zone, ...);
   z-solve(zone, ...);
   add(zone, ...);
   if (RUNTIME::isGPU(CU)) RUNTIME::synchronize();
   RUNTIME::commitTask();
   task = RUNTIME::getTask();
 } // while
} // parallel
```

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Computation Period: Code Transformation

INTRA-ZONE parallelism



Communication Period: Border Processing

```
for (zone=0; zone<NUM-ZONES; zone++) {</pre>
 east-zone = adjacency-east[zone]
 north-zone = adjacency-north[zone];
 east-AS = PLACEMENT::getAS (mesh[east-zone]]);
 north-AS = PLACEMENT::getAS (mesh[north-zone]);
 zone-AS = PLACEMENT::getAS (mesh[zone]);
 PLACEMENT::pack-face(tmpEast, east-AS, mesh[east-zone]);
 PLACEMENT::pack-face(tmpNorth, north-AS, mesh[north-zone]);
 if (PLACEMENT::isGPU(zone-AS)) {
    CUDA::setDevice(RUNTIME::GPU(zone-AS)):
   qpu-compute-border<<< grid, block, shared>>>(mesh[zone],
                                                  tmpEast,
                                                  tmpNorth);
 else if (PLACEMENT::isCPU(zone-AS)) {
    cpu-compute-border(mesh[zone], tmpEast, tmpNorth);
 PLACEMENT::unpack-face(tmpEast, east-AS, mesh[east-zone]);
 PLACEMENT::unpack-face(tmpNorth, north-AS, mesh[north-zone]);
```

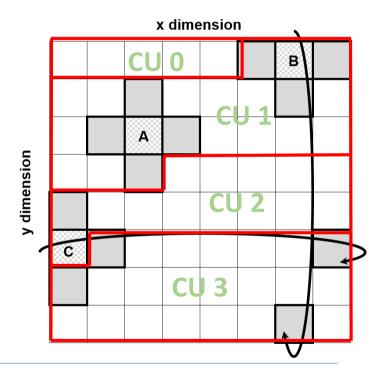
Communication Period: Data Packing

```
void PLACEMENT::pack-face(buffer, zoneAS, mesh-zone) {
  myAS = PLACEMENT::getAS();
 if (myAS!=zoneAS) {
   // remote packing of border data and transfer to myAS
     if (PLACEMENT::isGPU(zoneAS) {
       CUDA::setDevice(RUNTIME::GPU(zone-AS));
       gpu-pack-face<<<grid, block, shared>>>(...);
                                                        void cpu-pack-face(buffer, mesh-zone);
       CUDA::cudaMemCpy (buffer, ..., cudaDeviceToHost);
                                                        void cpu-unpack-face(buffer, mesh-zone);
     } else if (PLACEMENT::isCPU(zoneAS){
       cpu-pack-face(...);
                                                              gpu-pack-face(buffer, mesh-zone);
                                                    global
  } else {
                                                    global
                                                              gpu-unpack-face (buffer, mesh-zone);
    // pack border data
void PLACEMENT::unpack-face(buffer, zoneAS, mesh-zone);
```

In a hybrid execution the CUDA::cudaMemCpy is the source of overhead

Communication Period: Data placement and Communication

- Trade off between the number of data transfers and data placement
 - NCU =4
 - Zone B
 - Assigned to a CU where 1 adjacent zone is assigned to other CUs
 - Zone A
 - Assigned to a CU where all 4 adjacent zones are assigned to the same CU
 - Zone C
 - Assigned to a CU where 3 adjacent zones are assigned to other CUs



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Work Distribution Schemes For OpenMP+CUDA

- Baseline Schedulers
 - STATIC
 - DYNAMIC
- Performance Factor Conversion (PCF) Schedulers
 - PCF-STATIC
 - PCF-GUIDED
- Self Adaptive Schedulers
 - CLUSTERED GUIDED

STATIC scheduler

- Tasks are identified from 0 up to the number of tasks -1
- NTASKS = NUM ZONES;
- CU-WORK = NTASKS/NCU;
- If remaining tasks, those are assigned to lower CUs within the numbering
 - CPUs first, then the GPUs
- <start, end>: identifies the set of tasks assigned to a CU
 - start = initial task
 - end = final task
- Maximizes adjacency, so minimizes communications

DYNAMIC scheduler

- Fast CUs (e.g.: GPUs) will tend to get more work
- Slow CUs (e.g.: CPUs) will tend to get less work
- CHUNK = 1;
- Memorizes TASK-CU mapping
 - Avoids memory migration overheads
- Breaks adjacency, so will tend to increase the communications

PCF-STATIC scheduler

- Variant of STATIC scheduler
- Based on a <u>Performance Conversion Factor</u> (PCF)
 - PCF = relation between the computational power of CPU-based CUs and GPU-based CUs
 - Example
 - PCF = 2, means that GPU-based CUs are twice faster than CPU-based CUs
 - PCF = 1, means both CPU and GPU based CUs have same computation power

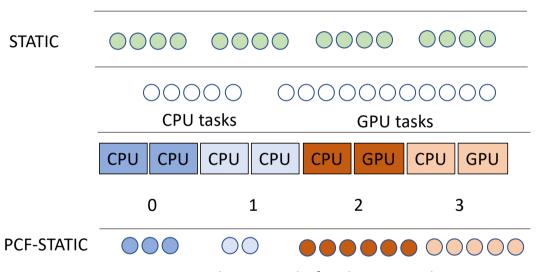
PCF-STATIC scheduler

- Divide in two parts the set of tasks
 - NTASKS = PCF x CPU-TASKS + CPU-TASKS = (PCF+1) x CPU-TASKS
 - GPU-TASKS = NTASKS CPU-TASKS
- Apply STATIC over CPU-TASKS and among all CPU-based CUs
- Apply STATIC over GPU-TASKS and among all GPU-based CUs
- Maximizes adjacency, so minimizes communications

PCF-STATIC scheduler

STATIC

- Example:
 - PCF = 2
 - NCU = 4
 - CPU-based CU = 2
 - GPU-based CU = 2
 - NTASKS = 16
 - CPU-TASKS = 5
 - **GPU-TASKS** = 11

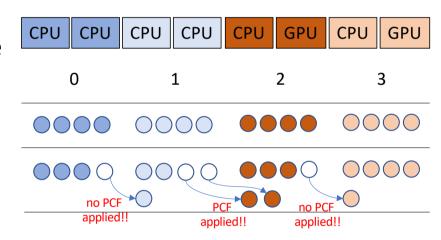


<start,end>: interval of tasks assigned to a CU

STATIC: <0,3> <4,7> <8,11> <12,15> PCF-STATIC: <0,2> <3,4> <5,10> <11,15>

PCF-GUIDED scheduler

- Initially, apply a STATIC scheduling
- Execute and monitor task execution time
- Adapt the work distribution so that it gets balanced
 - ALL-WORK = addition of all task execution times factorized with PCF
 - WORK-CU = ALL-WORK / NCU
 - Keep the assigned work per CU close to WORK-CU
- Maximizes adjacency, so minimizes communications



<start,end>: interval of tasks assigned to a CU

PCF-GUIDED scheduler

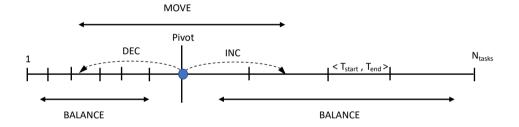
- Samples of execution time are taken from RUNTIME::executeTask() and RUNTIME::commitTask()
- Code scheme for work balance

```
#pragma omp parallel \
            num threads(RUNTIME::cpus+RUNTIME::gpus) \
            proc bind(true)
 unsigned int task;
  task = RUNTIME::getTask();
  while (task!=NO TASK) {
   unsigned int zone = task;
    unsigned int CU = RUNTIME::getCU();
    if (PLACEMENT::zonePlacement[zone]!=CU &&
        RUNTIME::isGPU(CU))
      PLACEMENT::migrateZone(CU);
    RUNTIME::executeTask();
     /* Computational Stages */
    if (RUNTIME::isGPU(CU)) RUNTIME::synchronize();
    RUNTIME::commitTask();
    task = RUNTIME::getTask();
 } // while
} // parallel
```

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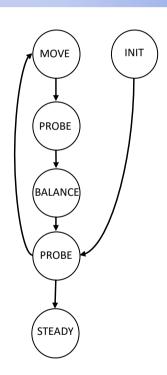
CLUSTERED GUIDED scheduler

- Set of tasks is divided in two clusters
 - One for CPU-based CUs, the other for GPU-based CUs
 - PIVOT: separating point for the two clusters
- At each instance of the scheduler, the PIVOT moves left/right to balance the work assigned to each cluster
 - Sort of a dichotomic search
- The scheduler balances the work distribution within each cluster



CLUSTERED GUIDED scheduler

- The scheduler evolves at runtime, switching between different states:
 - INIT: PIVOT is initialized (e.g.: PIVOT=NCPU). Applies a STATIC scheduling in both clusters.
 - MOVE: Moves PIVOT, according to where the maximum execution time has occurred.
 - PROBE: Samples execution time for each CU. Determines the maximum value observed in each cluster.
 - BALANCE: Applies a PCF-GUIDED scheduler with PCF=1 to each cluster.
 - STEADY: Records final configuration for work distribution.



CLUSTERED GUIDED scheduler

Data Structures:

 ${\bf Pivot:} \ {\bf Index} \ {\bf that} \ {\bf indicates} \ {\bf the} \ {\bf border} \ {\bf between} \ {\bf tasks} \ {\bf assigned} \ {\bf to} \ {\bf CPUs} \ {\bf and} \ {\bf tasks} \ {\bf assigned} \ {\bf to} \ {\bf CPUs} \ {\bf and} \ {\bf tasks} \ {\bf assigned} \ {\bf to} \ {\bf CPUs} \ {\bf and} \ {\bf tasks} \ {\bf assigned} \ {\bf to} \ {\bf CPUs} \ {\bf to} \$

DEC: Value to decrement the Pivot

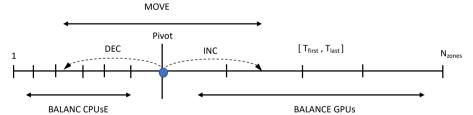
INC: Value to inclement the Pivot

TaskTime []: Vector of N_{zones} elements, each one describing the execution time of a task

CUtime []: Vector of N_{CUs} elements, each one describing the execution time of CU

FirstTask []: Vector of N_{CUs} elements, each one describing the T_{first} task assigned to a CU

LastTask []: Vector of N_{CUs} elements, each one describing the I_{Tast} task assigned to a CU

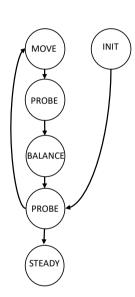


MOVE: T_{cpu} = max time for CPUs T_{gpu} = max time for GPUs if T_{cpu} > T_{gpu} INC = INC / 2 goingLEFT = false goingRIGHT = true pivot += INC if T_{gpu} > T_{cpu} DEC = DEC / 2 goingLEFT = true

goingRIGHT = false

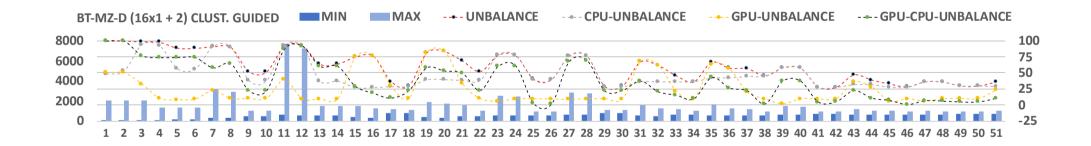
pivot-= DEC

```
BALANCE (CPUs/GPUs):
                                       Pivot = N<sub>CPUs</sub>
for cu = 1, N_{CUS}
                                      INC = DEC = N_{tasks} / 2
 TotalWork = CUtime[cu]
WorkPerCU = TotalWork / N<sub>CUs</sub>
for cu = 1, N_{CUS}
 First = FirstTask[cu]
 Last = LastTask[cu]
 Work = \sum_{First}^{Last} T_i
 DIFF = | Work - WorkPerCU |
 if (Work < WorkPerCU && DIFF > TH)
     while (Work < WorkPerCU) Last++; Work =+ T<sub>last</sub>
 else if ( Work > WorkPerCU && DIFF > TH )
     while (Work > WorkPerCU) Last--; Work =- T<sub>last</sub>
 LastTask[cu] = Last
 FirstTask[cu] = Last + 1
```

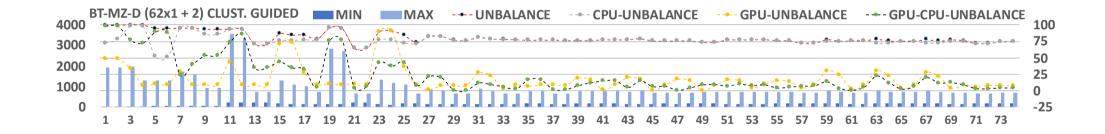


Number of steps to STEADY state: $log_2(N_{tasks}) \times 4$

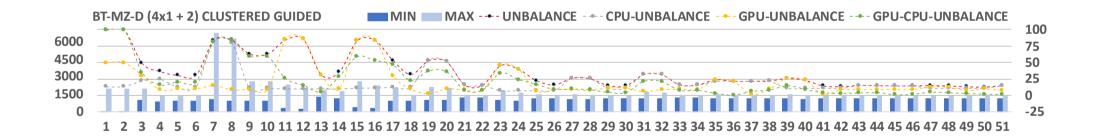
Examples of Clustered Guided



Examples of Clustered Guided



Examples of Clustered Guided



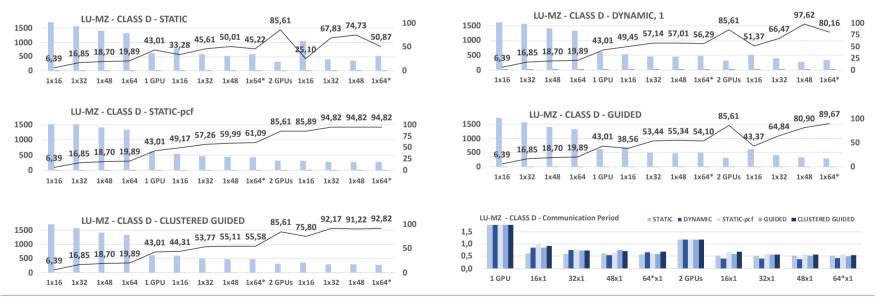
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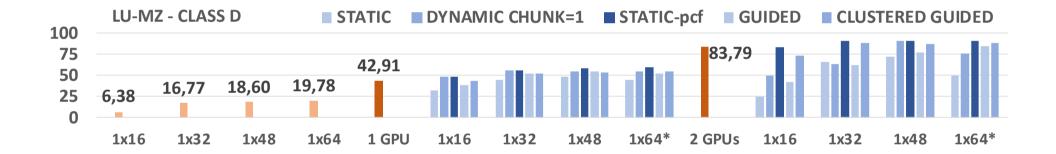
Environment

- AMD CTE @ BSC
 - AMD EPYC 7742 @ 2.250GHz (64 cores)
 - 2 x GPU AMD Radeon Instinct MI50 with 32GB
- Software stack
 - GCC 8.3.1-4
 - Radeon Open Compute (ROCm) Runtime software stack 3.5.0
- Hybrid NPB-MZ implementation
 - Parallel CUDA multi-gpu version of the NPB-MZ in C++
 - Parallel (OpenMP) implementation in Fortran of NPB-MZ
 - Runtime Libraries: libCU-rtl, libPLACEMENT-rtl, libSCHEDULING-rtl

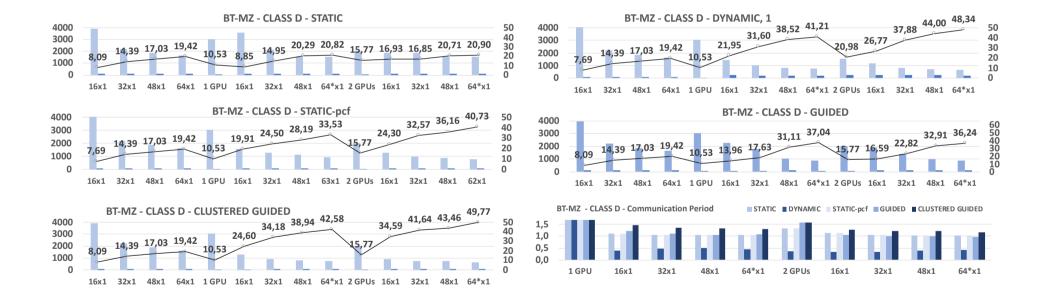
LU-MZ: Compute and Communication



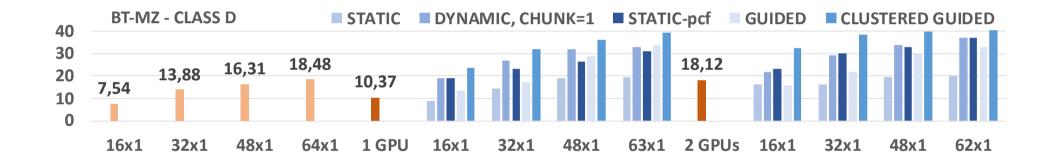
LU-MZ: Overall Performance



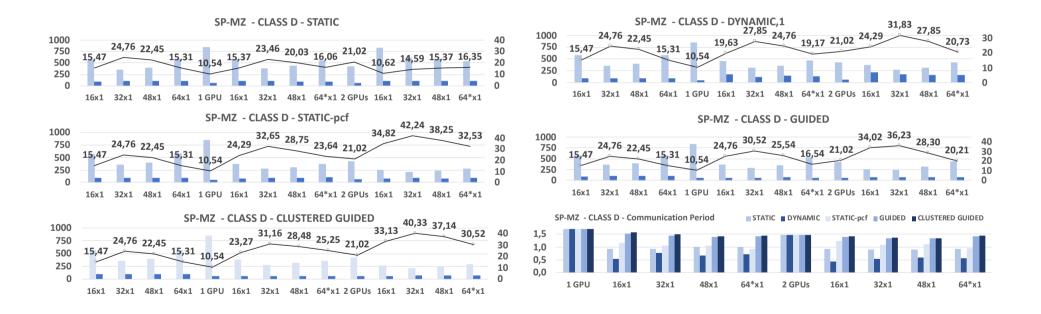
BT-MZ: Compute and Communication



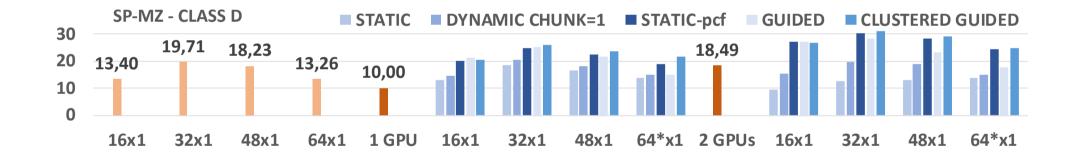
BT-MZ: Overall Performance



SP-MZ: Compute and Communication



SP-MZ: Overall Performance



Conclusions

- Case of study for hybrid computing (NPB-MZ), using OpenMP+CUDA
 - Methodology based on runtime implementation for bridging the two execution models
 - CU abstraction, AS abstraction at the programming model level
 - Work distribution schemes for hybrid executions
 - Based on rough performance comparison (PFC)
 - Monitoring task execution times (Clustered Guided)
- In general, the more GPUs in place, less space for using the CPUs
 - From a pure "FLOPS" perspective, we should try to use the CPUs for other purposes
 - Design runtime systems that solve programming limitations: memory allocators for dynamically changing data layouts, work distribution schemes, even code optimization

Heterogeneous Computing for Scientific Applications

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