Hackathon KAUST GPU 2020

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Overview

hpcscan is a C++ code for benchmarking HPC kernels (mainly for solving PDEs with FDM)

- Simple code struture based on individual test cases
- Easy to add new test cases
- Main class is Grid: multi-dimension (1, 2 & 3D) Cartesian grid
- Hybrid MPI/OpenMP parallelism
- All configuration parameters on command line
- Support single and double precision computation
- Compilation with standard Makefile
- No external librairies
- Follows C++ Google style code

Overview

hpcscan embeds several test cases

Current version 1.0

- General operations on grids
- Memory operations
- MPI communication
- FD computation
- Basic wave propagator

Possible additions for future versions

- Operations on matrices full and sparse
- FFT
- IO
- Compression

Compilation and validation

Compiling hpcscan
go to `./build` and `make` (by default compilation with single precision float)
To compile with double precision float, `make precision=double`

Validating hpcscan
go to `./script` and `sh runValidationTests.sh`

Table: `runValidationTests.sh` [1]

Machine	Compiler	Single prec.	Double prec.
Mars	g++ 9.3.0	764 PASS / 0 FAIL / 0 ERR / 20 WARN	764 PASS / 0 FAIL / 0 ERR / 20 WARN
Shaheen	icpc 19.0.5.281	764 PASS / 0 FAIL / 0 ERR / 20 WARN	764 PASS / 0 FAIL / 0 ERR / 20 WARN

Numbers can differ due to availability of features depending on the platforms

[1] Updated Nov 25, 2020

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Test platform - Shaheen II (KAUST)

Machine Shaheen II / Cray XC40

- Computing nodes Intel Haswell 2.3 Ghz dual socket (16 cores / socket)
- RAM 128 GB with Peak memory BW 136.5 GB/s
- Peak performance Single Prec. 2.36 TFLOP/s / Double Prec. 1.18 TFLOP/s
- Interconnect Cray Aries with Dragonfly topology
  - 60 GB/s optical links between groups
  - 8.5 GB/s copper links between chassis
  - 3.5 GB/s backplane within a chassis
  - 5 GB/s PCIe from node to Aries router

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Test Case Grid - Description

- Fill grid (W = coef)
- L1 error between grid W and R
- Get min. grid W
- Get max. grid W
- Update pressure W = 2*U - W + C*L (used in propagator)
- Medium Grid size 4 GB (1000 x 1000 x 1000 points)

Test Case Grid - Results

- CPU (Intel, no way to get AMD) and GPU kernels (V100)

Table: Bandwidth GB/s [2]

Machine	Algo.	Fill	L1 err.	Get max.	Get min.	Update Pres.
Shaheen CPU	Baseline	54	124	126	126	120
Ibex CPU	Baseline	92	217	224	224	198
Ibex GPU1	Cuda	497	274	700/221	700/221	673
Ibex GPU2	OpenAcc	270	-	-	-	-
Ibex GPU3	OpenMP	-	-	-	-	-

Table: Bandwidth GPoints/s

Machine	Algo.	Fill	L1 err.	Get max.	Get min.	Update Pres.
Shaheen CPU	Baseline	13.5	15.5	31.5	31.5	6.0
Ibex CPU	Baseline	23.0	27.1	56.0	56.0	9.9
Ibex GPU1	Cuda	124	34.5	175/55	175/55	33.7
Ibex GPU2	OpenAcc	67	-	-	-	-
Ibex GPU3	OpenMP	-	-	-	-	-

~~Reproduce results with ./hackathonTestCases/testCase_Grid/~~

[2] Updated Dec 1, 2020

Test Case Grid - Summary

Machine: Shaheen

- L1 Err., Get Min & Max: 125 GB/s close to peak BW (92 % Peak Mem. BW)
- Low perf for Fill: 54-58 GB/s (40-43 % Peak Mem. BW)
- Max Err. 72-91 GB/s (53-67 % Peak Mem. BW)
- Pressure update 6 GPoint/s (120 GB/s, 88 % Peak Mem. BW)

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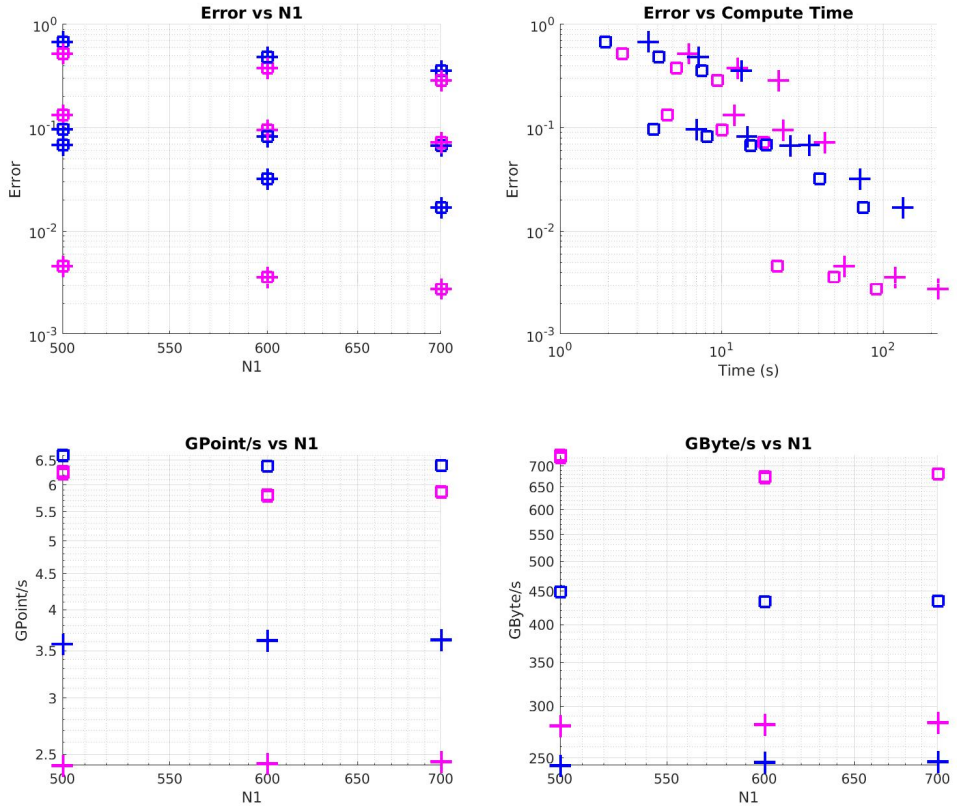
Test Case Propa - Description

- Seismic wave propagator
- 2nd order acoustic wave equation
- Time-domain Finite-difference
- Various FD order in space
- 2nd FD order in time
- Various grid size and time steps
- Total 18 configurations
- Comparison against analytical solution (Eigen mode)

Test Case Propa - Results

- **Machine: shaheen**
- 1 node / 32 threads
- CPU Baseline & cache blocking kernels [3]
- FD: Black O2, Blue O4, Pink O8, Red O12 / Square=CPU CacheBlk, Cross=Baseline

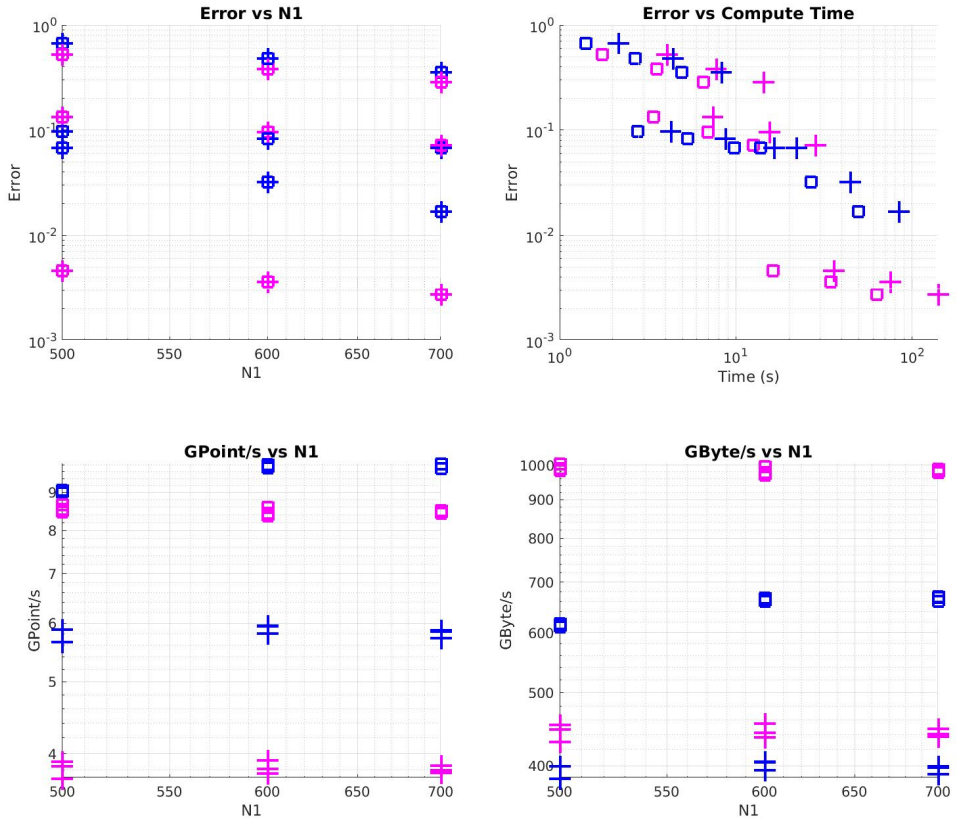


~~Reproduce results with `./hackathonTestCases/testCase_Propa/runShaheen.sh`~~

[3] Updated Nov 28, 2020

Test Case Propa - Results

- **Machine: Ibex Cpu**
- 1 node / 32 threads
- CPU Baseline & cache blocking kernels [4]
- FD: Black O2, Blue O4, Pink O8, Red O12 / Square=CPU CacheBlk, Cross=Baseline



~~Reproduce results with ./hackathonTestCases/testCase_Propa/runIbexCpu.sh~~

[4] Updated Dec 1, 2020

Test Case Propa - Results

Table: Best total time for 18 configurations [5]

Machine	Algo.	Time (s)	Speedup
Shaheen CPU	Baseline	826	0.5
Shaheen CPU	CacheBlk	388	1.0
Ibex CPU	Baseline	524	0.7
Ibex CPU	CacheBlk	265	1.5
Ibex GPU1	Cuda	XXX	Y.Y
Ibex GPU2	OpenACC	XXX	Y.Y
Ibex GPU3	OpenMP	XXX	Y.Y

[5] Updated Dec 1, 2020

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Conclusions and next steps

TO DO

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- KAUST ECRC and KSL for access and support on Shaheen II & Ibex