hpcscan version 1.1
Performance benchmarks on Shaheen II (KAUST)

December 2020

Content

Content

Introduction

All tests in single precision
Best performance is reported over 10 tries for each cases
Grids are 3D

Content

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

Content

Test Case Memory - Description

Benchmark objective

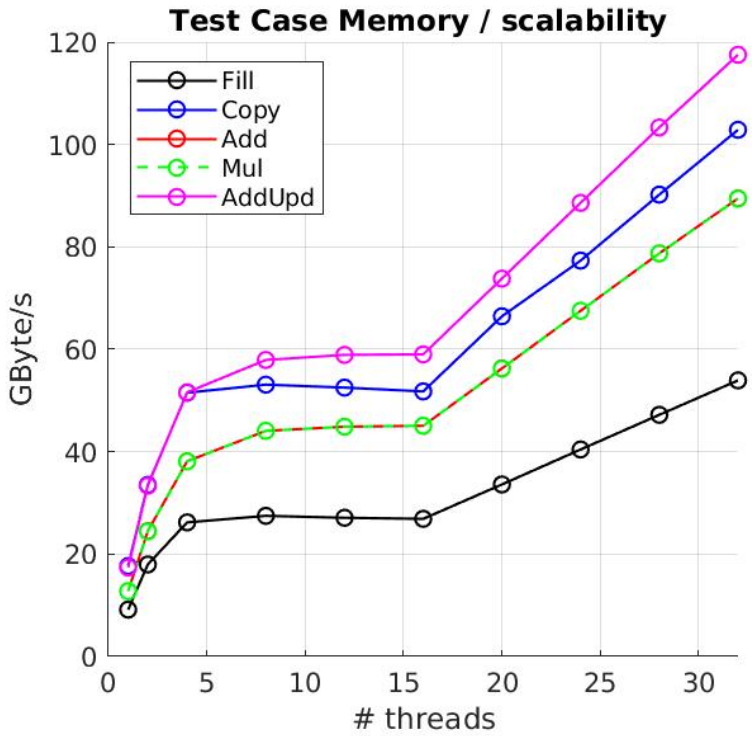
Measure GByte/s and GPoint/s for

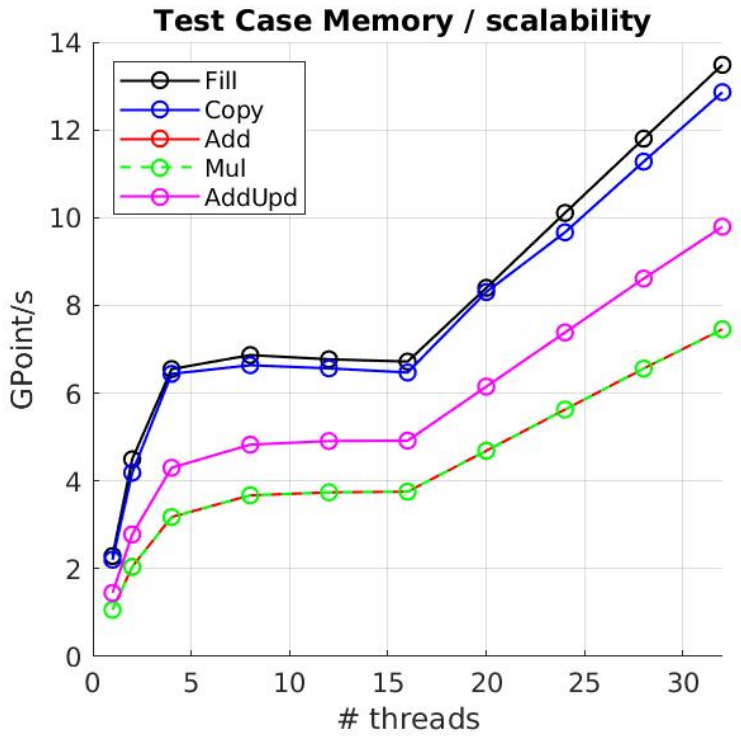
- Fill grid (W = coef)
- Copy grid (W = U)
- Add grids (W = U + V)
- Multiply grids (W = U * V)
- Add and update grids (W = W + U)

Benchmark configuration

- Scalability on 1 node with 1 to 32 threads
- Baseline kernel
- Grid size 4 GB (1000 x 1000 x 1000 points)
- Reproduce results with `./script/testCase_Memory/hpcscanMemory.sh`
- Elapsed time about 4 minutes

Test Case Memory - Results [1]





[1] Updated Dec 22, 2020

Content

Test Case Grid - Description

Benchmark objective

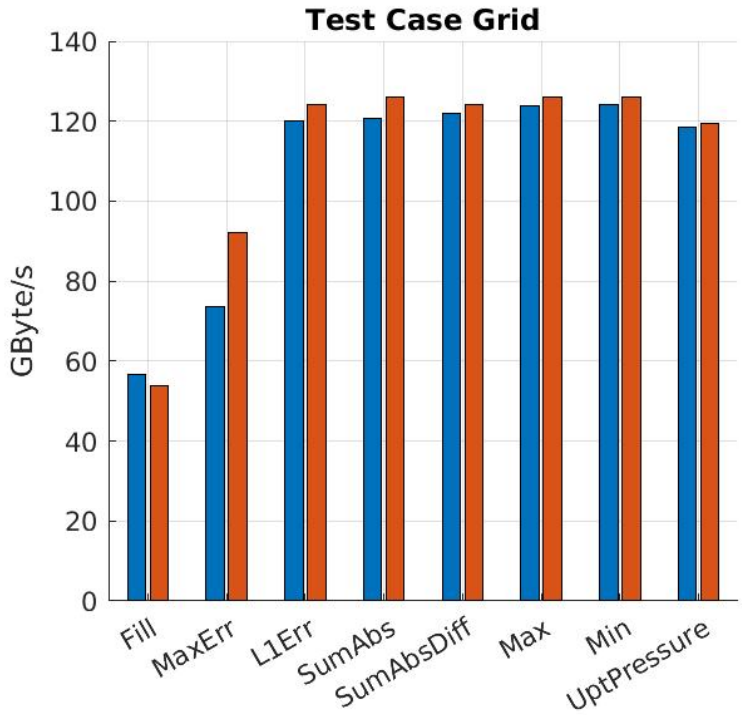
Measure GByte/s and GPoint/s for

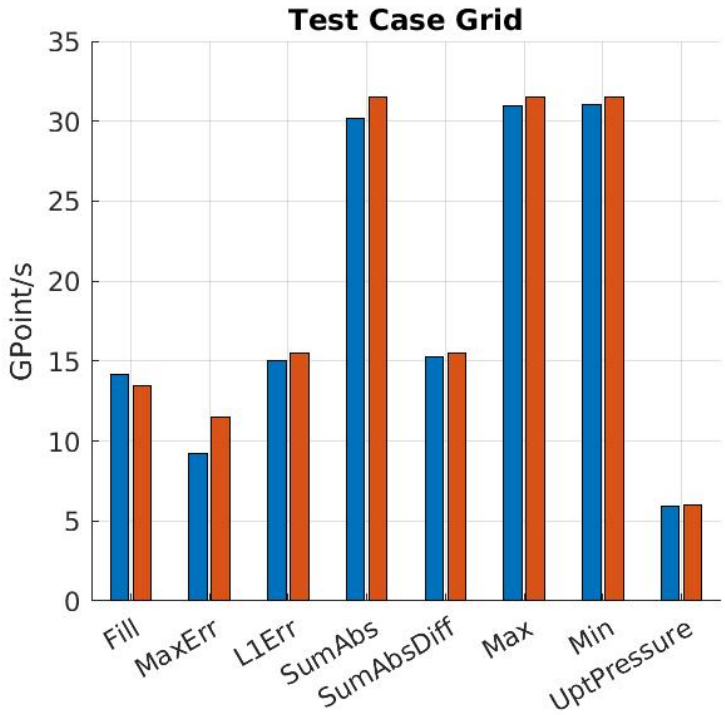
- Fill grid (U = coef)
- Max. diff (U-V)
- L1 norm between U and V
- Sum Abs(U) & Sum Abs(U-V)
- Get max. & Get min. grid U
- Update pressure (used in propagator)
- Boundary condition (free surface at all edges)

Benchmark configuration

- 1 node with 32 threads
- Baseline kernel
- 2 grid sizes
  - Small size 500 MB (500 x 500 x 500 points)
  - Medium size 4 GB (1000 x 1000 x 1000 points)
- Reproduce results with `./script/testCase_Grid/hpcscanGrid.sh`
- Elapsed time less than 1 minute

Test Case Grid - Results [2]





Blue small grid / Red medium grid
ApplyBoundaryCondition performs at 713/846 GBytes (89/105 Gpoint/s)

[2] Updated Dec 23, 2020

Content

Test Case Comm - Description

Benchmark objective

Measure GByte/s and GPoint/s for

MPI point to point communication

- Send with MPI_Send from proc X to proc 0 (Half-duplex BW)
- Send and receive with MPI_Sendrecv between proc X and proc 0 (Full-duplex BW)

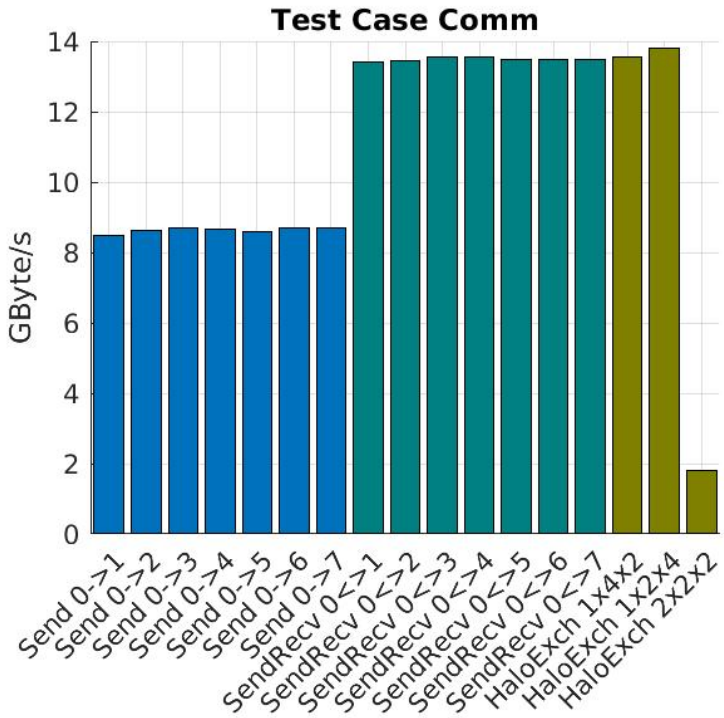
MPI collective communication

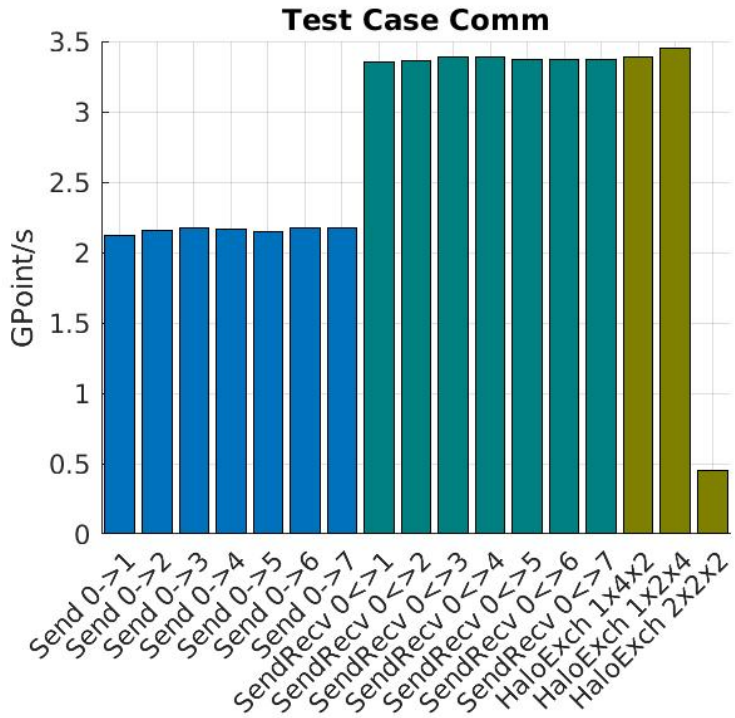
- Exhange of halos used in FD kernel with MPI_Sendrecv
- Domain decomposition with N1 x N2 x N3 subdomains

Benchmark configuration

- 8 nodes with 32 threads
- Baseline kernel
- Grid size 4 GB (1000 x 1000 x 1000 points)
- Subdomain decomposition: 1x4x2 / 1x2x4 & 2x2x2
- Reproduce results with `./script/testCase_Comm/hpcscanComm.sh`
- Elapsed time less than 1 minute

Test Case Comm - Results [3]





[3] Updated Dec 26, 2020

Content

Test Case FD_D2 - Description

Benchmark objective

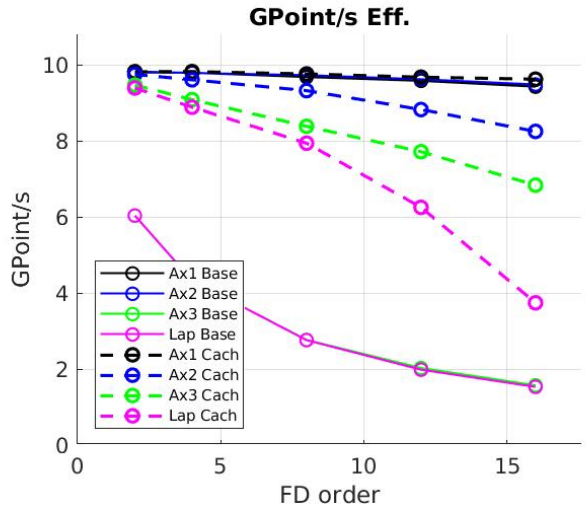
Measure GByte/s, GPoint/s & Gflop/s for

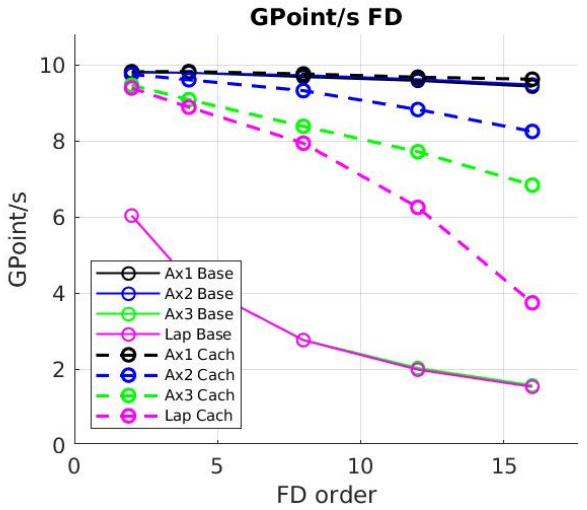
- Computation of second order derivatives with finite-difference stencil
- Directionnal derivatives
  - Axis 1, $W = \partial^2_{x1}(U)$
  - Axis 2, $W = \partial^2_{x2}(U)$
  - Axis 3, $W = \partial^2_{x3}(U)$
- Laplacian $W = \Delta(U)$
- Stencil orders 2, 4, 8, 12 & 16

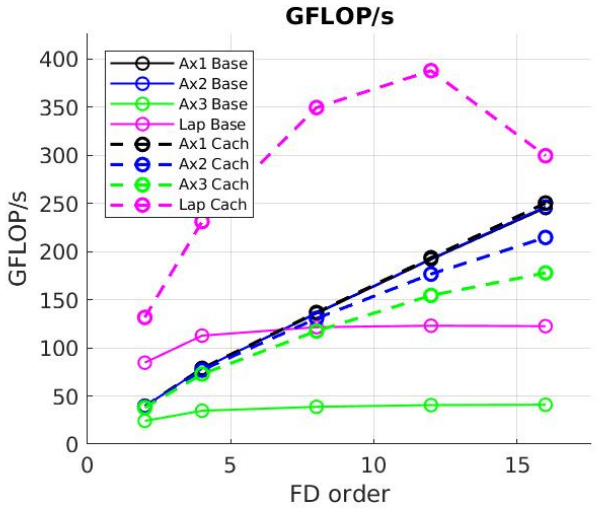
Benchmark configuration

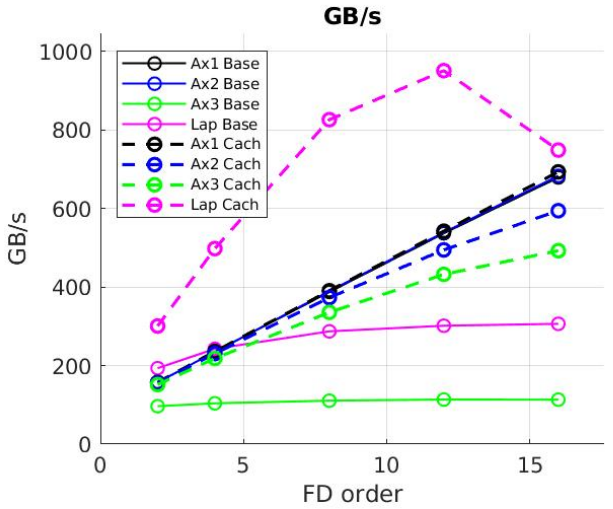
- 1 node with 32 threads
- 2 test modes
  - Baseline
  - CacheBlk
- Grid size 4 GB (1000 x 1000 x 1000 points)
- Reproduce results with `./script/testCase_FD_D2/hpcscanFD_D2.sh`
- Elapsed time about 2 minutes

Test Case FD_D2 - Results [4]









[4] Updated Dec 24, 2020

Content

Test Case FD_D2 - Description

Benchmark objective

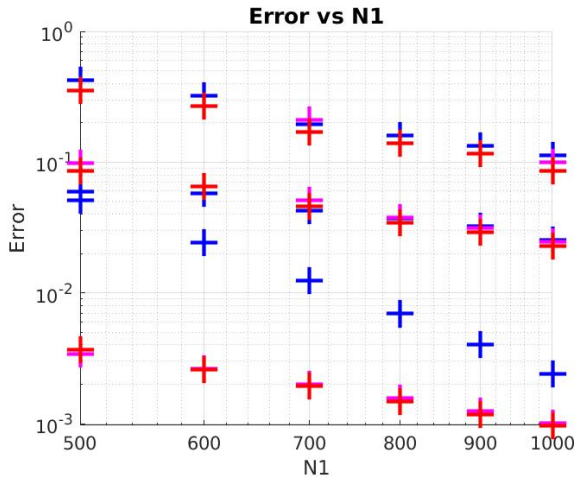
Measure GByte/s, GPoint/s & Gflop/s for

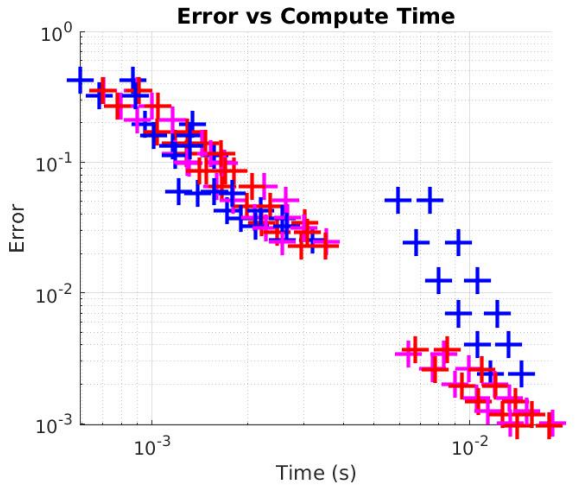
- Acoustic wave propagator
- Stencil orders 2, 4, 8, 12 & 16
- Time step 1, 0.5 & 0.1 of stability time step

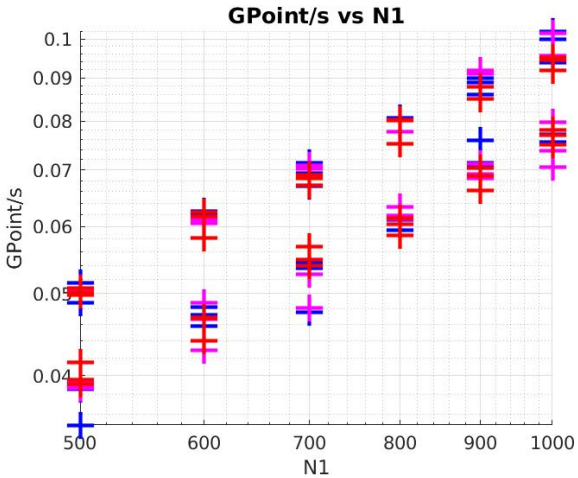
Benchmark configuration

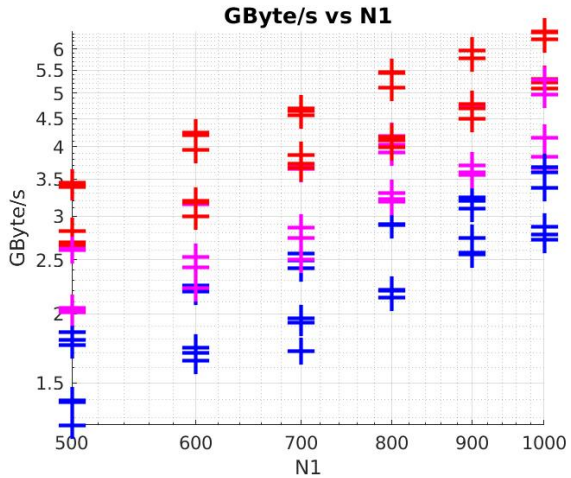
- 1 node with 32 threads
- Test mode CachBlk
- 2 propagator implementations
  - Ac2Standard
  - Ac2SplitComp
- Grid size from 500^3 (500 MB) to 1000^3 (4 GB)
- Reproduce results with `./script/testCase_PropaparamAnalysis/hpcscanPropaParamAnalysis.sh`
- Elapsed time about XX minutes

Test Case Propa - Results [5]









[5] Updated Dec 26, 2020

Test Case FD_D2 - Description

Benchmark objective

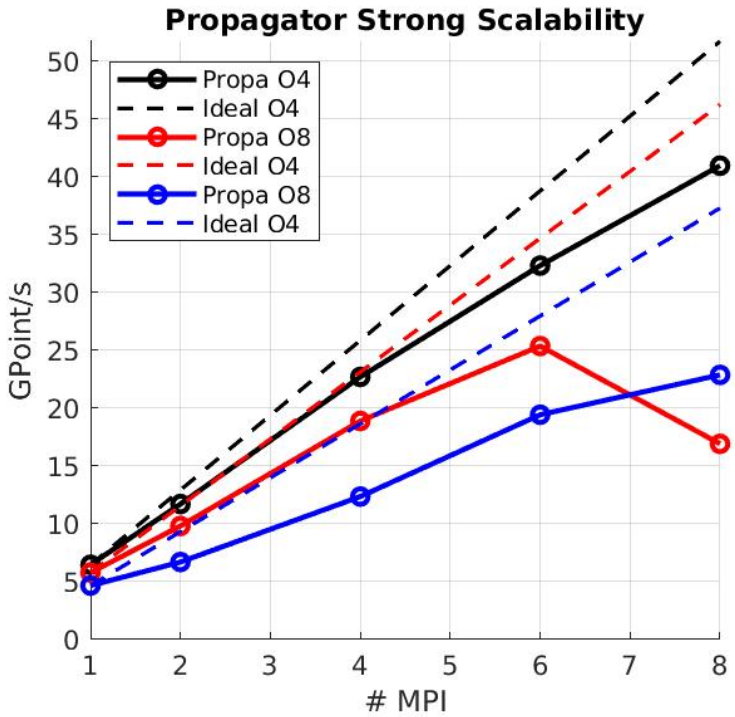
Measure GByte/s, GPoint/s & Gflop/s for

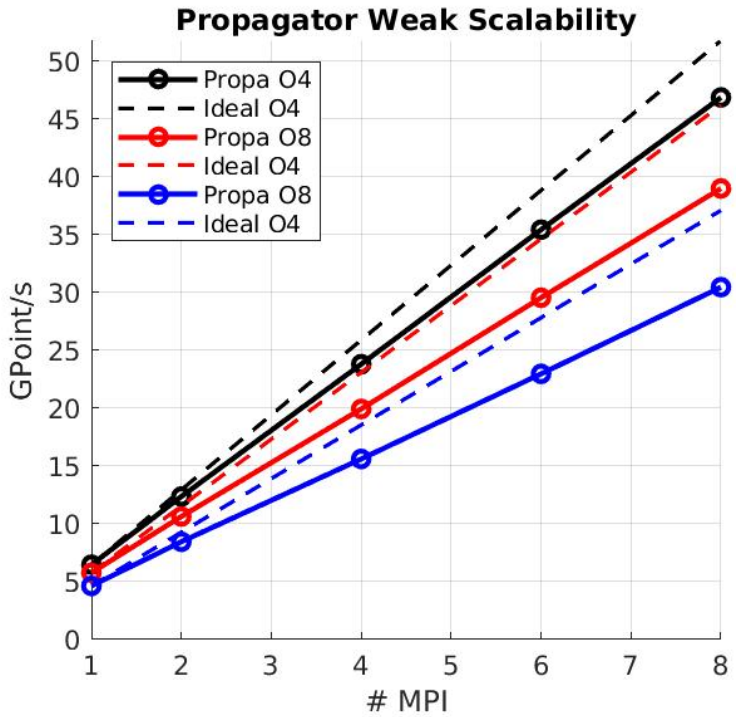
- Acoustic wave propagator
- Stencil order 8
- Strong and weak scalability

Benchmark configuration

- From 1 node to 8 nodes with 32 threads/node
- Test mode CachBlk
- Propagator implementation Ac2Standard
- Strong scalability: Grid size 1000^3 (4 GB)
- Weak scalability: Grid size from 1000x1000x1000 (4 GB) to 1000x4000x2000 (32 GB)
- Reproduce results with `./script/testCase_strongWeakScalability/hpcscanPropaStrongWeakScalability.sh`
- Elapsed time about 38 minutes

Test Case Propa - Results [6]





[6] Updated Dec 26, 2020

Content

Summary

Test Case Memory

- Measured memory BW between 91 to 122 GB/s (67-90 % of peak BW)
- Low BW 59 GB/s for Fill (43 % of peak BW)
- Multiply (= imaging condition) performs at 7.6 Gpoint/s

Test Case Grid

- 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)

Summary

Test Case Comm

- TO DO

Summary

Test Case FD_D2

- Large benefit of cache blocking
- Significant effect of grid dimnsion and index (very bad performance for n3 without cache blocking)
- Min BW 50 GFLOP/s (∂^2_{x3} O2) = 2 % peak BW [apparent Mem. BW 150 GB/s]
- Max BW 370 GFLOP/s (Δ O8) = 16 % peak BW [apparent Mem. BW 900 GB/s]
- Apparent Mem. BW 150-900 GB/s (110-660 % Peak Mem. BW) = shows data in-cache effect
- Typical stencils of interest for geophysical applications
  - Δ O4 BW = 8-10 GPoint/s
  - Δ O8 BW = 7-9 GPoint/s
  - Δ O12 BW = 3-5 GPoint/s
- Parallel efficiency with 8 nodes 55 to 86 % (depends on workload on Shaheen)

Summary

Test Case Propa

- TO DO

Content

Acknowledgements

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