hpcscan version 1.1
Performance benchmarks on Shaheen II (KAUST)

December 2020

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Introduction

All tests in single precision
Best performance is reported over 10 tries for each cases (unless stated otherwise)
Grids are 3D

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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 Memory - Description

Benchmark objective

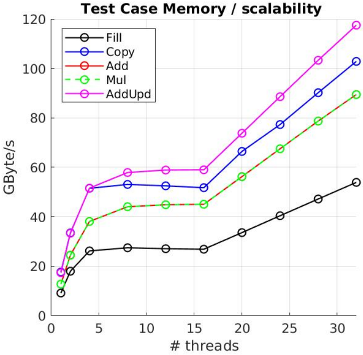
Measure GByte/s and GPoint/s for

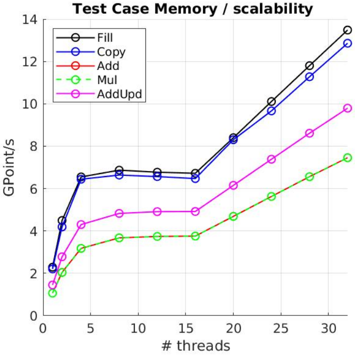
- Fill grid (W = coef)
- Copy grid (W = U)
- Add grids (W = U + V)
- Multiply grids (W = U * V)
- Add and update grids (W = W + U)

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

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Test Case Grid - Description

Benchmark objective

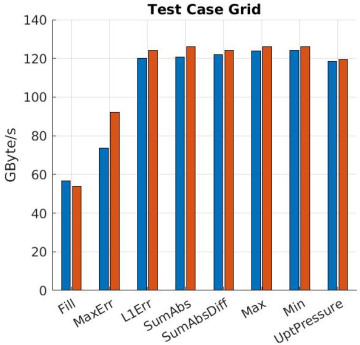
Measure GByte/s and GPoint/s for

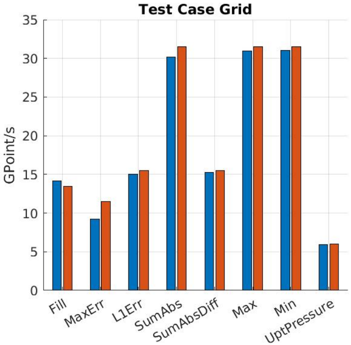
- Fill grid (U = coef)
- Max. diff (U-V)
- L1 norm between U and V
- Sum Abs(U) & Sum Abs(U-V)
- Get max. & Get min. grid U
- Update pressure (used in propagator)
- Boundary condition (free surface at all edges)

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

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Test Case Comm - Description

Benchmark objective

Assess inter-node communication bandwith

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)

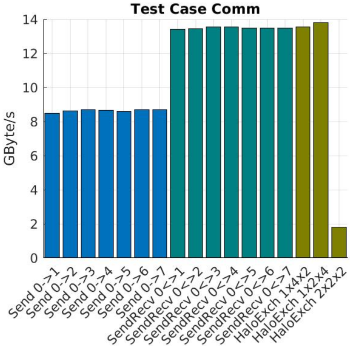
MPI collective communication

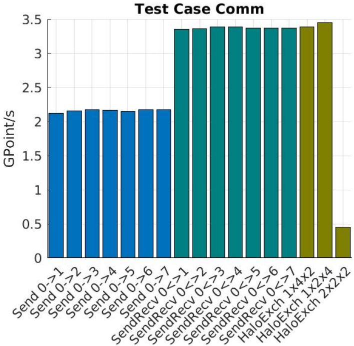
- Exhange of halos used in FD kernels with MPI_Sendrecv
- Effect of subdomain decomposition setttings

Benchmark configuration

- 8 nodes with 1 MPI/node & 32 threads/node
- Baseline kernel
- Grid size 4 GB (1000 x 1000 x 1000 points)
- FD order O8
- Subdomain decomposition settings: 1x4x2 / 1x2x4 & 2x2x2
- Reproduce results with `./script/testCase_Comm/hpcscanComm.sh`
- Total 3 configurations: Elapsed time less than 1 minute

Test Case Comm - Results [3]





[3] Updated Dec 26, 2020

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Test Case FD_D2 - Description

Benchmark objective

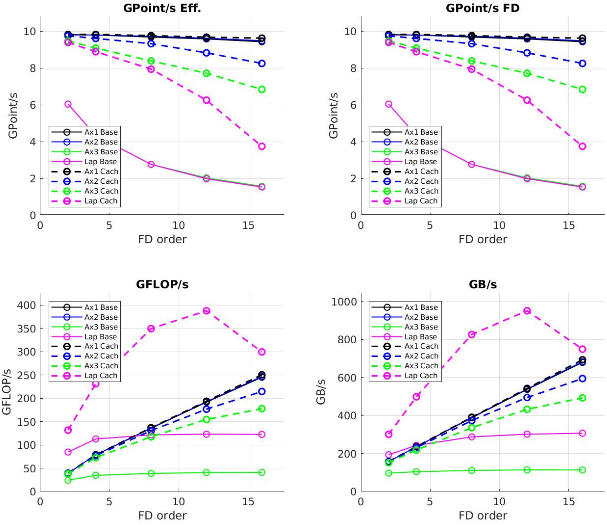
Assess performance of spatial second derivative computations with FD

- Directionnal derivatives
  - Axis 1, $W = \partial^2_{x1}(U)$
  - Axis 2, $W = \partial^2_{x2}(U)$
  - Axis 3, $W = \partial^2_{x3}(U)$
- Laplacian $W = \Delta(U)$
- Effect of FD stencil order
- Try different implementations of FD computation

Benchmark configuration

- 1 node with 32 threads
- 2 test modes: Baseline & CacheBlk
- Grid size 4 GB (1000 x 1000 x 1000 points)
- FD orders 2, 4, 8, 12 & 16
- Reproduce results with `./script/testCase_FD_D2/hpcscanFD_D2.sh`
- Total 10 configurations: Elapsed time about 2 minutes

Test Case FD_D2 - Results [4]



[4] Updated Dec 24, 2020

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Test Case Propa - Description

Benchmark objective

Find optimal configuration for the wave propagator regarding accuracy/cost

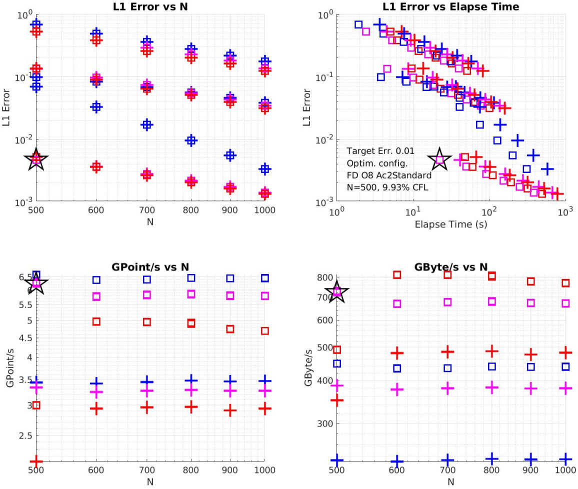
- Explore range of grid sampling
- Explore range of time step
- Explore range of FD order
- Try different implementations of the propagator

Benchmark configuration

- 1 node with 32 threads
- Test mode CachBlk
- 2 propagator implementations: Ac2Standard and Ac2SplitComp
- FD orders 4, 8 & 12
- Time step 100, 50 and 10% of stability time step
- Grid size from 500x500x500 (500 MB) to 1000x1000x1000 (4 GB)
- nt from 101 to 2311 (depending of the configuration) & ntry $= 4$
- Reproduce results with `./script/testCase_Propa/paramAnalysis/hpcscanPropaParamAnalysis.sh`
- Total 108 configurations: Elapsed time about 12 hours

Test Case Propa - Results [5]

Blue FD O4, Pink FD O8, Red FD O12 / Square=Ac2Standard, Cross=Ac2SplitComp



Target Err. 0.01
Optim. config.
FD O8 Ac2Standard
N=500, 9.93% CFL

[5] Updated Dec 28, 2020

Test Case Propa - Description

Benchmark objective

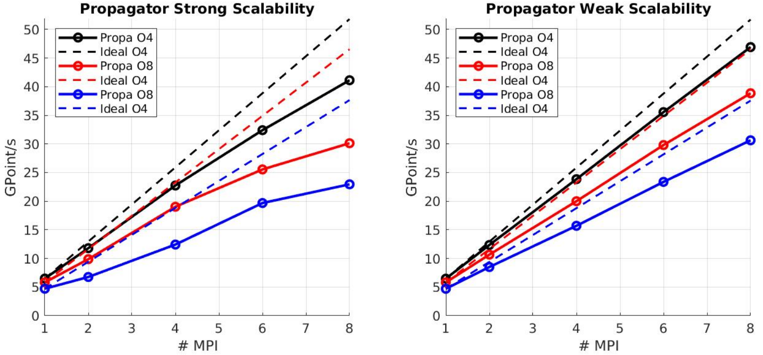
Assess the scalability of the wave propagator on multiple nodes

- Strong and weak scalability
- Effect of the FD stencil order

Benchmark configuration

- From 1 node to 8 nodes with 32 threads/node
- Test mode CachBlk
- Propagator implementation Ac2Standard
- FD orders 4, 8 & 12
- Strong scalability: Grid size 1000x1000x1000 (4 GB)
- Weak scalability: Grid size from 1000x1000x1000 (4 GB) to 1000x4000x2000 (32 GB)
- nt = 100
- Reproduce results with
  `./script/testCase_strongWeakScalability/hpcscanPropaStrongWeakScalability.sh`
- Total 30 configurations: Elapsed time about 1h 15min

Test Case Propa - Results [6]



[6] Updated Dec 28, 2020

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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

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Acknowledgements

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