Evaluating New Communication Models in the Nek5000 Code for Exascale

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Exascale ProGRAmming Models

Outline

- Parallelism, Programming Models and Legacy Applications at Exascale
- Nek5000 code
- Parallel Communication in Nek5000
  - Gather-Scatter Communication Operator
  - New MPI Gather-Scatter Communication Operator
  - New PGAS Gather-Scatter Communication Operator
- Conclusions

Parallelism at Exascale

- Tianhe-2 (#1 in Top500) has 3,120,000 cores in total, much larger number of processes at exascale → billion of processes.
- At exascale:
    - Interconnection networks with higher performance (smaller latency, larger bandwidth)
    - Emerging new network topologies, i.e. Slim Fly, and Cray Dragonfly
    - Support on NIC for communication operations without intervention of CPU

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Programming Models at Exascale

- Existing: parallel programming models are designed for tera and peta-scale eras.
- Good news: parallel programming models are being equipped with new features to effectively exploit exascale technology:
  - One-sided communication → use communication support from network
  - Non-blocking collectives → more asynchronous model, i.e. in linear solvers
  - Neighborhood collectives → use smart scheduler for communication on small group of processes
- PROBLEM: How many applications at EASC2015 use new features in programming models?

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Problem: Legacy Applications

- Communication in legacy codes was designed to allow for features that were not present during the initial development of the code, i.e. thousands of LOC for non-blocking communication.
- Development went so far that there is no turning back point. Communication code is so complex that it is very difficult to add new features.
- We need disruptive changes in codes to use new features in programming models.

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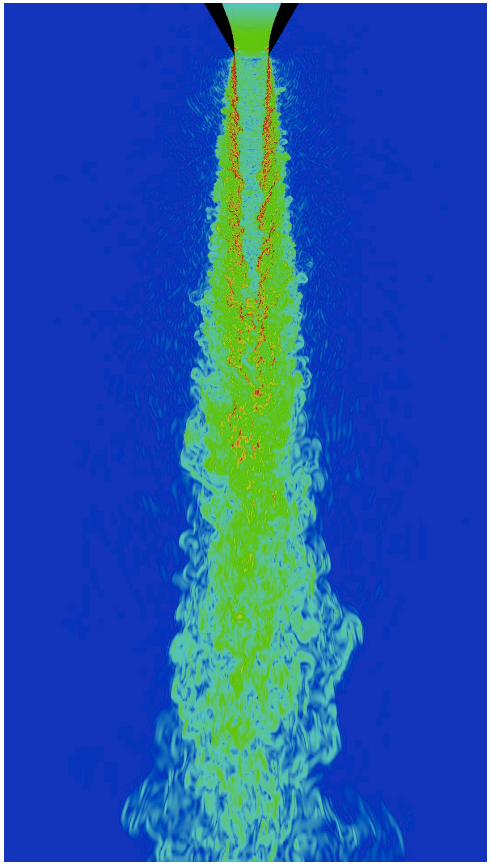
Nek5000 (our legacy applications)

- Nek5000 is a CFD code for the simulation of incompressible fluids. Nek5000 is used for reactor thermal hydraulics, astrophysics, combustion, oceanography, vascular flow modeling.
- It was developed in 80s and consists of 70,000 lines of code: 90% in Fortran77 (computation) and 10% in C (to handle communication).
- Communication implements halo exchange with 3 different algorithm with non-blocking MPI p2p comm (MPI1)
- Nek5000 communication kernel is very complex and obfuscated → very difficult to use new features in programming models



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Our Disruptive Change in Nek5000

- We designed a new communication kernel for Cartesian topology and structured grids.
- 7,000 loc → 500 loc → Code readability
- C, MPI C Bindings → Fortran, MPI Fortran Bindings → removed interoperability issue between C and Fortran
- No virtual topology → Cartesian virtual topology → neighborhood collectives possible in Nek5000

"All I'm saying is now is the time to develop the technology to deflect an asteroid."

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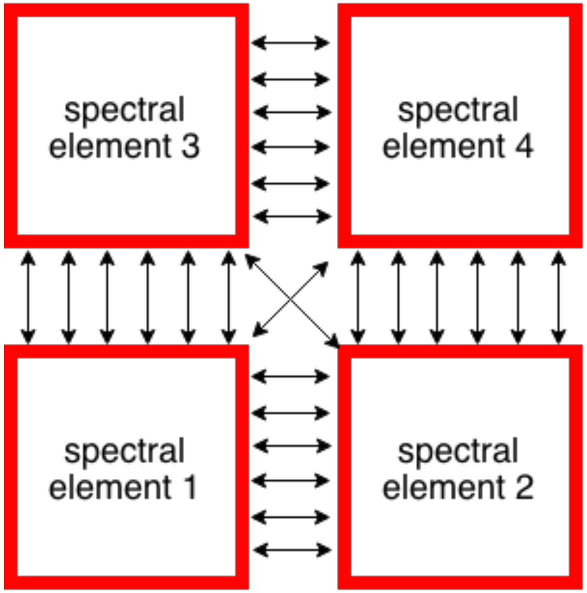
Parallel Communication in Nek5000

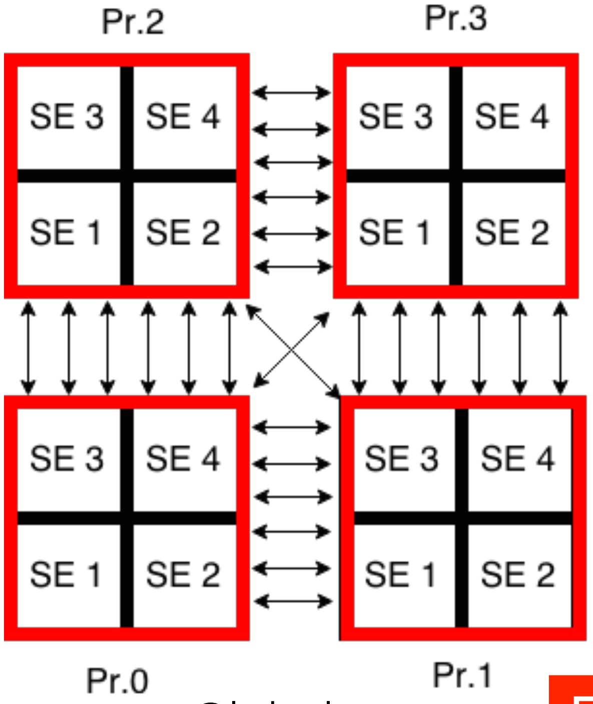
- Global reductions in the CG linear solver, i.e. calculation of inner products of auxiliary vectors.
- Point-to-point communication for a "halo exchange" in the so called gather-scatter operator
- Three old gather-scatter operator algorithms in Nek5000:
  - Pairwise (used for our comparison and fastest one)
  - Chrystal router
  - Allreduce

Gather-Scatter Communication Operator

- It is for communication of spectral element interface values:
  - values on shared (by elements on different processes) nodes have to be consistent



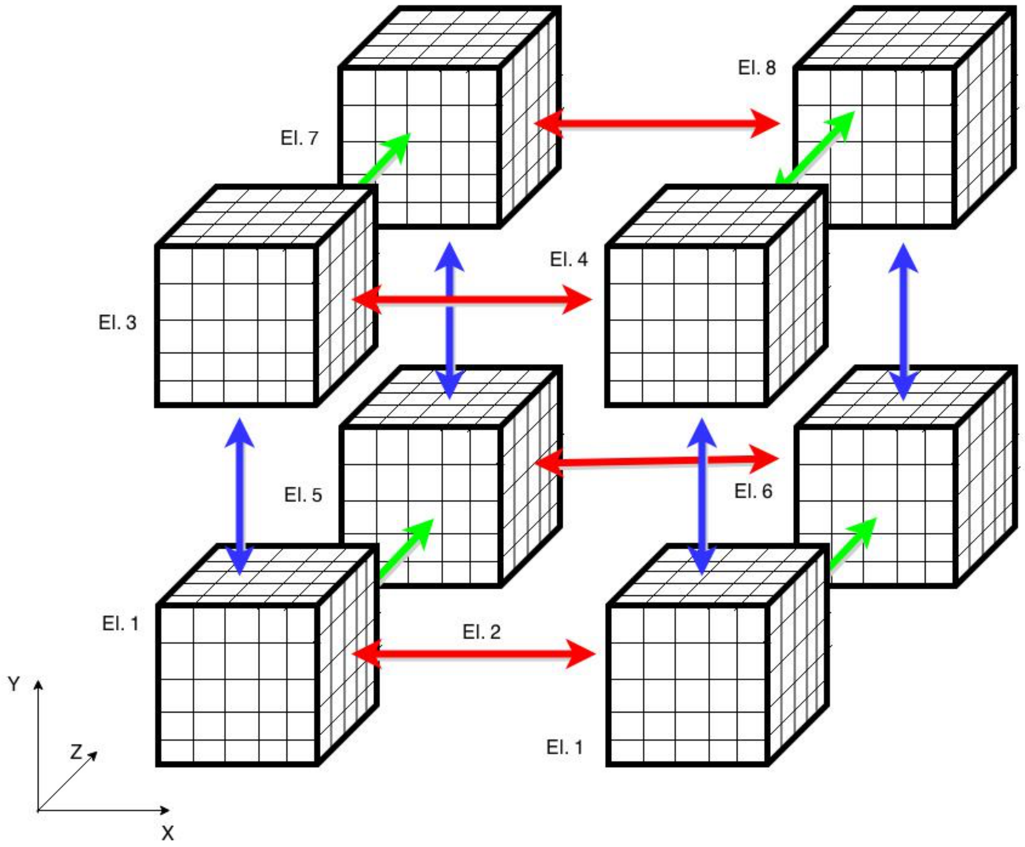
Local gs_op



Global gs_op

New Gather-Scatter Communication Operator

- Designed for Cartesian topology and uniform grids



- Local gs_op
  - synchronization between elements on one process
  - synchronization of all boundary points except those that are neighbors of elements on other processes
  - gs_op along X, Y, Z directions

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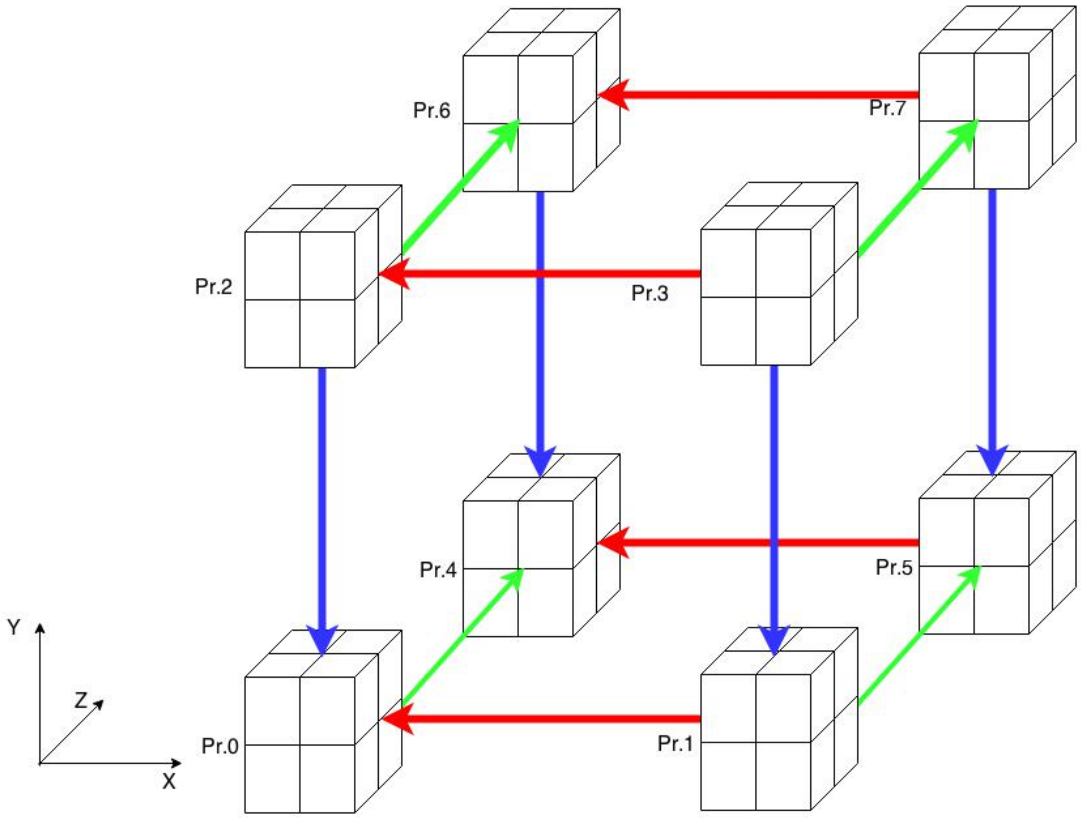
New Gather-Scatter Communication Operator

- Designed for Cartesian topology and uniform grids



- Global gs_op
  - synchronization of shared points between elements located on different processes
  - gs_op along X, Y, Z directions

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MPI Implementation

- New implementation uses Cartesian virtual topology
- Uses MPI blocking point-to-point communication (next step: non-blocking and neighborhood collectives)
- Old one uses non-blocking point to point collectives.

Test Environment

Beskow supercomputer at PDC, KTH:

- Cray XC40 system, Cray Aries interconnect;
- Cray Fortran77 and C/C++ compilers of version 5.2.40;
- Cray MPICH2 of version 7.0.4;
- Nekbone – skeleton version of Nek5000, with the same communication kernel

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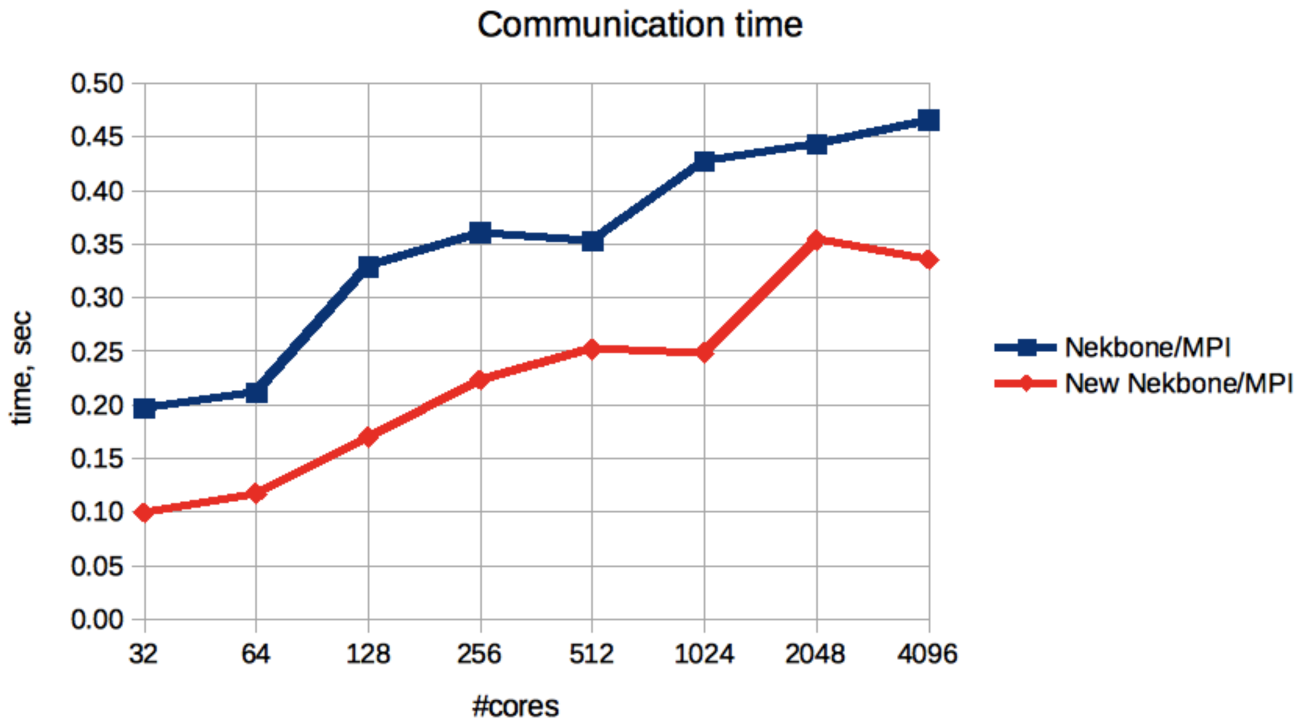
Comparison between Old and New MPI Communication in Nek5000/Nekbone (weak scaling)



The new Nekbone implementation is always faster than old. On average 37% faster.
This is expected as old Nekbone is designed for complex geometry.

1 MPI process per core
polynomial order – 10
# spectral elements per core - 256

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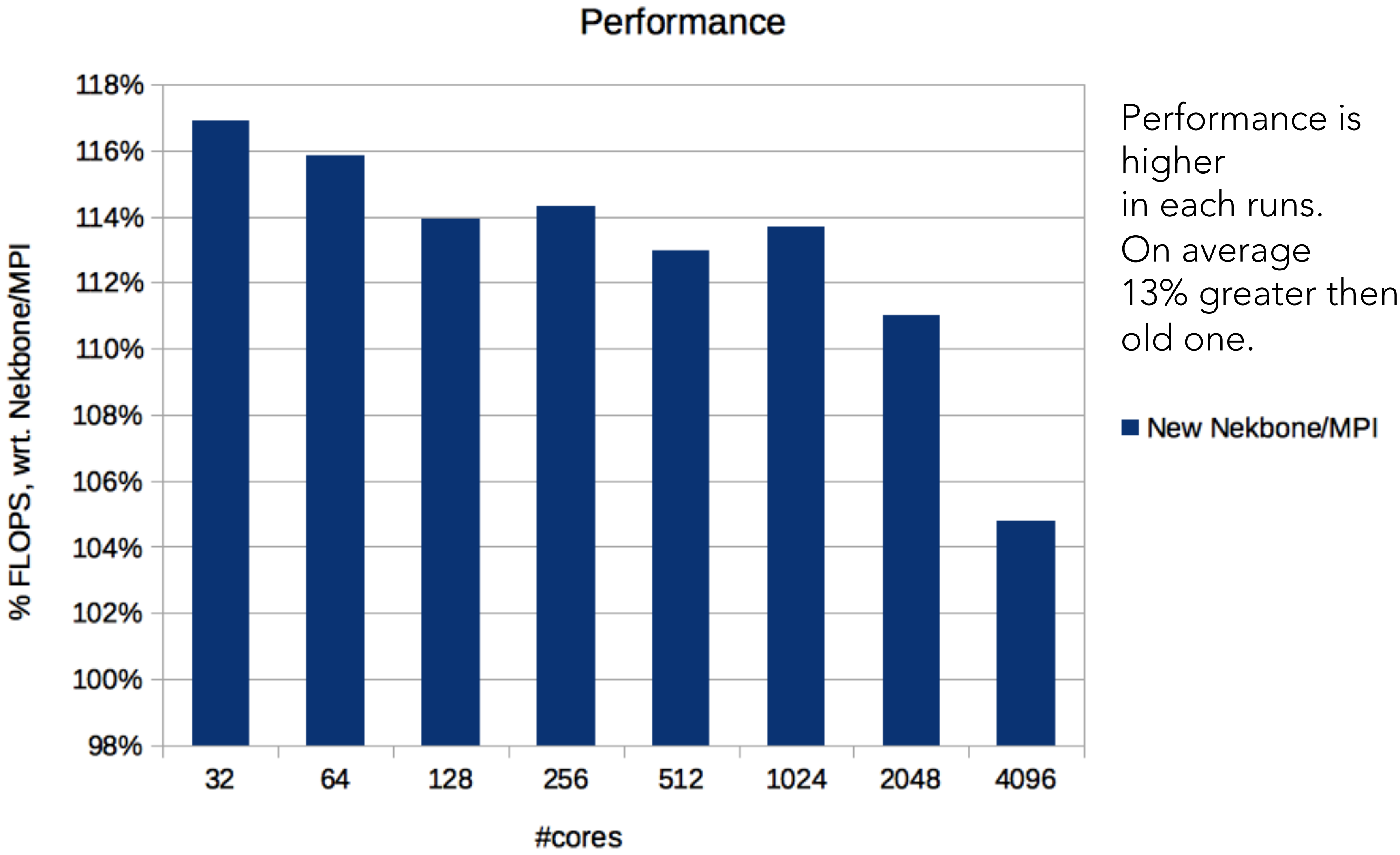
Comparison between Old and New MPI Communication in Nek5000/Nekbone (weak scaling)



Performance is
higher
in each runs.
On average
13% greater then
old one.

PGAS, GASPI and GPI-2

- Partitioned Global Address Space
  - Global memory space that is accessible for all the processes
  - One-sided communication (very fast when supported by network)
- GPI-2
  - Implementation of the GASPI standard of a PGAS API
  - Developed by Fraunhofer Institute for Industrial Mathematics ITWM

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GPI-2 Implementation

- Segment is a contiguous block of virtual memory. Segments may be globally accessible from every thread of every GPI-2 process.
- One-sided asynchronous communication: GPI-2 process specifies all communication parameters, both for the local and the remote side.
- GPI-2 offers the possibility to use different queues to handle communication requests.

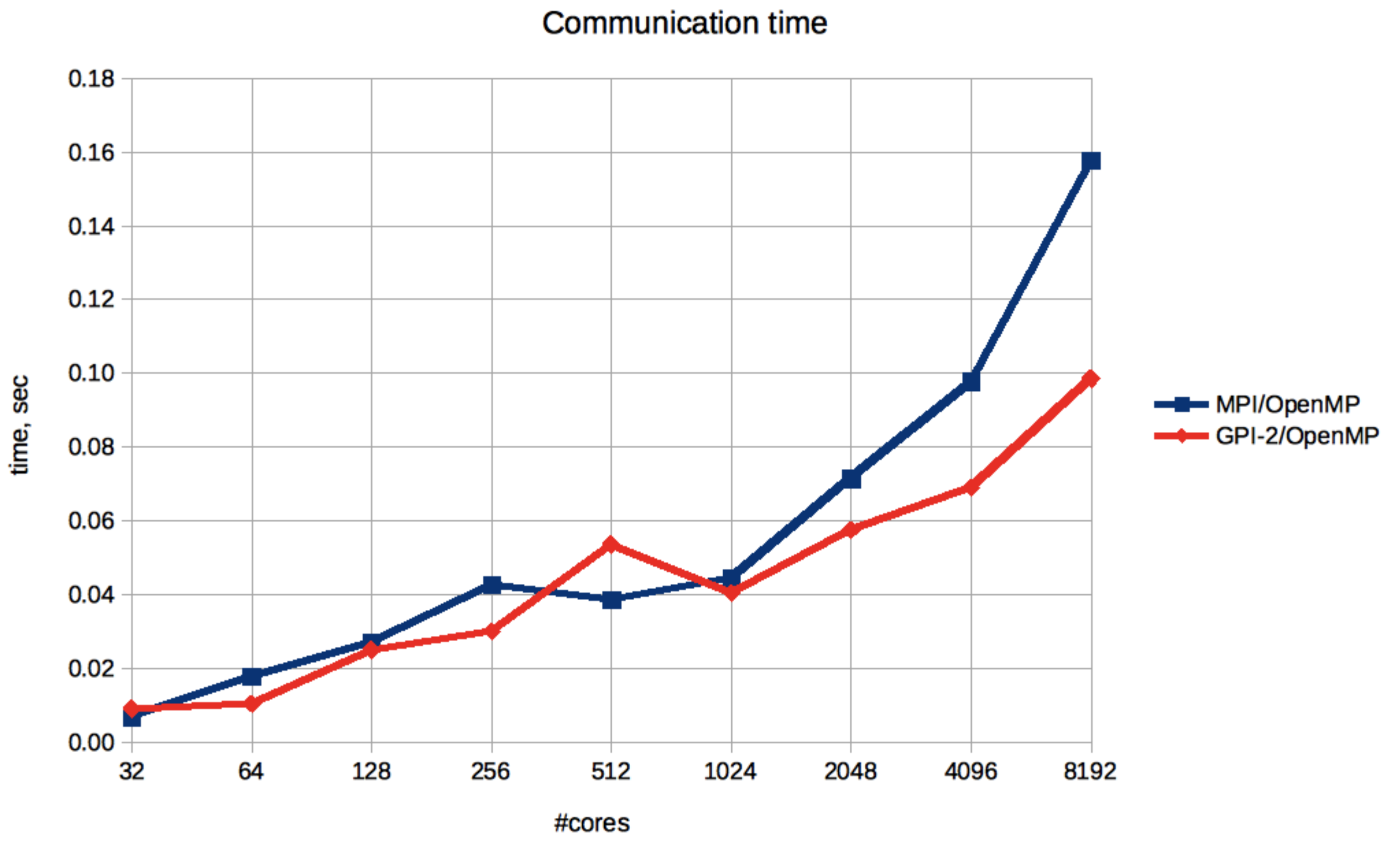
GPI-2 Implementation

- OpenMP directives are used in loops when evaluating A*x for the spectral elements, also in packing and averaging interface values, e.g.:

```
!$OMP PARALLEL DO PRIVATE(e,ur,us,ut,wk) SHARED(nelt,w,u,gxyz)
!$OMP& SCHEDULE(STATIC)
      do e=1,nelt
         call ax_e( w(1,e),u(1,e),gxyz(1,1,e),ur,us,ut,wk)
      enddo
!$OMP END PARALLEL DO
```

- Asynchronous communication allowed to overlap between computation + packing data and communication.

Comparison between New MPI and GPI-2 Communication in Nek5000/Nekbone (weak scaling)



GPI-2 version is always faster, except for 512 cores.
At 8192 cores GPI-2 is 60% faster than MPI.
Fair comparison would be with non-blocking MPI (in future).

1 GPI-2/MPI process per socket (16 cores)
polynomial order – 10
# spectral elements per process - 128

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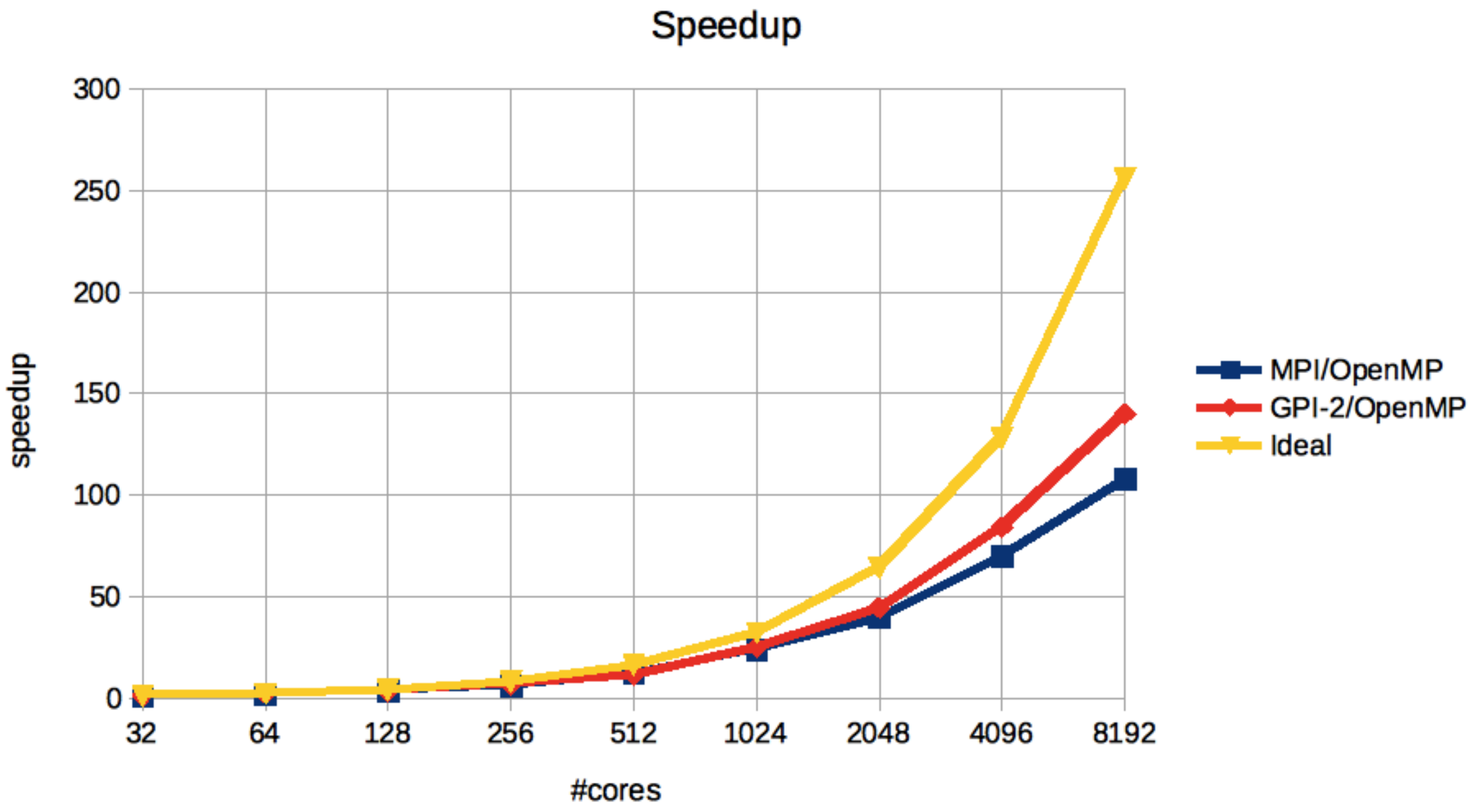
Comparison between New MPI and GPI-2 Communication in Nek5000/Nekbone (weak scaling)



At 8192 cores GPI-2 is 39% faster than MPI and 45% lower than ideal scaling, MPI – 58% lower than ideal scaling. Could be improved by adding more OpenMP directives to computations.

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Conclusions

- Going to exascale requires disruptive changes.
- New gather-scatter communication operator has approx. 500 lines of code, while the old one - 7000.
- New communication kernel can be used for co-design work as it is much easier than the old one.
- Communication time was decreased.

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Thank you!

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