UNIVERSITY OF CAMBRIDGE

Bringing a scientific application to the distributed world using PGAS

Performance, Portability and Usability of Fortran Coarrays

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Summary

We aim to investigate the

- performance,
- portability and
- usability

of Fortran 2008 coarrays for porting large, complex scientific applications to distributed memory.

Outline

- Coarrays & implementations of coarrays
- Synthetic benchmarks
- Porting a scientific code: TROVE

What are Coarrays

Coarrays are:

- a PGAS extension of Fortran,
- Fortran 2008 adds remote access to variables,
- Fortran 2015 adds collectives, atomics and teams.

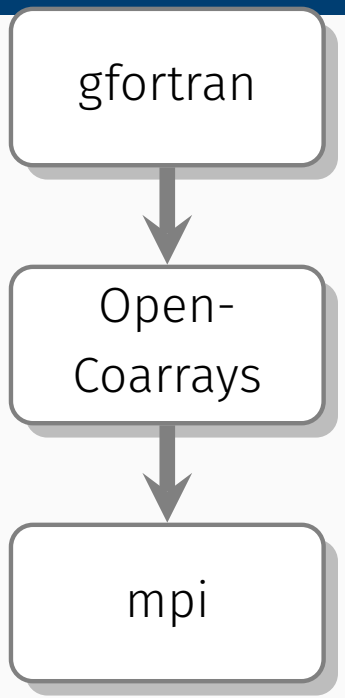
```
real :: x(10)[*]

x(:) = x(:)[1]
 !call mpi_get(x, 10, MPI_REAL, 1, disp, 10, MPI_REAL, mywin, ierr)

sync all
 !mpi_barrier(MPI_COMM_WORLD, ierr)

call co_sum(x, result_image=1)
 !mpi_reduce(x, x, 10, MPI_REAL, MPI_SUM, 0, MPI_COMM_WORLD, ierr)
```

Coarray implementations

	F2008	F2015	OpenMP	MPI
gfortran + OpenCoarrays	✓	✓	✓	✓
Intel Parallel Studio	✓	×	✓	✓
OpenUH + GASNet	✓	?	✓	
Cray	✓	✓	?	✓

Coarray implementations: gfortran + OpenCoarrays

- gfortran frontend generates calls to libcaf
  `_gfortran_caf_get (...)`
- OpenCoarrays supplies libcaf
- OpenCoarrays libcaf calls into a standard MPI library

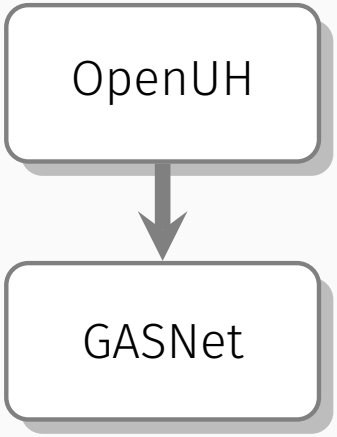


✓ gfortran + mpi are very widely supported
  ⇒ can run (almost) anywhere
✓ gfortran can compile most things
× MPI not the ideal target for implementing coarray support
× gasnet backend exists but is ‘unsupported’ (and doesn’t compile)

- Intel implementation uses a similar structure

Coarray implementations: OpenUH + GASNet

- OpenUH compiler frontend
- communication backends provided by GASNet



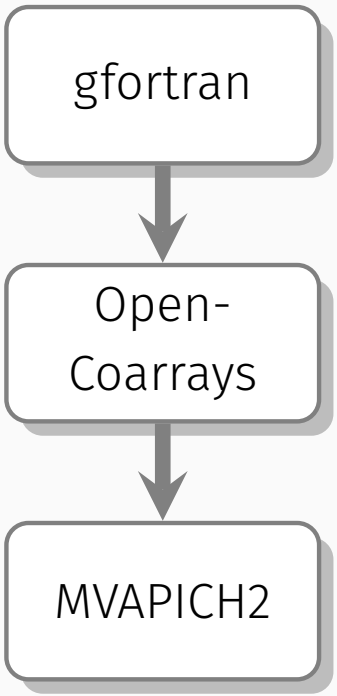
✓ potentially higher performance

× OpenUH as compliant with complex (nasty) science code

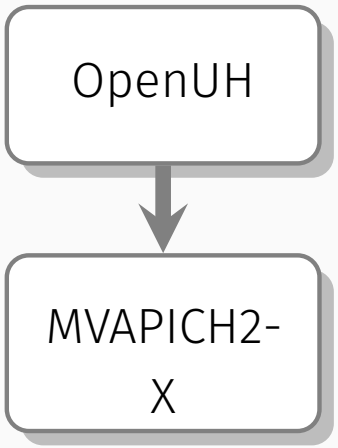
× OpenUH not simple to deploy

Coarray implementations: using MVAPICH2-X

Use MVPAICH2 MPI



Use MVPAICH2-X GASNet conduit



Synthetic Benchmarks

- EPCC Fortran Coarray micro-benchmark suite
- OSU microbenchmarks.

All measurements performed on with

- Intel Broadwell (E5-2650)
- Mellanox EDR

OpenCoarrays
: gfortran 7.1.0 + OpenCoarrays 1.8.10 + MVAPICH2 2.2

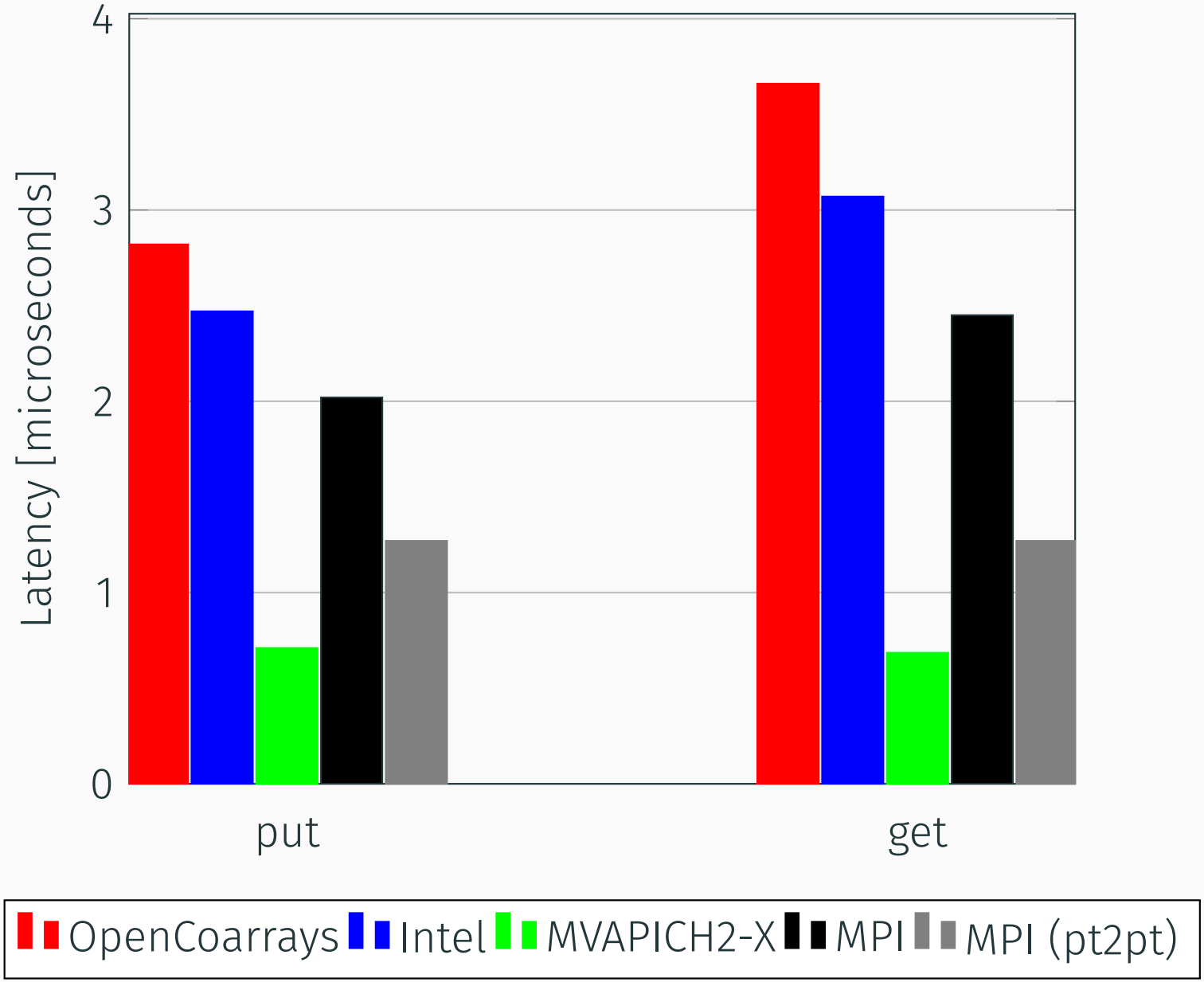
Intel
: Intel Parallel Studio (Intel compiler + Intel MPI) 17.4

MVPAICH2-X
: OpenUH 3.1.0 + MVPIACH2-X 2.2

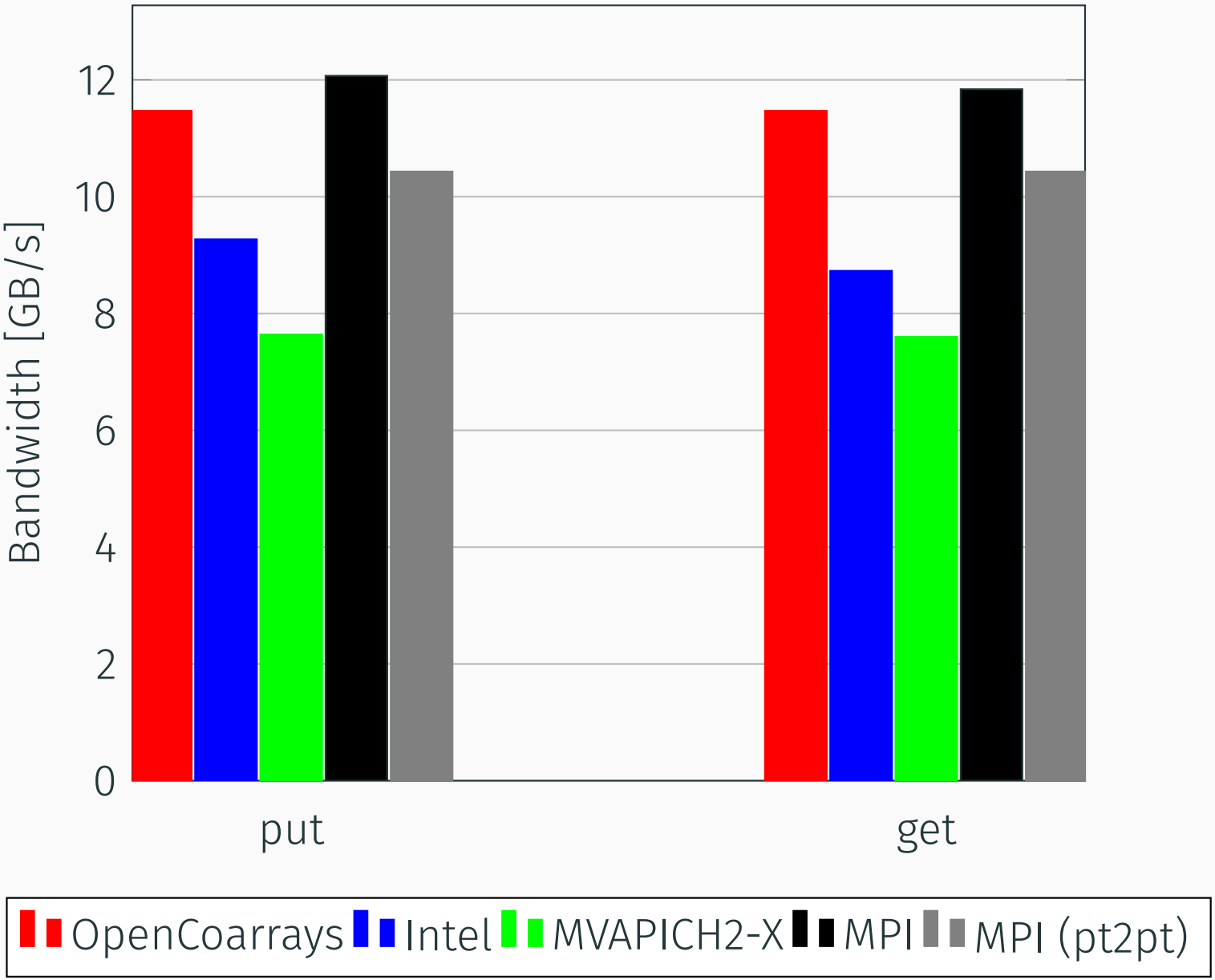
MPI put/get (using MPI-3 put and get)
: gfortran 7.1.0 + MVAPICH2-X 2.2

MPI (p2p) (using MPI send to fake puts and gets)
: gfortran 7.1.0 + MVAPICH2-X 2.2

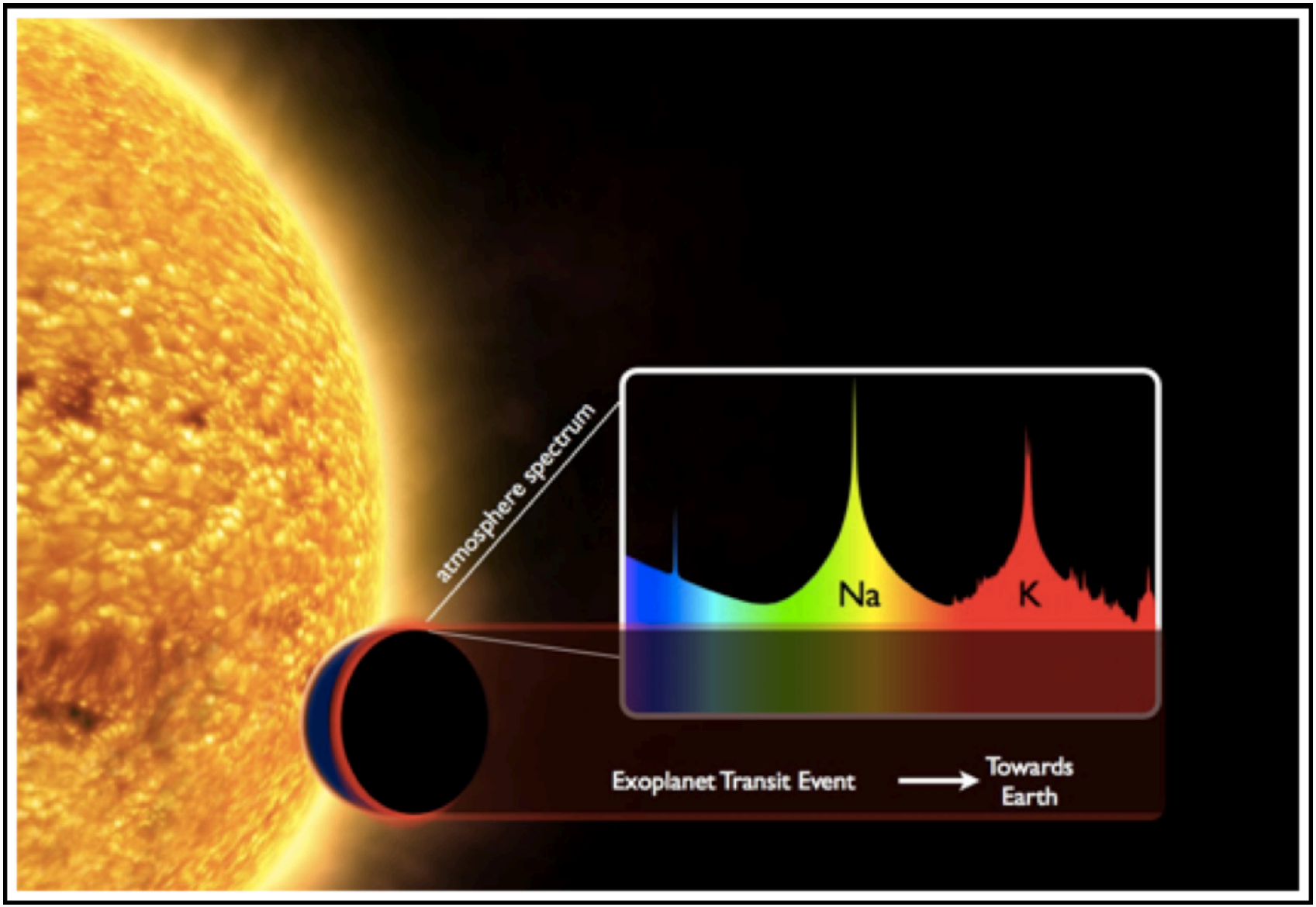
Synthetic Benchmarks: Latency



Synthetic Benchmarks: Bandwidth



TROVE


atmosphere spectrum
Na
K
Exoplanet Transit Event
Towards
Earth

TROVE

- part of the ExoMol (exoplanet molecular line search) project
- looking at the composition of atmospheres on exoplanets
- ultimately searching for aliens!

TROVE has been developed by Sergey Yurchenko (currently at UCL)

- under active development with many contributors
- written in modern Fortran
- developed targeting shared memory :-(
- $\sim$ 160k lines of code

TROVE: Why distributed memory

- TROVE has long run-times (>1M CPU Hours)
- Construction & diagonalisation of 1000s of matrices
- Matrices of size 1M x 1M
- Scientists want to compute bigger problems

Why Coarrays?

- Translating a large code base to distributed memory is daunting
- Maintainers prefer not to use MPI
- PGAS approach allows an ‘incremental’ approach

TROVE: code before

```
g = 0

$!omp parallel do private(h,phi,D) reduce(+:g)
do iterm = 1, N
  phi = !construct Hamiltonian
  D = !construct basis set
  h = matmul(transpose(D), matmul(phi, D))

  g = g + h
enddo
$!omp end parallel do

call diagonalize(g)
```

- Each loop iteration takes >10 seconds
  $\Rightarrow$ almost embarrassingly parallel

TROVE: code after

```
g = 0
do iterm = 1, N
  if (mod(iterm, num_images()) /= this_image()) cycle

  phi = !construct Hamiltonian
  D = !construct basis set
  h = matmul(transpose(D), matmul(phi, D))

  g = g + h
enddo

call co_sum(g)
call diagonalize(g)
```

- very few changes required from OpenMP
- scheduling is basic

TROVE: Results

Coarrays implementation works!

Before

Ideal scaling on 4 socket node

After

Ideal scaling on 4 nodes with 1 socket each

Problems

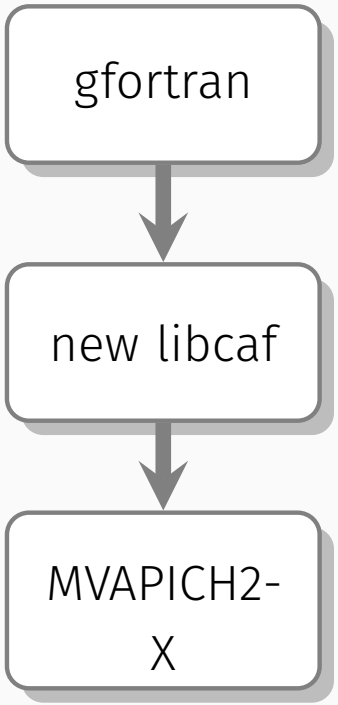
- TROVE not compatible with OpenUH
  $\Rightarrow$ can't use MVAPICH2-X :-(

Future Work

- Extracting more parallelism
- MPI interoperability

Wishlist

Building a coarray implementation with gfortran and an MVAPICH2-X based libcaf.



- gfortran frontend generates calls to libcaf
- a new implementation of libcaf
- this new libcaf calls MVAPICH2-X

  - combines the portable and friendly gfortran
  - with the high-performance of MVAPICH2-X

Thank you!