Overlapping communication and computation using the Intel MPI library's asynchronous progress control

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IXPUG Meeting, 13.-16.10.2020

Motivation

- Communication time can become bottleneck when scaling
- Overlap with computation: hide communication time
- Non-blocking MPI calls: communication **is not** progressing asynchronously
- Implementation in user code: possible, but lots of changes needed (e.g., calls to MPI_Test in computational loops)
- Promise of Intel MPI's progress control:
  - Progress handled internally
  - No change to user code needed

Intel MPI's asynchronous progress control

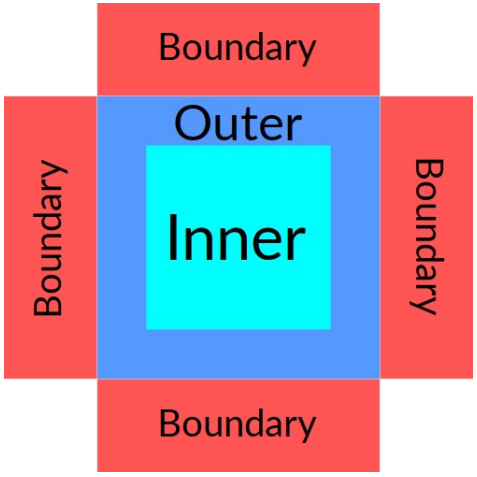
- Support for
  - Point-to-point operations
  - Blocking collectives
  - Non-blocking collectives (only Ibcast, Ireduce, Iallreduce)
- Only in release_mt and debug_mt variants
- Progress threads are spawned driving the communication
- Enable with I_MPI_ASYNC_PROGRESS=1
- Control pinning with I_MPI_ASYNC_PROGRESS_PIN
- Number of progress threads per MPI rank: I_MPI_ASYNC_PROGRESS_THREADS

Goals

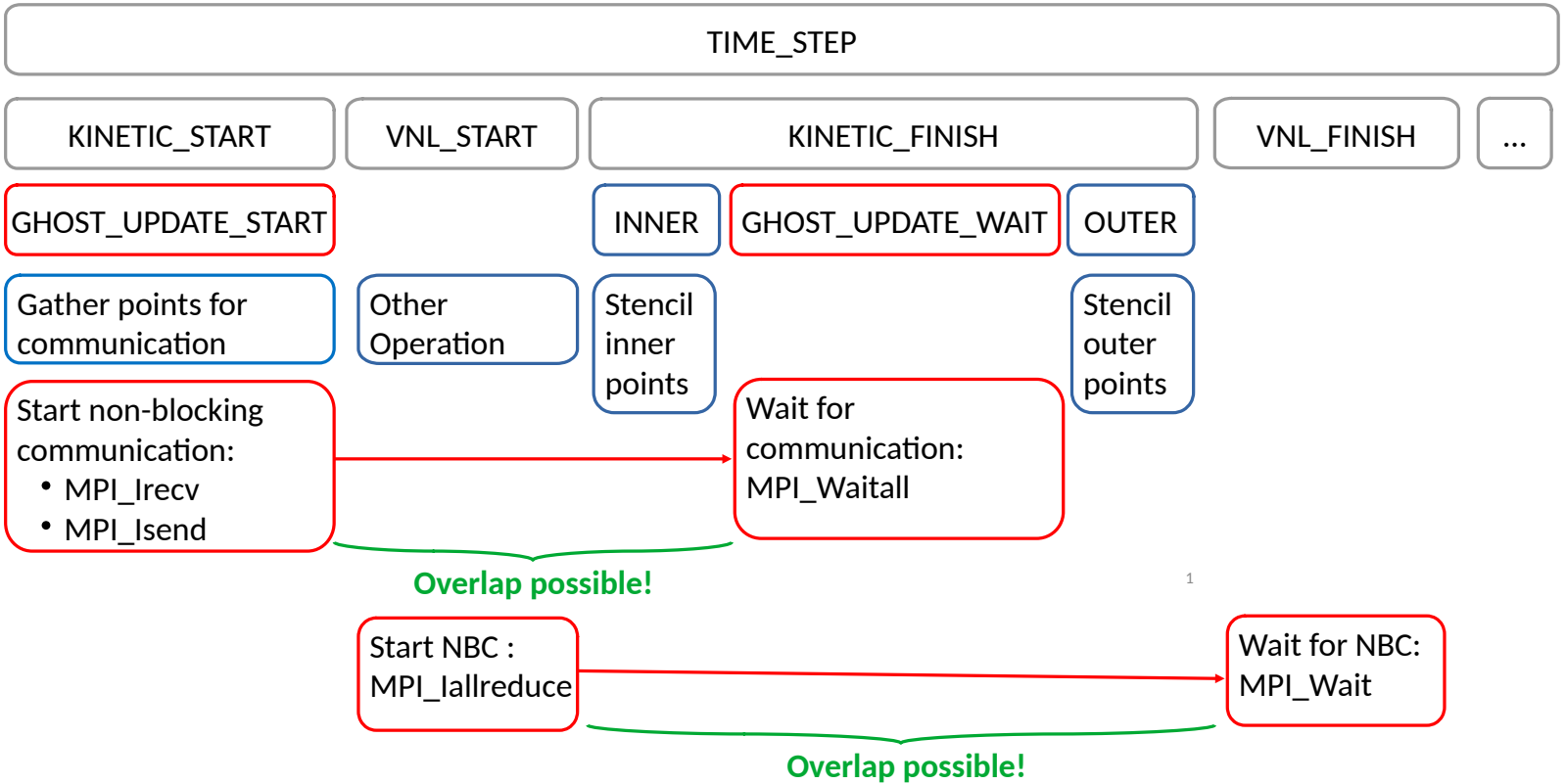
- Evaluate Intel MPI's asynchronous progress control for a real application
- Find best configuration
  - Fastest time to solution → compare full-node runs
  - Which combination MPI ranks & OpenMP threads fastest?
  - Spare cores for progress threads necessary?
  - Pinning necessary?
- Generalization to other codes

Application: Octopus

- Density functional theory code with pseudopotentials
- Real-space grid + finite differences
- Real-time time-dependent calculations
- Hybrid parallelization (MPI + OpenMP)
- Mainly Fortran, plus some C, plus some CUDA
- Open source: octopus-code.org
- Overlap of computation & communication:
  - Communication of boundary/ghost cells
  - Computation of inner part of stencil



Octopus: one time step



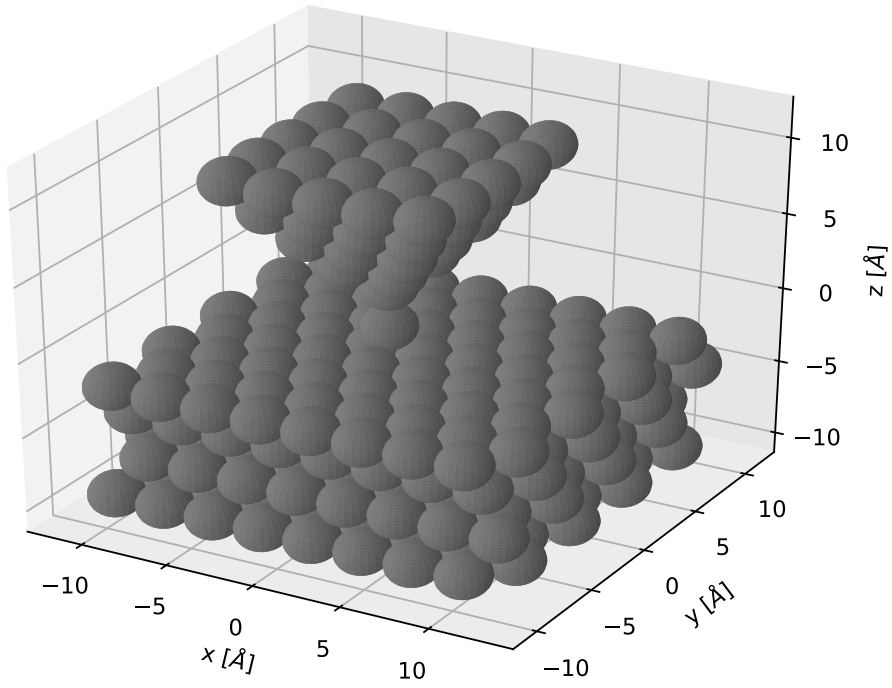
Benchmark clusters

MPCDF Max Planck Computing & Data Facility

- **Cobra** @ MPCDF
  - CPU: Intel Xeon 6148 Gold (Skylake)
  - 2x 20-core sockets/node = 40 cores/node
  - Interconnect: Omnipath (100 Gbit/s)
- **Raven** (interim system) @ MPCDF
  - CPU: Intel Xeon 9242 Platinum (Cascade lake AP)
  - 2x 48-core sockets/node = 96 cores/node
  - Interconnect: Infiniband HDR (100 Gbit/s)

Example system

- Silver tip over crystal
- Periodic in x and y
- 312 Ag atoms
- 3200 orbitals
- 2.4 M grid points

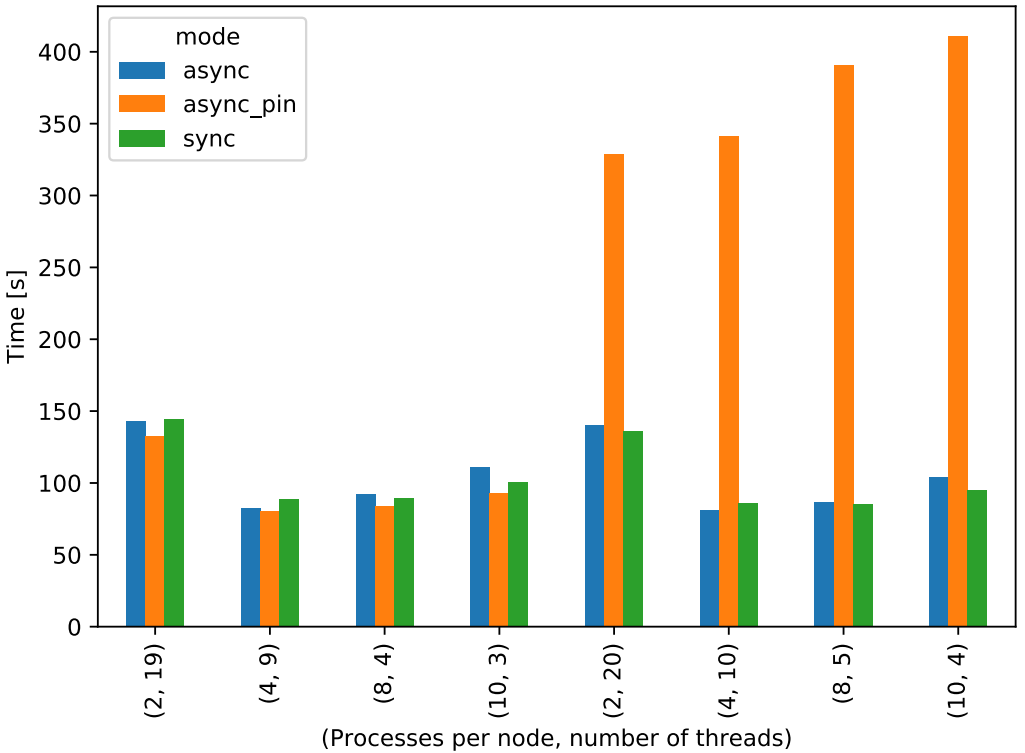


Results

Explanations

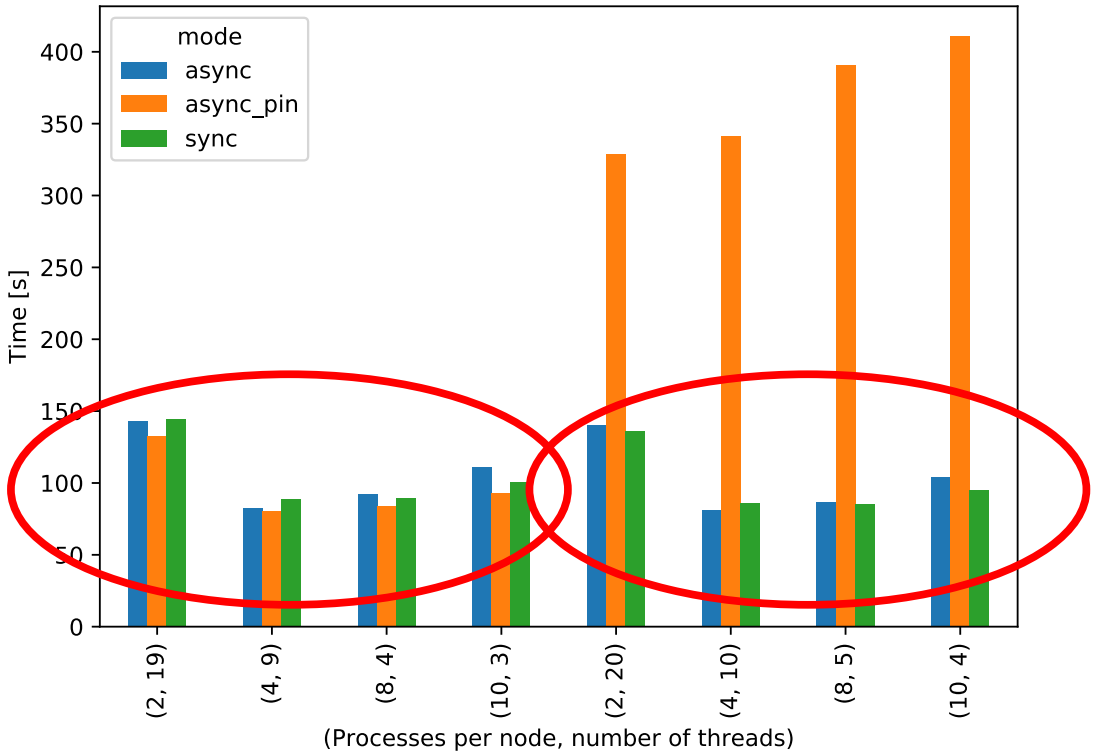
- 3 modes
  - sync: no asynchronous progress
  - async: asynchronous progress threads without pinning
  - async_pin: asynchronous progress threads with pinning
- Different combinations of MPI ranks x OpenMP threads for application
  - Full node: e.g. 1x40, 2x20, 4x10, 8x5, 10x4
  - Dedicated cores: e.g. 1x39, 2x19, 4x9, 8x4, 10x3
- Pinning using srun's cpu masks

Best combinations [cobra 40 cores/node]



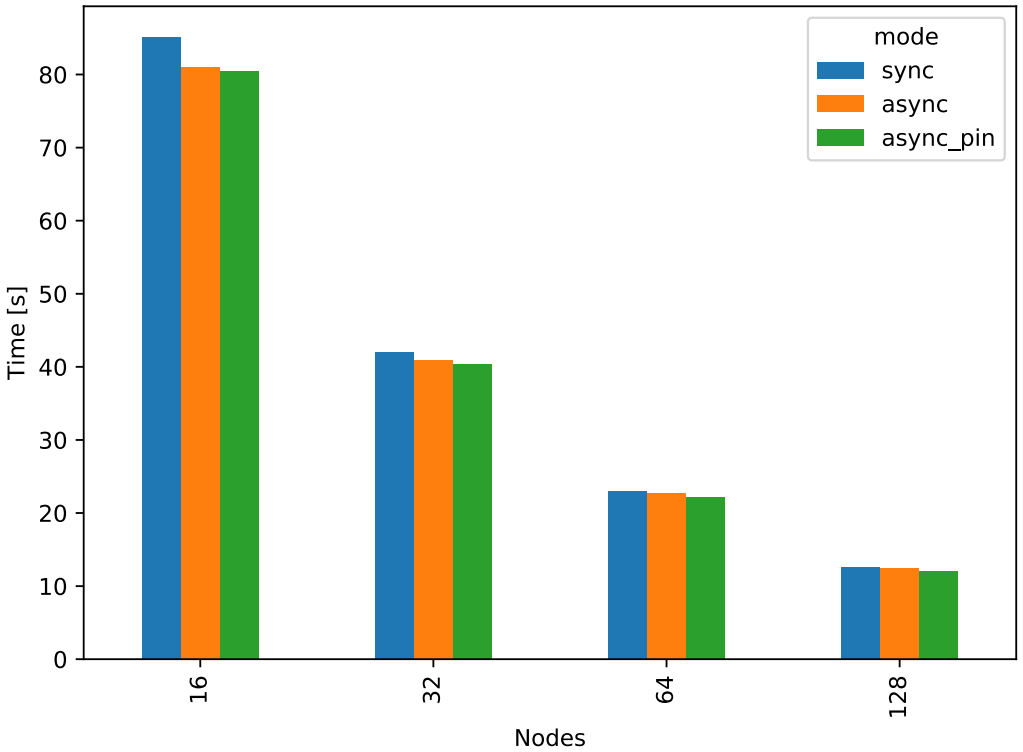
Best combinations [cobra 40 cores/node]

Dedicated cores
→ async_pin fastest



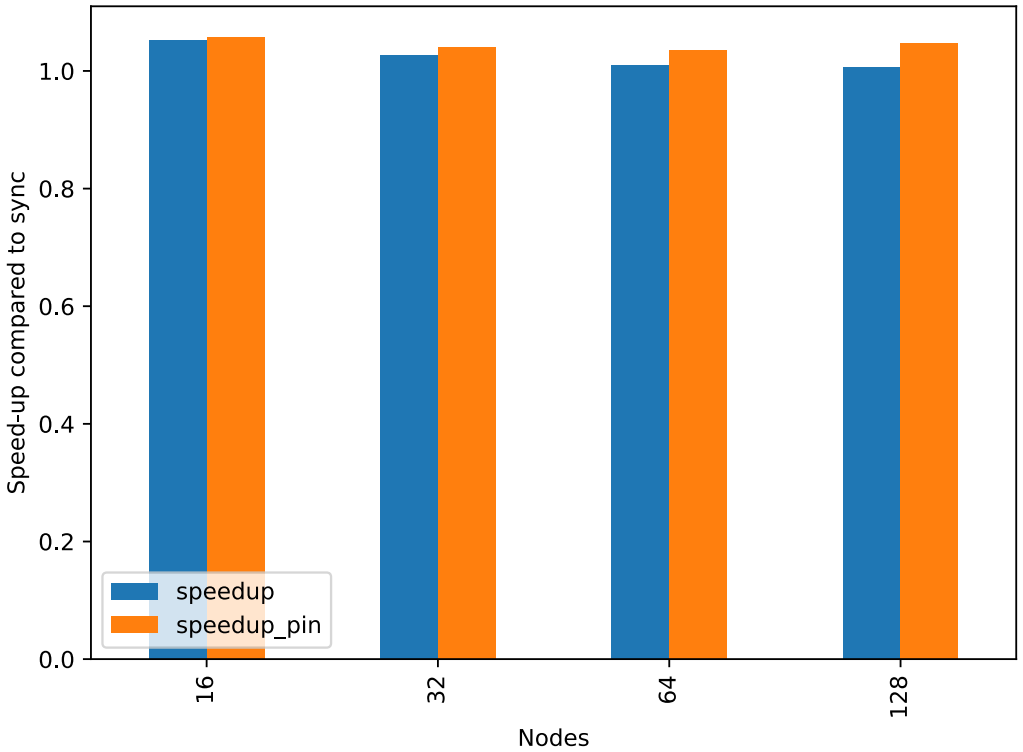
No dedicated cores
→ resource contention
if pinning enabled

Dedicated cores needed [cobra]



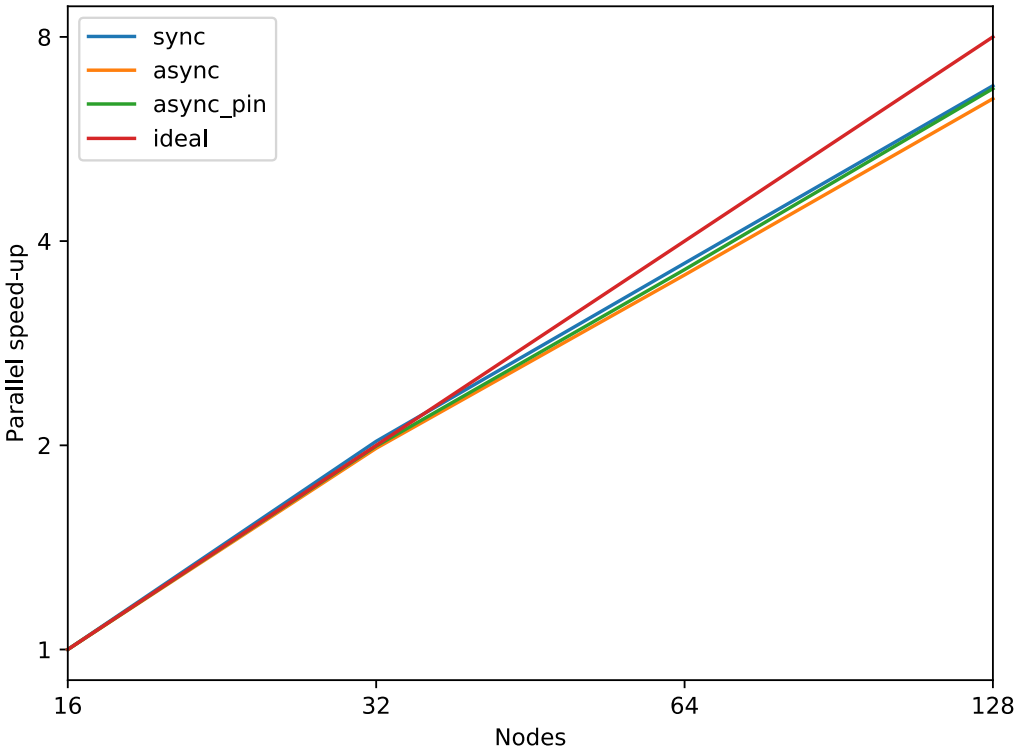
Fastest runs with pinning and dedicated cores!

Speed-up [cobra]



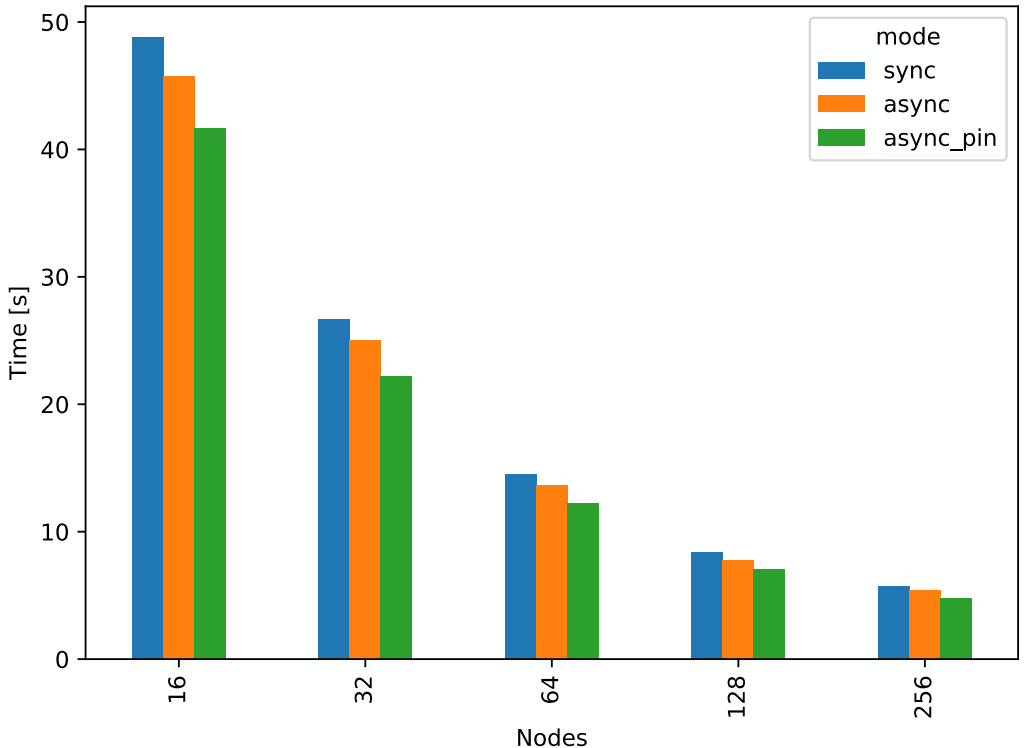
With pinning: speed-up of about 1.03x – 1.06x

Scaling of fastest runs [cobra]



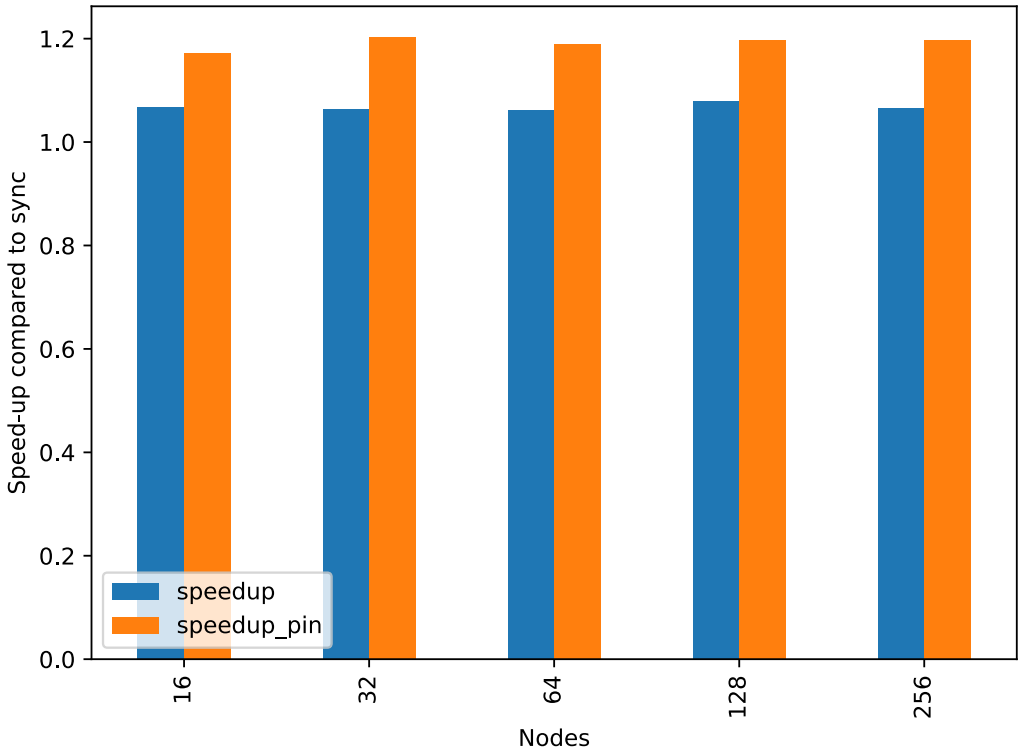
Good scaling: efficiency still 84% at 128 nodes (5120 cores)

Fastest runs [raven]



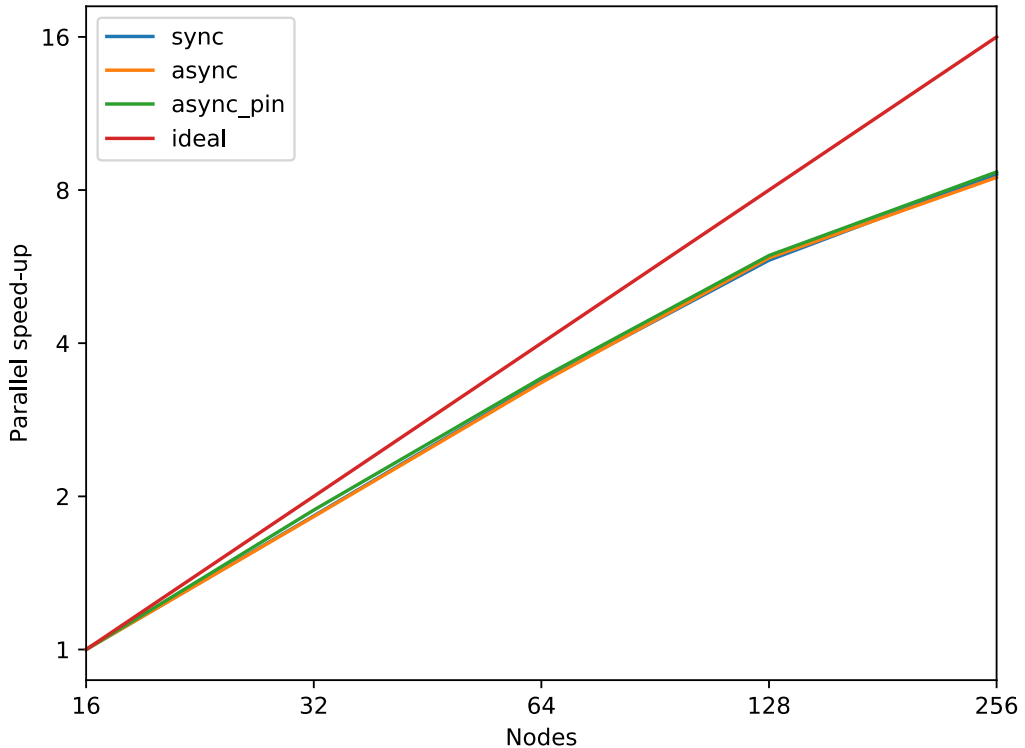
Fastest runs with pinning and dedicated cores!

Speed-up [raven]



With pinning: speed-up of about 1.17x – 1.20x

Scaling of fastest runs [raven]



Scaling efficiency:
74% at 128 nodes (12288 cores),
54% at 256 nodes (24576 cores)

Quantify overlap

- Difficult due to strong imbalance in communication volume (strange geometry)
- Compare average time in MPI functions
- On cobra, 16 nodes:
  - sync: 40.8 s of 89.7 s
  - async_pin: 33.1 s of 86.8 s

  → reduction of MPI time due to overlap

Generalization

- Stencil:
  - Split in inner & outer part needed
  - Benefit for other codes may be similar
  - Depends on stencil size (Octopus: 25 points)
- Hybrid codes probably benefit more
  - Less cores needed for progress threads
  - On cobra: on most node numbers, 8x4 best combination
    → 32 cores for compute, 8 for progress threads
  - Sacrificing a few cores probably ok for codes that are bound by memory bandwidth

Conclusions

- Intel MPI's asynchronous progress control allows overlap of computation & communication
- No change in user code needed for asynchronous progress
- Speed-up for octopus
  - Up to 1.05x on cobra (40-core Skylake nodes, Omnipath)
  - Up to 1.20x on raven (96-core Cascade Lake AP nodes, Infiniband)
- Lessons learned
  - Use release_mt/debug_mt
  - Dedicated cores needed
  - Do pinning right
  - Best potential for hybrid codes

Backup slides

Parallelization in Octopus

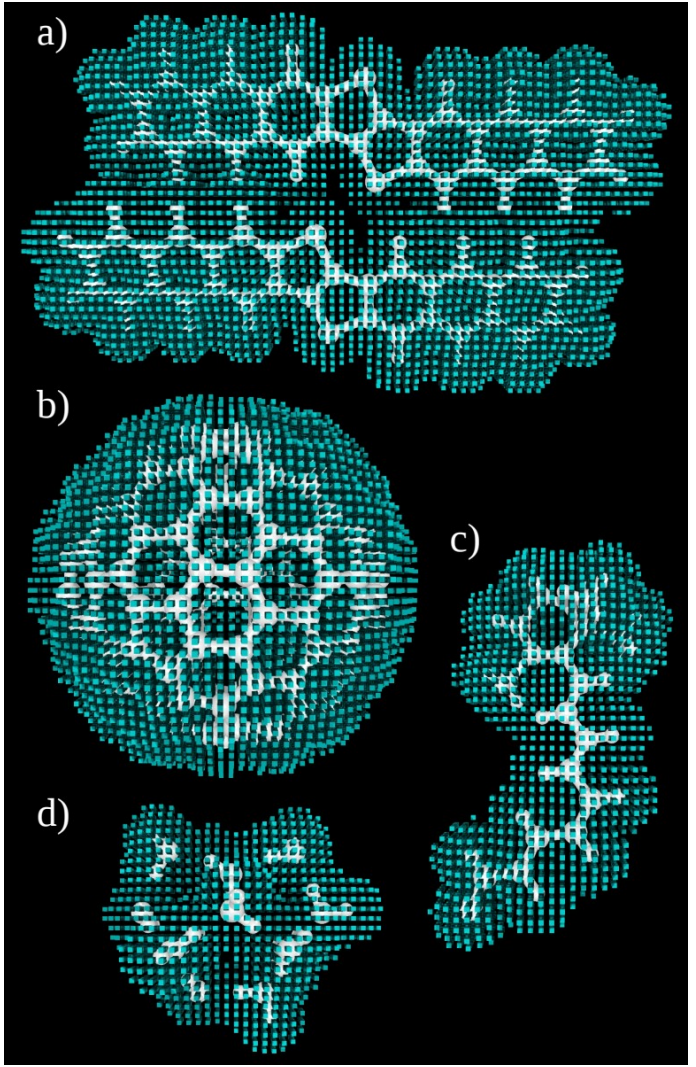
- Several dimensions
  - k points for periodic systems
  - States
  - Domain
- OpenMP parallelization also over domain loops
- Cobra: 2 nodes for domain (MPI + OpenMP)
  → 80 cores
- Raven: 1 node for domain (MPI + OpenMP)
  → 96 cores

Pinning: details

- Pinning needed for best results
  - Pin MPI rank + OpenMP threads next to progress thread
- Example: 4 MPI ranks, 9 OpenMP threads
  - Pin first rank to cores 0-8, second to 10-18, third to 20-28, fourth to 30-38
  - srun --cpu-bind=mask_cpu:0x1ff,0x7fc00,0x1ff00000,0x7fc0000000
  - Pin progress threads to dedicated cores 9, 19, 29, 39
  - export I_MPI_ASYNC_PROGRESS_PIN=9,19,29,39
- Slurm CPU mask:
  - Hexadecimal number, binary representation → enabled cores
  - 0x7fc00 = 0b11111111110000000000 (cores 10 to 18)

Data layout

- Real-space grid for FD
- Complicated shape possible, e.g. molecules



X. Andrade & A. Aspuru-Guzik, J. Chem. Theory Comput. (2013), 9, 10, 4360-4373

Data layout

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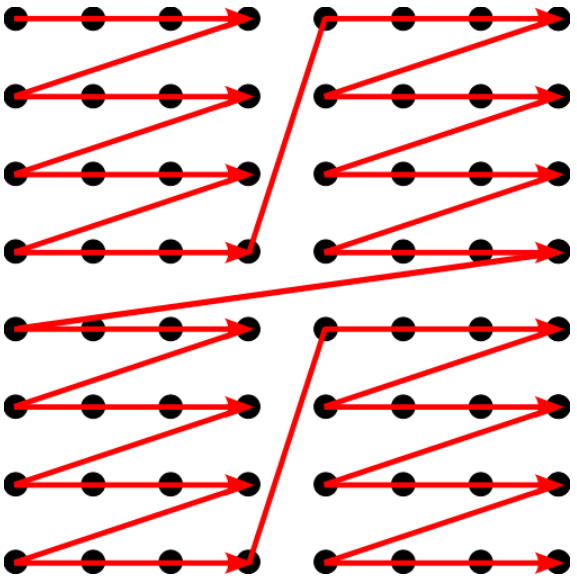
- Cache-aware mapping to 1D array



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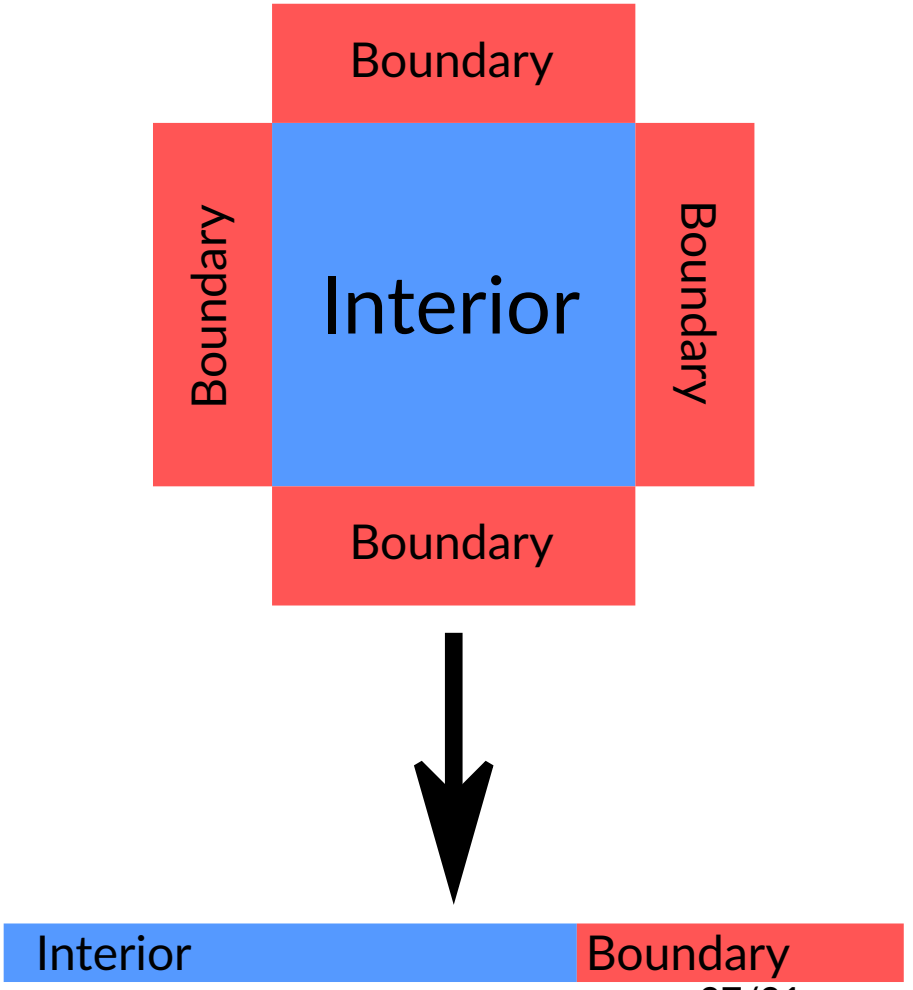
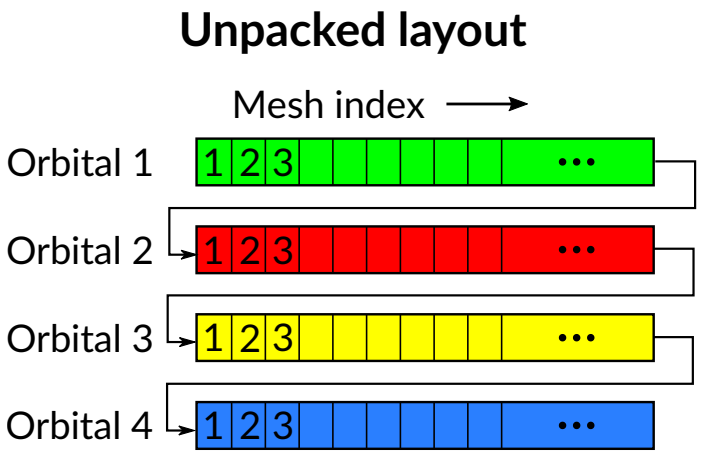
Data layout

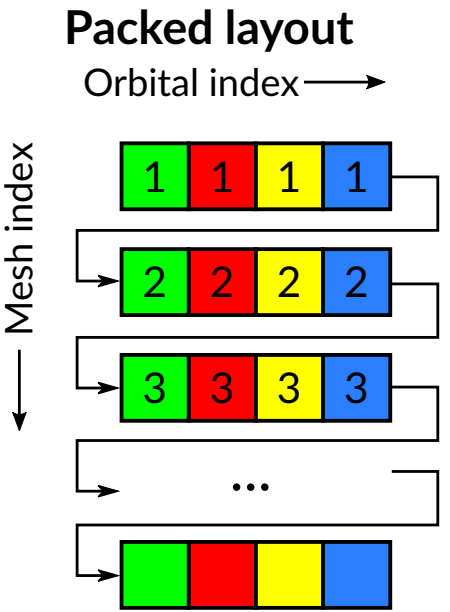
- Real-space grid for FD
- Complicated shape possible, e.g. molecules
- Cache-aware mapping to 1D array
- 1D data layout: 2 blocks
  - Interior points
  - Boundary/ghost points



Data layout II: batches

- Aggregate several orbitals into one batch
- Operations done over batches
- 2 layouts:
  - Unpacked
  - Packed → vectorization, GPUs

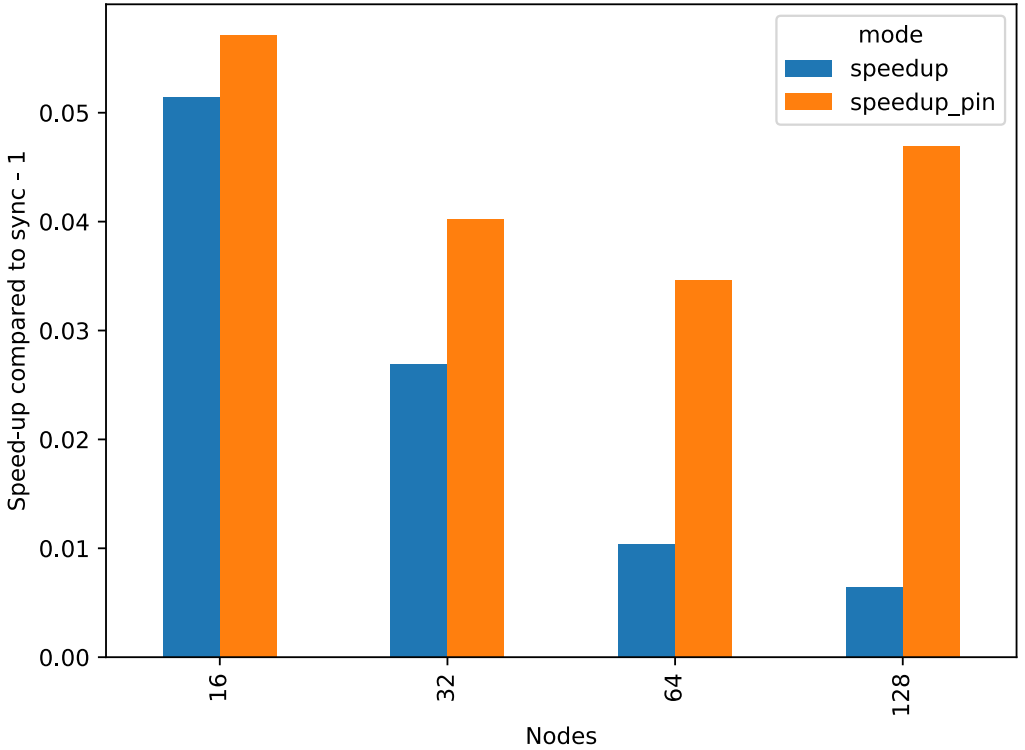




Best combinations [cobra]

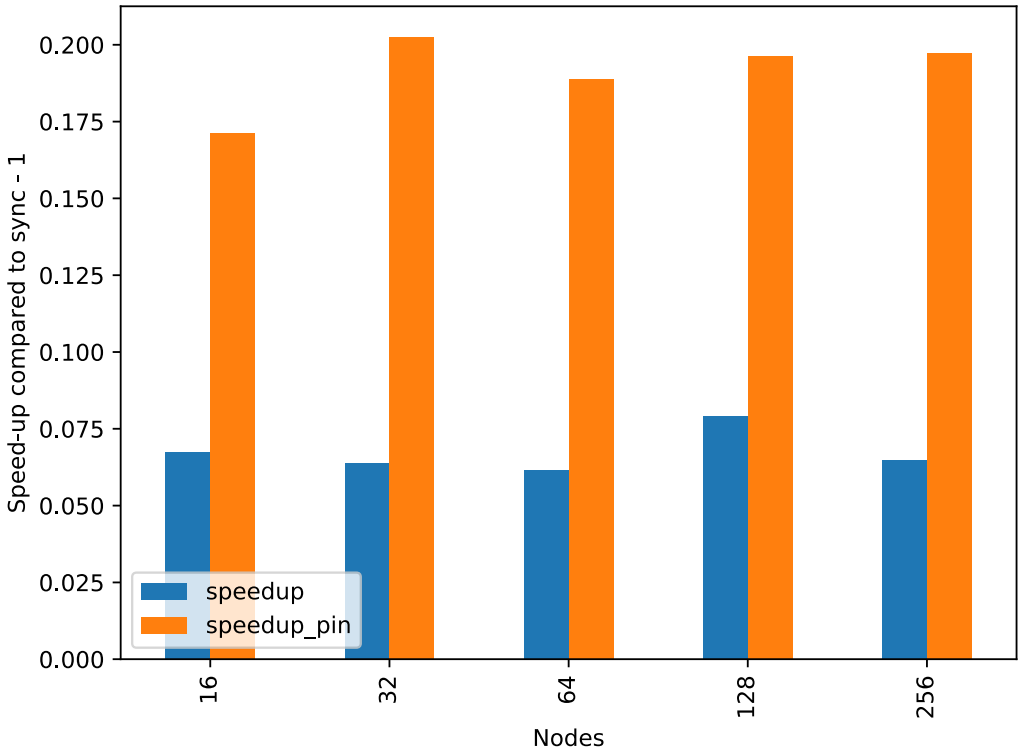
Nodes	sync	async	async_pin
16	8x5	4x10	4x9
32	8x5	4x10	8x4
64	8x5	4x10	8x4
128	8x5	4x10	8x4

Speed-up: zoom in [cobra]



With pinning: speed-up of about 1.03x – 1.06x

Speed-up: zoom in [raven]



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