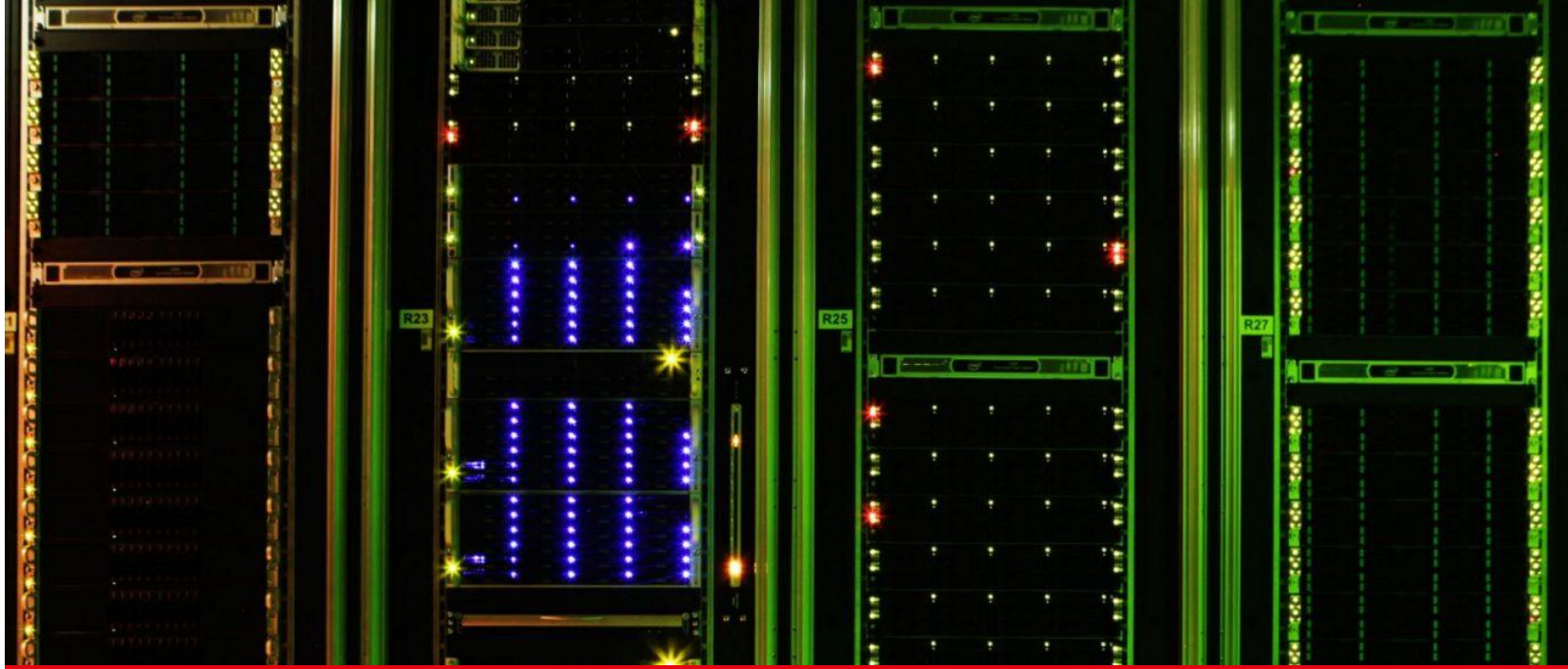
EPFL

EUROfusion



Parallel I/O in GENE-X Using ADIOS

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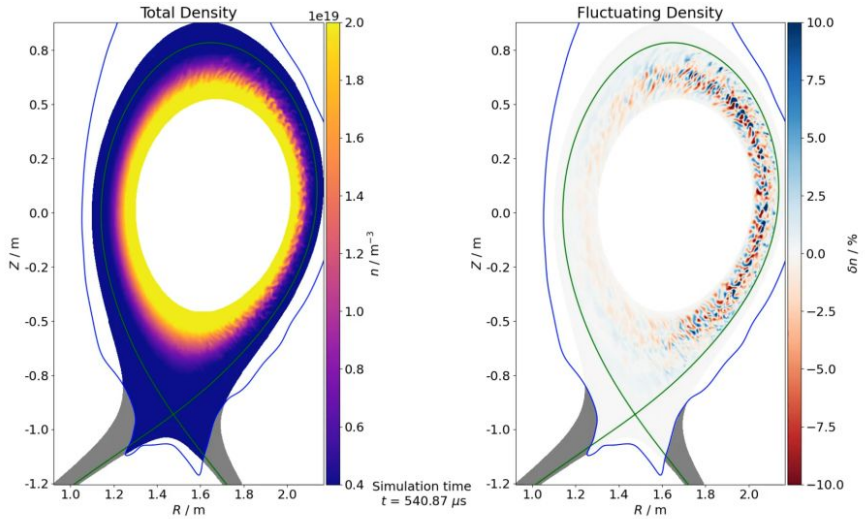
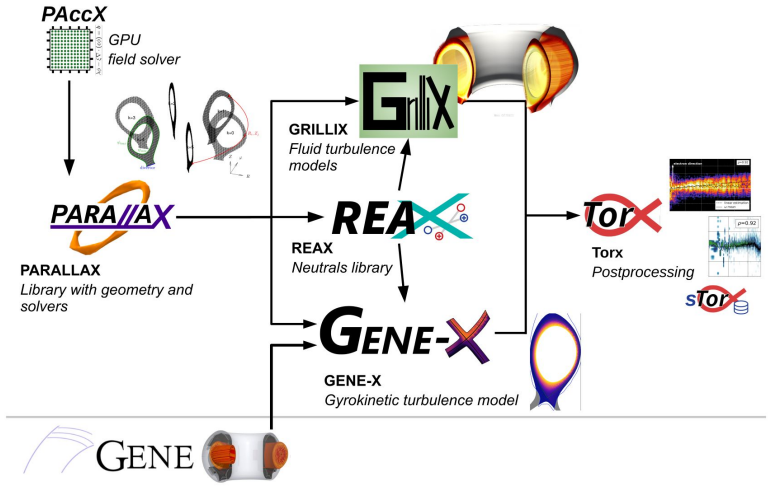
GENE-X Overview

GENE-X simulates turbulence in fusion devices

- Gyrokinetic + Electromagnetic equation, Eulerian grid, full-f, collisional
- Fortran 2008. MPI + OMP parallelization:
  - Strong scaling with 93% efficiency up to 512 nodes (~20K cores), good weak scaling

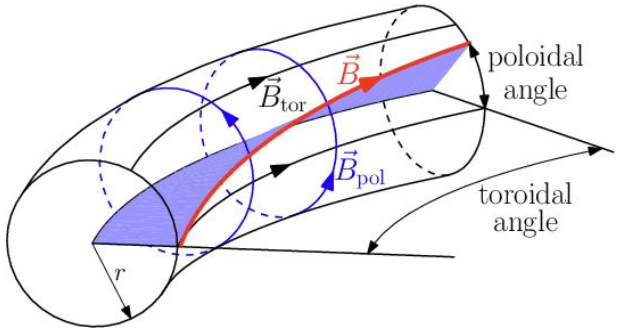


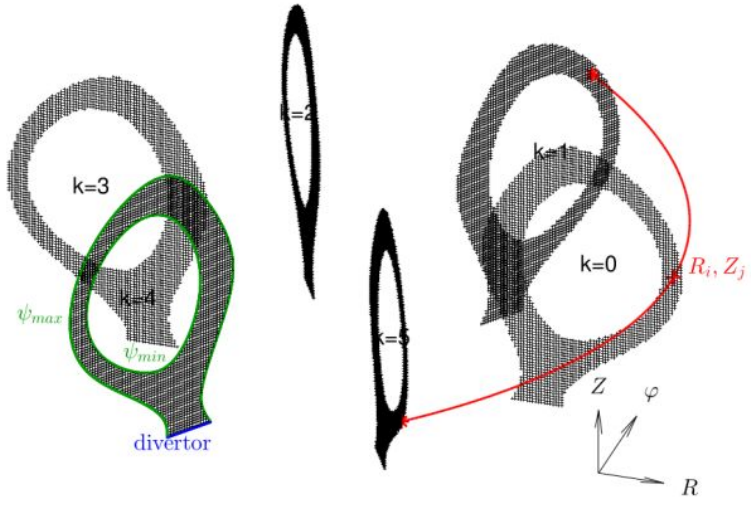


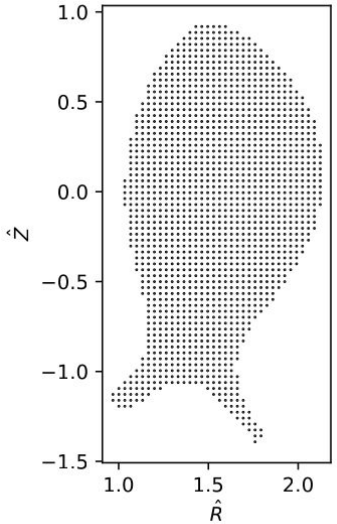
Source: P. Ulbl et al. (2024) “Towards first-principles simulations of the L- to H-mode transition with the global gyrokinetic turbulence code GENE-X”, TSVV4/1 Workshop 2024.

MPI Domain Decomposition

- Time evolution of a 5D distribution f, dims (RZ, phi, vpar, mu, alpha)
- Domain: tensor product of regular grids in all dims
- Spatial mesh: unstructured cartesian mesh for each phi (toroidal angle)
- MPI decomposition in phi, vpar, mu, alpha. OpenMP in RZ, no MPI.
- Typical sizes: (RZ: 1e5-1e7, phi: 32, vpar: 10-100, mu: 10-100, alpha: 2)







Source: P. Ulbl et al. (2024) “Towards first-principles simulations of the L- to H-mode transition with the global gyrokinetic turbulence code GENE-X”, TSVV4/1 Workshop 2024.

Current File I/O

- Spatial mesh
  - All phi planes created/read on all MPI procs
  - Writes only by MPI master to mesh.nc
- 5D state
  - Each MPI proc holds its own chunk of the state vector
  - Each MPI proc i writes its own chunk at time j to part_j/checkpoint_i.nc
- es_pot/A_par (RZ, phi)
  - Reduction to root on all phi sub-communicators. Write by MPI master
- 0/2D moments of 5D state
  - 0D (6 X alpha): collected across one species sub-communicator
  - 2D (RZ, phi, 8, alpha): collected across one phi-species sub-communicator
  - Reduction to MPI master on one sub-communicator and write

Limitations of Current I/O

- Spatial mesh
  - Not all meshes required on all procs
  - Assigned mesh chunks can be generated/read in parallel on each MPI proc
- 5D state
  - Writing generates many directories and files.
  - Restarting the simulation requires the same MPI configuration used during write.
- es_pot/A_par
  - MPI reduction not necessary, parallel I/O can be used on one sub-communicator
- 0/2D moments of 5D state
  - MPI reduction is not necessary, parallel I/O can be used

Previous attempts with parallel netCDF failed due to unknown runtime error

To get around the current limitations, we implement parallel I/O with ADIOS library

ADIOS

Adaptable Input/Output System from Exascale Computing Project (DoE, U.S.)

- Parallel file I/O for distributed arrays of arbitrary dimensions
  - Binary packed format (BP4, BP5)
  - HDF5 support
- Fortran/C/C++ bindings
- “BeginStep/EndStep” abstraction for time series data
- “Deferred Put/Get” abstraction: lazy evaluation to minimize low level ops
- Backends:
  - File: POSIX I/O, stdio, fstream
  - Network: MPI, RDMA

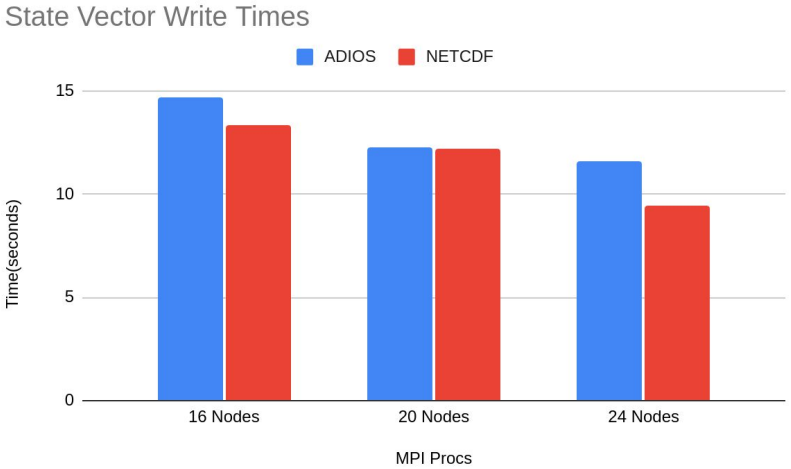
I/O Implementation With ADIOS

5D State Checkpoint

- Data+ghosts stored in contiguous 5D arrays local to each MPI process
- ADIOS write implementation:
  - Determine global/local sizes and offsets based on MPI config
  - Pack data into a continuous buffer for writing
  - Write a new output file or append a new step to an existing file, no parts directories
- ADIOS read implementation:
  - Determine global/local sizes and offsets based on MPI config
  - Read the latest data step into a continuous buffer and unpack the data
- Saved checkpoint is MPI config agnostic - read with different MPI config possible
- Possibility to play with numAggregators, numFiles at runtime
  - Default values: numAggregators = MPI nodes, numFiles = numAggregators

Read/Write 5D State: netCDF vs ADIOS

- Test on EPFL Jed, infiniband partition. Read and writes on /scratch
- (RZ, phi, vp, mu, spec) = (270K, 36, 80, 20, 2). 3 MPI configs
  - 16 Nodes: (1, 4, 1, 2, 2)
  - 20 Nodes: (1, 2, 5, 1, 2)
  - 24 Nodes: (1, 3, 2, 2, 2)
- Mean values over all nodes, for 20 runs

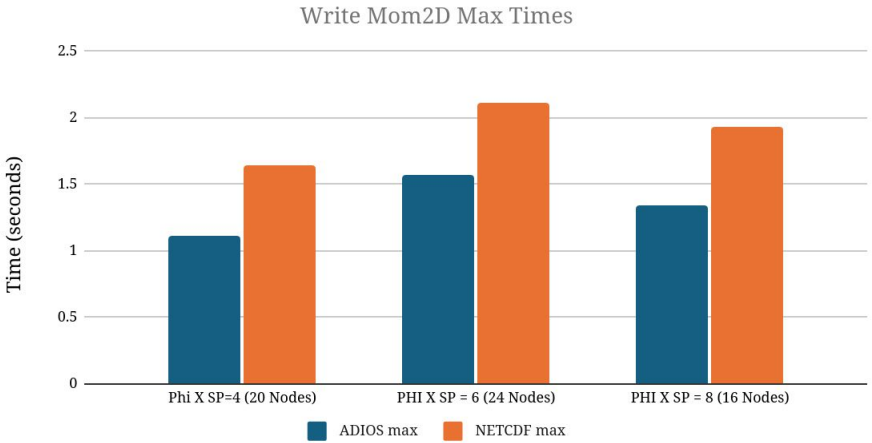


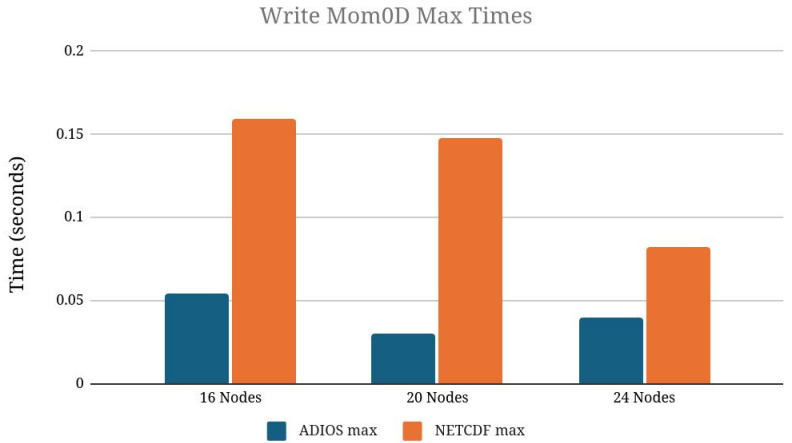
0D and 2D Moments

- Parallel write for moments using ADIOS, no reduction step:
  - Mom 0D: (6 X alpha), write using one species sub-communicator containing master
  - Mom 2D: (RZ, phi, 8, alpha), write using one phi-species sub-communicator
- No read implementation in netCDF or ADIOS

Write 0D/2D Moments: netCDF vs ADIOS

- Test on EPFL Jed, infiniband partition. Writes on /scratch
- Test params: (RZ, phi, vp, mu, spec) = (270K, 36, 80, 20, 2). 3 MPI configs
  - 16 Nodes: (1, 4, 1, 2, 2)
  - 20 Nodes: (1, 2, 5, 1, 2)
  - 24 Nodes: (1, 3, 2, 2, 2)
- Mean values over all nodes, for 20 runs
- Max times over all nodes as not all nodes participate in the exchange



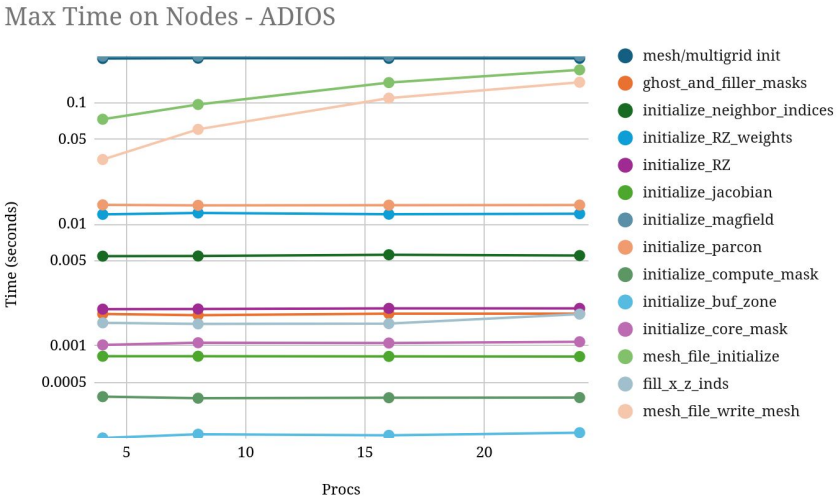


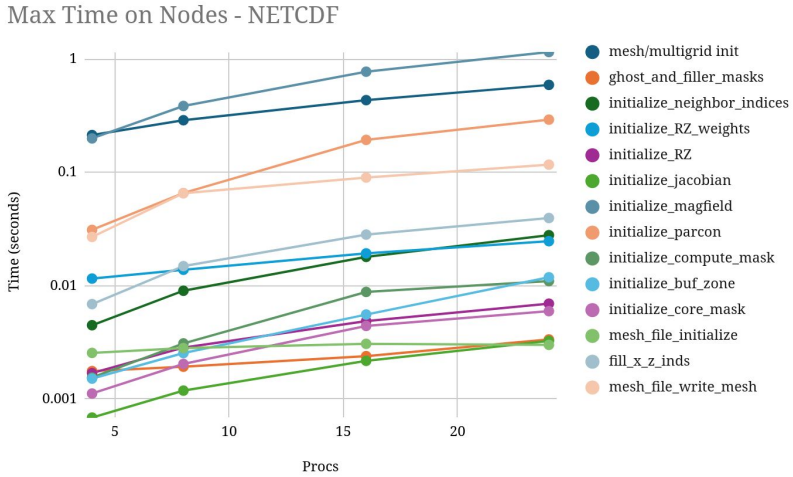
Mesh (Work in Progress)

- Current implementation:
  - Mesh built for all phi on all procs using PARALLAX (builds multigrids)
  - Only MPI master writes the mesh, multigrid info
- ADIOS based implementation:
  - Creating meshes for local phi doesn’t work, mesh data up to phi +2,-2 accessed.
  - Creating meshes for local + ghost phi range on each process.
  - Writing mesh only for local phi range (excluding ghosts) from a process.
  - (RZ, phi) shaped arrays written neatly by ADIOS, e.g. R/Z buffer, magnetic field
- Next steps: writing unstructured, hierarchical data related to multigrid

Mesh Init Time: ADIOS vs netCDF

- Tests conducted on Jed cluster, infiniband partition.
- (RZ, phi, vp, mu, spec) = (**270K**, **X**, 40, 16, 2). MPI config: (1, **X**, 1, 1, 1)
- **X**: 4, 8, 16, 24, 32
- ADIOS: average time across all (phi) nodes, 50 runs
- NETCDF: average time on master, 50 runs





Mesh Write: netCDF vs ADIOS

- Tests conducted on Jed cluster, standard partition. Write to /home
- (RZ, phi, vp, mu, spec) = (**270K**, **X**, 40, 16, 2). MPI config: (1, **X**, 1, 1, 1)
- **X**: 4, 8, 16, 24, 32
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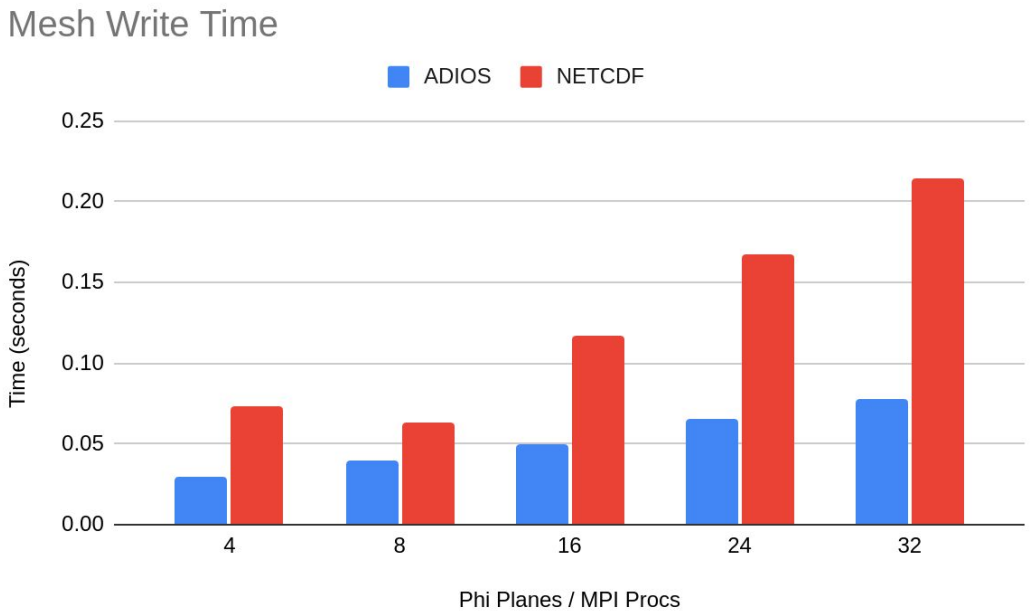

Summary

- Implemented ADIOS based I/O for spatial mesh, 5D state, 0/2D moments
- Speedup in mesh generation, mesh writing
- Slight slowdown in 5D checkpoint writing but speed up in reading
- Speedup in writing 0/2D moments
- Possible to restart simulation with a different MPI configuration
- Next steps: implementing mesh read, multigrid I/O, es_pot/A_par write

Thank you!

Mesh Init Time: ADIOS Speedup vs netCDF

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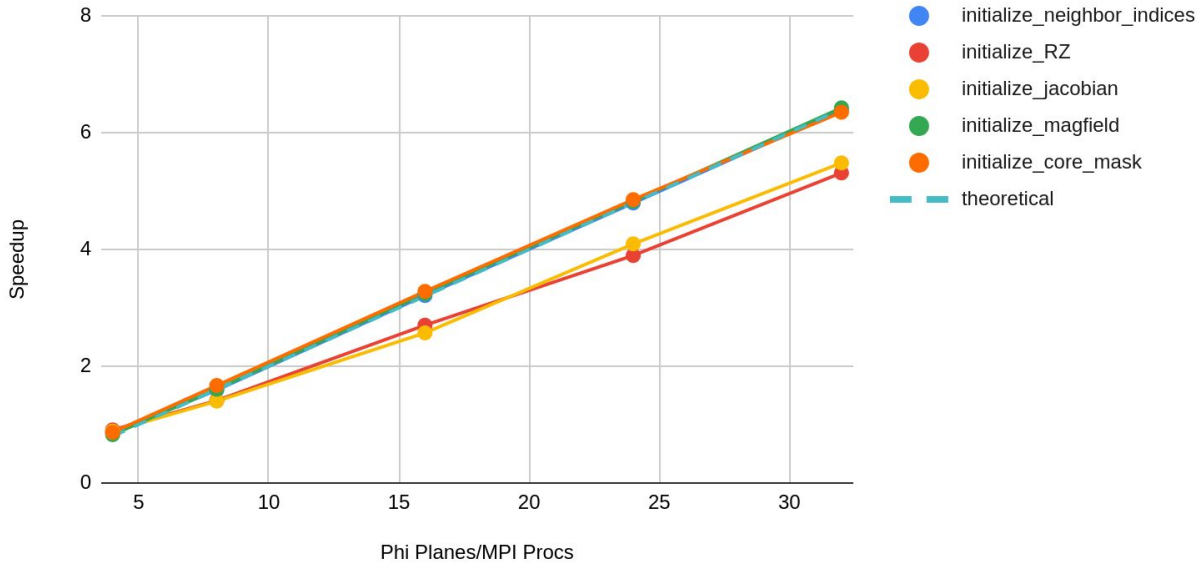

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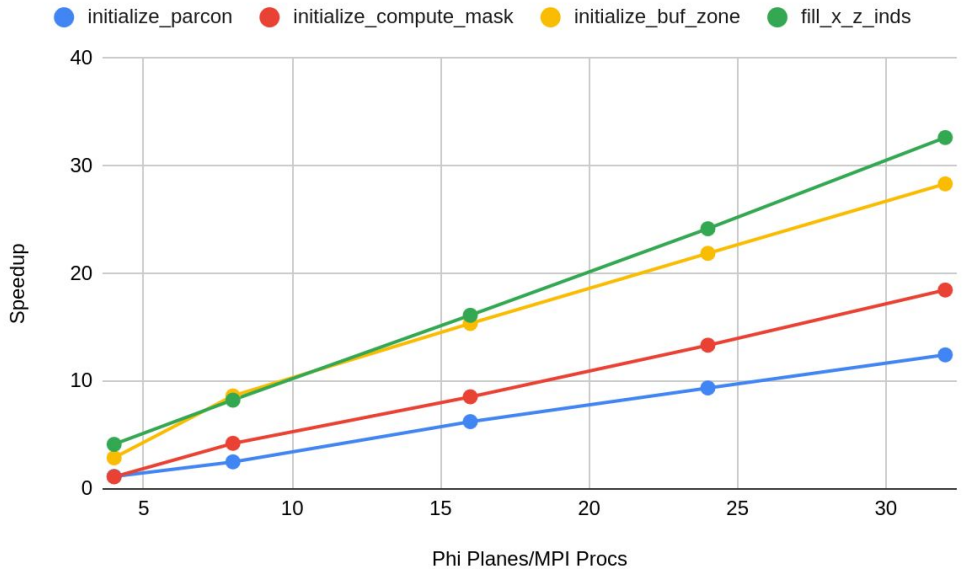

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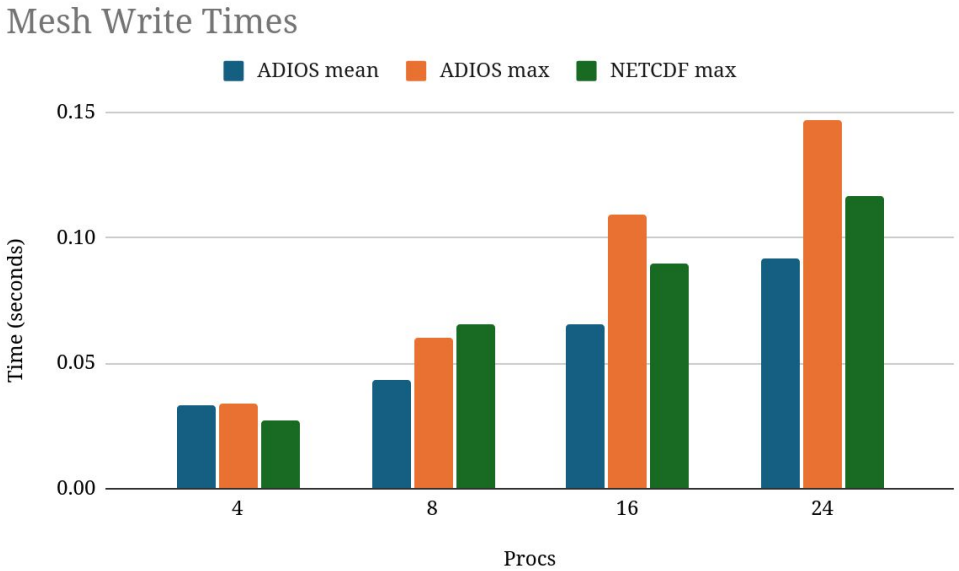

Mesh Init Time: ADIOS vs netCDF

adios					
	4	8	16	24	32
init_first_part	0.854958572	0.85705134	0.8563431516	0.8509147401	0.8497804452
initialize_RZ_domain	0.0000158475	0.00000885787	0.0000088520425	0.000008648669167	0.00000864859125
ghost_and_filler_masks	0.001920958	0.001863052923	0.001882407162	0.001828187382	0.00185232923
initialize_neighbor_indices	0.019397679	0.01817873297	0.01784290545	0.01788911952	0.01790065111
initialize_RZ_weights	0.06060214	0.06036289596	0.0602911834	0.06035665752	0.06016798763
initialize_RZ	0.002864023	0.0027012437	0.002593224014	0.002609399882	0.002582642998
initialize_vp_bsg	0.00316822225	0.00319293121	0.003201397196	0.00322651878	0.003221028761
initialize_jacobian	0.00095901075	0.000996864455	0.001038795685	0.0009725199533	0.0009614840256
initialize_magfield	0.4599644618	0.4595015625	0.4623392187	0.4646287057	0.4651894842
initialize_parcon	0.05584953	0.05184922977	0.05154521931	0.05168482959	0.05172708945
initialize_compute_mask	0.00206808825	0.0009552213425	0.0009796418087	0.0009841211433	0.0009773515287
initialize_buf_zone	0.00087600475	0.00046512104	0.000473519455	0.0004710492208	0.0004756471263
initialize_core_mask	0.00380840575	0.00354589999	0.003560439711	0.003569056783	0.003576467656
set_bsg_flags	0.000000636	0.0000006328125	0.0000006045975	0.0000006069841667	0.0000006567675
mesh_file_initialize	0.1151438505	0.1110297351	0.1477438678	0.1920398449	0.2559843296
fill_x_z_inds	0.0059884025	0.005810388898	0.005826820852	0.005849304162	0.005877692043
write_parallax	0.1612477895	0.1995761752	0.3329392955	0.4209620545	0.5678550485
mesh_file_write_mesh	0.0299476095	0.03957648549	0.04971448752	0.06587861621	0.07772146888

Mesh Init Time: ADIOS vs netCDF

netcdf					
	4	8	16	24	32
init_first_part	0.8322822097	0.9122345613	1.055840945	1.195848919	1.336582226
initialize_RZ_domain	0.00001540015	0.00000907994	0.00000931147375	0.000009376845833	0.00000931687375
ghost_and_filler_masks	0.002110708945	0.0021019893	0.002553898026	0.003006189112	0.003520346348
initialize_neighbor_indices	0.01674484507	0.02892006132	0.05731287841	0.08577917885	0.1143764987
initialize_RZ_weights	0.06017954972	0.06270466019	0.06914717026	0.07638419853	0.08806714
initialize_RZ	0.002604098615	0.00381579288	0.007007808245	0.01017058755	0.01371829844
initialize_vp_bsg	0.00322387016	0.003159375345	0.003211614508	0.00321811802	0.003207477323
initialize_jacobian	0.000852546775	0.001396652035	0.002670922839	0.003982811676	0.005272102918
initialize_magfield	0.3803545202	0.7387782497	1.499956439	2.241742322	2.989207912
initialize_parcon	0.06474757303	0.1301970669	0.3222760405	0.4847445977	0.6447891202
initialize_compute_mask	0.002330084765	0.004043642805	0.008381771997	0.01314121542	0.01807350873
initialize_buf_zone	0.00253728759	0.004020999653	0.007279010421	0.01030884915	0.0134821693
initialize_core_mask	0.003305013865	0.005925970655	0.01168614078	0.01732904997	0.02271425116
set_bsg_flags	0.000000683905	0.000000768595	0.00000072729125	0.0000007276341667	0.00000080250625
mesh_file_initialize	0.001217482015	0.000328629465	0.00023541758	0.0001231867367	0.0001159309106
fill_x_z_inds	0.02480439837	0.04797807351	0.0940138437	0.1414209391	0.191869545
write_parallax	0.02277475939	0.01223597045	0.00602845312	0.004210326838	0.003095064771
mesh_file_write_mesh	0.01835569328	0.007844673083	0.007353392543	0.006972715696	0.006729743577