Modernizing Legacy Codes for Next-Generation Storage Infrastructures

A Case Study of PALM on Intel DAOS

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Motivation: DAOS Software Stack

- approach: applications don't use DAOS API directly → **high level libraries**
- candidates for HPC: netCDF, HDF5, MPI, POSIX (!?)

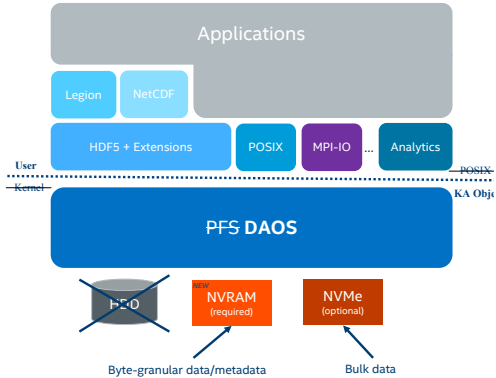

Figure: DAOS Software Stack

Source: A. Dilger DAOS: Scale-out Object Storage for NVRAM, Dagstuhl Workshop, May 2017

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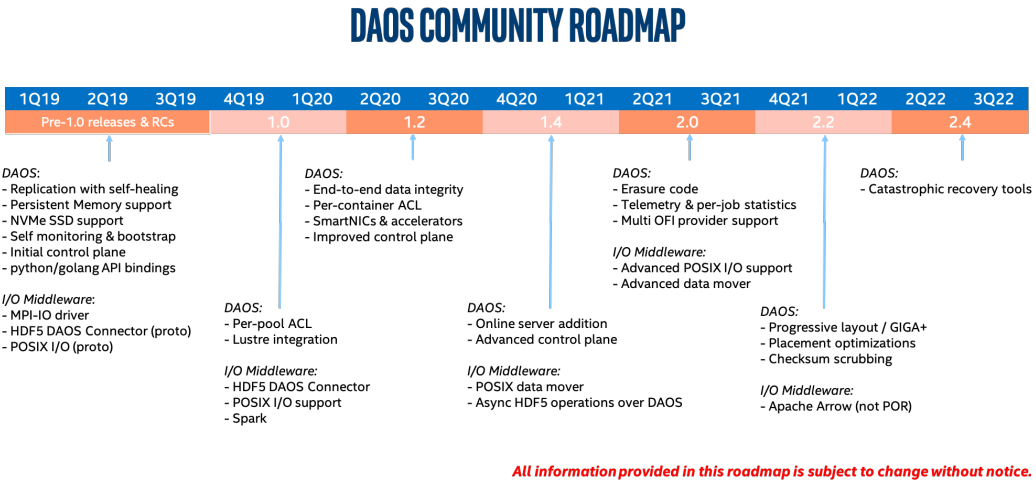

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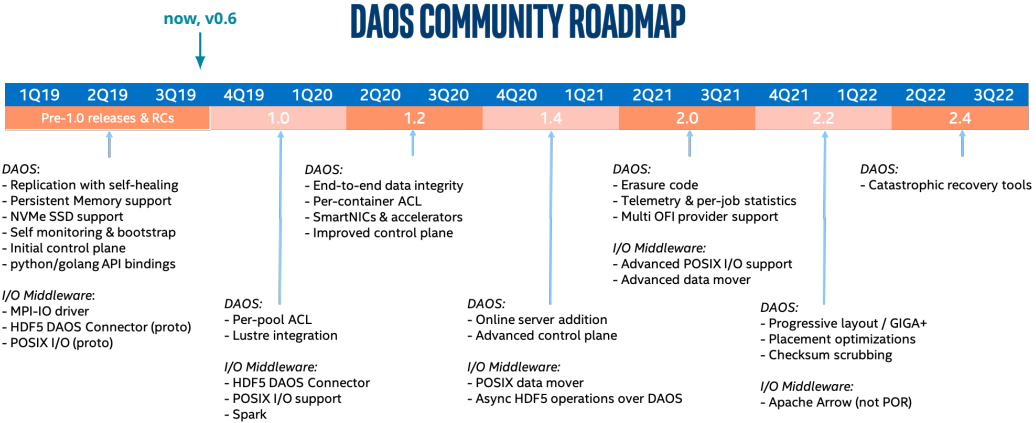

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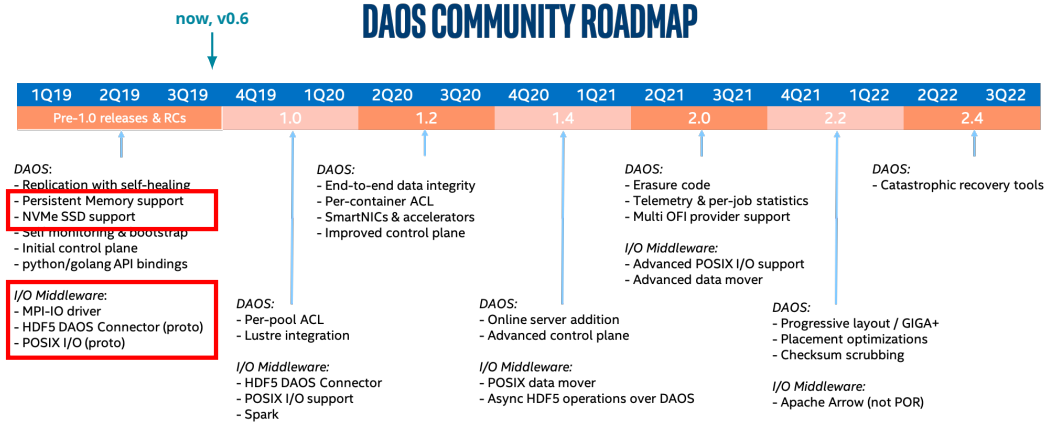

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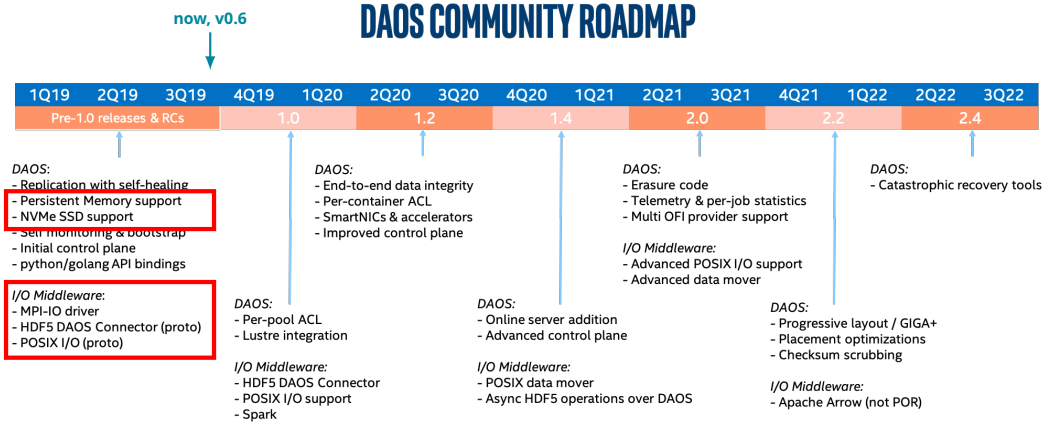

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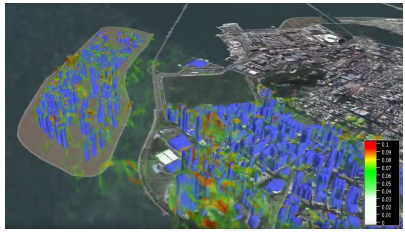
Outline

PALM Overview

- **Pa**rallelized **L**arge-Eddy Simulation **M**odel by IMUK @ Univ. Hannover
  - computes turbulent air flows, solves imcompressible Navier-Stokes equations
  - 3D compute domain, typical dimensions O(1k) x O(1k) x O(100)
  - since 1997, 200k+ lines of code, lots of modules



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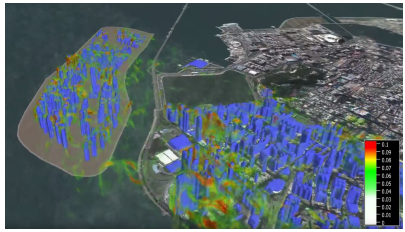
  - since 1997, 200k+ lines of code, lots of modules
  - Fortran 2003 (95) code base, GNU licenced
  - **MPI**/OpenMP parallelization, quite memory hungry
  - **netCDF** for data output



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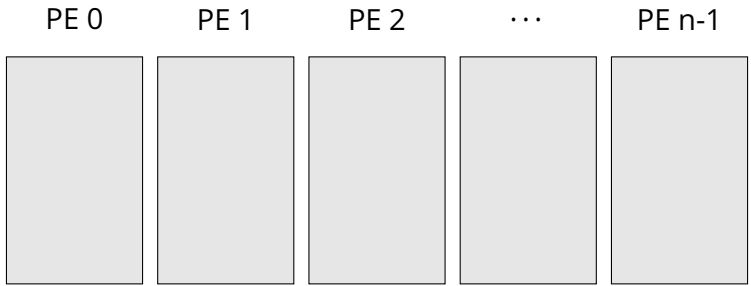

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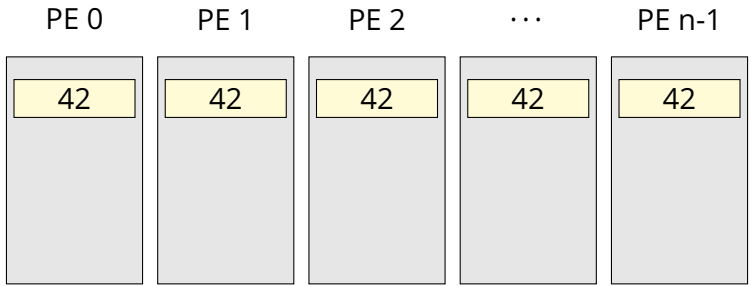

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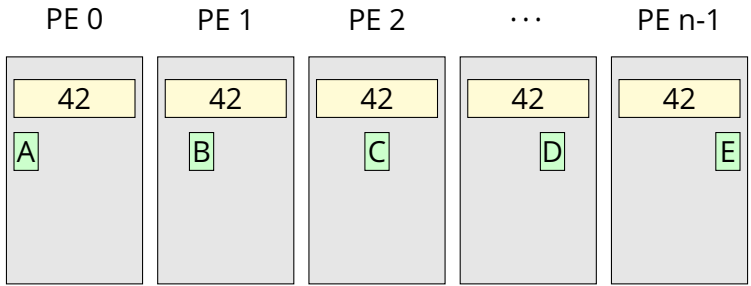

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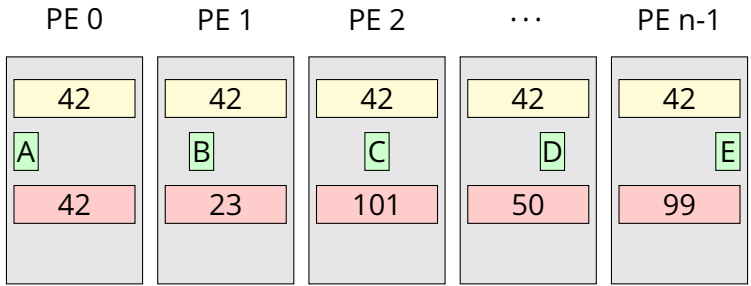

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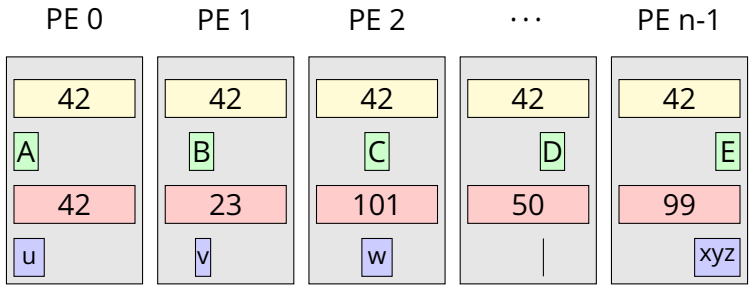
- **sgv** scatter/gatherv, like distributed but different shapes, globally indexed



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```
CALL wrd_write_string( 'topography' )
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```

- restore: read name from other hard-coded unit + large select statement

```
SELECT CASE ( restart_string(1:length) )
  ...
  CASE ( 'topography' )
    READ ( 13 )  topography
```

Checkpointing: Challenges

- raw binary data: hard to postprocess (useful for debugging)
- unformatted Fortran IO: "hidden" additional small writes
- one file per process
- PE-independent $\rightarrow$ complicated restore code
- interface to DAOS? Via POSIX!?
- **no abstraction**
- **no expressed parallelism**

Rewrite of PALM's Checkpointing

- new checkpointing abstraction layer

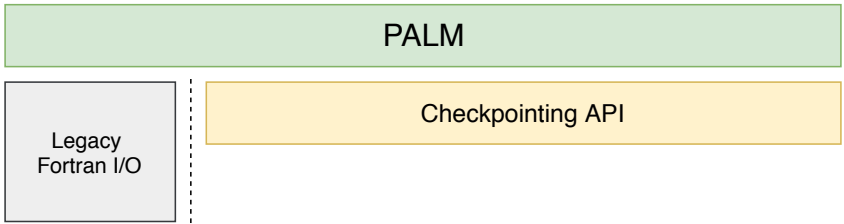
```
!-- optional call to define variable
CALL checkpoint_define('topography', topography, dt_replicated)

CALL checkpoint_write('topography', topography, dt_replicated)
CALL checkpoint_read('topography', topography, dt_replicated)
```

- enables to abstract from actual storage API
  - remove Fortran unformatted IO
  - use of *generic* functions
  - replace storage backend with modern technologies without application changes

Checkpointing Abstraction Layer

- new abstraction layer for PALM



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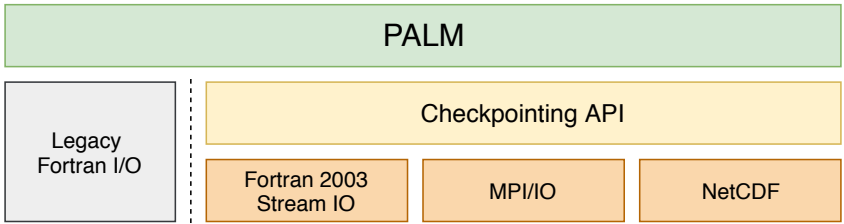
  - **ROMIO**: implementation of MPI's IO chapter
  - **netCDF**: IO for named and typed arrays; self-describing files; existing ecosystem



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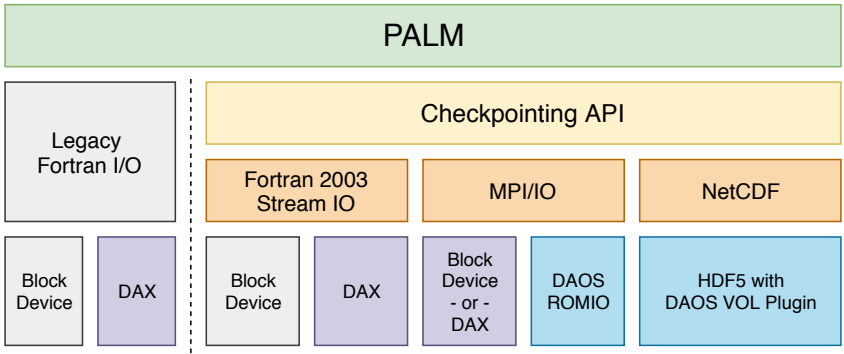

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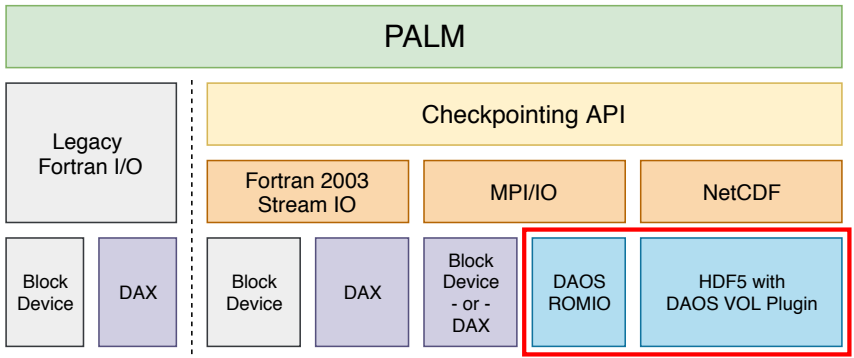

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- easy definition + data access
- **Danger**: performance pitfall

```
CALL NF90_REDEF( ncid )
CALL NF90_DEFVAR( ncid, label, datatype, id )
CALL NF90_ENDDEF( ncid )
```

Avoid transitions between definition and data mode!
Build batches of variable definitions, write in batch afterwards

Checkpoint Composition

- not all application data written to checkpoint
- typical composition (simplified) for $4096 \times 4096 \times 256$ compute domain

type	count	data (approx)
scalars	192	907 B
1D arrays	57	1.00 GB
2D arrays	21	1.25 GB
3D arrays	9	258.00 GB
4D arrays	1	806.25 KB
total	280	261 GB

Figure: share of checkpoint size per variable type

Experimental Results: HLRN IV

- evaluate new checkpointing framework on production system
- HLRN IV computer system, Göttingen
- **no DAOS** installation, but **Lustre** file system (4 MDT, 10 OSS, 100 OST)
- used 8 nodes: 2x Xeon Gold SKL 6148, 192 GB RAM, OmniPath, Intel MPI 19u4
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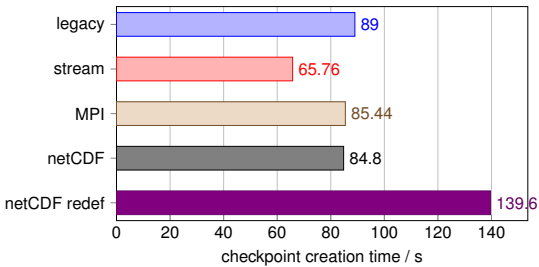

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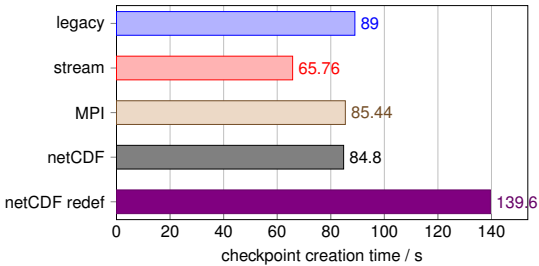

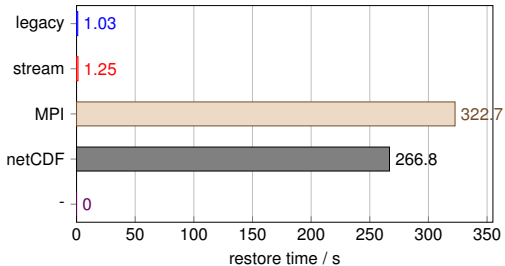

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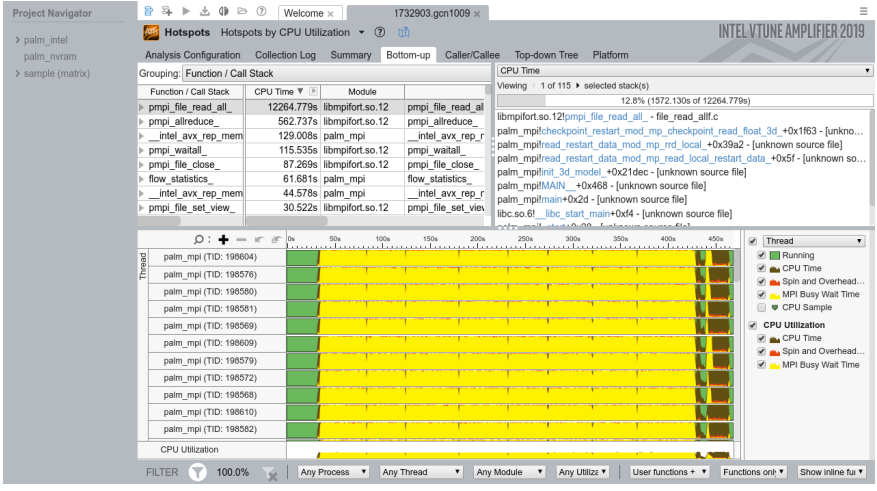

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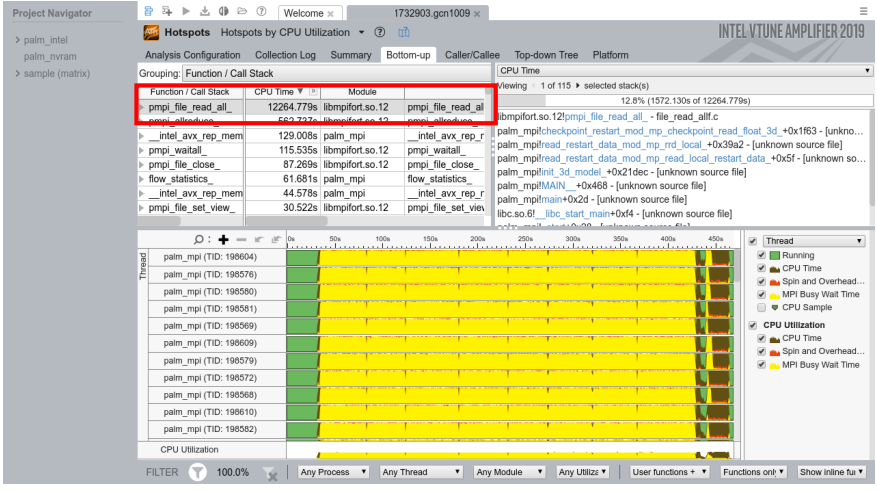

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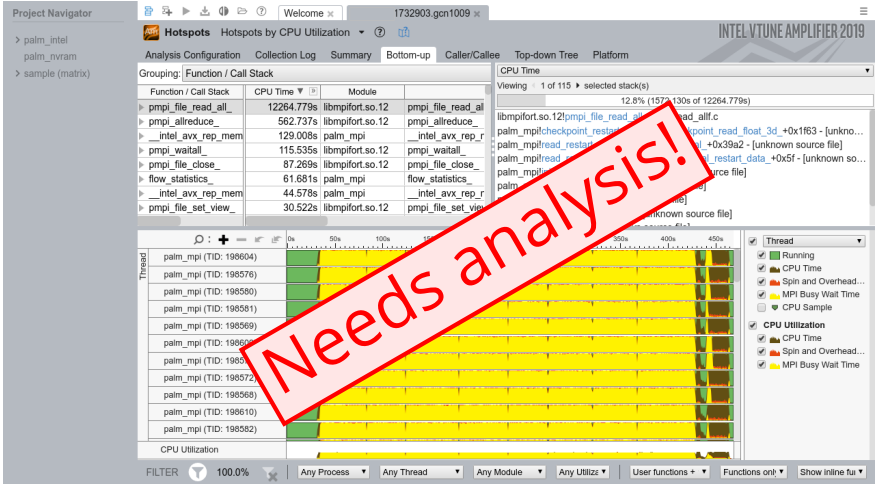

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netCDF

- our assumption: just built netCDF on top of DAOS-aware HDF5
- HDF5 VOL plugin for DAOS is work in progress, said to become stable this year, netCDF likely to need adjustments
- **DAOS currenty not useable via netCDF**

Experimental Results: DAOS Testbed

- single node:
  - dual Xeon Platinum 8260L (CL-SP, 24C/48T)
  - 6 TB Apache Pass (2 $\times$ 6 DCPMM), 768 GB DRAM
  - CentOS 7, gcc/gfortran 9.1
  - 32 MPI procs, domain size = 4096 $\times$ 4096 $\times$ 256
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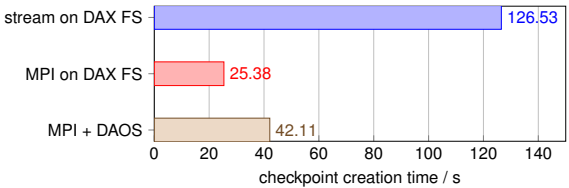

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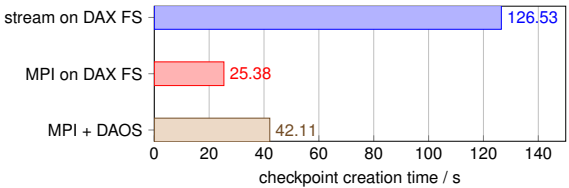

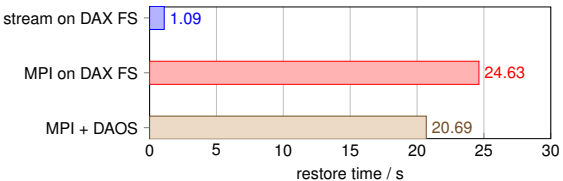

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- Usage:
  - permissions: required to use DAOS account to get access to pool
  - unmature tools: documented commands return *not implemented*
  - (1+x) threads per target, i.e. DCPMM, hog CPU cores $\rightarrow$ energy consumption!?
  - `first_core` option helpful

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CALL NF90_CLOSE(presentation)
```

Questions!?