The ABCs of Open MPI

Decoding the Alphabet Soup of the Modern HPC Ecosystem (Part 1)

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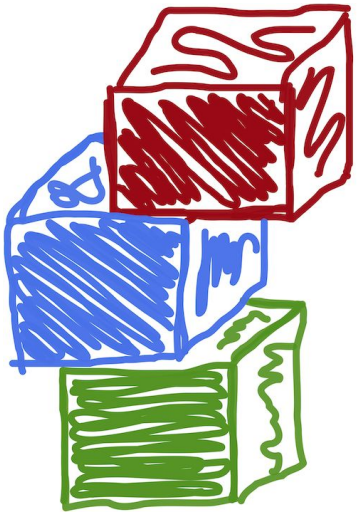


easybuild

Presented in conjunction
with the EasyBuild community

Webex Logistics

- This session is being recorded
- Ask questions in the Q&A panel

Overview

- Background
- PMIx: What is it?
- Building Open MPI
- A breakdown of Open MPI:
  - The run-time stuff
  - The MPI stuff
- Configuration / debugging tips
- The upcoming Open MPI v4.1.x series
- The upcoming Open MPI v5.0.x series

We'll get as far as we get today

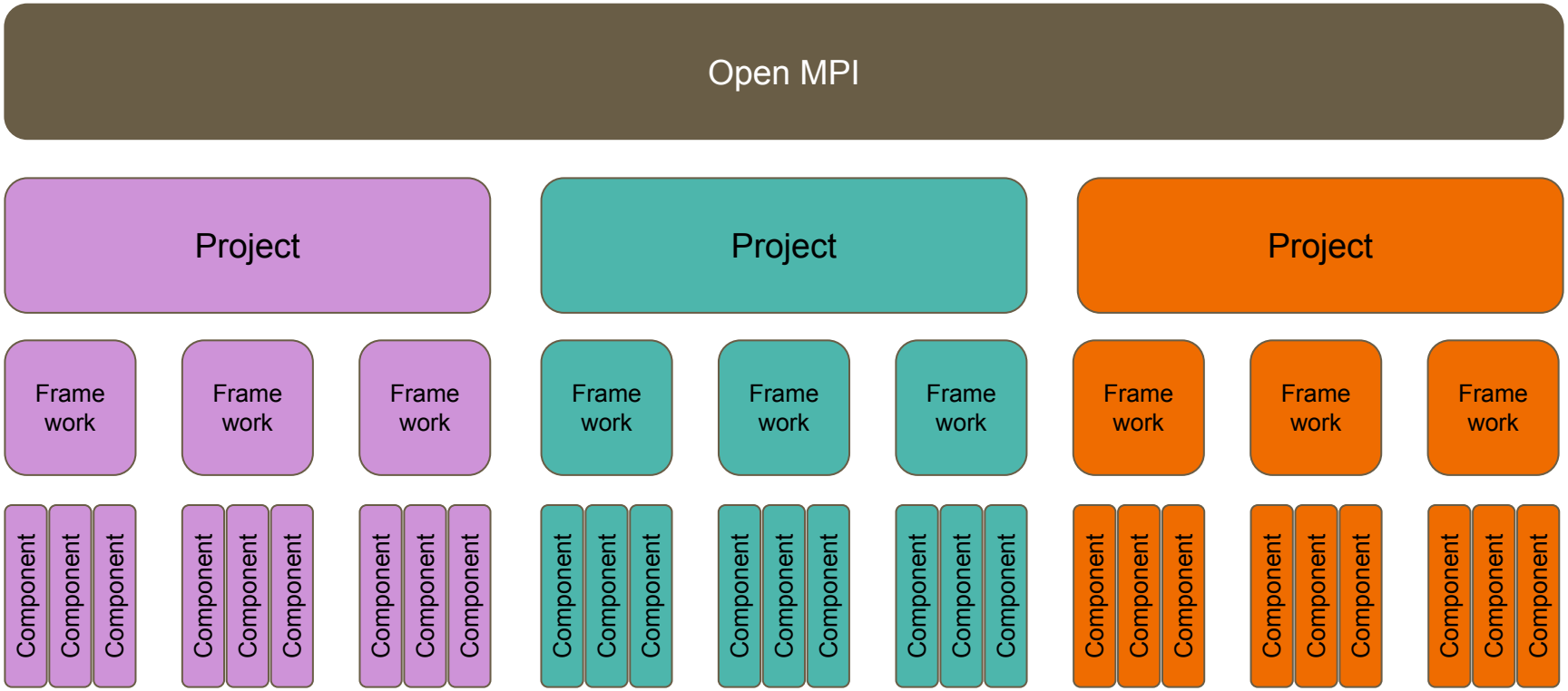
Next session: Wednesday, July 8

Background

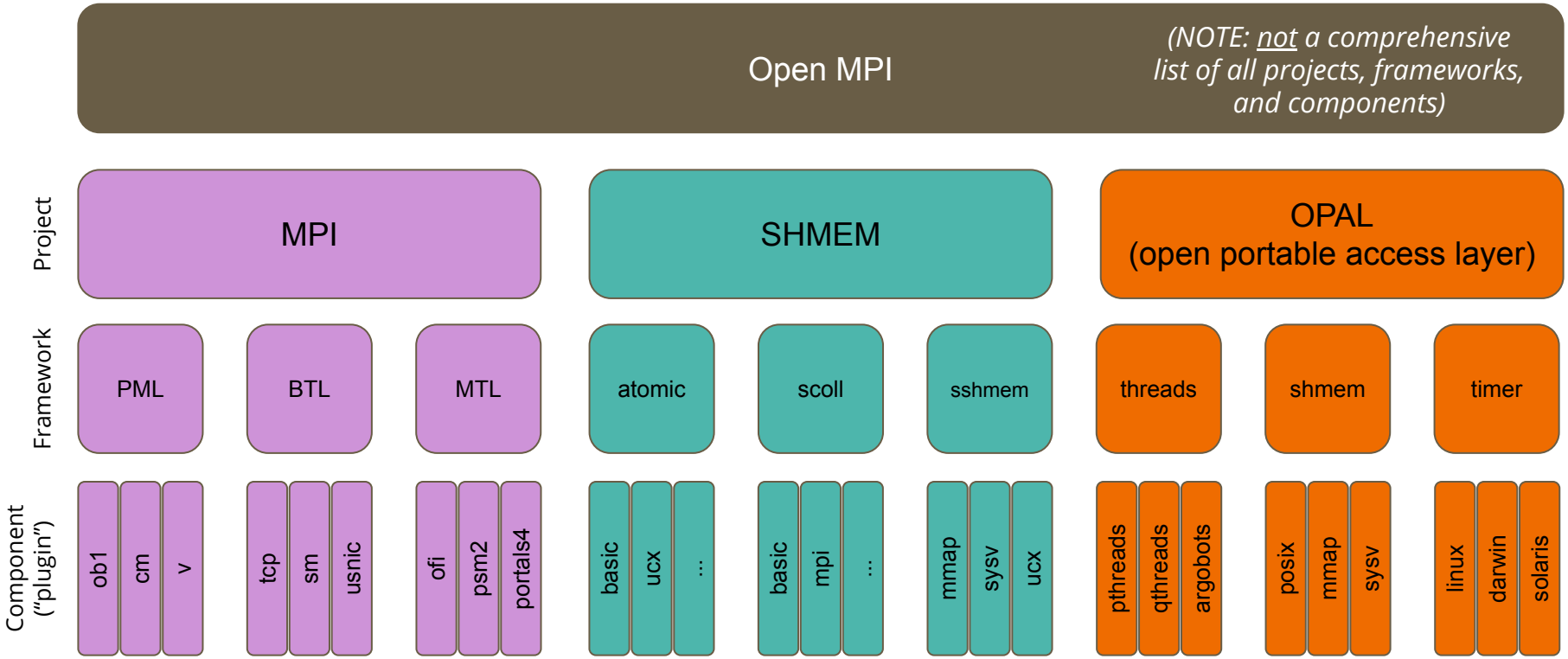
Open MPI Overall Architecture Terminology

- Modular Component Architecture (MCA)
  - Semantic architecture of the Open MPI software package
  - Hierarchy: Project → Framework → Component

Open MPI Overall Architecture Terminology



Open MPI Framework + Component Examples



Names of Frameworks and Components

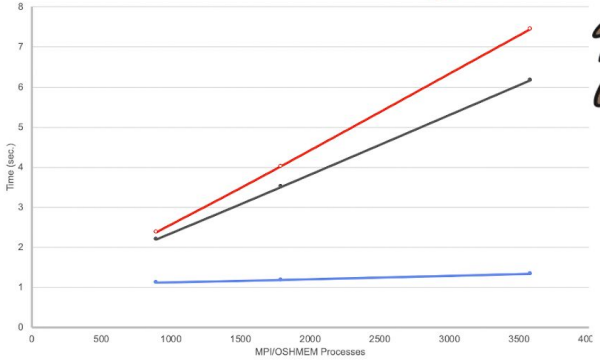
- The Open MPI community has proven to be terrible at naming things

- There are several frameworks and components with Star Wars-inspired names (i.e., that have nothing to do with their functionality)
  - Most famous: “`vader`” = shared memory message transport
  - A few non-Star-Wars science fiction names, too (e.g., Star Trek, Highlander)

PMIx: What Is It?

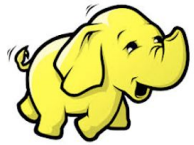
Origin: Changing Landscape

Launch time limiting scale



Programming model & runtime proliferation

Legion



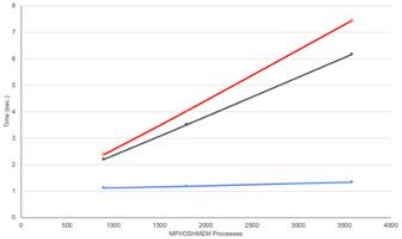
MPI
OpenMP

Hybrid applications

Model-specific tools

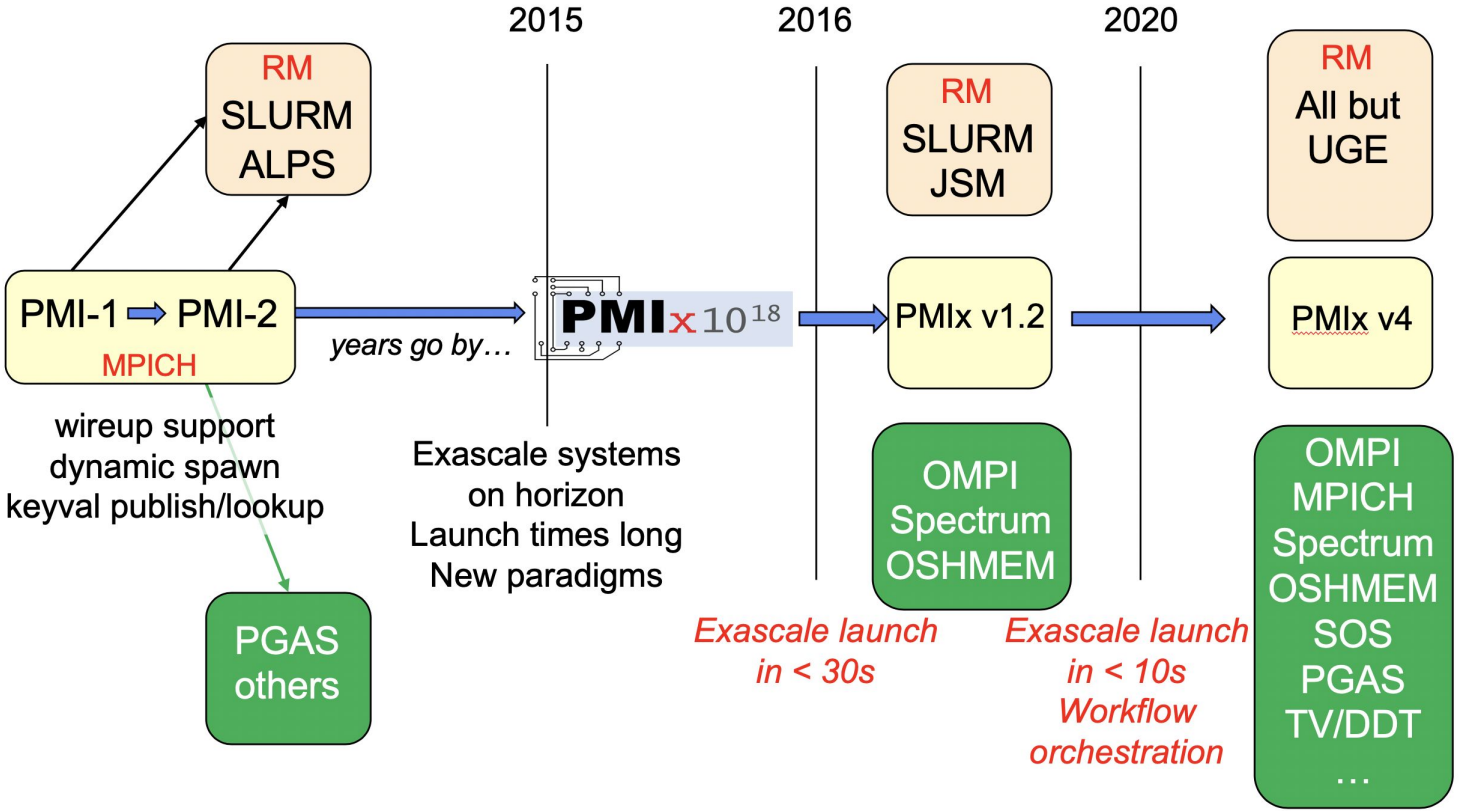
Container technologies

Start Someplace!



- Resolve launch scaling
  - Pre-load information known to RM/scheduler
  - Pre-assign communication endpoints
  - Eliminate data exchange during init
  - Orchestrate launch procedure

What is PMIx?


2015
2016
2020
RM
SLURM
ALPS
PMI-1 ➡ PMI-2
MPICH
wireup support
dynamic spawn
keyval publish/lookup
PGAS
others
years go by…
PMIx 10^18
Exascale systems
on horizon
Launch times long
New paradigms
RM
SLURM
JSM
PMIx v1.2
OMPI
Spectrum
OSHMEM
Exascale launch
in < 30s
RM
All but
UGE
PMIx v4
OMPI
MPICH
Spectrum
OSHMEM
SOS
PGAS
TV/DDT
…
Exascale launch
in < 10s
Workflow
orchestration

Three Distinct Entities

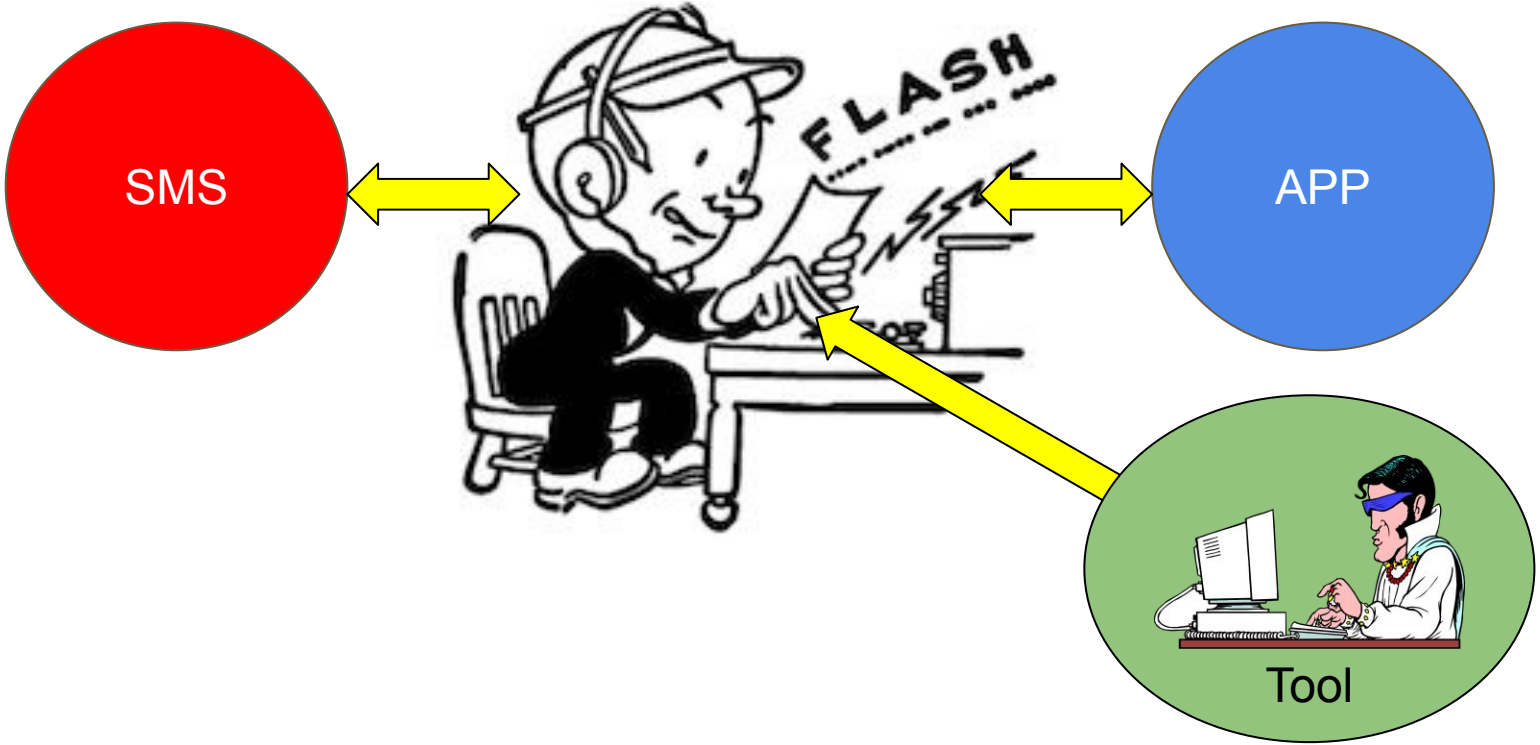
- PMIx Standard
  - Defined set of APIs, attribute strings
  - Nothing about implementation
- OpenPMIx Library
  - Full-featured implementation of the Standard
  - Intended to ease adoption
- PMIx Reference RTE (PRRTE) *v2.0 soon!*
  - Full-featured “shim” to a non-PMIx RM
  - Provides development environment

v4.0 soon!

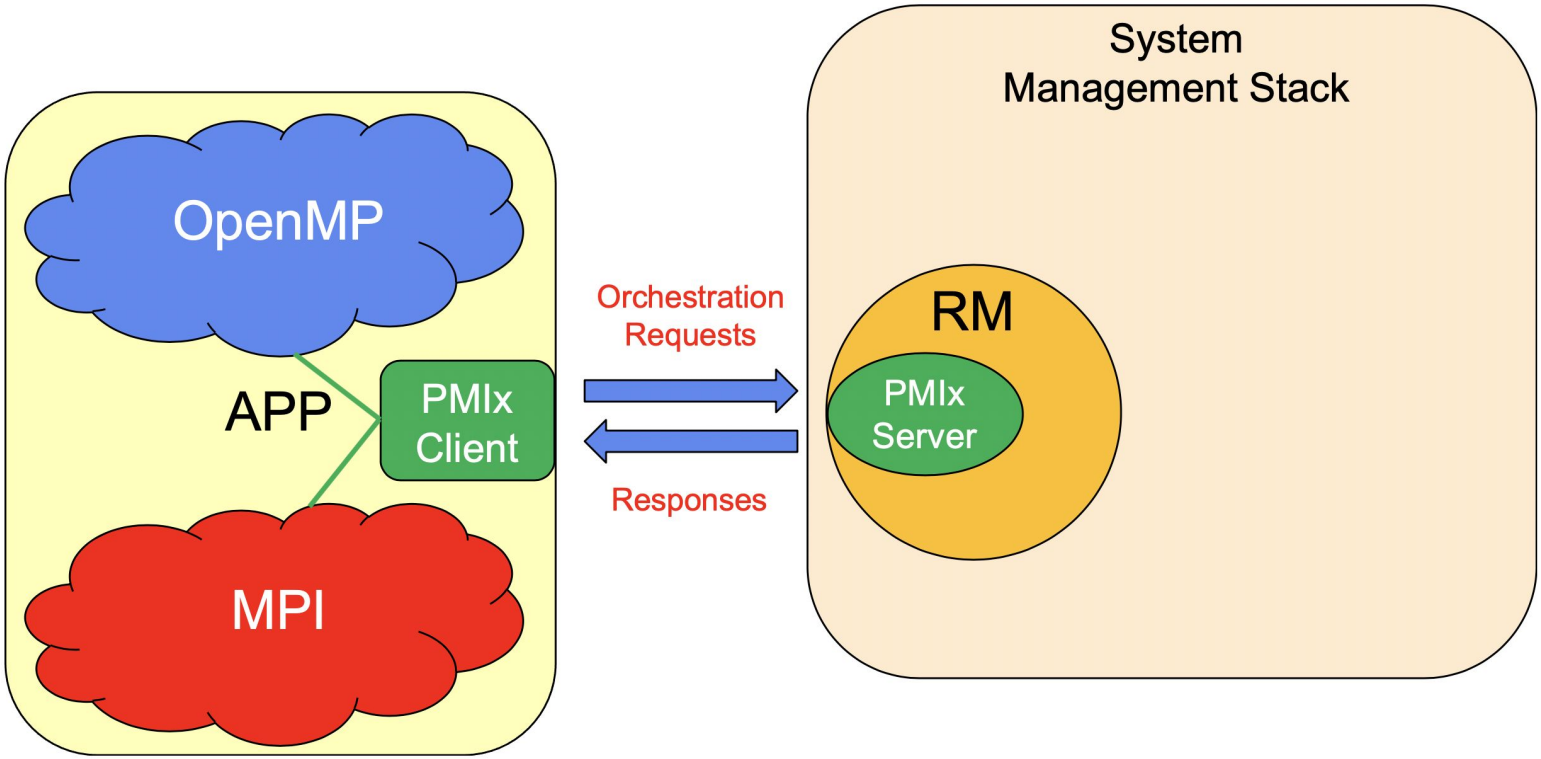
The Community

https://pmix.org
https://github.com/pmix

Messenger not Doer



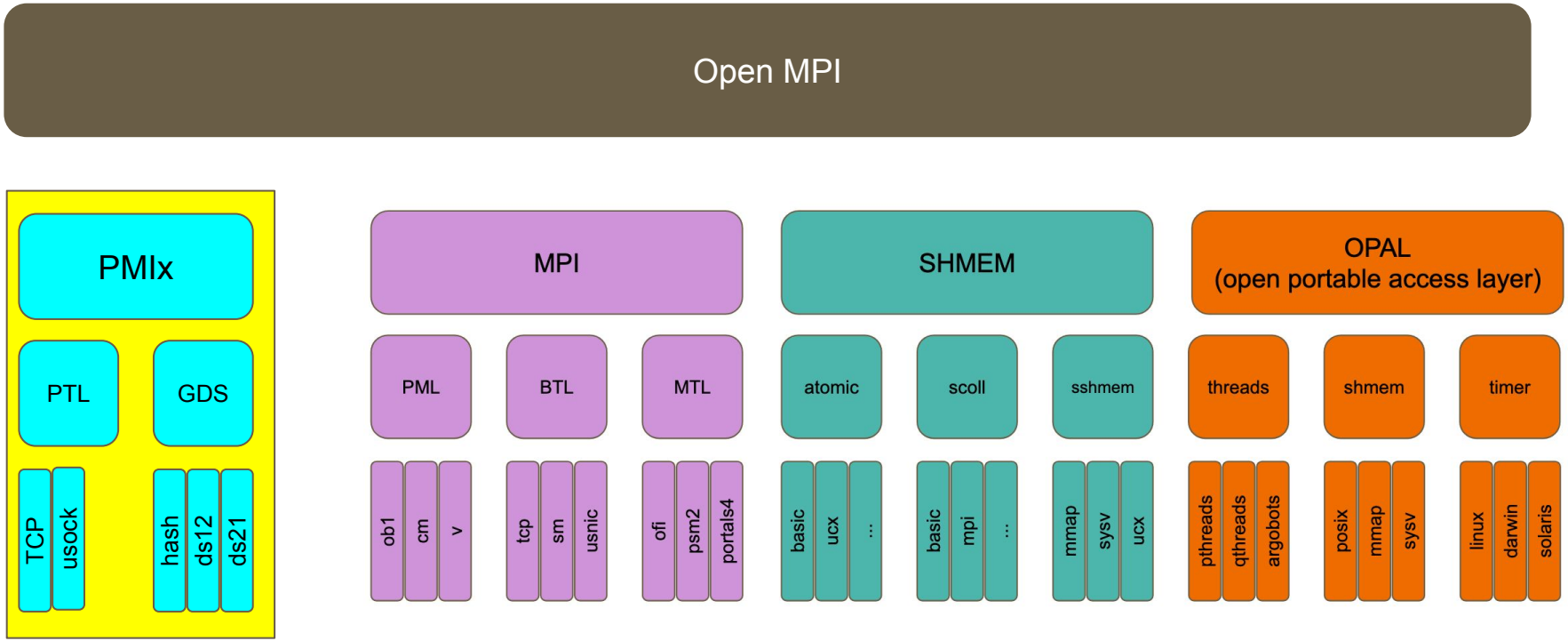
What Is Its Role?



"Doer" Exceptions

- Interactions with non-PMIx systems
  - Fabric manager, credential subsystems, storage systems
- Aggregate local collective operations
  - Fence, connect/disconnect
- Environment "support"
  - Inventory collection, process monitoring, logging

Where Does It Fit?



Building Open MPI

Tl;dr

```
wget \
  https://download.open-mpi.org/release/open-mpi/vx.y/openmpi-x.y.z.tar.bz2
tar xf openmpi-x.y.z.tar.bz2
cd openmpi-x.y.z

./configure --prefix=$HOME/my-ompi <options> |& tee config.out
# Most <options> typically deal with network communications
# libraries (e.g., libfabric, UCX)

make -j 8    |& tee make.out
make install |& tee install.out
```

Building from a Distribution Tarball vs. Git Clone

- Distribution tarballs are bootstrapped
- Building from a Git clone requires more tools
  - GNU Autotools
  - Flex
  - Pandoc (as of May 2020 git master / upcoming v5.0.0)

- See the `HACKING` file for more details about building from a Git clone

Configure Script Philosophies

- The configure script looks around your system
  - Searches for support for optional dependencies
  - If it finds them, builds support for them
  - If it does not find them, skip them (i.e., it's not an error)

- If user specifies `--with-FOO` (e.g., `--with-libfabric`)
  - The configure script will fail / abort if it cannot find / build support for FOO
- If user specifies `--without-FOO`
  - The configure script will (effectively) skip looking for FOO

- In short: *if a human asks for something that `configure` can't do, abort*

Specifying Compilers

- Via the usual GNU Autoconf method: shell variables
  - `CC` (C compiler)
  - `CXX` (C++ compiler)
  - `FC` (Fortran compiler)
    → `F77` and `F90` are no longer used!
    → `FC` is used to compile all Open MPI Fortran code

- Best practice: specify these values ***to the right of the configure token***
  - `./configure CC=/path/to/clang CXX=/path/to/clang++ FC=/path/to/gfortran …`
  - This way, these values end up in `config.log`

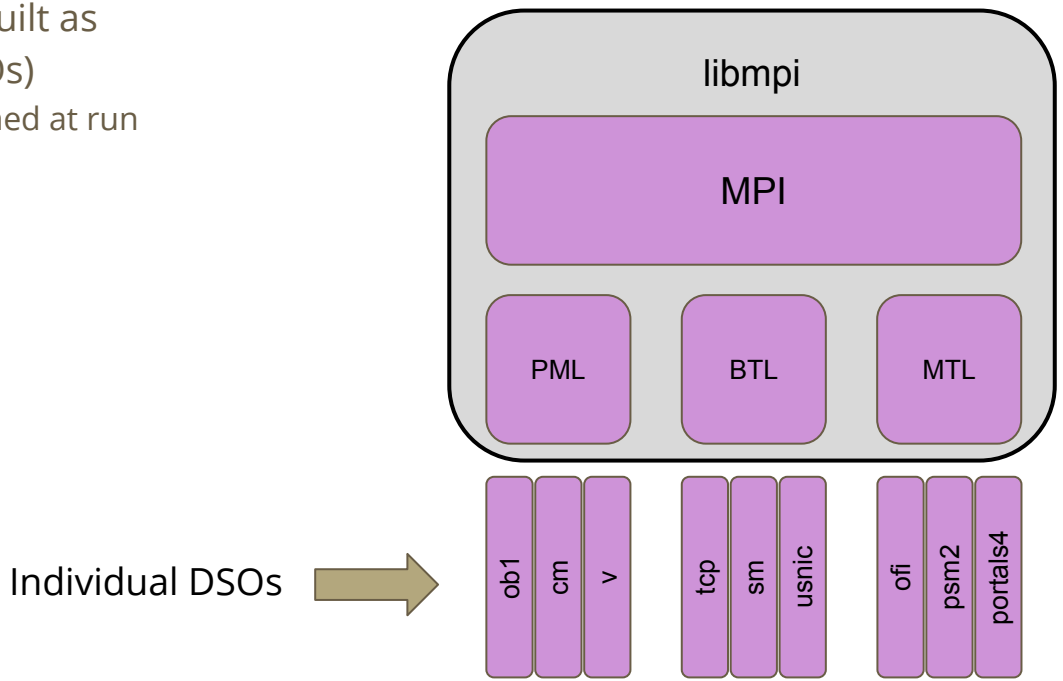
Project Libraries: Static or Shared?

- Open MPI supports building static and/or shared libraries
  - `--enable-static` / `--disable-static`
    - Referring to `libmpi.a`
  - `--enable-shared` / `--disable-shared`
    - Referring to `libmpi.so`

- Default (recomended):
  - `--disable-static`
  - `--enable-shared`

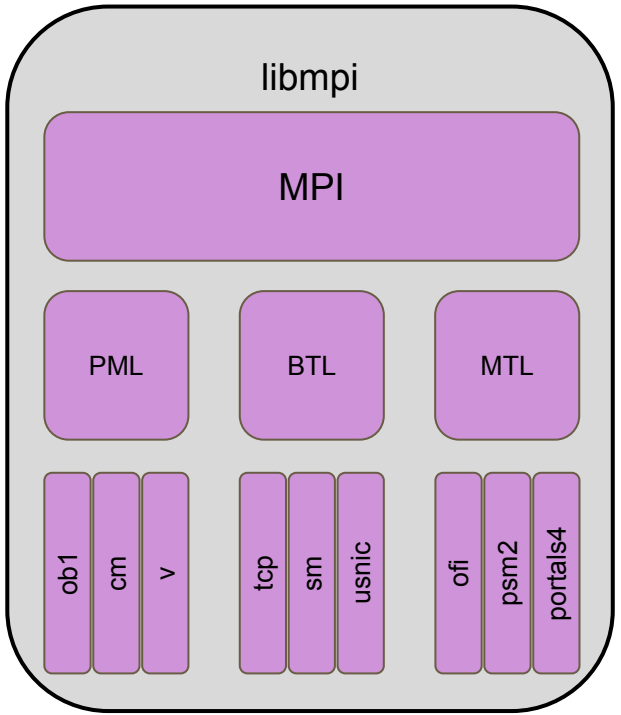
Components: DSO or Included?

- By default, components are built as Dynamic Shared Objects (DSOs)
  - Individual files that are opened at run time (e.g., via `dlopen()`)



Components: DSO or Included?

- By default, components are built as Dynamic Shared Objects (DSOs)
  - Individual files that are opened at run time (e.g., via `dlopen()`)
- But the components can also be included in their respective project library
  - `./configure --disable-dlopen ...`



Dependencies: libevent and hwloc

- Open MPI requires these two packages
  - Most modern Linux distros come with these packages
  - But installing the header files is not common
- Open MPI therefore (still) embeds full copies of these packages
  - If configure finds system-installed versions, it will use them (“external”)
  - If not, it will use the embedded copies (“internal”)

- Can use CLI options to force the “internal” or “external” versions:
  - `./configure --with-hwloc=/path/to/external/hwloc/install/tree …`
  - `./configure --with-libevent=internal ...`

Communication Libraries

The most common two libraries these days are Libfabric and UCX:

- Libfabric (“OpenFabrics Interfaces”)
  - `--with-libfabric[=LIBFABRIC_INSTALL_DIR]`
- UCX (Unified Communication X)
  - `--with-ucx[=UCX_INSTALL_DIR]`

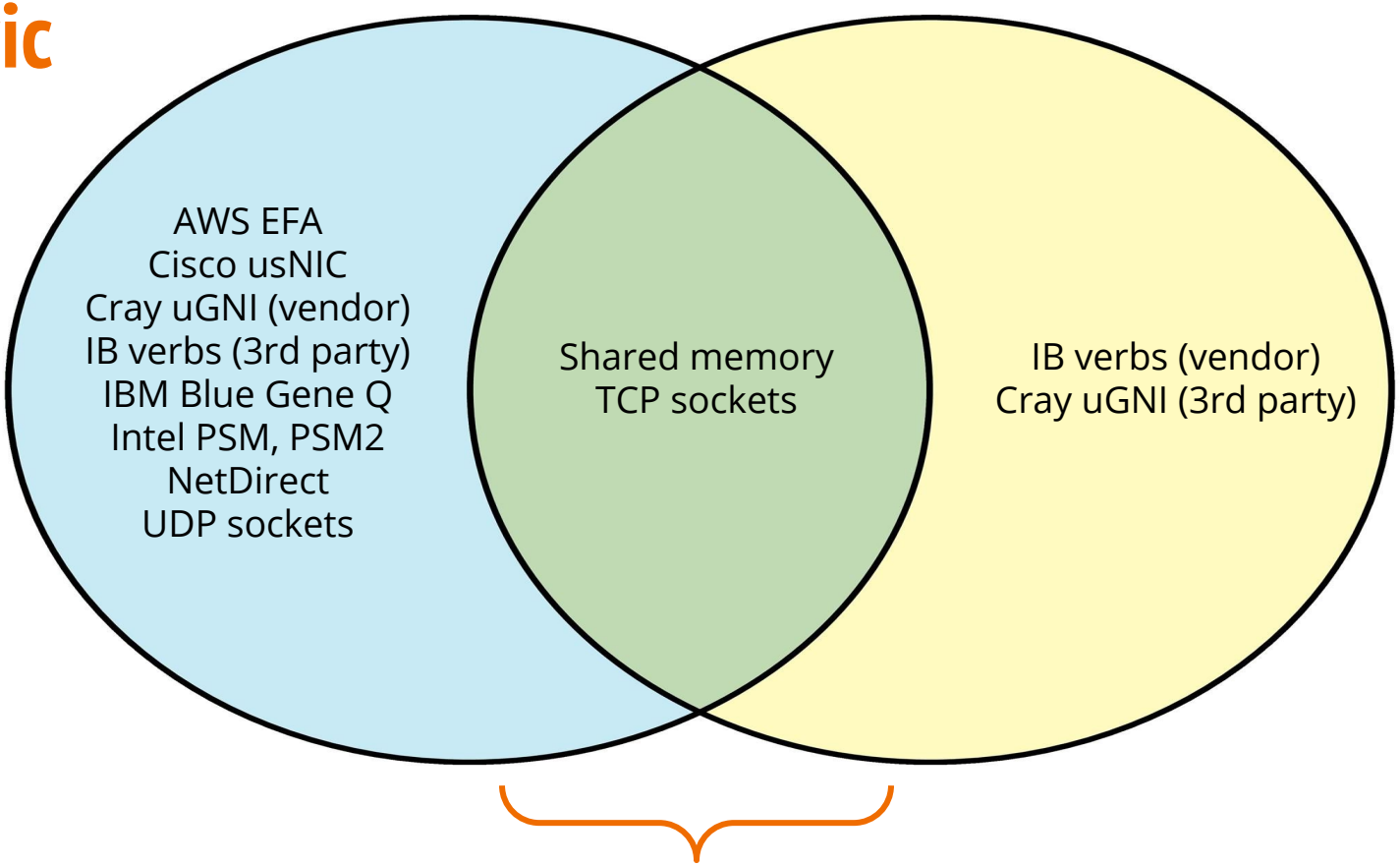
But other communication libraries are also availble, such as:

- PSM2 (OmniPath) and Portals4 are also supported
  - `--with-psm2[=PSM2_INSTALL_DIR]`
  - `--with-portals4[=PORTALS4_INSTALL_DIR]`

Libfabric ("OFI") and UCX

- Libfabric was originally created by network vendors who wanted an HPC network API that wasn't tied to the abstractions of InfiniBand
  - Cisco (usNIC)
  - Cray (uGNI)
  - Intel (PSM, PSM2)
- It has since grown to support many additional network types
  - AWS EFA (Elastic Fabric Adapter)
  - BlueGene Q
  - IB Verbs (IB, RoCE, iWARP)
  - NetDirect
  - POSIX TCP and UDP sockets
  - Shared memory

- UCX became the next generation, higher-abstraction InifiniBand support, supporting:
  - InfiniBand
  - RoCE
- It also grew to support additional network types:
  - Cray uGNI
  - POSIX TCP sockets
  - Shared memory



NOTE: Open MPI does not use Libfabric or UCX
for (pure) shared memory or TCP

Accelerators

Open MPI has CUDA support

- Nvidia (Mellanox) recommends building UCX with GDRcopy support
  - GDR = GPUDirect RDMA (there are multiple flavors of GPUDirect; this is the RDMA flavor)
  - Consult UCX documentation for GDRcopy build information
- Then build Open MPI with CUDA and UCX support
  - `./configure --with-cuda[=/path/to/cuda] --with-ucx[=/path/to/ucx]`
- PSM2 also supports CUDA

When built with CUDA support, Open MPI can send messages from / receive messages to GPU device memory without copying through main RAM

Open MPI Installation Details

- Use the `ompi_info` command to see information about your installation
- Useful CLI options:
  - `--parsable`: machine-friendly format
  - `--all`: see all available MCA run-time parameters

```
$ ompi_info
                 Package: Open MPI jsquyres@laptop Distribution
                Open MPI: 5.0.0a1
  Open MPI repo revision: v2.x-dev-7856-ge1e8b2a373
   Open MPI release date: Unreleased developer copy
                 MPI API: 3.1.0
           Ident string: 5.0.0a1
                 Prefix: /Users/jsquyres/bogus
 Configured architecture: x86_64-apple-darwin19.5.0
          Configured by: jsquyres
          Configured on: Sat Jun 20 13:46:35 EDT 2020
         Configure host: laptop
  Configure command line: '--prefix=/Users/jsquyres/bogus'
               Built by: jsquyres
               Built on: Sat Jun 20 14:00:44 EDT 2020
             Built host: laptop
             C bindings: yes
            Fort mpif.h: no
           Fort use mpi: no
      Fort use mpi size: deprecated-ompi-info-value
       Fort use mpi_f08: no
                ...
```

Questions?

That’s it for part 1!

Join us for part 2 in two weeks:
July 8, 2020
8am US Pacific / 11am US Eastern / 3pm UTC / 5pm CEST

Thank you!

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