MPI Malleability
Extending a production MPI implementation

Dr. Sonja Happ – ParTec AG

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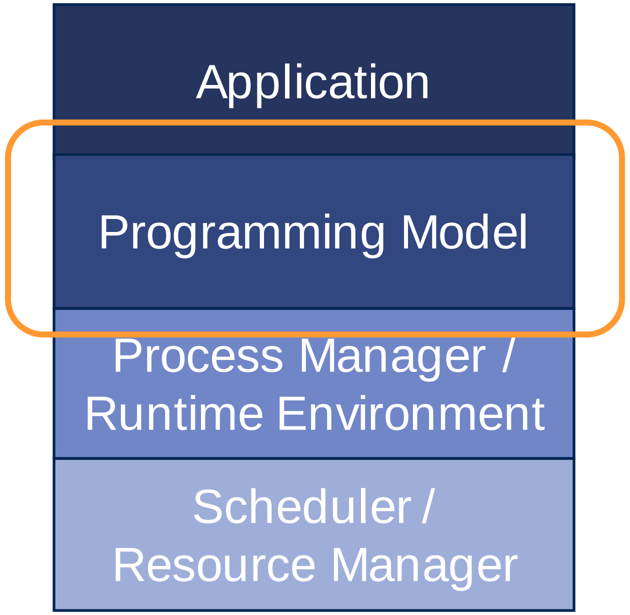
Computational Malleability in DEEP-SEA

- All layers of the HPC software stack involved
- DEEP-SEA enhances all layers with malleability features
  - Not all efforts can be covered here!

- Focus: MPI programming model
  - API and MPI library extensions
  - Interface with process manager

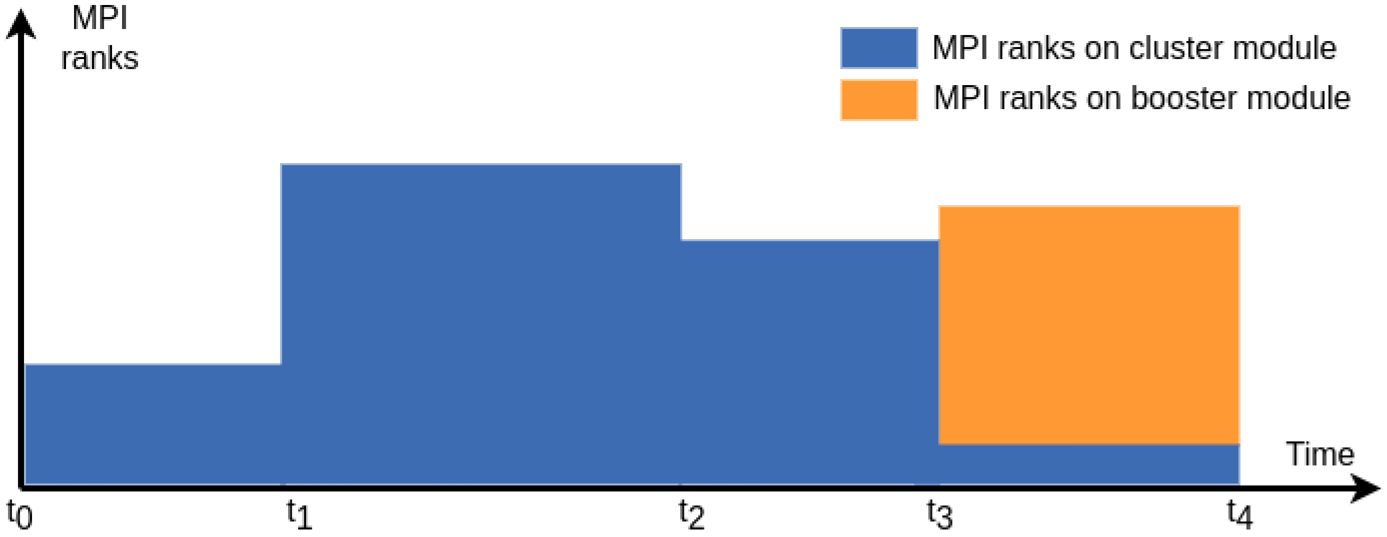
- Close collaboration with other EuroHPC19 projects


Application
Programming Model
Process Manager / Runtime Environment
Scheduler / Resource Manager

Malleability for MPI Applications

- Dynamic adaptation of number of MPI ranks
  - External constraints
  - Computational phases
  - Modular Supercomputing Architecture (MSA)

- Challenges
  - MPI interface for malleability
  - Exchange with process manager
  - Data re-distribution



Potential scenario:

t_0: Launch app with MPI ranks on cluster module

t_1: Expand app to use more ranks on cluster module (e.g. new app phase)

t_2: Shrink app to use less ranks on cluster module (e.g. energy constraint)

t_3: Shrink app to use much less ranks on cluster module and launch MPI ranks on booster module (e.g. new app phase)

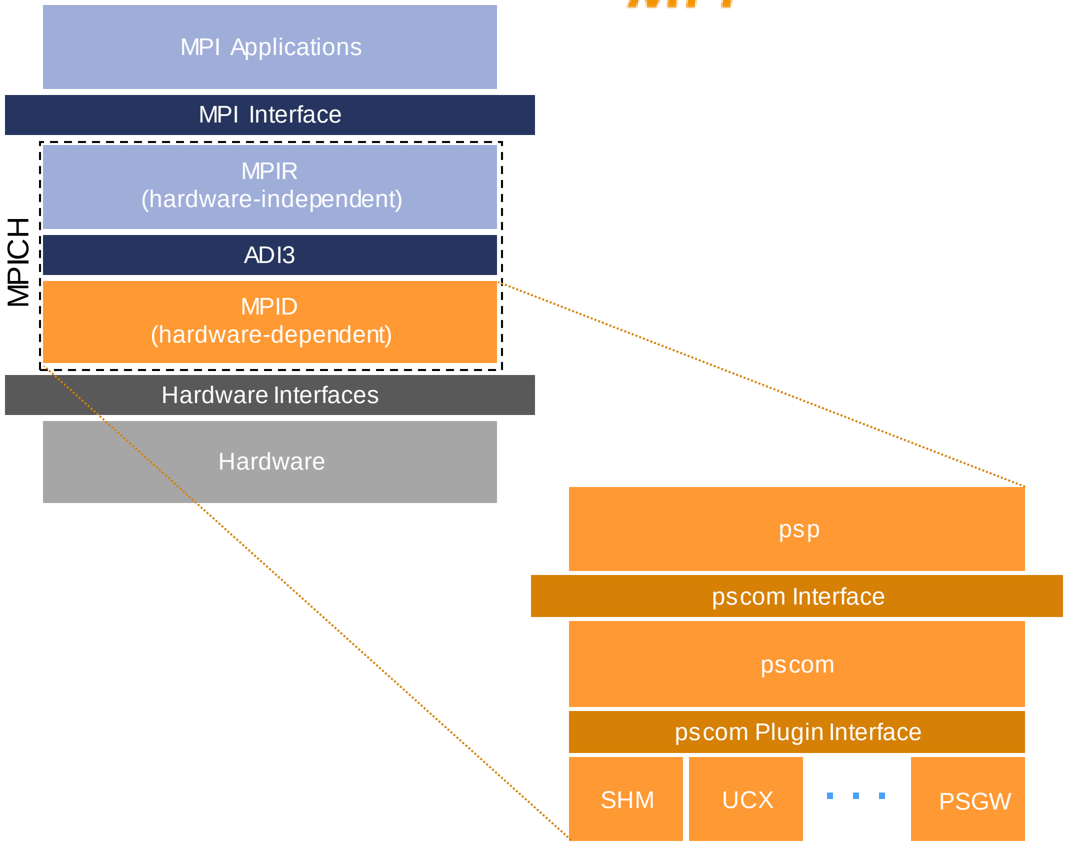
t_4: Finish app

ParaStation MPI

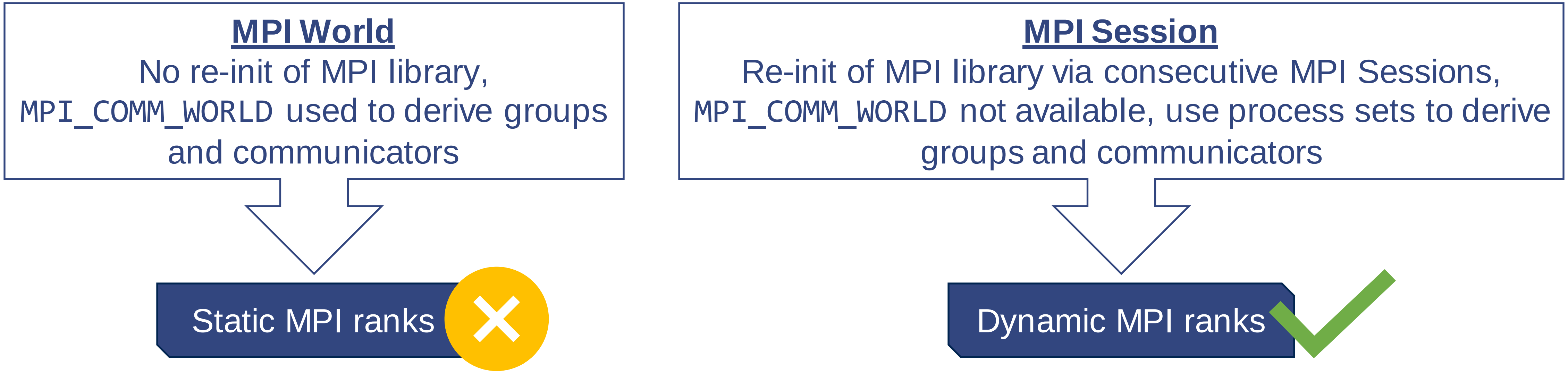
- Based on MPICH 4.1.2
  - Support MPICH tools for tracing, debugging, etc.
  - Integrates into MPICH on the MPID layer by implementing an ADI3 device
  - The PSP Device is powered by pscom – a low-level point-to-point communication library
  - Support the MPICH ABI Compatibility Initiative

- Support for various transports / protocols via pscom plugins
  - InfiniBand, Omni-Path, BXI, etc.
  - Concurrent usage of different transports

- Proven scalability



MPI Sessions for Malleability



MPI World
No re-init of MPI library, `MPI_COMM_WORLD` used to derive groups and communicators

Static MPI ranks ✗

MPI Session
Re-init of MPI library via consecutive MPI Sessions, `MPI_COMM_WORLD` not available, use process sets to derive groups and communicators

Dynamic MPI ranks ✓

- Exploit re-initialization ability of MPI Sessions
  - Re-init MPI library for changed processes
  - Update process sets during re-init to reflect changed MPI ranks

- Requirements for malleable MPI applications
  - Must use MPI Session model and process sets
  - Must not use MPI world model and `MPI_COMM_WORLD`

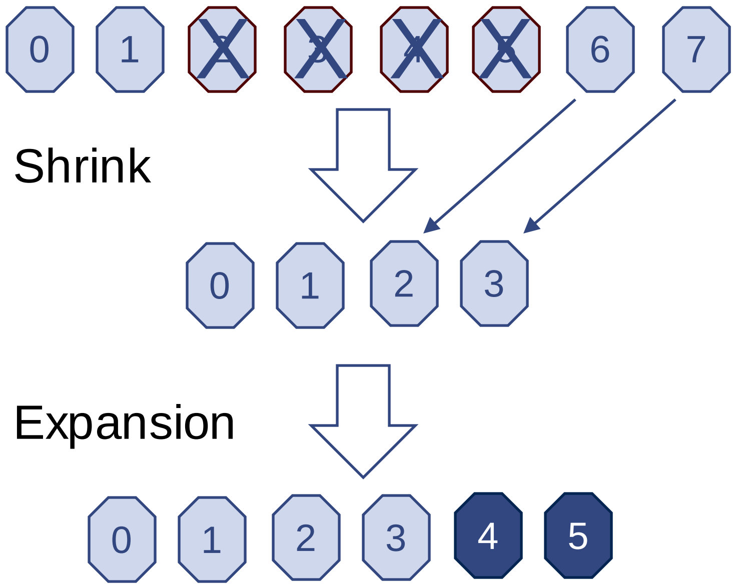
Getting ParaStation MPI ready for Malleability

- Enhancements for MPI Session implementation
  - Re-initialization of MPI library
  - Decoupling from MPI world model
  - Reference counting and checking on finalize
  - Error handling
  - PMIx Process Sets
- PMIx Spawn support

- All enhancements included in ParaStation MPI as of release 5.9.2-1
- Upstream: Many enhancements will be included in MPICH 4.2

MPI eXtensions for Malleability: Objectives

- Re-initialize MPI library
- Dense monotonic MPI rank numbering
- Allow users to
  - think in ranks and not nodes
  - select starting point
  - select ranks to exit for shrink
  - reuse utility functions
- Asynchronous resource allocation and spawning
- MPI-4 compatibility
- Rely on PMIx



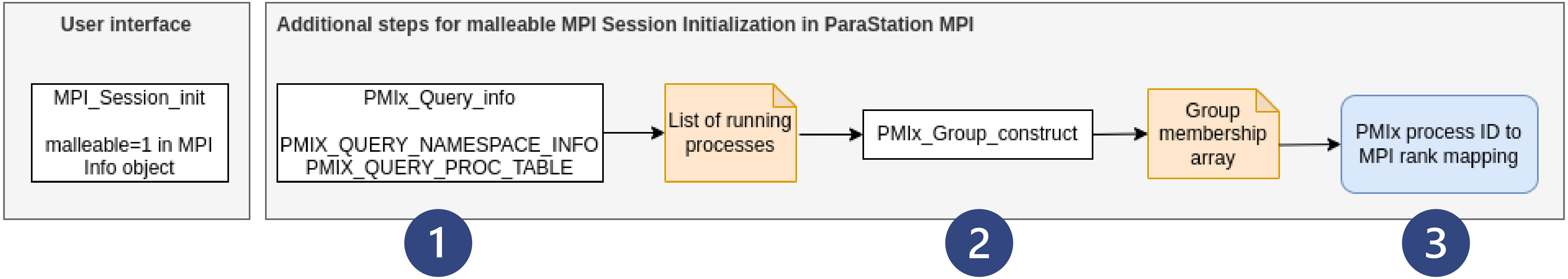
Shrink

Expansion

Proposal for 3 new MPI functions

Malleable Sessions with ParaStation MPI and PMIx

1. PMIx Query: Obtain information about all processes
2. Create PMIx Process Group for running processes
   - Process Group is destructed on `MPI_Session_finalize`
3. Obtain unambiguous mapping of PMIx process ID to MPI rank


User interface
MPI_Session_init
malleable=1 in MPI Info object
Additional steps for malleable MPI Session Initialization in ParaStation MPI
PMIx_Query_info
PMIX_QUERY_NAMESPACE_INFO
PMIX_QUERY_PROC_TABLE
List of running processes
PMIx_Group_construct
Group membership array
PMIx process ID to MPI rank mapping
1
2
3

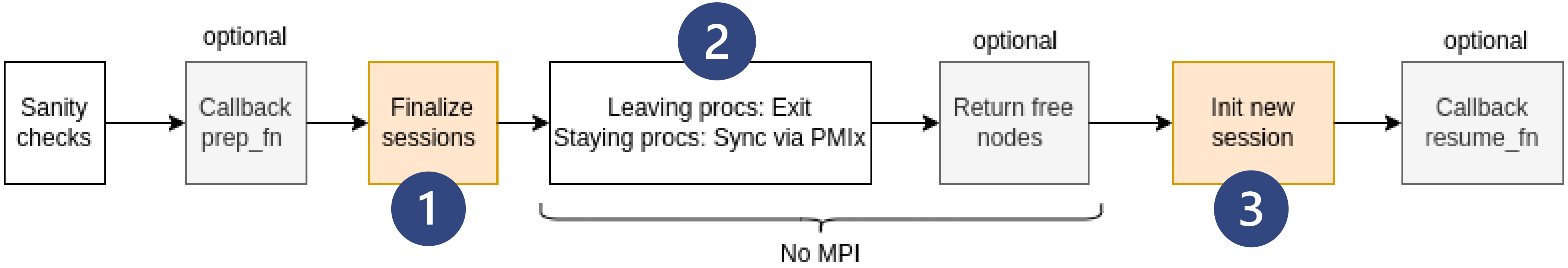
MPIX_Session_reinit

```
int MPIX_Session_reinit(int count, MPI_Session **session_array_in,
   MPI_Session *session_out, MPI_Info info,
   MPIX_Session_reinit_preparation_function *prep_fn, void *prep_userdata,
   MPIX_Session_reinit_resume_function *resume_fn, void *resume_userdata,
   int leave, MPI_Count nleave, int resize_allocation,
   MPI_Errhandler errhandler)
```

1. Finalize all existing MPI Sessions
2. Terminate processes that shall exit (shrink)
3. Initialize new MPI Session with updated rank-to-process mapping
   - Include new processes (expansion)
   - Exclude terminated processes (shrink)

Optional: Application-specific callbacks for session finalization and initialization

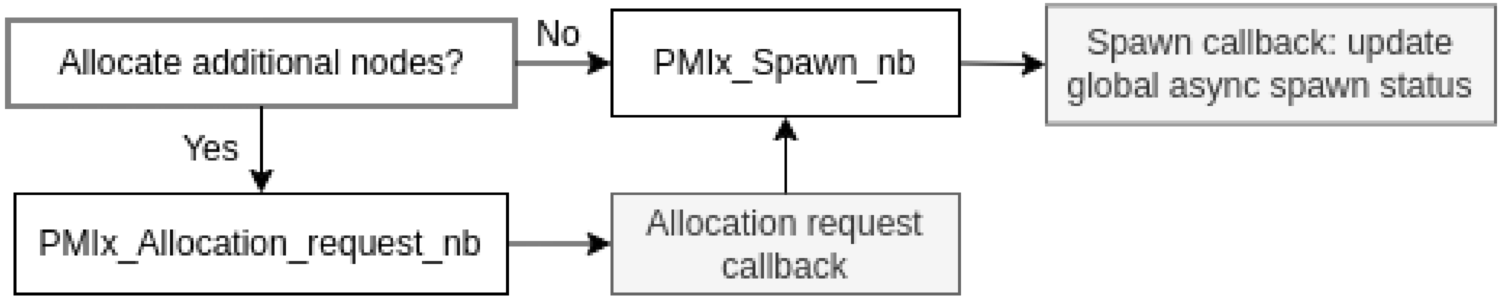
Optional: Return any free node(s)



MPIX_Spawn_async

```
int MPIX_Spawn_async(
   const char *command, char *argv[],
   int maxprocs, MPI_Info info,
   int root,int resize_allocation,
   MPI_Info *status)
```

- Trigger asynchronous spawn of new processes
- Optional: Allocate additional nodes and spawn processes on these nodes
- Most arguments like those of `MPI_Comm_spawn`
- Post-requirement: Call `MPIX_Session_reinit` to include additional processes in application progress


Allocate additional nodes?
No
PMIx_Spawn_nb
Spawn callback: update global async spawn status
Yes
PMIx_Allocation_request_nb
Allocation request callback

MPIX_Spawn_status

```
int MPIX_Spawn_status(MPI_Info *status)
```

- Obtain global status of asynchronous spawn
  - Async. spawn is available?
  - Process is spawned?
  - Status of global spawn operation?
  - Additional keys specific for ongoing or complete async spawn operation

- Future work: Relay external/ system constraints to MPI application via key value pairs, for example
  - Number of processes that can be spawned
  - Specific processes that should exit for shrink

Status and outlook

Status

- Testing with PMIx Reference Runtime Environment (PRRTE)
- Single-node tests successful
- Multi-node tests ongoing

Outlook

- Deployment on research HPC system (DEEP @JSC)
- Code review and release
- Discussion with MPI Forum

Thank you!

Dr. Sonja Happ

sonja.happ@par-tec.com

www.par-tec.com

ParTec AG
Possartstr. 20, 81679 Munich
Germany

www.deep-projects.eu

@DEEPprojects

@deep-projects

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Simplified example: Expansion

```c
int main(int argc, char *argv[])
{
    […] /* Init variables */
    /* Set malleable parameter in info object */
    MPI_Info_set(sinfo, "malleable", "1");
    /* Init session */
    MPI_Session_init(sinfo, MPI_ERRORS_ARE_FATAL, &session);
    […] /* Create MPI Objects and do work...*/
    if (!spawned) {
       /* Trigger the spawn */
       MPIX_Spawn_async((char *) "./my_app", MPI_ARGV_NULL,
                        /* spawn 2 processes */ 2, MPI_INFO_NULL,
                        /* rank 0 is the root */ 0, 0, &spawn_status);
       /* Wait for spawned processes to become ready */
       MPI_Info_get(spawn_status, "spawn_x_status", MPI_MAX_INFO_VAL, status, &found);
       while (strncmp(status, "complete", MPI_MAX_INFO_VAL) != 0) {
              MPIX_Spawn_status(&spawn_status);
              MPI_Info_get(spawn_status, "spawn_x_status", MPI_MAX_INFO_VAL, status, &found);
       }
       […] /* Clean-up old MPI objects */
       /* Re-init */
       sessions_for_reinit[0] = &session;
       MPIX_Session_reinit(1, sessions_for_reinit, &session_NEW, MPI_INFO_NULL,
                           MPIX_SESSION_REINIT_PREP_FN_NULL, NULL,
                           MPIX_SESSION_REINIT_RESUME_FN_NULL, NULL, 0, 0, 0, MPI_ERRORS_ARE_FATAL);
       […] /* Create new MPI objects and continue with work */
       MPI_Session_finalize(&session_NEW);
    } else {
       /* Spawned process, finalize session */
       MPI_Session_finalize(&session);
    }
}
```

Trigger async spawn

Know that new processes are available

Re-init complete, new processes are included