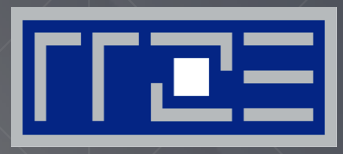
ERLANGEN REGIONAL COMPUTING CENTER



ESSEX: Sparse iterative solvers, asynchronicity and fault tolerance

Faisal Shahzad, Moritz Kreutzer and Gerhard Wellein

FFMK workshop „Application Interfaces for an Exascale OS”

December 8, 2014

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SPPEXA

FAU FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

Applications | Comp. Algorithms | Programming

Long-standing collaboration (15+ yrs)

Georg Hager
Erlangen Regional **Computing Center**

Parallelization, Optimization, Performance Engineering, Tools

M. Kreutzer

Programming

(Building blocks)

Achim Basermann
DLR, **Simulation and SW Technology**

Scalable Preconditioners, Eigenvalue Solvers, Solvers for Sparse Linear Systems

Jonas Thies

Comp. Algorithms

(JaDa, Pre-conditioner)

Gerhard Wellein
University of Erlangen
Dept. of **Computer Science**

Resilience, Performance Engineering, Parallelization, Optimization

Faisal Shazad

Programming

(Fault Tolerance)

ESSEX

Bruno Lang
University of Wuppertal
Applied Computer Science

Efficient Direct and Iterative Eigensolvers

L. Krämer

Comp. Algorithms

(FEAST)

Holger Fehske
University of Greifswald
Institute for **Physics**

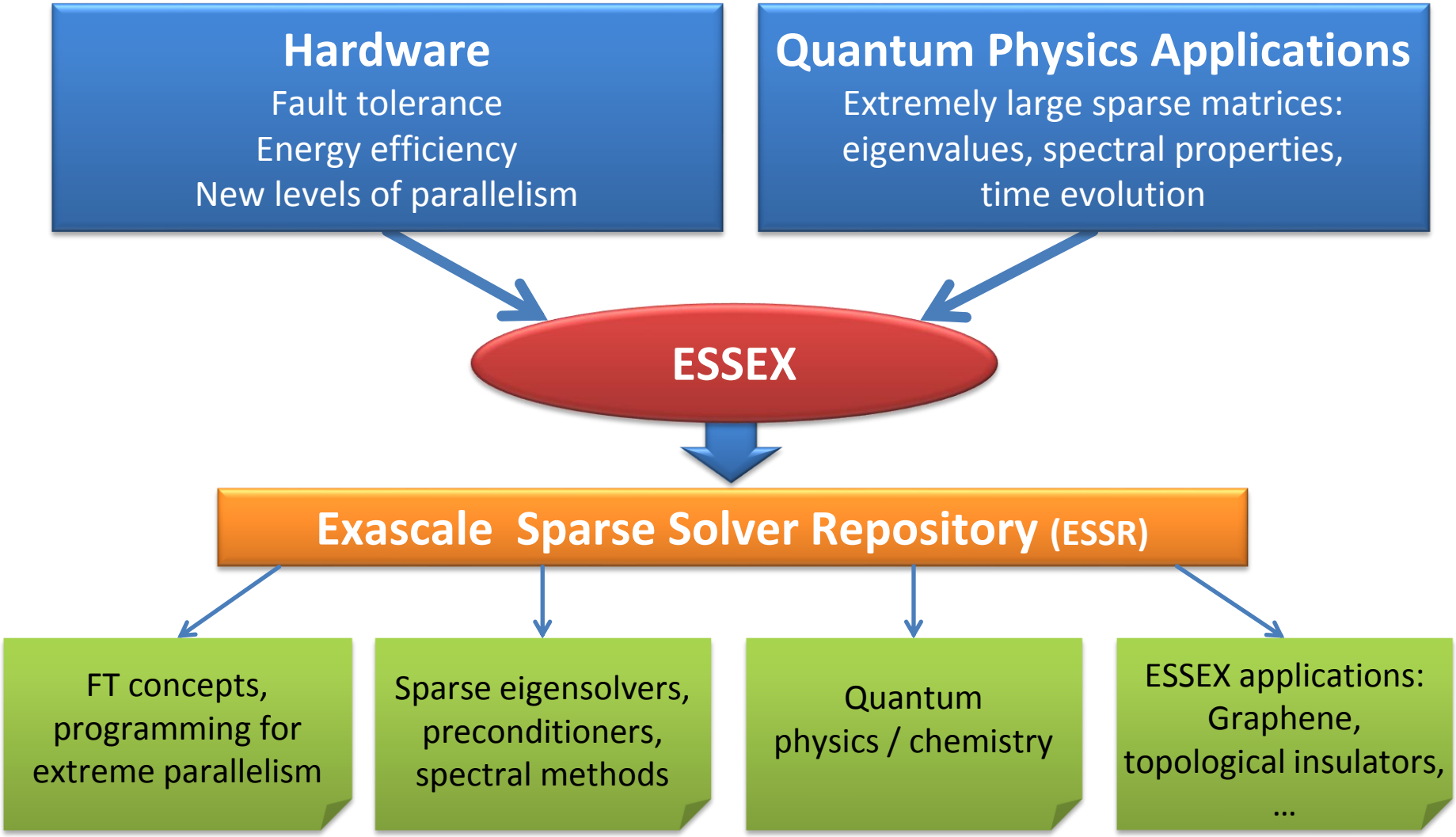
Complex Quantum Physics Applications, Numerical Methods

A. Alvermann
Comp. Algorithms /Applications (KPM, ChebTP)

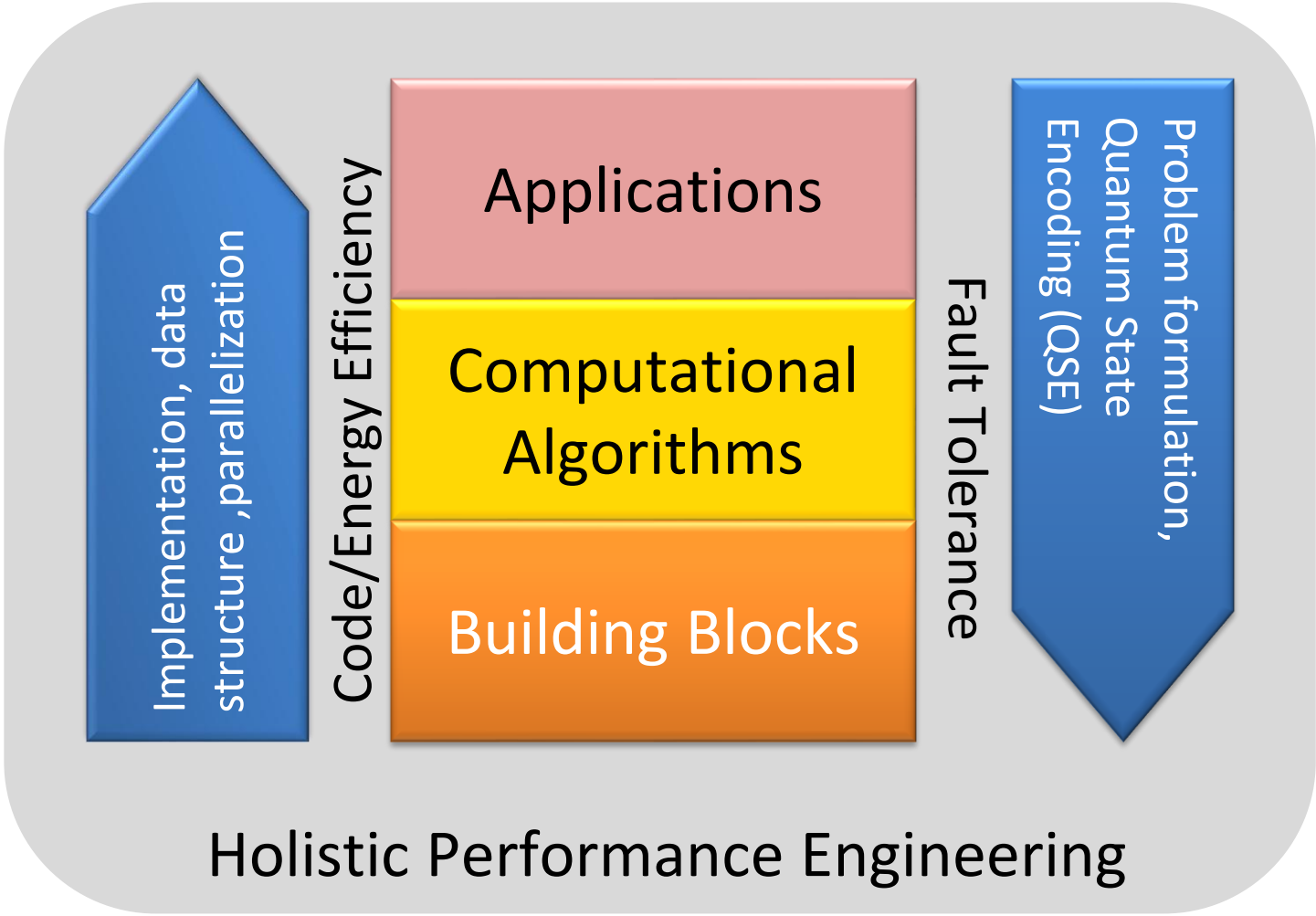
A. Pieper
Applications (Graphene, top. Insulators)

ESSEX - Equipping Sparse Solvers for Exascale

Equipping Sparse Scalable Solvers for Exascale (ESSEX)



ESSEX: “Co-Design” oriented project



Basic building blocks library: GHOST

General, Hybrid and Optimized Sparse Toolkit

- Basic tailored sparse matrix / vector operations
- CRS or **SELL-C-σ*** (**unified format**) storage schemes
- (Block-)SpMVM: SIMD intrinsic (AVX, SSE, MIC) & CUDA kernels
- Dense vector /matrices: row-/column-major storage

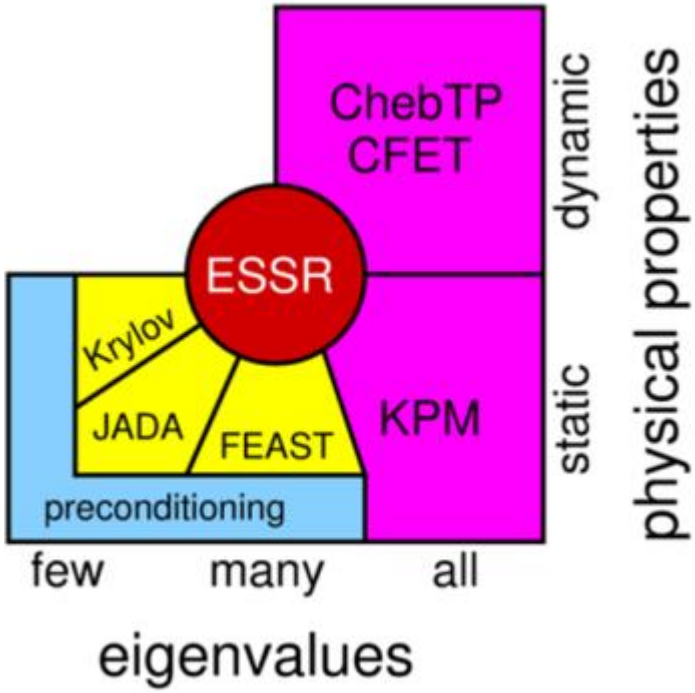
- **Supports** data & **task parallelism** (up to application level)
- MPI + OpenMP + **tasks for concurrent execution**
- **Generic and hardware-aware task management**

- **Application layer triggered checkpoint / restart**
- **Asynchronous checkpointing via tasks**
- **Various checkpoint locations (node, filesystem)**

*M. Kreutzer, G. Hager, G. Wellein, H. Fehske, and A. R. Bishop: *A unified sparse matrix data format for efficient general sparse matrix-vector multiplication on modern processors with wide SIMD units.* SIAM Journal on Scientific Computing **36**(5), C401–C423 (2014).

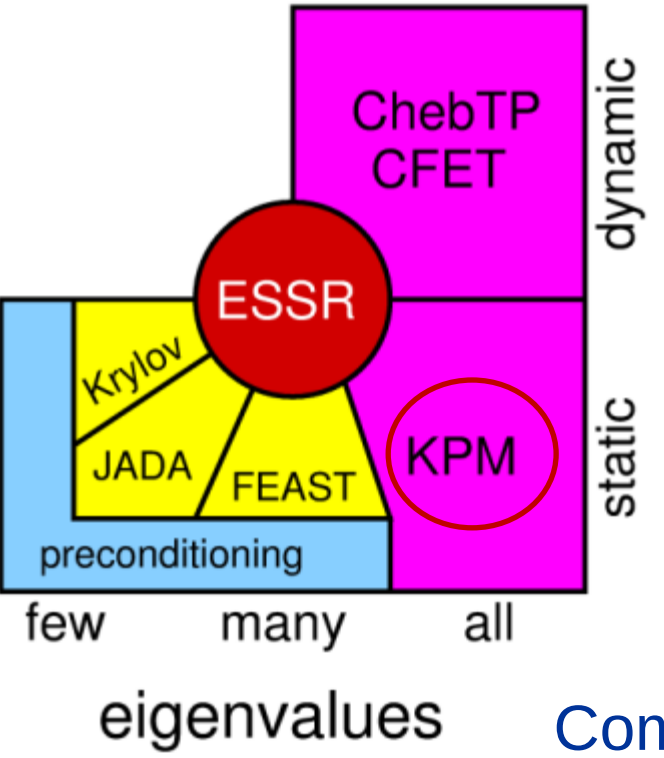
Our (ESSEX) effort –
get a simple solution first –
application driven –
No silver bullet

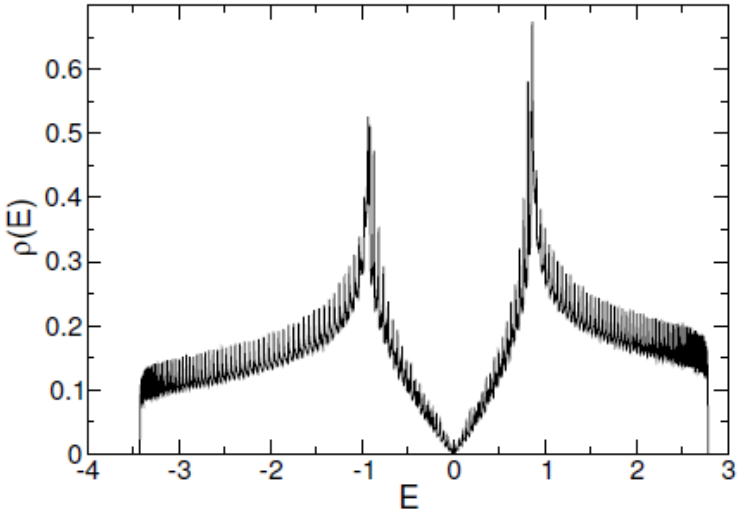
1. Iterative Solvers
   - Kernel Polynomial Method (KPM)
   - Jacobi Davidson (JADA)
2. Asynchronicity
   - Handling node-level parallelism
3. Fault Tolerance and Checkpointing/Restart



ESSEX: Computational challenges / methods

Cover most aspects of large sparse eigenvalue problem





$$X(\omega) = \frac{1}{N}\mathrm{tr}[\delta(\omega - H)X] = \frac{1}{N}\sum_{n=1}^{N}\delta(\omega - E_n)\langle\psi_n, X\psi_n\rangle$$

Compute approximation to complete eigenvalue spectrum of large sparse matrix A (with $X = I$)

A. Weiße, G. Wellein, A. Alvermann, and H. Fehske, Rev. Mod. Phys. **78**, 275 (2006).
The kernel polynomial method

ESSEX: Start with simple but efficient iterative algorithms ("Kernel Polynomial Method")

```
for r = 0 to R-1 do
  |v⟩ = |rand()⟩;
  Initialization &
  computation of μ0, μ1
  for m = 1 to M/2 do
    swap(|w⟩, |v⟩);
    |u⟩ = H|v⟩ ;
    |u⟩ = |u⟩ – b|v⟩ ;
    |w⟩ = –|w⟩ ;
    |w⟩ = |w⟩ + 2a|u⟩ ;
    η2m = ⟨v|v⟩ ;
    η2m+1 = ⟨w|v⟩ ;
  end
end
```

Application: R random configurations ($R=1,\ldots,10^2$) or iterative loop

Algorithm: Compute Chebyshev moments

Basic building blocks: spMVM and sparseBLAS1

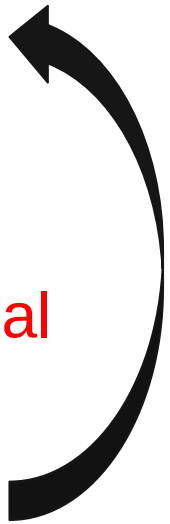
Checkpoint data: 2 vectors
Constant sparse matrix (H) – recompute

KPM approach can be implemented with only one global communication step

ESSEX: Iterative Eigensolvers – BJDQR

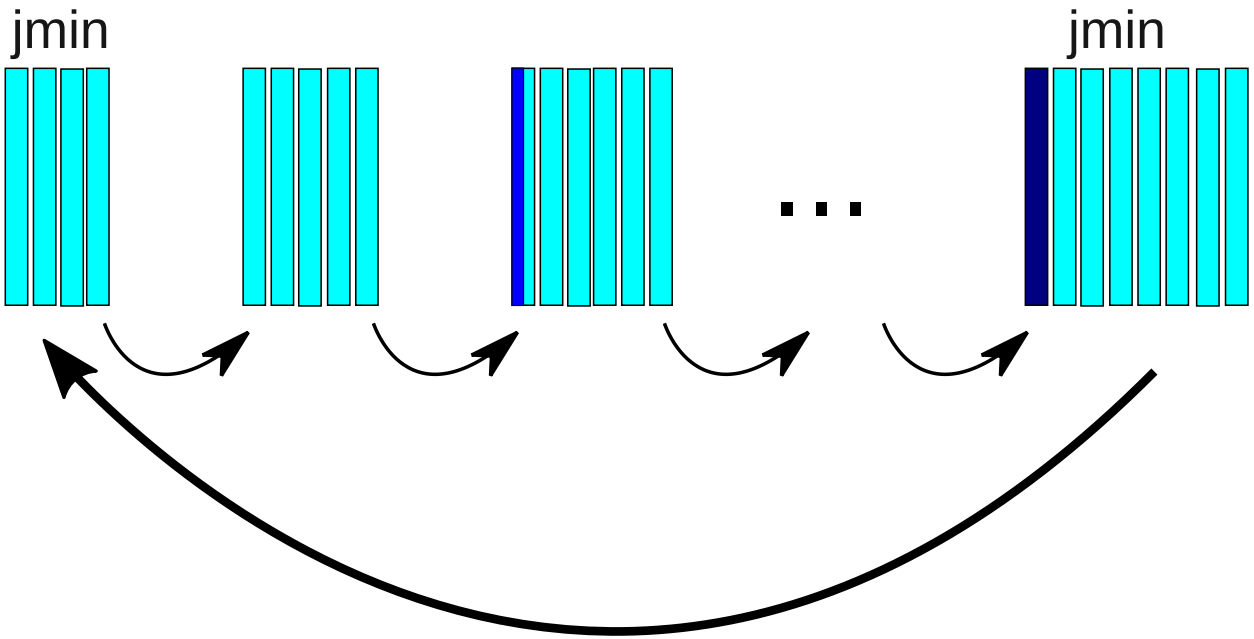
- Blocked Jacobi-Davidson QR Method

1: Setup initial subspace
2: while not converged do
3: Project the problem to a small subspace
4: Solve the small eigenvalue problem
5: Calculate an n_b approximations and their residual
6: **Lock** converged eigenvalues
7: Shrink subspace if required (**RESTART**)
8: Approximately solve the n_b correction equations
9: Block-Orthogonalize the new directions
10: Enlarge the subspace
11: end while



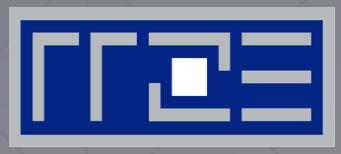
ESSEX: Iterative Eigensolvers – BJDQR

Converged eigenvectors (**LOCK**): incr. async. Backup in DP
Expanding subspace, full async. backup in SP after **RESTART**



RESTART: shrink subspace to **jmin** vectors

GHOST*: NODE-LEVEL ASYNCHRONICITY



Basic parallelization approach: MPI + X

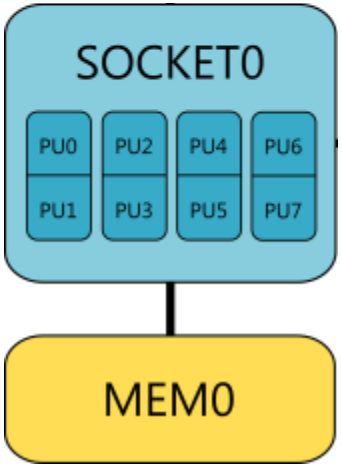
Motivation – Use X for many tasks at the same time

- Asynchronous Communication
- Asynchronous Checkpointing
- Concurrent worker teams (CPUs)
- Accelerators

Easy to use, low overhead, hardware-aware

*General, Hybrid and Optimized Sparse Toolkit
Developed by: Moritz Kreutzer, RRZE

Modern compute nodes



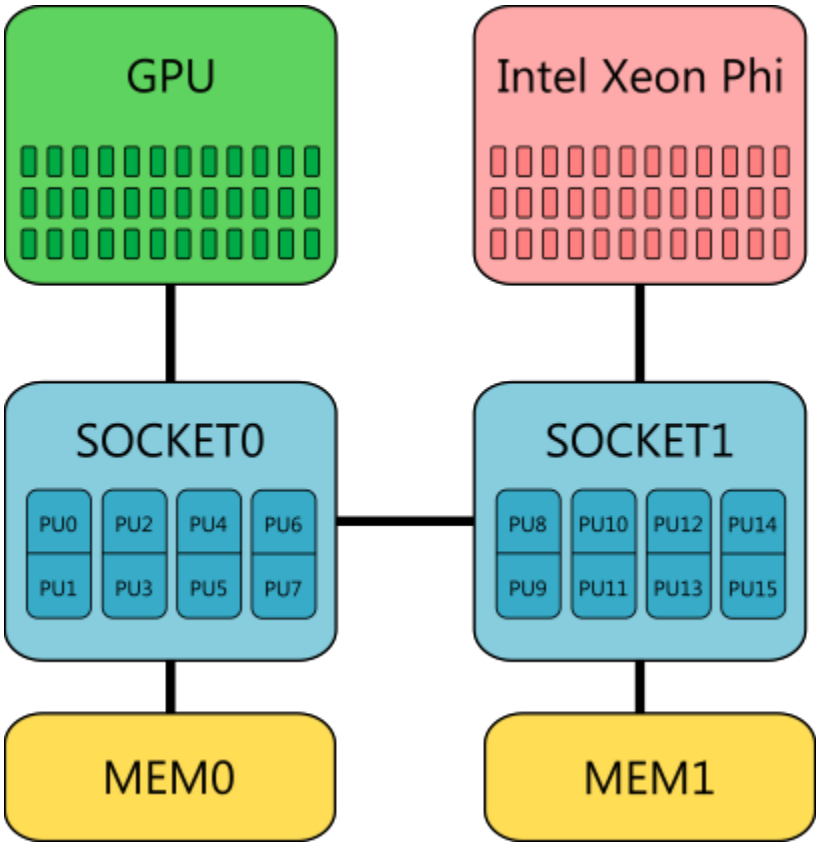
- Heterogeneous architectures on a single node
- Differ in programming paradigm
  - CPU: only native mode
  - GPU: only accelerator mode
  - Xeon Phi: accelerator or native mode
- Differ in performance

PU = processing unit

Work distribution

- Distinction between architectures via MPI processes:
  - exactly one process per GPU
  - at least one process per Xeon Phi
  - at least one process for all CPUs
- Each process gets assigned a weight deciding the share of work which depends on their relative performance
- Resource management:
  - Each process running inside an exclusive CPU set (no shared cores)
  - CPU sets may span several NUMA nodes

Example work distribution



- Amount of processes is the minumum: 3
- GPU is managed by a full core on the nearest socket
- CPU process spans two NUMA nodes
- Xeon Phi operated in native mode
  - one MPI process running on the coprocessor

Degrees of freedom in work distribution

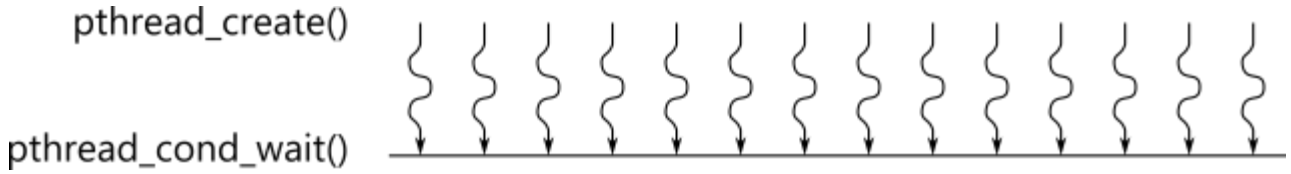
- More than one CPU processes
  - maybe favorable in order to avoid NUMA problems: one per NUMA node
  - one process per core/PU also possible (in case OpenMP is not present/desired)
- Number of PUs for GPU management
  - at least one, but the other PU on the same core may have problems in this case
- More than one process on the Xeon Phi

Resource management

- Each process stores idle/busy states and locality information of each of it‘s PUs (e.g. for initial state of CPU process)

PU	2	3	4	5	6	7	8	9	10	11	12	13	14	15
NUMA node	0	0	0	0	0	0	1	1	1	1	1	1	1	1
Idle	1	1	1	1	1	1	1	1	1	1	1	1	1	1

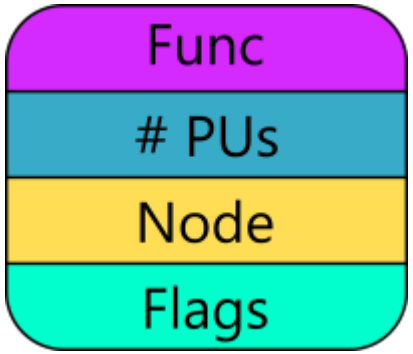
- One shepherd thread will be created per PU:



- The shepherd threads wait for tasks to be put in the task queue

Task processing

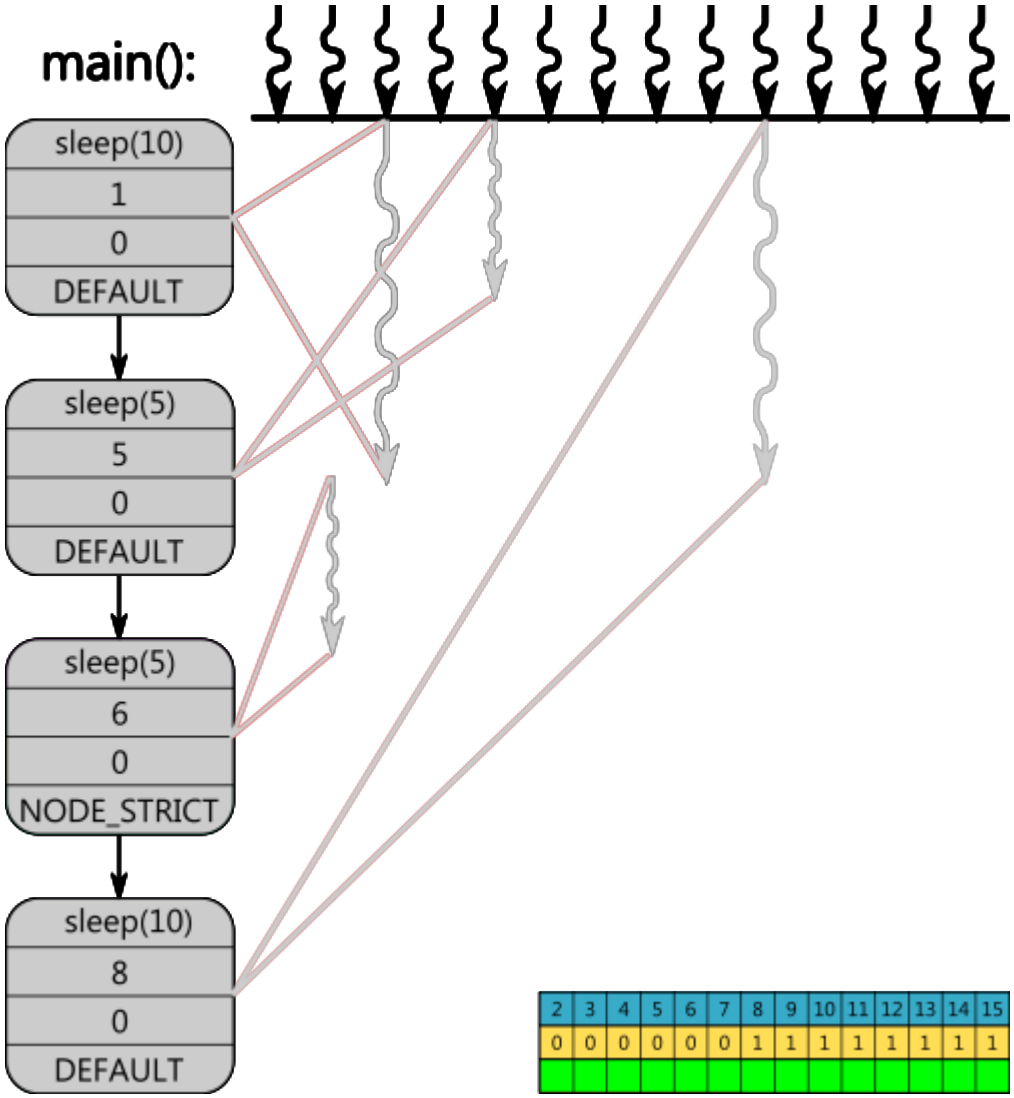
- A task is defined by
  1. A function callback along with parameters
  2. The number of PUs to process the task
  3. The preferred NUMA node to process the task
  4. Additional flags



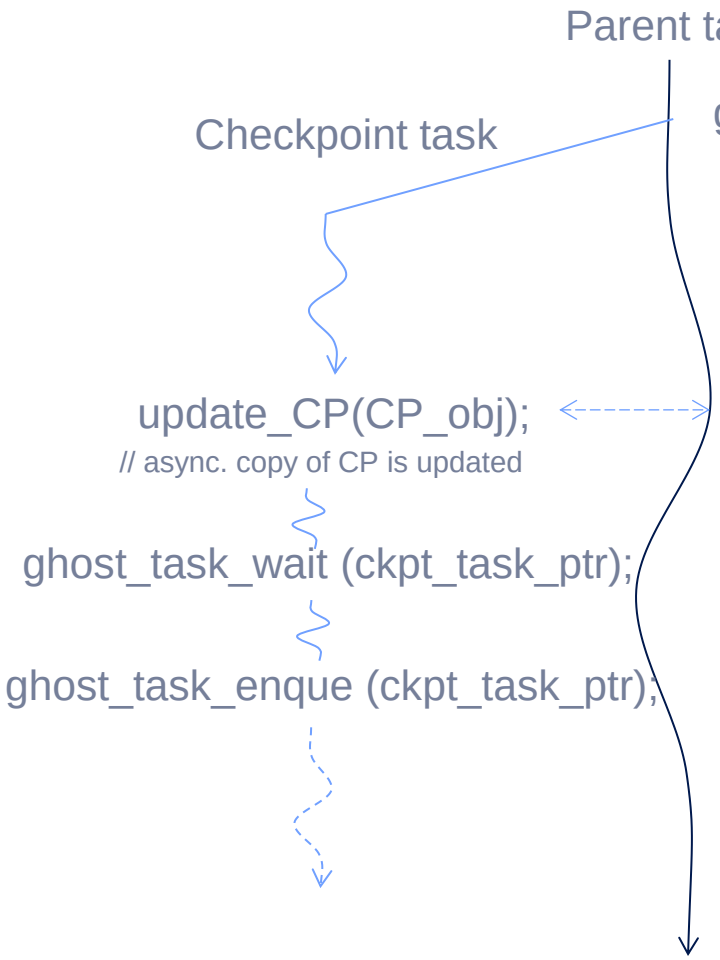
- Available flags (can be combined):
  - PRIO_HIGH: Put task to beginning of queue.
  - NODE_STRICT: Execute task only on the given NUMA node.
  - NOT_ALLOW_CHILD: Do not allow a child task to use the task‘s PUs.
  - NOT_PIN: Do not register the task in the PU map.

- All tasks line up in a single queue

Simple tasking example



Asynchronous checkpoints via GHOST-task thread:



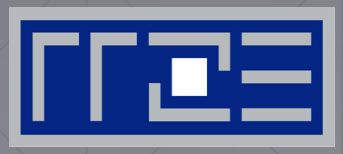
CP_obj:

- object of ckpt_t type
- ckpt_t class is defined by programmer
- checkpoint object contains the aynchronous copy of the checkpoint

CP_func:

- This function takes an updated copz of CP_obj as argument and writes to PFS..

FAULT TOLERANCE AND ASYNCHRONOUS CHECKPOINTING



Pragmatic approach:

- Hide costs for checkpointing
  - Asynchronous
  - Remote Node checkpoints / hierarchical
  - Restart from node local data if possible

- Prototype experiences with GPI – Application based FT with CR

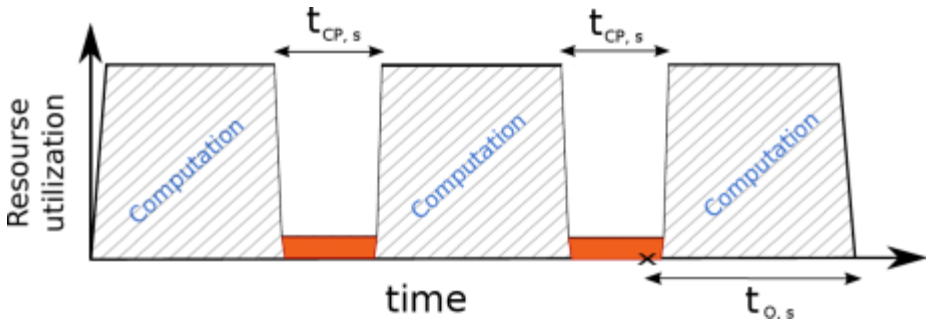
Checkpoint/Restart optimizations

1. Application level checkpointing
   - Minimal checkpoint data
2. **Asynchronous checkpointing**
3. **Multi-level checkpointing (PFS/remote node/localFS)**
4. Checkpoint compression
5. …

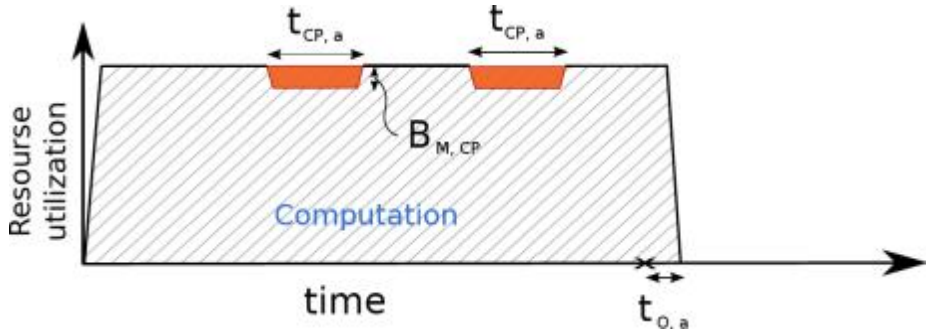
Hide / avoid costs of computational costs of checkpoints

Synchronous vs. asynchronous checkpointing

- Synchronous checkpointing:
  - Computation halts for I/O time
  - High execution time overhead



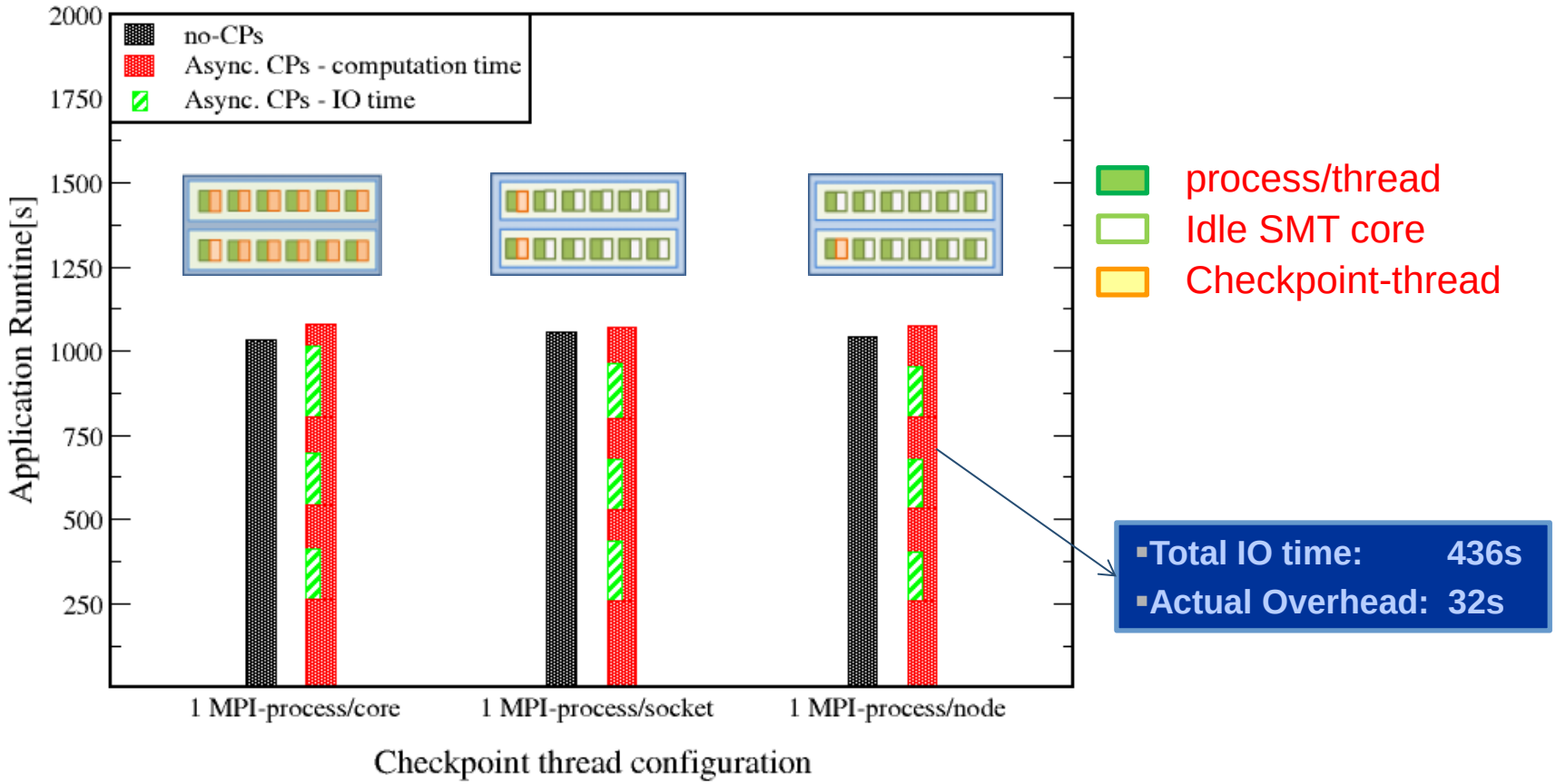
- Asynchronous checkpointing:
  - Dedicated threads for performing asynchronous I/O
  - Low execution time overhead
  - Checkpoint location: flexible (e.g. using SCR)
  - In-memory copy required.



Asynchronous Checkpointing

- Hybrid (MPI-OpenMP) configuration performance comparison

Cluster: LiMa, num. of nodes = 32, PFS = LXFS, Aggregated CP size = 200 GB/CP



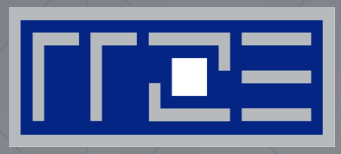
Asynchronous checkpoints – Remote node

- Memory mapped – local filesystem

- Checkpoint data by
  - Exchanging MPI messages
    - Portable
    - May interfere with regular communication
      → Low priority checkpoint message scheduling?
  - **`rsync /remotenode/localFS`**
    - Generality? → efficient via IB?
    - May use (slow) alternative data path (e.g. GBit – if available)

  - Failed node detection?!
  - Restart MPI within same batch job and ignore FT in communication layer?!

APPLICATION DRIVEN AUTOMATIC FAULT TOLERANCE (AFT)



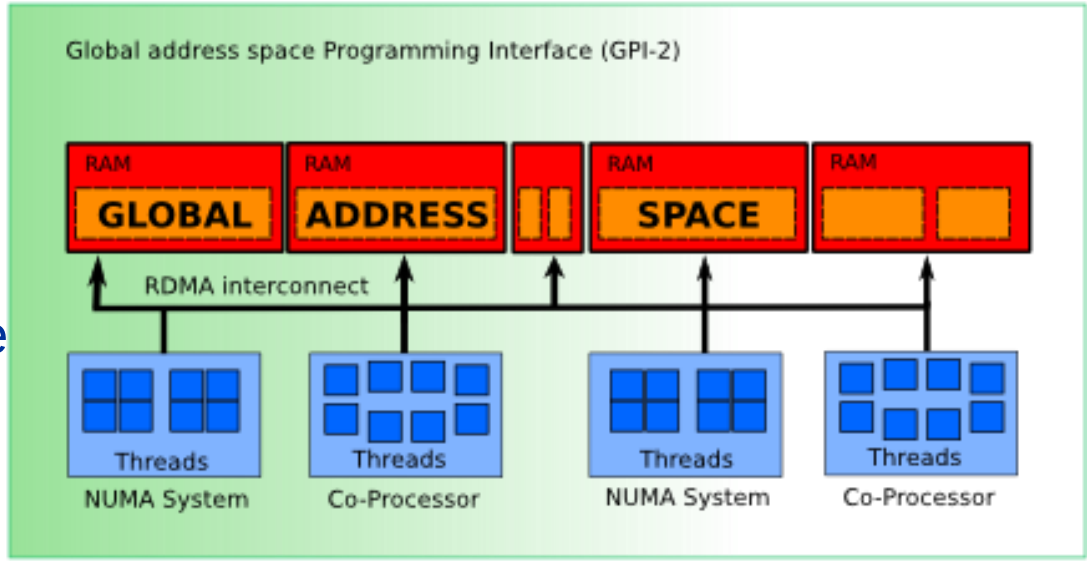
Our (naïve) approach:

- Regular asynchronous Checkpoints (FS or remote node)
- Node failure detected by communication library (Communication library in valid state after node/process loss)
- Spare nodes are available – application replaces lost node
- Application driven restart from last checkpoint

AFT: GPI Introduction

- Current version: **GPI-2** (see http://www.gpi-site.com/gpi2/)
  Developed by Fraunhofer IWTM
- Implements **GASPI** standard: http://www.gaspi.de/software.html
  (Global Address Space Programming Interface)
- PGAS programming model

- Two memory parts
  - Local memory:
    local to each GPI process
  - Global memory: Accessible
    for other processes



- Enables fault tolerance
  - via providing TIMEOUT for every communication call.

AFT: GPI - Application requirements

- **Algorithm based on PGAS model**

- **For effective fault tolerance**
  - No global synchronization, barriers
  - Each GPI-process communicates with certain subset of GPI-processes (e.g. neighbors)
  - In case of failures, rest of the processes detect errors in results and correct them accordingly.

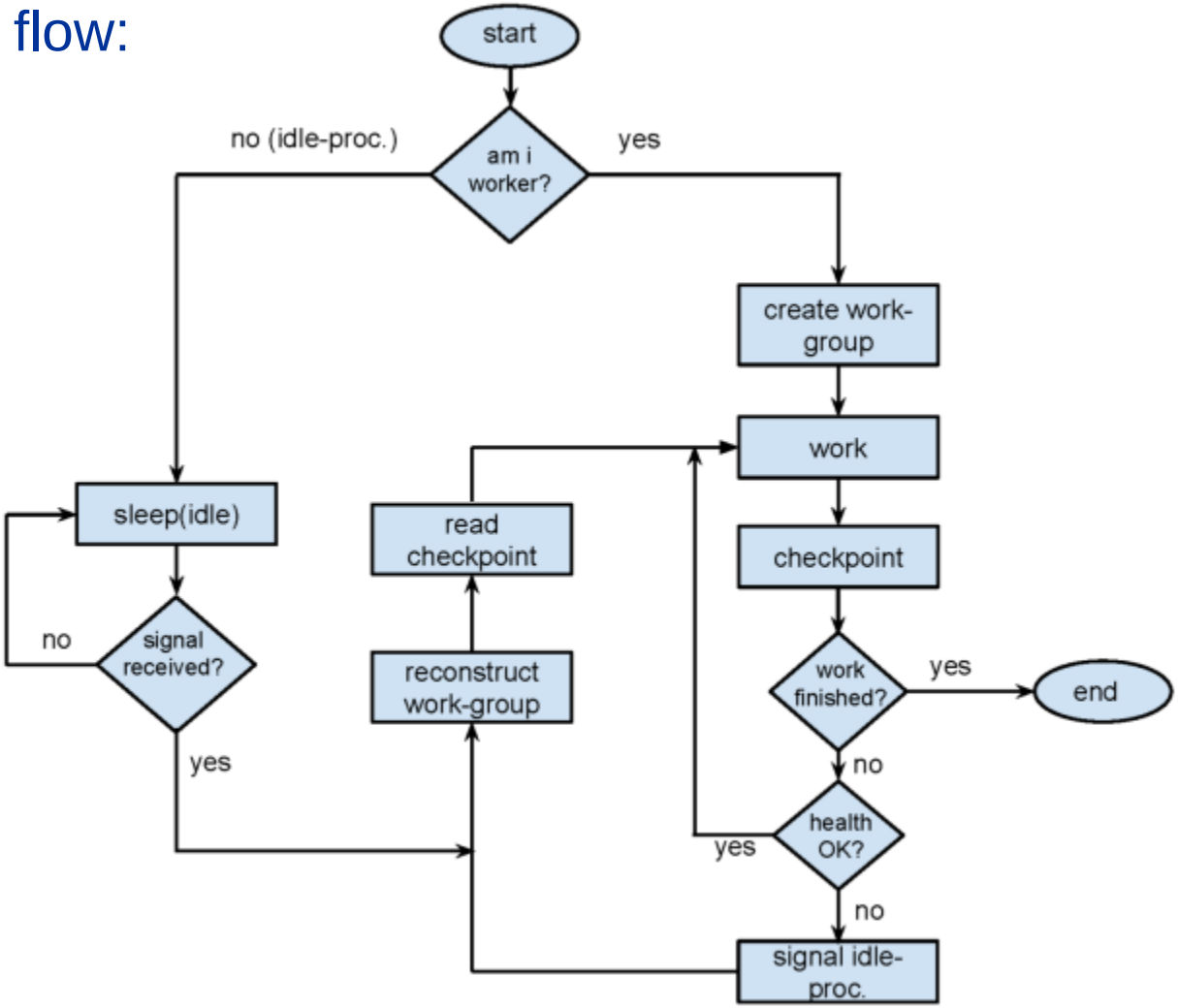
- **Algorithm driven FT based applications**

Prototype FT implementation

- Idea:
  - Running the program with ‚n+m‘ processes, where ‚m‘ is the number of idle processes.
  - Program initially utilizes ‚n‘ processes for work (work-group)
  - In case of a failed process in ‚work-group‘, an idle process is added to the ‚work-group‘.
  - Processes in newly established ‚work-group‘ restart the work from last checkpoint.

Prototype FT implementation: LBM

- Program flow:



Toy FT implementation: Health Check

- What GASPI provides:
  - A process local copy of ‚health check vector‘.
  - After each read/write from a process, the health check vector entry of that particular process is locally updated.
  - The entires of health vector are either 0 or 1.

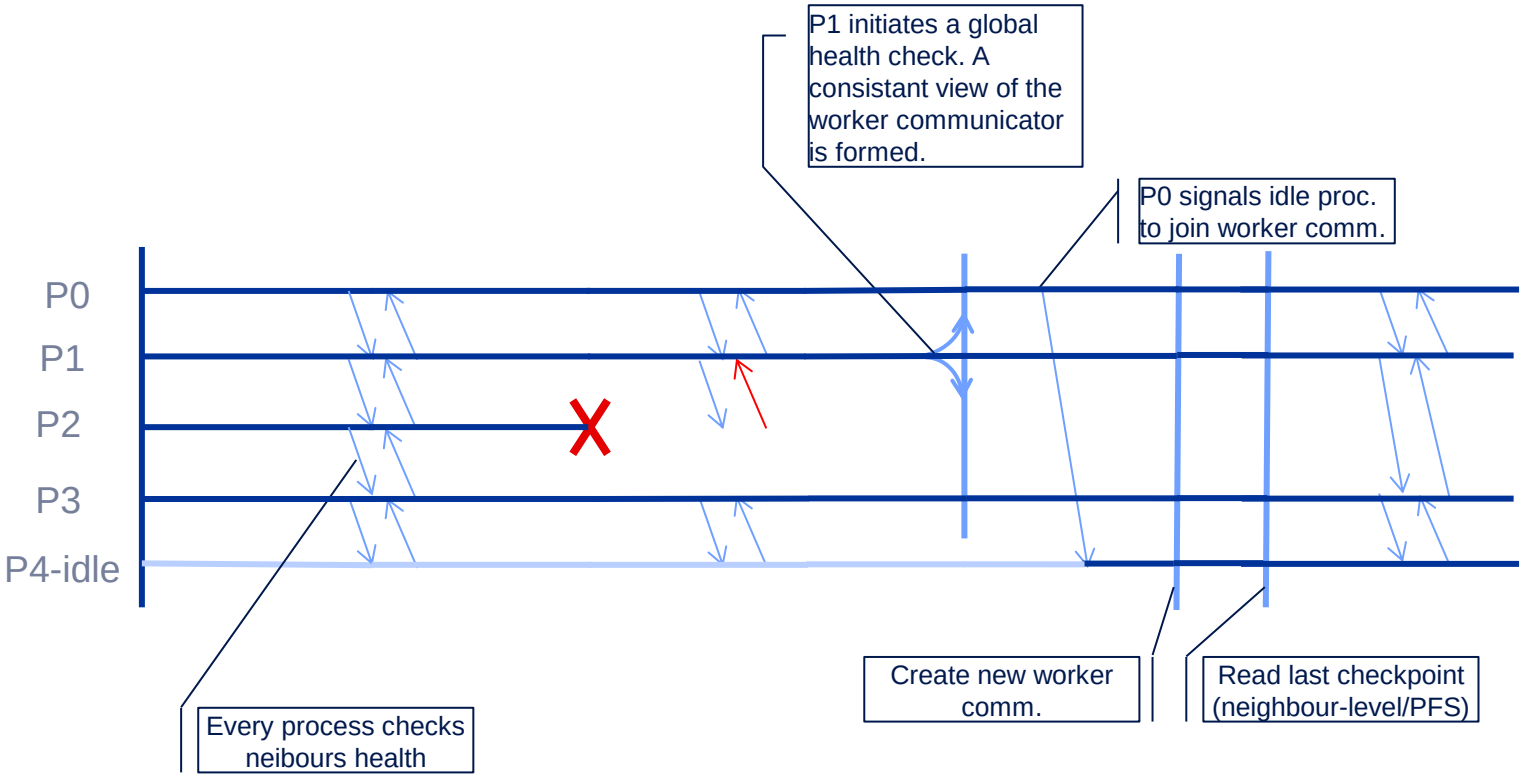
- User side:
  - User can copy this ‚health vector‘ via gaspi_state_vec_get() routine.
  - Deletion of old comm., creation of new comm., new communication structure, (checkpoint/restart) -> user responsibility

Prototype FT implementation: LBM

- Health check routine

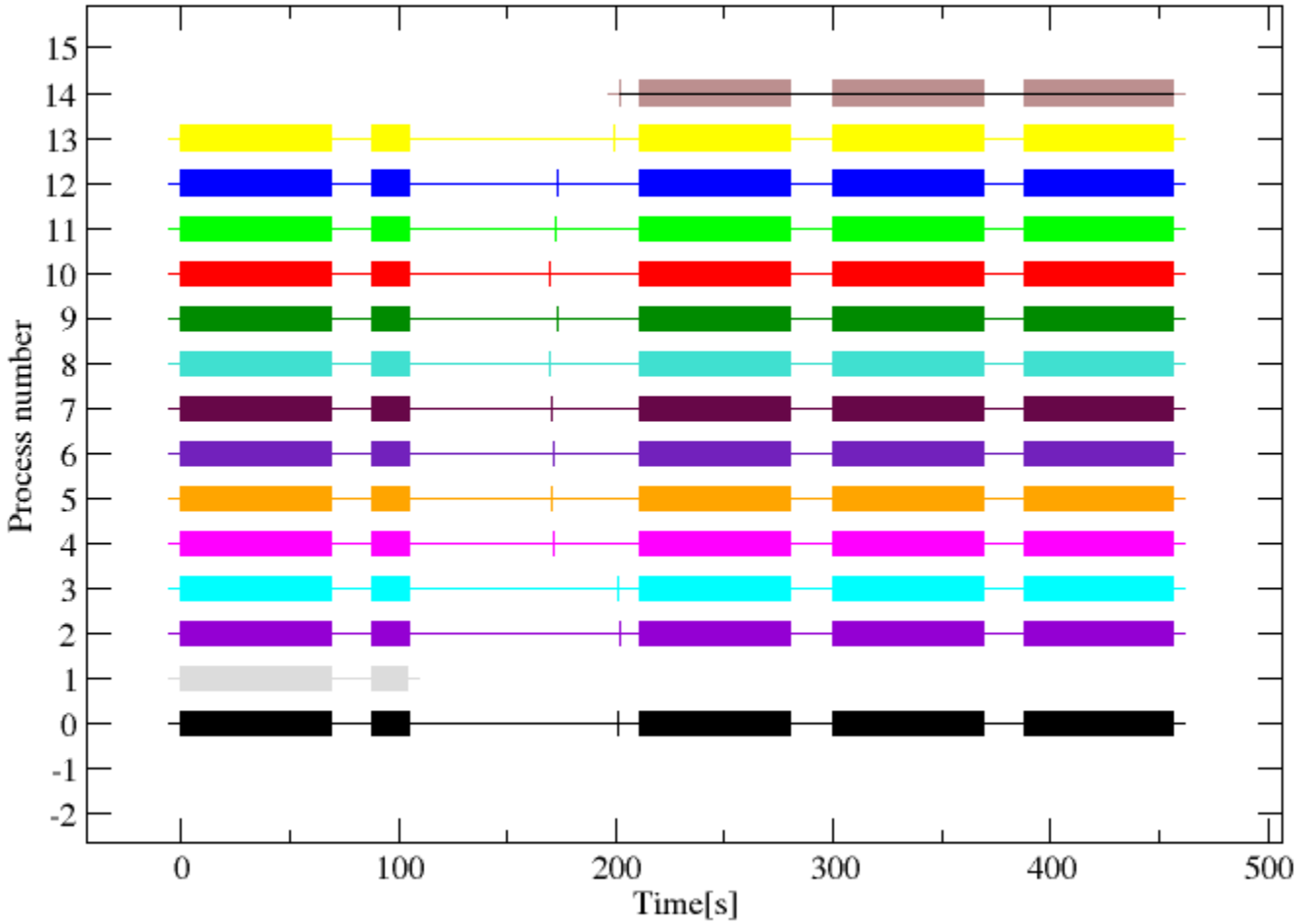
```
void send_msg_to_check_state(gaspi_state_vector_t health_vec, gaspi_rank_t *avoid_list){
    for(int i=0; i<numprocs; ++i){
        if(avoid_list[i]!=1)
        {
            ASSERT(gaspi_write(0, 0, i, 0, 0, sizeof(int), 0, GASPI_BLOCK));
        }
    }
    gaspi_return_t retval;
    retval = gaspi_wait(0, GASPI_BLOCK);
    ASSERT(gaspi_state_vec_get(health_vec));

    for(int i=0; i<numprocs; ++i){
        if(health_vec[i]==1){
            avoid_list[i]=1;
        }
    }
    if(myrank==0)    print_health_vec(health_vec);
}
```

Toy FT implementation: local health check



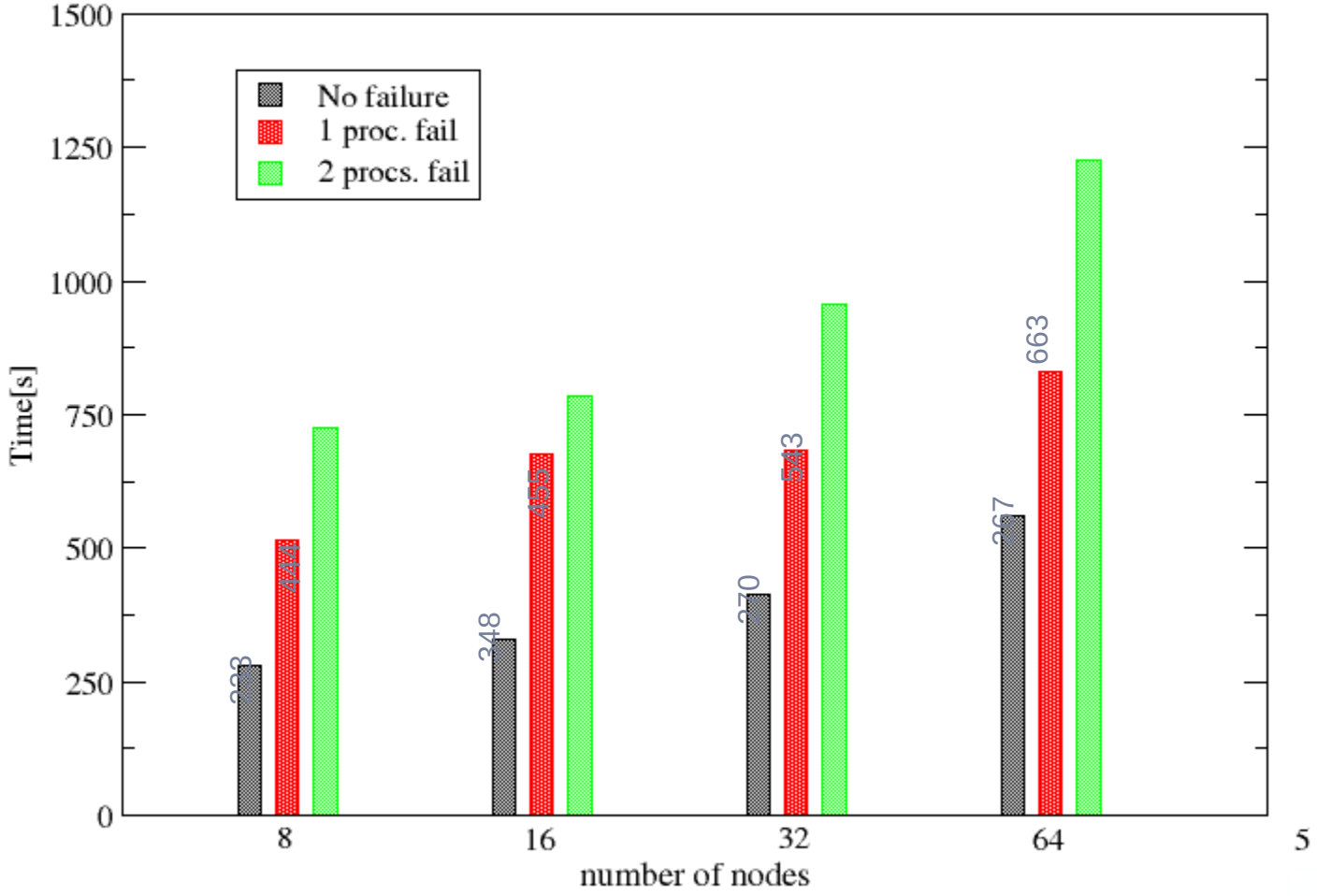
Toy FT implementation: LBM Benchmarks (I)

- Global health check, 16 nodes 1 failure



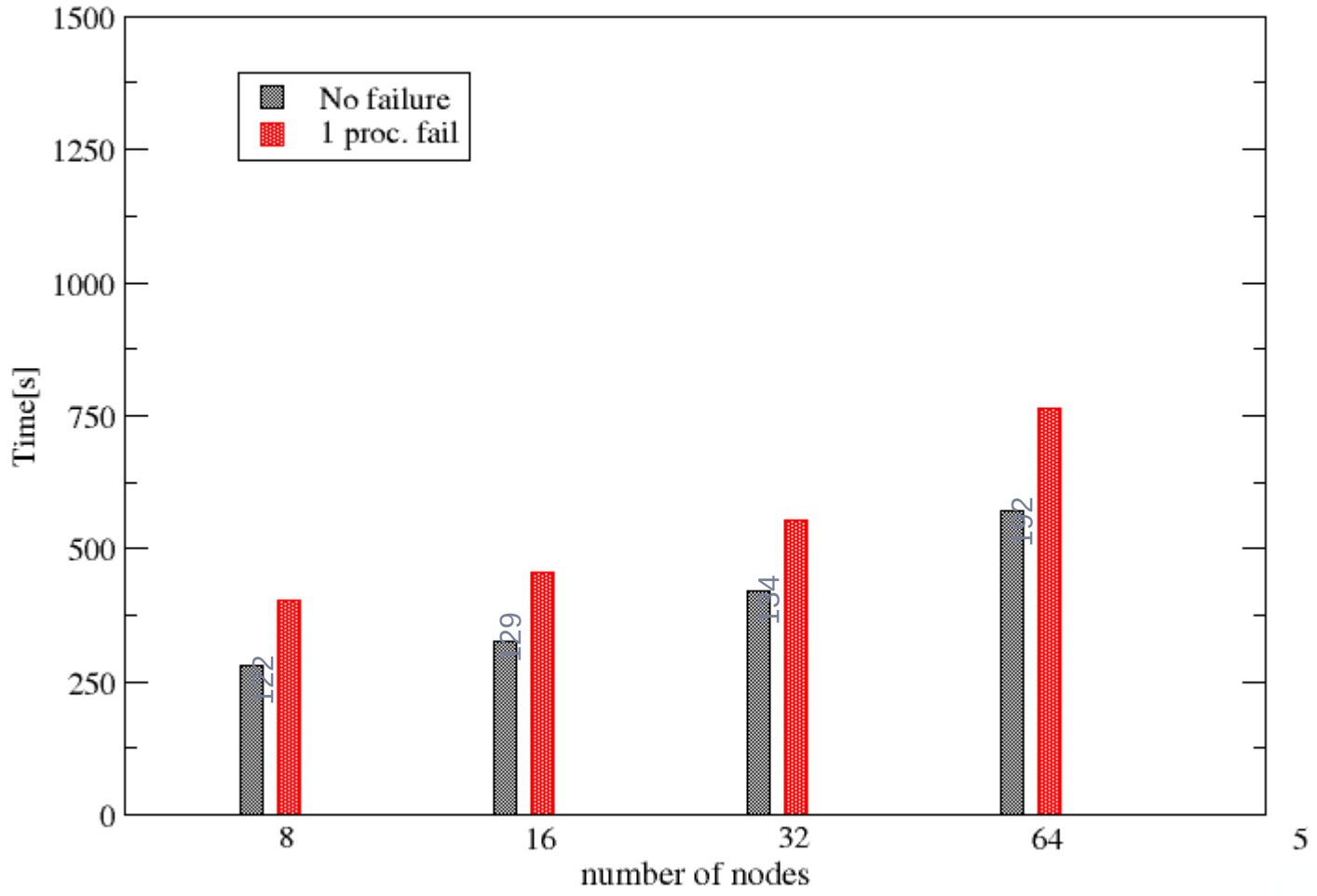
Toy FT implementation: LBM Benchmarks (II)

- Recovery time scaling, LOCAL Health check



Toy FT implementation: LBM Benchmarks (III)

- Recovery time scaling, GLOBAL Health check



GPI fault recovery overhead:

- Timeout returns for communication after failure
  - Only the communication to/from the failed process contibutes to this overhead.
- Global health vector update to have consistant view of the health vector across all processes
- Rebuilding worker communicator
  - Process 0 signals the idle processes, which then joins the creation of new comm.
- Checkpoint fetching from neighbour (or PFS) and reinitializing

Prototype FT implementation: SPMVM

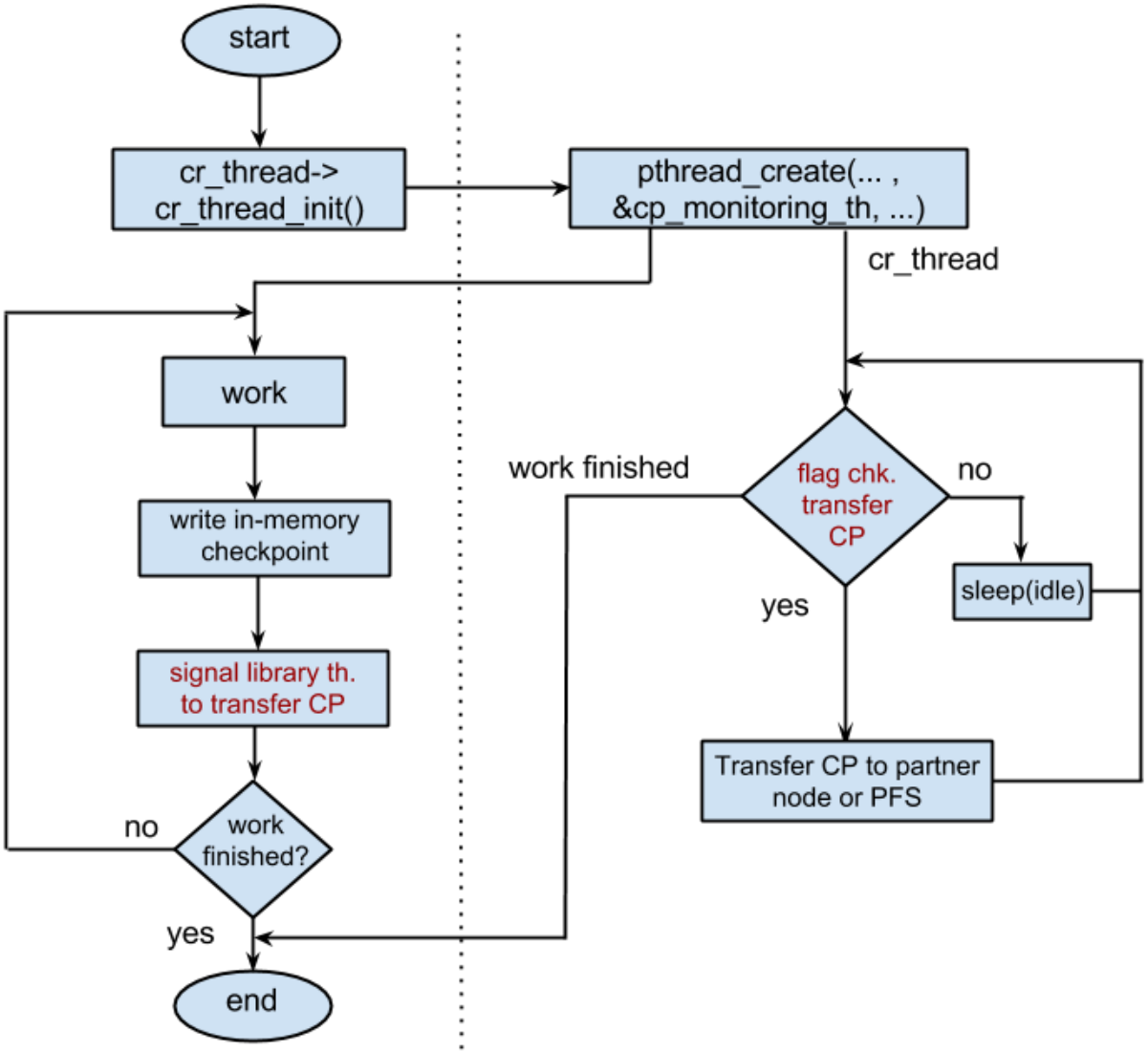
- Each process has point-to-point communication with many other processes.
- This communication pattern of a matrix is checkpointed at the start once.
- Restart:
  - ‚Recovery-process' reads the matrix data & communication pattern of the dead-process.
  - Remaining processes redirect all communication from dead-process to recovery-process.

Neighbor level checkpointing for GPI (I)

- Development of Multi-level checkpointing infrastructure.
  - Based on library calls
  - Library thread responsible for transfering data in-between nodes and PFS.
  - Independent of communication library (MPI/GPI)

- Multi-level checkpointing with various layers of the application.
  - Different checkpoint frequency on various layers.

Neighbor level checkpointing for GPI (II)



Testing:

- Tested successfully up to 1000+ cores with 1-2 failures.
- Challenges using higher number of cores:
  - Seg. fault during deletion of old comm/ recreat new comm.
  - Issue using barrier for new comm.
  - Both issues are under investigation by Frauenhofer IWTM.

  → Bug in GPI library has been detected and will be fixed in next release.
- Future optimizations:
  - Reduction in health check time.

Concluding remarks:

Asynchronicity: User controlled node-level resource management still lacks simple and efficient support from OS.

FT: If you use checkpointing

- do it asynchronously (dedicated threads) – keep data in memory? – reduce interference with regular communication?
- use application specific knowledge
- restarting at runtime is a challenge with current communication libraries → You feel like a test pilot
- GPI is on a reasonable way – MPI-ULFM?

FT: Exascale “modus operandi” still unclear:

- Pool of spare nodes?
- Continue wit remaining set

GHOST will become public available this year

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If you are interested in testing, you are very welcome

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ask us: https://blogs.fau.de/essex/

SPPEXA

Thank you!

Questions?

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