A Scalable and Extensible Checkpointing Scheme for Massively Parallel Simulations

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Abstract

Realistic simulations in engineering or in the materials sciences can consume enormous computing resources and thus require the use of massively parallel supercomputers. The probability of a failure increases both with the runtime and with the number of system components. For future exascale systems it is therefore considered critical that strategies are developed to make software resilient against failures. In this article, we present a scalable, distributed, diskless, and resilient checkpointing scheme that can create and recover snapshots of a partitioned simulation domain. We demonstrate the efficiency and scalability of the checkpoint strategy for simulations with up to 40 billion computational cells executing on more than 400 billion floating point values. A checkpoint creation is shown to require only a few seconds and the new checkpointing scheme scales almost perfectly up to more than 30 000 (215) processes. To recover from a diskless checkpoint during runtime, we realize the recovery algorithms using ULFM MPI. The checkpointing mechanism is fully integrated in a state-of-the-art high-performance multi-physics simulation framework. We demonstrate the efficiency and robustness of the method with a realistic phase-field simulation originating in the material sciences.

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1 Introduction

Modern simulation software must scale to massively parallel computing clusters to provide sufficient memory and computational power. Many algorithms that are used to model the respective physical processes take the form of explicit stencil codes that can be executed in parallel. Since processor clock rates have ceased to improve, only additional parallelism can be used to deliver more computational power. With the increasing number of concurrently working processing units, the probability of a failure in the system in a certain time period rises as well. This problem is observed in studies of real world systems (Schroeder and Gibson, 2006; Taerat et al., 2008; Zheng et al., 2011; Martino et al., 2014), examined in theory (Herault and Robert, 2015) and discussed as a grand challenge in the upcoming exascale era of supercomputing (Dongarra et al., 2011; Cappello et al., 2014).

There are different categories of errors that may affect a running system including hardware and software faults or network issues. The error types can additionally be divided into hard errors like hardware outages that cause the affected system or application to crash and soft errors like bitflips that can be introduced by cosmic radiation and may not be noticed by the system but cause wrong results. In the following, we discuss only hard errors with a focus on process faults.

Since modern simulation software applications may run for several hours or even days, as e.g. in (Hötzer et al., 2015; Hötzer et al., 2016; Steinmetz et al., 2016; Bartuschat et al., 2016; Bartuschat and Rüde, 2015), they are likely exposed to outages. Hence, applications that are not prepared to handle these errors might fail or lead to wrong simulation results.

There are different approaches to develop resilient applications. Two major categories are checkpoint-restart and algorithm-based techniques. Checkpoint-restart methods are based on creating regular snapshots of the simulation data that can be recovered after a failure. The simulation then continues from the recovered backup. Consequently, this approach is suited for schemes that yield a sequence of well-defined states. Hence, it especially fits explicit time stepping schemes like the phase-field method proposed in (Hötzer et al., 2015) or the Lattice Boltzmann method (LBM) (Krüger et al., 2016). Algorithm-based resilience techniques are based on application dependent algorithms to recompute the data that may have been lost due to a failure.

In this work, we propose a scalable checkpoint-restart method to prepare long running simulation applications with schemes that yield a sequence of well-defined states for hard faults in parallel systems and exemplarily apply them to a large-scale phase-field simulation application.

1.1 Outline

At best, a resilience technique should at the same time be robust, introduce low overhead in terms of memory and runtime and be flexible and easy to implement into existing frameworks. To fulfill these requirements, we present and
implement a resilient, diskless and distributed checkpointing scheme to regularly create snapshots of the simulation data. A checkpoint-restart mechanism with diskless snapshots requires the application to be able to recover from faults during runtime. Therefore, we use the User Level Failure Mitigation (ULFM) extension to the current MPI standard developed by the MPI Forum that enables applications running with MPI to recover from runtime faults (Bland et al., 2012a,b, 2013). This approach allows us to solely rely on in-memory checkpoints without the need for persistent storage and therefore requires only low overhead to create and restore the snapshots. Using appropriate data structures, we can distribute the snapshots to restrict the memory overhead and to rebalance the workload after process faults to maintain low runtimes.

1.2 Contribution

In this work we show that

(i) our in-memory checkpointing implementation scales almost perfectly to \(2^{15}\) MPI processes and only takes a few seconds to create a snapshot of a simulation domain consisting of roughly 40 billion cells and more than ten times as many floating point values (see figure 5);

(ii) we approximately spend less than 4% of the runtime on checkpoint creation using a theoretically optimal checkpointing frequency on a system with a mean time between failures (MTBF) of one hour (see figure 6);

(iii) the data recovery process scales equally and takes less than a second in all of our test scenarios since it does not involve any communication (see figure 7);

(iv) we are able to continue a phase-field simulation from the last checkpoint after process faults during runtime using a ULFM MPI implementation.

The rest of the paper is structured as follows: Section 2 summarizes some related work regarding faults in HPC systems. In section 3 we will introduce the software design and data structures of our framework. Section 4 covers a proposal for an extension to the current MPI standard that was developed by the MPI Forum and provides the user the means to stabilize the parallel environment after process faults. In section 5 we first describe strategies that can be employed to recover an application after a fault in the underlying system. The section then covers the algorithmic details of the checkpointing and recovery schemes that we implemented in the course of this work. In section 6 we briefly introduce a real-world application based on the phase-field model that is used to demonstrate and benchmark the covered resilience techniques. Finally, in section 7 we present the results of various benchmarks.
2 Faults in Parallel Systems

The increasing complexity and size of modern HPC infrastructure and corresponding software raises questions about the stability of long running applications.

As we are reaching the exascale era of supercomputing, the frequency of faults is expected to rise (Cappello et al., 2014; Dongarra et al., 2011). Once the MTBF is in the order of the runtime of a simulation then it becomes likely that a failure strikes. Restarting such applications until successfully completed may incur high cost.

The reliability of actual HPC systems has been studied in e.g. (Schroeder and Gibson, 2006; Taerat et al., 2008; Zheng et al., 2011; Martino et al., 2014). In (Schroeder and Gibson, 2006), the data from 22 different HPC systems at the Los Alamos National Laboratory over the course of nine years from 1996 – 2005 is collected. The authors conclude that failure rates in HPC systems seem to be roughly proportional to the number of processors in the systems and rather not depend on the type of the employed hardware. This is still an interesting outcome, although the system sizes are hardly comparable to state-of-the-art clusters. To better understand the link between system outages and job interruptions, (Zheng et al., 2011) examines the reliability, availability and serviceability logs as well as the jobs logs that have been collected over 273 days from a 40-rack Blue Gene/P system with about 163,000 cores in total on more than 40,000 nodes. The authors observe that jobs with a larger size, i.e. a larger number of processes tended to be more affected by system failures than jobs that have smaller size but longer execution times.

In (Herault and Robert, 2015) a theoretical model is presented to show that the failure rate of a parallel system is proportional to the number $N$ of employed nodes. Defining $\mu$ as the MTBF of the system and $\mu_{\text{ind}}$ as the MTBF of an individual node, the authors show that

$$\mu = \frac{\mu_{\text{ind}}}{N}$$

(1)

assuming that $\mu_{\text{ind}}$ is equal on all nodes.

Although the results of the studies are hardly comparable in a quantitative fashion, they show a similar trend and therefore support our assumption: the number of components that is employed when running parallel applications is linked to the MTBF.

3 Exascale Simulation Software Design

While the strategies we present in this work are generically applicable, the actual implementation benefits from a framework that provides sufficient flexibility, extensibility, and appropriate data structures. Likewise, we show that our approach to resilience is suited to be implemented in large, complex and scalable simulation frameworks. In particular, we demonstrate that it can be used
and is fully operational in current computing practice. To demonstrate this, we will implement our fault tolerance techniques in the simulation framework WALBERLA (Götz et al., 2008; Donath et al., 2009; Feichtinger et al., 2009; Godenschwager et al., 2013; Bartuschat and Rüde, 2015; Schornbaum and Rüde, 2016; Bauer et al., 2016).

WALBERLA (widely applicable Lattice Boltzmann from Erlangen) is a parallel HPC software framework for multi-physics simulations mainly targeting applications based on the LBM. It provides efficient data structures, communication schemes, load balancing and implements performance critical optimizations like SIMD vectorization and intra-node multithreading.

Besides its support for the LBM to perform fluid simulations and the integrated *pe physics engine* (Götz et al., 2008; Iglberger and Rüde, 2009; Preclík and Rüde, 2015) which can be used to study particle-laden flows, WALBERLA’s modularity also allows to implement general stencil algorithms on structured grids.

It is written in C++ and can be employed on all kinds of machines and operating systems as it supports the major compilers and scales from desktops up to large HPC clusters. It uses OpenMP for shared memory parallelization and MPI for distributed memory communication, while both can be combined in a hybrid approach to run multiple OpenMP threads per MPI process.

### 3.1 Domain Partitioning

WALBERLA partitions the simulation domain into blocks that may carry arbitrary data including classes that are provided by the framework to fit the needs for certain applications like the LBM, C++ standard library data structures or data structures defined by the user.

Each block is assigned to one process. However, a process may own more than one block. Each process is only responsible to execute the simulation on the blocks assigned to it. Consequently, mechanisms like load balancing are realized by distributing the workload in terms of whole blocks.

The structure that holds all the blocks is completely distributed. Thus, every process only carries the data of its assigned blocks and only knows of the blocks that are in their direct neighborhood. No information about the global domain partitioning are stored. This has two implications: the memory allocated on a certain process only depends on the number of blocks on that process and the data is not stored redundantly in any way, i.e. if block data is lost on one process, it cannot be restored by others. This way WALBERLA is able to scale perfectly with system size, as the memory requirement of each process is independent of the number of processes that run the simulation.

WALBERLA can perform simulations on nonuniform grids (Schornbaum and Rüde, 2016). It provides mechanisms to refine the domain during the setup phase or adaptively during runtime (Schornbaum and Rüde, 2017). Each block can be refined into eight equally sized blocks in parts of the domain that require a higher resolution while a 2:1 balance of the refinement levels of neighboring blocks has to be maintained. It is possible to trigger the refinement during the
simulation, for example if it is not known beforehand where the domain will require higher resolution. It is possible to register callbacks that define rules, determining when a block has to be refined for example to keep the simulation stable. As areas with higher resolution require more computational power, this flexible nonuniform partitioning also has the advantage that less computational power is wasted because only parts of the domain that really require finer grids are refined.

Additionally, WALBERLA enables the user to perform runtime load balancing. Different load balancing algorithms can be applied via callback functions. To efficiently handle the data redistribution, the implementation uses a lightweight proxy block data structure without simulation data during the load balancing process. As soon as the load is sufficiently balanced, the actual simulation data is migrated.

### 3.2 Communication

Parallelization and communication in WALBERLA are realized by OpenMP for shared memory within a node and MPI for distributed memory between nodes. It is also possible to run WALBERLA applications using a hybrid OpenMP / MPI approach. In this case, the library spawns OpenMP threads on every MPI process when needed. In order to hide the actual communication interface from the user, an extra communication layer is introduced, that wraps calls to MPI. This layer allows for optimizations - for example if block data were exchanged between two blocks that reside on the same process. In this case MPI functions do not have to be called since memcopy can be used instead. In WALBERLA, data is communicated by packing and unpacking it to and from buffers, which are sent and received via MPI respectively. With hybrid OpenMP / MPI, the data can be packed and unpacked in parallel via multiple OpenMP threads. This allows for example to create and send packages for every face, edge and corner of a block in different threads.

### 4 Resilience in MPI

The communication system that is employed by a parallel application plays an important role regarding faults in the underlying environment. It is likely that processes become aware of faults in a parallel system through failing communication. Since MPI is one of the most common communication systems in parallel applications and is also used in WALBERLA for distributed memory communication it is the focus of this section.

The current MPI specification (version 3.1) does not include mechanisms to deal with failures that are caused by the underlying system (MPI Forum, 2015). It is rather the implementation that shall be responsible for such failures and resolve them without letting the user notice them at all. Yet, some failures like for example process faults might not be resolvable by the implementation and will therefore result in an error raised by the affected MPI routine.
## ULFM Error Codes and Routines

| Error Code | Explanation |
|------------|-------------|
| MPI_ERR_PROC_FAILED | Returned when an MPI function cannot operate failure-free due to process failure. |
| MPI_ERR_PROC_FAILED_PENDING | Returned when a non-blocking receive function that accepts messages from MPI_ANY_SOURCE was posted and no send message has matched, while there are potential sending processes that are known to have failed. |
| MPI_ERR_REVOKED | Returned if a communication routine is used on a revoked communicator. |
| MPI_Comm_revoke( comm ) | Marks a communicator as revoked. If a communicator is revoked, all MPI functions that attempt to use it will immediately return the error code MPI_ERR_REVOKED without performing any communication. Also, all currently running communication routines on the communicator will exit with this error code. |
| MPI_Comm_shrink( comm, newcomm ) | Creates a new communicator that discards all failed processes. In general, ranks are assigned to different processes on the new communicator. |

Table 1: Summary of some of the new MPI error codes and routines introduced by the ULFM extension.

The practice of insulating the user from the error handling process is more or less rescinded by an extension to the MPI specification called User Level Failure Mitigation (ULFM) that was recently proposed by the MPI Forum (Bland et al., 2012a,b, 2013). It targets the recovery from failures like processor faults that result in unresponsive processes.

ULFM offers a lot of flexibility as it does not define a particular recovery mechanism but rather provides the user with routines to bring the MPI environment into a stable state. That means that the user may employ any recovery strategy using the repaired MPI infrastructure including checkpoint-rollback or algorithm-based recovery techniques. The user is also able to reach different levels of recovery. Possibly not all workers in a master-worker environment have to be aware of other workers being hit by a fault. In this case, comparably expensive collective failure reporting routines can be avoided while they might be essential in other, homogeneous applications where all processes might for example take part in collective communication.

Table 1 shows a summary of the subset of new MPI routines introduced by ULFM that is relevant for our implementation. The recovery pipeline we implement can be divided into three steps:
(i) As soon as a process failure is signaled by an MPI routine the communicator is revoked via `MPI_Comm_revoke()`. A failure is either signaled

- directly (via `MPI_ERR_PROC_FAILED` or `MPI_ERR_PROC_FAILED_PENDING`), if a process tries to communicate with a failed process or
- indirectly (via `MPI_ERR_REVOKED`), if a process does not directly communicate with a failed process, but another process does, and revokes the communicator.

This step is necessary since we need to inform all processes that a fault has happened.

(ii) The communicator is shrunk via `MPI_Comm_shrink()` in order to discard all failed processes from the old communicator. The new communicator is no longer revoked.

(iii) An application-level recovery mechanism is started. In our case, the last checkpoint is recovered.

Although the extension is a proposal and not yet part of the actual standard, an implementation of a subset of the proposed concepts already exists in form of a fork of the OpenMPI implementation. This allows for testing and preliminary integration into production software like waLBerla.

5 A Scalable Checkpoint-Recovery Scheme

In this section we will introduce the checkpoint-rollback recovery strategy as implemented in waLBerla. We will discuss the general approaches, advantages and disadvantages of checkpoint-rollback recovery and also briefly introduce algorithm-based recovery techniques as an alternative to the chosen approach. Then in the second part of this section we will describe the details of our implementation.

5.1 Recovery Strategies

If a fault in a parallel system affects a component that is simultaneously used by an application it might lead to lost data, errors or crashes during the program’s runtime. Especially for long running simulations a restart can be very costly. However, regarding massively parallel software it is likely that only a fraction of the used components is actually affected by the failure. Thus, respective applications might recover by dismissing or replacing the erroneous components and recovering potentially lost data from backup or by recomputing.

In this subsection, we aim to present some of the techniques and algorithms that can be used to restore lost data and to continue the execution despite failures in the system. First of all, we will examine checkpoint-rollback recovery. Finally, we will give a brief overview of algorithm-based recovery techniques.
5.1.1 Checkpoint-Rollback.

The most widely used and most straightforward techniques to recover from process failures regarding HPC applications are based on restorable checkpoints of an application state (Herault and Robert, 2015; Elnozahy et al., 2002; Young, 1974; Daly, 2006; Chandy, 1975; Treaster, 2005). When a failure happens, the application rolls back to the last valid checkpoint and recomputes the data that was lost due to the failure and the rollback. The major advantages of this technique are its simplicity and that it can be used as a general-purpose method as it is not tailored to a specific algorithm. The latter point is a benefit of the checkpoint-rollback technique introduced in this work. This way, fault tolerance is not limited to certain algorithms, but available for all applications that use the framework’s data structures. In our case this includes LBM algorithms as well as the phase-field method that will be employed as an example application later in this work.

The idea of checkpoint-rollback recovery can be realized in many different ways depending on the underlying application. Some (parallel) applications might require a coordinated checkpointing algorithm, meaning that the processes must create a snapshot of the application’s state at the same time in order to assure a certain consistency between all processes. For other applications, an uncoordinated scheme, where all processes create checkpoints but not necessarily at the same time might be sufficient. The latter technique has the advantage that the processes do not have to spend time to coordinate the checkpoint and that potentially shared I/O resources are not simultaneously used by all of them. As a tradeoff, hierarchical strategies might be employed like for instance checkpointing in groups of processes.

As orthogonal criteria, the data to be stored, the type of storage and the level of redundancy may differ. Some strategies might consider dumping the entire application memory (system-level checkpoints) while others only store particular data structures chosen at application level (application-level checkpoints), which might save resources in terms of storage space and checkpointing duration. On the other hand, a system-level checkpointing mechanism might decrease the complexity of the application itself as external tools can be used more easily.

While it might be beneficial to store the snapshot to disk in order to restart the whole application at a later point in time or to inspect the data offline, time can be saved by only backing up the data in the main memory of different processes, provided the system can tolerate failures without halting the application. For some techniques, tradeoffs between redundancy of the data can be made by storing parts of it on only some processes. This also poses a tradeoff between resource savings and resilience of the system as only some processes carry a certain part of the domain and a fault will result in ultimate loss of data if all processes of that group fail.

The checkpointing scheme that we implement in the course of this paper can be seen as a coordinated application-level scheme with in-memory checkpoints. As the cell updates in stencil based algorithms depend on the cells’ neighbors, the checkpoints must be created at the same time during the simulation (coor-
dinates). Only this way we can ensure that the simulation stays stable after a rollback. To keep the memory footprint low, only data structures, that cannot be recreated automatically from other snapshot data are stored during a checkpoint. The implementation allows for flexible redundancy schemes by offering the user the option to register callback functions with custom rules defining the number of snapshot copies and the processes they shall be stored on. Section 5.2 contains more details on the implementation of the checkpointing scheme.

5.1.2 Algorithm-Based Fault Tolerance.

One alternative to checkpoint-rollback recovery are so called algorithm-based fault tolerance (ABFT) techniques. They are not based on checkpoints of the domain but aim to recover lost data using application specific algorithms. This has the advantage that in general little to no time is spent during failure-free periods and therefore the computation time without faults does not increase significantly. However, as ABFT depends on the application, the recovery algorithms must be designed carefully and are in general not usable on other applications. In many cases, no ABFT algorithms are known.

A successful example of ABFT in numerical linear algebra is the recovery of matrix entries via checksums. By storing additional vectors that contain the checksums of a matrix’ rows and columns, lost or corrupt entries can often be reconstructed (Huang and Abraham, 1984; Bosilca et al., 2009; Yao et al., 2011).

Another successful ABFT approach to recover data loss in parallel multigrid algorithms is presented in (Huber et al., 2016). The idea is introduced for the Laplace equation

\[-\Delta u = 0 \text{ in } \Omega \subset \mathbb{R}^3, \quad u = g \text{ on } \partial\Omega.\]

but extends to more general problems where geometric multigrid can be used. Just as the checkpoint-rollback algorithm of this article it only assumes that the domain is partitioned in blocks, whose data may be lost when a process fails. However, different from a checkpointing algorithm that reloads redundantly stored data, the ABFT technique is based on a fast recomputation of lost data. This is especially attractive when the state information of a complex solution process is partly lost. The specific technique relies on the ghost layer data being stored redundantly so that the lost data can be recomputed by a local multigrid algorithm when the missing data is reinitialized and the ghost layer data is used as Dirichlet boundary conditions for the recovery computation. In (Huber et al., 2016) this class of recovery algorithms is analyzed and improved by using the so-called superman strategy. Here the local recovery is accelerated by realizing excess parallelization. If additionally, an asynchronous control is employed, where the healthy processors are not halted during recovery, but let continue the iteration, then the recovery does not lead to any slowdown as compared to the unperturbed fault-free computation.

We now return to the phase-field simulations as described in (Bauer et al., 2015; Hötzer et al., 2016b) and that are based on an explicit time stepping. Here the various fields can be recovered from partial checkpoint data or possibly...
algorithm-based by exploiting physical correlations. Depending on the field and the available checkpoint data, the fields can be recovered without information loss, otherwise the state of the fields is calculated in an approximated way using e.g. analytic equations. For example in the phase-field model used here, one of the concentration fields can be recovered without loss of information if the other concentration fields are available by exploiting mass conservation. In the case that the concentration fields are not available, the field state can be calculated using the phase-fields and the Gibbs energies in an approximate fashion. Similarly, the phase-fields can be recovered from partial checkpoint data. Also the temperature fields can be recovered in an approximate fashion if the checkpoint does not exist by using analytic profiles.

5.2 Implementation

We implement a diskless and coordinated application-level checkpointing strategy to achieve a flexible, robust and scalable solution regarding faults in the underlying system. The method builds on the ability to tolerate faults during runtime. We reach this by using the prototype ULFM MPI implementation that was introduced in section 4. In this section, we will present the architecture and algorithms of our specific approach.

5.2.1 Checkpoints.

Diskless Checkpointing. The chosen strategy employs in-memory checkpoints. This means that the data is backed up by distributing it to the main memory of the processes. Obviously, in-memory checkpoints lead to data loss as soon as a process or node that carries the respective memory faults or the application terminates. Therefore, it is crucial that a respective implementation is capable of recovering from a fault during runtime. If the whole application terminated, no backup would be left to be restored. However, one could for instance additionally implement checkpointing to disk at a lower frequency to protect the simulation against failures that strike the whole system.

The main advantage of in-memory checkpoints is that they are not limited to possibly slow I/O of disk storage and are not affected by other nodes in the cluster using the same device to write and read data at the same time. This way it is possible to maintain relatively low overhead.

Custom Data Structures. The checkpointing frequency and execution is maintained by a callback, which is automatically invoked with a parametrized period between two iterations. During the setup, this checkpointing callback accepts callbacks for every entity that needs to be backed up. Obvious entities that need to be backed up and therefore need to be registered are the blocks of the domain, including their simulation data as well as metadata like information about neighboring blocks. Others are for instance timers that need to be reset to the timestamp of the last valid checkpoint.
All entities that shall be restorable after a fault, must provide three callback functions: one that creates a snapshot, one that restores the snapshot after a fault and one that swaps the snapshot buffers. The latter one will be explained later in this section. In this way, each entity is responsible for the snapshot creation of its own data. This has three advantages: there is no need for a class or function that can snapshot arbitrary data, the snapshots are highly customizable for every entity and their data stays decoupled from the checkpointing mechanism. On the other hand, this means that the three callback functions need to be implemented individually for different entities.

**Redundancy.** As stated in previous sections, the domain partitioning that is implemented in waLBerla results in fully distributed data structures that evidently lie in main memory. Opposed to disk storage, main memory is in general erased as soon as the respective process or node faults. In order to securely store the data, we therefore need to employ a certain level of redundancy. When one process fails, its data must be backed up somewhere else. As we want to use in-memory snapshots, that means the data must be available on another process that is still alive. Otherwise the backup is entirely lost and the application cannot recover from the failure. However, for large scale simulations it is in general not possible to store the backup in an all-to-all fashion, meaning that every process stores a backup of the data of all other processes. A lower level of redundancy must be implemented - only some copies of the backups from one process are made and stored in the memory of some other processes. This unfortunately leads to a certain tradeoff regarding resilience of the system: it cannot always be guaranteed that there is a backup available in the part of the system that survived a fault. In other words, if all processes that carry the backup of a failed process fail as well, that data is lost. Indeed, with the growing number of nodes in modern parallel systems, the probability for data loss shrinks, if the data is well distributed. The risk can for instance be minimized by storing backups on different nodes that are rather unlikely to fail at the same time.

To decouple the distribution scheme from the actual checkpointing and recovery routines and to offer the user the flexibility to implement custom distribution algorithms, the respective functions that determine the distribution rules can be registered as callbacks. The user needs to choose a scheme that determines the ranks that the current process shall send its copies to and the ranks it will receive copies from. An example for a distribution callback that stores one copy of the backup at the ‘opposing’ rank (shifted by $N_{proc}/2$) can be seen in algorithm 1. Since nodes typically carry consecutive MPI ranks, this method guards against single-node failures.

To improve the performance, each process carries one copy of its own checkpoint. This way, less data has to be exchanged during the checkpointing step and no data has to be exchanged during the recovery process (without load balancing) as can be seen in figure 1.
Figure 1: Illustration of a pair-wise checkpointing strategy. At time step $t_1$ each process creates a snapshot of its part of the domain and exchanges a snapshot with its partner process. The processes now carry a distributed checkpoint of the whole domain. After the fault, the living processes restore the checkpoint from $t_1$. This is possible without inter-process communication since each process stored a snapshot of its own domain. $P_0$ is now responsible for the data that was processed by $P_1$ before the fault.

**Resilient Checkpointing.** When the checkpointing callback functor is invoked to create a snapshot, it calls all registered callbacks responsible for the checkpoint creation of the respective entities like blocks and timers. This way, one after another, all instances that have been attached via a respective callback create snapshots of their data.

In order to make sure that the snapshots of all data structures are consistent on all processes, the mechanism must be robust to faults during the checkpointing process. If for instance a snapshot of the domain has been successfully created while the snapshot of a timer that is used to influence time dependent properties of the simulation was not, the simulation might not behave as expected when the application rolls back to that data.

To solve this problem, we implement a double-buffer model for the snapshot creation and recovery. Two snapshot buffers instead of one are maintained by each entity that requires data exchange between processes to create a redundant backup of its data (no exchange is needed for instance if the entity’s data is equal on all processes in the same iteration). One of those buffers serves as a read-only container, carrying the snapshot that shall be restored upon a fault. This buffer must not be touched during the snapshot creation. The other one is writable and shall be used when a new checkpoint is created. After a snapshot has been created in the writable buffer, all processes perform a handshake to check if any process faults occurred before or during the checkpoint creation. If there was a fault, the read-only buffer still carries a valid snapshot from the last checkpoint.
Algorithm 1 Program flow of a pair-wise snapshot distribution. The function determines the rank the current process shall send its data to and the rank it receives its data from, so that the respective send and receive schedules can be invoked.

Function PairwiseSnapshotDistribution

determine the number of processes $N_{\text{proc}}$
determine the rank of the current process
if $N_{\text{proc}} > 1$ then
    shift = $N_{\text{proc}}$/2
    sendTo = (rank + shift) mod $N_{\text{proc}}$
    if shift > rank then
        recvFrom = $N_{\text{proc}}$ − (shift − rank)
    else
        recvFrom = rank − shift
    end
end
return (sendTo, recvFrom)
end

which is then recovered. If there were no faults and all processes succeeded creating the checkpoint, the buffers can be swapped to update the read-only buffer with the new checkpoint. Here, the already mentioned callback function that shall swap these buffers comes into play: its purpose is to swap the buffers (preferably by swapping the pointers accessing them to avoid copying data) so that the former read-only buffer becomes the writable one that will be used the next time a snapshot is created and the writable buffer becomes read-only. Since there is no communication involved, the buffer swapping procedure cannot be affected or interrupted by faults in the system. The full resilient checkpointing algorithm is shown in algorithm 2.

5.2.2 Fault Propagation and Recovery.

With a working checkpointing implementation in place, we will now cover what happens when a fault actually strikes. The recovery can be divided into two steps: the stabilization of the MPI environment and the recovery of the lost data.

In the course of this paper, we extended WALBERLA by mechanisms to recover from faults using the ULFM extension of the MPI standard that has been discussed in section 4. This means, failures are detected by the MPI library and signaled to WALBERLA via errors that are raised by MPI routines. After a failure happens, a process will notice it as soon as it tries to communicate with a dead process via an MPI function.

Although almost all MPI communication routines are wrapped by respective WALBERLA library functions, MPI routines could still be called directly from an application. Therefore, if errors were checked via return codes, some of them might bypass the WALBERLA library. Also, it is very cumbersome to handle return codes throughout a large code base or application. Fortunately, the MPI standard provides the routine MPI_Comm_set_errhandler() to register a callback function to a communicator that is called when an MPI function on
Algorithm 2 Program flow of the resilient checkpointing procedure using the double-buffer model.

Function CreateResilientCheckpoint

| forall registered entities do |
| create checkpoint in writable buffer |
| end |

// The following handshake has two purposes: // - it assures that all processes // finished checkpointing // - it is used to inform all processes // of potential faults in the system. call Handshake

if process(es) failed then
    // Since no buffers have been swapped yet, // the read-only buffer still carries // the previous snapshot. call RecoverLastCheckpoint
else
    // A fault cannot prevent the buffers // from being swapped since no // communication is necessary here. forall registered entities do |
    | swap checkpoint buffers |
end
end

that communicator raises an error. This way it is possible to handle MPI errors in one place.

After a fault has happened, we must first revoke the affected communicators to inform all processes of the fault and secondly we need to shrink them to stabilize the MPI environment. A straightforward approach would be to simply call `MPI_Comm_revoke()` and `MPI_Comm_shrink()` and restore the snapshots in the registered callback function and return from the callback in order to continue the application. However, this has a severe drawback: as it is not predictable when, respectively where in the code a fault strikes, different processes might resume the application at different places and with different states which most likely results in chaotic behavior.

Therefore, we use a different approach that ensures a deterministic recovery process. Instead of triggering the recovery mechanism directly, the callback only throws an exception. This exception is then caught in the main program loop as shown in algorithm 3.

There are two main steps to be performed in the catch block. First, the parallel environment must be brought back into a consistent state. We achieve this by calling the respective ULFM MPI routines (`MPI_Comm_revoke()` and `MPI_Comm_shrink()`). During this process, information about the fault can be collected. In our case, this includes information of the rank reassignment that may happen during `MPI_Comm_shrink()`. Both, the information on the fault as well as the method that was used to distribute the checkpoint data are used to determine how the checkpoint shall be restored. An algorithm that calculates
Algorithm 3  Recovery mechanism via exception handling in the main program loop. The checkpoint recovery also adapts the current iteration step.

Function RecoveryMechanism

\[
\text{while current step} < \text{number of steps do}
\]

\[
\begin{align*}
\text{try} \\
\text{single step} \\
\text{catch ProcessFaultException} \\
\text{stabilize parallel environment} \\
\text{recover last checkpoint}
\end{align*}
\]

\[
\text{end}
\]

\[
\text{end}
\]

the correct rank assignment for the recovery is shown in algorithm 4.

Then all snapshots can be restored. This typically also involves setting the current iteration step to the value it had when the snapshot was created. That way, the main program loop can be continued from the restored checkpoint.

5.2.3 Memory Usage.

The described approach increases the memory consumption of the respective application. It is affected by two factors. Depending on the redundancy scheme, additional copies of the simulation data need to be stored in main memory. For the pair-wise checkpointing scheme as discussed above, assuming that each process carries the same amount of data (i.e. the domains of all processes are of equal size), the memory consumption triples: each process needs to store the actively used domain, a snapshot of its own and one of its partner’s domain. If the resilient checkpointing algorithm using the double-buffer model is implemented, each snapshot creates a footprint of twice its size. In this case, the memory usage of the pair-wise checkpointing scheme increases by a factor of five. In general, the per process memory usage of the scheme calculates as

\[
\text{Mem} = S(1 + 2R)
\]

where \( S \) is the memory consumption of the local domain (assuming it is equal on all processes) and \( R \) the number of copies (\( R = 2 \) for the pair-wise scheme). Therefore it rises linearly with the redundancy.

In typical long-running LBM or phase-field applications the memory capacity of each node is not fully exhausted. In this sense the applications are run close to the strong scaling limit. Using a scalable framework like WALBERLA, this does not pose a problem as more computing resources can be easily added without decreasing the parallel performance. Therefore the memory increase of the checkpointing method is not an issue for the targeted applications.

5.2.4 Load Balancing.

After the recovery, the workload of a failed process is shifted to the surviving process that restored the respective snapshot of the dead process’ data. Thus,
Algorithm 4 Program flow of a pair-wise snapshot recovery distribution. Every backed up block on a process also contains its origin in form of a rank. If this rank is passed to the shown function, the function returns the rank, the data shall be restored on. The result is equal on all processes. Therefore a process can plug in the origins of its backed up blocks and compare the result to its own rank. If it is equal, that process needs to restore the respective block and add it to its own.

// \(N_{\text{proc}} - 1\): number of processes before the fault
// \(R_{t-1}\): a rank of a process that existed before the fault
// \(P(R_{t-1})\): the process with rank \(R_{t-1}\) before the fault
// \(R_{\text{reassignment}}()\): a function that returns a process’ new rank,
// given its rank before the fault

Function PairwiseSnapshotRecovery\((R_{t-1}, R_{\text{reassignment}})\)

// Ranks on surviving processes do not necessarily equal the ranks before faults. Therefore, the process that was identified via rank \(R_{t-1}\) before the fault could either
// - still carry rank \(R_{t-1}\) \((R_t = R_{t-1})\)
// - carry a different rank \((R_t \neq R_{t-1})\)
// - or not exist anymore.
if \(P(R_{t-1})\) has not survived then
  // We need to find the rank \(R_{t-1}^{\text{backup}}\) that received the checkpoint data from \(R_{t-1}\).
  // For the pairwise checkpointing scheme as shown in algorithm 1
  // this works as follows:
  shift = \(N_{\text{proc}} - 1\)/2
  \(R_{\text{backup}}^{t-1} = (R_{t-1} + \text{shift}) \mod N_{\text{proc}}\)
  if \(P(R_{\text{backup}}^{t-1})\) has not survived then
    // Checkpoint not restorable as only one copy was made.
    call Abort
  else
    // Determine the new rank \(R_t^{\text{backup}}\) of \(P(R_{\text{backup}}^{t-1})\).
    \(R_t^{\text{backup}} = R_{\text{reassignment}}(R_{\text{backup}}^{t-1})\)
    return \(R_t^{\text{backup}}\)
  end
else
  // Determine the new rank \(R_t\) of \(P(R_{t-1})\).
  \(R_t = R_{\text{reassignment}}(R_{t-1})\)
  return \(R_t\)
end

we can expect a load imbalance right after the recovery process. This may severely increase the runtime of the application or lead to processes running out of memory. Especially if multiple faults occur, we need to introduce an additional load balancing step. Efficient and scalable load balancing techniques are already presented in (Schornbaum and Rüde, 2017) and implemented in the WALBERLA framework.

Still, even with a load balancing algorithm in place, the presented checkpointing technique naturally results in an increased average work load for the surviving processes. This load increase could be circumvented by respawning the dead processes and reintegrating them into the system. MPI offers rou-
tines including `MPI_Comm_spawn()` that can be used for this purpose. There are different approaches that might be employed. Especially for applications that rely on a constant number of worker processes, spare processes could be injected when the application is started. Their purpose is to stay idle first and replace dead processes after failures in the system. This way, the application can withstand a defined number of failures with a constant number of processes. It would also be possible to restart the dead processes and reintegrate them into the parallel application during runtime. The latter approach could also be used apart from a failure scenario to add available resources from a cluster system to a long running simulation as soon as they are available or release some processes if the cluster requires them for other applications.

5.2.5 Checkpointing Frequency.

An essential parameter that needs to be adapted regardless of the chosen scheme is the frequency of the checkpoints. In (Young, 1974; Daly, 2006; Herault and Robert, 2015) the authors derived different but similar approximations to the optimal checkpointing frequency $f_{opt}$.

A first-order approximation to the optimal checkpointing interval $T_{fo}$, i.e. the time between two checkpoints is derived in (Herault and Robert, 2015). The goal is to minimize the time that is spent checkpointing as well as the time that it takes to recompute values after a rollback to the last valid checkpoint. The resulting first-order approximation is given by

$$\frac{1}{f_{opt}} = T_{fo} \approx \sqrt{2\mu C}$$

where $\mu$ is the MTBF of the underlying system and $C$ the time it takes to create a valid checkpoint of the domain. The model fits applications that perform a co-ordinated checkpointing scheme. It is important to note that this approximation is only valid if the MTBF $\mu$ is large compared to the time spent checkpointing ($C$).

The approximation has to be used carefully as it gives only a rough estimate for a theoretical system and relies on some assumptions including a constant MTBF $\mu$ and checkpointing duration $C$ during the life time of an application. Also, it might be hard to estimate $\mu$ for a specific target system. In this sense the estimate (3) may only serve as an orientation to experiment with different checkpointing intervals.

6 Phase-Field Method as an application to Real-World computational materials design

To demonstrate the practicability of the proposed strategies, we employ them to a phase-field simulation as discussed in detail in (Hötzer et al., 2015). In this section we briefly summarize the phase-field method.
The properties of materials are related to their microstructure. For the development of tailored materials, it is of high interest to understand the fundamental mechanisms controlling the microstructure evolution. To investigate the mechanisms under the influence of different physical effects, the phase-field method has been established as powerful tool (Hötzer et al., 2016a).

During the directional solidification of ternary eutectic alloys, various patterns consisting of three solid phases $\alpha$, $\beta$ and $\gamma$ evolve from the melt $\ell$ (Dennstedt and Ratke, 2012). Due to the wide range of forming patterns in the microstructure, ternary eutectic alloys are interesting for technical products and scientific investigations (Hötzer et al., 2016a; W. Kurz, 1975). The setup for the simulation of directional solidification is schematically depicted in figure 2. By applying a moving temperature field with a constant gradient, the solidification direction and velocity are controlled.

To investigate the directional solidification of ternary eutectic alloys, the phase-field model based on the Grand potential approach from (Choudhury and Nestler, 2012) is used. The evolution equations for the $N = 4$ phase-fields $\partial \phi_\alpha / \partial t$, for the $K = 3$ chemical potentials $\partial \mu / \partial t$ and for the analytic moved temperature gradient $\partial T / \partial t$ are given as:

$$\tau \epsilon \frac{\partial \phi_\alpha}{\partial t} = -\epsilon T \left( \frac{\partial a(\phi, \nabla \phi)}{\partial \phi_\alpha} - \nabla \cdot \frac{\partial a(\phi, \nabla \phi)}{\partial \nabla \phi_\alpha} \right)$$

Figure 2: Setting to simulate the ternary eutectic directional solidification based on (Hötzer, 2017). Thereby, the melt $\ell$, consisting of three components, solidifies in the three phases $\alpha, \beta$ and $\gamma$. In dashed blue the moving window technique with the block-structured grid is highlighted. Below, in red the moving analytic temperature gradient is shown.
\[
\frac{T}{\epsilon} \frac{\partial \omega(\phi)}{\partial \phi_\alpha} - \frac{\partial \psi(\phi, \mu, T)}{\partial \phi_\alpha} - \frac{1}{N} \sum_{\beta=1}^{N} (r_\beta + \Gamma_\beta),
\]
\(\quad := \Gamma_\alpha\)
\[
\frac{\partial \mu}{\partial t} = \left[ \sum_{\alpha=1}^{N} h_\alpha(\phi) \left( \frac{\partial c_\alpha(\mu, T)}{\partial \mu} \right) \right]^{-1}
\[
\left( \nabla \cdot \left( M(\phi, \mu, T) \nabla \mu - J_{st}(\phi, \mu, T) \right) \right)
\[
- \sum_{\alpha=1}^{N} c_\alpha(\mu, T) \frac{\partial h_\alpha(\phi)}{\partial t}
\[
- \sum_{\alpha=1}^{N} h_\alpha(\phi) \left( \frac{\partial c_\alpha(\mu, T)}{\partial T} \right) \frac{\partial T}{\partial t},
\]
\[
\frac{\partial T}{\partial t} = \frac{\partial}{\partial t} \left( T_0 + G(z - vt) \right) = -Gv.
\]

The evolution equation for the chemical potentials (5) alone results in 1 384 floating point operations per cell and 680 Bytes that need to be transferred from main memory (Bauer et al., 2015). Further details of the phase-field model are presented in (Hötzer et al., 2015; Choudhury and Nestler, 2012). The discretizations in space with a finite difference scheme and in time with an explicit Euler scheme are specified in (Hötzer et al., 2016). To efficiently solve the evolution equations on current HPC systems, the model is optimized and parallelized as proposed in (Bauer et al., 2015). Besides explicit vectorization and parallelization with MPI, a moving window approach is implemented on top of the block structured grid data structures of waLBerla as depicted in figure 2. This allows to reduce the total simulation domain to just a region around the solidification front. Typical simulations in representative volume elements may require between 10 000 to 20 000 compute cores for multiple hours (Hötzer et al., 2015). A typical phase-field simulation of the directional solidification of the ternary eutectic system Al-Ag-Cu is shown in figure 3. The 12 000 \times 12 000 \times 65 142 voxel cell domain is calculated on the SuperMUC system with 19 200 cores within approximately 19 hours.

Based on this highly parallel and optimized solver, the eutectic solidification of idealized systems and real ternary alloys like Al-Ag-Cu were investigated in large scale domains and the experimentally assumed growth of spirals could be demonstrated (Hötzer et al., 2016b, 2015).

7 Benchmarks

In this section, we present benchmarks to illustrate the performance of our checkpointing implementation. First, we introduce the application parameters. Then we discuss different aspects of the checkpointing scheme, explain and present the respective performance results.
7.1 The test cases

To benchmark the checkpointing scheme of section 5.2, we simulate the directional solidification of a ternary eutectic system using the implementation presented in (Bauer et al., 2015) of the phase-field model introduced in section 6. For the simulation parameters, the values of (Hötzer et al., 2016b) to study spiral growth are used. To resolve spiral growth, large domain sizes and millions of time steps are required, resulting in massively parallel and long-running simulations. Since we expect such large-scale simulations to be subject to hardware failures in future setups, the scenario is suited to demonstrate resilience techniques. However, as noted in section 5.1, the checkpointing algorithm is not
bound to a specific algorithm and can therefore also be applied to other applications using different data structures. In this sense, the block data items that are exchanged among the processes are black-boxes to the implementation. They solely need to implement respective serialization and deserialization routines.

The moving window depicted in figure 2 is realized by adding information about the current absolute coordinates of the domain to the block data. By simply adding this data to the checkpoint, there is no additional work involved but implementing the serialization and deserialization routines for the cell coordinates.

The domain is set to a fixed size in the z-direction while different sizes are employed in the x- and y-directions. This is achieved either by varying numbers of cells per block or by varying the number of blocks in the respective directions. The model requires 12 floating point values per cell.

The tests are performed on the clusters listed in table 2.

### 7.2 System Size and Scaling

Resilience in parallel systems gets more crucial with large numbers of processes as already discussed in section 2. As a consequence, it is important that the implemented technique scales well to massively parallel systems. In fact, this is what we can expect from the proposed scheme: the amount of data to be

| Processor Type                    | LSS cluster (LSS at FAU Erlangen) | Emmy cluster (RRZE at FAU Erlangen) | SuperMUC Phase I, Thin Nodes (Leibniz Supercomputing Centre Garching) |
|-----------------------------------|-----------------------------------|-------------------------------------|-------------------------------------------------|
| Processor (cores)                  | Xeon E7-4830 (8)                  | Xeon 2660v2 (10)                     | Xeon E5-2680 (8)                                 |
| Base frequency (GHz)               | 2.13 GHz                          | 2.20 GHz                            | 2.70 GHz                                        |
| Compute nodes                      | 8                                 | 560                                 | 18 (islands) × 512 (nodes)                       |
| Processors per node                | 4                                 | 2                                   | 2                                               |
| Memory per node (GB)               | 256 GB                            | 64 GB                               | 32 GB                                           |
| Interconnect technology            | InfiniBand QDR                    | InfiniBand QDR                      | InfiniBand                                      |
| MPI                               | OpenMPI 1.7 (ULFM Fork)           | Intel MPI 5.1                       | IBM MPI 1.4                                     |

Table 2: Test systems that are used during the benchmarks. The LSS cluster is mainly used to test the runtime fault tolerance of the implementation by installing ULFM. On the SuperMUC system, the intra-island topology is based on a non-blocking tree while the inter-island topology is only based on a 4:1 pruned tree. Therefore the connection quality is expected to decrease when moving from one to multiple islands.
exchanged between processes during a checkpoint depends on the redundancy and not on the overall number of processes. If we choose the number of copies that are backed up to be constant, the strategy scales, i.e. the duration of the checkpointing step stays constant and independent of the number of processes. However, in practice it also depends on the network topology as we can see in our benchmark results.

To demonstrate the scalability of the checkpointing scheme, we set up a weak scaling experiment (Padua, 2011) by fixing the number of blocks per process while increasing the size of the domain and therefore the number of processes. As discussed, in this scenario, we expect the time it takes to create a snapshot to be independent of the number of overall processes in the system. We perform the weak scaling with a different number of cells per block in multiple benchmarks. The domain size is kept constant in the $z$-direction. As the number of blocks is not always an integer multiple of the number of processes, we also plot the average number of blocks per process. In our setups, it varies roughly between 5 and 6 blocks per process.

We perform the experiment on different machines. The results from the Emmy cluster, where we use up to 64 nodes with up to 1280 MPI processes in total can be found in figure 4.

On the SuperMUC system, we performed the benchmark on up to 2048 nodes, with 32768 MPI processes for the largest scenario. The results can be found in figure 5.

Both benchmarks show, that the algorithm scales almost perfectly, i.e. independently of the number of employed processes. The time increases only
slightly with the increasing number of processes. In the SuperMUC scaling we can see a sudden increase in the checkpointing duration. This is expected since the simulation spans to multiple islands from that point on. As in our setup the pair-wise checkpointing strategy locates the backups of a process pair on two different islands, the slower data exchange increases the duration of the checkpoint creation. This can be avoided by altering the distribution strategy or by pinning the MPI ranks in a proper order to force that no backups are sent to a different island. On the other hand, having the backup pairs on different islands guards against failure of an entire island. With increasing number of islands (two islands for $2^{14}$ processes, four islands for $2^{15}$ processes) the checkpointing duration stays stable.

### 7.3 Overhead

Although, in theory, the checkpointing duration scales perfectly this does not necessarily mean its time consumption is negligible. Recall the approximation to the theoretical optimal checkpointing frequency $f_{\text{opt}}$ from (3).

In fact, the overall time that should be spent on checkpointing according to the approximated optimal checkpointing frequency depends indirectly on the number of processes in the system as this number is related to the MTBF. This relation was shown in (1).

As the MTBF of a parallel system $\mu$ is expected to decrease if its size increases, the optimal checkpointing frequency $f_{\text{opt}}$ will increase. Thus, although the checkpointing duration itself would stay constant, the frequency and therefore the overhead would grow with larger systems if the optimal checkpointing frequency was employed.
Not only the frequency, but also the size of the data packages influences the checkpointing duration. This means, larger per-process workloads are also expected to increase the time spent checkpointing. However, an increased absolute checkpointing duration also increases the optimal checkpointing period.

To get an estimate for the overhead that would be introduced if the checkpointing frequency was set to the theoretical optimal value that was shown in (3), we plug the measured durations from the scaling on the SuperMUC system into the respective formula. We then compute the overhead by dividing the respective checkpointing duration $C$ by the approximation to the optimal checkpointing interval $T_{opt} = 1/f_{opt}$:

$$\text{OVERHEAD} = \frac{C}{T_{opt}} = \frac{C}{\sqrt{2\mu C}}. \quad (7)$$

In figure 6 we plot the function for different hypothetical MTBFs $\mu$ and using measured values for the checkpointing duration $C$.

![Graph of the overhead due to checkpointing using an approximation to the optimal checkpointing frequency. The overhead function depends on the MTBF of the system $\mu$ and the checkpointing duration $C$. (a) and (b) mark the checkpointing time for the SuperMUC scenario of figure 5 for $2^{13}$ and $2^{15}$ processes respectively.](image)

Looking up the measured checkpointing time for two scenarios from the SuperMUC benchmark, we can see that using the approximated optimal checkpointing frequency, the time spent checkpointing lies below 3% for MTBFs of down to one hour.
7.4 Recovery

Since the block data that needs to be restored during the recovery already resides on the respective processes, the recovery does not involve any inter-process communication (as illustrated in figure 1). The time is only spent on deserialization of the data. As the data resides in main memory, we do not expect the time spent during the recovery process to have a large impact on the runtime. Still, a load balancing step is in general necessary to maintain the performance of the application after a failure.

To measure the time it takes to recover the block data, we simulate a failure by erasing the block data from all processes and forcing them to restore the block data of the partner process from the last checkpoint. This way, each process is then responsible for the block data of another process. No process is actually killed during this procedure.

The benchmark is performed on the Emmy cluster and the results can be seen in figure 7.

![Figure 7: Weak scaling of the recovery duration for different block sizes on the Emmy cluster. The average number of blocks per process slightly varied for different numbers of processes due to the test setup.](image)

As we can see from the benchmark, the results are as expected. The recovery scales almost perfectly since there is no communication involved and it only takes several milliseconds to restore the data. Compared to the runtime of a typical simulation, the time that is spent on recovery can be neglected.

7.5 Fault Tolerance

To test the fault resilience of the application, we install the OpenMPI ULFM implementation on both, desktop machines and the LSS cluster at the Chair
for System Simulation in Erlangen and simulate process faults via kill signals from within the application (using the C library function `raise()` and from the outside (using the `kill` command).

Figure 8 illustrates a test on the LSS cluster where we simulate the directional solidification using the ULFM MPI implementation. In the depicted scenario, each process carries six blocks with $20^3$ cells per block. During the simulation we send kill signals to four MPI processes using the `kill` command. The application then recovers from the process faults during runtime and successfully restores the last snapshot of the simulation data using the pair-wise checkpointing scheme as described in section 5.2. This way the simulation is continued without halting and restarting the application.

![Figure 8](image)

(a) time step 2500  (b) time step 5600  (c) time step 9950

Figure 8: Phase-field simulation of the direction solidification of the ternary eutectic system Al-Ag-Cu in a $160 \times 160 \times 120$ voxel cell domain, run with 64 MPI processes on two nodes of the LSS cluster. During the simulation we send kill signals to four MPI processes. The affected blocks are highlighted in figure 8b. Blocks that reside on the same process are equally colored. After the processes fault, the simulation restores the last checkpoint during runtime and then proceeds.

It should be noted, that the OpenMPI fork that implements ULFM is still experimental (Bland et al., 2013, 2015). Still, the fork serves as a tool to provide a proof of concept implementation - regarding the MPI library itself as well as applications using it.

8 Conclusion

In this work, we show how to extend a simulation framework by resilience features while still maintaining performance and scalability. We propose a distributed and diskless checkpointing algorithm that can be combined with the runtime recovery mechanisms of the ULFM MPI extension to provide a fast and scalable method to implement resilience in modern applications. Using a double-buffer model, we make the checkpointing procedure itself resilient to process failures.

Applying the approach to the simulation of a real material system, we show that it only introduces minor runtime overhead and scales almost perfectly. In the largest benchmark scenario with a domain consisting of about 40 billion cells...
and more than ten times as many floating point values, the checkpoint creation
takes less than 7 seconds using $2^{15}$ MPI processes. Since the recovery phase
does not require inter-process communication, it scales and takes less than a
second in all performed benchmarks. Using an approximation to the optimal
checkpointing frequency, we show that the checkpoint creation only creates an
overhead of less than 4% of the application’s runtime in a theoretical system
with a MTBF of one hour.

In future work, we aim to apply the proposed mechanisms to other engi-
neering problems with different data structures in order to illustrate the direct
transfer. Also, we plan to experiment with different distribution algorithms than
the proposed pair-wise checkpointing scheme. As mentioned in section 5.2.4 it
would be interesting to implement mechanisms allowing the creation of new
processes after faults as soon as the respective resources are available. While
the concepts can be exhibited to further tackle load imbalance, the technique
can also be used apart from a failure scenario.

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References

Bartuschat, D., Fischermeier, E., Gustavsson, K., and Rüde, U. (2016). Two
computational models for simulating the tumbling motion of elongated par-
ticles in fluids. Computers & Fluids, 127:17 – 35.

Bartuschat, D. and Rüde, U. (2015). Parallel multiphysics simulations of
charged particles in microfluidic flows. Journal of Computational Science,
8:1 – 19.

Bauer, M., Hötzer, J., Jainta, M., Steinmetz, P., Berghoff, M., Schornbaum, F.,
Godenschwager, C., Köstler, H., Nestler, B., and Rüde, U. (2015). Massively
parallel phase-field simulations for ternary eutectic directional solidification.
In Proceedings of the International Conference for High Performance Com-
puting, Networking, Storage and Analysis, SC ’15, pages 8:1–8:12, New York,
NY, USA. ACM.

Bauer, M., Schornbaum, F., Godenschwager, C., Markl, M., Anderl, D., Köstler,
H., and Rüde, U. (2016). A Python extension for the massively parallel mul-
tiphysics simulation framework waLBerla. International Journal of Parallel,
Emergent and Distributed Systems, 31(6):529–542.
Bland, W., Bosilca, G., Bouteiller, A., Herault, T., and Dongarra, J. (2012a). A proposal for User-Level Failure Mitigation in the MPI-3 standard. *Department of Electrical Engineering and Computer Science, University of Tennessee*.

Bland, W., Bouteiller, A., Herault, T., Bosilca, G., and Dongarra, J. (2013). Post-failure recovery of MPI communication capability. *The International Journal of High Performance Computing Applications, 27*(3):244–254.

Bland, W., Bouteiller, A., Herault, T., Hursey, J., Bosilca, G., and Dongarra, J. J. (2012b). An Evaluation of User-level Failure Mitigation Support in MPI. In *Proceedings of the 19th European Conference on Recent Advances in the Message Passing Interface*, EuroMPI’12, pages 193–203, Berlin, Heidelberg. Springer-Verlag.

Bland, W., Lu, H., Seo, S., and Balaji, P. (2015). Lessons learned implementing User-Level Failure Mitigation in MPICH. In *2015 15th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing*, pages 1123–1126.

Bosilca, G., Delmas, R., Dongarra, J., and Langou, J. (2009). Algorithm-based fault tolerance applied to high performance computing. *Journal of Parallel and Distributed Computing, 69*(4):410 – 416.

Cappello, F., Geist, A., Gropp, W., Kale, S., Kramer, B., and Snir, M. (2014). Toward exascale resilience: 2014 update. *Supercomputing Frontiers and Innovations, 1*(1).

Chandy, K. M. (1975). A survey of analytic models of rollback and recovery strategies. *Computer, 8*(5):40–47.

Choudhury, A. and Nestler, B. (2012). Grand-potential formulation for multi-component phase transformations combined with thin-interface asymptotics of the double-obstacle potential. *Physical Review E, 85*(2).

Daly, J. T. (2006). A higher order estimate of the optimum checkpoint interval for restart dumps. *Future Generation Computer Systems, 22*(3):303–312.

Dennstedt, A. and Ratke, L. (2012). Microstructures of directionally solidified Al–Ag–Cu ternary eutectics. *Transactions of the Indian Institute of Metals, 65*(6):777–782.

Donath, S., Götz, J., Bergler, S., Feichtinger, C., Iglberger, K., and Rüde, U. (2009). waLBerla: The need for large-scale super computers. In Wagner, S., Steinmetz, M., Bode, A., and Brehm, M., editors, *High Performance Computing in Science and Engineering, Garching/Munich 2007: Transactions of the Third Joint HLRB and KONWIHR Status and Result Workshop, Dec. 3–4, 2007, Leibniz Supercomputing Centre, Garching/Munich, Germany*, pages 459–473. Springer Berlin Heidelberg, Berlin, Heidelberg.
Dongarra, J., Beckman, P., Moore, T., Aerts, P., Aloisio, G., Andre, J.-C., Barkai, D., Berthou, J.-Y., Boku, T., Braunschweig, B., Cappello, F., Chap- 
mman, B., Chi, X., Choudhary, A., Dosanjh, S., Dunning, T., Fiore, S., Geist, 
A., Gropp, B., Harrison, R., Hereld, M., Heroux, M., Hoisie, A., Hotta, K., 
Jin, Z., Ishikawa, Y., Johnson, F., Kale, S., Kenway, R., Keyes, D., Kramer, 
B., Labarta, J., Lichnewsky, A., Lippert, T., Lucas, B., Maccabe, B., Mat-
zuoka, S., Messina, P., Michielse, P., Mohr, B., Mueller, M. S., Nagel, W. E., 
Nakashima, H., Papka, M. E., Reed, D., Sato, M., Seidel, E., Shalf, J., Skin-
ner, D., Snir, M., Sterling, T., Stevens, R., Streitz, F., Sugar, B., Sumi-
moto, S., Tang, W., Taylor, J., Thakur, R., Trefethen, A., Valero, M., Van 
Der Steen, A., Vetter, J., Williams, P., Wisniewski, R., and Yelick, K. (2011). 
The international exascale software project roadmap. *The International Jour-
nal of High Performance Computing Applications*, 25(1):3–60.

Elnozahy, E. N. M., Alvisi, L., Wang, Y.-M., and Johnson, D. B. (2002). A 
survey of rollback-recovery protocols in message-passing systems. *ACM Com-
puting Surveys*, 34(3):375–408.

Feichtinger, C., Götz, J., Donath, S., Iglberger, K., and Rüde, U. (2009). 
WaLBerla: Exploiting massively parallel systems for lattice Boltzmann sim-
ulations. In Trobec, R., Vajteršic, M., and Zinterhof, P., editors, *Parallel 
Computing: Numerics, Applications, and Trends*, pages 241–260. Springer 
London, London.

Godenschwager, C., Schornbaum, F., Bauer, M., Köstler, H., and Rüde, U. 
(2013). A Framework for Hybrid Parallel Flow Simulations with a Trillion 
Cells in Complex Geometries. In *Proceedings of the International Conference 
on High Performance Computing, Networking, Storage and Analysis*, SC ’13, 
pages 35:1–35:12, New York, NY, USA. ACM.

Götz, J., Feichtinger, C., Iglberger, K., Donath, S., and Rüde, U. (2008). Large 
scale simulation of fluid structure interaction using Lattice Boltzmann meth-
ods and the ‘physics engine’. *ANZIAM Journal*, 50(0):166–188.

Herault, T. and Robert, Y. (2015). *Fault-Tolerance Techniques for High-
Performance Computing*. Springer Publishing Company, Incorporated, 1st 
edition.

Hötzer, J., Jainta, M., Bauer, M., Steinmetz, P., Kellner, M., Köstler, H., Rüde, 
U., and Nestler, B. (2016). *High Performance Computing in Science and En-
eering – Garching/Munich 2016*, chapter Study of complex microstructure 
evolution in ternary eutectic alloys with massive parallel large-scale phase-
field simulations. Bayerische Akademie der Wissenschaften.

Huang, K.-H. and Abraham, J. A. (1984). Algorithm-based fault tolerance for 
matrix operations. *IEEE Transactions on Computers*, 33(6):518–528.

Huber, M., Gmeiner, B., Rüde, U., and Wohlmuth, B. I. (2016). Resilience for 
Massively Parallel Multigrid Solvers. *SIAM Journal on Scientific Computing*, 
38(5).
Hötzer, J. (2017). Massiv-parallele und großskalige Phasenfeldsimulationen zur Untersuchung der Mikrostrukturentwicklung.

Hötzer, J., Jainta, M., Steinmetz, P., Nestler, B., Dennstedt, A., Genau, A., Bauer, M., Köstler, H., and Rüde, U. (2015). Large scale phase-field simulations of directional ternary eutectic solidification. *Acta Materialia*, 93(0):194 – 204.

Hötzer, J., Kellner, M., Steinmetz, P., and Nestler, B. (2016a). Applications of the phase-field method for the solidification of microstructures in multicomponent systems. *Journal of the Indian Institute of Science*.

Hötzer, J., Steinmetz, P., Dennstedt, A., A., G., Kellner, M., Irmak, S., and Nestler, B. (2017). Influence of growth velocity variations on the pattern formation during the directional solidification of ternary eutectic Al–Ag–Cu. *Acta Materialia*.

Hötzer, J., Steinmetz, P., Jainta, M., Schulz, S., Kellner, M., Nestler, B., Genau, A., Dennstedt, A., Bauer, M., Köstler, H., and Rüde, U. (2016b). Phase-field simulations of spiral growth during directional ternary eutectic solidification. *Acta Materialia*, 106:249 – 259.

Hötzer, J., Tschukin, O., Said, M., Berghoff, M., Jainta, M., Barthelemy, G., Smorchkov, N., Schneider, D., Selzer, M., and Nestler, B. (2016). Calibration of a multi-phase field model with quantitative angle measurement. *Journal of Materials Science*, 51(4):1788–1797.

Iglberger, K. and Rüde, U. (2009). Massively parallel rigid body dynamics simulations. *Computer Science - Research and Development*, 23(3):159–167.

Krüger, T., Kusumaatmaja, H., Kuzmin, A., Shardt, O., and Silva, G. (2016). *The Lattice Boltzmann Method*. Springer-Verlag GmbH.

Martino, C. D., Kalbarczyk, Z. T., Iyer, R. K., Baccanico, F., Fullop, J., and Kramer, W. (2014). Lessons learned from the analysis of system failures at petascale: The case of Blue Waters. In *44th Annual IEEE/IFIP International Conference on Dependable Systems and Networks, DSN 2014, Atlanta, GA, USA, June 23-26, 2014*, pages 610–621.

MPI Forum (2015). MPI: A Message-Passing Interface Standard. Version 3.1. Technical report, MPI Forum.

Padua, D. (2011). *Encyclopedia of Parallel Computing*. Springer Science & Business Media.

Preclik, T. and Rüde, U. (2015). Ultrascale simulations of non-smooth granular dynamics. *Computational Particle Mechanics*, 2(2):173–196.

Schornbaum, F. and Rüde, U. (2016). Massively Parallel Algorithms for the Lattice Boltzmann Method on NonUniform Grids. *SIAM Journal on Scientific Computing*, 38(2):C96–C126.
Schornbaum, F. and Rüde, U. (2017). Extreme-scale block-structured adaptive mesh refinement. *CoRR*, abs/1704.06829. Submitted to SIAM SISC.

Schroeder, B. and Gibson, G. A. (2006). A large-scale study of failures in high-performance computing systems. In *Proceedings of the International Conference on Dependable Systems and Networks*, DSN ’06, pages 249–258, Washington, DC, USA. IEEE Computer Society.

Steinmetz, P., Yabansu, Y., Hötzer, J., Jainta, M., Nestler, B., and Kalidindi, S. (2016). Analytics for microstructure datasets produced by phase-field simulations. *Acta Materialia*, 103:192–203.

Taerat, N., Naksinehaboon, N., Chandler, C., Elliott, J., Leangsuksun, C. B., Ostrouchov, G., and Scott, S. L. (2008). Using log information to perform statistical analysis on failures encountered by large-scale HPC deployments. In *Proceedings of the 2008 high availability and performance computing workshop*.

Treaster, M. (2005). A survey of fault-tolerance and fault-recovery techniques in parallel systems. *CoRR*, abs/cs/0501002.

W. Kurz, P. R. S. (1975). *Gerichtet erstarrte eutektische Werkstoffe: Herstellung, Eigenschaften und Anwendungen von In-situ-Verbundwerkstoffen*. Springer.

Yao, E., Chen, M., Wang, R., Zhang, W., and Tan, G. (2011). A new and efficient algorithm-based fault tolerance scheme for a million way parallelism. *CoRR*.

Young, J. W. (1974). A first order approximation to the optimum checkpoint interval. *Communications of the ACM*, 17(9):530–531.

Zheng, Z., Yu, L., Tang, W., Lan, Z., Gupta, R., Desai, N., Coghlan, S., and Buettner, D. (2011). Co-analysis of RAS log and job log on Blue Gene/P. In *25th IEEE International Symposium on Parallel and Distributed Processing, IPDPS 2011, Anchorage, Alaska, USA, 16-20 May, 2011 - Conference Proceedings*, pages 840–851.