Malleability for HPC

ZIH-Colloquium | June 23, 2022 | Josef Weidendorfer
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The Role of the Future Computing Group at LRZ

Understand best options – not just for the next system
Recommendations internally (for system purchase and operation)
and externally (for supporting LRZ users)

User Requirements

- Compute Demands | Ease of Use

Technology HW & SW

- Cost-Effective | Sustainable/Green

Future Computing Group

Analyse, Predict

Recommend

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Outline

- Definition / Motivation
- LAIK: a runtime for elastic HPC codes
  - Overview
  - Examples
  - Directions
- Ongoing efforts
Definition “Malleable”

American Heritage Dictionary

Capable of being shaped or formed

For this talk (HPC context)

The property of a parallel code to be able to take advantage of changes in available compute resources during run time
Benefits of Malleable Codes for Compute Centers

Improved usage model
• Quick job submission (for interactivity) by on-demand shrinking of running jobs
• Shrinking instead of killing running jobs if a high-priority jobs comes in

Better resource utilization
• Reduce fragmentation on a system (alternative to back-filling to use idle resources)
• Dynamic migration to more adequate resources when they become available

Better operation
• Dynamic migration to enable quick maintenance (similar to VMs)
• Ability to react on predicted node failures ("pro-active" fault tolerance)
Outline

• Definition / Motivation
• LAIK: a runtime for elastic HPC codes
  • Overview
  • Examples
  • Directions
• Ongoing efforts
Envelope: German research project on self-organizing systems (2017 – 2019)
KIT, TUM, JGU Mainz, RWTH Aachen

- Pro-active fault tolerance
  - Retreat application from node before (predicted) failure
  - Application-integrated approach: needs support for malleability
Original Focus

• Enable “easy” porting of MPI codes for malleability

• Shrink / expand based on external requests
  • Process IDs (ranks) not integral part of API
    • Library controls number of processes, knows how to distribute data
      (application specifies partitioner algorithm)
    • Constrain to iterative codes using “owner computes” paradigm
  • Automatic re-partitioning on resource size changes

• Enable fault tolerance
  • pro-active (react to predicted failure in the future)
  • reactive (cope with spontaneous failure)
Basic Idea

- Data is stored in multiple global (multi-dimensional) arrays, distributed over processes
  - Processes declare local access wish for array elements for compute phases
  - Value changes are globally propagated on demand

- Any communication = value updates of array elements

- We want to specify the communication requirements in an **abstract** way
  - Not based on MPI ranks, but: what data needs to be locally available for computation
  - Requirements declared once → calculate communication schedules
    - executed multiple times on demand
LAIK

- SPMD, can co-exist with MPI / OpenMP
  - a LAIK entity (process) is a Unix Process
- C API, runs on Linux & MacOS
- [github.com/envelope-project/laik](https://github.com/envelope-project/laik)
- Communication backends as plugins: currently MPI, TCP
Index Spaces, Partitionings, Partitioners

- Example: disjunctive partitioning

- General partitioning: multiple processes per index

- Custom partitioner algorithms supported
  - can use another partitioning as input (e.g. with ghost layer)
Communication Schedule on Update, same Container
Communication Schedule on Update, same Container (2)

Needed: reduction operation (can be custom)
Data Containers

- Memory for data arrays, known to LAIK
- Same type for each index in a container
  - Type needed for reductions
- Layout: how are indexes locally ordered in memory
  - Application can specify custom layouts

- Explicit allocation
  - Specify set of partitionings to reserve space for, LAIK allocates
  - Get memory address for a local index (application knows layout)
  - Trigger Update: can only involve partitionings specified in allocation

- Repartitioning: allocate new, copy (= Update), free old
Application Structure (suggested, not enforced)

• Sequence of compute phases
  • Trigger adequate updates on phases changes

• Mark program points where resource size changes are allowed
  • Global synchronization
  • Results in re-runs of partitioner algorithms
    • Take joining / leaving processes into account
    • Data redistribution is “just” an update from old to new partitioning
Example: 2D Jacobi

- Two matrices, 5 point stencil
- Partitionings: “Init”, “Read with halos”, “Write” (disjunctive)
- Phases

Task Graph

- Init
  - init1
  - read
- Iter 1
  - write
- Iter 2
  - write
  - read

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LAIK Update Object

- Declaration
  - Before/after partitionings of same index space
  - Do update into same or different allocation?
  - Reduction operation
- Contains calculated communication schedule as instruction stream
  - Different abstractions possible: <RunUpdate>, <MPISend, …>
  - To be run by the communication backend (or stack of backends)
- Pre-optimize as much as possible
  - Can include code generation
  - Can be done off-line using pre-calculated partitionings in files (Metis runs)
LAIK Update Object (2)

Partial Specialization

- Information which may not be known at declaration time
  - backend to use, hardware available, machine topology
  - data container (from/to), type info, layout, memory addresses
- whenever new info becomes available, run optimization
  - can be done locally, as long as all LAIK processes agree on basics
Benefits of instruction stream approach

- Optimization passes are decoupled code
- Application-specific passes possible
- Easy selection via external configuration
- Instructions can be backend-specific (backend executes instruction stream)
  - Enables layers of backends, which pass instruction stream down
    e.g. Smart NIC-support: reduction offloading, resource reservation
- Variants of instruction streams to react dynamically
  - Change of job priority from job scheduler
LAIK Update Object (4): Optimization Passes

Examples

• Lower abstraction:
  “send indexes 1-5 from container X” → “send 5 ints at 0xX”
• Merge multiple sends between same peers into one send
• Copy pieces into pre-allocated network buffers
• Different reduction algorithms depending on size / topology
• Detect Pattern & replace with MPI collective (All-to-All)

Provided functionality for Passes

• Can create backend-specific calls to early resource alloc/free
• Reordering via attaching ordering labels
Porting of LULESH (Shock Hydrodynamics)

- Incremental porting from MPI code
  - Small steps, easy to check for correctness
  - Eliminate 2800 lines of comm code (~50%)
  - Almost no changes in main loop of reference code
- Performance/scalability similar to MPI
- Added elasticity and external control
LULESH: Weak Scaling

- Normalized time per iteration
MPI Communication for Kernels

- Kernel 2: communicate neighbors’ corner data, and do local reduction (sum)
LAIK Model: Just Update

- Kernel 2: one partitioning with overlapping access at edges: triggers reduction on update

use SUM reduction
Fault Tolerance for spontaneous Failures

Regular “in-memory” checkpointing, to neighbor node
Extend partitioning for redundancy, copy into “checkpoint” containers
Fault Tolerance for spontaneous Failures

1) Regular “in-memory” checkpointing, to neighbor node
   Extend partitioning for redundancy, copy into “checkpoint” containers

2) Node failure: Transition execution only partially completed
   • Values do not get updated correctly
   • Still, application can proceed (just “wrong values”)
     • Failure handling can be delayed to later point
       (or skips computation)
Fault Tolerance for spontaneous Failures

1) Regular “in-memory” checkpointing, to neighbor node
   Extend partitioning for redundancy, copy into “checkpoint” containers

2) Node failure: Transition execution only partially completed
   Failure handling can be delayed to later point

3) Rollback to previous checkpoint
   Copy back, only working if redundancy was enough
   • Without failed processes, data distribution may be different, but can proceed
   • Eventually with Re-balancing step

Evaluated via (1) “TCP backend”, (2) ULFM MPI implementation
Memory Consumption

- "Standard Release": delete old checkpoint only after next checkpoint successful
- “Early Release”: delete old checkpoint before creating next checkpoint (higher risk!)
At SC19

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Other Directions LAIK

• Automatic load balancing
• Alternative for virtual topology
  • LAIK knows communication matrix for updates
  • Developer can specify which updates should be as fast as possible
• Other communication backends
  • Shared memory: 2-copy → 1-copy → 0-copy
  • RDMA on libfabric (allows direct resource reservation): less handshakes, better asynchrony
• Show that API works with requirements from real-world applications
  • More ports

Understand what is needed in MPI to best support these features
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Efforts

MPI

• TRR Invasic / EU DEEP-SEA
  Research on extending MPI for elasticity, proposal to MPI forum
  (by Isaias Compress Urena, Michael Gerndt)
• Ongoing discussion in MPI WG Malleability
  • Very flexible, covers different use cases

PMIx

• Updates for malleability
• Pushed by work in EU DEEP-SEA
Process Interactions on Malleable Allocations

Management Network

Consolidated Allocation
- Existing Allocation
- Expansion Allocation

HPC Network

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Adaptation Step 1
Adaptation Step 2
Adaptation Step 3

New Adapted Allocation

Expansion Allocation

Preexisting Allocation

1: Reallocation Message

SLURMCTLD

Scheduler Plugin

MPI Process

Node

SRUN

SLURMCTLD

SLURMSTEPD

MPI

Rank 0 (0)

Rank 1 (1)

Rank 2 (2)

Rank 3 (3)

Rank 4 (4)

Rank 5 (5)

Rank 6 (6)

Rank 7 (7)

Rank 0 (8)

Rank 1 (9)

Rank 2 (10)

Rank 3 (11)

Rank 4 (12)

Rank 5 (13)

Rank 6 (14)

Rank 7 (15)
Adaptation Step 4
Adaptation Step 5
Adaptation Step 6
Efforts

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PMIx
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PMIx in DEEP-SEA System Software

- PMIx enables interoperability
- Programming models:
  - MPI, GPI2, GPI-Space, OmpSS
- Tools support:
  - Trace analyzers, memory analyzers, monitors
- Network endpoints setup:
  - Tools over management network
  - HPC network
- Heterogeneous task mappings

- Integration primarily with Slurm