TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

# Top-Down Performance Analysis Methodology for Workflows

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# Workflows Matter

Common use cases today are not limited to single applications

- Pre- and post-processing
- Heterogeneous applications in multiple jobs
- Multi-phase calculations as separate jobs

The obvious job is not always the problem job

A single job is not always the problem

I/O captures inter job dependencies and communication

- I/O is to workflows what MPI is to individual parallel jobs

# I/O: More than POSIX

New Score-P feature: I/O recording (POSIX, ISO C, HDF5, NetCDF, MPI I/O)

Instrumenting high-level I/O interfaces allows better attribution of costs

- High level interfaces may be asynchronous, distributed, filtered
- Small high-level operations may produce large actual changes, or vice versa

# Approach

Display overall summary of the behavior of a workflow

- Distribution of time among constituent jobs
- Breakdown of workflow into I/O, communication, and computation components
- Dependencies among jobs

Display summary of each job's behavior

- Distribution of time among job steps
- Breakdown of each job into I/O, communication, and computation components

Display each job step (single application run)'s behavior

- Breakdown into I/O, communication, and computation components
- Access to full trace data in Vampir

# Implementation

Convert OTF2 traces to high-level summary profiles

- Categorize each function as I/O, communication, or computation
- Hierarchical view of I/O handles accessed
- Summary of job properties

Generate summary of entire workflow from SLURM accounting database

- Jobs and steps involved
- Submission parameters and dependencies
- Submission, start, and end times

Visualize results

- Identify I/O dependencies
- Build timeline and dependency information
- Link profile view of each job step to detailed trace view in Vampir

# Identifying I/O dependencies

Jobs reading/writing the same I/O handle

In particular, may-read after may-write

Of particular interest: identifying independent steps in the workflow

These steps can potentially be run simultaneously if the allocation is large enough

Problems: false sharing, filtering for relevance

- Files may be opened with overly permissive permissions
- /dev, /proc, /sys etc. may create false dependencies
- Scaling problems: one sample run had 28k files, of which ~500 were not in the above directories

# Example Workflow: GROMACS

Well-known molecular dynamics software

Typical workflow:

- Set up simulation environment
- Add solvent medium
- Generate initial molecular model (e.g. of a protein)
- Energy minimisation
- Initial equilibration
- Actual molecular dynamics computation

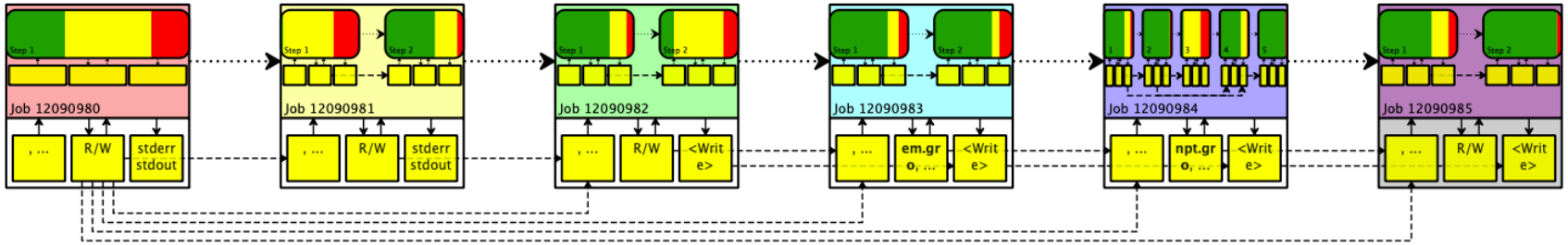
Steps communicate with each other via filesystem

Dependencies are implicit

Not preconfigured to use any off-the-shelf workflow managers

# GROMACS in more depth

## Dependency Graph

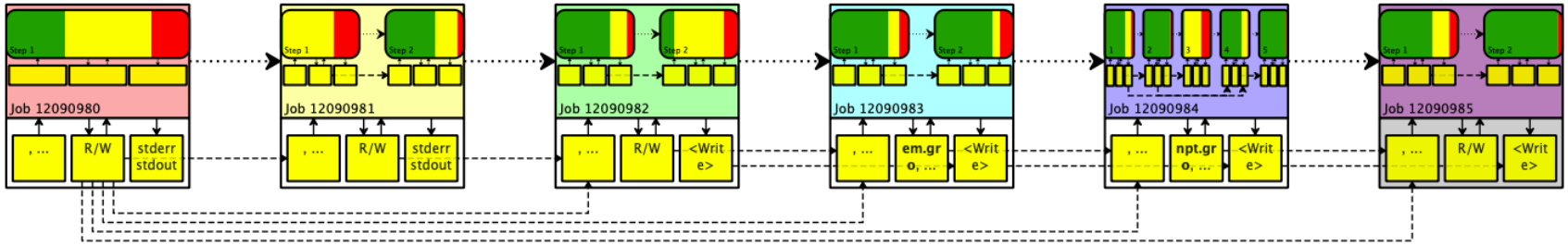



Legend

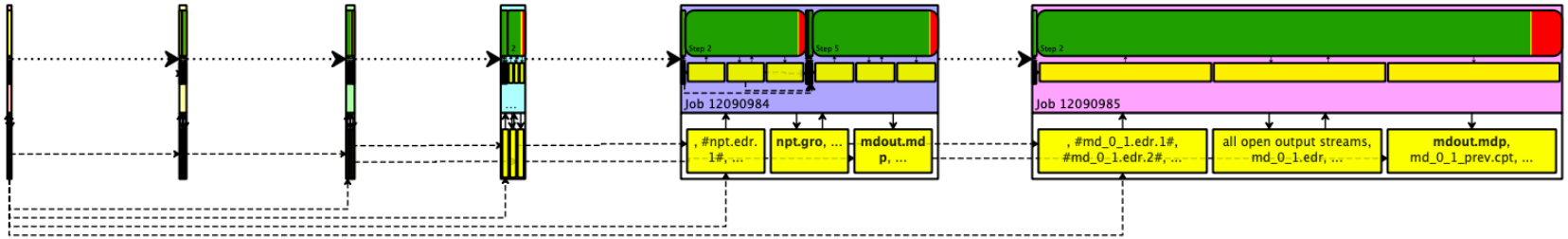

Dependency

# GROMACS in more depth

## Dependency Graph




## Timeline



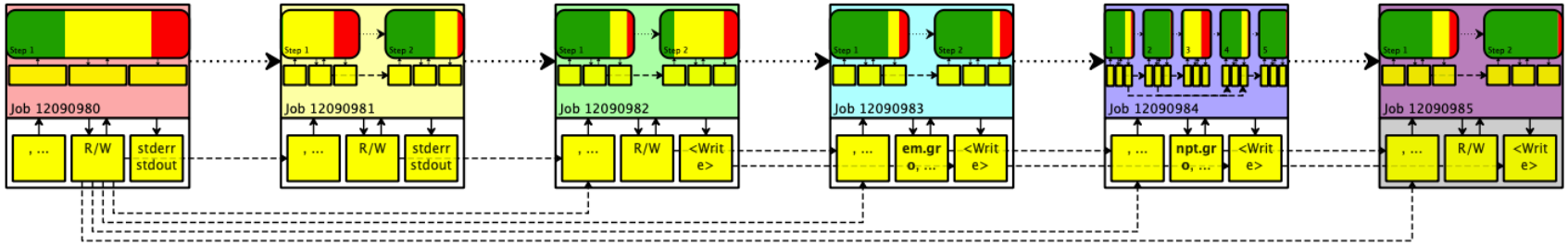

### Legend

Compute | I/O | MPI

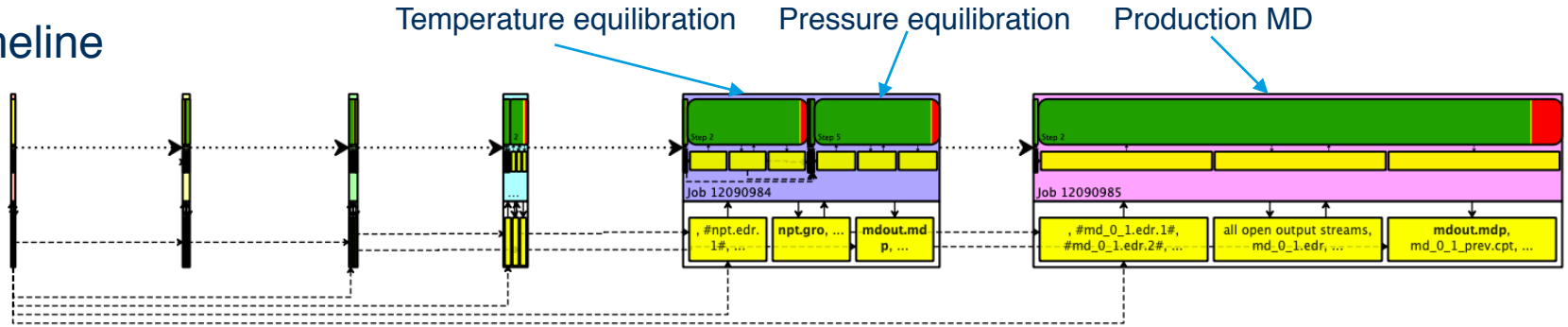
Dependency

# GROMACS in more depth

## Dependency Graph



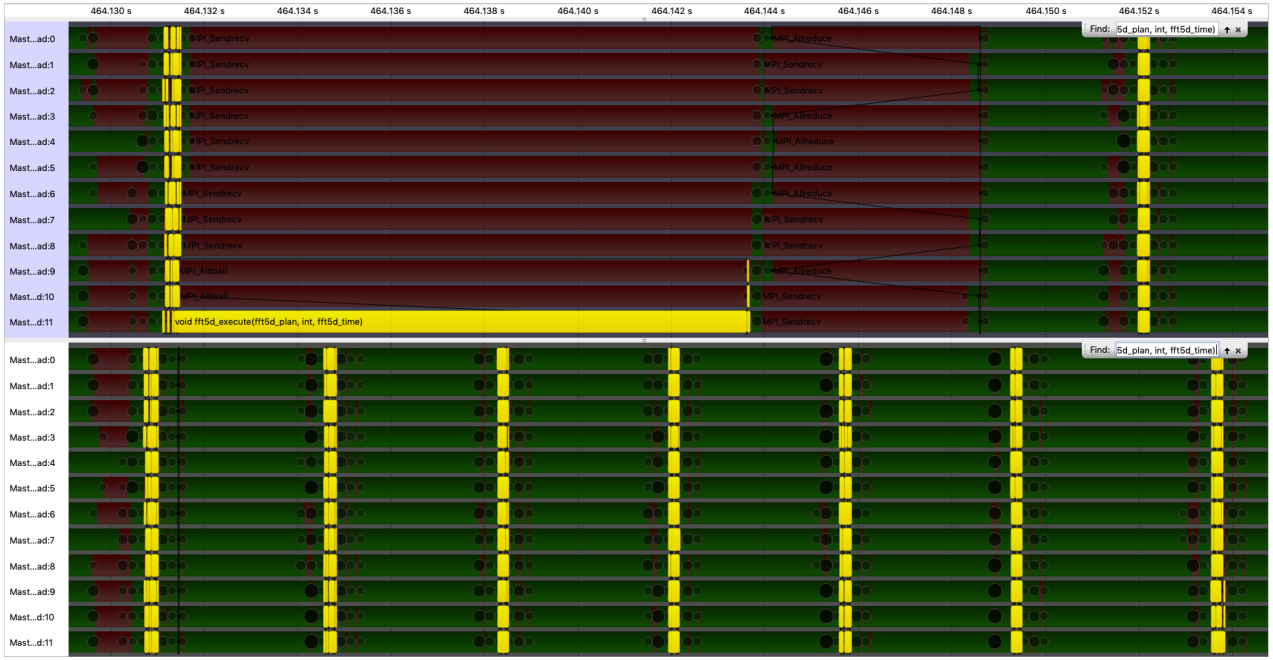

## Timeline




### Legend


Dependency

# GROMACS: finding load imbalance




Top: dynamic load balancing disabled, FFT code (yellow) imbalanced across ranks
Bottom: dynamic load balancing enabled, FFT code remains balanced

Result: reduces MPI share from ~10% to ~5% in the production MD step

# Integration with Workflow Managers: Cromwell and GATK

Many workflows use something other than pure SLURM and shell scripts to manage dependencies

Especially true when these workflows are more complex DAGs

Sample workflow manager: Cromwell

- Supports a wide variety of back ends, including but not limited to SLURM
- Supports a flexible enough specification to allow us to insert measurement hooks
- Has off-the-shelf example workflows that provide real-world non-linear dependencies

# Cromwell hooks

## Backend configuration

```
    slurm {
      actor-factory =
"cromwell.backend.impl.sfs.config.ConfigBackendLifecycleActorFactory"
      config {

                    …
        String scorep = ""
        """
        script-epilogue="/usr/bin/env bash /home/wwilliam/wdl-testing/slurm-epilog.sh"

        submit = """
            sbatch -J ${job_name} -D ${cwd} -o ${out} -e ${err} -t ${runtime_minutes} -
p ${queue} --export=ALL \
            ${"-n " + cpus} \
            --mem-per-cpu=${requested_memory_mb_per_core} \
            --wrap "/usr/bin/env bash ${scorep} /usr/bin/env bash ${script}"
        """
        kill = "scancel ${job_id}"
        check-alive = "squeue -j ${job_id}"
        job-id-regex = "Submitted batch job (\\d+).*"
      }
```

# Cromwell hooks

## Score-P wrapper

```
#!/bin/bash

set -e
echo "Job $SLURM_JOB_ID"
export BASE_DIR=$PWD
export OUTPUT_DIR=$PWD/experiments
export SCOREP_EXPERIMENT_DIRECTORY=$OUTPUT_DIR/$SLURM_JOB_ID/$SLURM_JOB_ID
export SCOREP_ENABLE_TRACING=true
export SCOREP_ENABLE_PROFILING=false
export SCOREP_TOTAL_MEMORY=3700MB
echo "Job $SLURM_JOB_ID"
export SCOREP_FILTERING_FILE=/home/wwilliam/SimpleVariantDiscovery/test.filter

install_scorep_dir=/home/wwilliam/scorep-install-java
bin_scorep_dir=$install_scorep_dir/bin
lib_scorep_dir=$install_scorep_dir/lib
profiler=/home/wwilliam/workflow-analysis/vendor/otf2_cli_profile/build/otf-profiler
export LD_LIBRARY_PATH=$lib_scorep_dir:$LD_LIBRARY_PATH
mkdir -p $OUTPUT_DIR/$SLURM_JOB_ID
$@
pushd $SCOREP_EXPERIMENT_DIRECTORY

if [ "$SCOREP_ENABLE_TRACING" = "true" ]
then
    $profiler -i $SCOREP_EXPERIMENT_DIRECTORY/traces.otf2 --json -o $SCOREP_EXPERIMENT_DIRECTORY/result
fi
popd
```

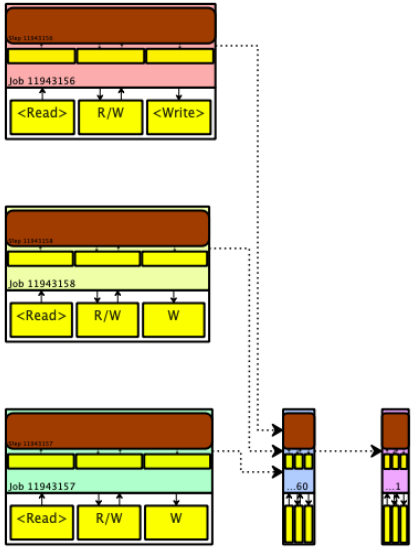
# Cromwell hooks

## Epilog script

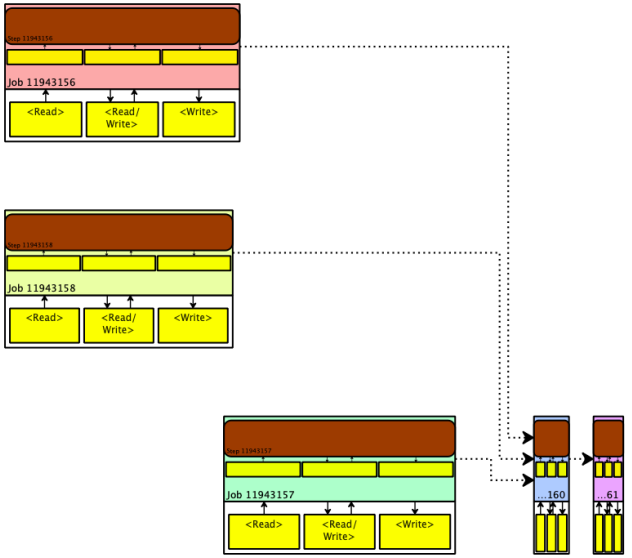
```
#!/bin/bash

module load Python/3.6.6-foss-2019a

cd ../experiments
SLURM_JOB_ID=`ls`
python /home/wwilliam/workflow-analysis/vendor/JobLog/joblog.py $SLURM_JOB_ID
$SLURM_JOB_ID
```

# GATK Sample Workflow: Joint Calling Genotypes

## Duration scaled dependency graph




## Timeline




Input data: one set of files per genetic sample

Process each input appropriately and independently

Merge and process results

# Implementation Issues

GATK is written in Java; Score-P support is still experimental for Java tracing

As with many real-world workflows, GATK doesn't use MPI

Common parallelisation approach: more jobs in the workflow

Will need to evaluate GUI scalability

- Number of jobs
- Number of files

# Future Work

Formalized metrics of workflow quality

Visualization of these quality metrics

Automate recommendations for workflow tuning

# Evaluating overall workflow performance

Multiple criteria possible depending on site policy and goals:

- Goodness of fit (how efficiently does the workflow use its allocated resources?) E.g. typical shared environments with many smaller workflows sharing a large machine
- End-to-end time (if we're maximally generous with resources, how fast can we make this workflow?) E.g. weather forecasting
- Energy efficiency

# Visualizing Workflow Quality

Goodness of fit: visualise allocated vs. used resources

- Scale box height
- Do we need log scaling options for time and size?
- How to distinguish large number of small jobs from single large jobs space-efficiently?
- Do we care how much of each partition we're using?

End-to-end time: identify and visualise workflow's critical path

- Based on current I/O pattern? Based on best case from trace analysis?

Important modelling question: how does average queue time scale with:

- Size of allocation
- Duration of allocation

# Steps towards optimisation

Define scope of valid optimisations

- Restructuring workflow (script-level dependency changes)
- Changing filesystems for important steps
- Changing scaling of various steps
- Optimizing a single application
- Restructuring inter-app communication patterns
- Redesigning entire workflow (wholesale redesign of poorly performing apps, creating new apps/merging existing ones, redefining intermediate data requirements)

# Conclusion

Implemented:

- Measurement infrastructure for HPC workflow tracing
- Initial visualiser for workflow performance
- Job dependency analysis based on SLURM information, I/O, and timing

Tested on:

- GROMACS with custom run scripts
- GATK JCG workflow under Cromwell

Visualizer available in upcoming Vampir release

Trace-to-profile tool and job log tool available on GitHub

# Questions?

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