Leveraging the checkpoint-restart technique for optimizing CPU efficiency of ATLAS production applications on opportunistic platforms

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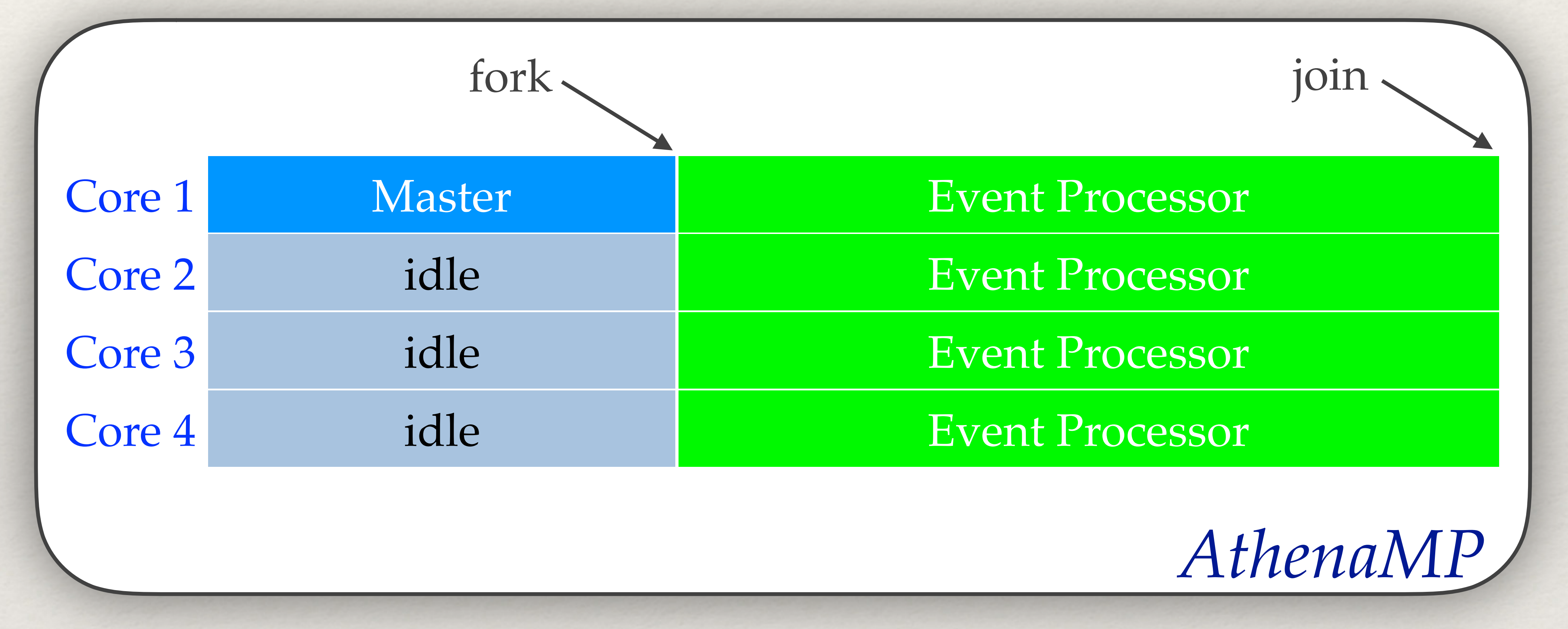
Introduction

- ATLAS uses **AthenaMP** (multi-process version of its data reconstruction, simulation and analysis framework Athena) for running production workloads on multi-core platforms

- The sequential phase of an Athena MP job (initialization in the master process) includes:
  - Loading of shared libraries
  - Reading of the detector geometry and conditions data from external databases
  - Building transient representation of the detector geometry
  - Initialization of algorithms and services



Core 1	Master	Event Processor
Core 2	idle	Event Processor
Core 3	idle	Event Processor
Core 4	idle	Event Processor

- In some cases the **<u>initialization step takes as long as 10-15 minutes</u>**, which has a visible negative impact on overall CPU efficiency of the job

Introduction (contd.)

- ATLAS runs large number of production jobs with similar configuration parameters
  - E.g. jobs within one Geant4 Simulation production task share the same configuration
  - The only difference between jobs within such task is which events they need to process

- For such jobs, instead of going through the same initialization phase over and over again, we can consider the following scenario:
  - **Step 1:** run one job from the task through the initialization step and then **checkpoint** it;
  - **Step 2: distribute** the generated **checkpoint image** over to the compute nodes;
  - **Step 3: restart** production jobs from the checkpoint image instead of running them through the initialization phase.

- This presentation contains some preliminary results of applying this strategy to ATLAS Geant4 Simulation jobs on a Volunteer Computing system and an Intel KNL supercomputer

Checkpointing Tool

- **DMTCP** (Distributed MultiThreaded Checkpointing) **http://dmtcp.sourceforge.net/**
  - Checkpoints a single host or distributed computation in user space
  - Does not require kernel-level access
  - Minimum runtime overhead
- Has been used for testing the checkpoint-restart mechanism for CMSSW and Geant4 MT
  - See the presentation by P Elmer in ACAT 2013
- For our tests so far we have been using DMTCP 2.4.5
  - Integrated into ATLAS software releases as an external package

Making checkpoint images in AthenaMP

- The **master AthenaMP process checkpoints itself** just before forking event processors
  - Using DMTCP API from within C++ code
- Once the checkpoint image has been created, the master process exits immediately
- The checkpoint image together with other auxiliary files (e.g. automatically generated script for restarting) is put into a tarball for later usage
- In order to activate this mechanism we introduced a special `--checkpoint` command-line option to ATLAS Job Transform
  - **Job Transform** is a python wrapper used for running Athena jobs in production

Restarting AthenaMP from a checkpoint image

- The location of a checkpoint image is provided to the transform via `--restart` command-line option

- The transform unpacks the checkpoint tarball into job's run directory and initiates restart by running the restart script

- The first thing AthenaMP does after restart is to update a few configuration parameters: numbers of processes to fork, input file name and the number of events to process
  - This information is provided to AthenaMP by the transform

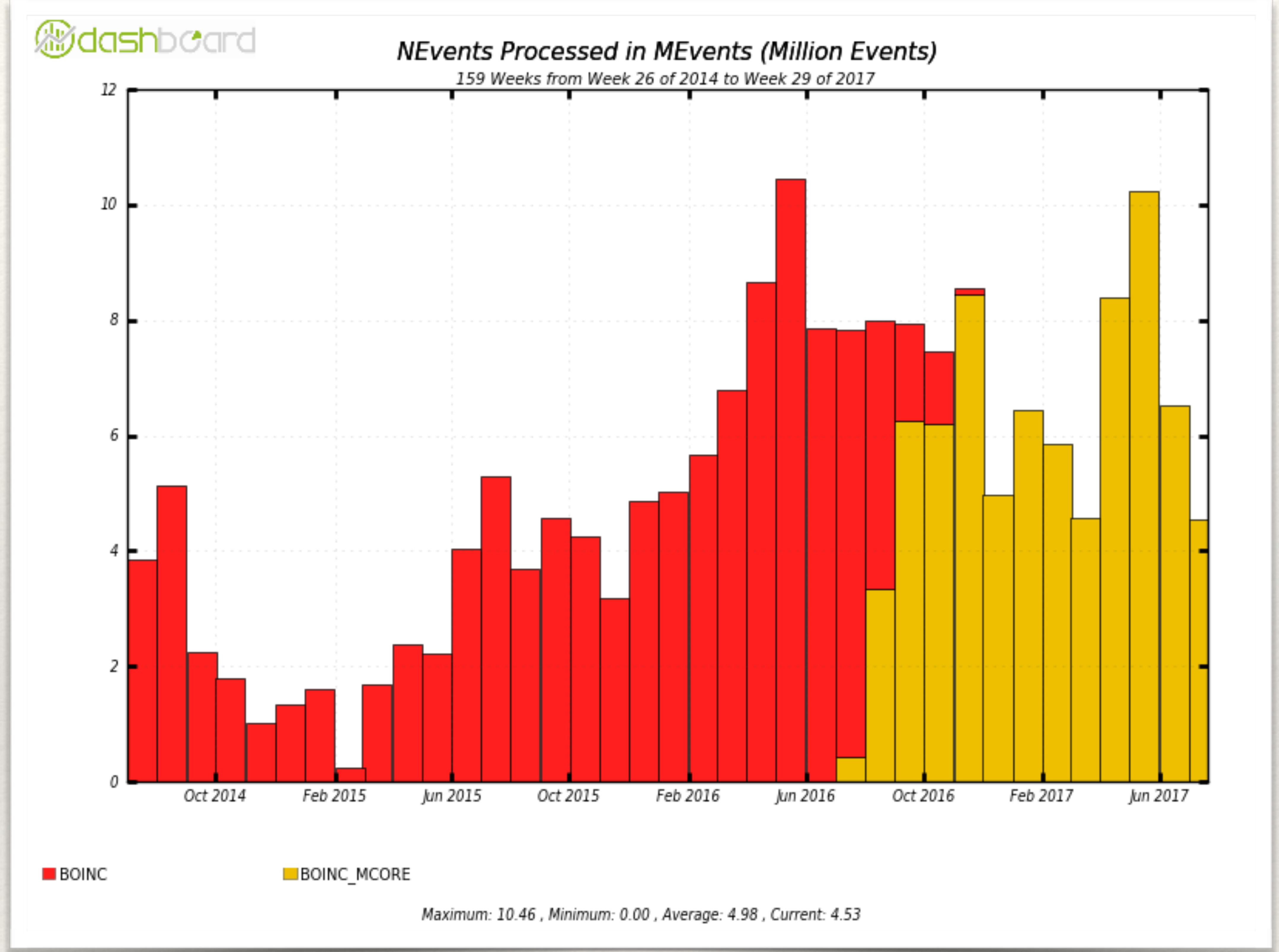
- After that the job proceeds as usual

Portability of checkpoint images

- It is desirable to generate one checkpoint image for a large set of jobs (e.g all jobs within the same production task) and then use it for launching jobs on heterogenous platforms at various sites
    - ATLAS software is built against SLC6 for production usage
- This is non-trivial, for DMTCP expects to see the same platform at restart as the one seen at checkpoint
- In order to overcome this limitation, we can leverage VM/container technology
    - Create checkpoint image within VM/container and restart within the same VM/container
- We followed this strategy for testing AthenaMP checkpoint-restart on BOINC
    - Volunteer computing platform used by the ATLAS@Home project

Testing on ATLAS@Home

- **ATLAS@Home**
  - A volunteer computing project started in 2014
    - An outreach tool to get the public involved in ATLAS
  - Volunteers run Geant4 simulation inside a VM
  - Based on BOINC platform used in many volunteer computing projects
    - Built-in support for virtualization using VirtualBox
  - ATLAS@Home is integrated into the ATLAS workflow management system
    - From the outside it looks like a normal "Grid" site
  - ATLAS@Home is currently an equivalent of a T2 site



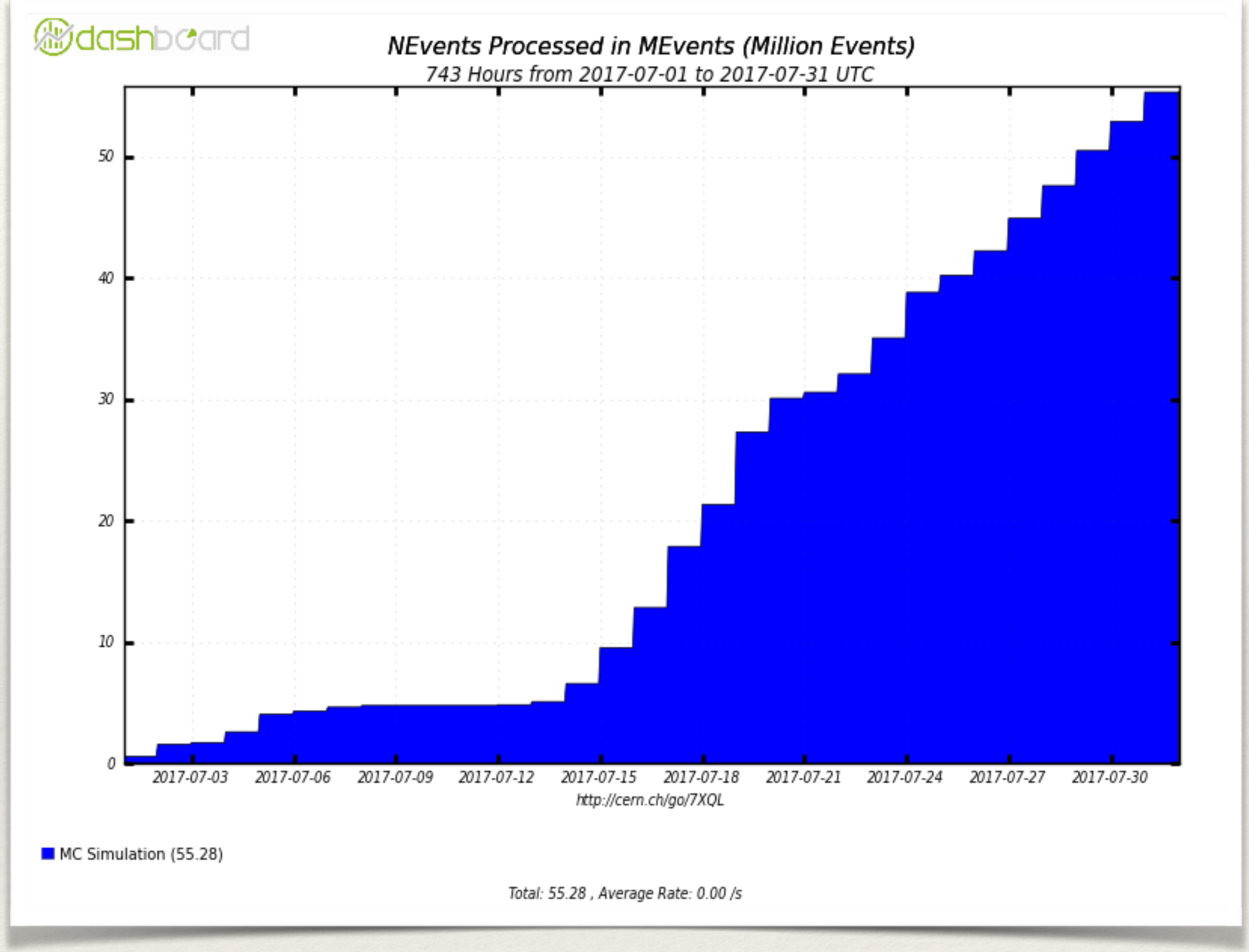
Events processed on ATLAS@Home per month since the start of the project. The colors show the transition from single-core (red) to multi-core (yellow) jobs

Testing on ATLAS@Home (contd.)

- ATLAS@Home makes a good choice for a prototype platform to test checkpoint-restart
  - Since jobs run in a VM, we are in a complete control of the environment
  - Volunteers often complain of long initialization times due to reading of external databases
  - Jobs in ATLAS@Home/BOINC run for 1-2hr, which makes fast initialization rather important
- Volunteers download a VM disk image once and use it for each job
  - We create an image with all the necessary software cached in the CVMFS cache
- For checkpointing tests we created a tarball with a compressed checkpoint image and saved it in the VM image
- ***Preliminary tests demonstrated that AthenaMP can restart from the checkpoint image in 15-20 sec, while in case of regular initializations we measured ~4 min for jobs with fast database connections and 10-15 min for jobs with slow database connection***

Testing on Intel KNL

- **Cori HPC @ NERSC**
  - The 5th most powerful supercomputer in the world on the November 2016 list of Top 500 HPC-s
  - Cori Phase 1: 2.4K Intel Xeon "Haswell" nodes
  - **Cori Phase 2**: 9.7K Intel KNL nodes
    - 68 cores per node @ 1.4 GHz
    - Each core has 4 hardware threads and two 512-bit-wide vector processing units
    - Each node has 96 GB DDR4 + 16 GB MCDRAM (multi-channel DRAM) memory
  - In July 2017 ATLAS simulated 55M events with Geant4 on Cori Phase 1&2.



Events simulated on Cori Phase 1&2 in July 2017

Testing on Intel KNL (contd.)

- On Cori KNL we tested AthenaMP restarts from locally generated compressed and uncompressed images
- Cori compute nodes represent a homogenous environment, so we don’t have to worry about image portability
- The image tarballs were unpacked into run directories prior to submitting jobs to the batch system
- The job startup time was measured between launching AthenaMP until the moment it forked event processors
- The table contains results obtained by running 300 singe-node jobs

	Image size	Startup time (sec)	Startup speedup vs regular AthenaMP
Regular AthenaMP	N/A	663.1 ± 22.8	1
Compressed image	550MB	50 ± 9.7	13.3x
Uncompressed image	1.8GB	20.8 ± 9.1	31.5x

Summary/Outlook/Acknowledgements

- DMTCP was successfully tested by ATLAS for checkpoint-restarting Geant4 Simulation jobs
- First tests with production jobs on ATLAS@Home/BOINC and Intel KNL demonstrated that by restarting from checkpoint images we can considerably speedup job startup times
- However, there is still a long way to go before we can declare our readiness to use the checkpoint-restart technology in production
  - Automation of the process
  - Validation of the results
- The authors would like to thank our volunteer testers in ATLAS@Home (*Yeti* and *MAGIC*) for running the jobs for us and providing useful feedback