Multithreaded simulation for ATLAS: challenges and validation strategy

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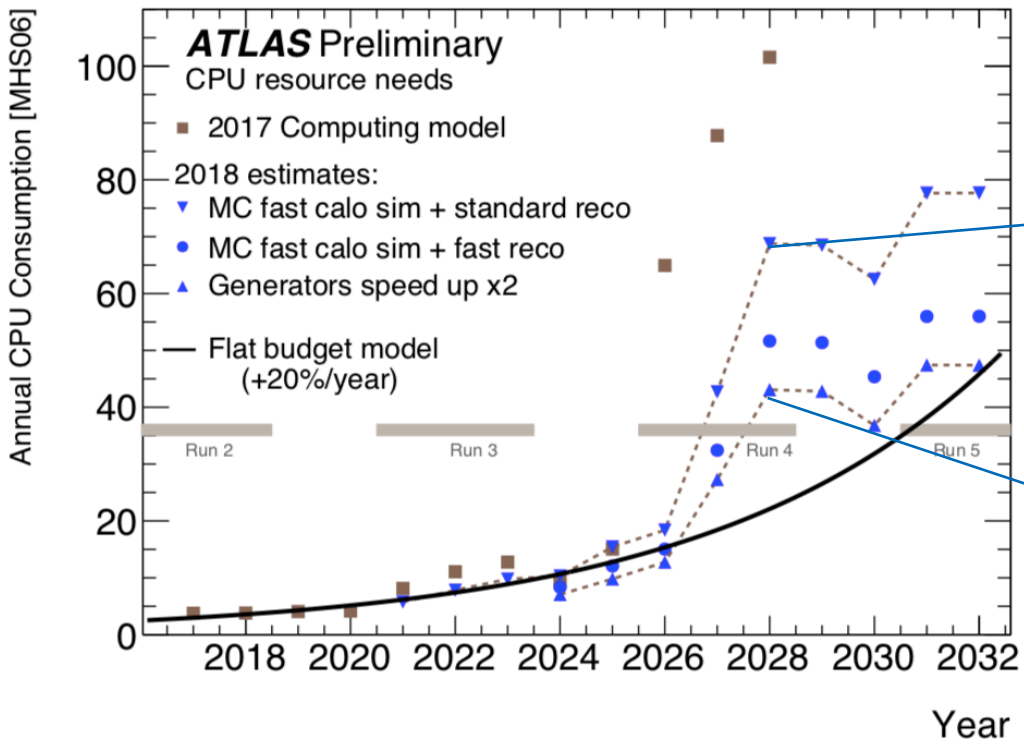
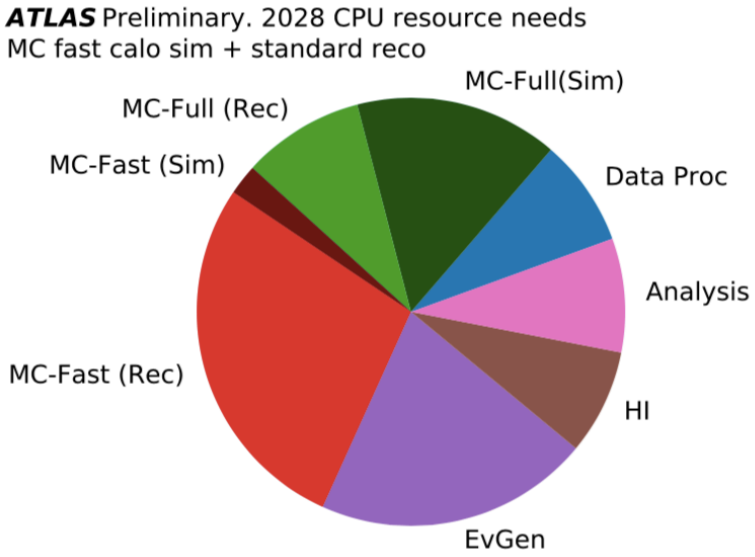
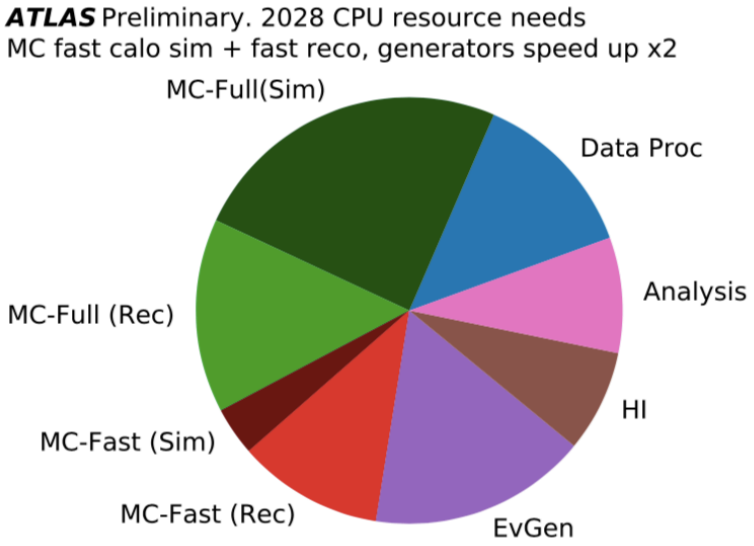
Computing complexity challenges

[ATLAS public]



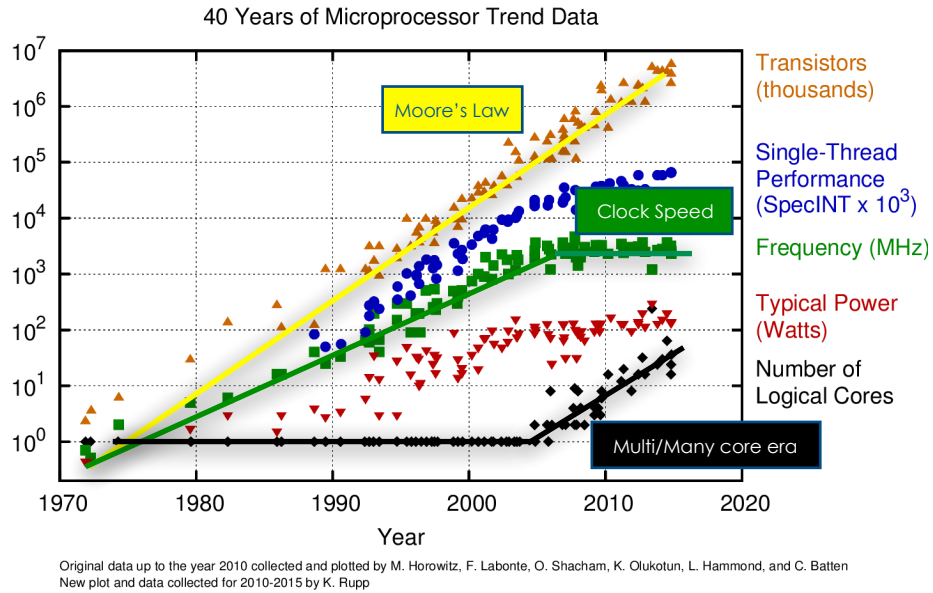




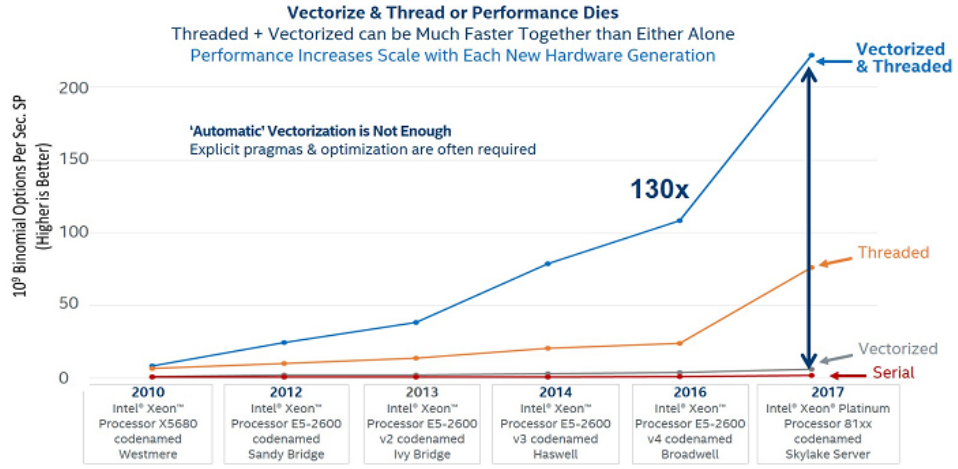
- In Run3, 50% of simulation will rely on fast techniques (aim to reach ~75%), but full Geant4 simulation will be heavily used regardless
- In Run 4, Full Simulation is expected to be the largest CPU consumers (20-25%)
  - Together with FastSim and FastReco it amounts to ~40% of all expected CPU consumption.
- Any performance optimizations of ATLAS simulation have a big impact on the overall picture.

Why multi-threading?

- Evolution trend of faster single-threaded CPU performance broken **more than 10 years ago**
- Increase of **CPU cores** and more execution units to overcome stagnation in CPU Clock Speed
  - low power core sharing a pool of memory
- **We need 'Multi-Threaded (MT)' design** to run effectively on modern architectures and profit from multi-core designs
  - MT approach is critical for heterogeneous architectures (e.g. GPU HPCs)
  - This approach scales better with respect to the multi-processing approach (AthenaMP) especially on the architectures that are foreseen to be used in the next LHC runs
- Production ready MT simulation is considered **CRITICAL** for Run 3 and **BLOCKER** for Run 4
  - to exploit the HL-LHC successfully
- What about **vectorization**?



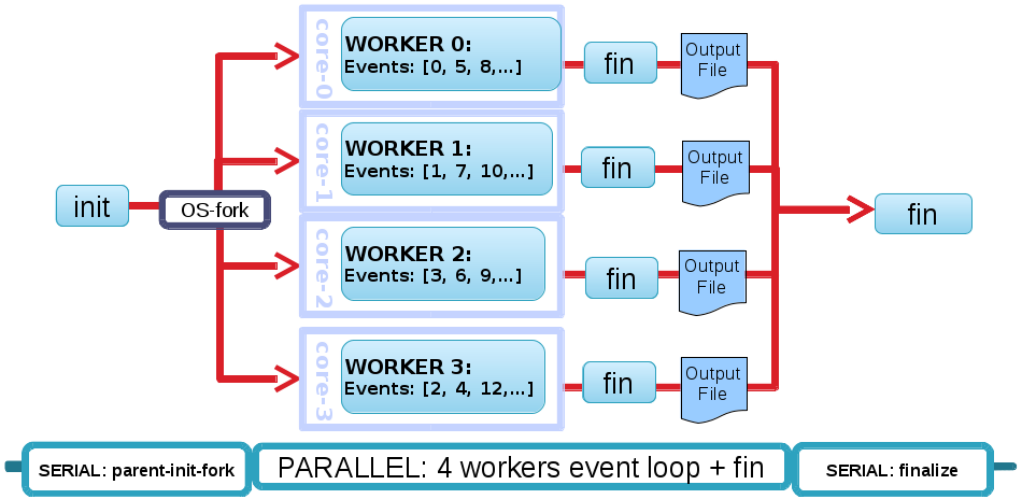
History of Intel chip introductions by clock speed and number of transistors

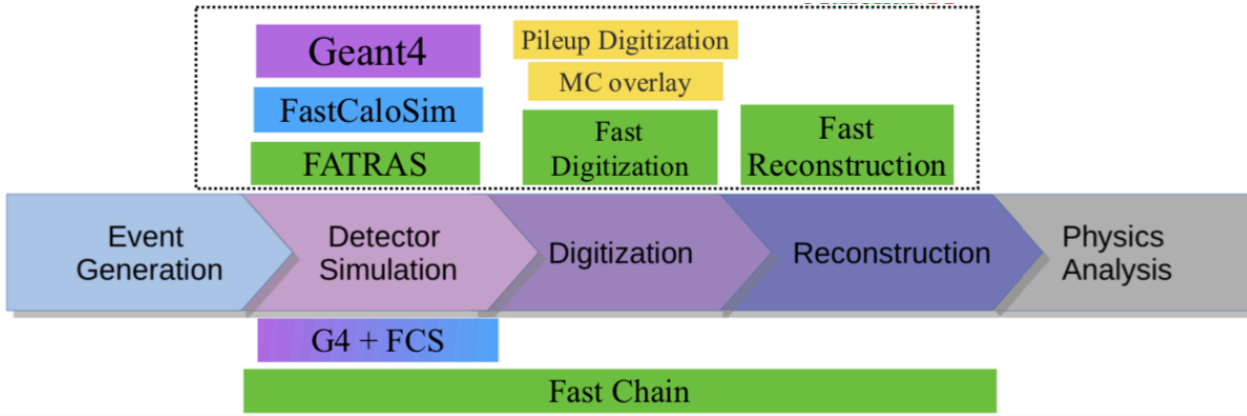


Why multi-threading?

- The amount of **MC samples** producible already **limits** physics analysis
  - with the upcoming runs and increased luminosity will be worse
- The current model, **AthenaMP,** relies on Linux's *copy-on-write* mechanism for sharing memory pages between forks:
  - doesn't scale for Run-3 and beyond
- Ongoing effort to migrate **ATLAS** computing model to ***multi-threaded* AthenaMT**
  - Finer-grained *task parallelism*, minimised memory footprint
  - Only execute() is concurrent
  - *Scheduler-driven*, by dependency graph
- **Simulation**, **Digitization** and **Reconstruction** moving to MT paradigm using the AthenaMT/GaudiHive infrastructure.
  - Better scaling in terms of memory footprint (leverage new architectures)
  - Easy the investigation of heterogeneous computing architectures (e.g. use GPUs, FPGAs etc)

Schematic View of ATLAS AthenaMP



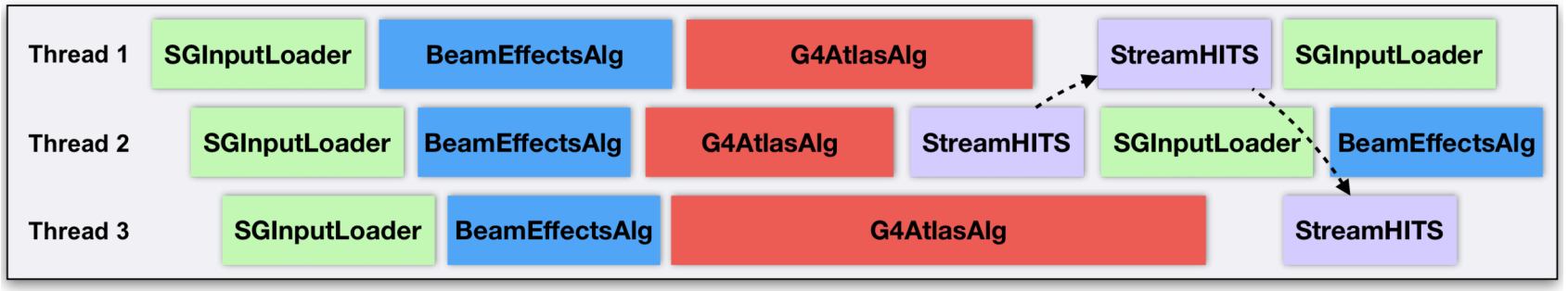


AthenaMT and Geant4MT

- **AthenaMT** is based on **GaudiHive**, a multi-threaded, concurrent-execution extension to Gaudi :
  - Concurrency model based on **TBB**
  - Scheduling is driven by data-flow
  - Events processed in multiple threads

- **Geant4** has its own approach to parallel processing
  - Master-slave concurrency model, using **pthreads**
  - Provides event-level parallelism
  - Thread safety achieved using **thread-local storage**
    - Main Geant4MT components must be thread-local

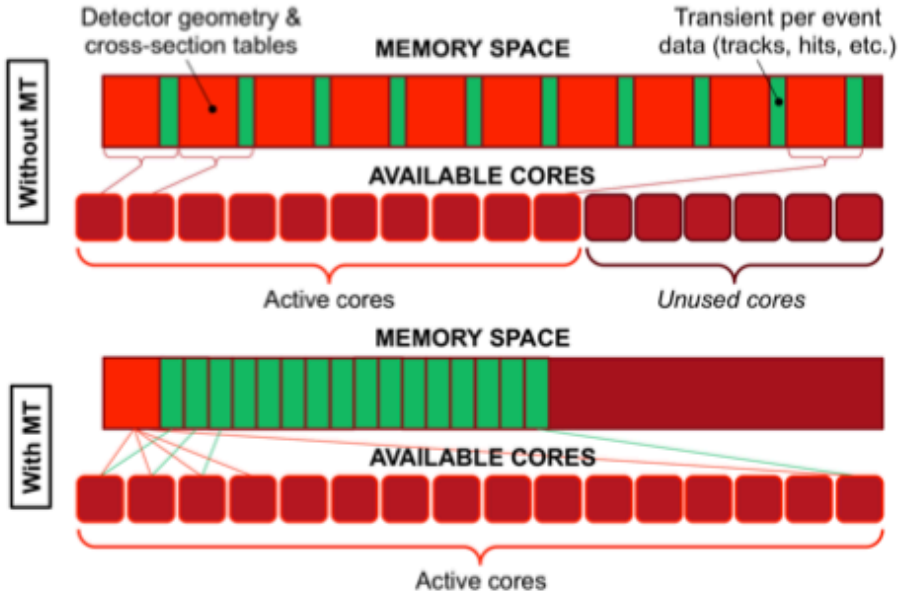
- **GaudiHive** provides **task locality, not thread locality**
    - Cannot easily pin a Gaudi component to a specific thread
    - Must decouple the Gaudi components from the Geant4 core functionality
    - Initialization is very tricky: G4 requires that thread-local objects are initialized in their threads at the right time



Thread coupling AthenaMT and G4MT

- **Geant4MT** has been successfully integrated in **AthenaMT**
  - Inter-event rather than intra-event parallelism:
    - memory saving coming from sharing geometry and cross-section tables between threads

- **Segfaults** during execution or finalization of MT jobs, due to the way TBB starts new threads:
  - When **finalizing** a MT job:
    - TBB creates extra-threads that are not catched by the ThreadPoolSvc -> no call to G4ThreadInitTool::initThread
      - Crashes when G4ThreadInitTool::terminateThread is called for those threads



- During **execution** of a MT job:
  - In some cases **TBB can spawn new threads** even after initialization is complete
  - The simulation was aborted because the geometry was released after the initialization but it is always needed to initialize new threads

Case study: Differences in LAr Hits

- Differences in the LAr Hits affecting ***very rarely*** the energy*:*

```
Ex:
Py:diff-root         INFO comparing [22] leaves over entries...
000.LArHitContainer_p2_LArHitEMB.m_energy.6891 3484255171L -> 1336771523L => diff= [22.27205722%]
Py:diff-root         INFO Found [630943] identical leaves
Py:diff-root         INFO Found [1] different leaves
```

- LArG4SimpleSD instances are contained in SDWrapper, which has a common hit collection container for all SDs.
- The SDWrapper is a derived G4VSensitiveDetector, and instances of SDWrapper are contained in a thread ID-keyed map.
- Problem was likely localized to ProcessHits.

```
LArCalorimeter/LArG4/LArG4Barrel/src/LArBarrelCalibrationCalculator.cxx
LArCalorimeter/LArG4/LArG4Barrel/src/LArBarrelPresamplerCalculator.cxx
```

Strategy for MT debugging

Simulation with 10 ttbar events,
sequential mode vs *MT with* 5 threads

Strategy for MT debugging

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Increment the messaging level to DEBUG (~7GB for 10 ttbar evts)

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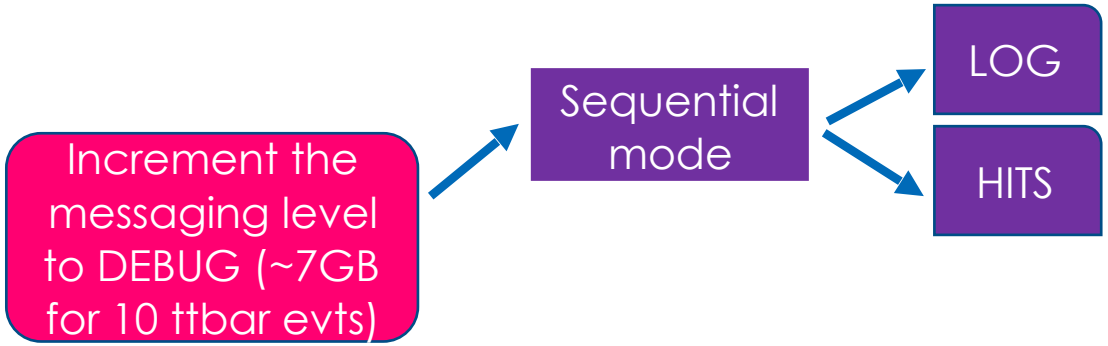

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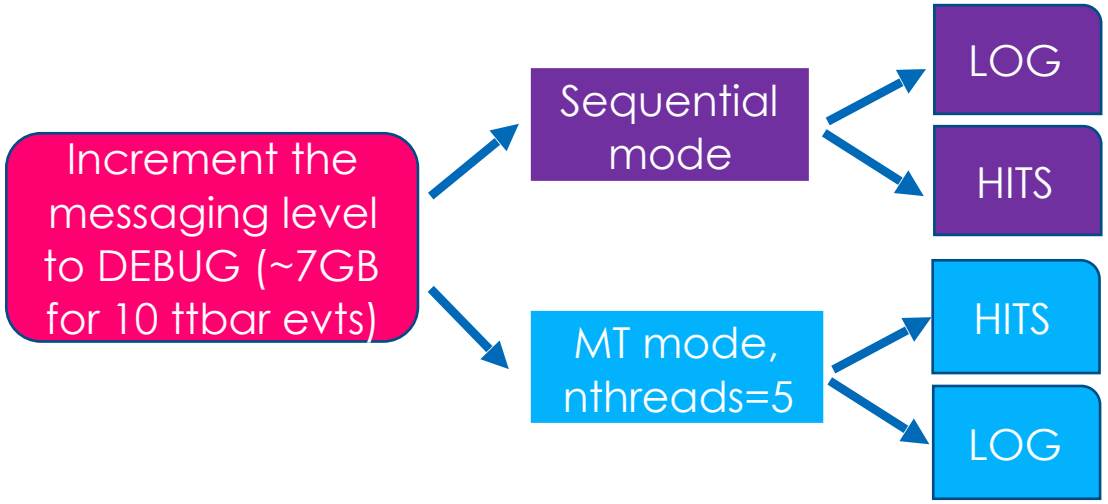

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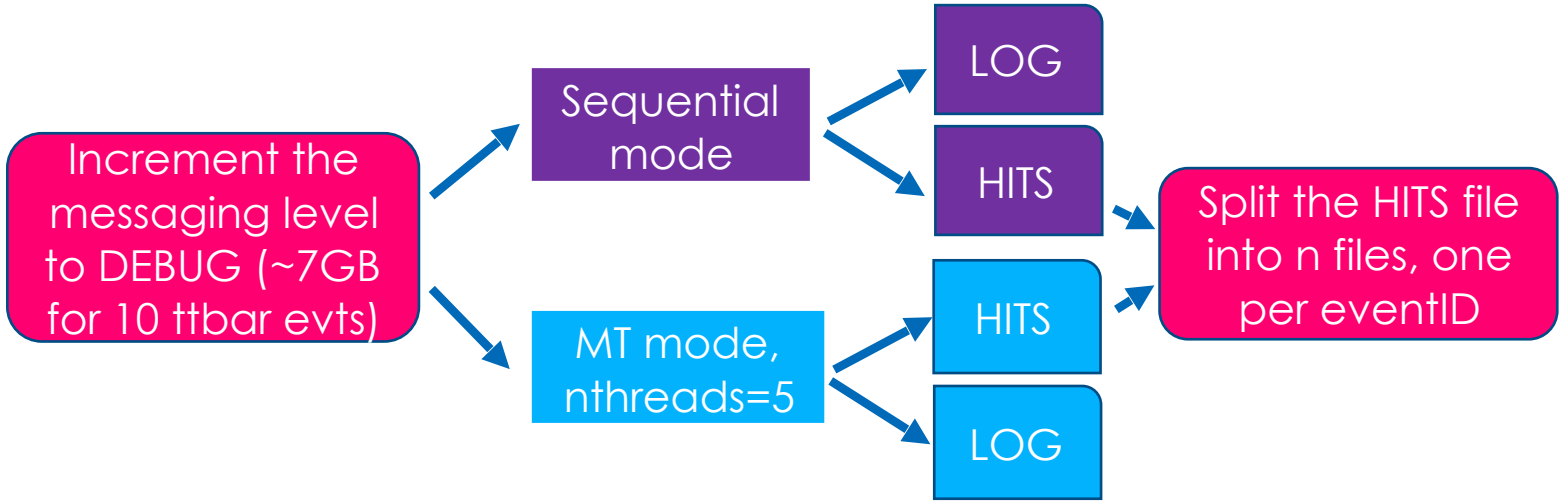

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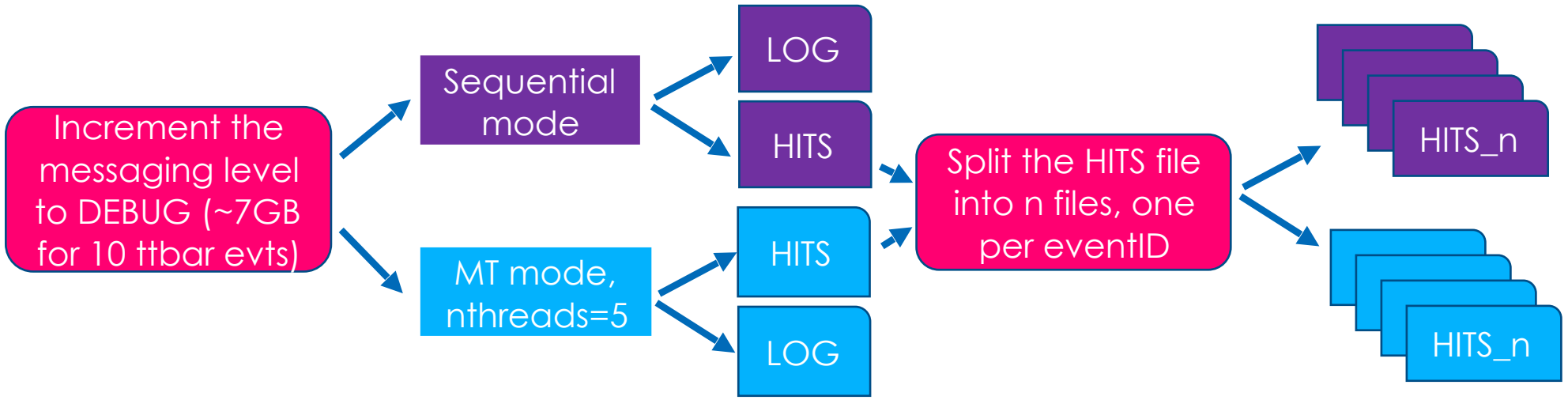

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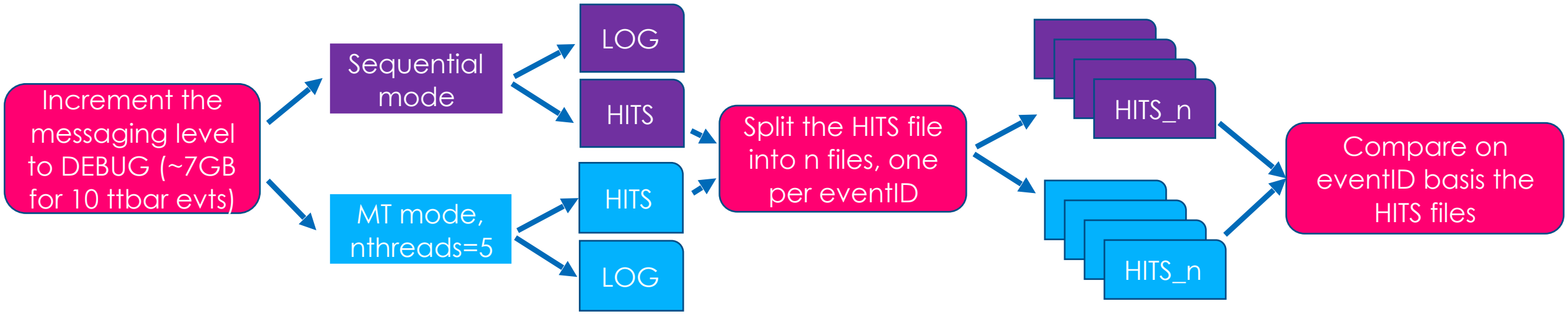

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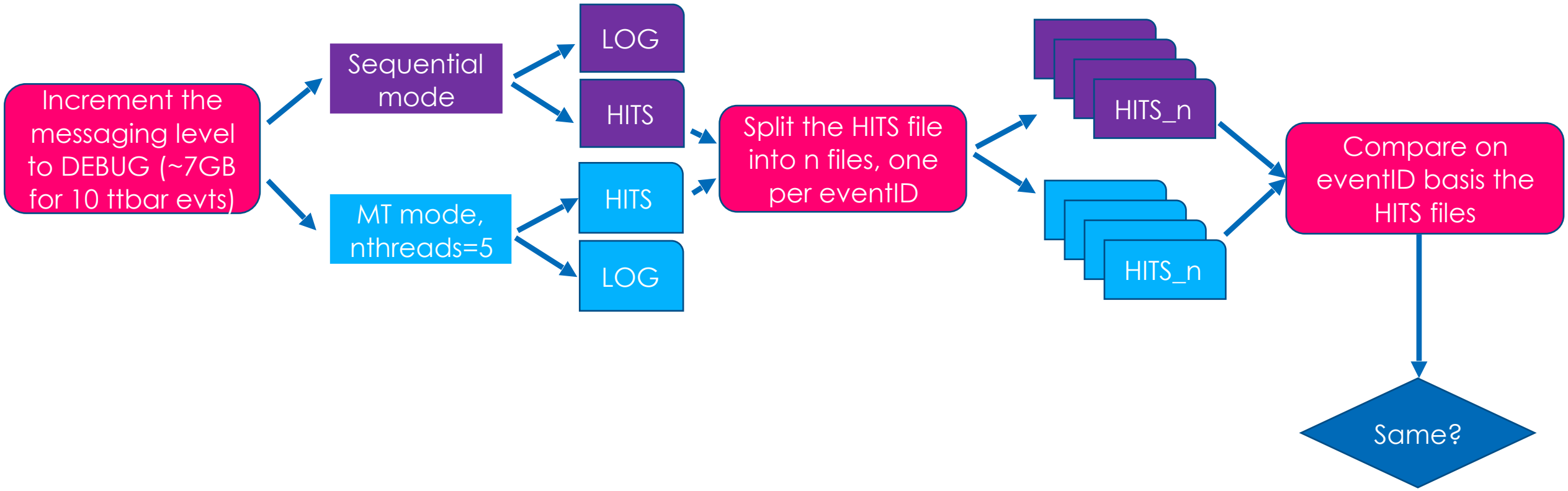

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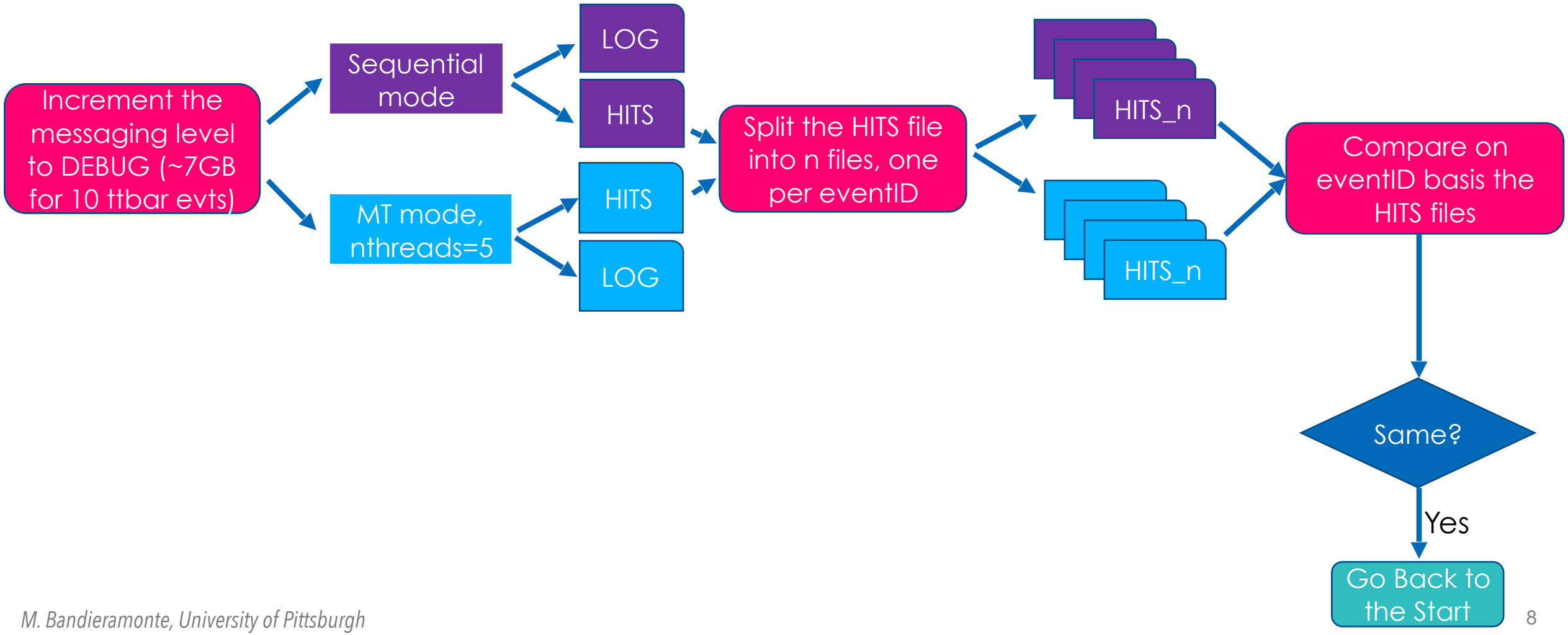

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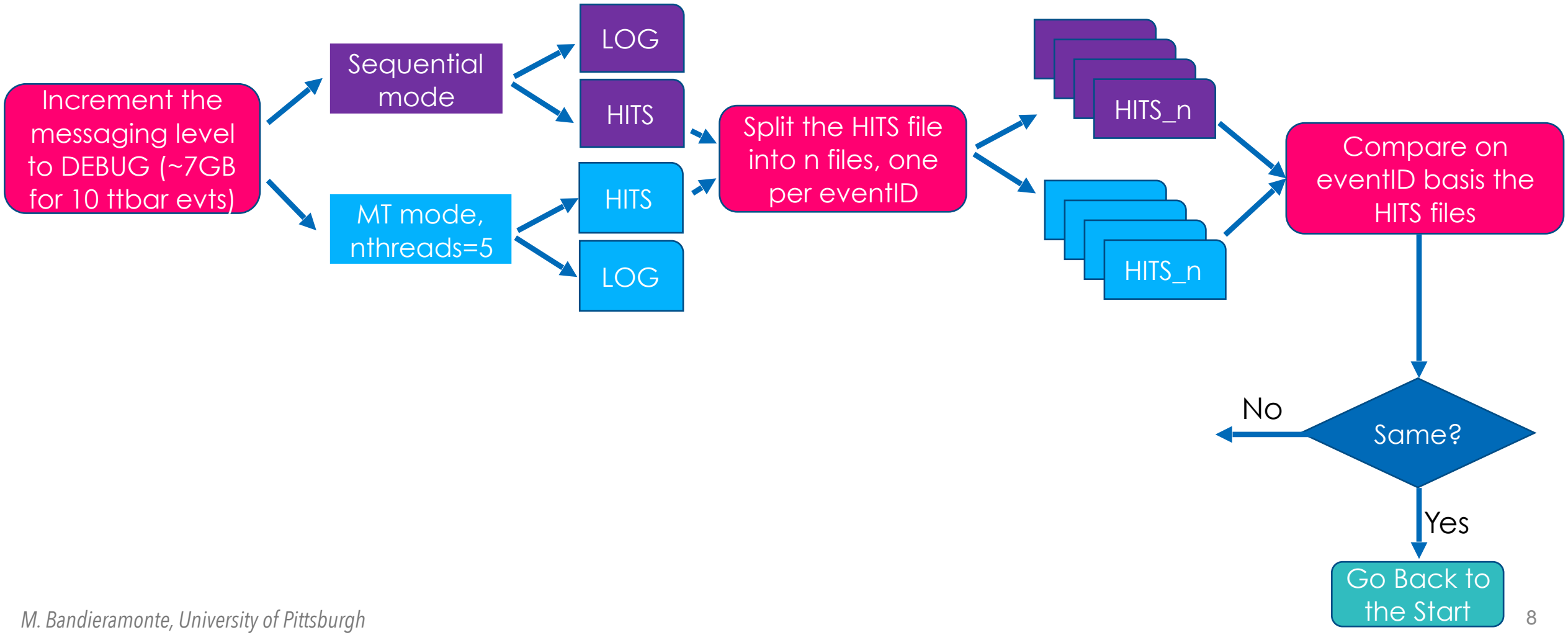

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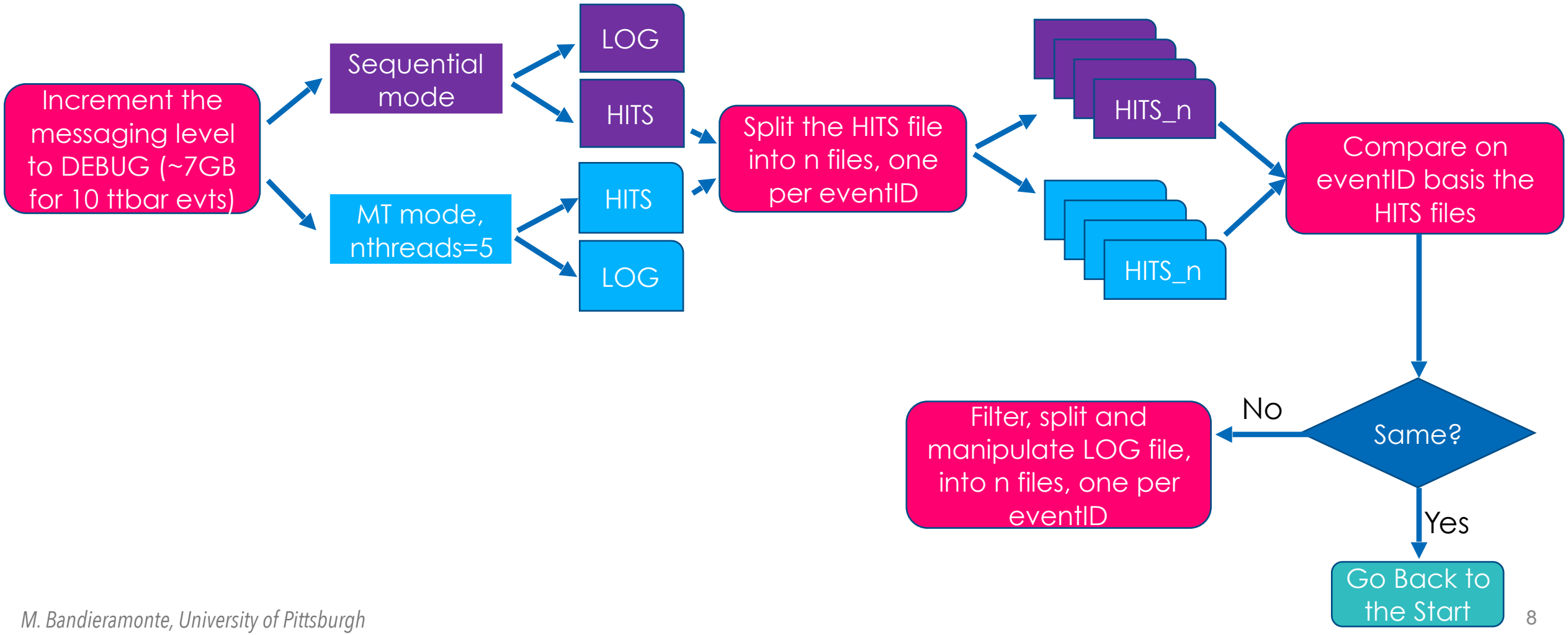

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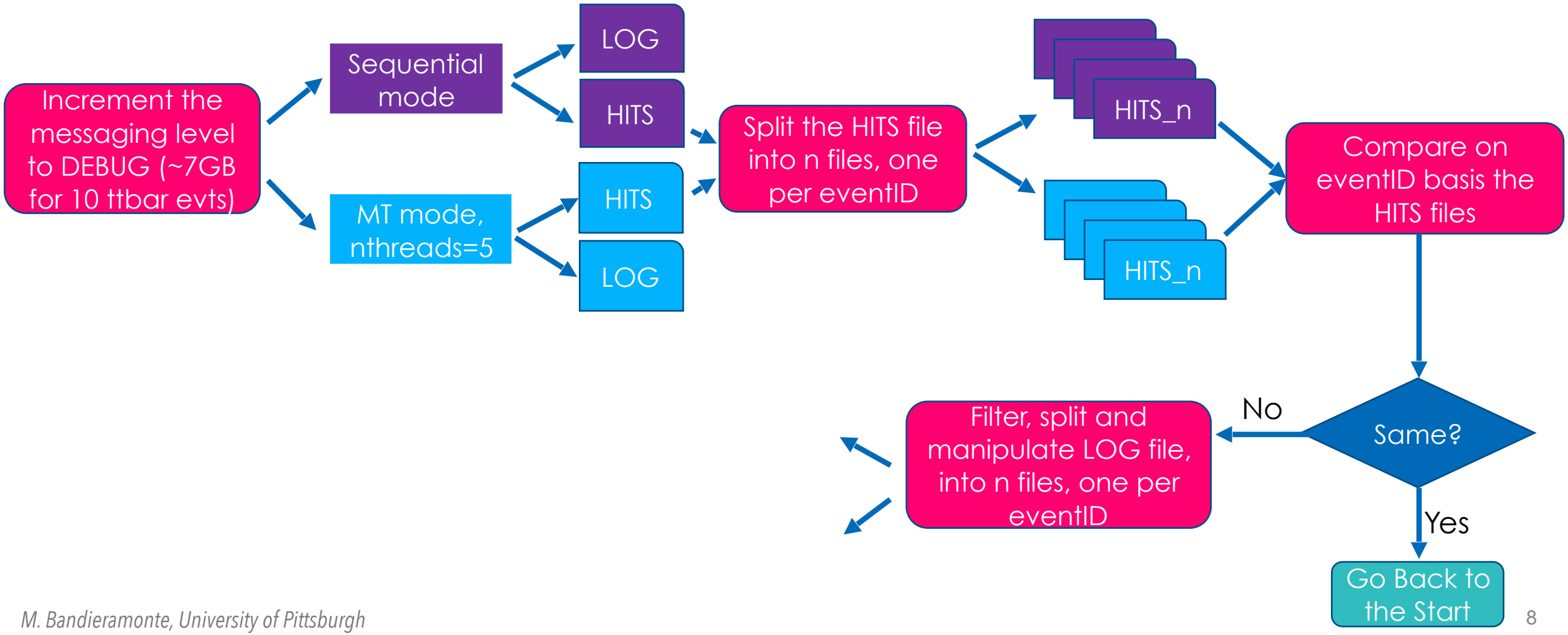

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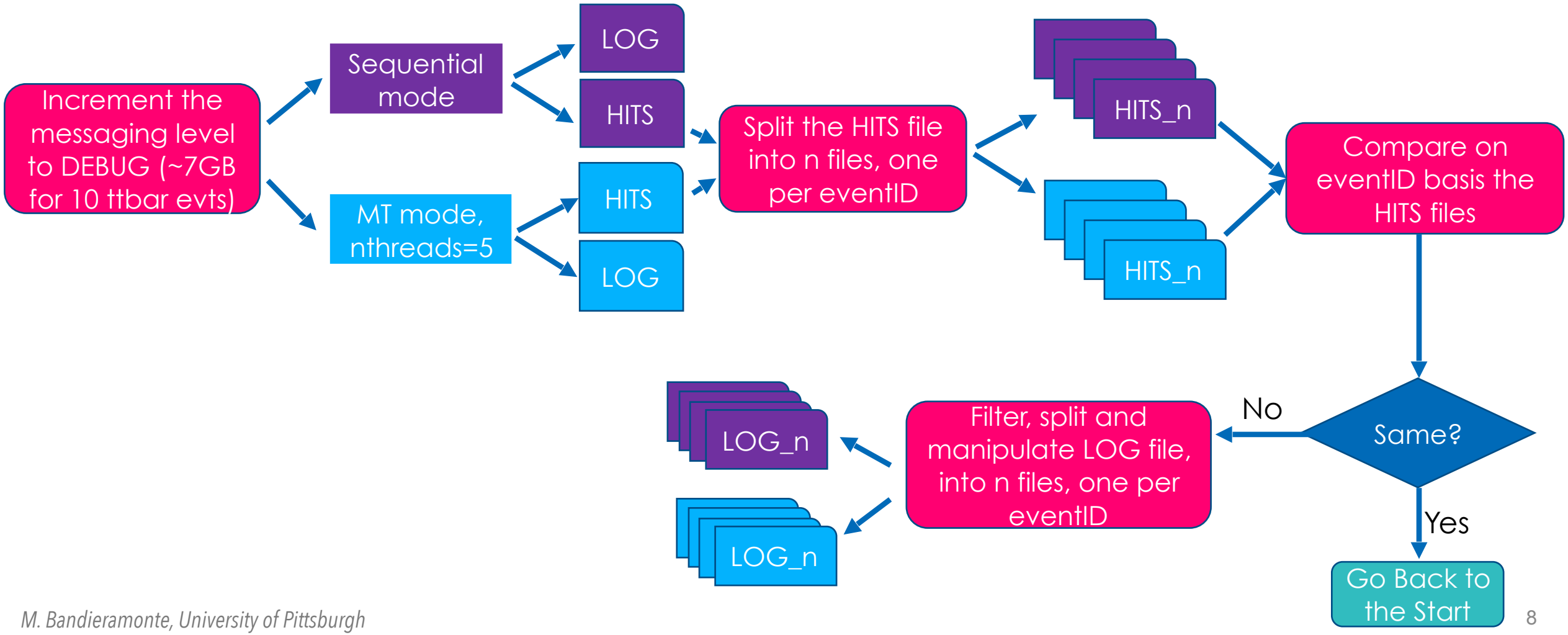

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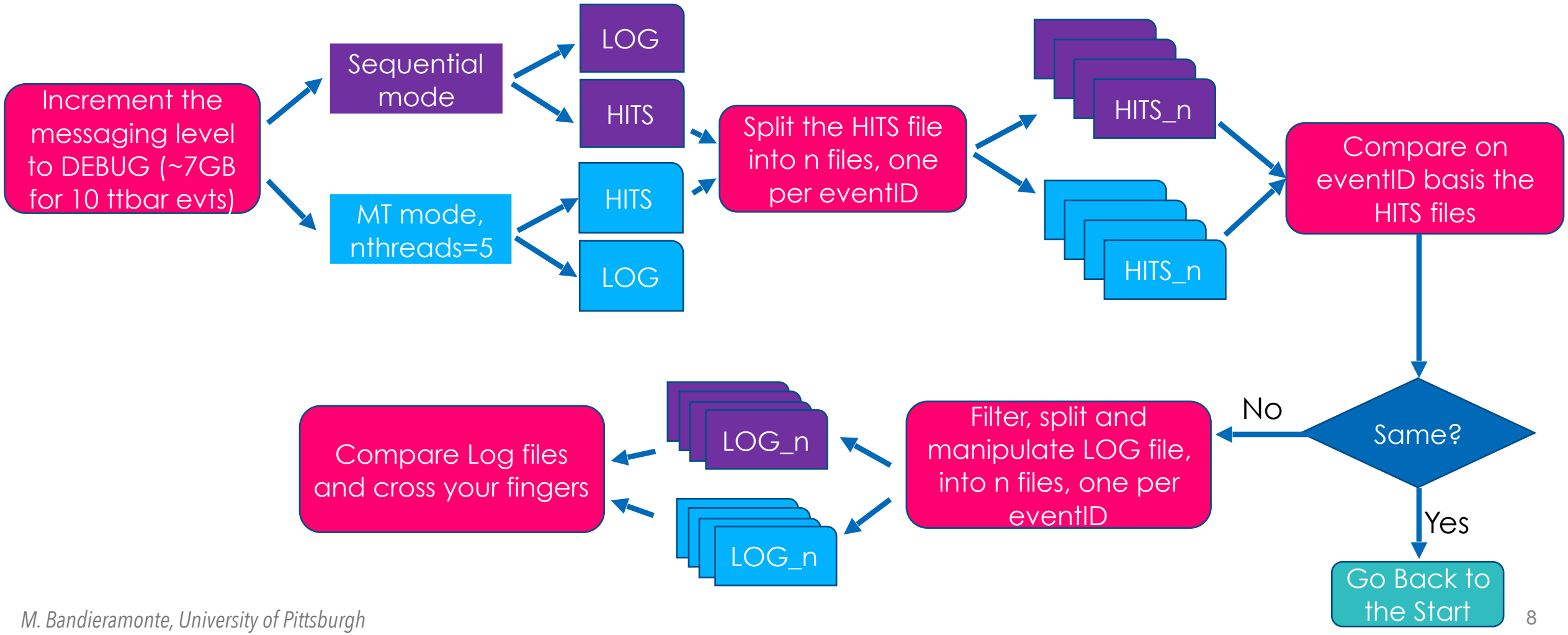

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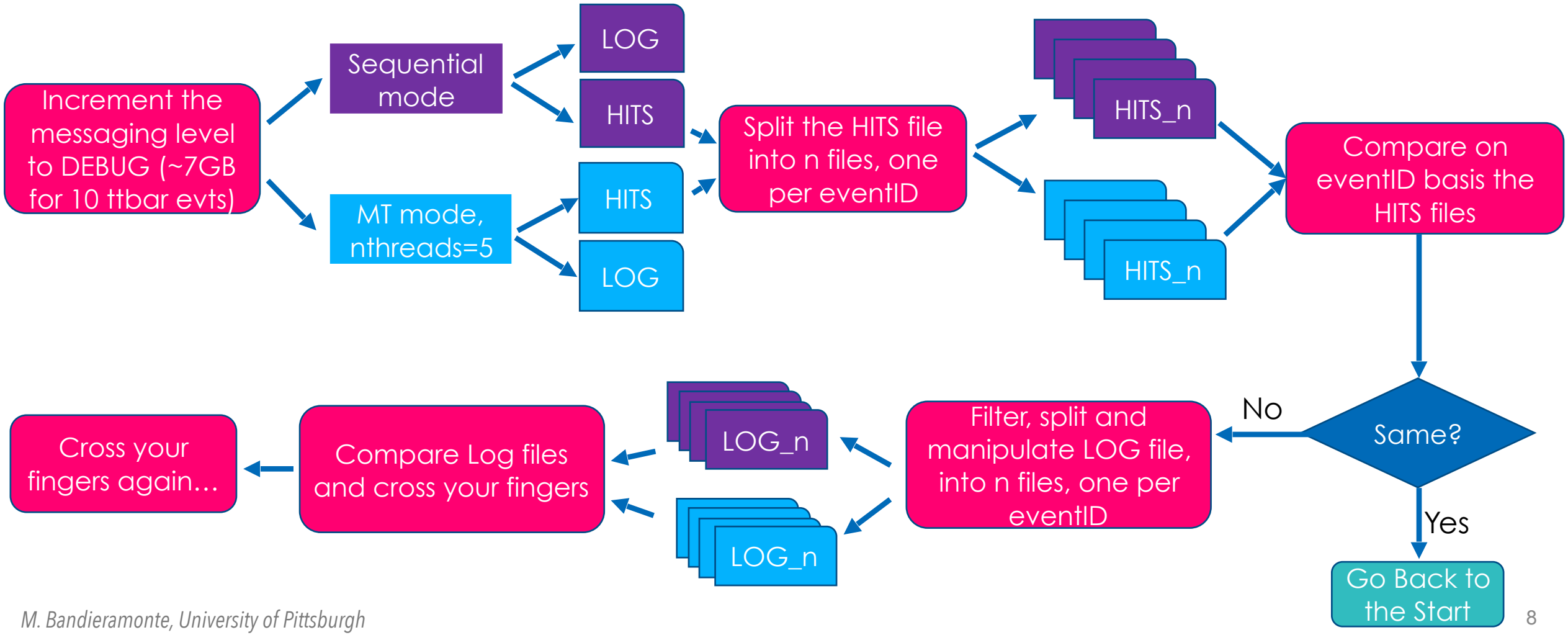

Strategy for MT debugging

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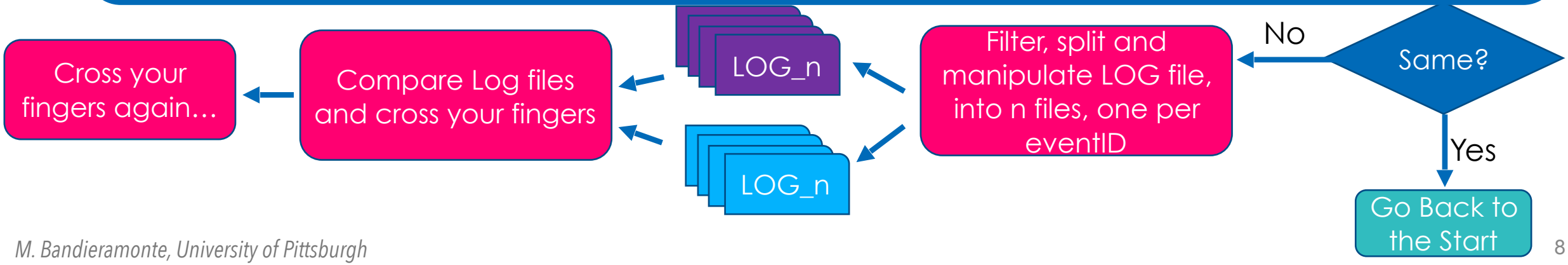
EMBPresamplerCalculator

```
10673650 EMBPresamplerCa...  DEBUG  module,x0,y0,current0 from map 5 0.541834 0.234809 [-1.03946-] {+1.08644+}
10673651 EMBPresamplerCa...  DEBUG    Energy for sub step 0.0246629
10673652 EMBPresamplerCa...  DEBUG  set current map for module 5
10673653 EMBPresamplerCa...  DEBUG  module,x0,y0,current0 from map 5 0.523319 0.204478 [-1.00652-] {+1.04875+}
10673654 EMBPresamplerCa...  DEBUG    Energy for sub step 0.0246629
10673655 EMBPresamplerCa...  DEBUG  set current map for module 5
10673656 EMBPresamplerCa...  DEBUG  module,x0,y0,current0 from map 5 0.504805 0.174147 [-0.973578-] {+1.01106+}
10673657 EMBPresamplerCa...  DEBUG    Energy for sub step 0.0246629
10673658 EMBPresamplerCa...  DEBUG  set current map for module 5
10673659 EMBPresamplerCa...  DEBUG  module,x0,y0,current0 from map 5 0.48629 0.143817 [-0.932291-] {+0.970216+}
10673660 EMBPresamplerCa...  DEBUG Hit Energy/Time [-0.175662-] {+0.179722+} 87.253
```



The problem & the fix

PsMap is a singleton and ***SetMap()*** method was not thread-safe:

- set the current "Current map" in its private member **m_curr**
- store the module in **m_module**.

LArBarrelPresamplerCalculator.cxx

```
m_psmap->SetMap(imodule);
m_psmap->Map()-> GetAll(x0,y0,&gap,&current0,&current1,&current2);
```

PsMap.cxx

```
void PsMap::SetMap(int module)
{
  if (m_module==module) return;
  m_module=module;
  […]
  if (m_theMap.find(code) != m_theMap.end())
    m_curr = m_theMap[code];
  else {
        m_curr=0;
  }
}
```

- ! **Data race** in the *LArBarrelPresamplerCalculator:*
  - **SetMap** could be called by another thread before the current values were obtained

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LArBarrelPresamplerCalculator.cxx

```
CurrMap* cm = m_psmap->GetMap(imodule);
```

PsMap.cxx

```
CurrMap* PsMap::GetMap(int module) const
{
  [..]
  auto it = m_theMap.find(code);
  if (it != m_theMap.end())
    return  it->second;
  else {
        return nullptr;
  }
}
```

- **! Data race** in the *LArBarrelPresamplerCalculator:*
  - **SetMap** could be called by another thread before the current values were obtained
- Remove **`SetMap()`** function and **`m_curr`** and **`m_module`** members
- Implement **`CurrMap* GetMap(imodule) const`** method

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}
```

Tested with 100 ttbar with MT 10 threads → Solved!

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- Remove **`SetMap()`** function and **`m_curr`** and **`m_module`** members
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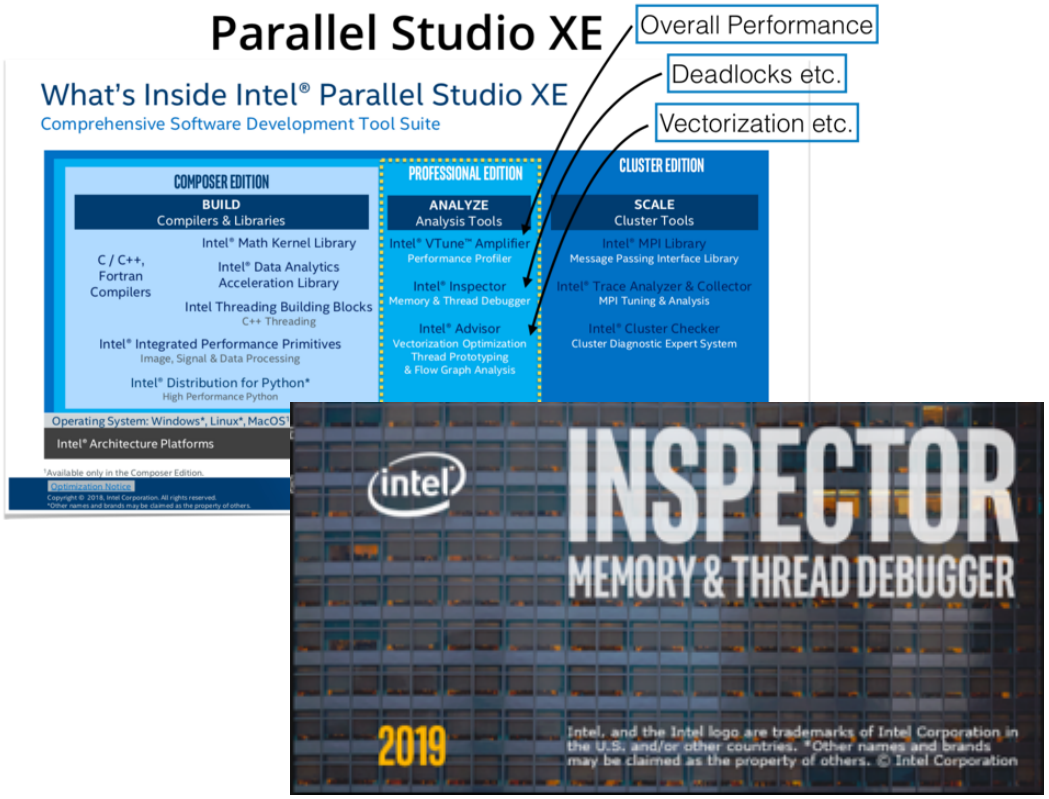
Tools to detect thread related issues




```
[mbandier@p05614910w96644 g4mt_tests]$ inspxe-cl -help
Intel(R) Inspector Command Line tool
Copyright (C) 2009-2018 Intel Corporation. All rights reserved.

Usage: inspxe-cl <-action> [-action-option] [-global-option] [[--] target [target options]]

Type 'inspxe-cl -help <action>' for help on a specific action.

Available actions:
    collect
    collect-with
    command
    convert-suppression-file
    create-breakpoints
    create-suppression-file
    export
    finalize
    help
    import
    knob-list
    merge-states
    report
    version

[mbandier@p05614910w96644 g4mt_tests]$ inspxe-cl -help collect
-c, -collect=<string>          Choose an analysis type.

Usage: inspxe-cl -collect=<string> [-action-option] [-global-option] [--] <target> [<target options>]

  <string> gives the analysis type to perform on <target>. Use -knob-list to
  list the knobs for an analysis type. Available analysis types:
    Name  Description
    mi1   Detect Leaks
    mi2   Detect Memory Problems
    mi3   Locate Memory Problems
    ti1   Detect Deadlocks
    ti2   Detect Deadlocks and Data Races
    ti3   Locate Deadlocks and Data Races

Action options:
-app-working-dir=<string>      Specify a directory where the application will be
```

```
[mbandier@p05614910w96644 g4mt_tests]$ inspxe-cl -collect ti2 -knob stack-depth=16  -- python /build2/mb/build/install/AthSimulation/22.0.0/InstallArea/x86_64-slc6-gcc62-opt/bin/athena.py "--threads=4" "runargs.AtlasG4Tf.py" "SimuJobTransforms/skeleton.EVGENtoHIT_MC12.py"
```

Data races in AthenaMT

- Collection of data races detected in AthenaMT simulation with **Intel Inspector**:

ATLASSIM-3991	Data race 1 - read/write		OPEN
ATLASSIM-3992	Data race 2 - read/write		OPEN
ATLASSIM-3993	Data race 3 - read/write		OPEN
ATLASSIM-3994	Data race 4 - read/write		RESOLVED
ATLASSIM-3995	Data race 5 - read/write		OPEN
ATLASSIM-3996	Data race 6 - read/write		OPEN
ATLASSIM-3997	Data race 7 - read/write		RESOLVED
ATLASSIM-3998	Data race 8 - read/write		OPEN
ATLASSIM-3999	Data race 9 - read/write		OPEN
ATLASSIM-4005	Data race 10 - read/write		OPEN
ATLASSIM-4015	Data race 11 - write/write - libRIO.so and AtlasFieldSvc		OPEN
ATLASSIM-4016	Data race 12 - write/write - libG4AtlasAlgLib and libGaudiCoreSvc		OPEN

Description

Data race of read-write type:

```
Description: Read
Source: char_traits.h:262
Function: compare
Module: libstdc++.so.6
Variable: tileVolumeString

Call Stack:
libstdc++.so.6!compare - char_traits.h:262
libTileGeoG4SDLib.so!find - basic_string.h:2025
libTileGeoG4SDLib.so!ProcessHits - TileGeoG4SD.cc:61
libG4tracking.so!Hit - G4VSensitiveDetector.hh:122
libG4tracking.so!ProcessOneTrack - G4TrackingManager.cc:126
libG4event.so!DoProcessing - G4EventManager.cc:185
libG4AtlasAlgLib.so!ProcessEvent - G4AtlasWorkerRunManager.cxx:179
libG4AtlasAlgLib.so!execute - G4AtlasAlg.cxx:325
libGaudiPythonLib.so!execute - Algorithm.h:51
libGaudiKernel.so!sysExecute - Algorithm.cpp:496
libGaudiHive.so!execute - AlgoExecutionTask.cpp:60
```

```
Description: Write
Source: char_traits.h:290
Function: copy
Module: libTileGeoG4SDLib.so
Variable: tileVolumeString

  Code snippet:
   288      if (__n == 0)
   289        return __s1;
  >290      return static_cast<char_type*>(__builtin_memcpy(__s1, __s2, __n));
   291        }
   292

Call Stack:
libTileGeoG4SDLib.so!copy - char_traits.h:290
libTileGeoG4SDLib.so!_ZN8G4StringC4EPKc - G4String.icc:39
libTileGeoG4SDLib.so!ProcessHits - TileGeoG4SD.cc:61
libG4tracking.so!Hit - G4VSensitiveDetector.hh:122
libG4tracking.so!ProcessOneTrack - G4TrackingManager.cc:126
libG4event.so!DoProcessing - G4EventManager.cc:185
libG4AtlasAlgLib.so!ProcessEvent - G4AtlasWorkerRunManager.cxx:179
libG4AtlasAlgLib.so!execute - G4AtlasAlg.cxx:325
```

Problem:

```
static const G4String tileVolumeString("Tile");
```

Was not thread-safe, substituted with:

```
static const char * const tileVolumeString = "Tile" ;
```

That is initialised before the first call

Lock Hierarchy Violations

- Collection of lock hierarchy violations detected in AthenaMT simulation with **Intel Inspector**:

- It happens when two threads are trying to access and lock two critical sections in a different order. Possible deadlock.

Thread 1:

```
Description: Lock owned
Source: gthr-default.h:748
Function: __gthread_mutex_lock
Module: libAthAllocators.so
Variable:  block allocated at ArenaBase.cxx:148

Code snippet:
   746  {
   747    if (__gthread_active_p ())
  >748      return __gthrw_(pthread_mutex_lock) (__mutex);
   749    else
   750      return 0;

Call Stack:

libAthAllocators.so!__gthread_mutex_lock - gthr-default.h:748
libAthAllocators.so!allocator - ArenaBase.icc:40
libGeneratorObjectsTPCnv.so!_ZN2SG21ArenaHandleBaseAllocTINS_18ArenaPoolA
libGeneratorObjectsAthenaPoolPoolCnv.so!createTransient - TPConverter.icc
libGeneratorObjectsAthenaPoolPoolCnv.so!PoolToDataObject - T_AthenaPoolCu
libAthenaPoolCnvSvcLib.so!createObj - AthenaPoolConverter.cxx:68
libAthenaBaseComps.so!makeCall - AthCnvSvc.cxx:565
```

Thread 2:

```
Description: Lock owned
Source: gthr-default.h:748
Function: __gthread_mutex_lock
Module: libAthAllocators.so
Variable: block allocated at ArenaBase.cxx:30
Code snippet:

   746 {
   747 if (__gthread_active_p ())
  >748 return __gthrw_(pthread_mutex_lock) (__mutex);
   749 else
   750 return 0;


Call Stack:

libAthAllocators.so!__gthread_mutex_lock - gthr-default.h:748
libStoreGateLib.so!clearStore - SGImplSvc.cxx:309
libStoreGateLib.so!clearStore - SGHiveMgrSvc.cxx:49
libAthenaServices.so!clearWBSlot - AthenaHiveEventLoopMgr.cxx:1310
libAthenaServices.so!drainScheduler - AthenaHiveEventLoopMgr.cxx:1260
libAthenaServices.so!nextEvent - AthenaHiveEventLoopMgr.cxx:850
```

Click to edit

AthenaMT & Geant4MT validation

- **Recent progress highlights**:
  - **Output** validation:
    - Fixed: thread-unsafety causing difference in HITS of LAr sensitive detector (~1-2%)
    - Fixed: thread-unsafety causing difference in HITS of Tile sensitive detector (~1-5%)
    - Fixed: simulation with CaloCalibrationHit (~50% of Dead material hits)

We can now run reliably full single-threaded and multi-threaded simulations, results are fully consistent **(read identical) !** physics validation in progress.

- Confirmed reproducibility of simulation with **SUSY/Exotics G4Extensions** enabled:
  - We currently have six packages which add support for additional particles and physics processes to Geant4
    - Charginos - Stable and Decaying Charginos – OK ✓
    - Gauginos - OK ✓
    - Neutralinos - Decaying - OK ✓
    - Monopoles - OK ✓
    - Quirks - Postponed - lack of samples (no associated physics analysis) ✗
    - RHadrons - waiting for samples ✗
    - Sleptons - Stable, Decaying taus, Decaying light - OK ✓

AthenaMT vs AthenaMP benchmarks

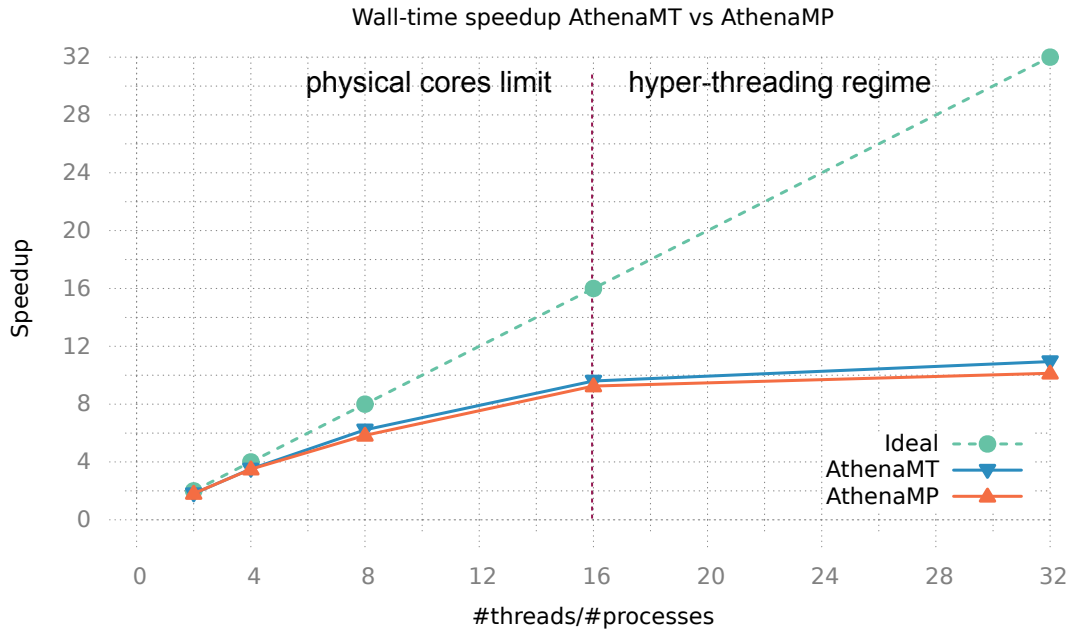
```
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Byte Order:            Little Endian
CPU(s):                32
On-line CPU(s) list:   0-31
Thread(s) per core:    2
Core(s) per socket:    8
Socket(s):             2
NUMA node(s):          2
Model:                 79
Model name:            Intel(R) Xeon(R)
                         CPU E5-2620 v4 @ 2.10GHz
Test on 100 ttbar events, with prom
Athena, r2019-09-30T2130,master

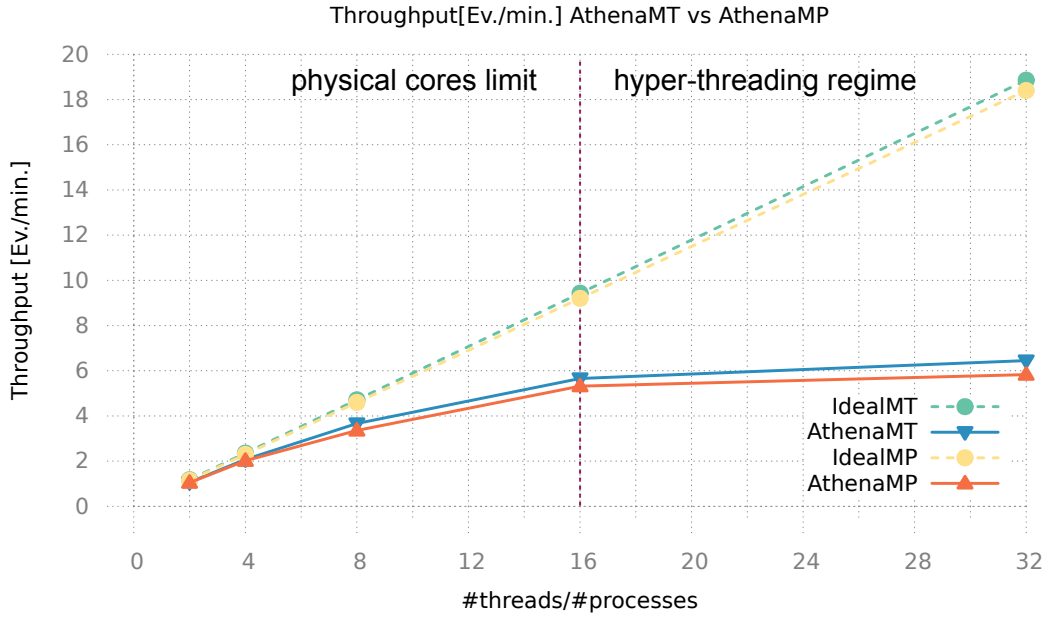
results are AVG of 5 separate runs (from 1-32
threads/processes) - the machine was quiet all the
time (me as only user)
```

$$\text{AthenaMT Speedup}_{th\_n} = \text{Wall-time}_{th\_1} / \text{Wall-time}_{th\_n}$$

$$\text{AthenaMP Speedup}_{proc\_n} = \text{Wall-time}_{proc\_1} / \text{Wall-time}_{proc\_n}$$

Wall-Time [min.]	1 thread/process
AthenaMT	169.6733333
AthenaMP	173.9166667





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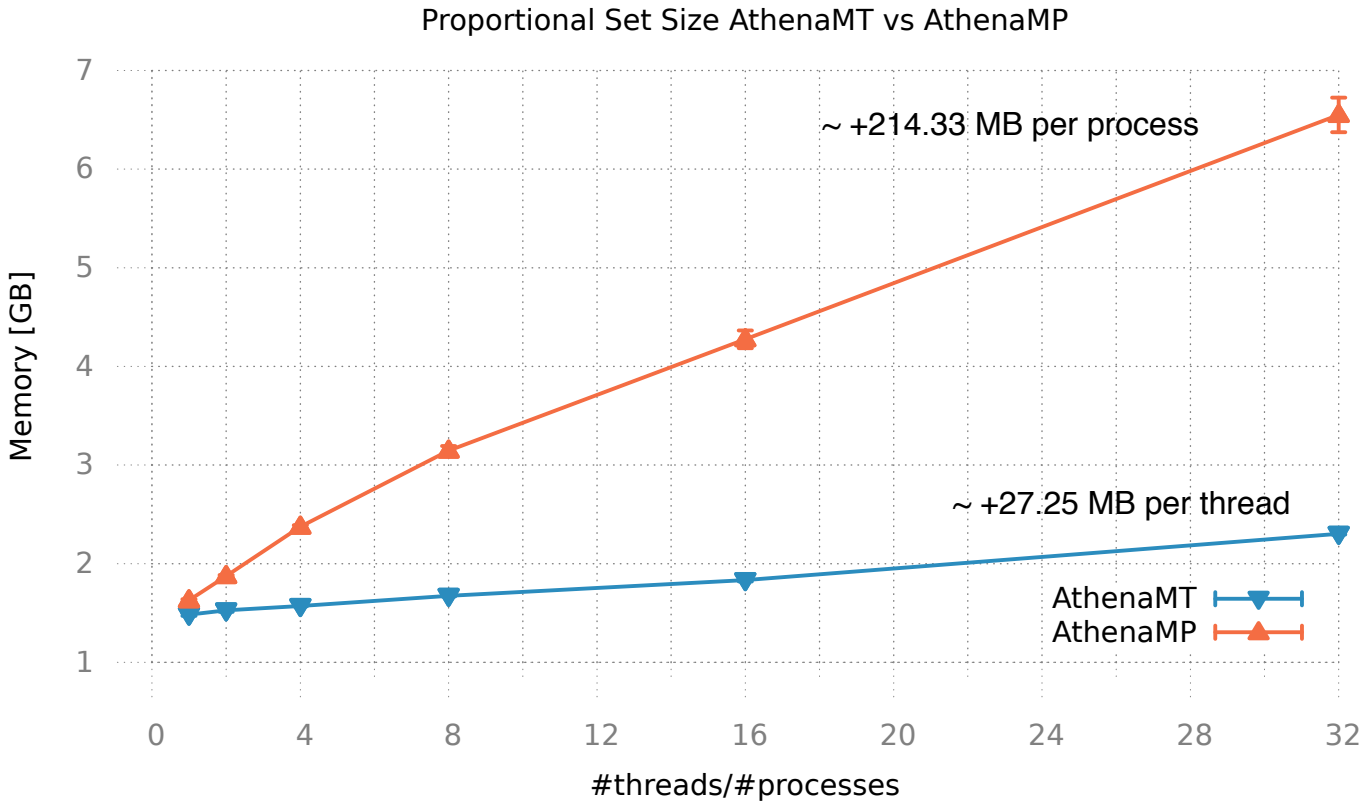
PSS[GB]	1 thread/process
AthenaMT	1.482771301
AthenaMP	1.628312683



The Proportional Set Size (PSS) is the portion of main memory occupied by a process and is composed by the private memory of that process plus the proportion of shared memory with one or more other processes

AthenaMT vs AthenaMP benchmarks

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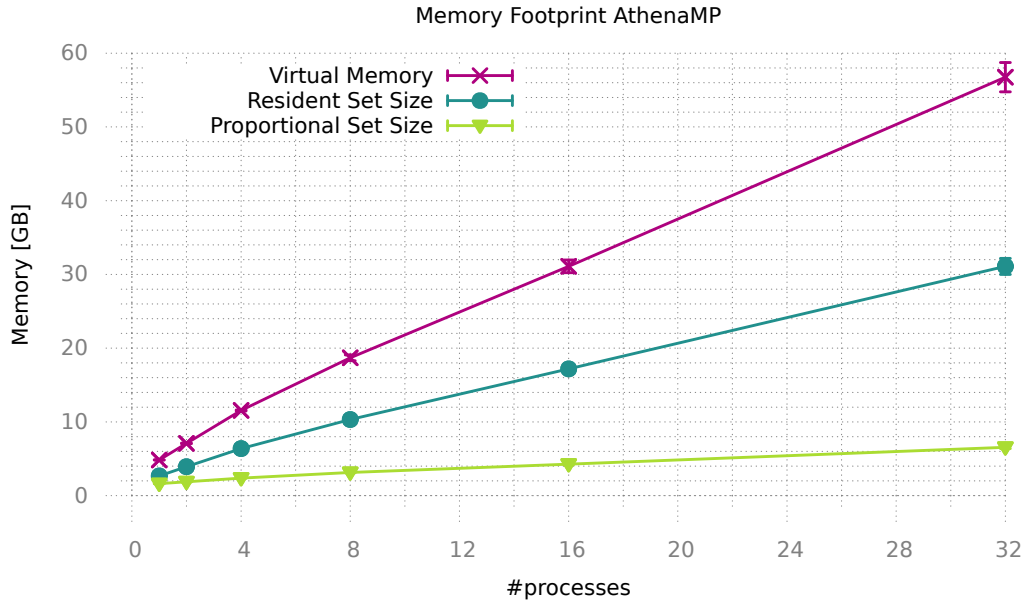

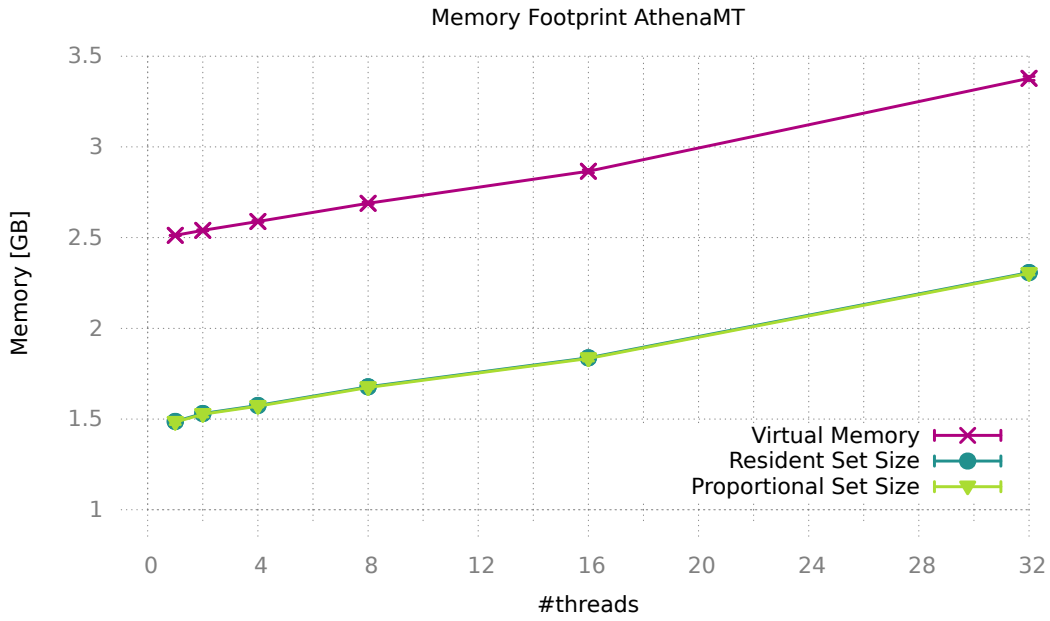

Summary

- **The Athena Multi-threaded simulation with Geant4MT is fully functional**
  - Outside of ISF:
    - The G4 single threaded vs multi-threaded output has been confirmed to be identical
    - 100k grid test were ran with 8 cores without reported issues (physics validation in progress)
  - Inside ISF:
    - simulation runs correctly in multi-threaded mode with 1 thread and the output has been validated
- Next steps
  - *Solve the thread-unsafely issues and assure that G4MT simulation works with more than one thread and that the results are reproducible*

Thanks for your attention.

Marilena Bandieramonte
marilena.bandieramonte@cern.ch

Backup slides

AthenaMT vs AthenaMP benchmarks

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