MultiThreading in GEANT4 A SIMULATION TOOLKIT

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A lot of material by J. Pipek

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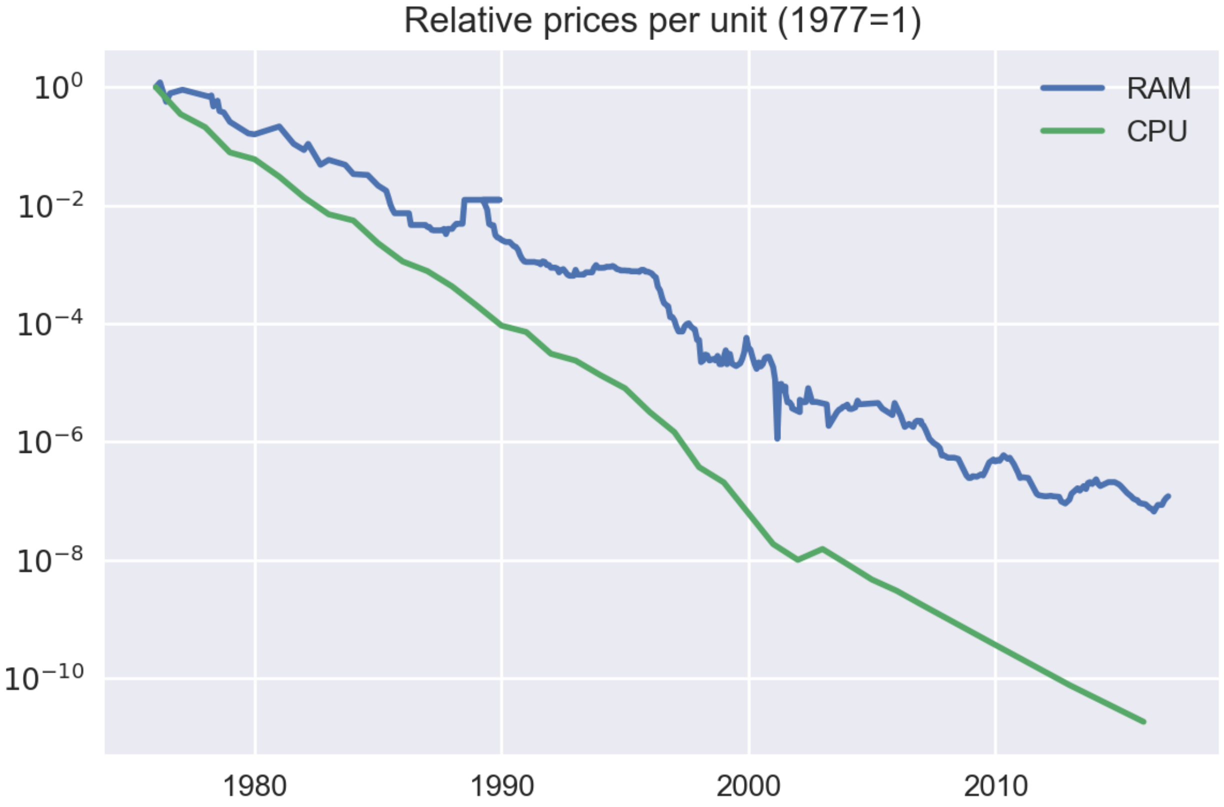
Part I: Motivation

Motivation: performance/$

- Multi-core CPUs
- Expensive memory



slower

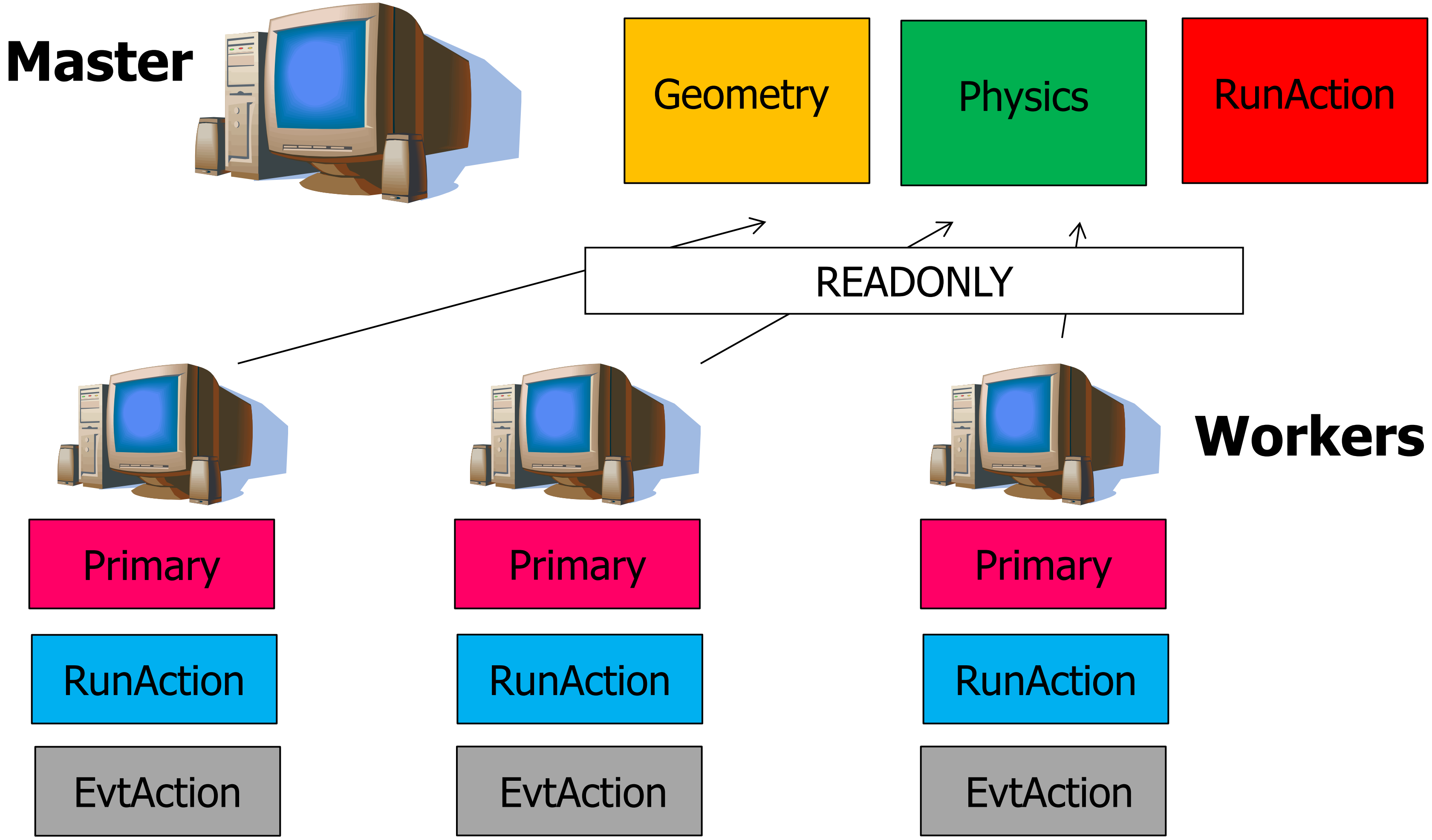
fast

⇒ Memory optimization is more and more important!

Processes vs. threads

- **Processes** are separate instances of running computer programs that have their exclusive execution context, memory and other system resources.
- **Threads** are parallel "independent" executions within a process. They **share** the same memory space and system resources (of the process).

Concept for multi-thread …



Master

Geometry

Physics

RunAction

READONLY

Workers

Primary

RunAction

EvtAction

Primary

RunAction

EvtAction

Primary

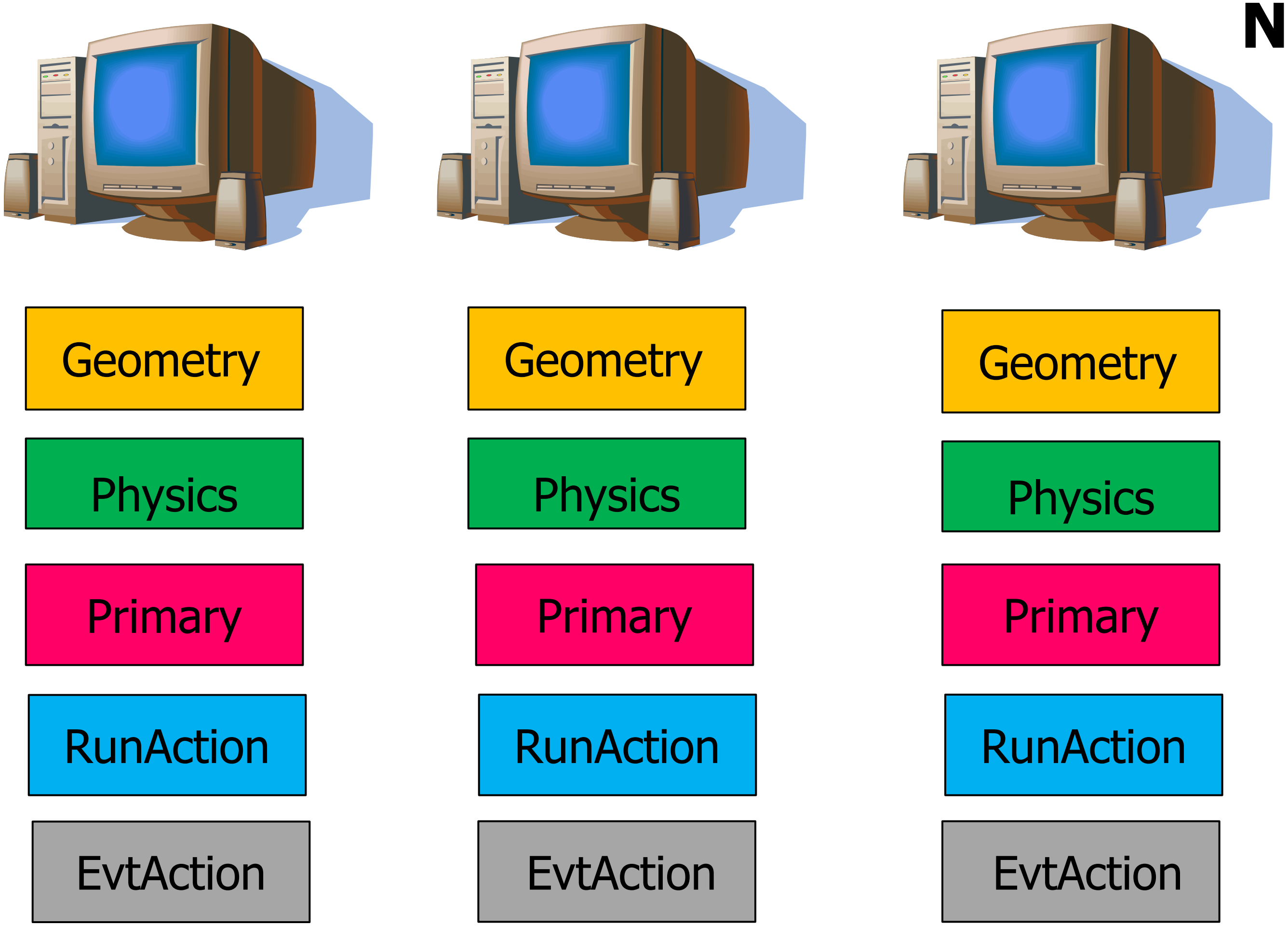
RunAction

EvtAction

… vs. parallelisation

Remember....

Nodes



Geometry	Geometry	Geometry
Physics	Physics	Physics
Primary	Primary	Primary
RunAction	RunAction	RunAction
EvtAction	EvtAction	EvtAction

- Each node hosts a complete simulation
- Many copies of geometry and physics tables
- More memory-thristy

Situation of Monte Carlo sims

- Single-particle simulation is trivially parallelizable!
- Each event can be simulated independently
  - not too much per-event state
  - not too much memory necessary for computation
- A lot of **“static” data**
  - complicated geometries (+ their optimization)
  - physics tables (cross-section data)
  - electromagnetic fields (if present)

⇒ We can benefit a lot from efficient memory sharing!

Solutions: threads

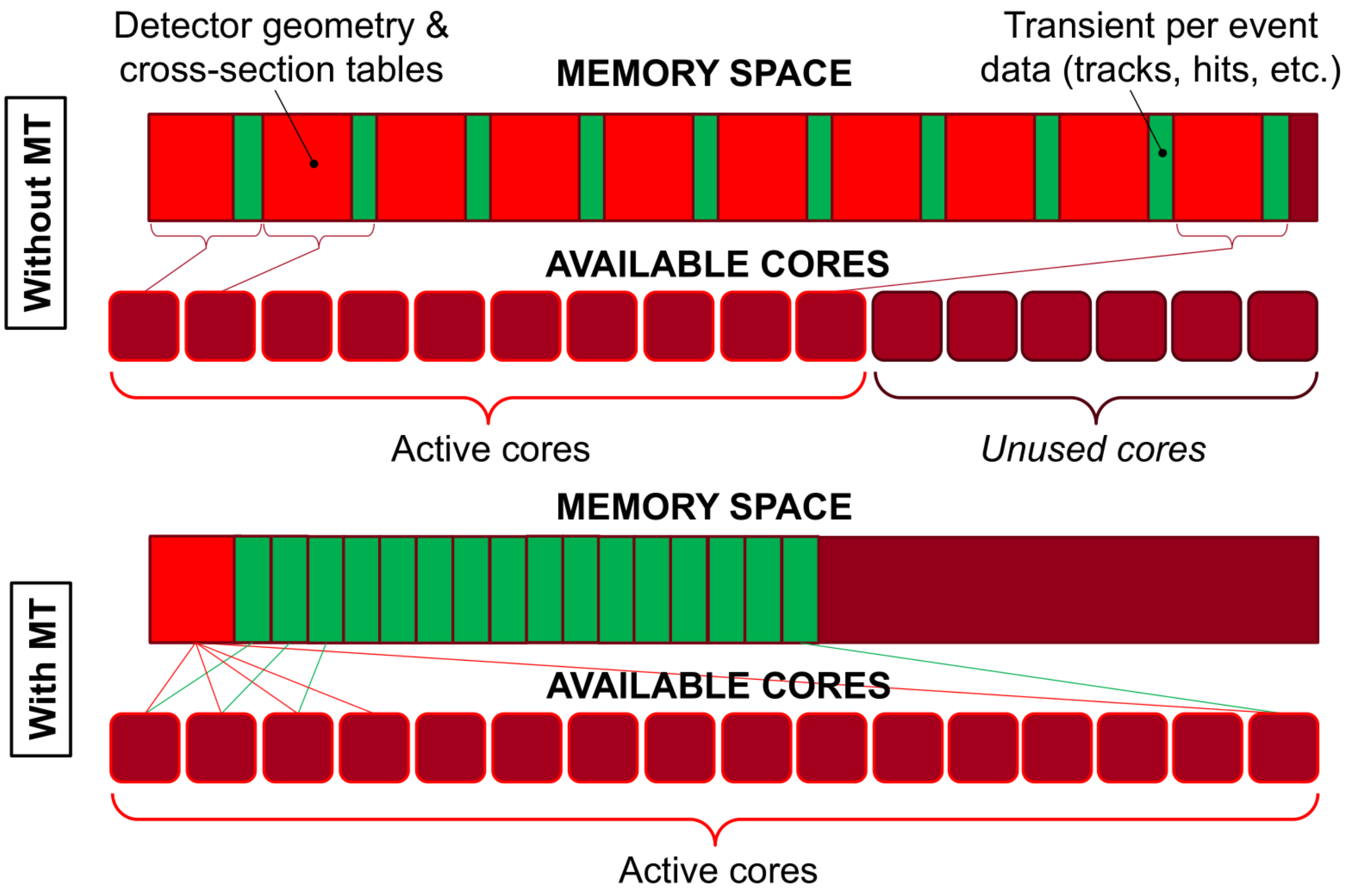
Advantages:

- memory & resource effectivity (sharing)
- in-process synchronization

Disadvantages:

- difficult to write properly
- difficult to debug (indeterministic behaviour)
- race conditions / dead-locks
- thread synchronization costs

Memory in MT applications



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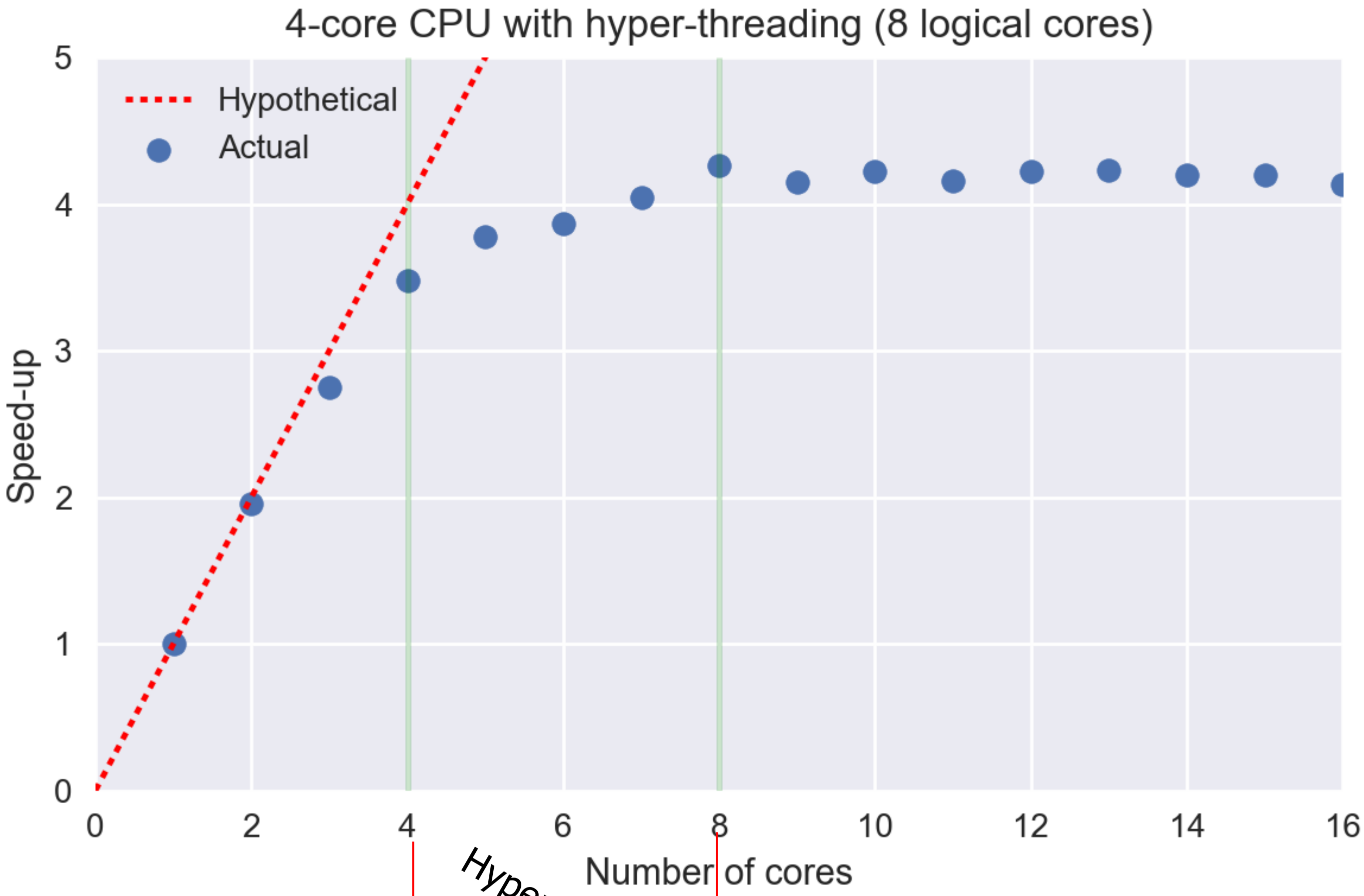
Performance in MT mode



Real physical cores

Hyper-threading

No further gain ☹

Part II: Multi-threading in Geant4

Execution modes in Geant4

- **Sequential mode**
  - everything run in one thread only
  - accepts both user actions and action initialization to support old code (Geant4 < 10.0)
- **Multithreaded mode**
  - "master" thread for the application
  - events simulated in multiple "worker" threads
  - accepts only action initialization
  - Recently supported also in **Windows OS**
    - Starting from Geant4 10.5

Good news: The same code may support both modes!

Multithreading in Geant4

Main thread ("master")

- initialization of geometry and physics
- user interface
- start worker threads
- distribute events
- merge results

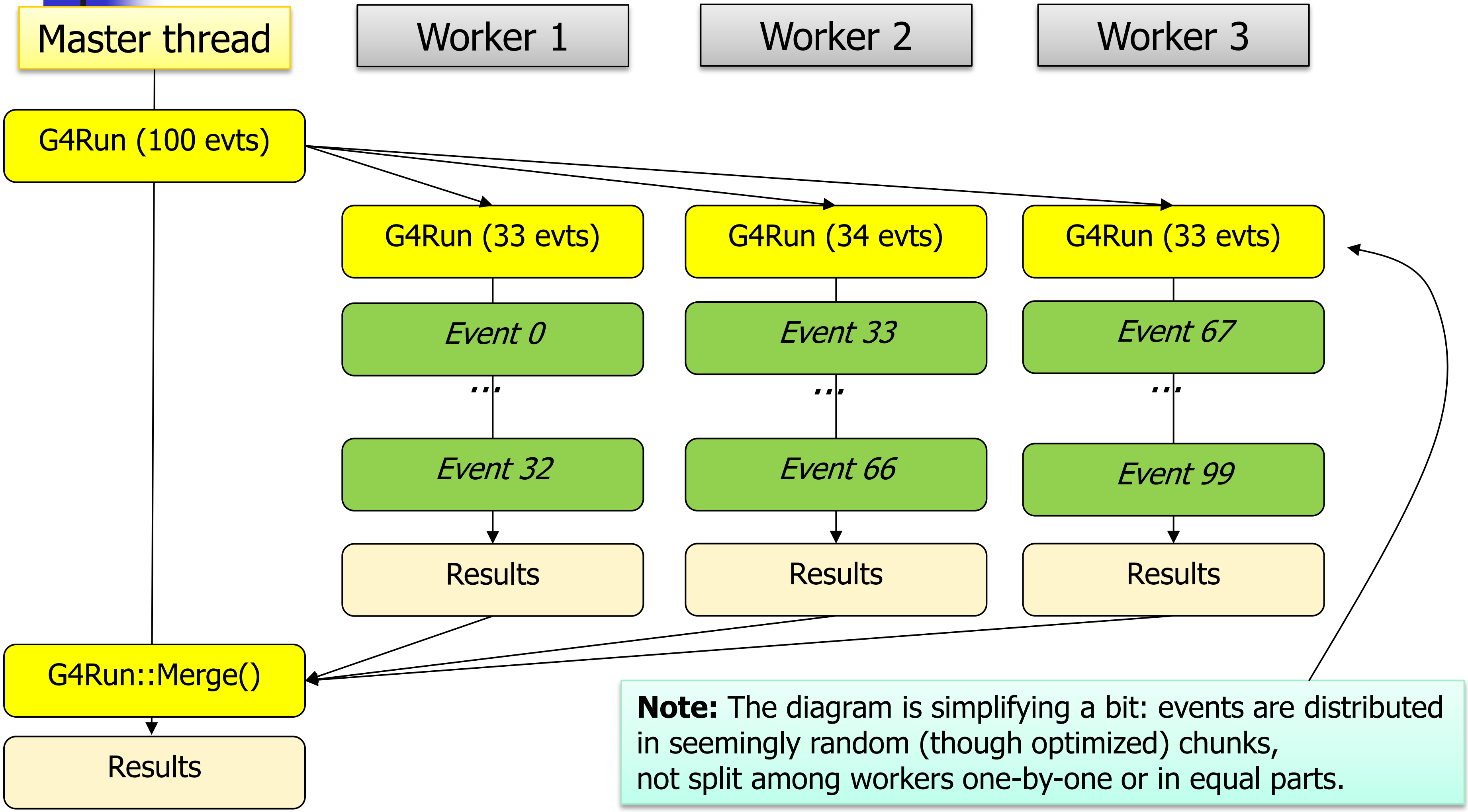
SPLIT

RESPONSIBILITIES

Worker threads

- event simulation
- partial results
- user actions

Event processing

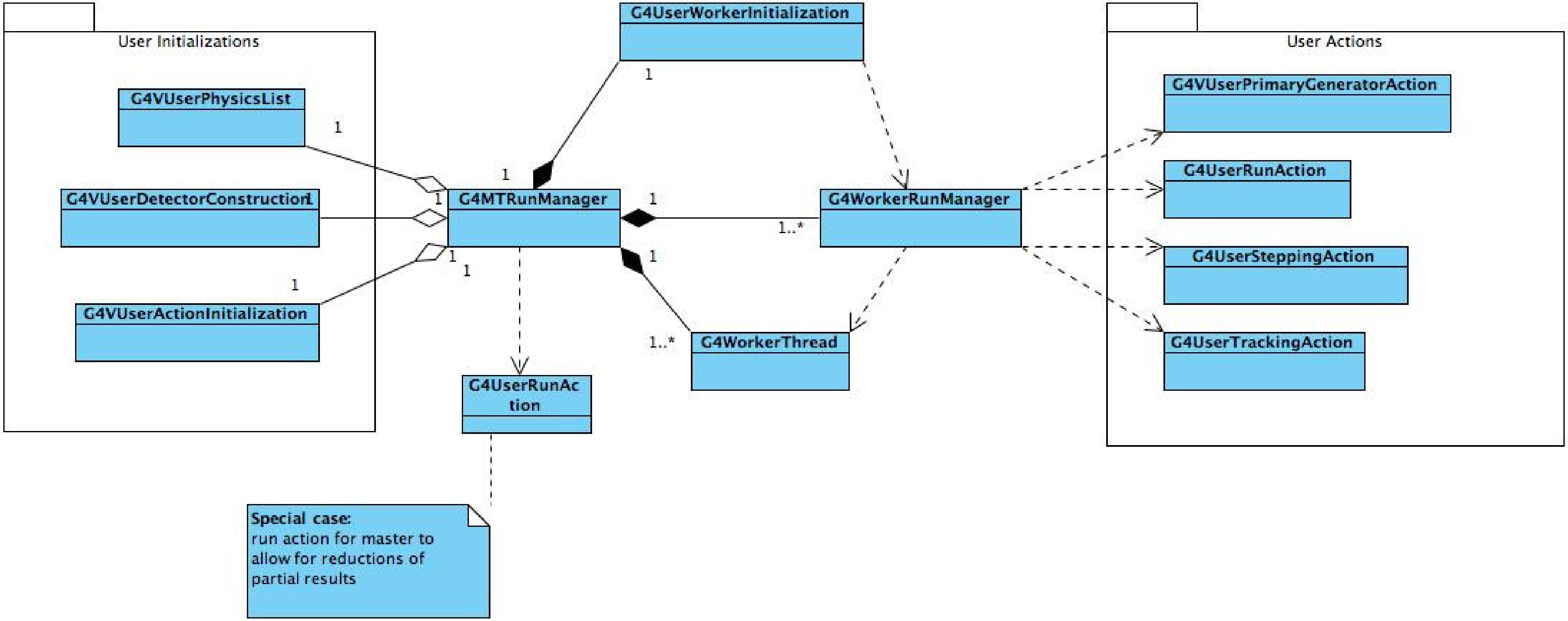


Note: The diagram is simplifying a bit: events are distributed in seemingly random (though optimized) chunks,
not split among workers one-by-one or in equal parts.

G4MTRunManager

- Substitute for sequential **G4RunManager**
  - inherits from it
  - disables the SetUserAction() methods
- **Additional** responsibilities
  - start worker threads
  - distribute events among the workers
  - take care about merging of runs

Run manager relations



Special case:
run action for master to allow for reductions of partial results

G4UserRunAction in MT mode

This action (unlike the rest) can apply in both **worker** and **master** threads:

- To distinguish where you are, use IsMaster() method
- If you have behaviour for master, register the instance in G4VUserActionInitialization::BuildForMaster()

```
void MyActionInitialization::Build() const {
    SetUserAction(new MyRunAction());
    // ...other actions
}

void MyActionInitialization::BuildForMaster() const {
    SetUserAction(new MyRunAction());
    // Only run action
}
```

Note: This, in principle, can be a different class

Merging of runs

- Usually tricky
- Geant4-native tools automatically
  - **command-based scoring**
  - **g4analysis** (histograms summed, trees in separate files)
- Custom data require manual approach
  - in G4Run::Merge() (of your custom “MyRun”)
  - in G4RunEventAction::EndOfRunAction()

```
void MyRunAction::EndOfRunAction(const G4Run* run) {
    // ...
    // Merge accumulables
    G4AccumulableManager* accumulableManager = G4AccumulableManager::Instance();
    accumulableManager->Merge();
    // ...
```

main() for both modes

- CMake setting
  -DGEANT4_BUILD_MULTITHREADED=ON/OFF
- Preprocessor macro G4MULTITHREADED

```
#include <G4MTRunManager.hh>
#include <G4RunManager.hh>

int main() {
    #ifdef G4MULTITHREADED
        G4MTRunManager* runManager = new G4MTRunManager;
    #else
        G4RunManager* runManager = new G4RunManager;
    #endif
    // ..
}
```

Set the number of threads

- Default number of threads: 2
- Change this using
  - UI command:
    - `/run/numberOfThreads 6`
    - `/run/useMaximumLogicalCores`
  - C++ code: `runManager->SetNumberOfThreads(4)`
  - Environment variable (highest priority): G4FORCENUMBEROFTHREADS=4
- **`G4Threading::G4GetNumberOfCores()`** tells the actual number of logical cores
- Further tweaking options available (advanced)

Note: Must be done in pre-initialize stage

Multithreaded G4cout

- If you use `G4cout` for output, it's relatively synchronized and each message is prepended with the thread number
  - **Note:** this does not work with `std::cout` (another reason not to use it!)

```
### Run 0 starts.
G4WT1 > EventAction: absorber energy/time scorer ID: 0
G4WT1 > EventAction: scintillator energy/time scorer ID: 1
G4WT0 > EventAction: absorber energy/time scorer ID: 0
G4WT0 > EventAction: scintillator energy/time scorer ID: 1
 Run terminated.
Run Summary
  Number of events processed : 10000
  User=21s Real=11.36s Sys=1.59s
```

Multithreaded G4cout

- To buffer the output from each thread at a time, so that the output of each thread is grouped and printed at the end of the job

```
/control/cout/useBuffer true|false
```

- To limit the output from threads to one selected thread only:

```
/control/cout/ignoreThreadsExcept 0
```

- To redirect the output from threads in a file:

```
/control/cout/setCoutFile coutFileName
/control/cout/setCerrFile cerrFileName
```

Part III: Thread-aware coding

Good news!

You don't have to care (too much) about threading issues, **provided that** you:

- Don't manually open **external files**
- Use **g4analysis / command-based scoring** for output
- Avoid **static** variables and fields (especially in user actions)
- Correctly **merge runs** if using accumulables or hits
- Use the **`G4(MT)RunManager`** trick in main() (see above)
- Use **`G4VUserActionInitialization`**
- Don't **experiment** with Geant4 kernel
  (especially not in user actions)

If you don't meet these conditions, you must write **thread-aware code**.

Writing thread-safe code

- Find out which variables are modified inside the **worker threads**:
  - these must **not** be **`static`**!
  - use **`G4ThreadLocal`** if possible
  - split the classes if necessary
- Variable “locality”:
  - don’t use global variables
  - don’t use static class fields
  - prefer local variables to class fields
- Be careful about deleting pointers
- Use mutexes & locks when you access a shared resource

Shared resources and mutex'es

- **Mutex** is an object variable that can be locked so that only one thread can use it at the same time.
- **Lock** is an act of locking the mutex:
  - locking an open mutex succeeds immediately
  - locking a locked mutex blocks and waits until it is available again
- Manipulation with **shared resources** should be encapsulated by locking/unlocking a particular mutex

Mutex'es and locks in Geant4

- **Mutex** is best created as static object inside an anonymous namespace (class **G4Mutex**)

```
namespace { G4Mutex myMutex = G4MUTEX_INITIALIZER; }
```

- **G4AutoLock** is a "clever" implementation of the locking mechanism:
  - you just create it with mutex address as parameter
  - when the object is destroyed (end of function or block), the mutex is automatically freed

```
{
    G4AutoLock(&myMutex);
    // ... (do something)
}   // Now, the mutex is freed.
```

Drawbacks and caveats of locking

- Synchronization & locking is not CPU **costly**
- Using multiple locks can lead to a **dead-lock**:
  - Threads need mutexes A and B to proceed
  - Thread1 has locked mutex A
  - Thread2 has locked mutex B
  - **No thread can acquire the second lock!!!**

Alternatives:

- There are more sophisticated threading tools
- Avoid using shared resources as much as possible

G4AutoDelete

- If you don't know when to properly delete an object in threads (typical case!), you can register it with **`G4AutoDelete`**

```
#include "G4AutoDelete.hh"
// ...
G4AutoDelete::Register(aPointer);
// ...
```

- This will ensure that the object is deleted when the worker thread ends.

Thread-safe I/O

- Geant4's scoring and g4analysis are **thread-safe**
- Custom **output** (alternatives):
  - Have one file per thread (or per each instance of user action class)
  - Have only one file and guard the procedure by mutex, add some caching mechanism
- Custom **input**:
  - Read everything in master thread and share the data as read-only
  - Reading on demand – protect by mutex, add some caching mechanism

Example: read particles

```
namespace { G4Mutex myMutex = G4MUTEX_INITIALIZER; }
MyFileReader* MyPrimaryGenAction::fileReader = nullptr;

MyPrimaryGenAction::MyPrimaryGenAction(G4String fileName) {
        G4AutoLock lock(&myMutex);
        if (!fileReader) fileReader = new MyFileReader(fileName);
        particleGun = new G4ParticleGun(1);
        // ...Define particle properties
}

MyPrimaryGenAction::~MyLowEPrimaryGenAction() {
        G4AutoLock lock(&myMutex);
        if (fileReader) { delete fileReader; fileReader = 0; }
}

void MyPrimaryGenAction::GeneratePrimaries(G4Event* anEvent) {
        G4ThreeVector momDirection;
        G4AutoLock lock(&myMutex);
        momDirection = fileReader->GetAnEvent();
        particleGun->SetParticleMomentumDirection(momDirection);
        // ...Set other particle properties
}
```

Conclusion

- Geant4 offers an optimized multithreaded mode (optional)
- Multithreading is powerful but a complex and potentially **dangerous** tool

Hands-on session

- Task 4
  - Task4e: Try to run in sequential and MT

- **`http://202.122.35.42/task4`**