OAK RIDGE National Laboratory

Optimizing Dynamical Cluster Approximation on the Summit supercomputer

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U.S. DEPARTMENT OF ENERGY

SciDAC: Computational Framework for Unbiased Studies of Correlated Electron Systems

- I would like to thank:

  Giovanni Balduzzi (PhD. Student, ETH Zurich)
  Urs Hähner (PhD. Student, ETH Zurich)
  Ying Wai Li (NCCS, ORNL)
  Thomas Maier (CNMS, ORNL)
  Thomas Schulthess (Director, CSCS, ETH Zurich)

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- *This research used resources of the **O**ak Ridge **L**eadership **C**omputing **F**acility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.*

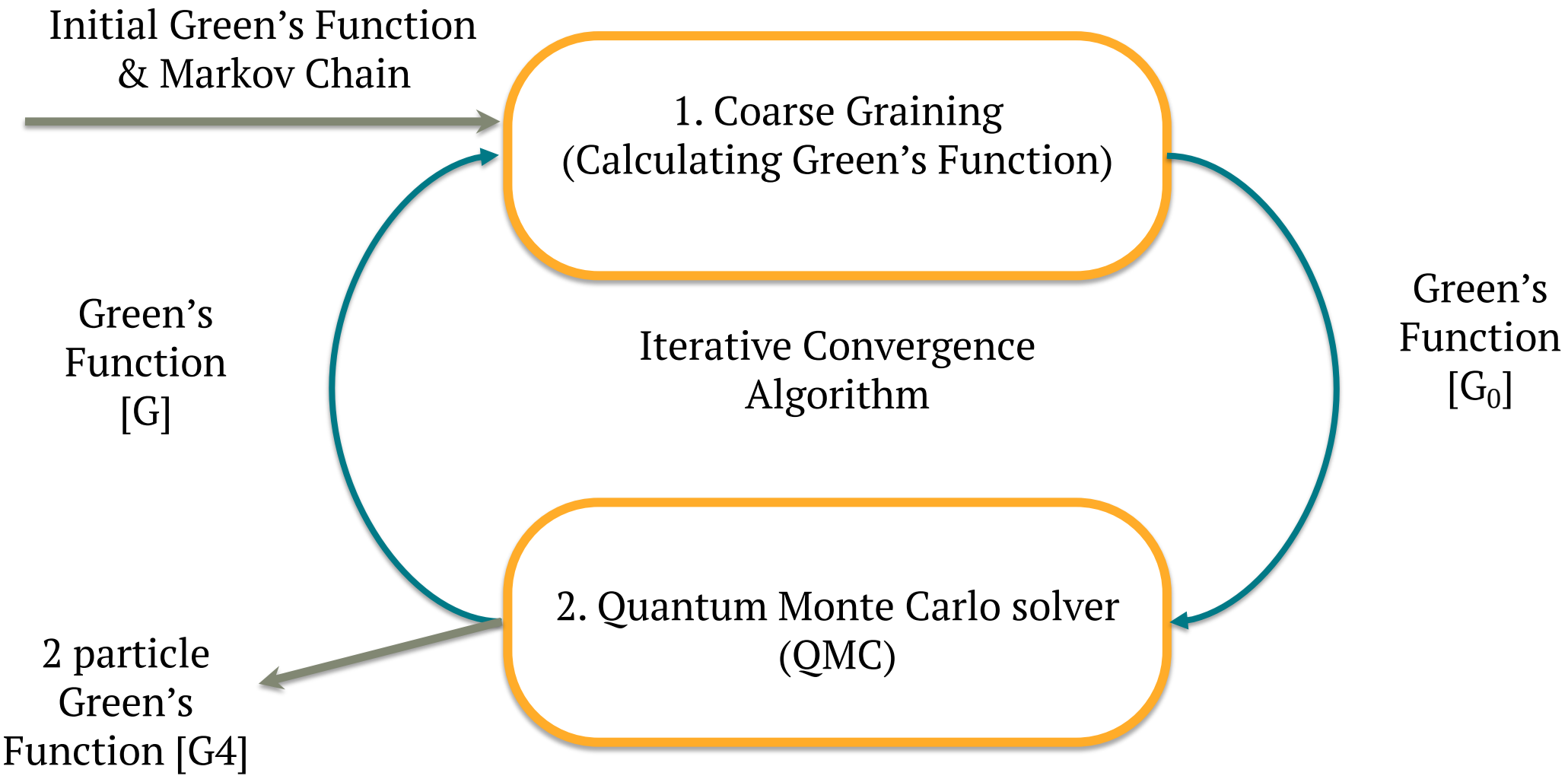
Overview : DCA++

- DCA++ → Dynamical Cluster Approximation
- Numerical simulation tool — predict behaviors of co-related quantum materials (such as **superconductivity**, **magnetism**)
- DCA++ — computes **many-body Green's function** — material's properties can be calculated from this function.
- Iterative self consistent algorithm — two primary kernels
  - **Coarse graining** of single particle *Green's function* (reduces complexity of infinite size lattice problem)
  - **Quantum Monte Carlo** solver

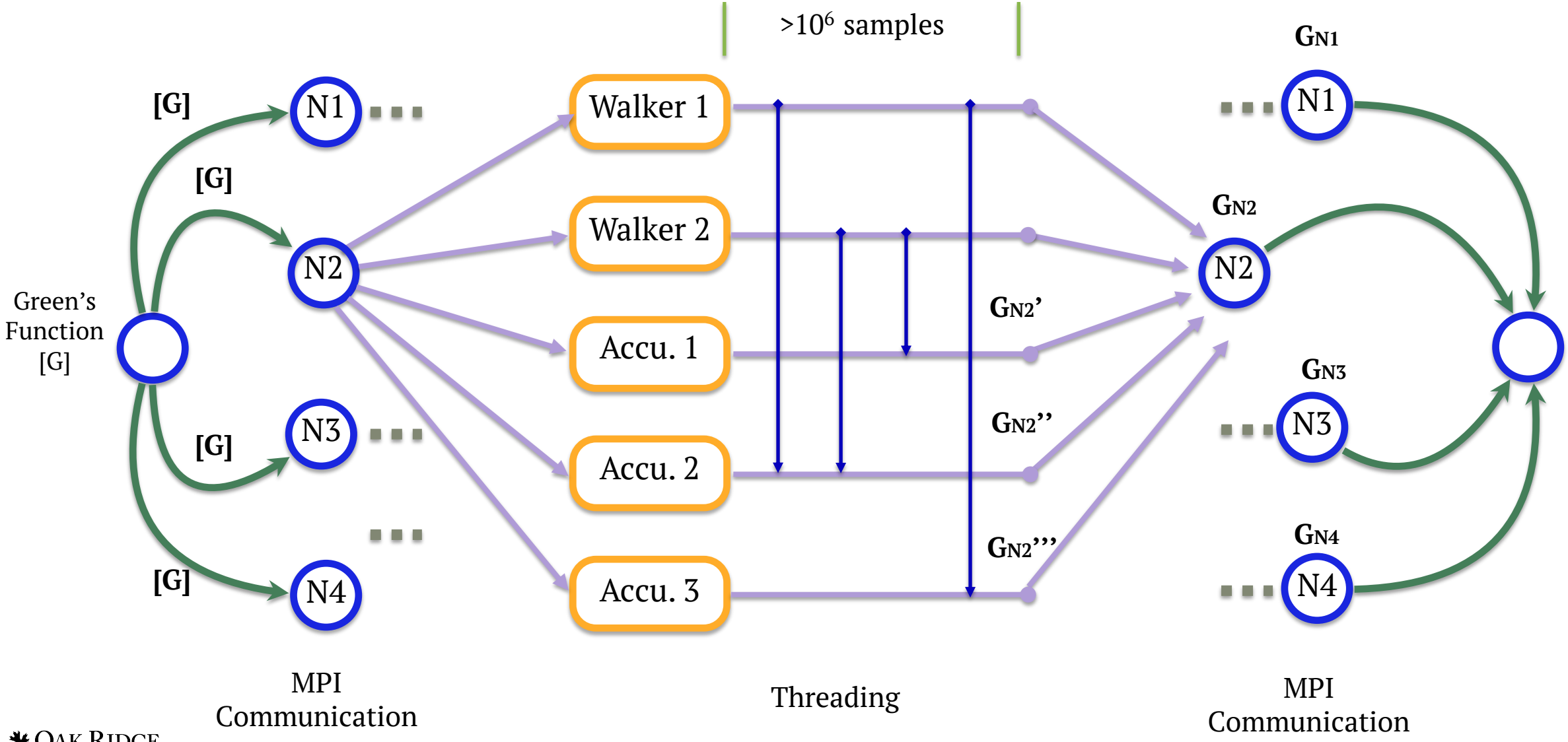
DCA++ ran on Titan – 18600 nodes at16 Petaflop rate (peak), sustained 1.3 Petaflop rate [Gordon Bell 2009]

DCA++: A software framework to solve correlated electron problems with modern quantum cluster methods. *U. Hähner, et al. .CPC 2019.*

DCA++ : Primary kernels workflow

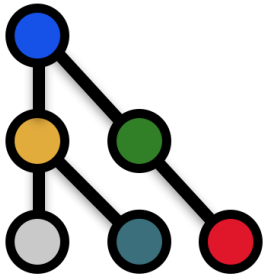


DCA++ : Quantum Monte Carlo Solver



Walkers running on GPU : Accumulators run on the CPU

Profiling DCA++ on Titan

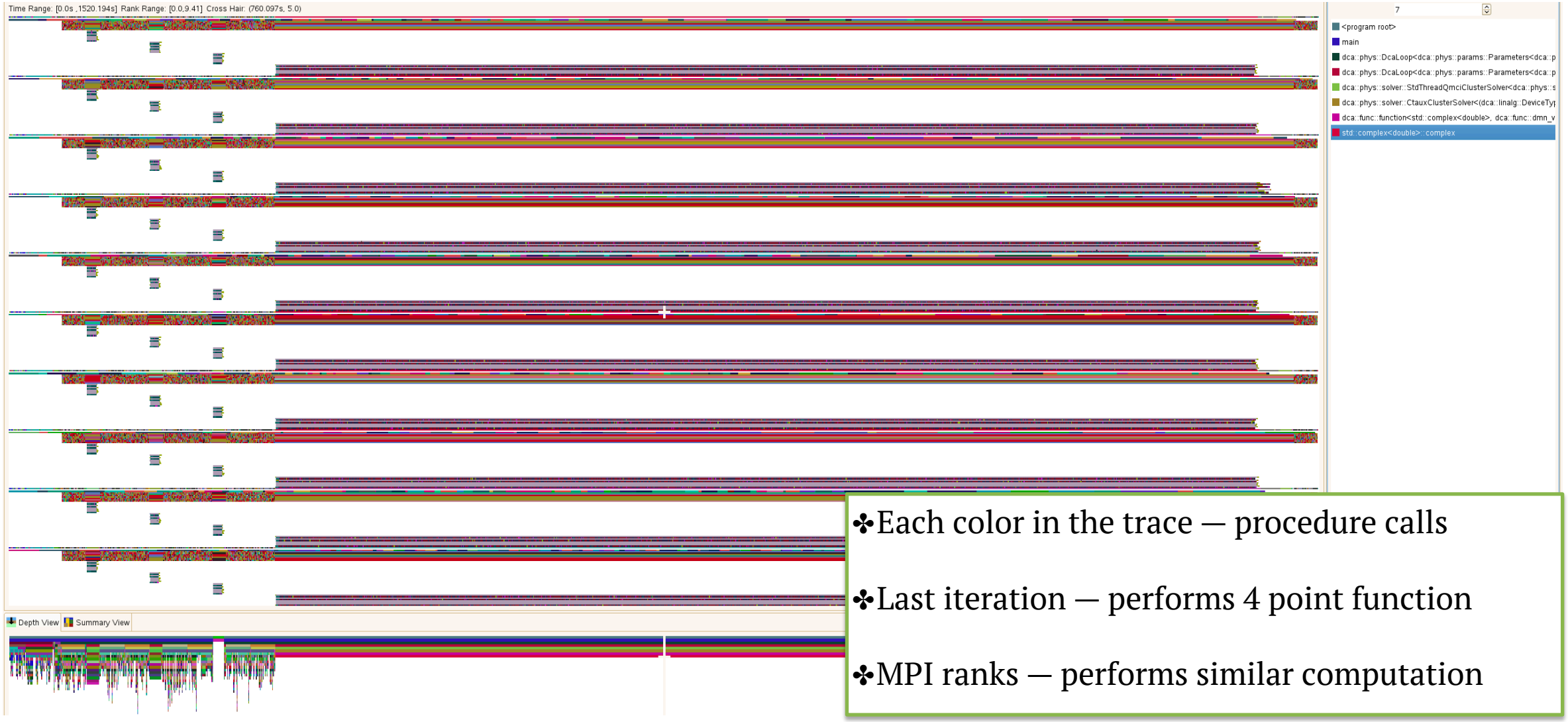


- **Profiler used**: HPCToolkit [Visualizer: HPCTraceviewer]

- **DCA++ code**:
  - Synthetic dataset (realistic to the science)
  - Beta: 20
  - Number of Titan nodes used: 10
  - Number of MPI ranks used: 10 (1 rank per node)
  - Iterations: 4 (till convergence)
  - Last iteration step — performs the 4 point function

- **Acknowledgment**: Dr. John Mellor Crummey & Dr. Laksono Adihanto (Rice U.)

Profiling DCA++ on Titan (using HPCToolkit)



MPI Ranks + Threads

Iterations [execution time]

- Each color in the trace — procedure calls
- Last iteration — performs 4 point function
- MPI ranks — performs similar computation

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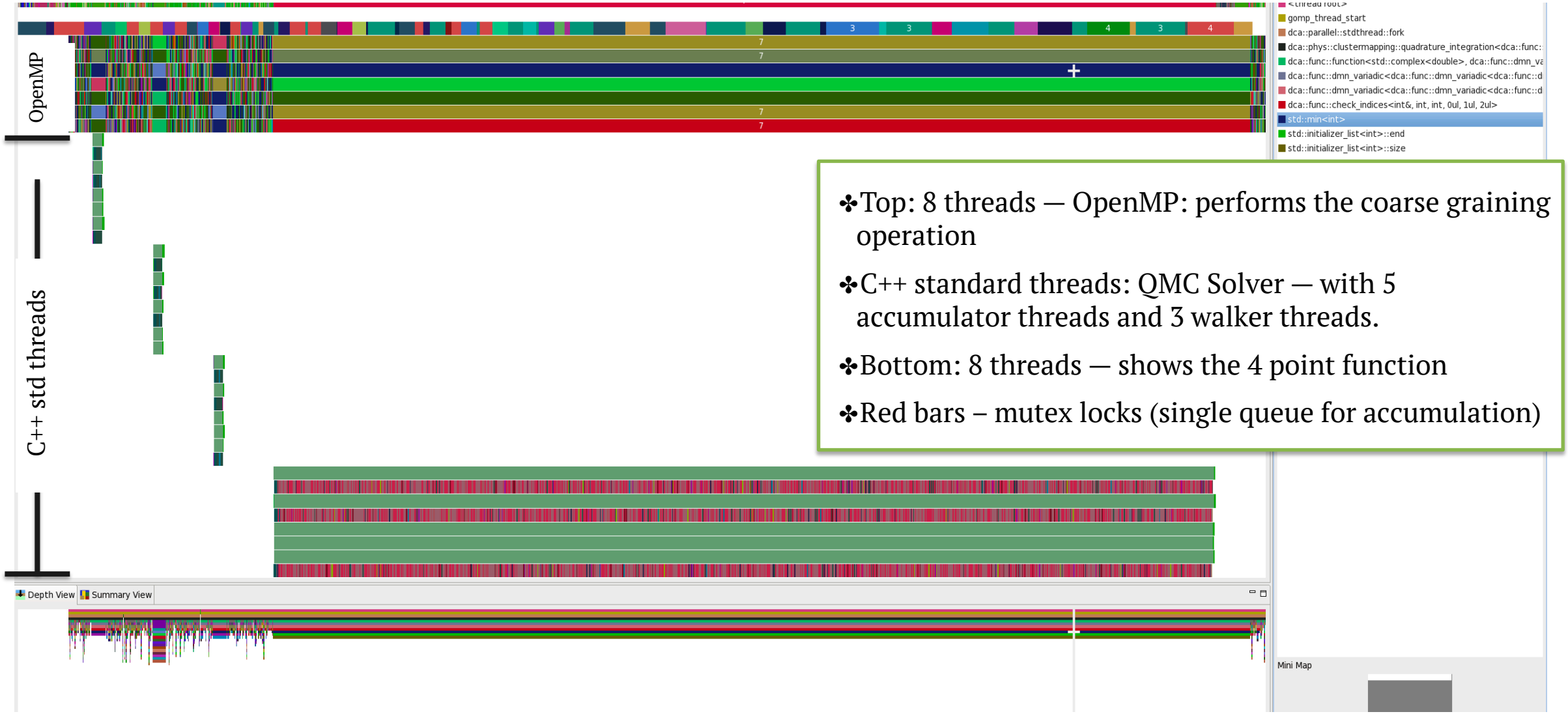
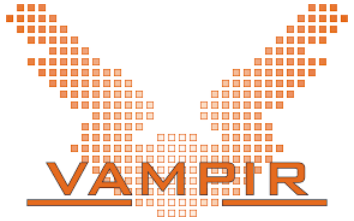
Profiling DCA++ on Titan (using HPCToolkit)



- Top: 8 threads — OpenMP: performs the coarse graining operation
- C++ standard threads: QMC Solver — with 5 accumulator threads and 3 walker threads.
- Bottom: 8 threads — shows the 4 point function
- Red bars – mutex locks (single queue for accumulation)

Profiling DCA++ on Titan



- **Profiler used**: ScoreP [Visualizer: VAMPIR]

- **DCA++ code**:
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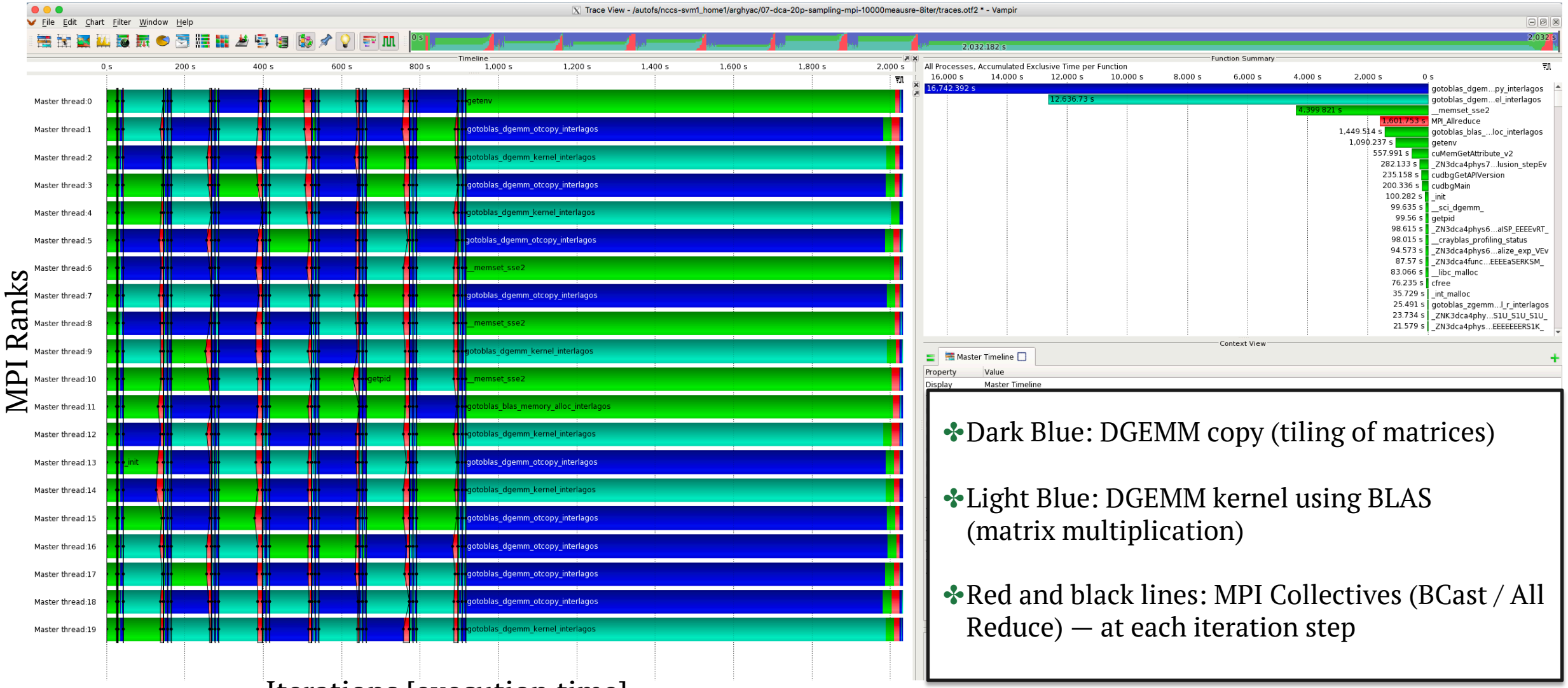
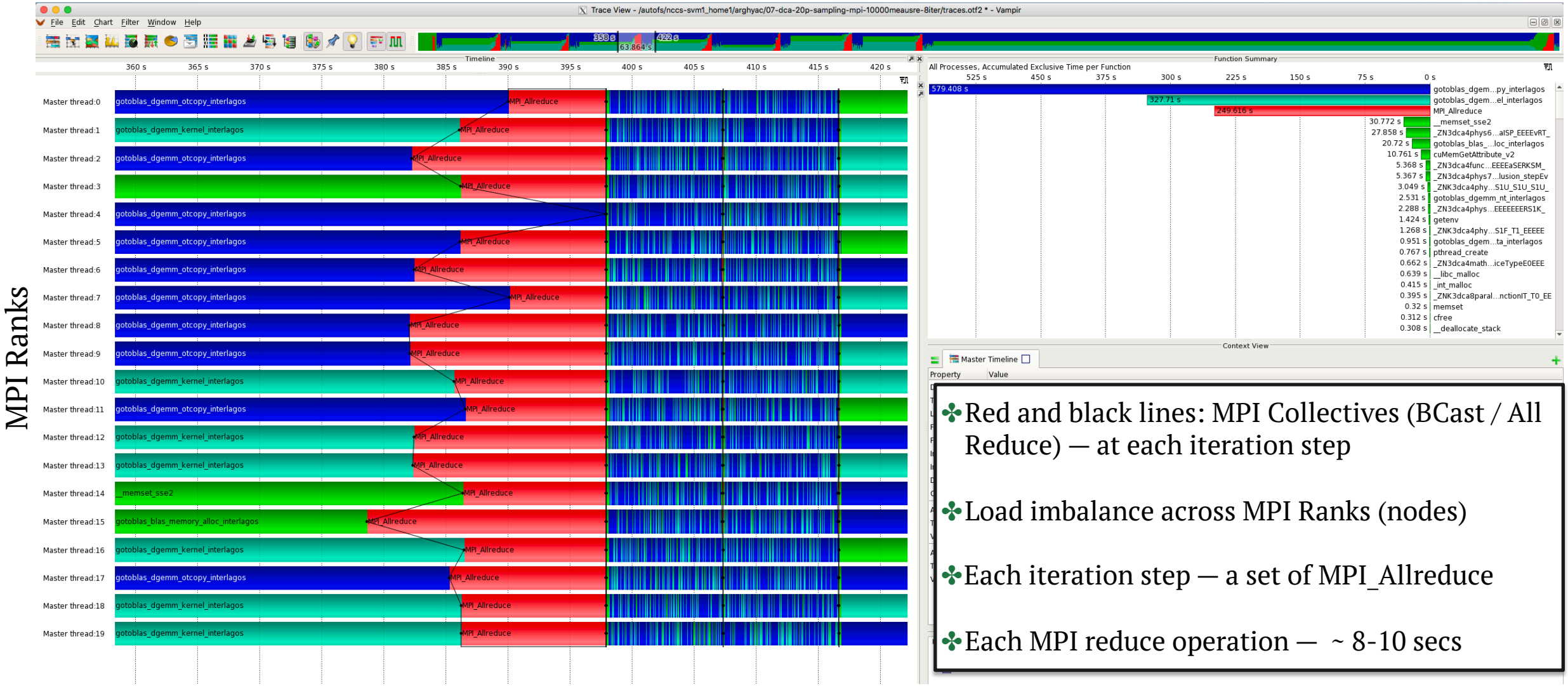
- **Acknowledgment**: Ronny Brendel (T.U. Dresden / ScoreP ; Currently: NVIDIA)

Profiling DCA++ on Titan (using ScoreP)



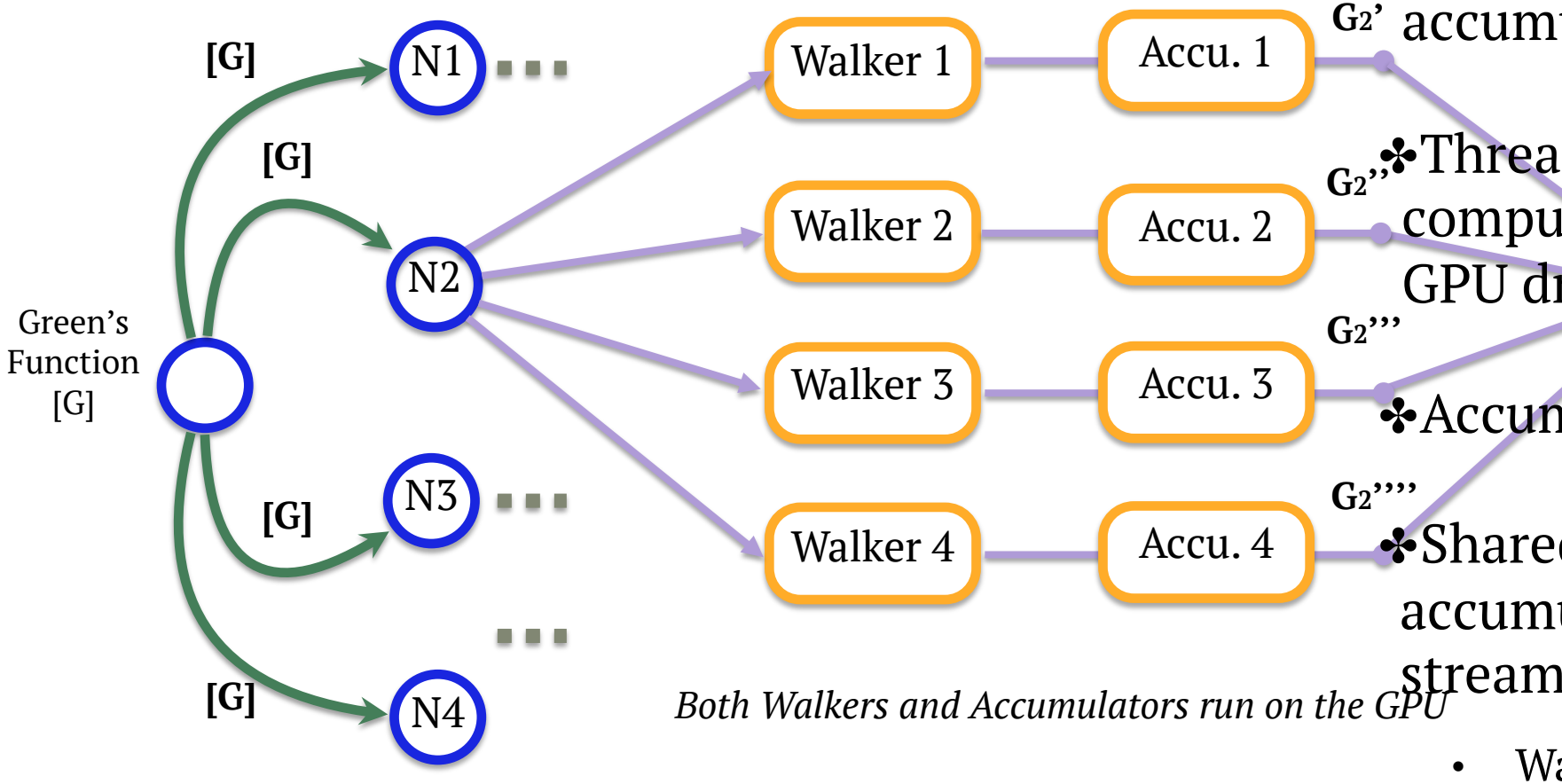
- Dark Blue: DGEMM copy (tiling of matrices)
- Light Blue: DGEMM kernel using BLAS (matrix multiplication)
- Red and black lines: MPI Collectives (BCast / All Reduce) — at each iteration step

Profiling DCA++ on Titan (using ScoreP)



- Red and black lines: MPI Collectives (BCast / All Reduce) — at each iteration step
- Load imbalance across MPI Ranks (nodes)
- Each iteration step — a set of MPI_Allreduce
- Each MPI reduce operation — ~ 8-10 secs

Quantum Monte Carlo Solver (new code)



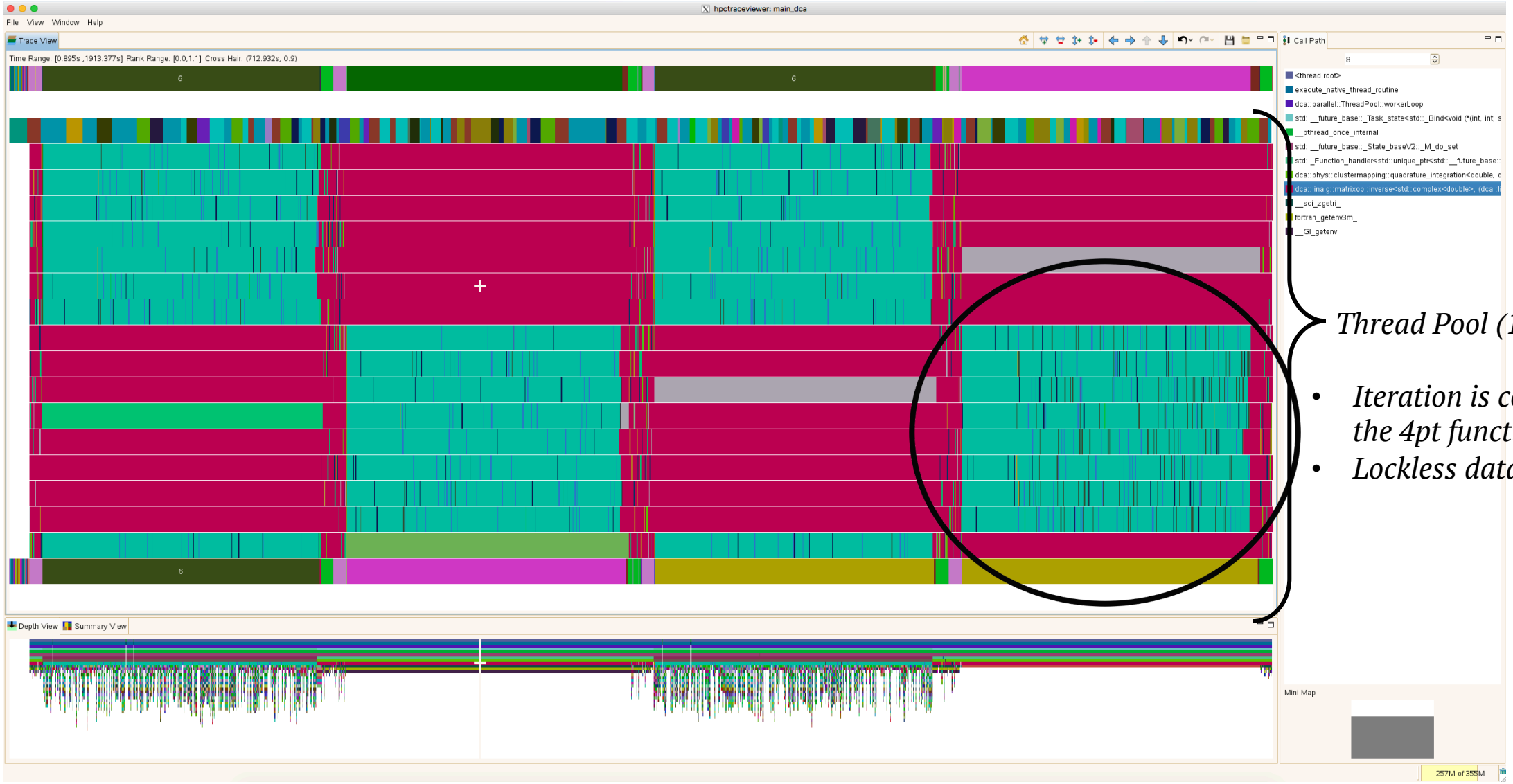
Both Walkers and Accumulators run on the GPU

"Walker – Accumulator" mapping: 1:1

- ✤Lockless data structure for the accumulator queue
- ✤Thread pool for the CPU computation coarse graining / GPU driver threads
- ✤Accumulation now on the GPUs
- ✤Shared walker / accumulators: accumulation on a separate GPU stream
  - Walkers continue random walk

Profiling DCA++ on Titan (using HPCToolkit)

MPI Ranks + Threads



Thread Pool (16 threads)

- *Iteration is computing the 4pt function*
- *Lockless data structure*

Iterations [execution time]

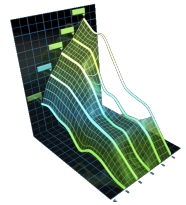
Profiling old / improved DCA++ on Summit

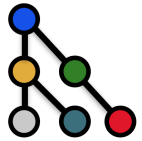
- **Profiler used**:

  NVProf (CUDA Toolkit)

  TAU (SciDAC Institute) – Ongoing Collaboration

  HPC Toolkit (Rice University)– Ongoing Collaboration





- **Versions of DCA++ code (compare and contrast)**:
  [Both codes are now publicly available: *https://github.com/CompFUSE/DCA*]

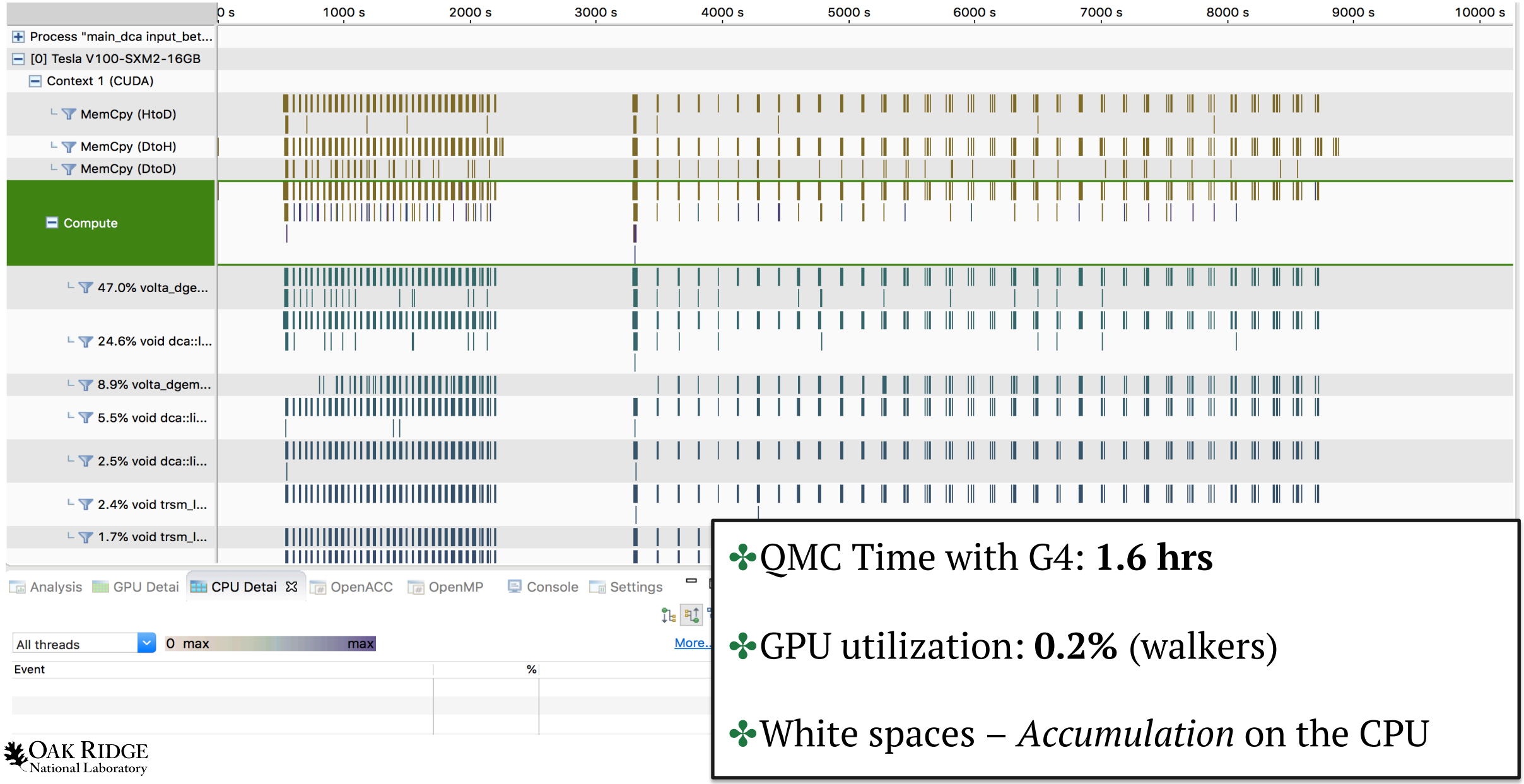
  - Old Code [pre SciDAC] – version 1.0.0
  - New Code [March 10th , 2019] – Ongoing

Input Parameters [large case]

- **Beta**: 50
- **Initial self-energy**= “T= 0.02/dca_sp.hdf5”
- **Iterations**: 2
- **Do-finite-qmc**: true (coarse graining is ON) – Turned off for production run
- **Measurements:** 1020
- **Cluster size:** 24
- **Initial configuration size**: 3300
- **Walkers**: 7 (=h/w threads mapped)
- **Accumulator**: 5
- **Shared Walker / Accumulator**: false
- **G4**: ON (last iteration)

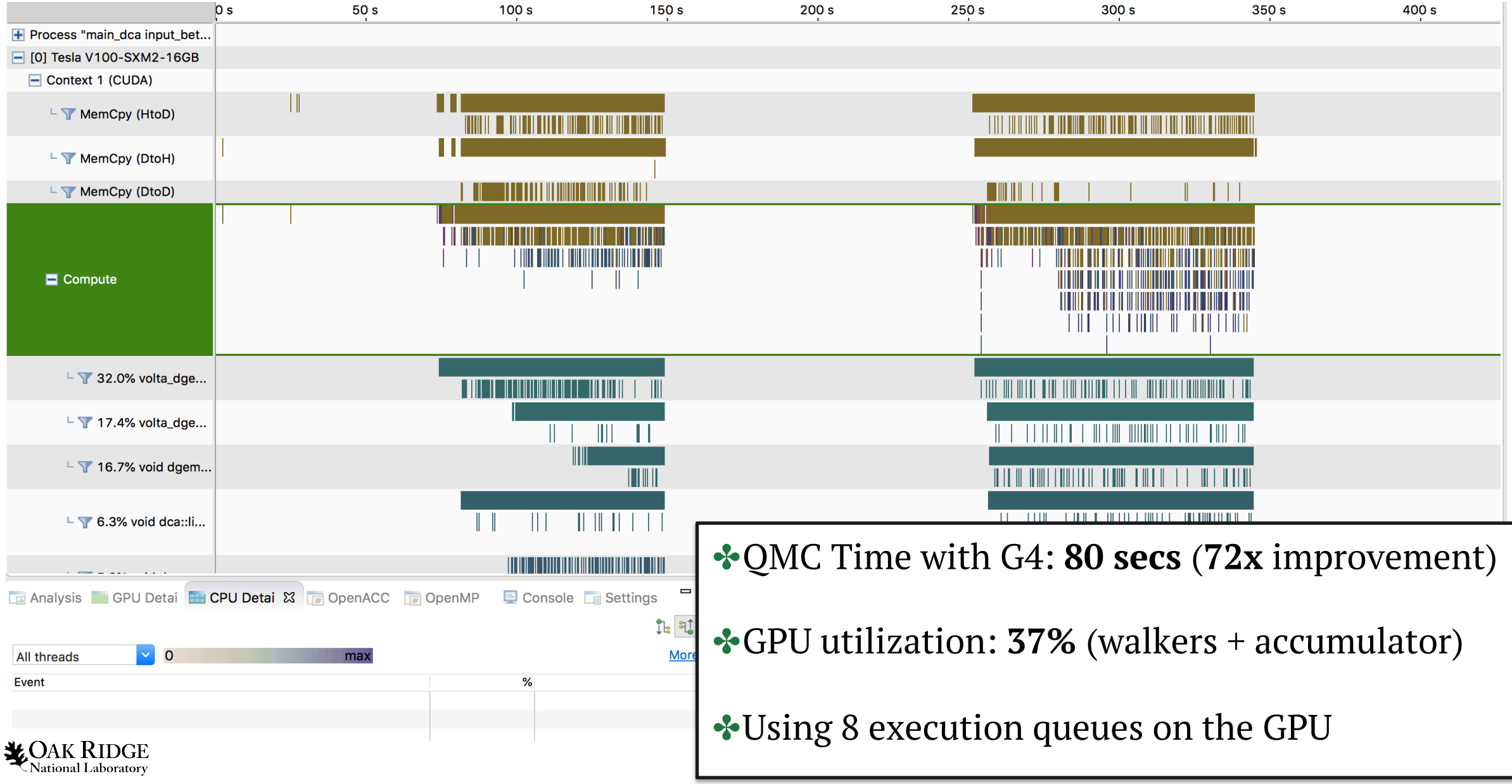
- Summit: 1 node :: 6 MPI ranks :: 1 rank/rs :: 1 rank/gpu :: smt1 :: 7 h/w threads /rs

DCA++ Profile [Old Code]



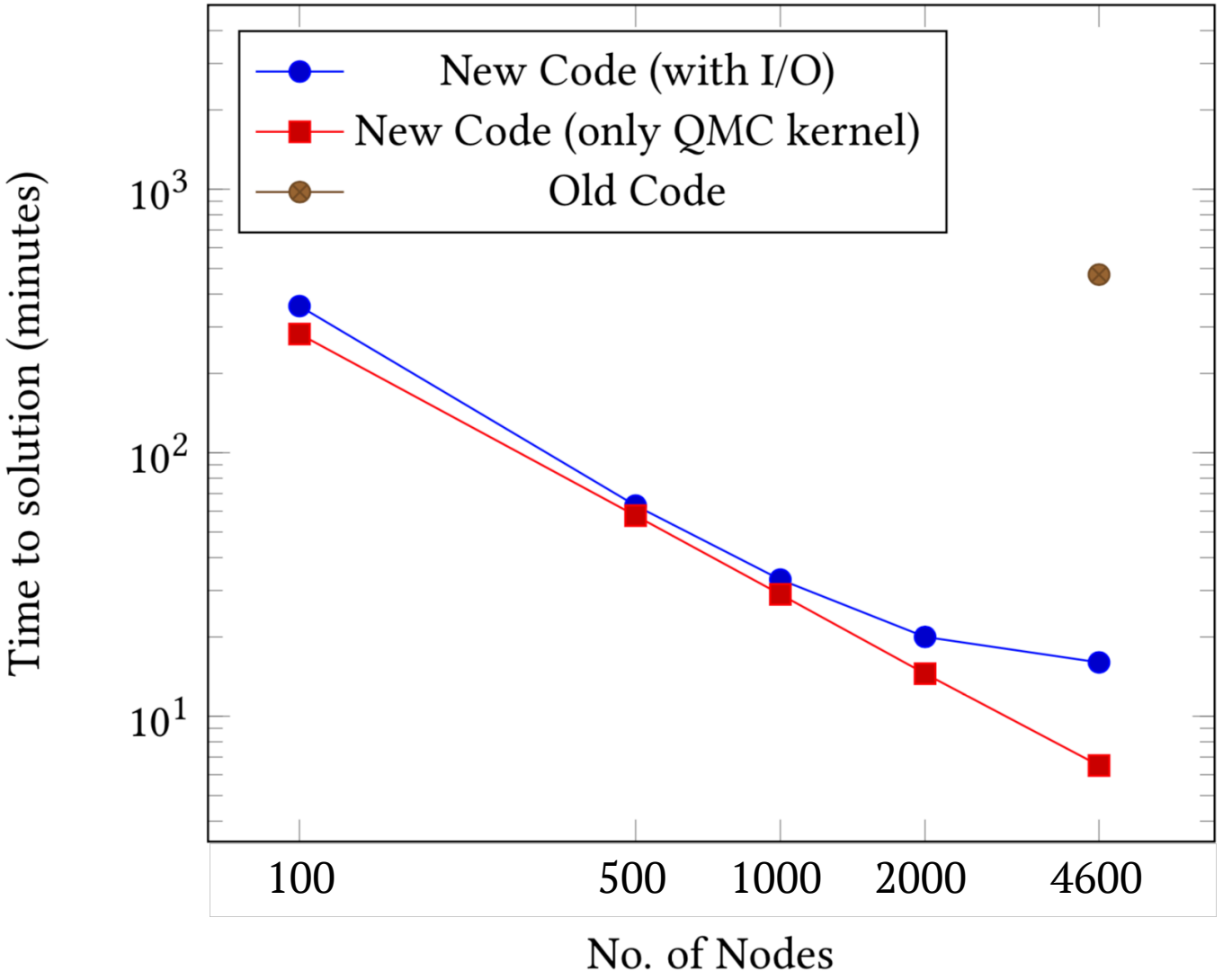
- QMC Time with G4: **1.6 hrs**
- GPU utilization: **0.2%** (walkers)
- White spaces – *Accumulation* on the CPU

DCA++ Profile [New Code]



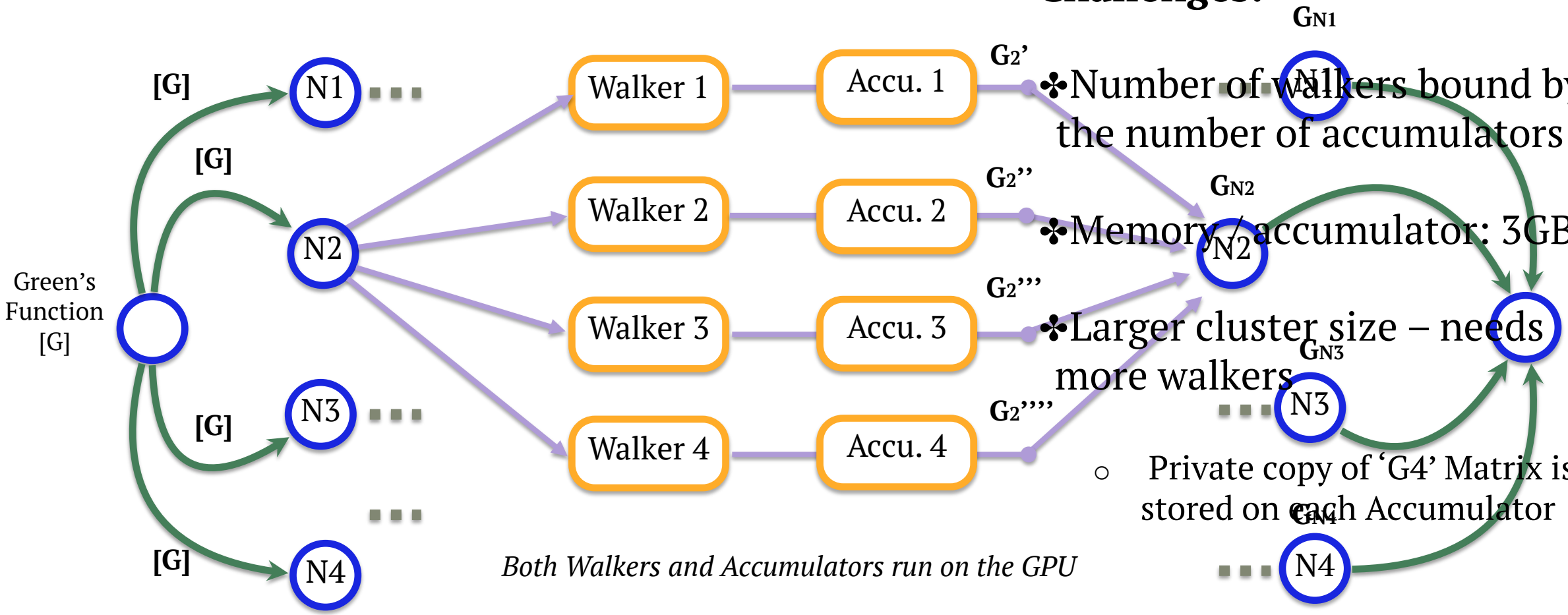
- QMC Time with G4: **80 secs** (**72x** improvement)
- GPU utilization: **37%** (walkers + accumulator)
- Using 8 execution queues on the GPU

DCA++ at scale on Summit (*INCITE*)



- Strong scaling : production run
- Cluster size: 6 ([6 0] [0 6])
  - 80M Measurements
- 1 MPI Process / GPU
- ~ 3000 Measurements / rank
  - **46% GPU** utilization
- Entire Summit (4600 nodes)
  - Old Code – **9.65 hrs.**
  - New 'Improved' Code – **6.5 mins.**
- Sustained performance: **43 PFLOPS**
- Peak performance: 73.5 PFLOPS
- Peak power: **9MW** [for 4600 nodes]

Quantum Monte Carlo Solver (new code)



Both Walkers and Accumulators run on the GPU

"Walker – Accumulator" mapping: 1:1

Challenges:

- Number of walkers bound by the number of accumulators
- Memory / accumulator: 3GB
- Larger cluster size – needs more walkers
  - Private copy of 'G4' Matrix is stored on each Accumulator

Ongoing efforts : SciDAC

- Single-band Hubbard model –> *2 / 3 – band Hubbard Model*
- Memory challenges for accumulators
- Use of mixed precision (*half*-, *single*- and *double* precision) [Tensor cores]
- Collaboration with TAU:
  - TAU/CUDA initialization and CPU/GPU timestamp sync. on Power9 + NVIDIA (Summit)
  - Updated CUDA support – multi-GPU nodes
  - TAU data organization – for GPU streams
  - Continuous Integration – performance database (past / future developments)
- *Autocorrelation* time based on system size and number of measurements
  - Time it takes for two measurements to be decorrelated and hence not biased configurations

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