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Creating the Next Generation of Stable, Interoperable and Performant Simulator – A Call for Open Standards

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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We need models of varying fidelity
How many tools do we need for all of them?

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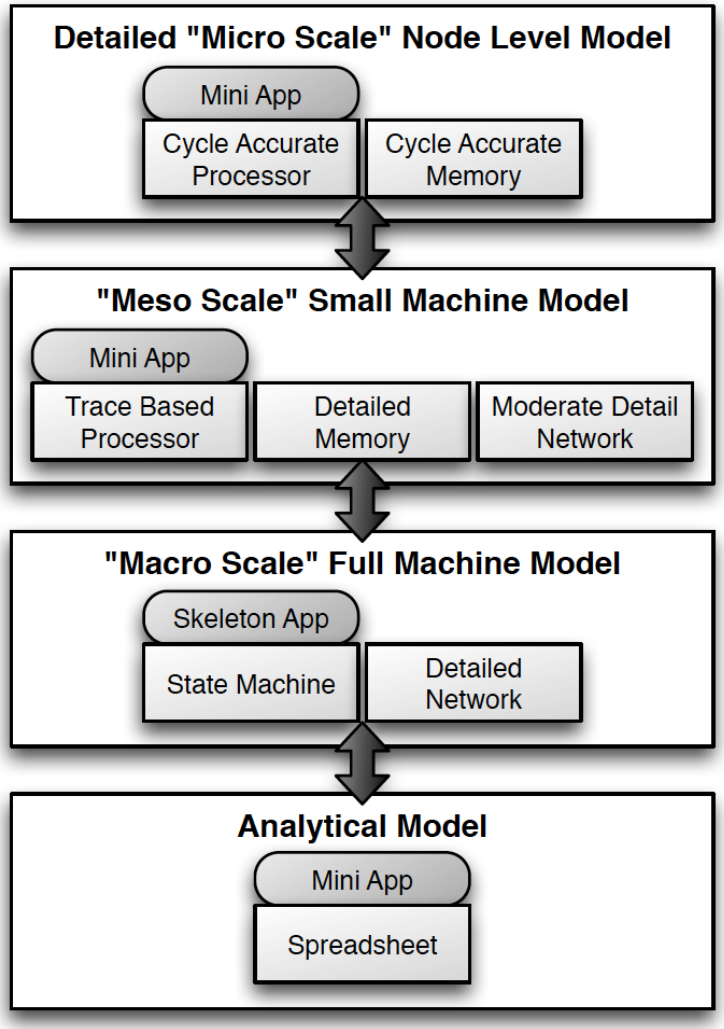
- High fidelity
  - What you care about only at exists at cycle-accurate detail
    - Cache reuse policies in memory
    - Flit-level flow control
  - Validation of lower fidelity models
- Medium fidelity
  - Coarse-grained modeling of architecture at system scale
    - Adaptive routing without flit detail
    - Scaling of collectives with network congestion
  - Validation of constitutive models at scale
- Constitutive models
  - Potentially good accuracy with right fitting
  - Rapid parameter space exploration



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SST
Structural Simulation Toolkit

We need models of varying fidelity
How many tools do we need for all of them?

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SST
Sonic Screwdriver Toolchain

How do we defeat the Daleks?

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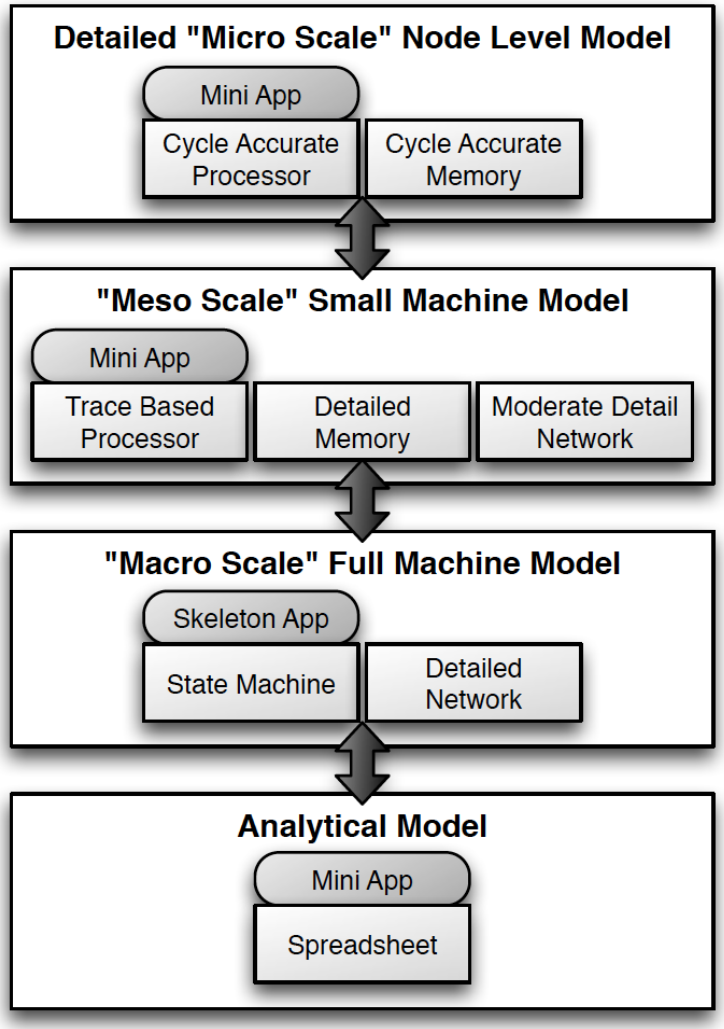
- Common Core
  - Scale up performance = scale up performance simulation = parallel simulation (PDES)
- Composability
  - Define standards for composing models that speak same language and share the same notion of time
- Community
  - Concerted effort to define standards and reuse code



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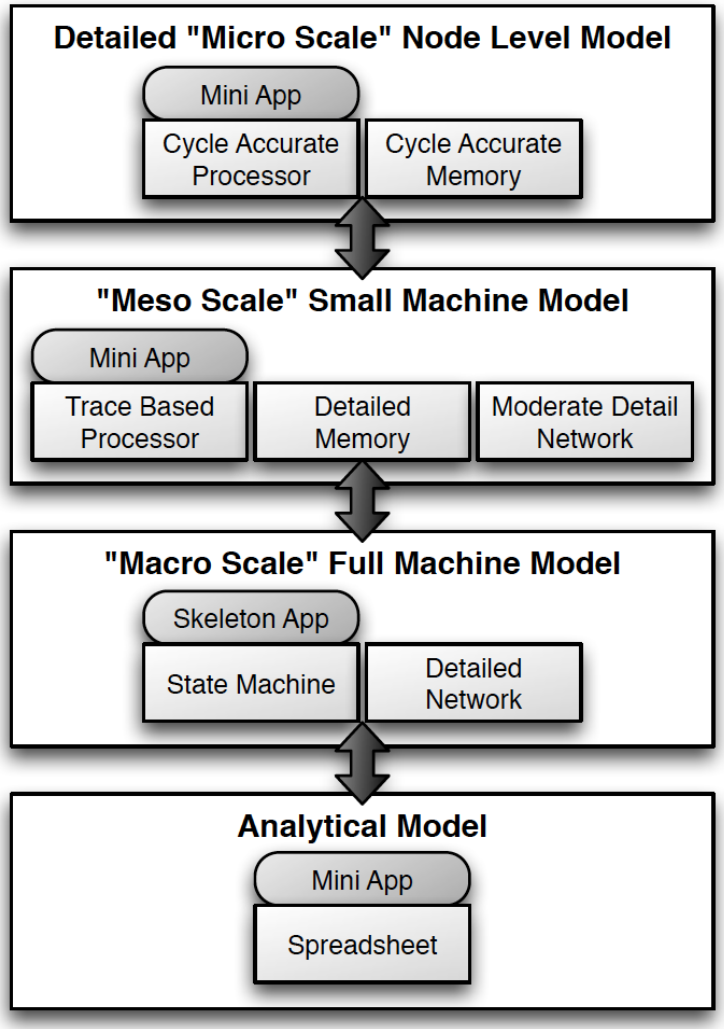

What is the major source of suffering in parallel discrete event simulation (PDES)?

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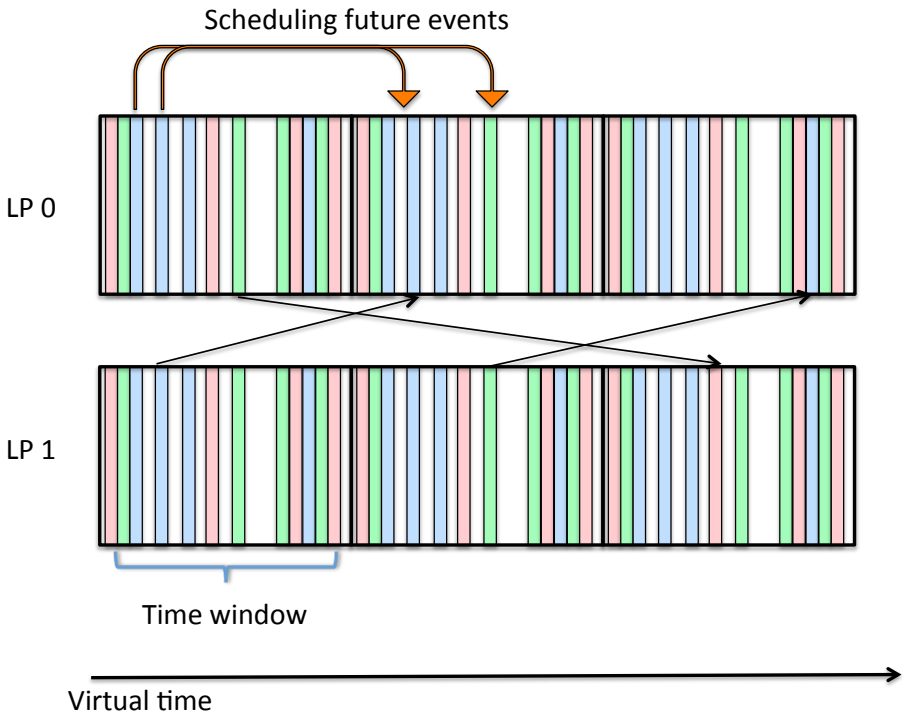
- Scale up machines = scale up simulations of machines = PDES
- Need event management and scheduling
  - Avoid time-order violations!

Dependencies between events



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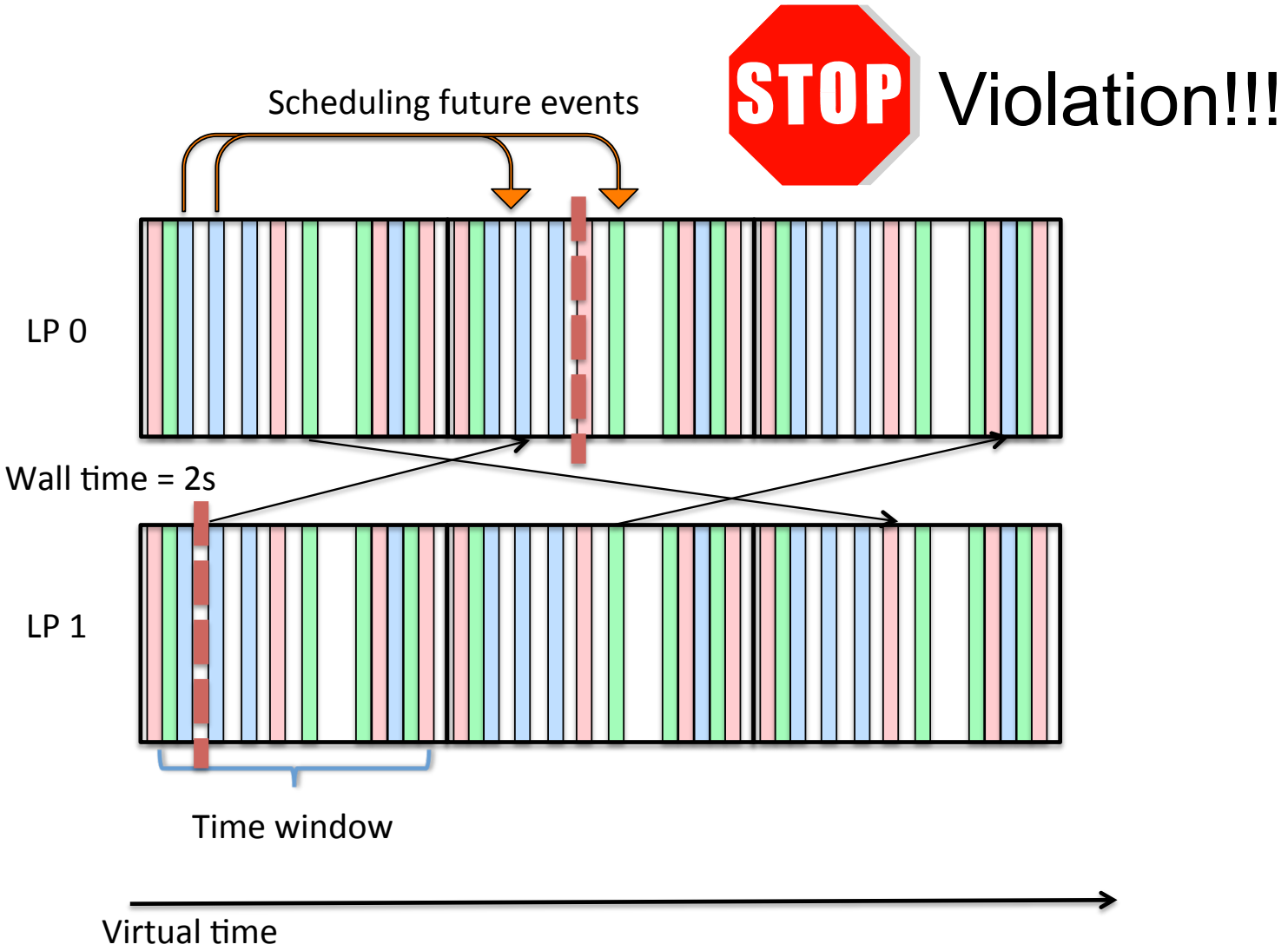

What is the major source of suffering in parallel discrete event simulation?

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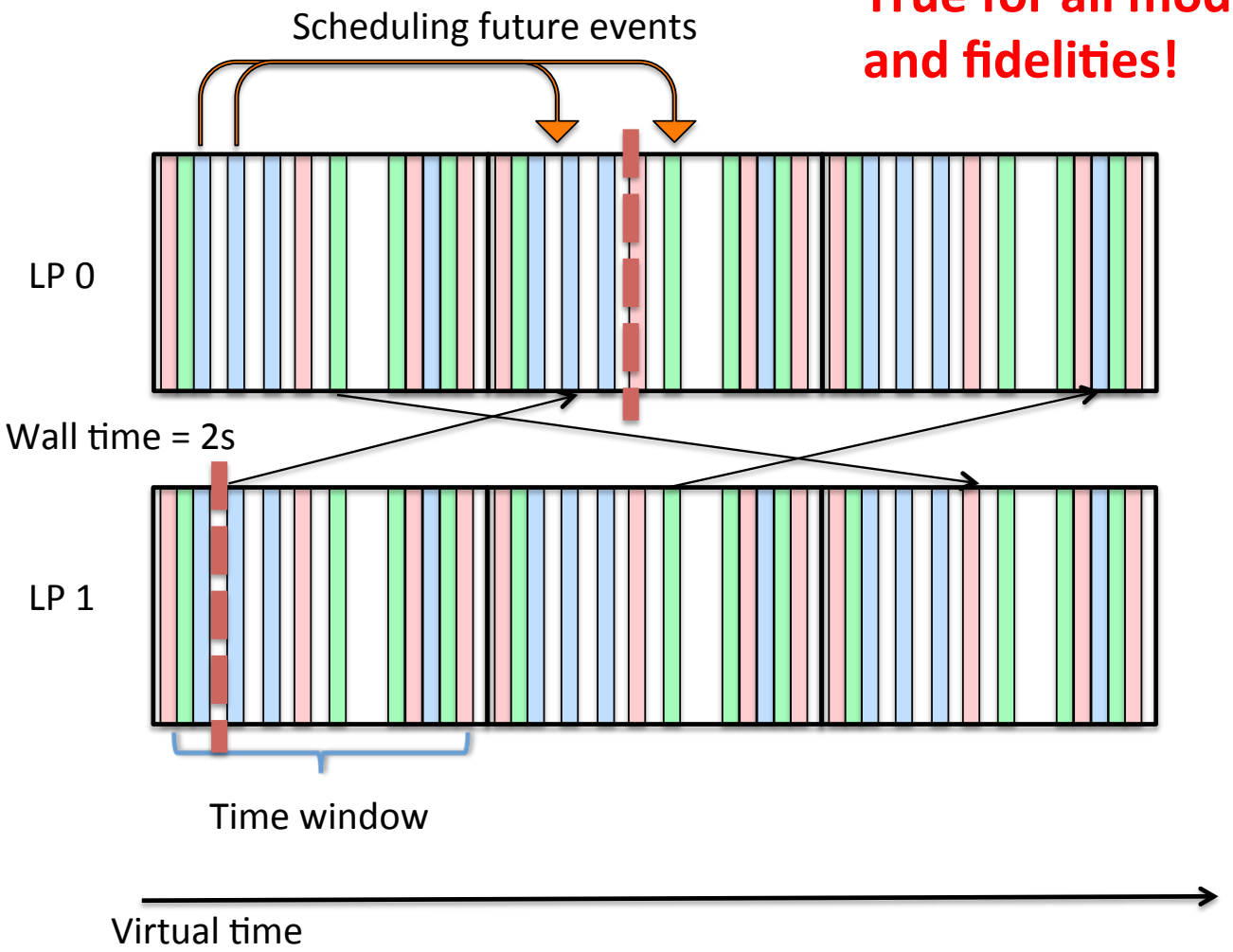
True for all models and fidelities!



What is the major source of suffering in parallel discrete event simulation?

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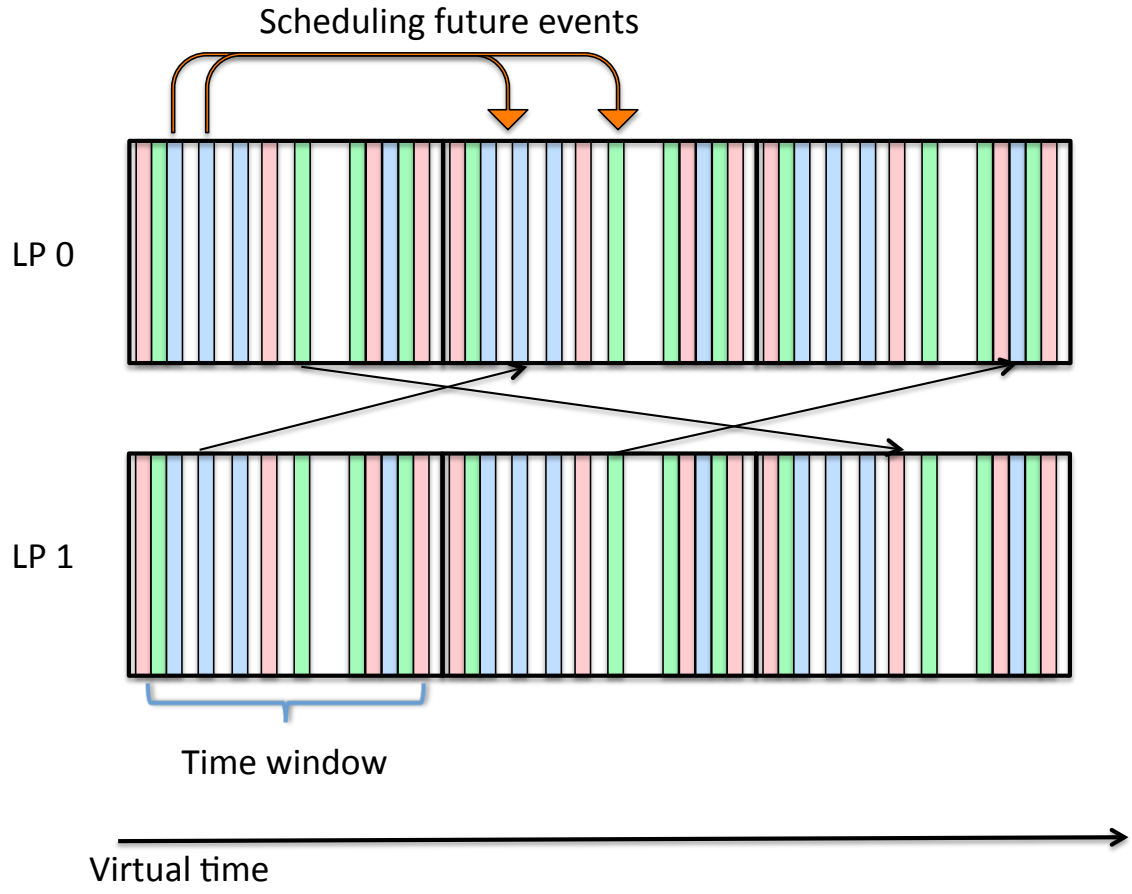
- Parallelism possible mainly from lookahead (safe time window) based on virtual latency between components



Solutions to the problem exist, but are non-trivial: Why rewrite over and over?

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- "Naïve" conservative time-stepping algorithm
  - Global, collective communication
  - Communication optimizations to lower prefactor, but has scalability limits

while $t < t_{termination}$ **do**
  Run all events until $t + \delta$
  Log event sends to $S = \{N^{LP0}_{events}, N^{LP0}_{bytes}, N^{LP1}_{events}, \ldots\}$
  MPI_ReduceScatter with SUM array S
  MPI_ReduceScatter returns N^{total}_{events}, N^{total}_{bytes}
  $N^{left}_{bytes} = N^{total}_{bytes}$
  for $msgNum < N^{total}_{events}$ **do**
    MPI_Recv(void*, MPI_ANY, N^{left}_{bytes})
    $N^{left}_{bytes} = N^{left}_{bytes} - msgSize$
  end for
  Determine t^{local}_{min}
  MPI_Allreduce(t^{global}_{min}, t^{local}_{min})
  $t = t^{global}_{min}$
end while

Solutions to the problem exist, but are non-trivial: Why rewrite over and over?

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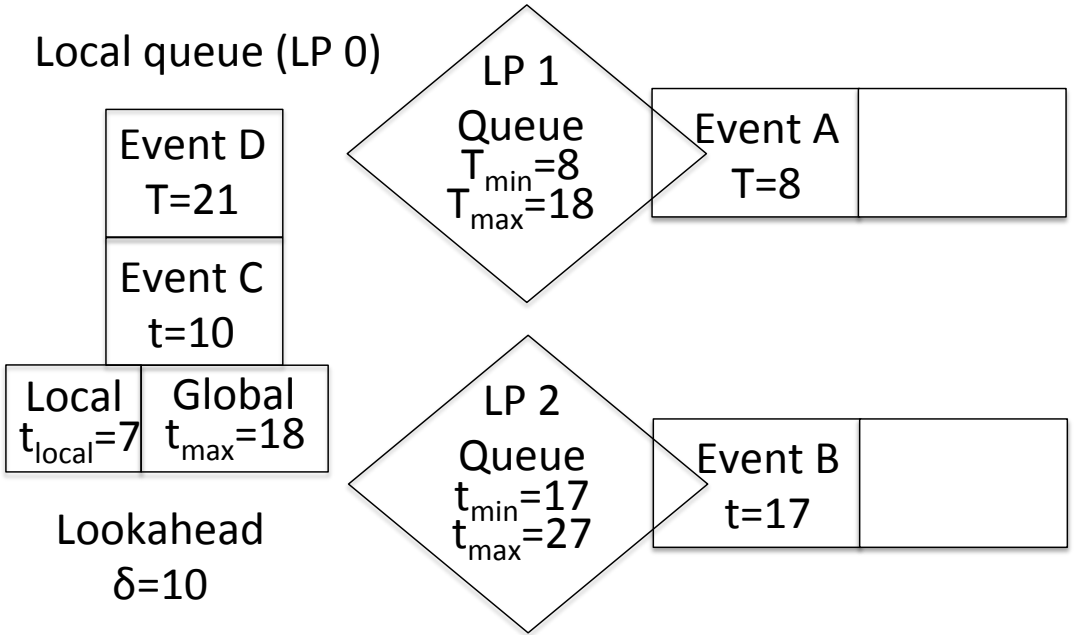
- Conservative algorithm with event queues: Optimization to limit communication for LP's that are "connected"
  - Local, point-to-point communication
  - More difficult to implement



What makes us write ad-hoc code instead of leverage existing code?

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- Lack of standards
- Lack of documentation
- Huge monolithic code bases
- Compatibility across platforms
- A million and one dependencies
- Physical models dependent upon simulation framework

Experiments we care about are model-driven – simulator is a tool to get us what we really care about!

Design considerations for an optimal high fidelity (cycle-level) simulator

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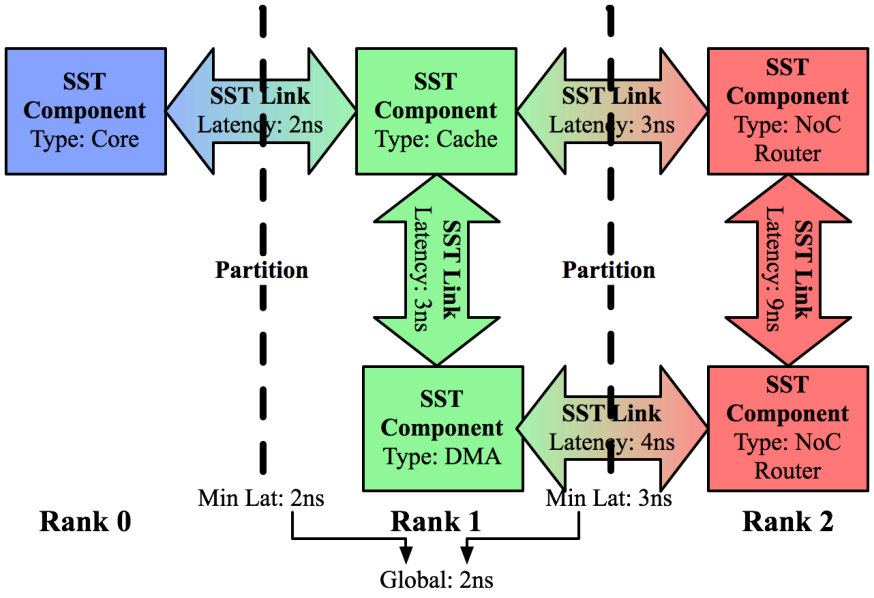
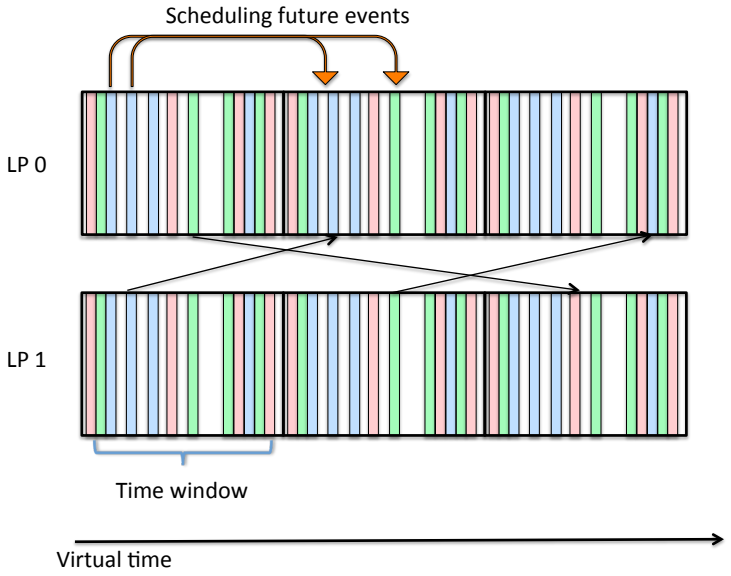
- Many events per time window
- No major time gaps (generally always have events)
- Components with different link latencies and clocks
- Domain specific synchronization algorithms



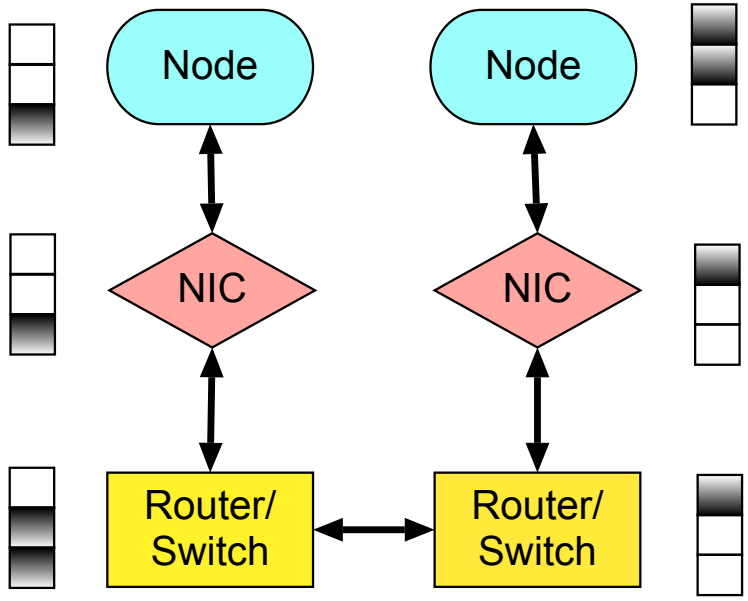


Design considerations for an optimal coarse-grained structural simulator

Sandia National Laboratories

- May have a few events per time window – or might have a lot
- Can have large gaps - time windows with no events in them
- Huge number of components, but with the same link latency

Abstract machine model with congestion via buffers and queues



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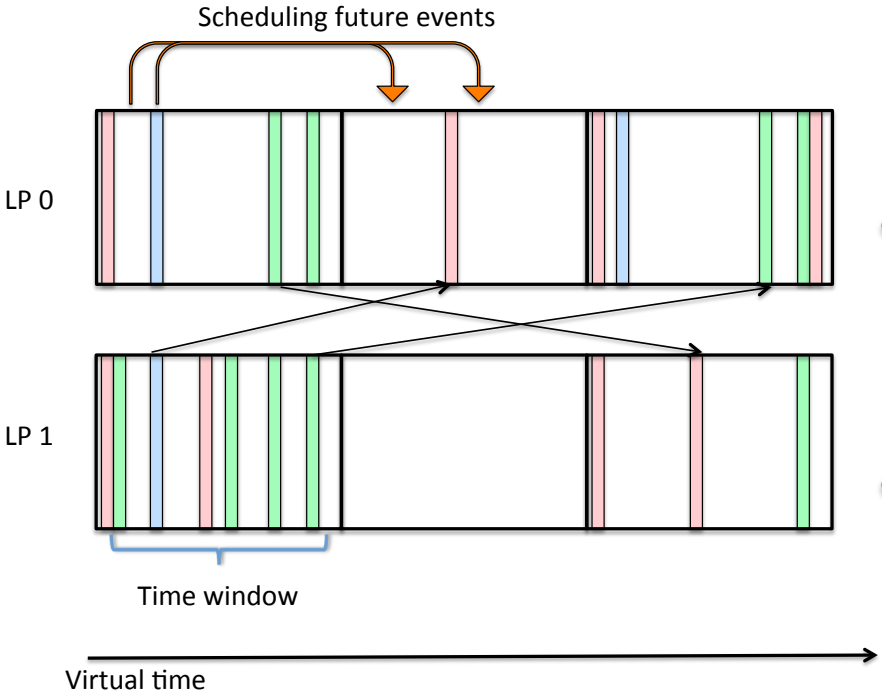


```
int USER_MAIN(int argc, char **argv)
{
 MPI_Init(&argc, &argv);

 ...

 for (int iter=0; iter < niter; ++iter){
   MPI_Isend(left_block, nelems_left_block, MPI_DOUBLE,
       row_send_partner, row_tag, MPI_COMM_WORLD, &reqs[0]);
   MPI_Isend(right_block, nelems_right_block, MPI_DOUBLE,
       col_send_partner, col_tag, MPI_COMM_WORLD, &reqs[1]);
   MPI_Irecv(next_left_block, nelems_left_block, MPI_DOUBLE,
       row_recv_partner, row_tag, MPI_COMM_WORLD, &reqs[2]);
   MPI_Irecv(next_right_block, nelems_right_block, MPI_DOUBLE,
       col_recv_partner, col_tag, MPI_COMM_WORLD, &reqs[3]);

   do_dgemm('T', 'T', nrows, ncols, nlink, 1.0, left_block, nrows,
      right_block, ncols, 0, product_block, nrows);
  }

  ...

  MPI_Finalize();
}
```

MPI calls start generating network traffic

Compute call might take 5ms but link latencies in the network are only 100ns!

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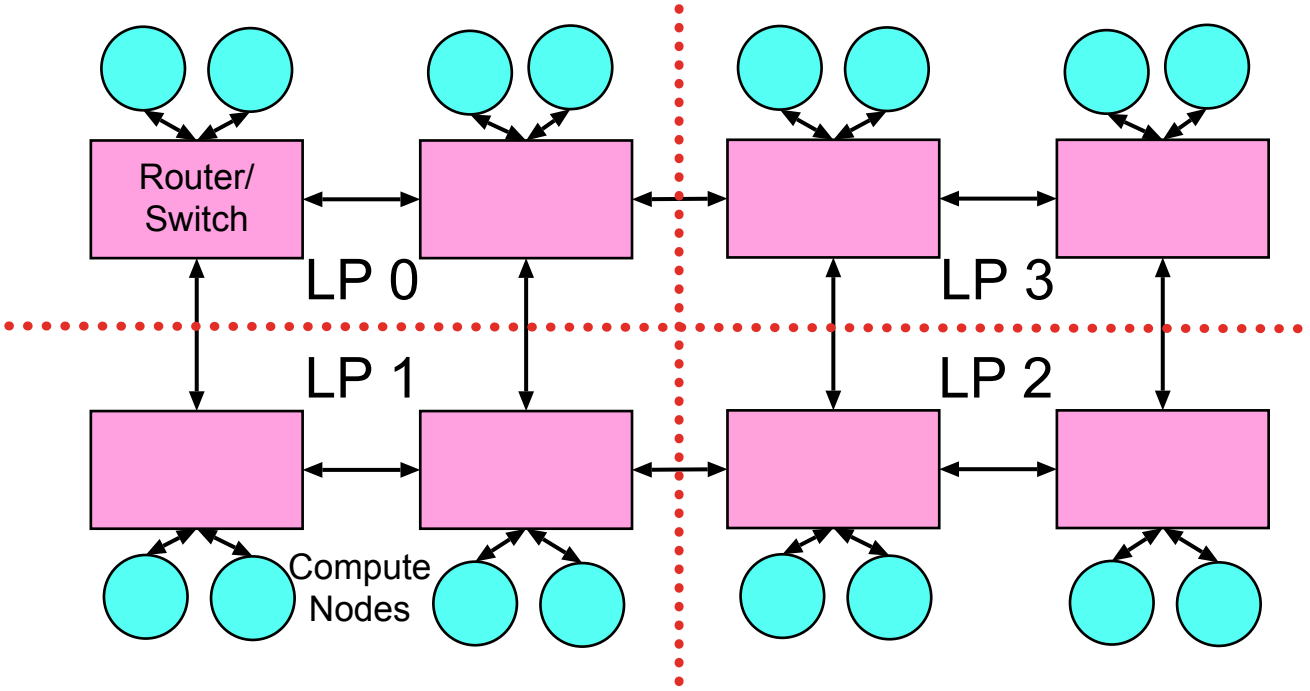
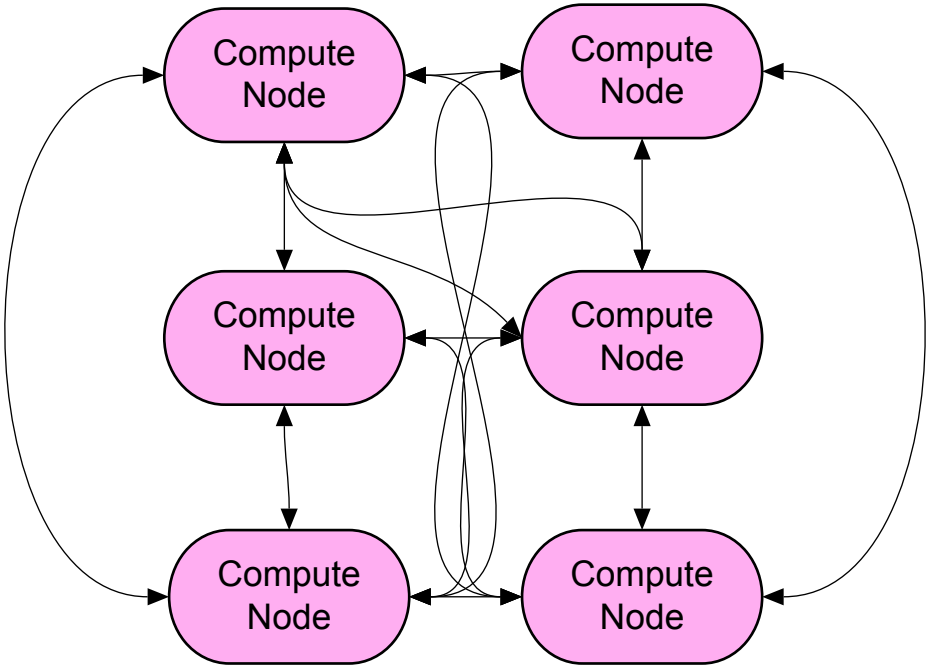


Design considerations for a simulator based on analytical models

- Only a few events per time window
- Many different components, but all connected to each other



$$\Delta T = \alpha + \beta N$$

α = Latency

β = Inverse bandwidth

N = Message size

Unifying elements across all fidelities

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- Sending network messages
  - Portability layer to network APIs
  - Serialization library for event objects
- Local/global virtual time
  - Event ordering and correctness
  - Model input and statistics collection
- Partitioning components across parallel workers
  - Mapping of LPs to physical nodes
  - Optimize partition for cheaper communication
- Managing/scheduling events
  - Map/calendar/heap data structures
  - Cancel events

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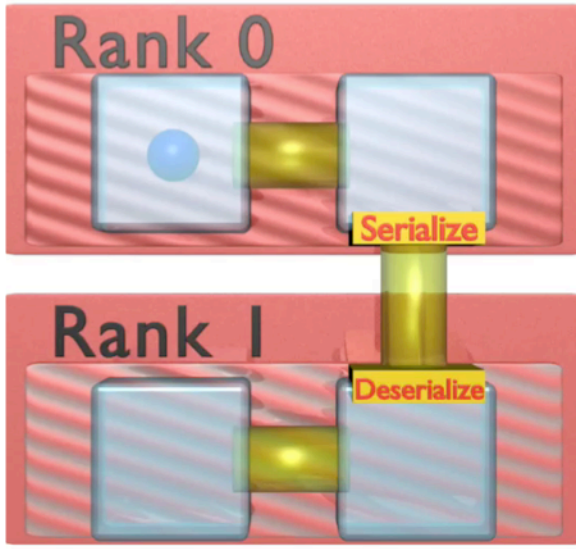

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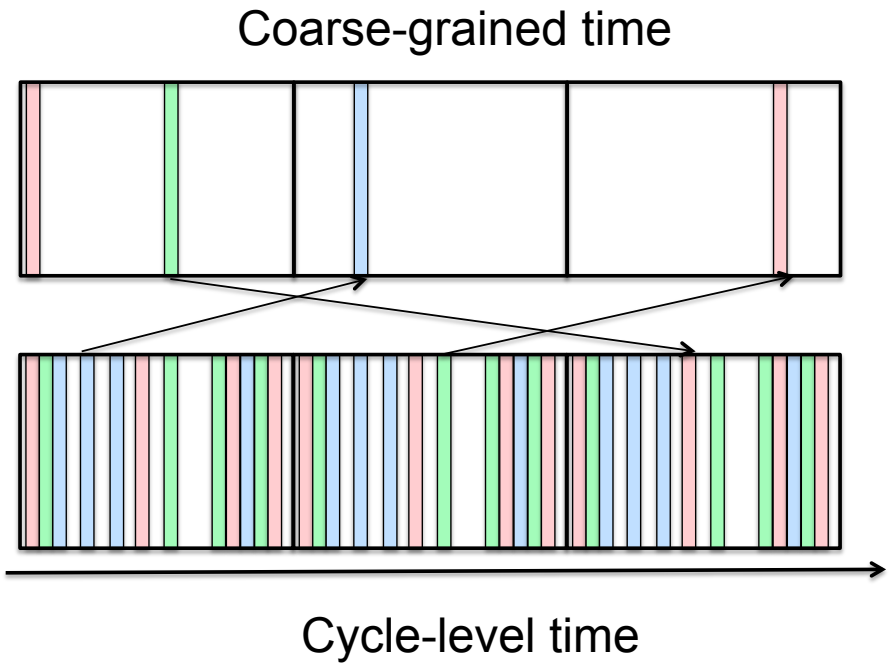

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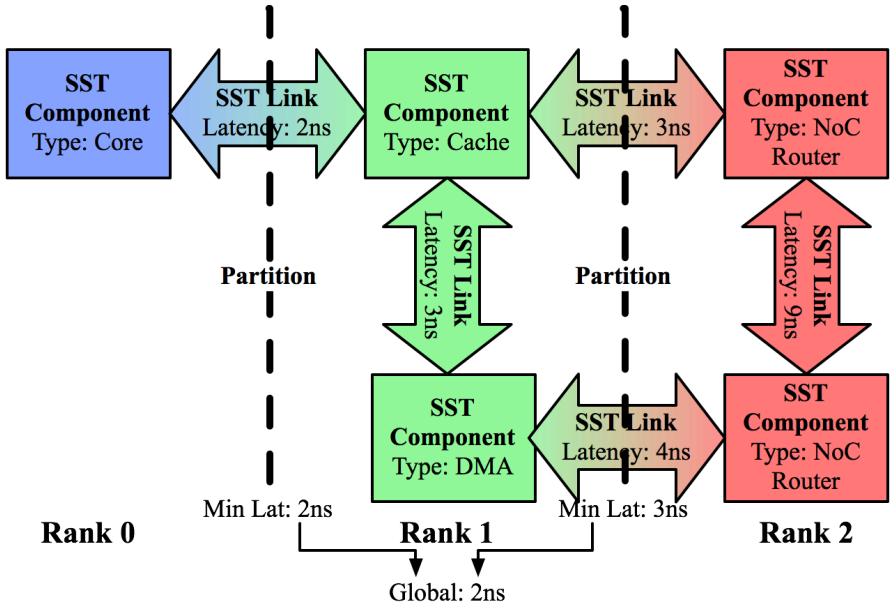

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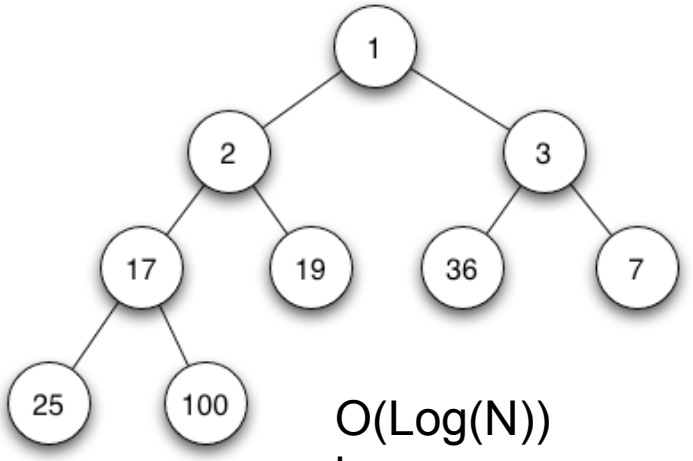

O(Log(N)) heap

T=1,T=2, T=3	T=7		T=17, T=19
T=25			T=36
			T=100

O(1) calendar

Disunifying elements across fidelities: partitioning strategy and parallel algorithm

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- Partitioning strategy
  - Cycle-level has heterogeneous components – partitioning really requires intelligent graph partitioner
  - Coarse-grained has many homogenous components – partitioning still requires intelligent partitioner, but more about minimizing graph connectivity than best link latency
- Parallel algorithm
- Global assumptions on interoperability components
  - Can any memory subsystem model interact with any processor or network model? Or are event messages only “self-compatible”?

Polymorphic components can be tuned for different problems

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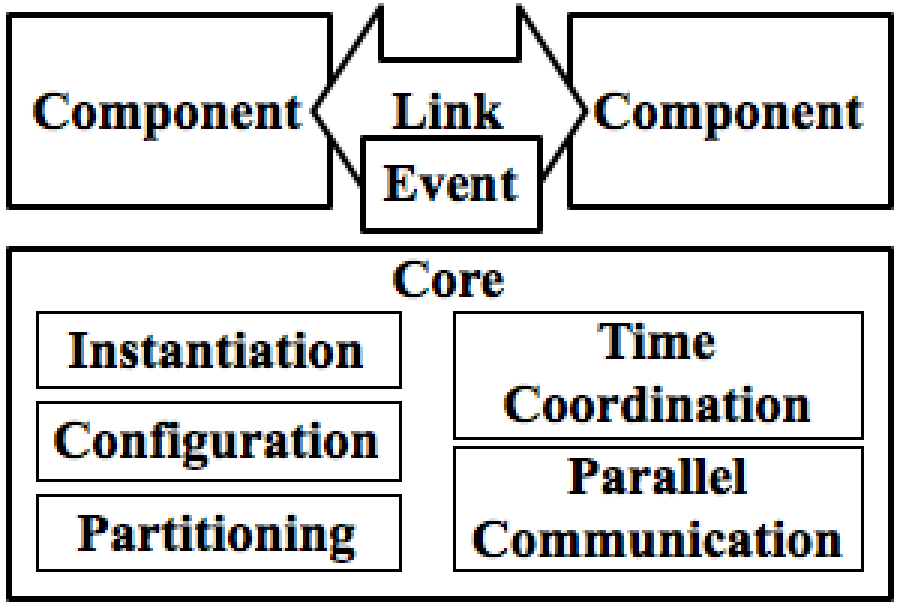
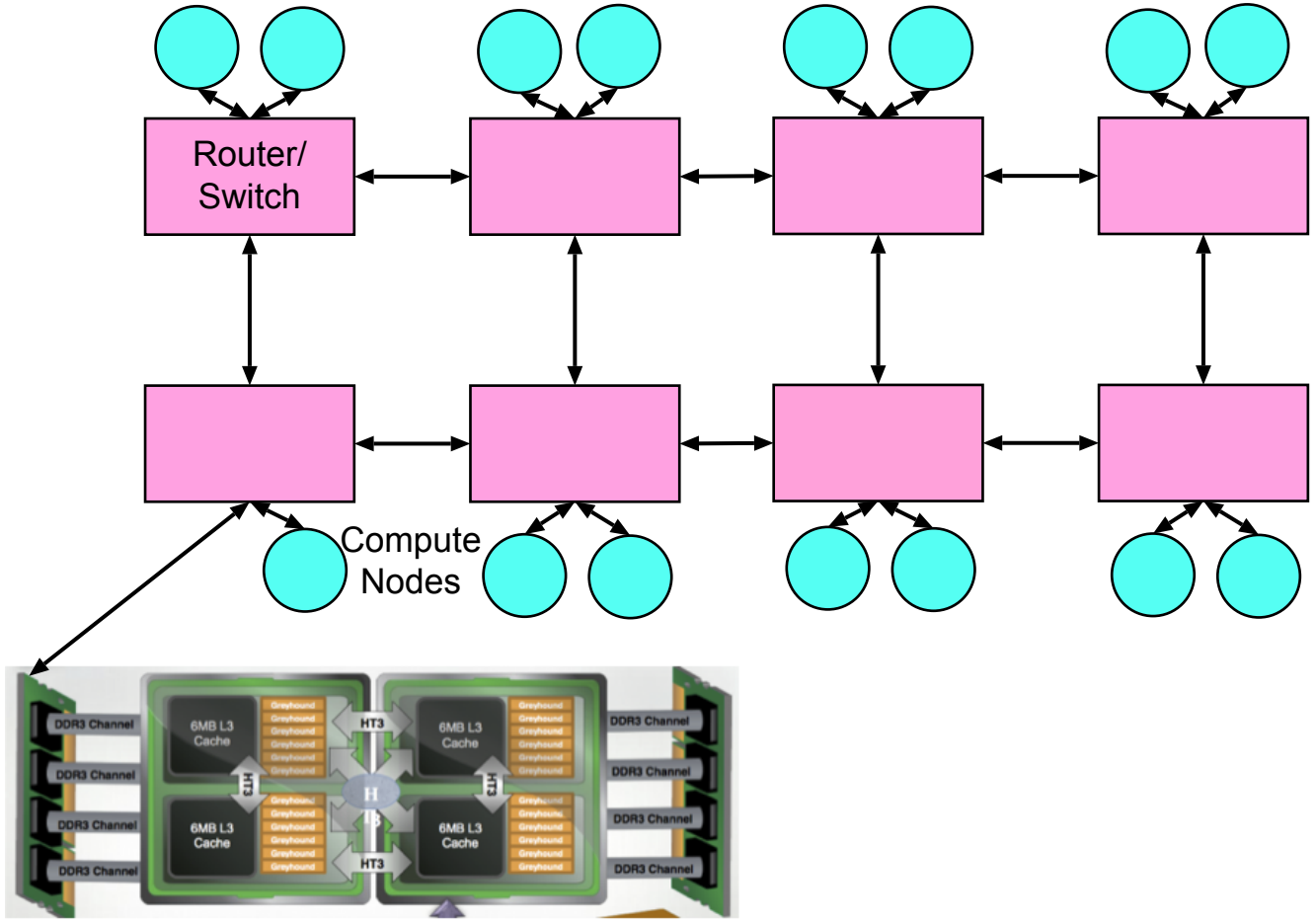
- Components don't need to be aware of partitioning strategy
- Components don't need to be aware of parallel algorithm



Challenge problem: mixing fidelities

LP with heavy-weight node operating on different time scales, but look ahead determined by coarse-grained links!



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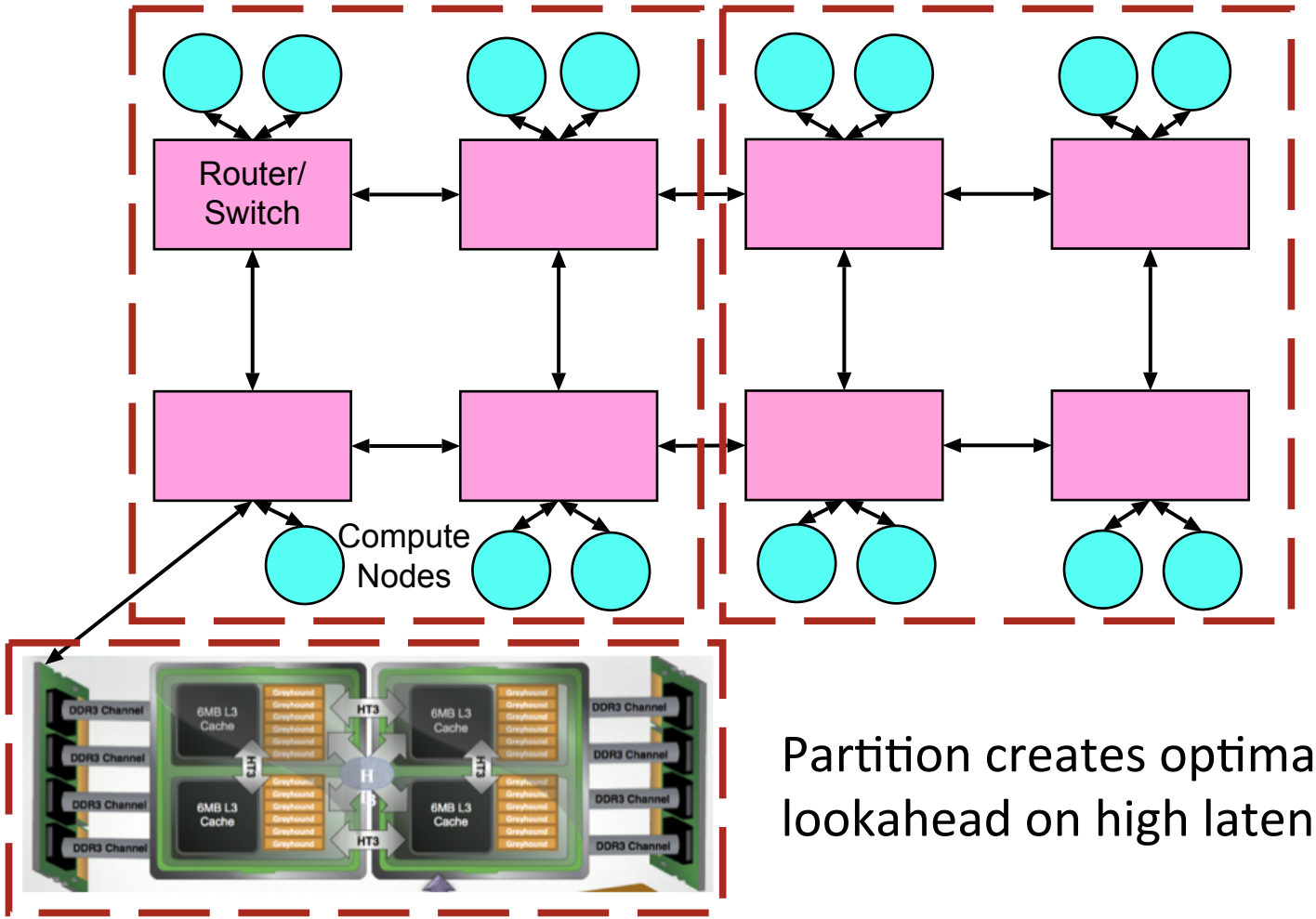
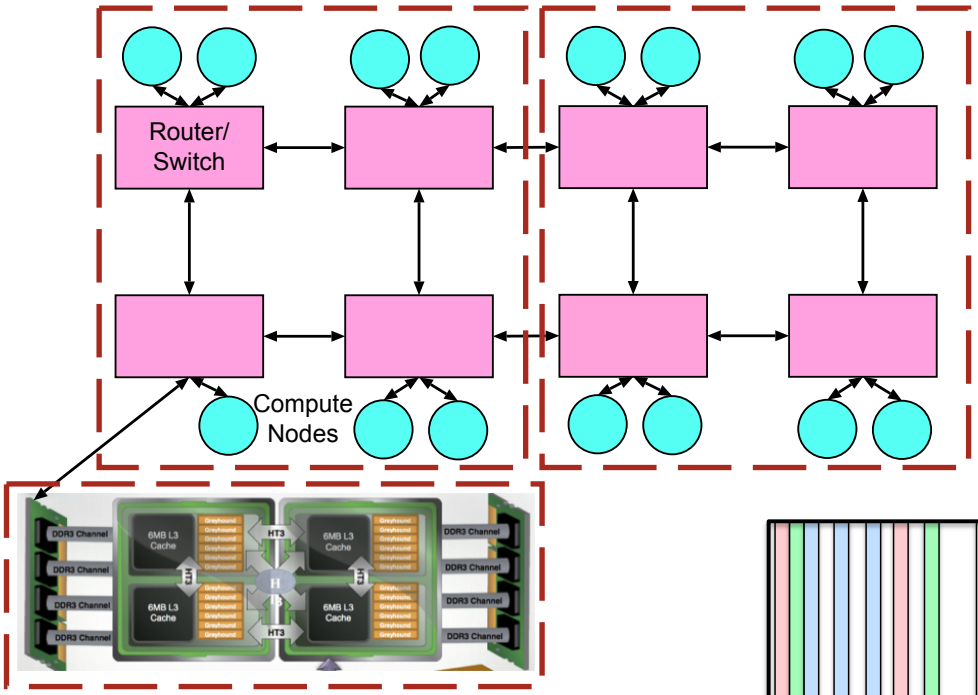
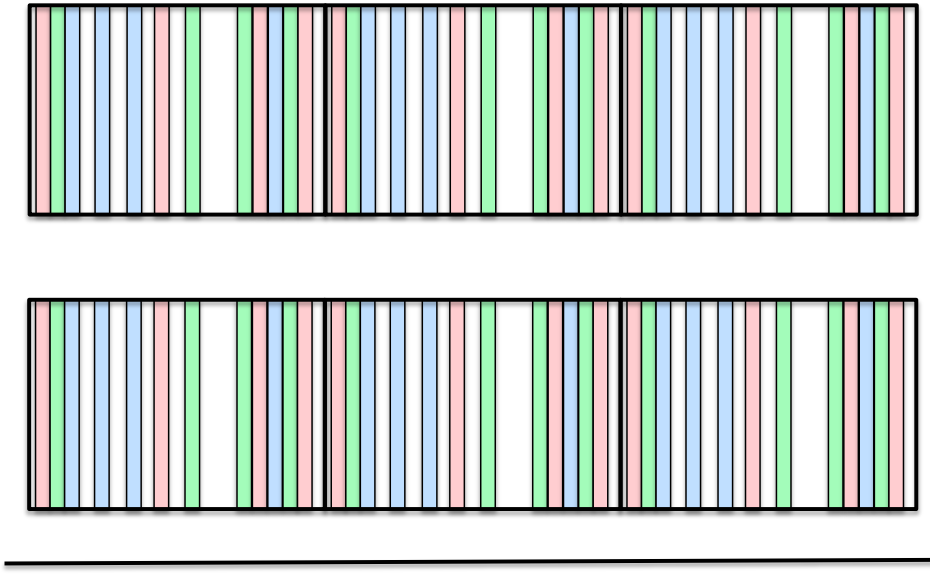


Partition creates optimal lookahead on high latency links

Challenge problem: mixing fidelities



Good partitioning balances number of events per LP



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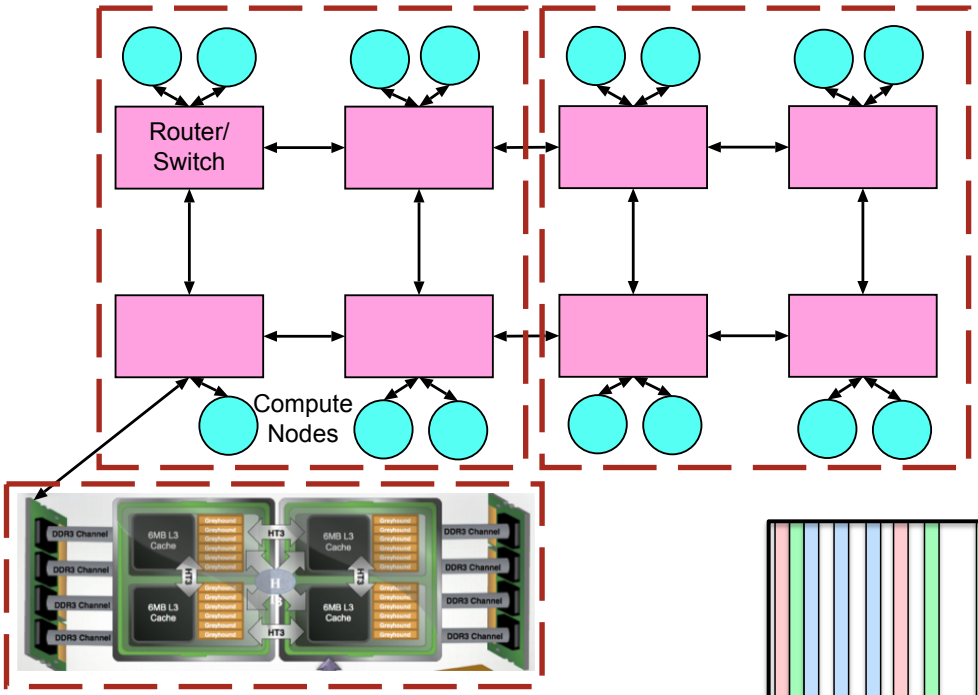

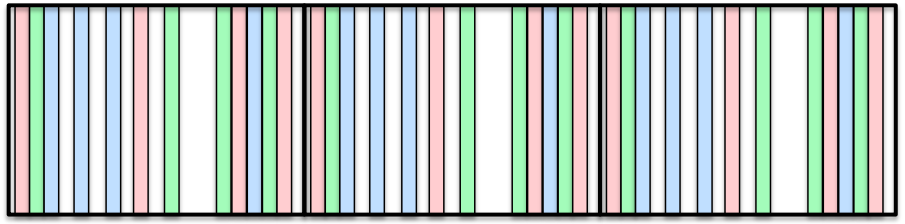

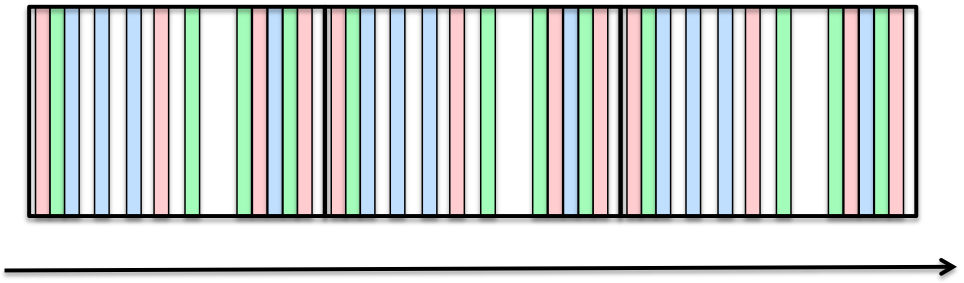

Simulator core problem, not a domain-specific problem

Challenge problem: histogram of message delays in PDES run

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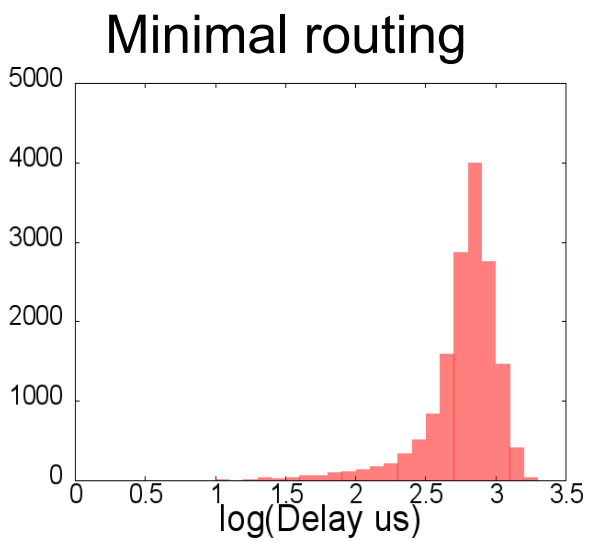
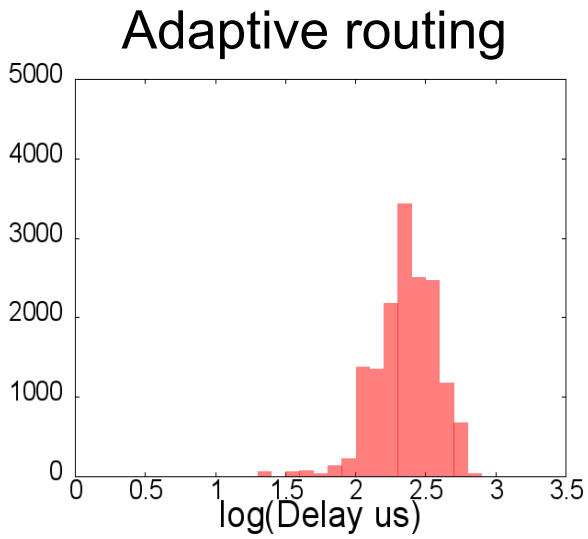
- Tag packet going out, going in with time
  - Add single field to existing network message object
  - Notion of global time
- Histogram object that reduces/collects data
  - hist->add_one(delay)
  - Object must output usable data format/figure at end of simulation
  - Data must be reduced across LPs





Challenge problem: histogram of message delays in PDES run

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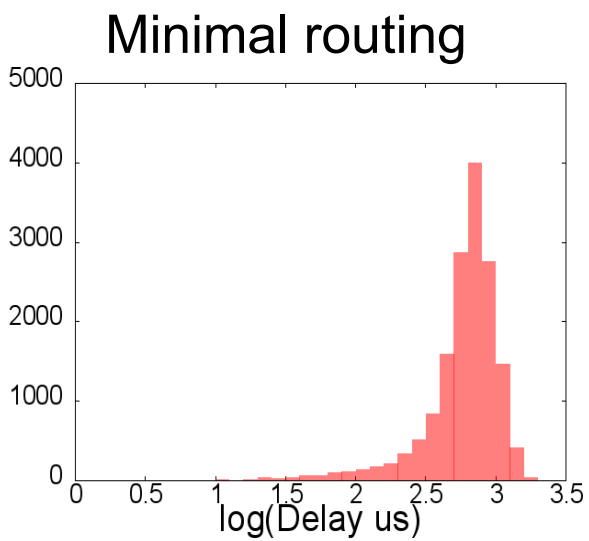
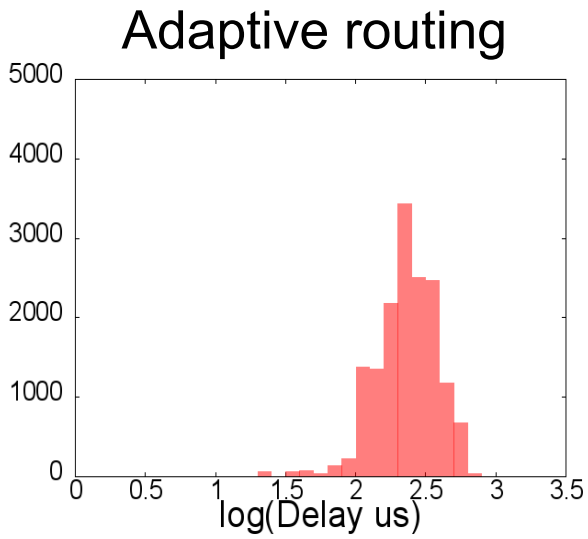
Majority of work should already be done for us in common core!





MODSIM is Camp David, not Sinai

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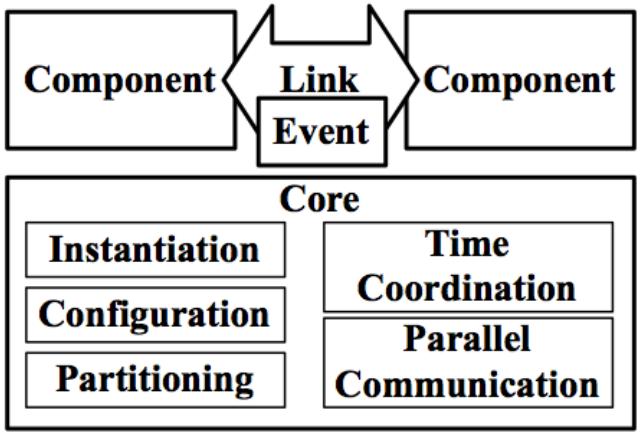
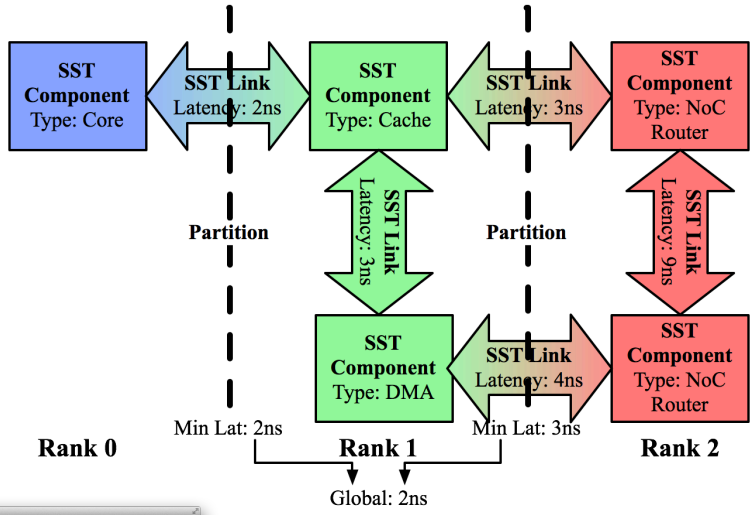
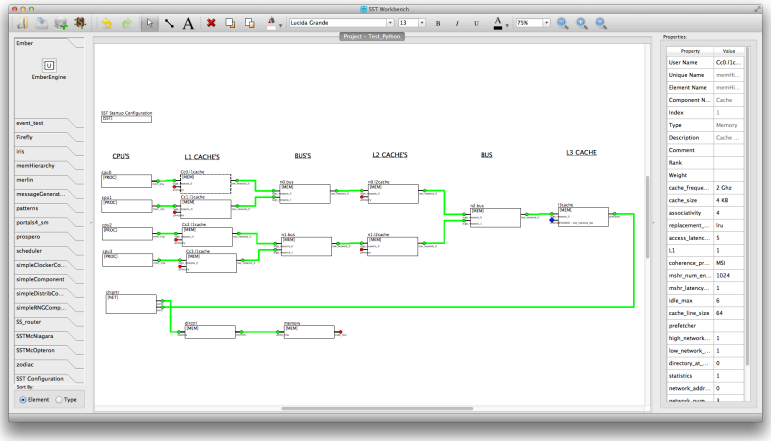
Structural simulation toolkit at Sandia (SST) is a jumping off point for discussing universal simulation standards, not C++ framework written on stone tablets!







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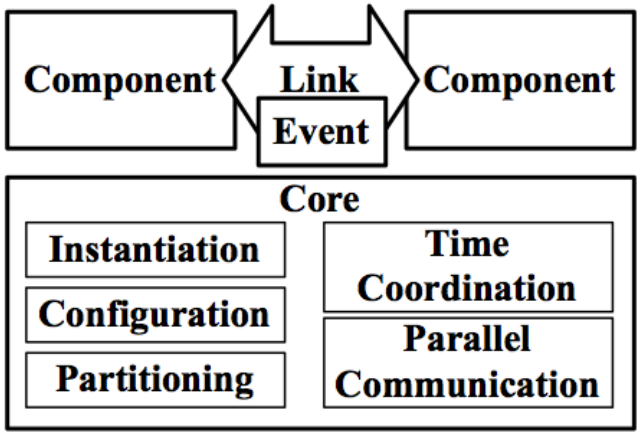
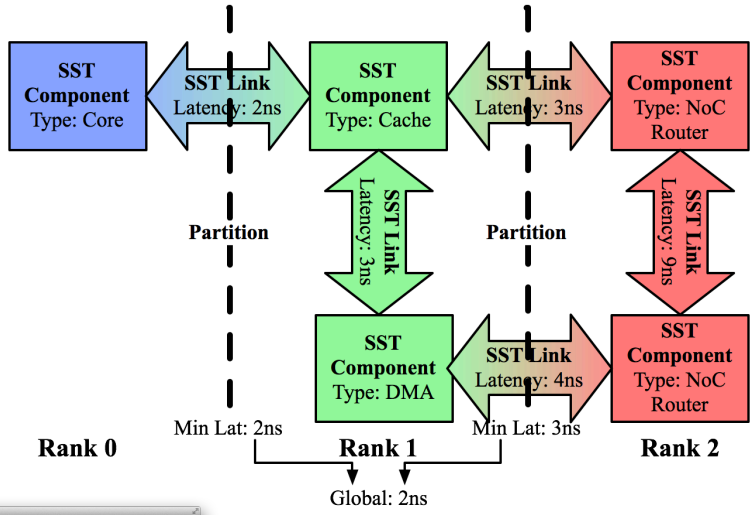
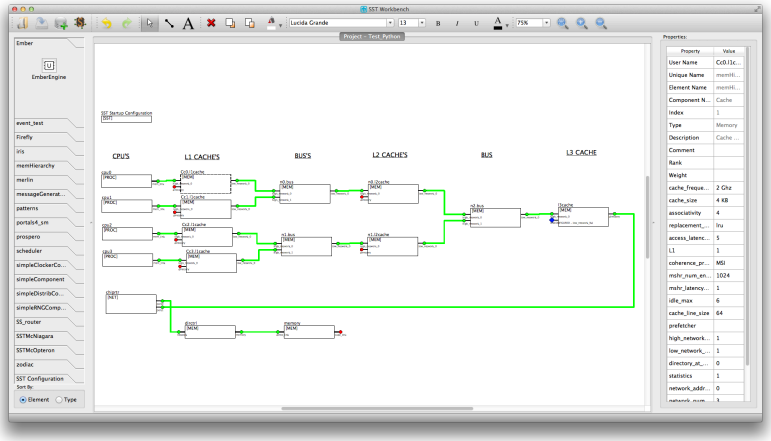
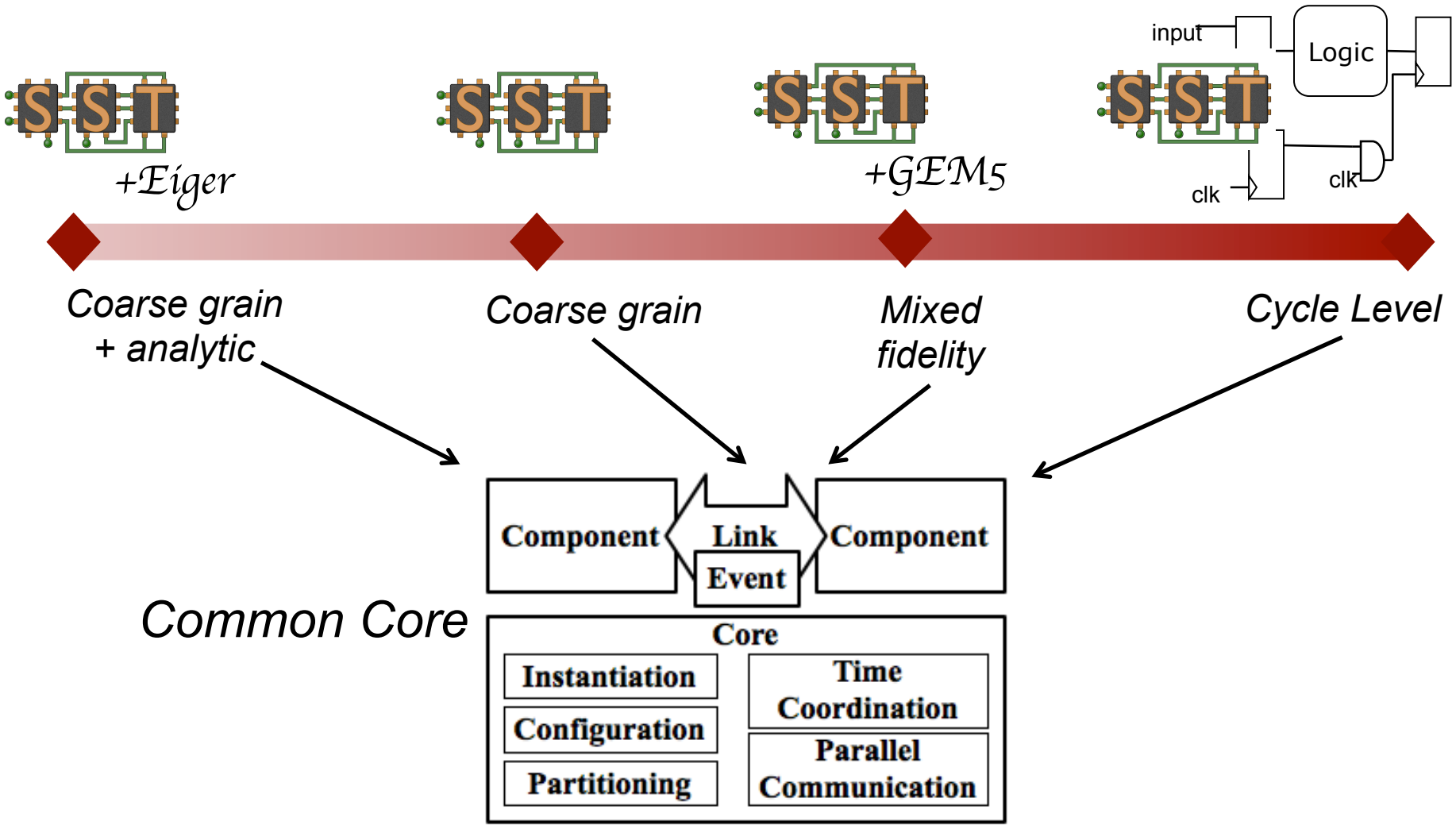
We think our PDES core is mature and lightweight enough to make your life easer – enable you to use your own code, not force you to use ours!







Range of simulation: success stories so far



MODSIM Summary

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- Gaps:
  - Lack of standards, lack of code reuse
- Bigger picture and potential collaborators:
  - Everyone? Anyone who wants to scale experiments through PDES or wants to compose models mixing different fidelity/physics
- What would make it easier to leverage results from other groups?
  - If you find yourself writing a PDES core, who you gonna call…
- ***Development/adoption of standards will be driven by collaboration and refined through use cases***