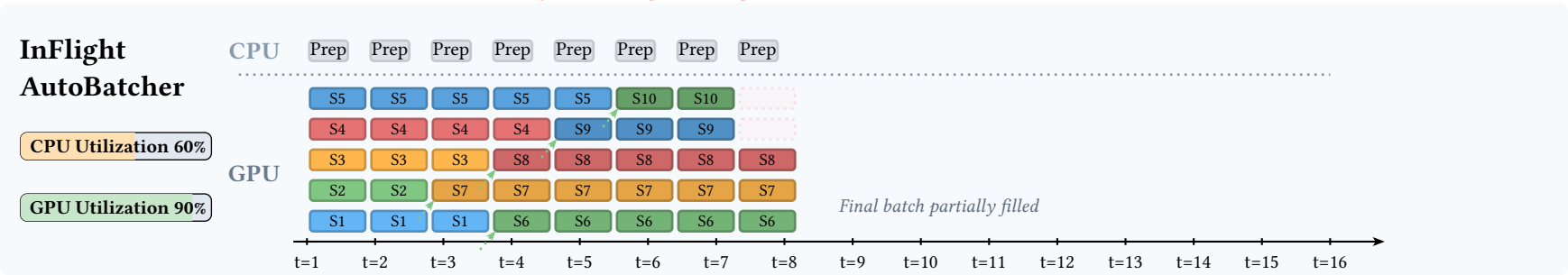
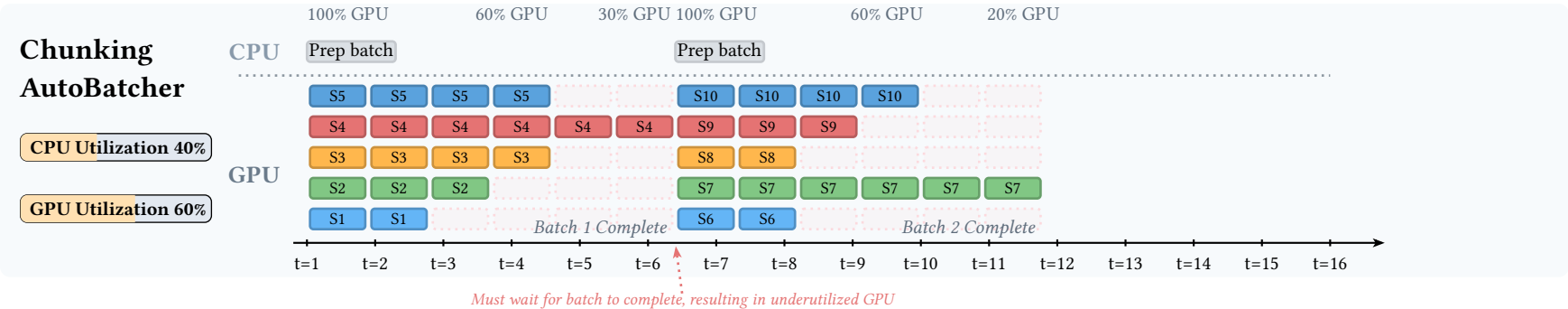
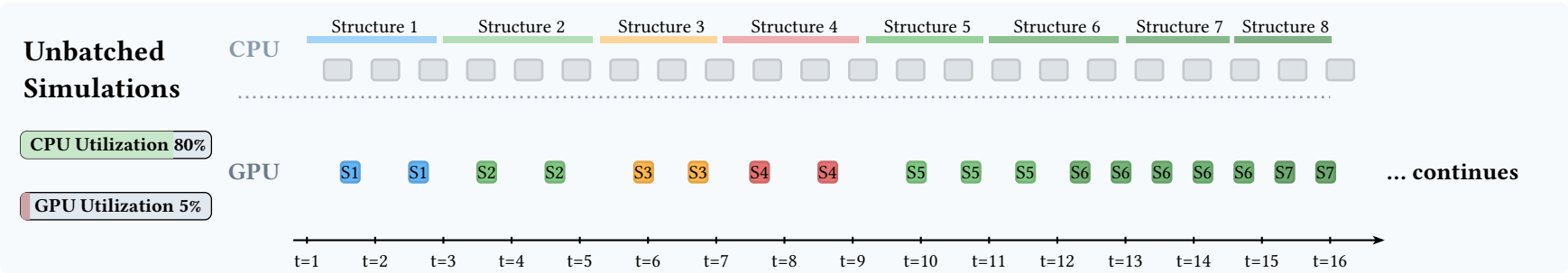


GPU Batching Strategies for Atomistic Simulations

Comparison of Unbatched vs. ChunkingAutoBatcher vs. InFlightAutoBatcher



In-flight batching achieves highest GPU utilization and maximizes predictions per unit time

Unbatched: Each simulation runs sequentially with most calculations on CPU and minimal GPU utilization
Chunking: Fixed-size batches improve GPU utilization but can't adapt to varying simulation completion times
In-flight: Dynamic reallocation eliminates GPU idle time by immediately adding new structures when others complete. Color changes indicate in-flight structure replacement.