# Visuals on the House: Optimizing HPC Workflows with No-Cost CPU Visualization


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## Abstract


The rise of heterogeneous resources in modern HPC systems has driven the scientific community beyond the exascale threshold. However, relying on GPUs for simulations often leaves CPUs underutilized. *In situ* techniques reduce data movement by operating in-memory but still involve blocking operations. We propose copying GPU-based timestep data to host memory, allowing CPUs to **concurrently handle visualization and analysis**, thus enabling simulations to continue without interruption.


## Implementation

- Inline Visualization and Analysis (GPU Blocking)
- Concurrent Visualization and Analysis (sim on the GPU, vis on the CPU)

```cpp
// Thread pool to manage non-blocking threads
ThreadPool::ThreadPool(size_t numThreads) : stop(false), activeTasks(0) {
    for (size_t i = 0; i < numThreads; ++i) {
        workers.emplace_back(&ThreadPool::workerThread, this);
    }
}

ThreadPool::~ThreadPool() {
    {
        std::unique_lock<std::mutex> lock(queueMutex);
        stop = true;
    }
    condition.notify_all();
    for (std::thread &worker : workers) {
        worker.join();
    }
}

void ThreadPool::enqueue(std::function<void()> task) {
    int taskID = taskIDCounter++;
    {
        std::unique_lock<std::mutex> lock(queueMutex);
        tasks.push(std::move(task));
        ++activeTasks;
    }
    condition.notify_one();
}

void ThreadPool::waitForCompletion() {
    std::unique_lock<std::mutex> lock(queueMutex);
    completionCondition.wait(lock, [this]() { return tasks.empty() && (activeTasks == 0); });
}

void ThreadPool::workerThread() {
    while (true) {
        std::function<void()> task;
        {
            std::unique_lock<std::mutex> lock(queueMutex);
            condition.wait(lock, [this] { return stop || !tasks.empty(); });
            if (stop && tasks.empty()) {
                return;
            }
            task = std::move(tasks.front());
            tasks.pop();
        }
        task();
        --activeTasks;
        completionCondition.notify_all();
    }
}

int ThreadPool::getTaskIDCounter() const {
    return taskIDCounter.load();
}
```

## Use Case

The GABLS1 benchmark simulates an atmospheric boundary layer (ABL) driven by a uniform geostrophic wind and a prescribed surface, and is used for weather forecasts, climate models, and our understanding of atmospheric phenomena.

## Next Steps

- Preliminary results are promising
- Run at scale on ALCF and JSC resources: 70 (280 GPUs), 140 (560 GPUs), 280 (1120 GPUs) nodes planned.

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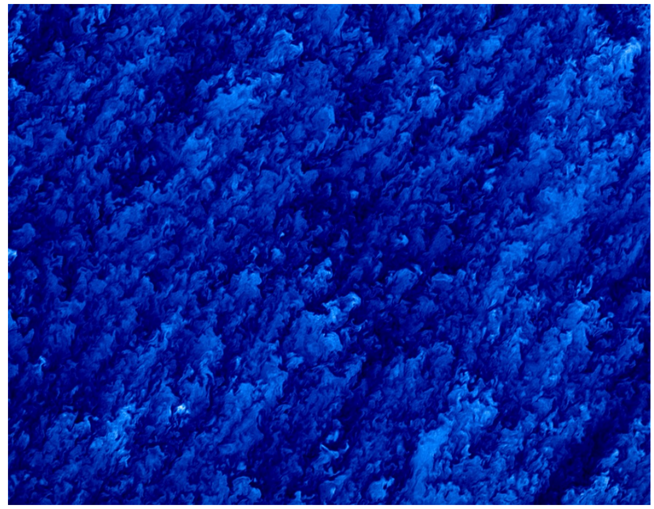
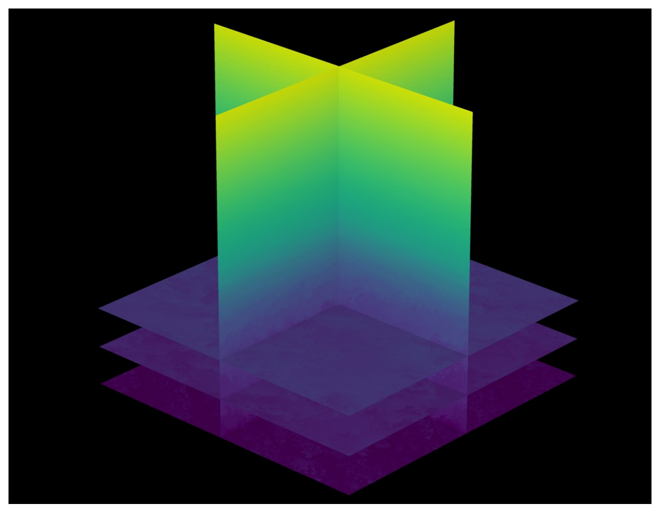


The GABLS case (MFEV/SMG model) simulated with NekRS, showcasing the turbulence fine structures in the X-Z plane at y = 100 m.



Slices of potential temperature in the GABLS case, highlighting the stratification of the Atmospheric Boundary Layer

## References


[1] A. C. Bauer, H. Abbasi, J. Ahrens, H. Childs, B. Geveci, S. Klasky, K. Moreland, P. O'Leary, V. Vishwanath, B. Whitlock, et al. In situ methods, infrastructures, and applications on high performance computing platforms. In Computer Graphics Forum, vol. 35, pp. 577–597. Wiley Online Library, 2016. 1

[2] R. J. Beare, M. K. MacVean, A. A. M. Holtslag, J. Cuxart, I. Esau, J.C. Golaz, M. A. Jimenez, M. Khairoutdinov, B. Kosovic, D. Lewellen, T. S. Lund, J. K. Lundquist, A. McCabe, A. F. Moene, Y. Noh, S. Raasch, and P. Sullivan. An Intercomparison of Large-Eddy Simulations of the Stable Boundary Layer. Boundary-Layer Meteorology, 118(2):247–272, Feb. 2006. doi: 10.1007/s10546-004-2820-6 2

[3] N. El-Sayed and B. Schroeder. To checkpoint or not to checkpoint: Understanding energy-performance-i/o tradeoffs in hpc checkpointing. In 2014 IEEE International Conference on Cluster Computing (CLUSTER), pp. 93–102. IEEE, 2014. 1

[4] M. Isakov, E. d. Rosario, S. Madireddy, P. Balaprakash, P. Carns, R. B. Ross, and M. A. Kinsy. Hpc i/o throughput bottleneck analysis with explainable local models. In SC20: International Conference for High Performance Computing, Networking, Storage and Analysis, pp. 1–13, 2020. doi: 10.1109/SC41405.2020.00037 1

[5] B. Kosovic and J. A. Curry. A large eddy simulation study of a quasi steady, stably stratified atmospheric boundary layer. Journal of the At mospheric Sciences, 57(8):1052 – 1068, 2000. doi: 10.1175/1520-0469 (2000)057<1052:ALESSO>2.0.CO;2 2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