

6 ESSENTIAL WAYS

To Optimize HPC Software with MPI and OpenMP

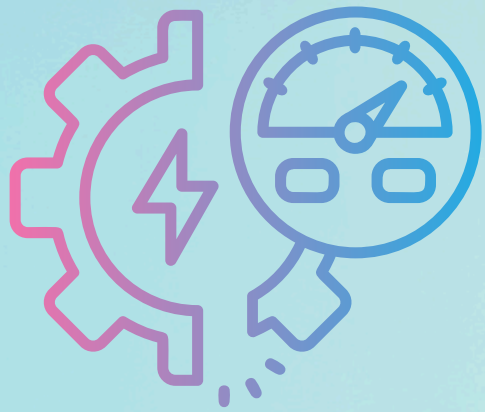


01

UNDERSTAND WHY OPTIMIZATION MATTERS

Optimization is about making programs **run faster**, **use fewer resources**, and **scale efficiently** on supercomputers.

- Saves CPU hours and energy costs
- Enables larger, more complex scientific simulations
- Maximizes the potential of hardware and software investments



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ACCELERATE WITH OPENMP

OpenMP optimizes work within a single node using threads.

🔧 Optimization tips:

- Apply **#pragma omp parallel** for to loops.
- Use reduction to safely combine results.
- Control thread placement with **OMP_NUM_THREADS** and **OMP_PLACES**.
- **Avoid false sharing** by aligning per-thread data.



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PROFILE AND MEASURE PERFORMANCE

Measure before tuning!

🧰 Tools:

- **perf**, **mpiP**, or **Intel VTune** for CPU/MPI profiling
- **HPCToolkit** or **Score-P** for tracing hybrid performance

📊 Metrics:

- Execution time
- Speedup (T_1 / T_p)
- Efficiency (S / P)
- Strong & Weak scaling efficiency

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PARALLELIZE WITH MPI



MPI (Message Passing Interface) enables distributed computing.

🔑 Key tips:

- Use non-blocking communication (**MPI_Isend**, **MPI_Irecv**) to overlap computation.
- Minimize synchronization and redundant messages.
- Organize ranks logically with **MPI_Cart_create** for topology-aware efficiency.

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COMBINE MPI + OPENMP FOR HYBRID POWER



Hybrid programming = **MPI between nodes** + **OpenMP within nodes**.

⚙️ Run setup example:

```
export OMP_NUM_THREADS=8  
mpirun -np 4 --bind-to core ./hybird_app
```

💡 Goal: fewer MPI processes, more threads per process = balanced memory and communication load.

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APPLY ADVANCED OPTIMIZATIONS



🚀 Boost efficiency with:

- **Cache blocking** for better data reuse
- **Loop fusion** to reduce memory access
- **Asynchronous I/O** to minimize waiting
- **Roofline modeling** to identify bandwidth vs compute limits

More Information

In HPC, every cycle counts. Optimize locally, scale globally.

Learn more: mpi-forum.org | openmp.org