Load Balancing and Data Migration in a Hybrid Computational Fluid Dynamics Application

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High Performance Computing

Computer Science

Scientific Computing

Center for Simulation and Modeling (SaM)

HPC researchers/consultants

★ ★ ★ ★ ★

Educational

Research

Technical

521 users

Sciences

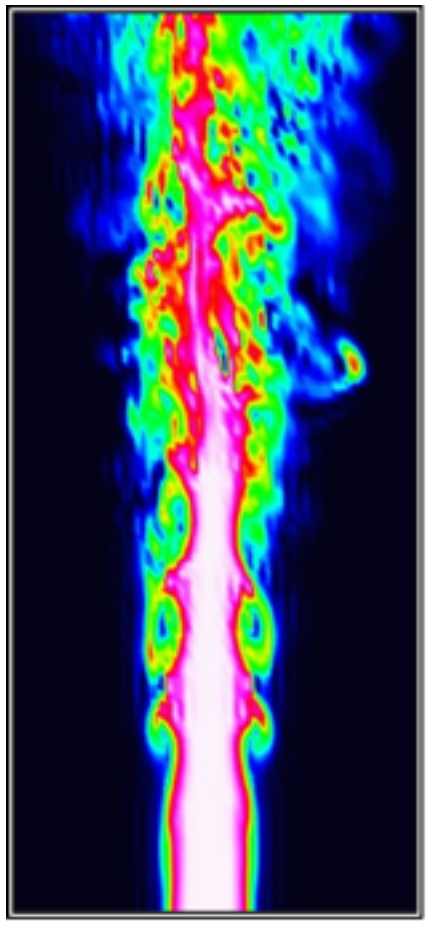
Health

Engineering

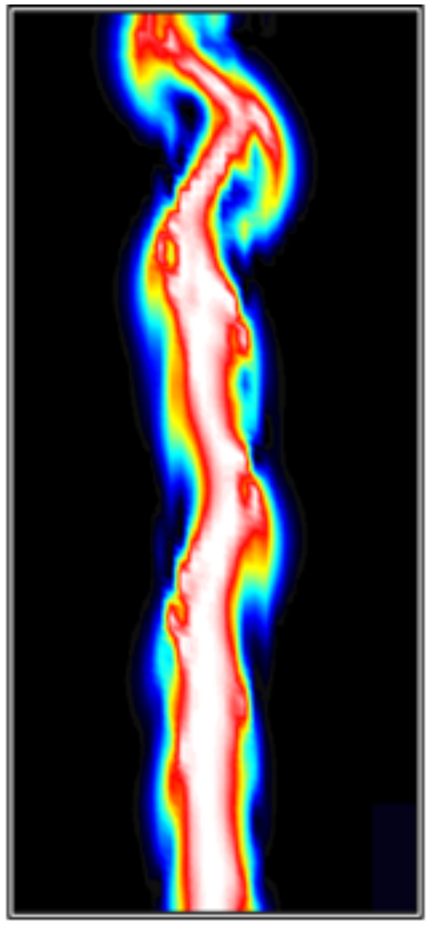
8,040 cores

91% utilization in 2014

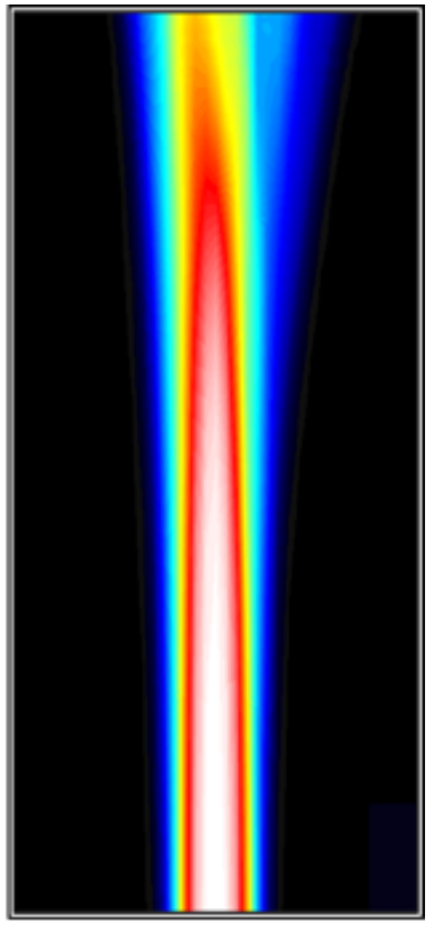
IPLMCFD


Direct Numerical Simulation

(DNS)


Large Eddy Simulation

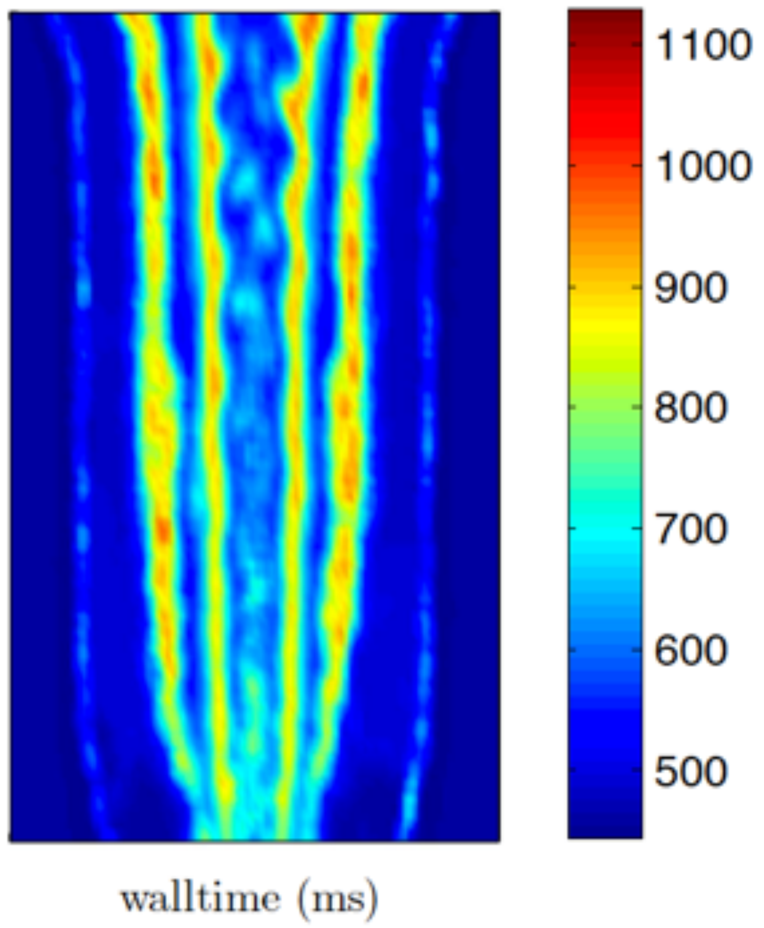
(LES)

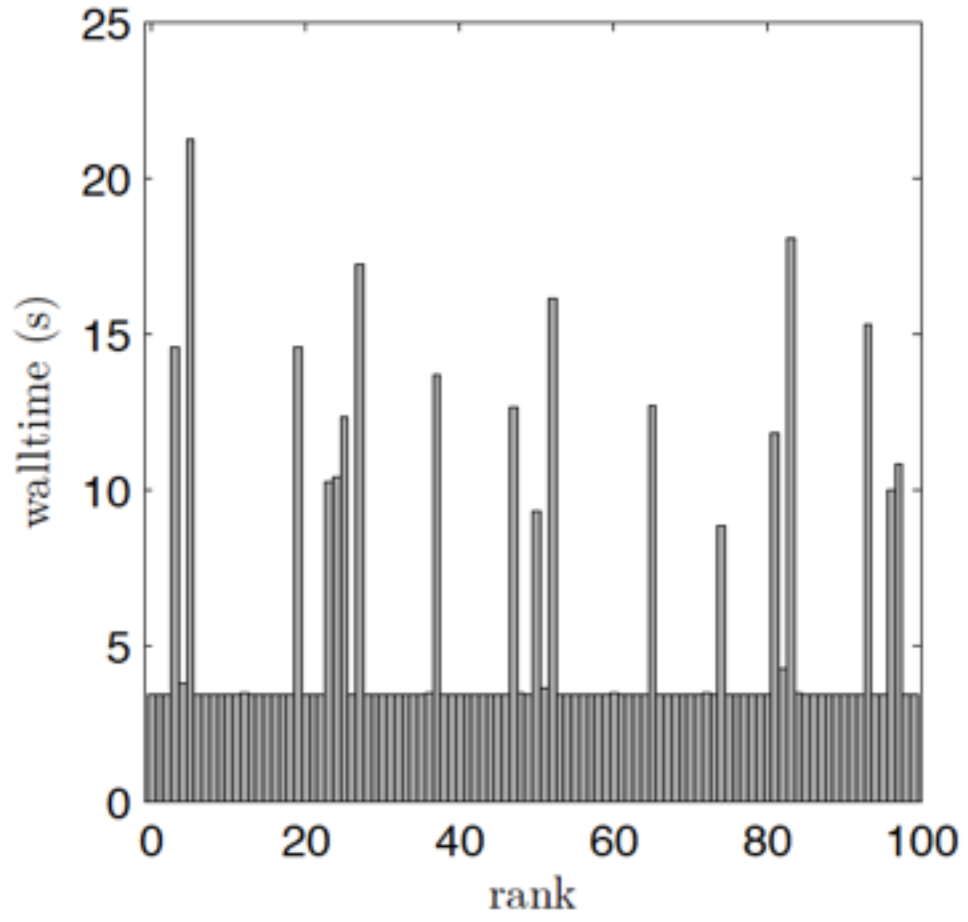

Reynolds Averaged Simulation

(RANS)

- A massively parallel solver for turbulent reactive flows.
- LES via filtered density function (FDF).

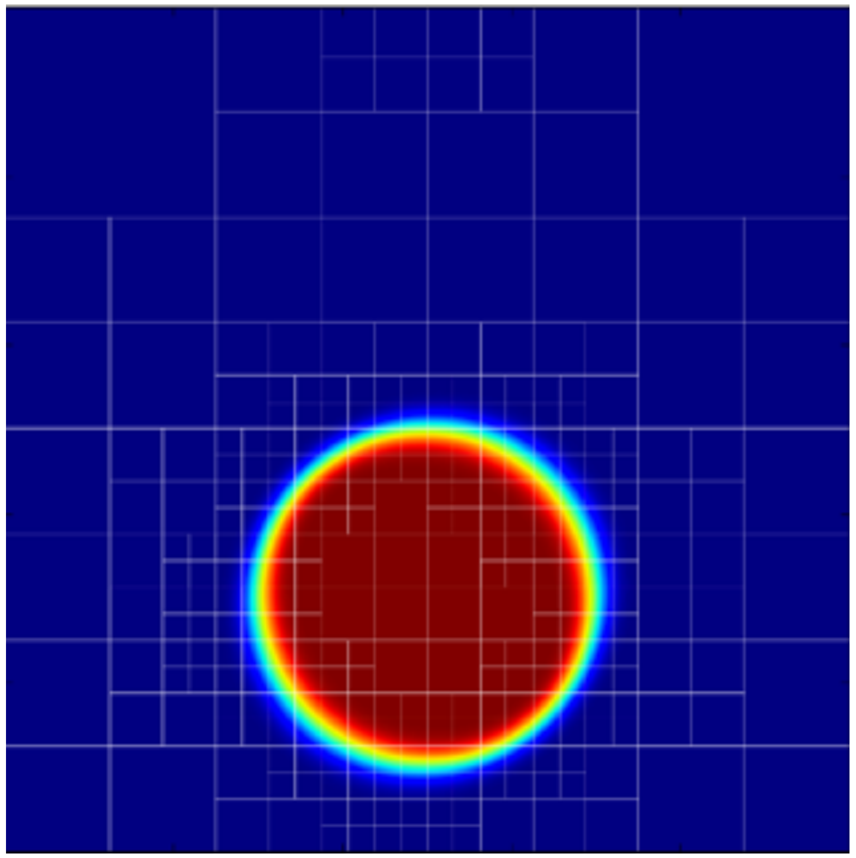
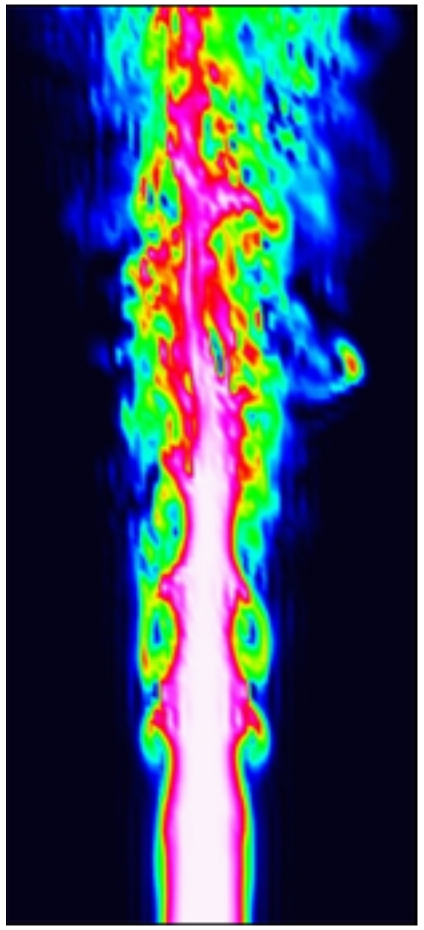
Load Imbalance





- IPLMCFD uses a graph partitioning library (METIS) to redistribute work.
- Requires to split execution between calls to repartition cells.

Reasons for Load Imbalance in CFD

Traditional	IPLMCFD
 Langer *et al*, SBAC-PAD, 2012.	
Adaptive Mesh Refinement	Chemical Reaction

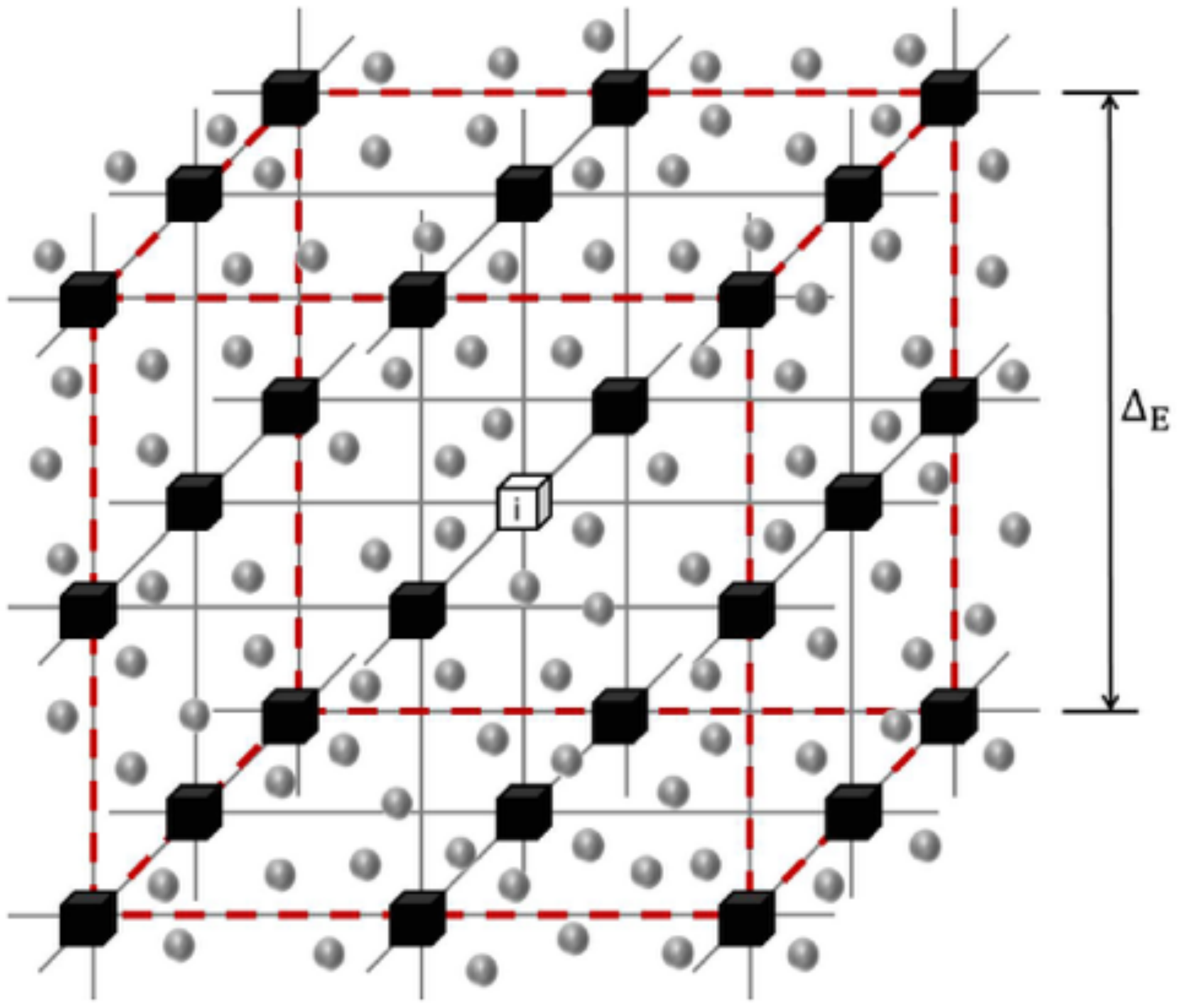
- Approaches:
  - ❖ Task-parallel
  - ❖ Zoltan
  - ❖ Charm++

Agenda

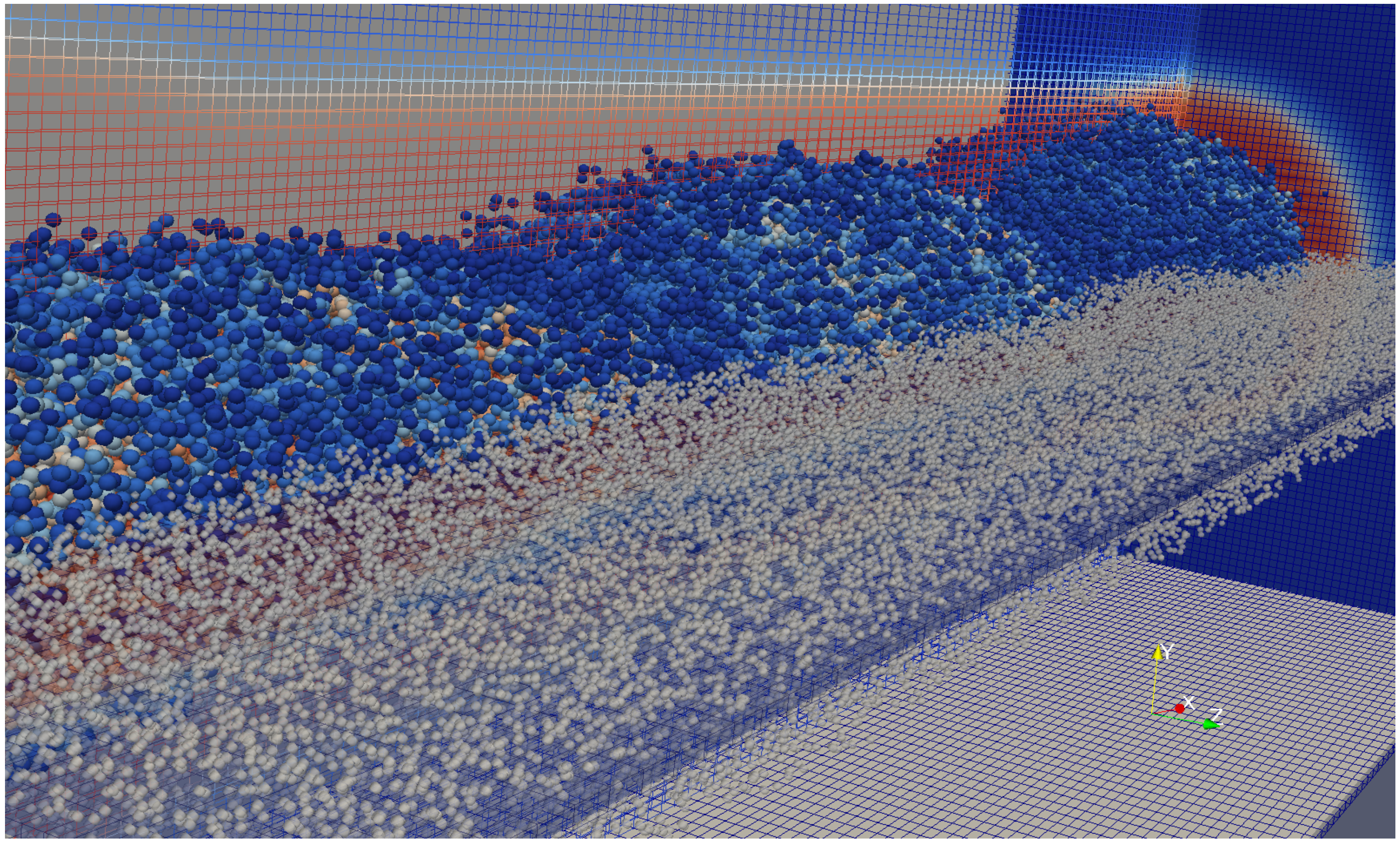
- IPLMCFD: A Hybrid Computational Fluid Dynamics Application
- Zoltan Library
- PaSR Benchmark
- Zoltan vs Charm++ Comparison

Hybrid CFD Application

- IPLMCFD: Irregularly Portioned Lagrangian Monte Carlo Finite Difference.
- Domain divided into cells, the atomic distribution unit.
- Ensemble of cells:
  - Same number of FD points.
  - Same number of MC particles.

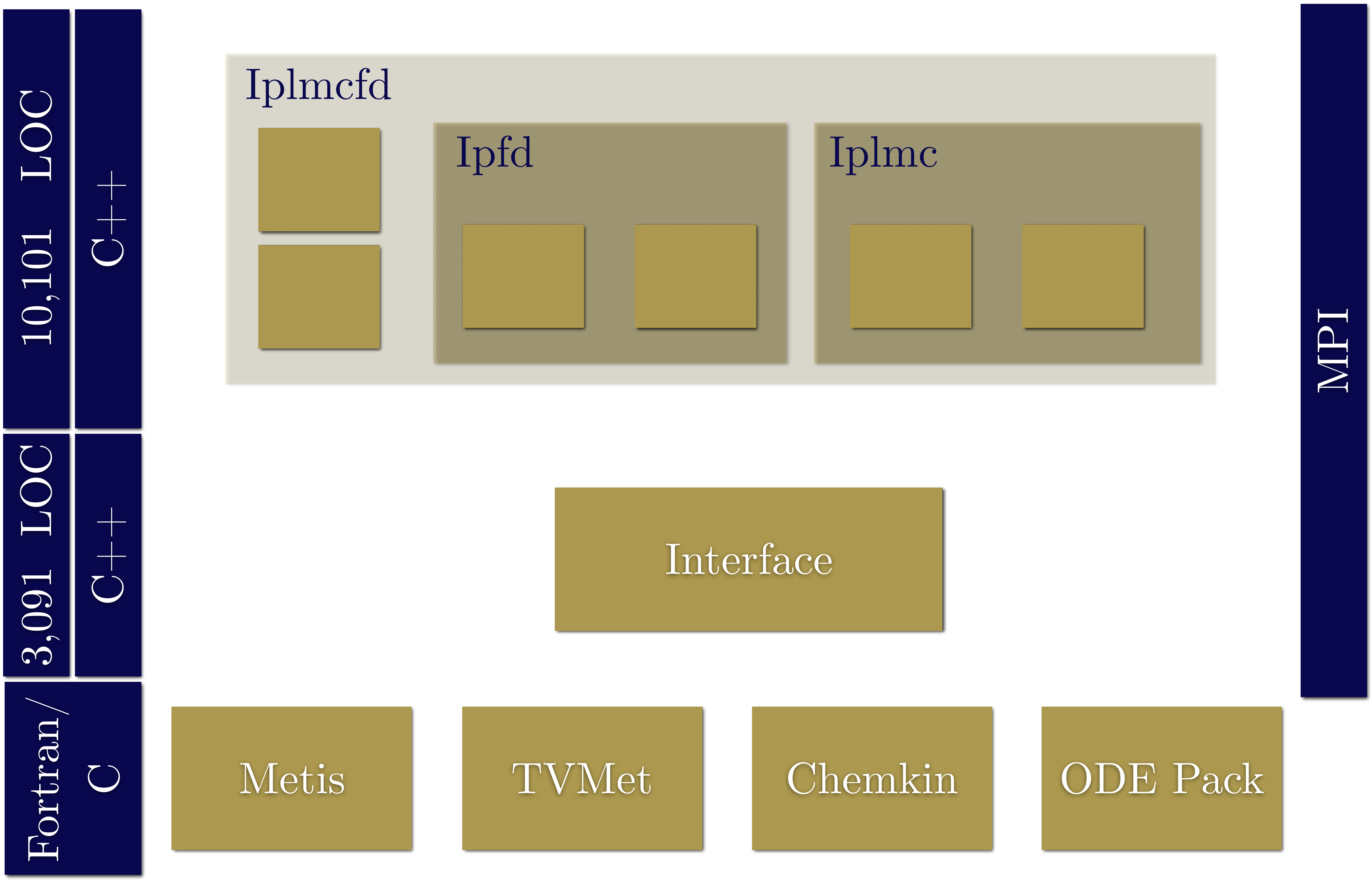


Computational Fluid Dynamics



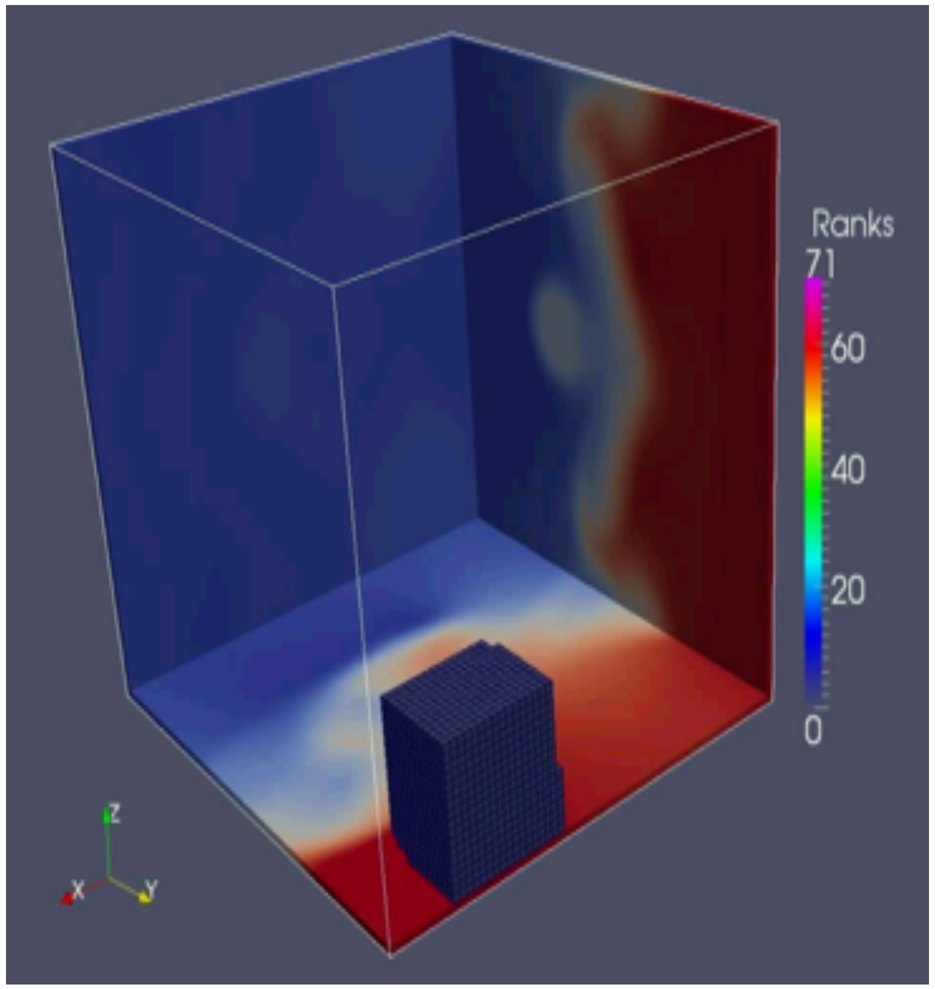
# Grids	# Particles	# Species	Required Memory GBs	GFLOP per iteration	# Iterations	Serial Run-time (1 GFLOP/s)
10^6	6×10^6	9	1.69	29.5	60,000	20.5 days
10^6	6×10^6	19	2.48	90.7	60,000	63 days
5×10^6	50×10^6	19	24.0	544.7	220,000	3.8 years

Code Structure



IPLMCFD

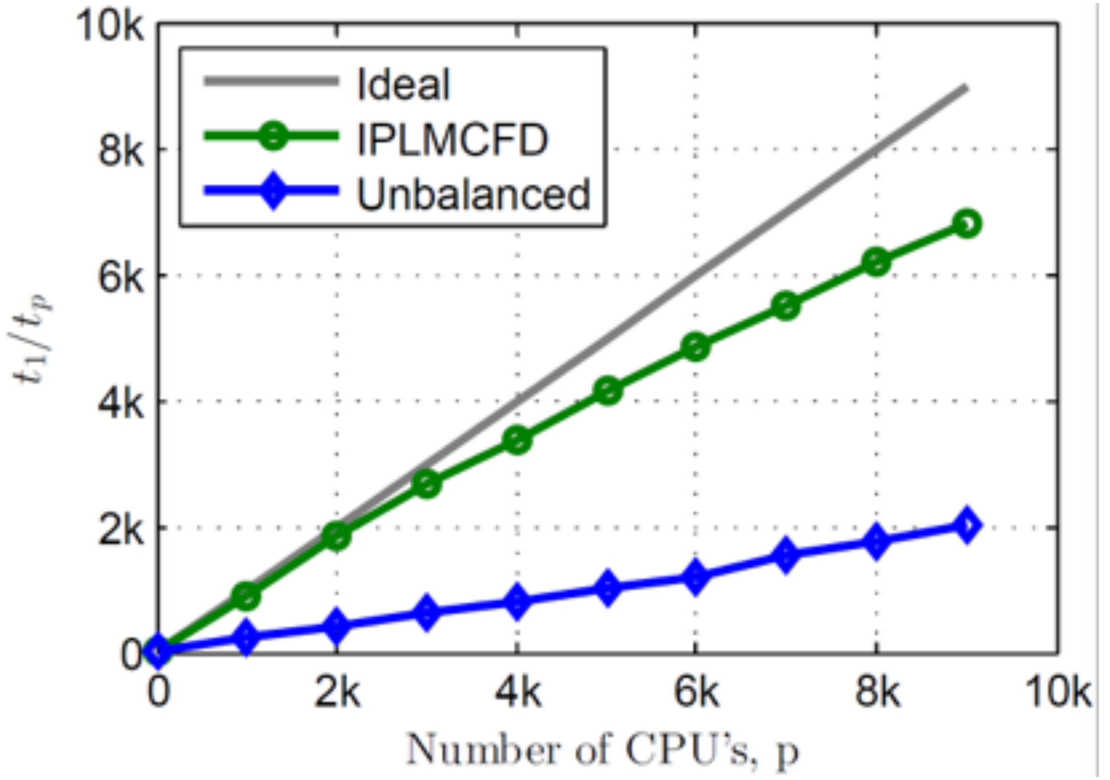
- A scalable algorithm for hybrid Eulerian/Lagrangian solvers.
- Goals:
  - Balance the computational load among processors through weighted graph partitioning.
  - To minimize the number of adjacent elements assigned to different processors (minimize the edge-cut).
- Irregularly shaped decompositions:
  - Disadvantages:
    - Nontrivial communication patterns
    - Increased communication cost.
  - Advantage (major):
    - Evenly distributed load among partitions.

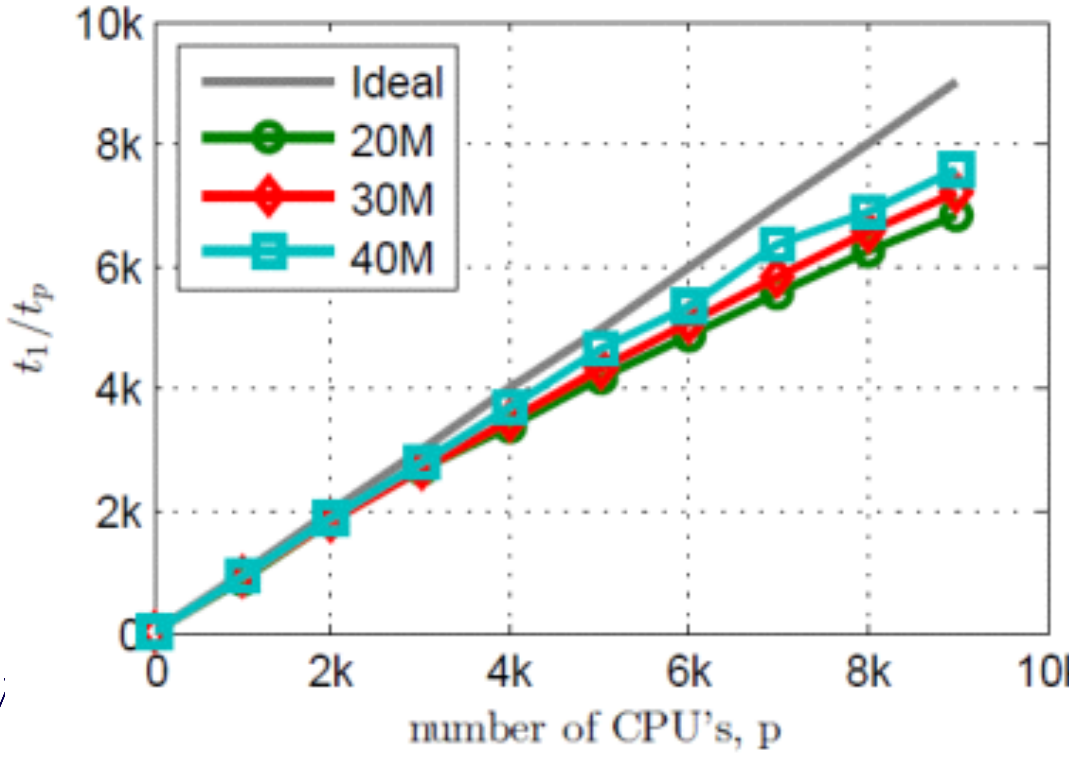


P. H. Pisciuneri *et al.*, *SIAM J. Sci. Comput.*, vol. 35, no. 4, pp. C438-C452 (2013).

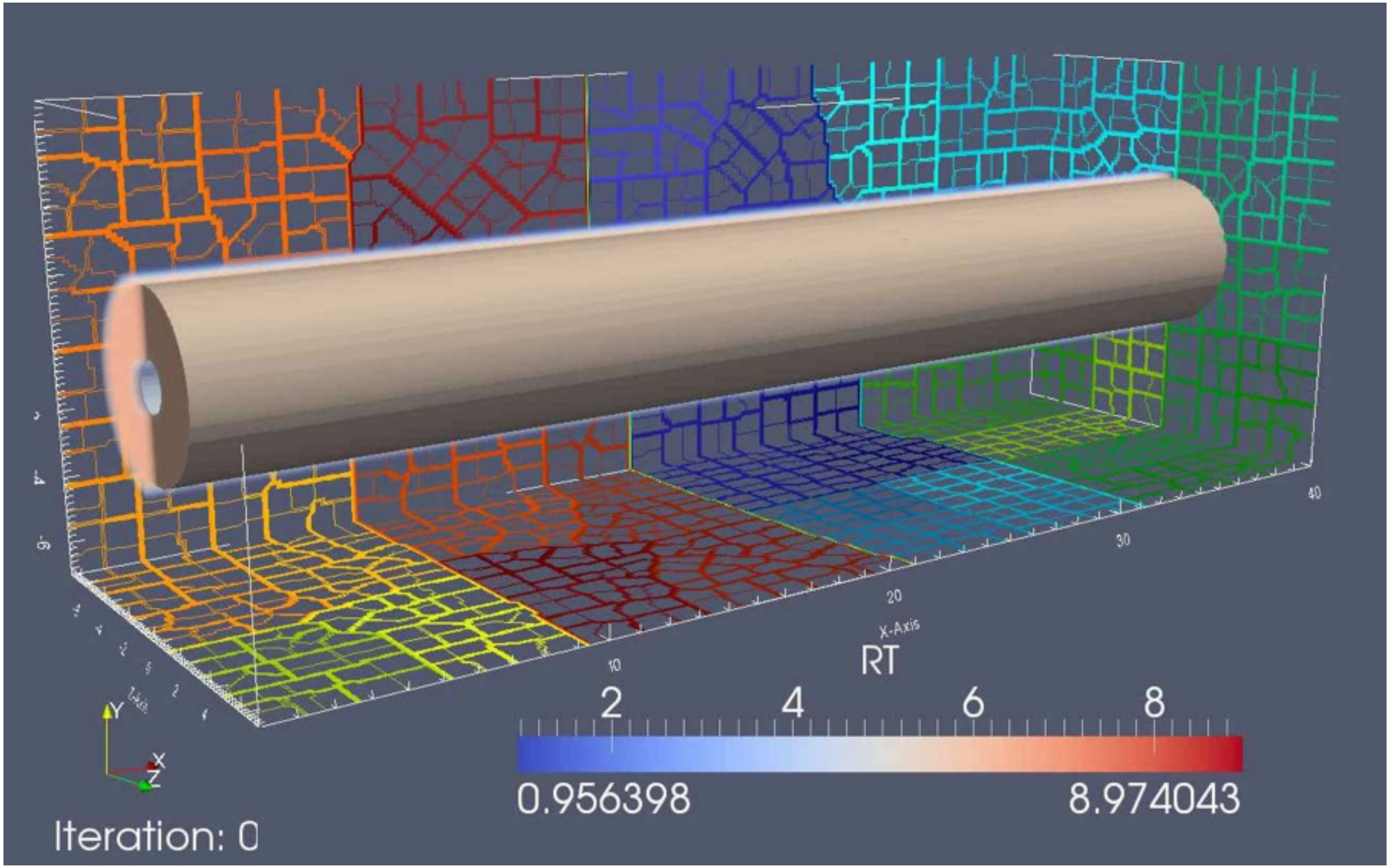
Strong Scaling

- Geometry:
  - 2.5 million FD points
  - 20 million MC particles
  - Chemistry: 9 species, 5-step
- Top:
  - Unbalanced: 22% efficiency (9K cores)
  - IPLMCFD: 76% efficiency (9K cores)
- Bottom:
  - Performance of IPLMCFD improves as the number of MC particles increases
  - IPLMCFD: 84% efficiency at 9k processors for 40M particles
- Timing:
  - The average of 10 iterations immediately after load balancing



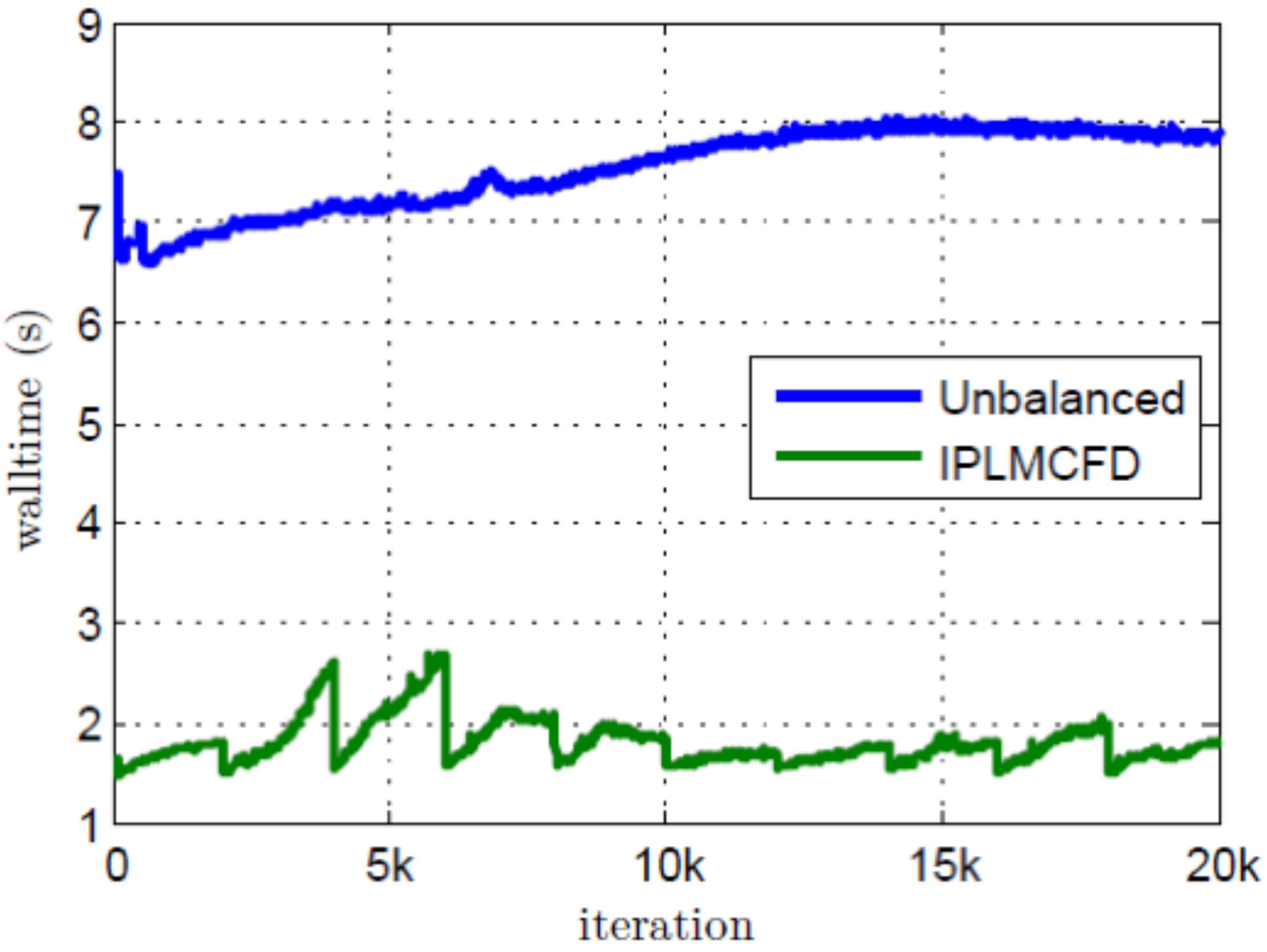


Simulation of a Premixed Flame



Temporal Performance of IPLMCFD

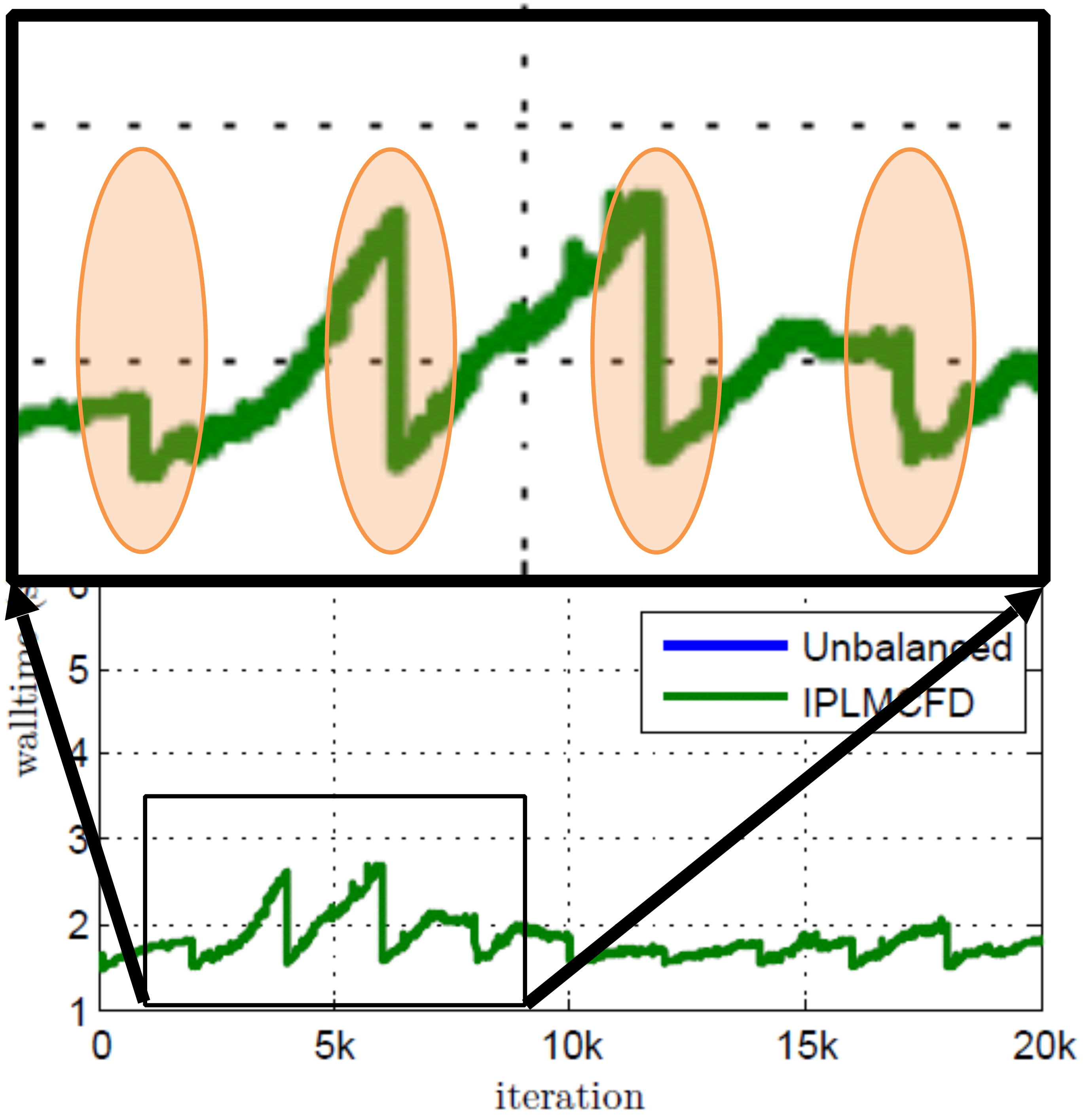
- Unbalanced: approx. static performance
- IPLMCFD: variable performance
  - Load balancing is performed approx. every 2000 iterations
  - Optimal performance immediately after load balancing
  - Performance degrades in time
- Potential walltime savings afforded by IPLMCFD for this example:



$\boxed{T_{\text{Unbalanced}} - T_{\text{IPLMCFD}} = 30 \text{ hours}}$

Cost of Repartitioning

- **Naïve approach:**
  - Immediately before load-balancing checkpoint the entire simulation
  - Restart the simulation with a new decomposition
  - Costly, involves:
    - Writing to shared filesystem
    - Simulation cleanup
    - Simulation startup
    - Reading from shared filesystem
  - Does not scale
  - $O(10^2 - 10^3)$ iterations in cost
- **Optimal approach:**
  - Repartitioning should be handled in memory
  - The new partition is aware of the previous partition, thus minimal data movement and interruption



Zoltan

- "*A toolkit of parallel combinatorial algorithms for unstructured and/or adaptive computations*".
- Sandia-OSU collaboration since 2000.
- Part of Trilinos package.
- Zoltan2 project in C++.

Dynamic load balancing
Parallel repartitioning

Data migration tools

Distributed data directories

Unstructured communication

Dynamic memory management

Zoltan IPLMCFD

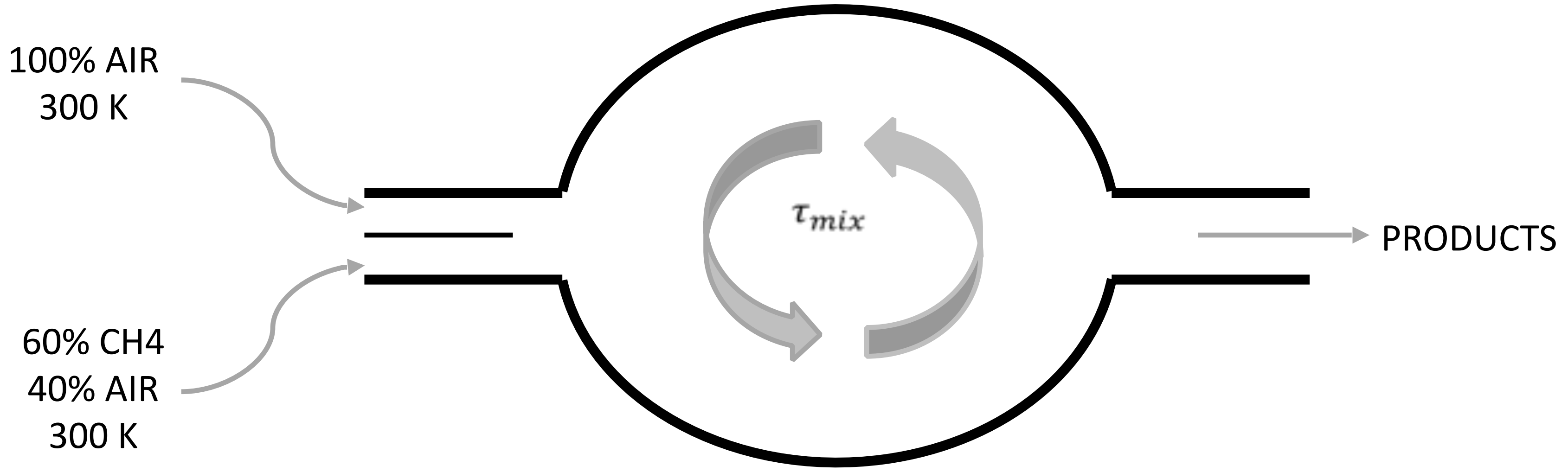
- Zoltan's callback function interface.
- Methodology:
  - ❖ Atomic unit $\longrightarrow$ cell (irregular subdomains).
  - ❖ Data registration $\longrightarrow$ number of objects, object weights.
  - ❖ Graph management $\longrightarrow$ number of edges, edge weights.
  - ❖ Migration $\longrightarrow$ pack/unpack functions.
  - ❖ Load balancing $\longrightarrow$ partition, repartition, refinement.
  - ❖ Global information $\longrightarrow$ distributed data directory.

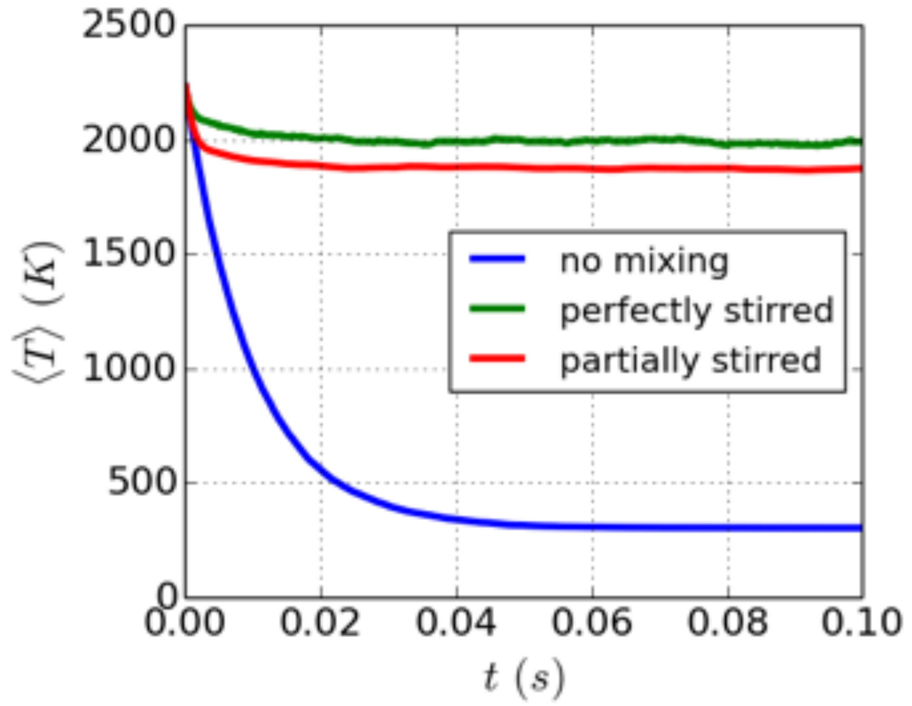
Charm++ IPLMCFD

- Goal: fully exploit Charm++ features.
- Methodology:
  - ❖ Atomic unit $\longrightarrow$ subdomain (regular subdomains).
  - ❖ Containing class $\longrightarrow$ 3D chare *array*.
  - ❖ Process-based data $\longrightarrow$ chare *group*.
  - ❖ Communication $\longrightarrow$ outermost level.
  - ❖ Structured control flow $\longrightarrow$ Structured Dagger.
  - ❖ Migration $\longrightarrow$ PUP methods.

Partially Stirred Reactor (PaSR)

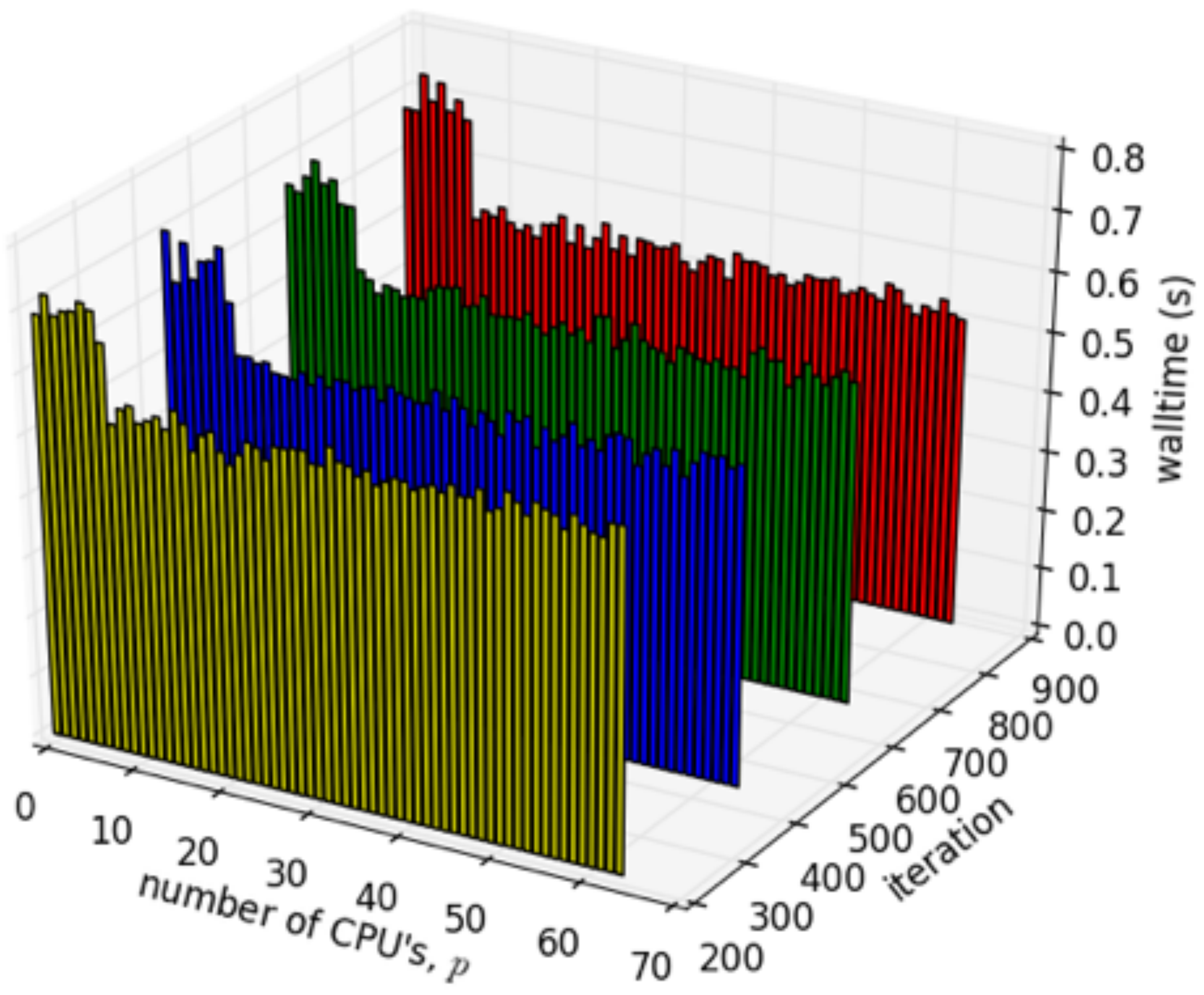
- Parameters:
  - IC: Stoichiometric mixture of methane&air reacted until equilibrium (T≈2230 K)
  - Simulation duration: $t_{end}=10\ \tau_{res}$
- Realizability:
  - Lower bound, no mixing
  - Upper bound, perfectly stirred



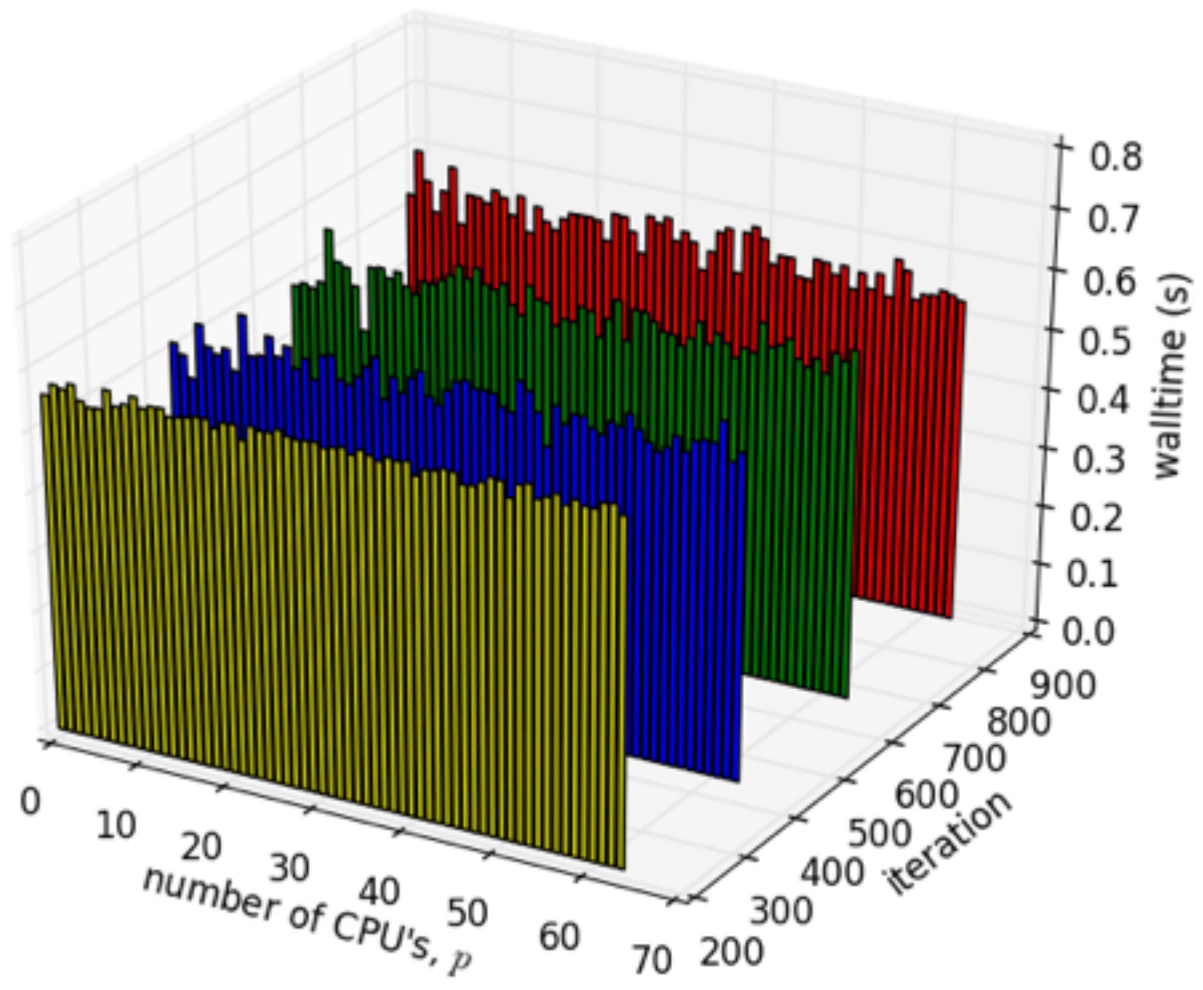


Dynamic Load-Balancing

Static Partition



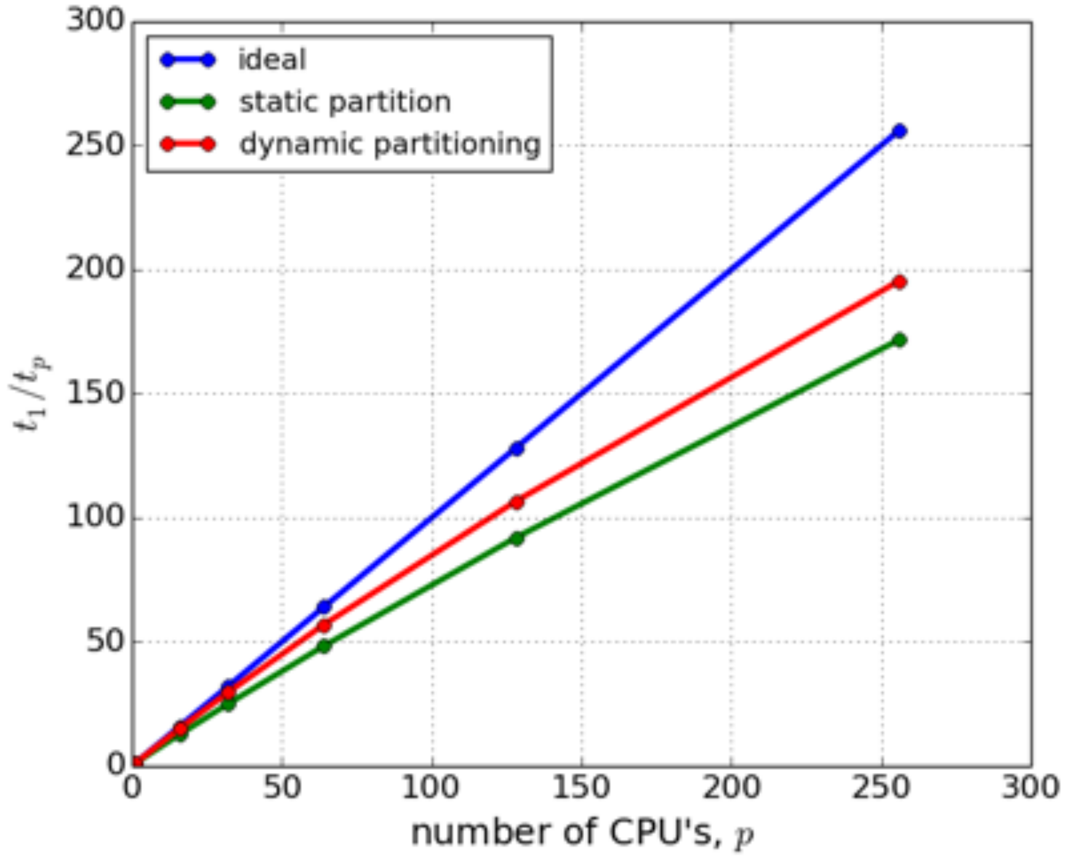
Dynamic Partitioning



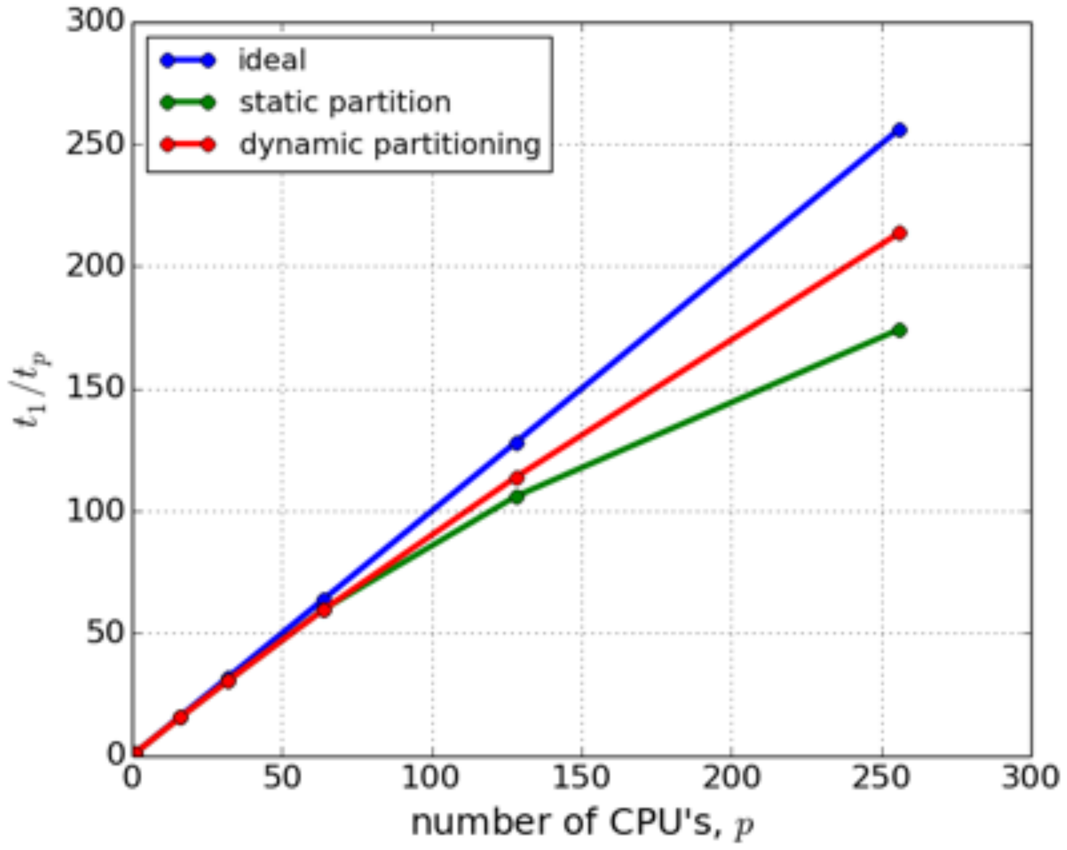
Strong Scaling

- Parameters:
  - ❖ 10,000 particles
  - ❖ Chemistry: 9 species, 5-step
- Timings over the entire simulation (Stampede)
  - ❖ The Zoltan and Charm++ timings include all overhead associated with repartitioning and data migration

ZOLTAN



Charm++



Programming Effort

	Zoltan IPLMCFD	Charm++ IPLMCFD
Startup	39	0
Object Graph Management	80	0
Data Migration	427	61
Load Balancing	40	3
Measured in lines of code (LOC)		

Charm++ Wishlist

- MPI $\longrightarrow$ Charm++ migration guide:
  - Instructions on using Charm++ with build systems.
  - Translating common MPI programming patterns.
  - Dealing with communication operations.
  - Highlighting opportunities for improvement.
- Parallel I/O documentation.
- Accelerator programming documentation.

Conclusions

- Competitive performance between Zoltan and Charm++ for adaptive simulations of turbulent reactive flows.
- Charm++ alleviates programming effort of infrastructure for adaptive computation.

Thank You!

Q&A