Dynamic Load Balancing of High Performance Computing Applications

Echtzeit-AG, 25 Nov 2014, TU Dresden

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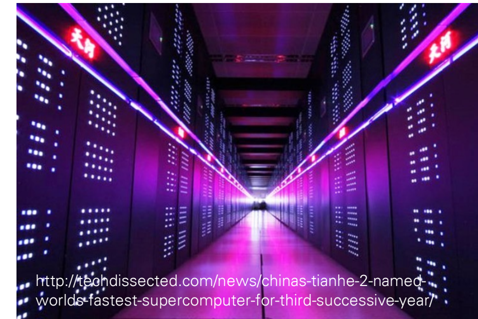
Outline

- **Introduction**
- Dynamic Load Balancing
  - Objectives
  - Metrics: Workload, Load Balance
  - Typical Approach
- Partitioning Methods
- Software Stack
- Experiences with COSMO-SPECS+FD4
- Conclusion

Introduction: High Performance Computing

- Large number of computers (nodes) tightly coupled with fast network
- "Supercomputers": fastest available HPC systems
- Batch scheduling of compute jobs
  - Applications request a fixed amount of nodes and time
- Typical programming model
  - Message Passing Interface (MPI)
  - Combined with OpenMP, OpenCL, CUDA, … within a node
- Current hot topics: energy efficiency, fault tolerance, heterogeneity, programmability

Tianhe-2, CN
16 000 nodes
384 000 cores
+ 48 000 Phi
54,9 PFLOPS
17,8 MW

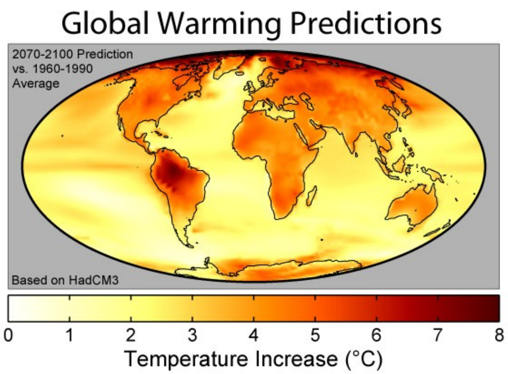


Titan, USA
18 688 nodes
299 008 cores
+ 18 688 GPUs
27,1 PFLOPS
8,2 MW

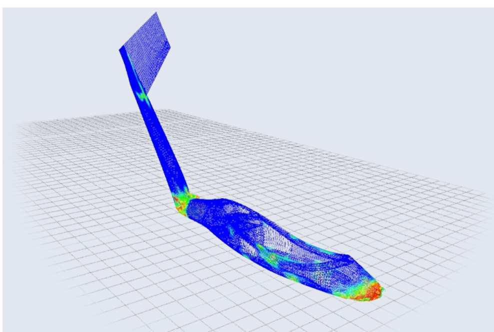
Sequoia, USA
98 304 nodes
1 572 864 cores
20,1 PFLOPS
7,9 MW

K Computer, JP
88 128 nodes
705 024 cores
11,3 PFLOPS
12,6 MW

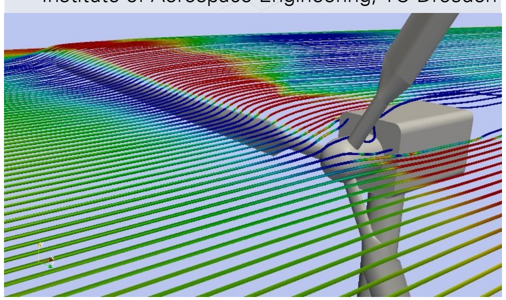
Introduction: High Performance Computing Applications



http://commons.wikimedia.org/wiki/File:Global_Warming_Predictions_Map.jpg



Institute of Aerospace Engineering, TU Dresden

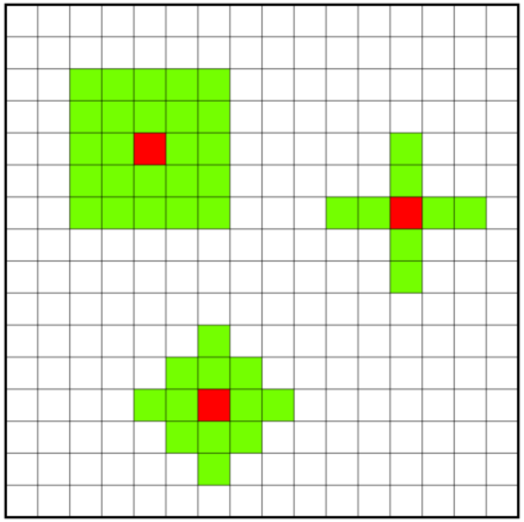


http://civsweb01.purduecal.edu/fipse/?page_id=247

- A few examples of HPC applications:
  - Earth sciences: weather/climate prediction, earthquake simulations
  - Structural mechanics: vehicle design, crash simulation, civil engineering
  - Computational fluid dynamics: wind tunnel, turbine flow
  - Molecular Dynamics: drug design, structural biology, material science
- Many HPC applications are simulations based on partial differential equations
- Discretized in space and time to allow the approximate numerical solution

Introduction: Discretization and Parallelization

- Grid represents distribution of unknowns in space
- Stencil computations to advance from one time step to the next
  - Data dependencies to neighbor cells only



Introduction: Discretization and Parallelization

- Grid represents distribution of unknowns in space
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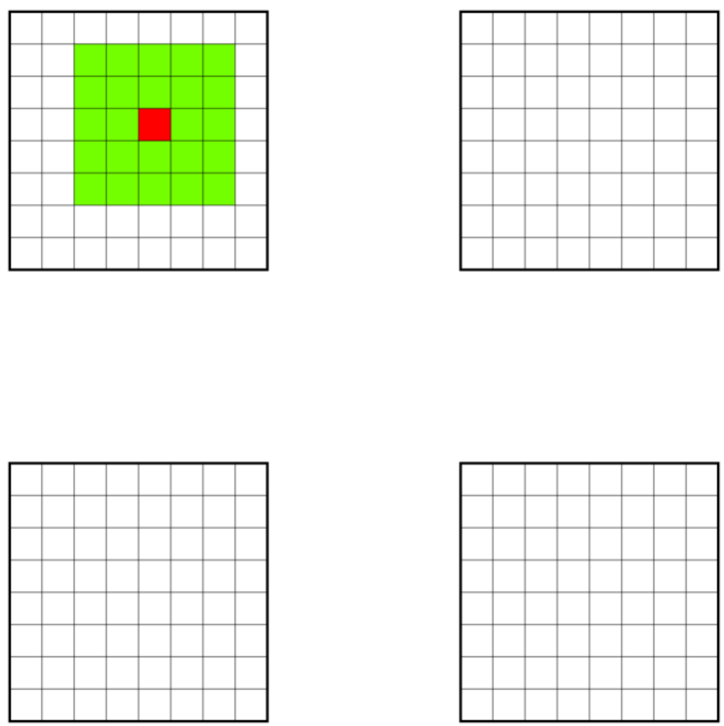
- Parallelization by spatial decomposition of the grid (partitioning)
  - Load-balanced and minimal communication



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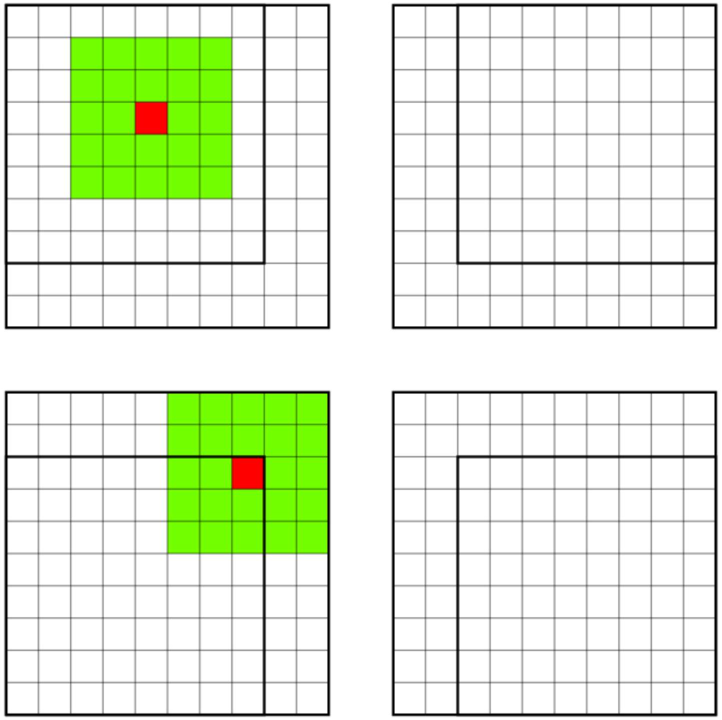
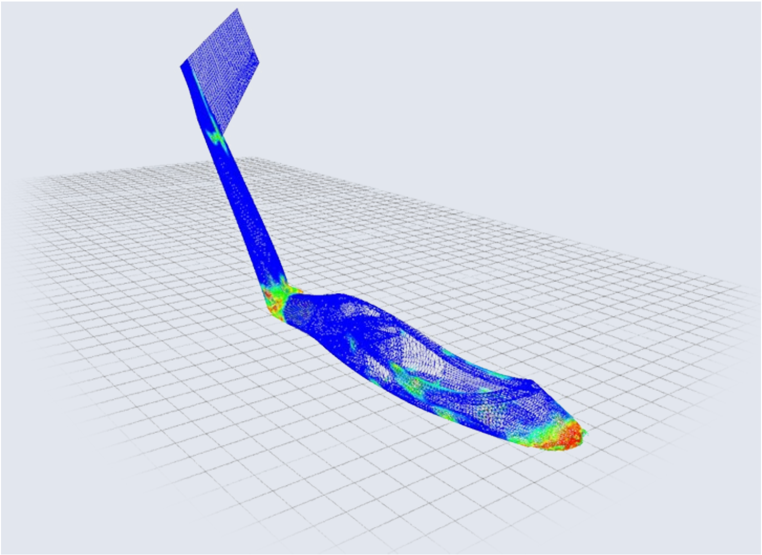


Introduction: Unstructured Grids

- Rectangular grids are the most simple case
- Triangular meshes or arbitrary grid structures are also used
- Complex geometries are better represented



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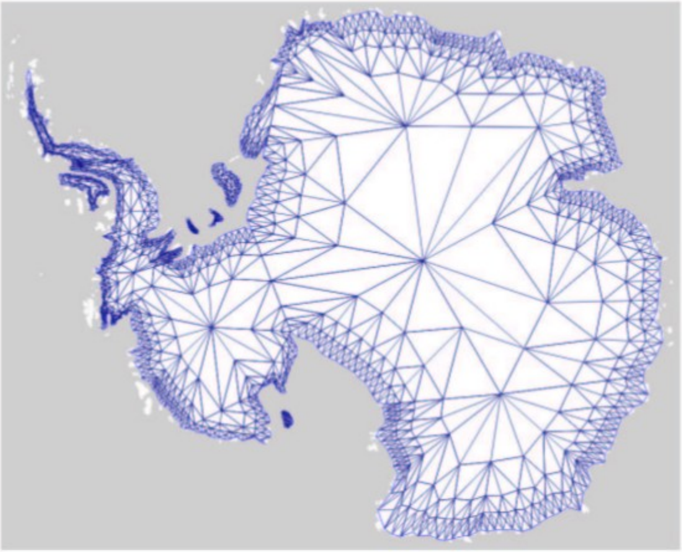
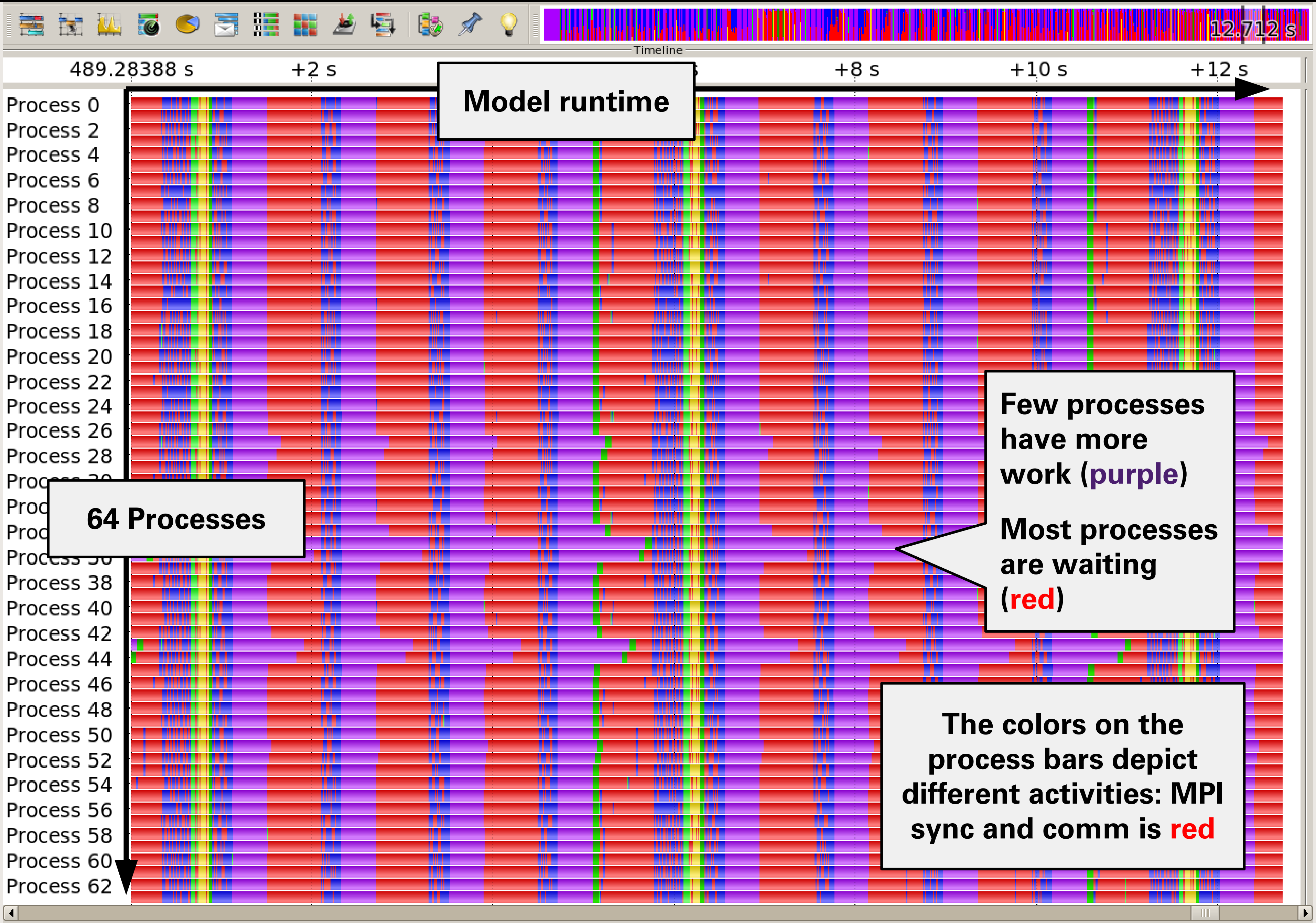


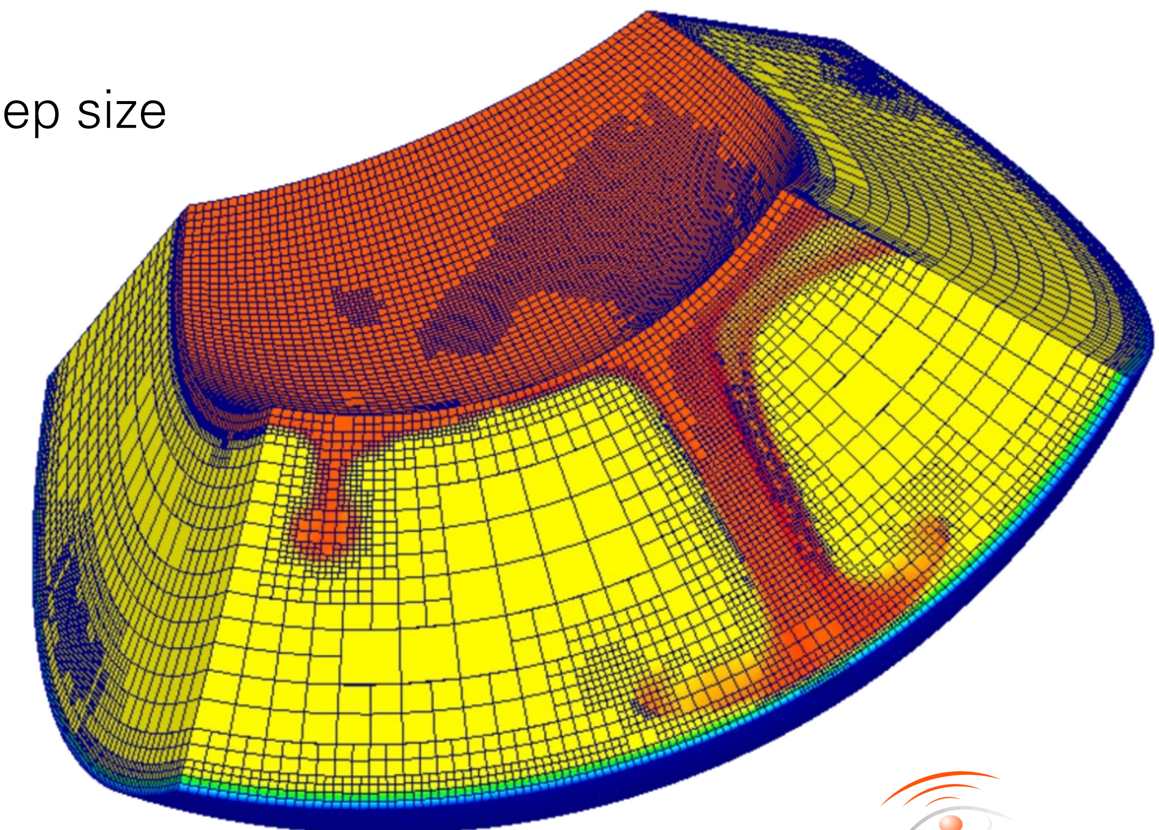
Behrens, *Multilevel optimization by space-filling curves in adaptive atmospheric modeling,* Frontiers in Simulation, 2005

Load Imbalance Visualized



Introduction: Sources of Imbalances

- Adaptive grids / Adaptive mesh refinement (AMR)
  - Adapt the spatial grid resolution dynamically to the simulation, e.g. shock waves, flame fronts, cracks, ...
- Adaptive time stepping
  - Same, but for time step size



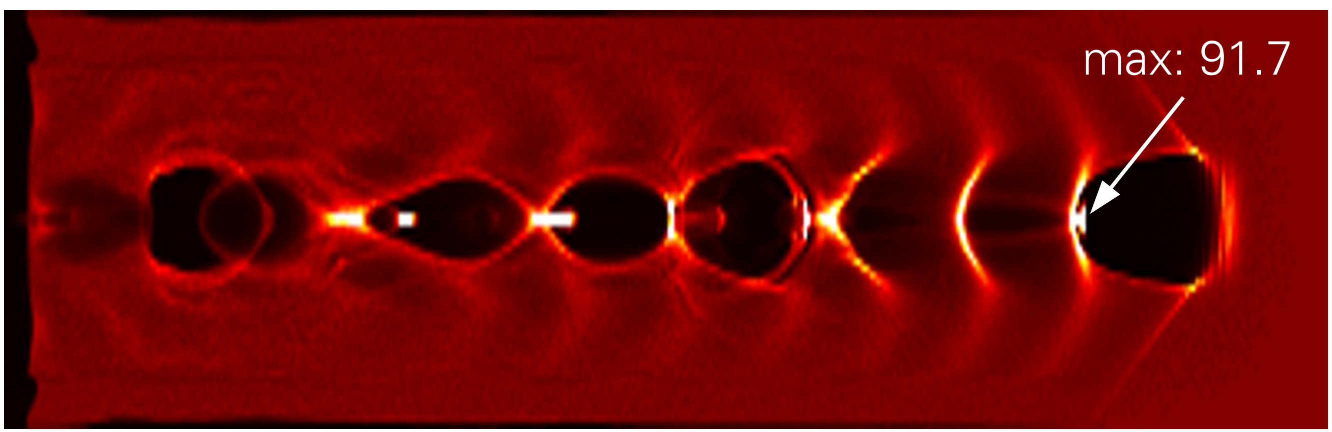
Adaptive refinement of thermal plumes in the mantle convection simulation Rhea

Burstedde et al., *ALPS: A framework for parallel adaptive PDE solution*, J. Phys. Conf. Ser. 180, 2009

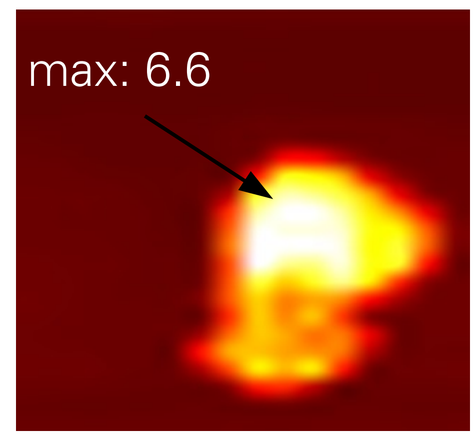
Introduction: Sources of Imbalances

- Model-inherent sources
  - Computational effort per grid cell varies with the model variables
  - Particle-in-Cell: number of particles per grid cell
  - Cloud microphysics: presence of droplets, temperature

Laser wakefield acceleration simulation (LWFA) with particle-in-cell code PIConGPU



Cloud simulation COSMO-SPECS



Workload relative to avg

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  - **Objectives**
  - Metrics: Workload, Load Balance
  - Typical Approach
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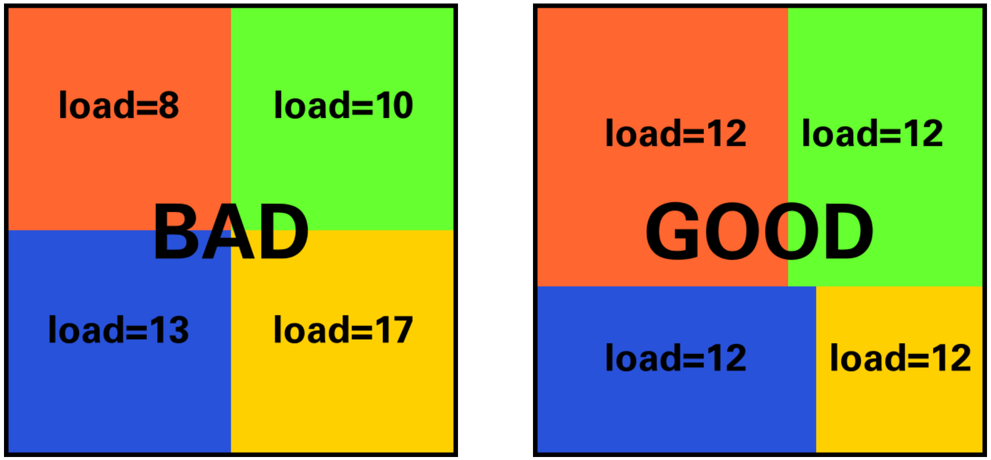
Dynamic Load Balancing: Objectives

- Four objectives of dynamic load balancing

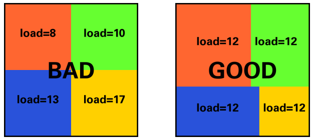
Dynamic Load Balancing: Objectives

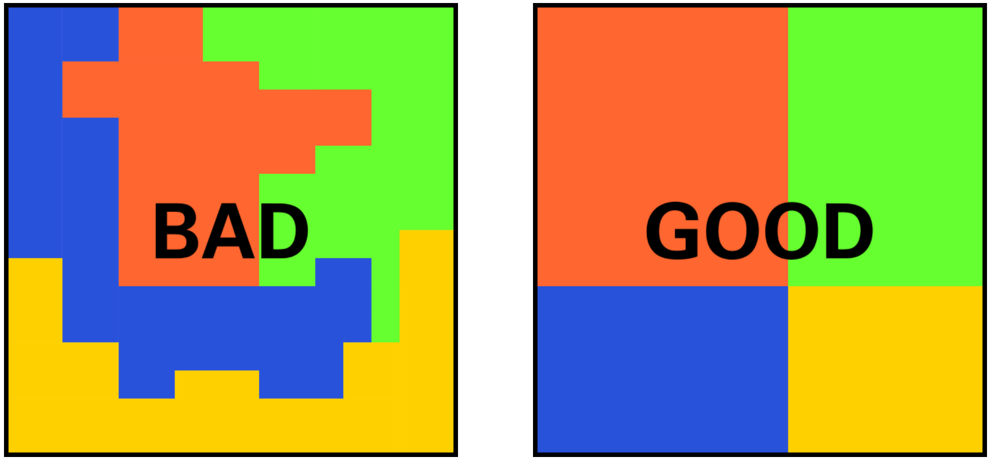
- Four objectives of dynamic load balancing
  - Balance workload



Dynamic Load Balancing: Objectives

- Four objectives of dynamic load balancing
  - Balance workload
  - Reduce communication between partitions (due to data dependencies)





Dynamic Load Balancing: Objectives

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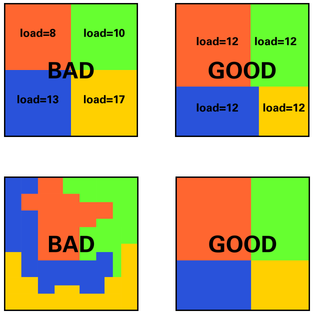

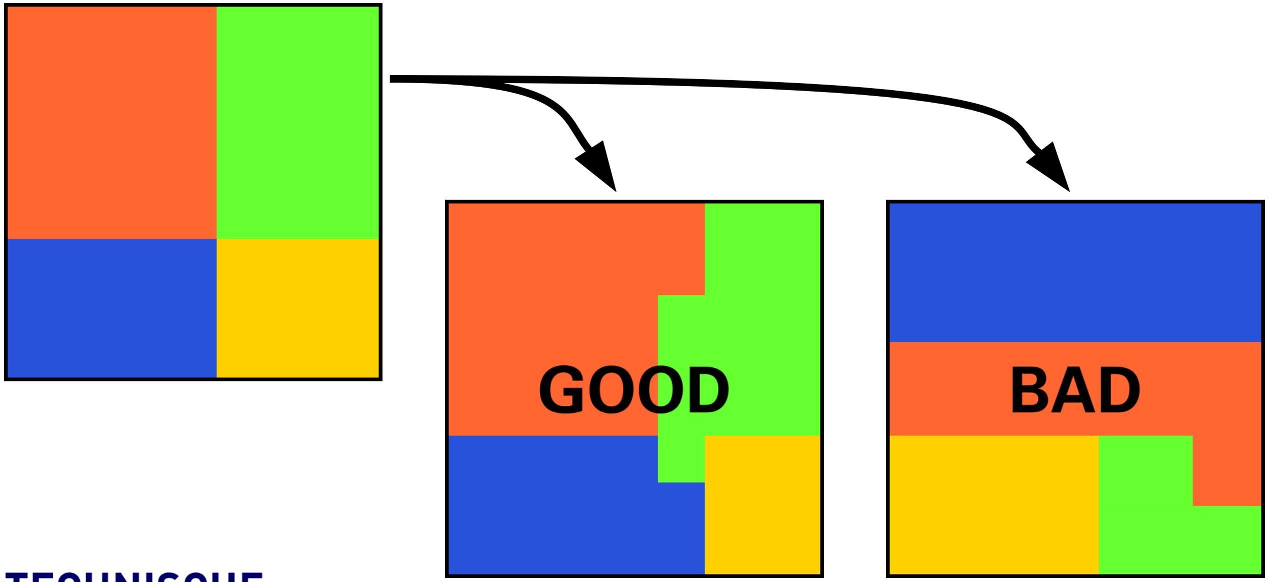

Dynamic Load Balancing: Objectives

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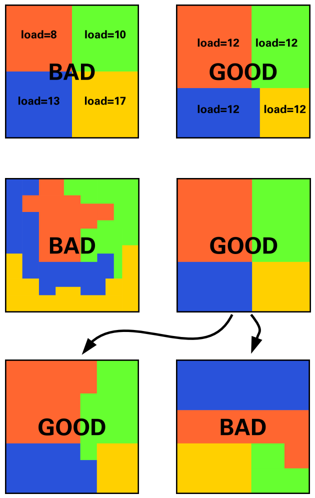
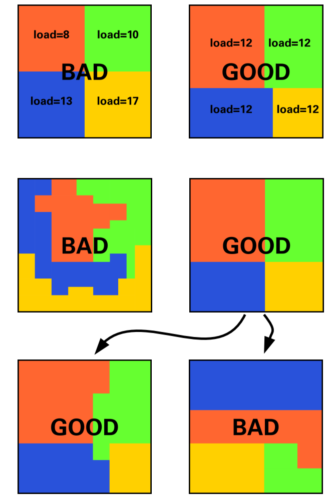
  - Compute partitioning as fast as possible



Dynamic Load Balancing: Objectives

- Four objectives of dynamic load balancing
  - Balance workload
  - Reduce communication between partitions (due to data dependencies)
  - Reduce migration, i.e. communication when changing the partitioning
  - Compute partitioning as fast as possible
- Contradictory goals
- Optimal solution for first two goals is NP-complete
- Existing methods (heuristics) provide different trade-offs between the four objectives



Teresco, Devine, Flaherty, *Partitioning and Dynamic Load Balancing for the Numerical Solution of Partial Differential Equations*, LNCSE, vol. 51, pp. 55-88, 2006.

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  - **Metrics: Workload, Load Balance**
  - Typical Approach
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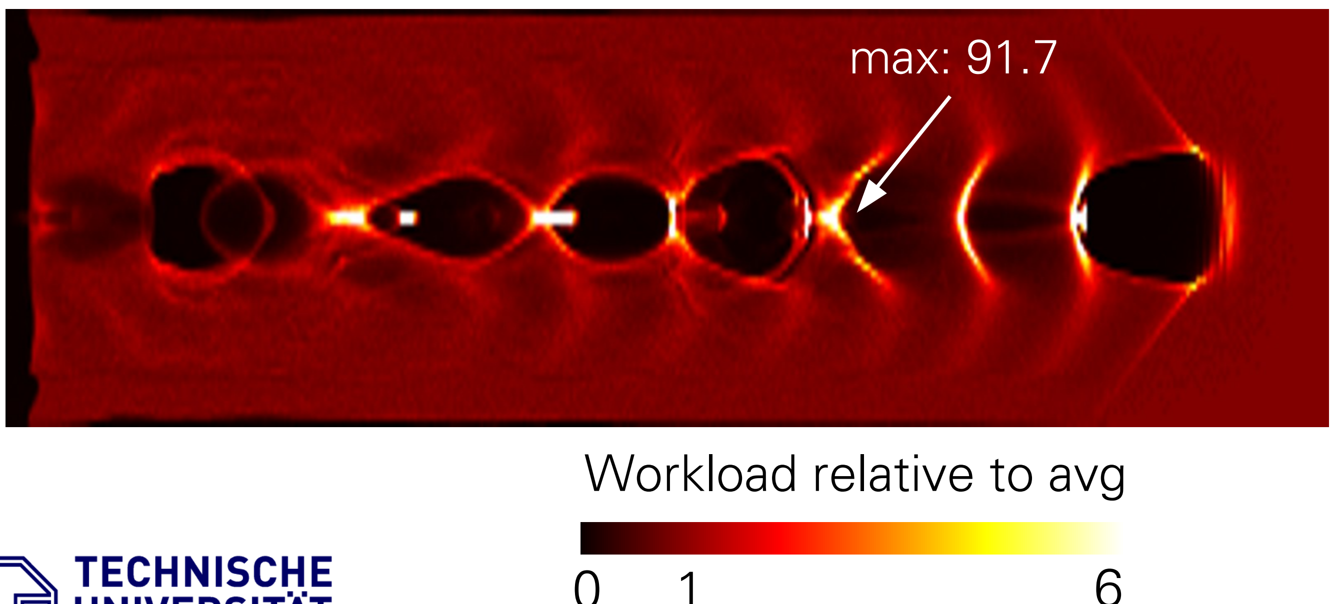
Dynamic Load Balancing: Metrics

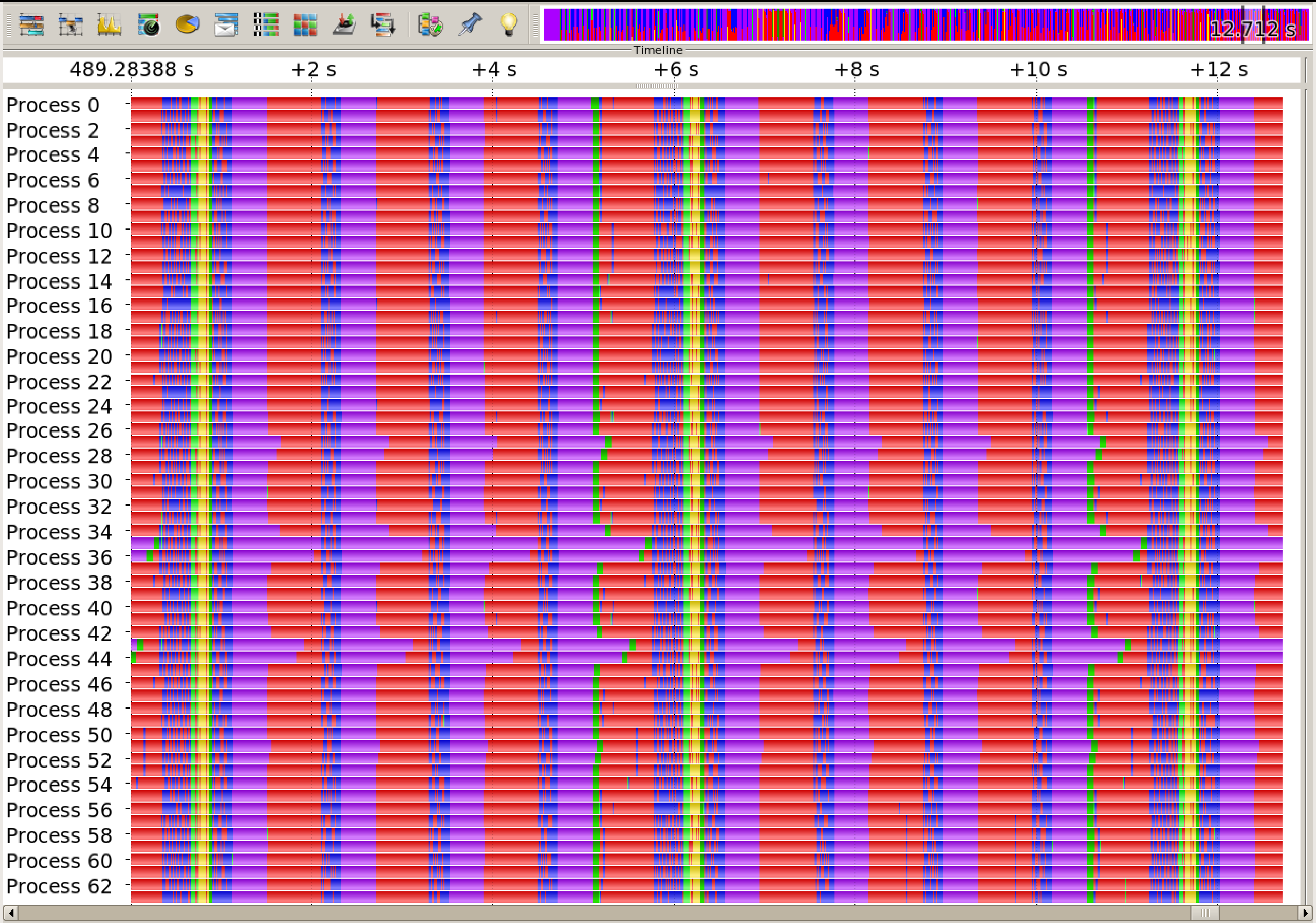
- Workload / weight of a single grid cell
- Needs to be estimated for the future time step(s)
  - Typical: Measurement of current load (time, cycles, ...) and assume load will change slightly only (*principle of persistence*)
  - Derive suitable indicators from model-specific variables (i.e. number of particles in grid cell)

Watts, Taylor, *A Practical Approach to Dynamic Load Balancing*, IEEE Trans. Par. Distr. Sys., vol 9, pp. 235-248, 1998.

Muszala, Alaghband, Hack, Connors, *Natural Load Indices (NLI) for scientific simulation*, J. Supercomp., vol 59, pp. 1-22, 2010.



How to measure Load Balance?



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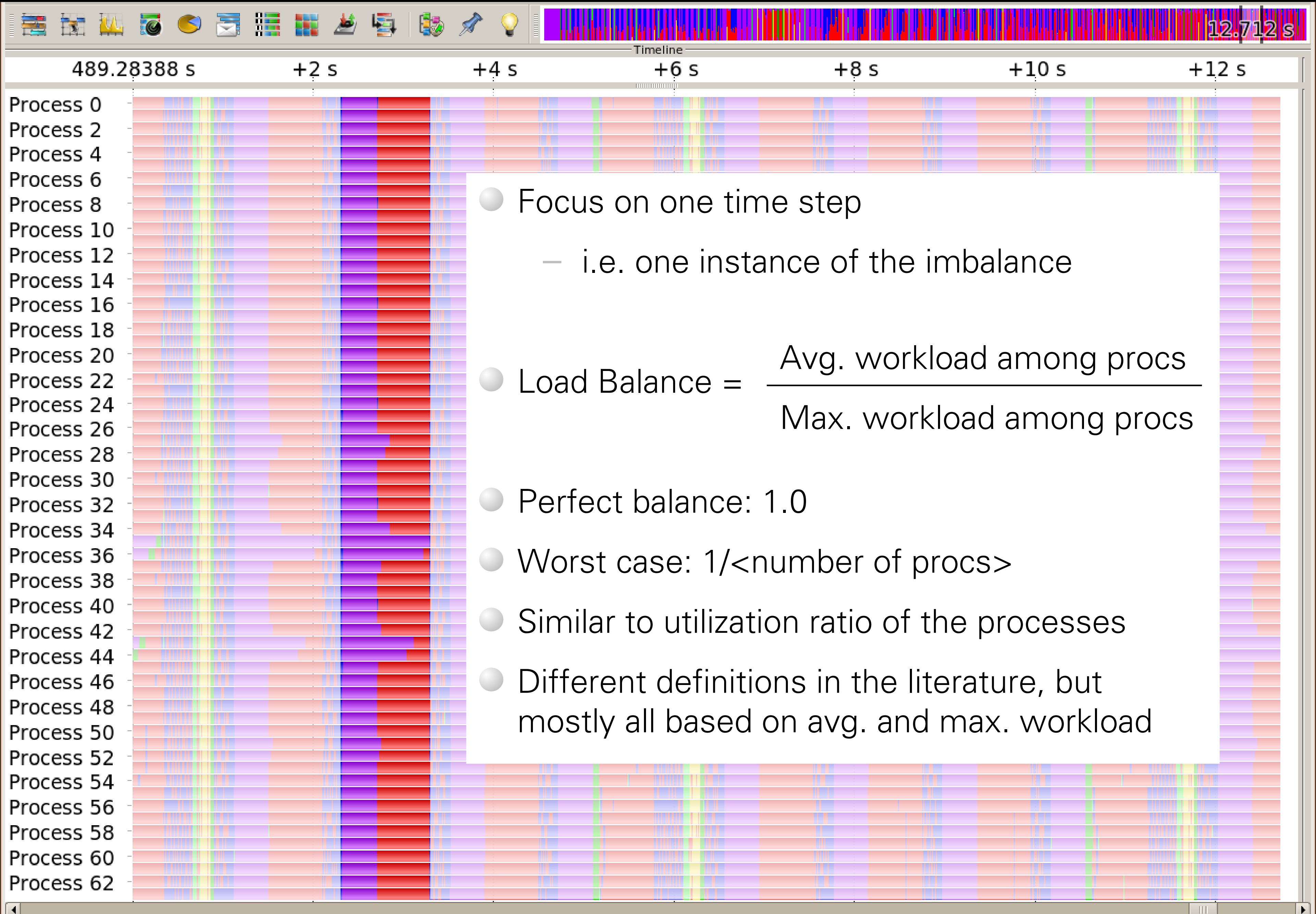

- Focus on one time step
  - i.e. one instance of the imbalance
- Load Balance = $\frac{\text{Avg. workload among procs}}{\text{Max. workload among procs}}$
- Perfect balance: 1.0
- Worst case: 1/<number of procs>
- Similar to utilization ratio of the processes
- Different definitions in the literature, but mostly all based on avg. and max. workload

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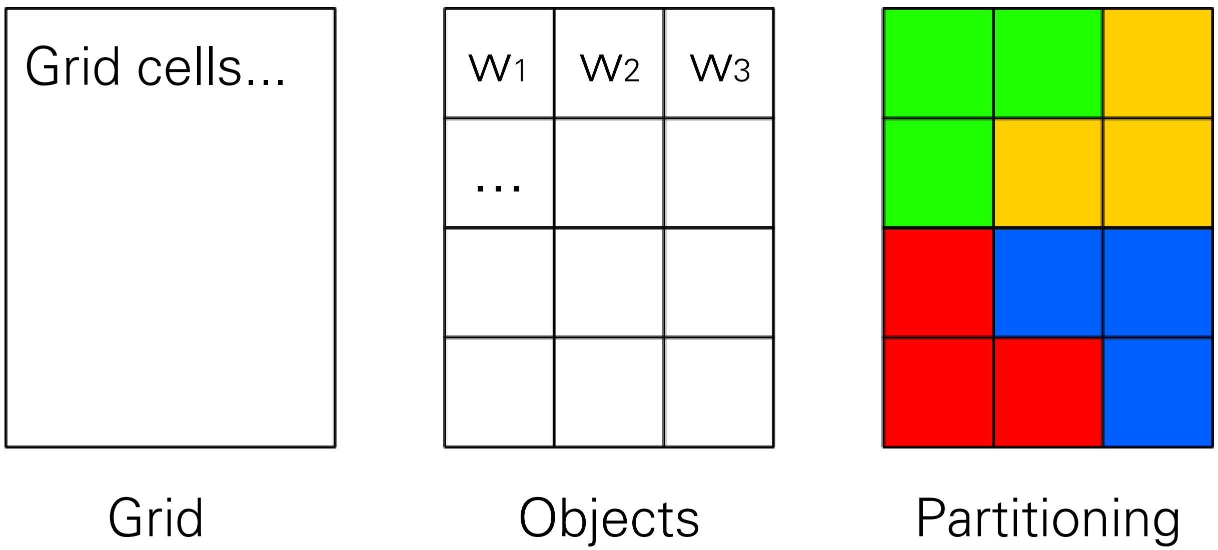
Dynamic Load Balancing: Typical Approach

- Decompose the grid in *objects* for assignment to processes and migration between processes
  - Object = Single grid cell or block of grid cells
  - Workload / weight of a single object: w_i



Dynamic Load Balancing: Typical Approach

- Object size determines granularity
  - Too small objects: high overhead for management of objects and load balancing
  - Too large objects: too coarse grained to reach good load balance
- Estimation for required granularity when running on P processes
  - $\max(w_i) \leq \sum w_i / P$
  - To run efficiently on large number of processes: decrease $\max(w_i)$ (i.e. object size) or increase $\sum w_i$ (i.e. problem size) sufficiently
- Objects size may also influence cache efficiency of the computations

Dynamic Load Balancing: Typical Approach

FOR timeStep = 1 **TO** numberOfTimeSteps

Determine load balance for this time step
(based on indicators or estimation from last time step)

IF loadBalance < tolerance **THEN**

Determine workload of each object for this time step
(based on indicators or estimation from last time step)

Call partitioning method — **4: Partitioning**

Migrate objects — **3: Migration**

END IF

Exchange ghost cells with neighbors — **2: Communication**

Compute model equations — **1: Load balance**

NEXT

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Partitioning

- Partitioning = Assignment of objects to processes
  - Objectives of load balancing should be satisfied
- Input:
  - Number of processes P
  - Weight of all objects w_i (to optimize load balance)
  - Information about neighborship of objects (to optimize communication)
  - Current partitioning (to optimize migration)
- Output:
  - Mapping of objects to processes

Partitioning: Classification of Methods

Partitioning Methods

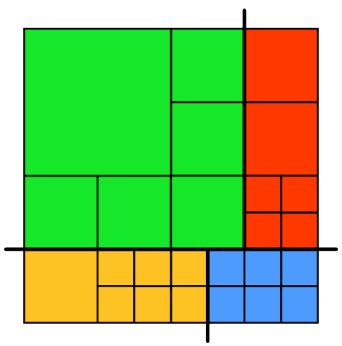
Geometric Methods

Need spatial coordinates and object weights

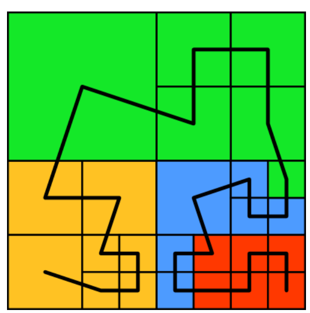
Graph-based

Consider object decomposition as a weighted graph

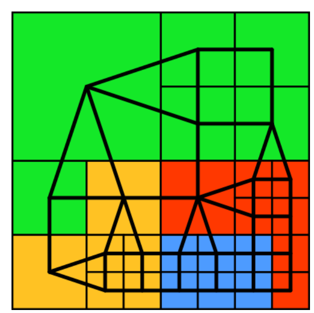
Recursive Bisection



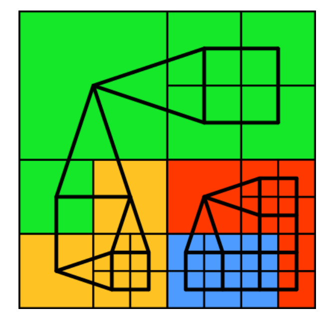
Space-Filling Curves



Global Graph-based



Local Graph-based



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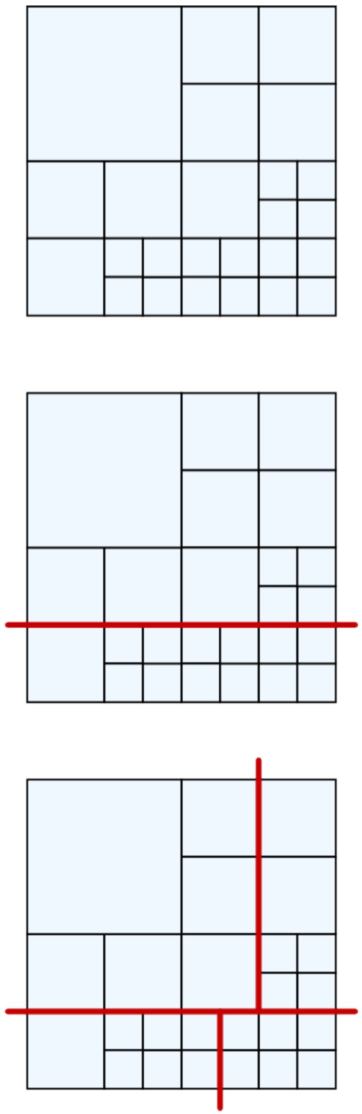
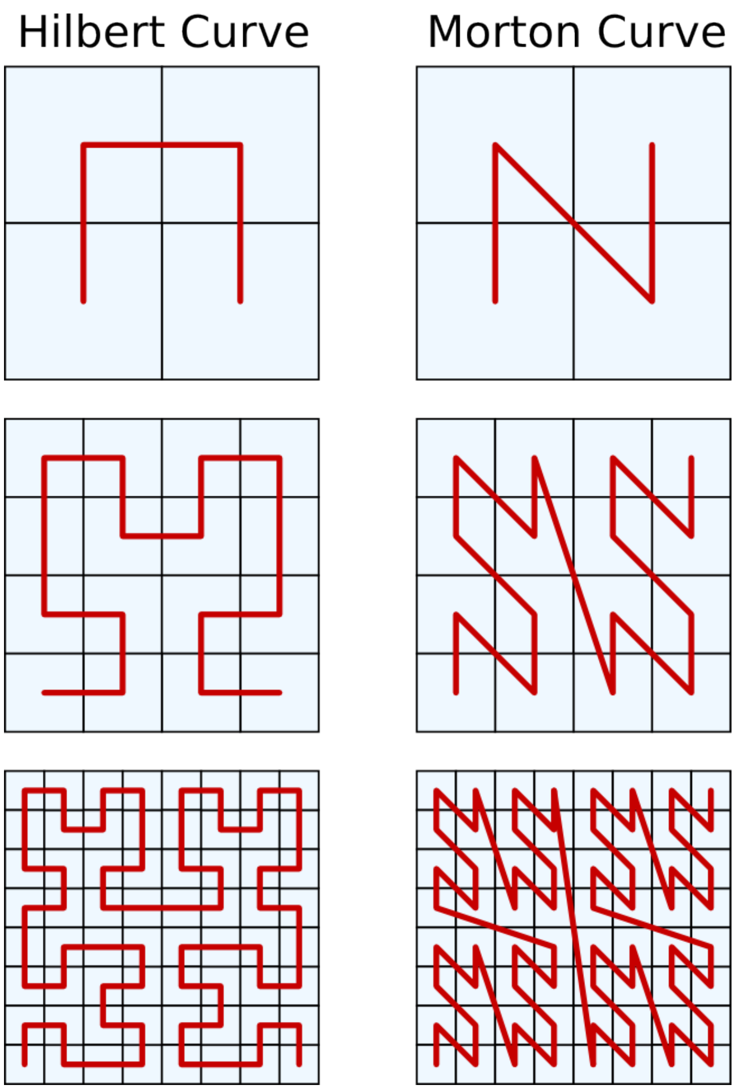
Partitioning: Recursive Bisection



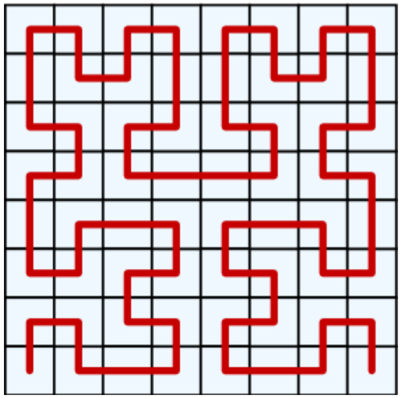
- Cut the grid in two equal weighted parts
- Apply this algorithm recursively for each part until number of desired partitions is reached
  - Processor count ≠ 2^n: cut in more than 2 parts or cut in unequal parts
- Very fast, but moderate scalability
- Requires fine granularity to reach good balance
- Moderate optimization of communication costs
- Versions:
  - Recursive Coordinate Bisection (RCB)
  - Unbalanced Recursive Bisection (URB)
  - Recursive Inertial Bisection (RIB)

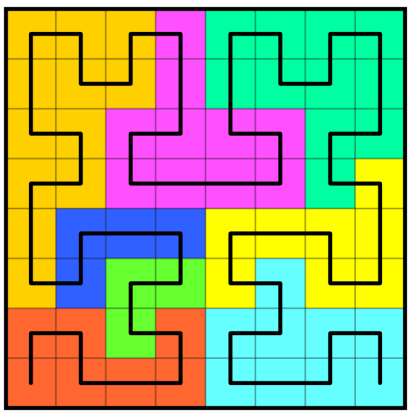
Partitioning: Space-Filling Curves (SFCs)



- 1D traversal of the grid
- nD → 1D mapping / ordering
- Data locality
  - Points close on the curve are also close in the nD grid
- Self-similarity
  - Constructed recursively from a start template in *O*(log n)
- Most prominent for load balancing:
  - Hilbert curve (higher locality)
  - Morton curve (faster)

Partitioning: Space-Filling Curves (SFCs)





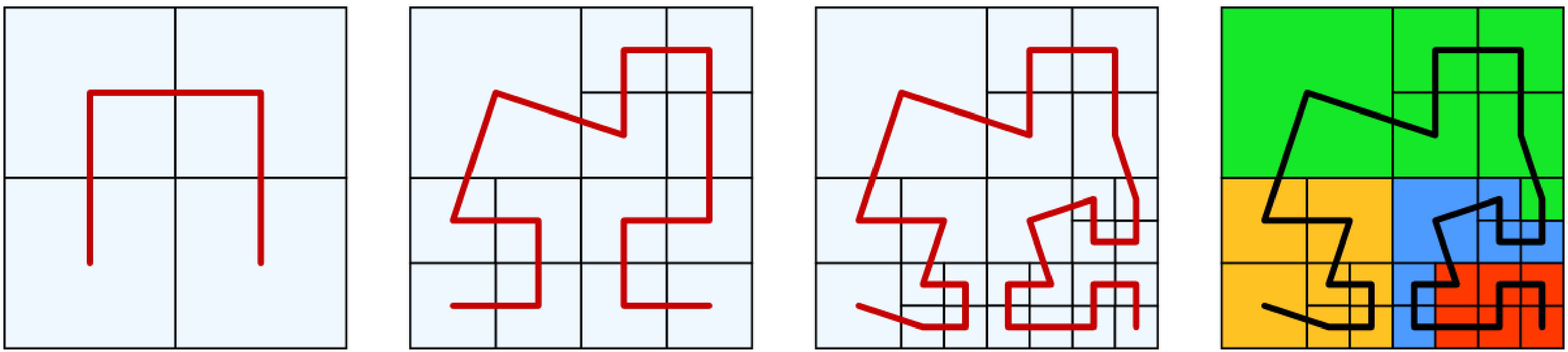
- Partitioning is reduced to 1D
- 1D partitioning is core problem of SFC partitioning
  - Decompose object chain into consecutive parts
- Two classes of existing 1D partitioning algorithms:
  - Heuristics: fast, parallel, no optimal solution
  - Exact methods: slow, serial, but optimal
- SFC implicitly optimizes for low communication and migration
  - SFC locality leads to moderate communication costs
  - Migration typically between neighbor ranks

Pilkington, Baden, *Dynamic partitioning of non-uniform structured work-loads with spacefilling curves*, IEEE T. Parall. Distr., vol. 7, no. 3, pp. 288-300, 1996.

Pinar, Aykanat, *Fast optimal load balancing algorithms for 1D partitioning*, J. Parallel Distr. Com., vol. 64, no. 8, pp. 974-996, 2004.

Partitioning: Space-Filling Curves for Mesh Refinement

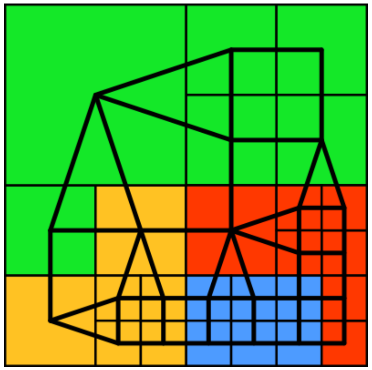
- Space-Filling Curves are well suited for structured adaptive mesh refinement (AMR) due to their self-similarity



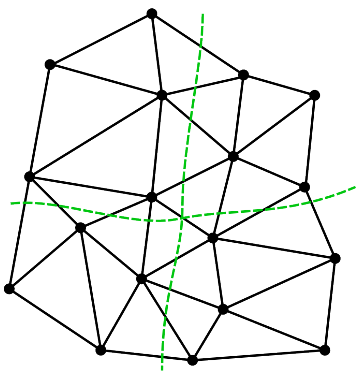
Start template | Refine | Refine | Partition

Burstedde et al., *ALPS: A framework for parallel adaptive PDE solution*, J. Phys. Conf. Ser. 180, 2009

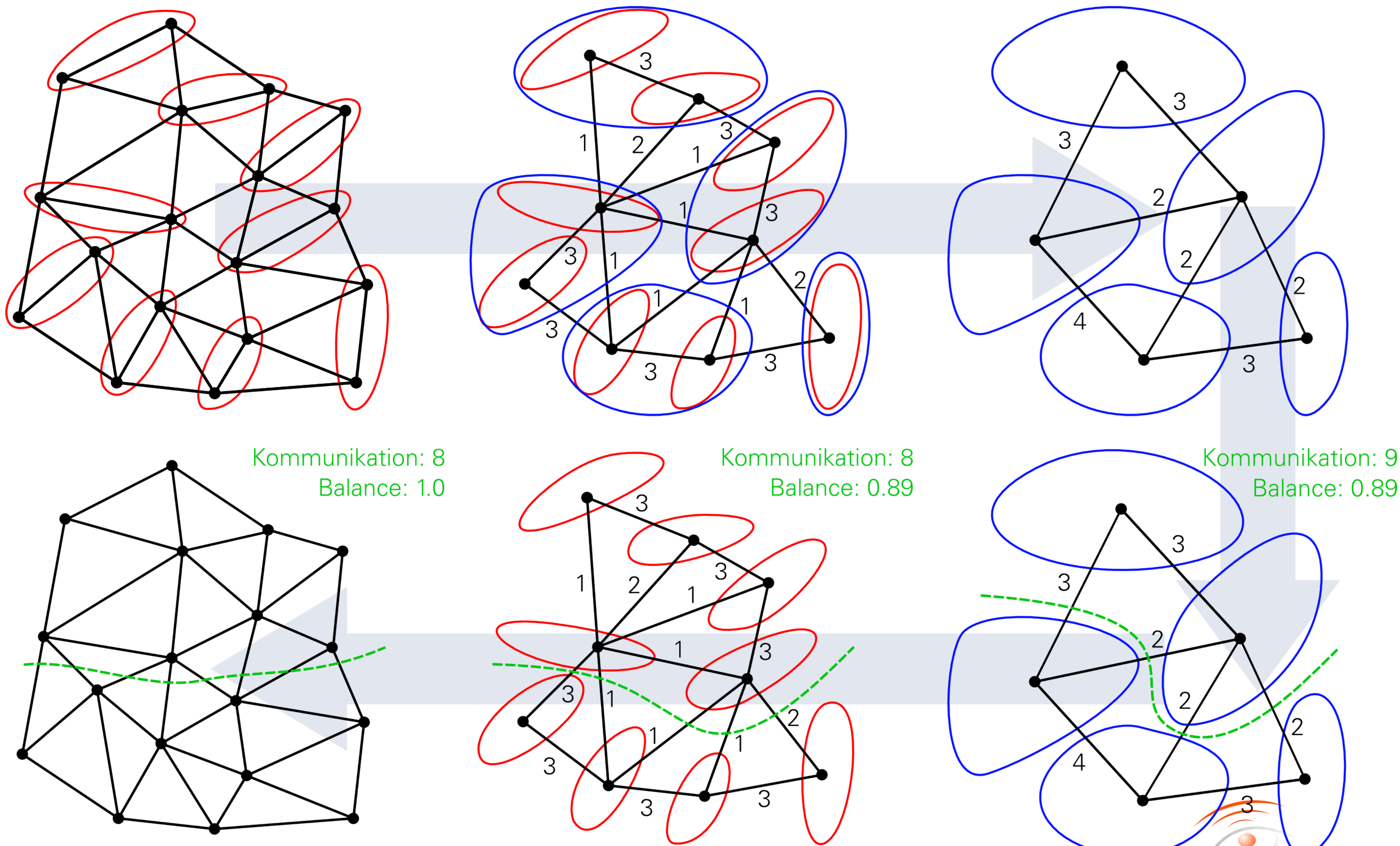
Partitioning: Global Graph-based Methods



- View the decomposition as a weighted graph
  - Vertex weight: object's workload
  - Edge weight: comm. costs between objects
- Works for irregular grids
- Very good optimization of communication costs
- Very time consuming, hard to parallelize efficiently
- High migration costs
- Different heuristics / many publications
  - Greedy graph partitioning (fast, but worse quality)
  - Recursive spectral bisection (very slow)
  - Multilevel graph partitioning (widely used)



Partitioning: Multilevel Graph Partitioning



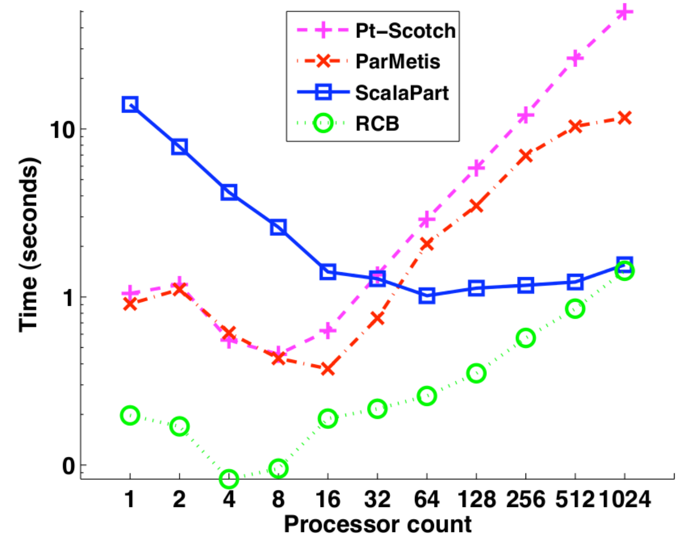
Schloegel, Karypis, Kumar, *Parallel static and dynamic multi-constraint graph partitioning*. Conc. Comp.: Pract. Exper., vol 14, pp. 219-240, 2002.

Partitioning: More Advanced Global Graph-based Methods

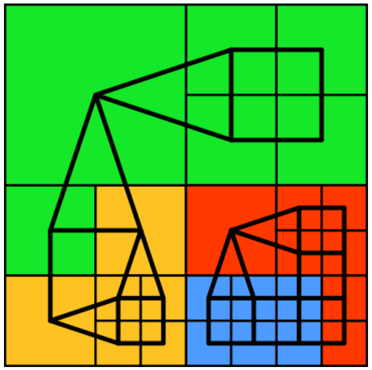
- Multilevel hypergraph partitioning
  - Edges connect more than two nodes
  - Accurate model of communication and migration costs leads to higher quality
  - More expensive
- Multilevel + coordinate mapping + geometric method (ScalaPart)
  - Graph is mapped to a grid to get coordinates of vertexes
  - Fast geometric method + border refinement
  - Much better scalability

Catalyurek et al., *A repartitioning hypergraph model for dynamic load balancing*, J. Par. Distr. Comp., vol. 69, pp. 711-724, 2009.

Kirmani, Raghavan, *Scalable parallel graph partitioning*, SC 2013.



Partitioning: Local Graph-based Methods

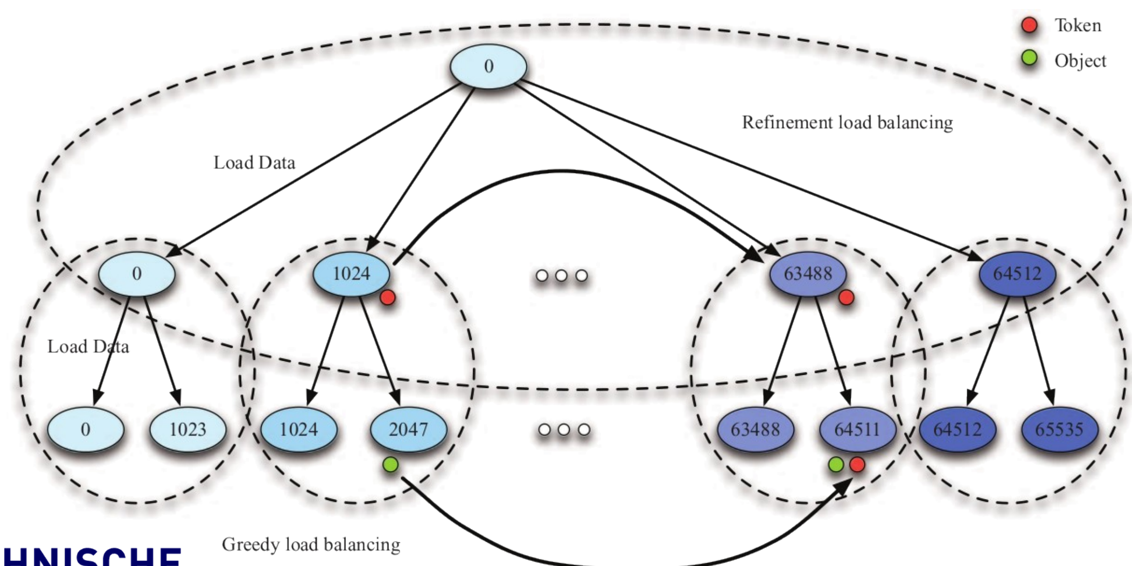


- Only subsets (i.e. neighborships) of existing partitions exchange objects
- Requires an initial partitioning
- Requires multiple iterations (with different subsets) to reach good balance
- Sufficient for small workload changes or as refinement step for other methods
- Typically very fast, but depends on number of iterations
- Scalable by design: only local actions
- Algorithms
  - Diffusion algorithms
  - Work-stealing algorithms

Partitioning: Hierarchical Methods

- Organize processes in hierarchy
  - I.e. derived from network or application topology
- Apply partitioning method independently in each level
- Better scalability than centralized approaches
- Less memory requirements than (serial) methods
- Most promising methods for large scale

Teresco, Faik, Flaherty: *Hierarchical Partitioning and Dynamic Load Balancing for Scientific Computation,* LNCS vol. 3732, pp. 911-920, 2006.

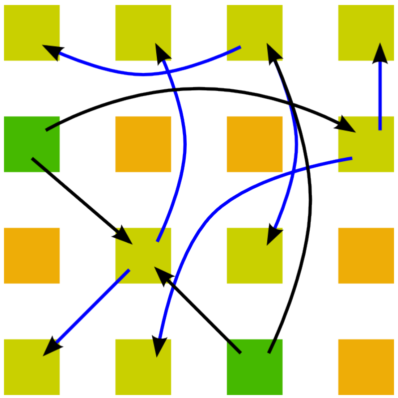


Zheng, Bhatele, Meneses, Kale, *Periodic hierarchical load balancing for large supercomputers.* Int. J. High Perf. Comp. App., vol. 25, pp. 371-385 2011.

Partitioning: GrapevineLB Distributed Load Balancer

Menon, Kale, *A Distributed Dynamic Load Balancer for Iterative Applications*, SC 2013.

- Does not fit in classification
  - Does not use communication topology information
- Local migration decisions based on knowledge about some underloaded processes
  - Information is spread with a randomized epidemic (gossip) algorithm, only a few rounds
  - Every overloaded process knows about some randomly chosen underloaded processes
- Objects are transferred to random processes that are known to be underloaded
  - They may reject the object if they already received enough load
- Runtime comparable to diffusion, but much better load balance



Partitioning: Scalability Challenges

- Large number of processes and objects
- Serial algorithms not sufficient
  - Large memory and network usage when collection weights of 1M-1G objects at one process
  - Even the simplest heuristic would be too slow
- The challenge is to find algorithms that
  - Leave weights distributed or communicate them only sparsely (e.g. within neighborship)
  - Nevertheless achieve global balance (without a detailed global view)

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- Introduction
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- **Software Stack**
- Experiences with COSMO-SPECS+FD4
- Conclusion

Software Stack: Application Layer

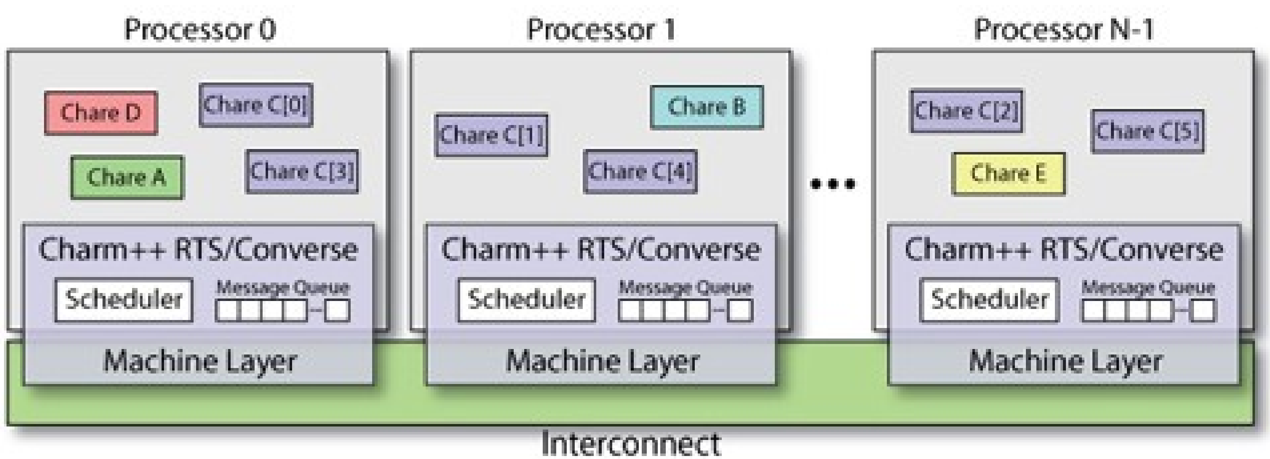
- Dynamic load balancing in HPC applications is usually hand-coded in the application
- Huge coding effort when introducing load balancing to a big/real HPC application
- 3rd party libraries to compute partitioning
  - ParMetis: multilevel graph, diffusion, multiconstraint
  - Jostle, PT-Scotch, DibaP: multilevel graph
  - Zoltan: geometric, hypergraph, hierarchical, can use ParMetis and PT-Scotch

Software Stack: Runtime / Framework Layer

- MPI is static, no load balancing
- MPI-based frameworks
  - Frameworks for parallel PDEs: PETSc, FD4, ...
  - Adaptive mesh refinement frameworks: ALPS, GrACE, Chombo, Racoon, ...
- Load balancing of virtual MPI processes: Adaptive MPI
- Alternative runtime systems: Charm++, PREMA

Huang et al., *Performance Evaluation of Adaptive MPI*, PPoPP 2006

Acun et al., *Parallel Programming with Migratable Objects: Charm++ in Practice*, SC 2014



Charm++ system view

https://charm.cs.illinois.edu/tutorial/CharmRuntimeSystem.htm

Software Stack: Operating System Layer

- Typical HPC system: OS reduced as much as possible
- Single-System Image (SSI) OS's allow load balancing and transparent process migration in a cluster
  - Used for load balancing between different applications, but not within an application
- Systems
  - Kerrighed, (open)Mosix, OpenSSI
- Few installations with ~100 nodes
- No experience with large state-of-the-art HPC systems
- FFMK seeks to migrate (oversubscribed) MPI processes for load balancing

Lottiaux et al., *OpenMosix, OpenSSI and Kerrighed: A Comparative Study*, INRIA Research Report 5399, 2004.

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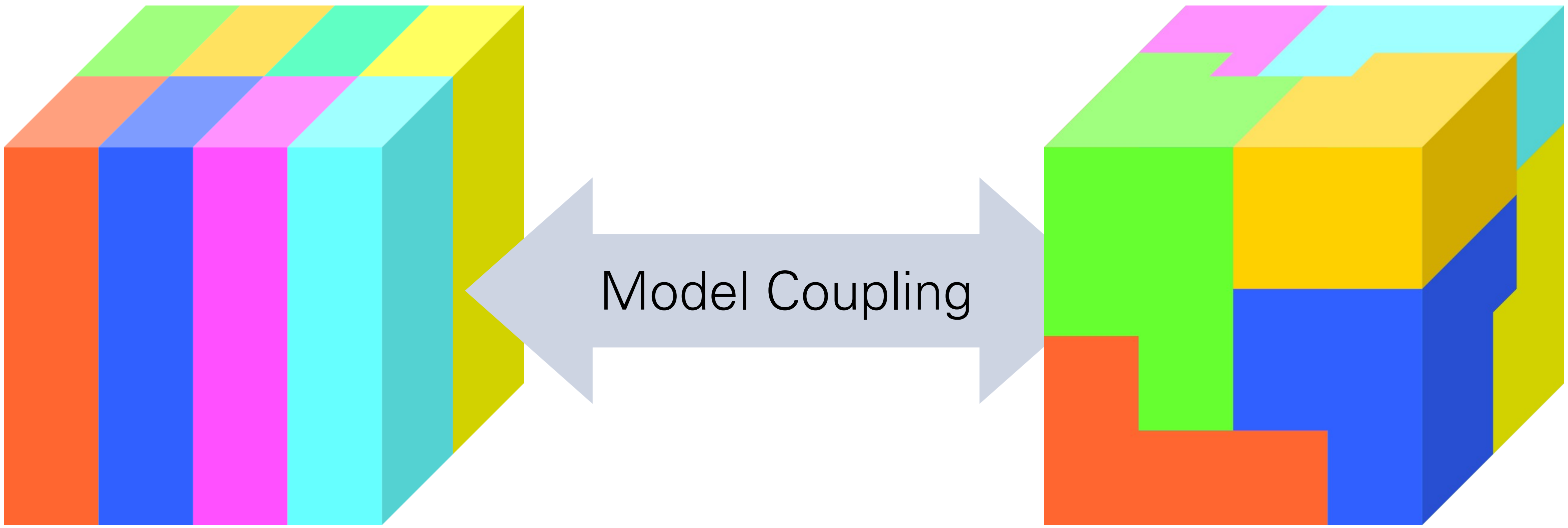
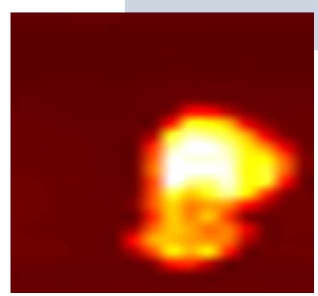
COSMO-SPECS+FD4: Parallelization and Coupling Concept

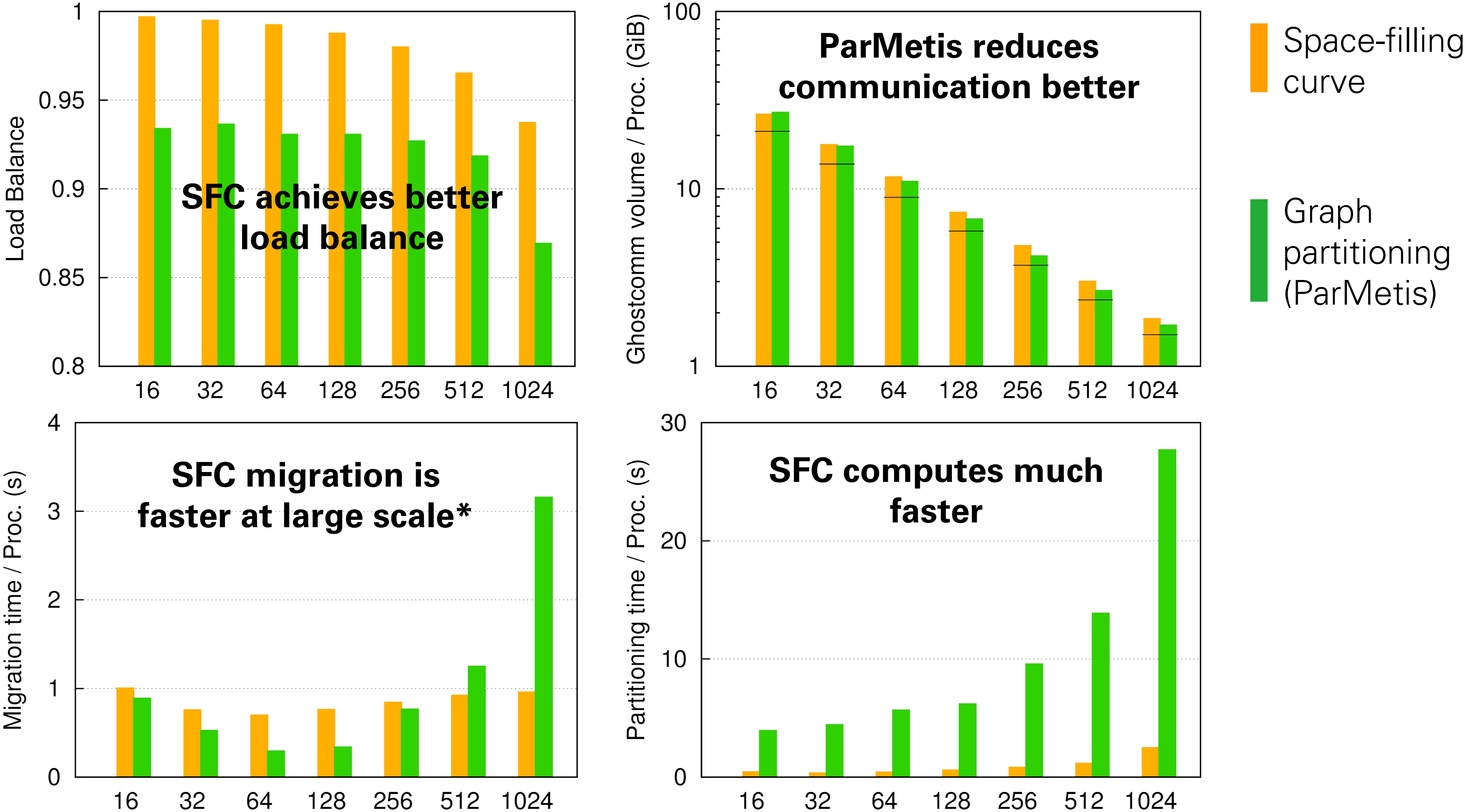
COSMO Atmospheric Model | **Cloud Microphysics Model**



COSMO Atmospheric Model	Cloud Microphysics Model
Large (legacy) Codebase	Block-based 3D Decomposition
2D Decomposition	Dynamic Load Balancing
Static Partitioning	

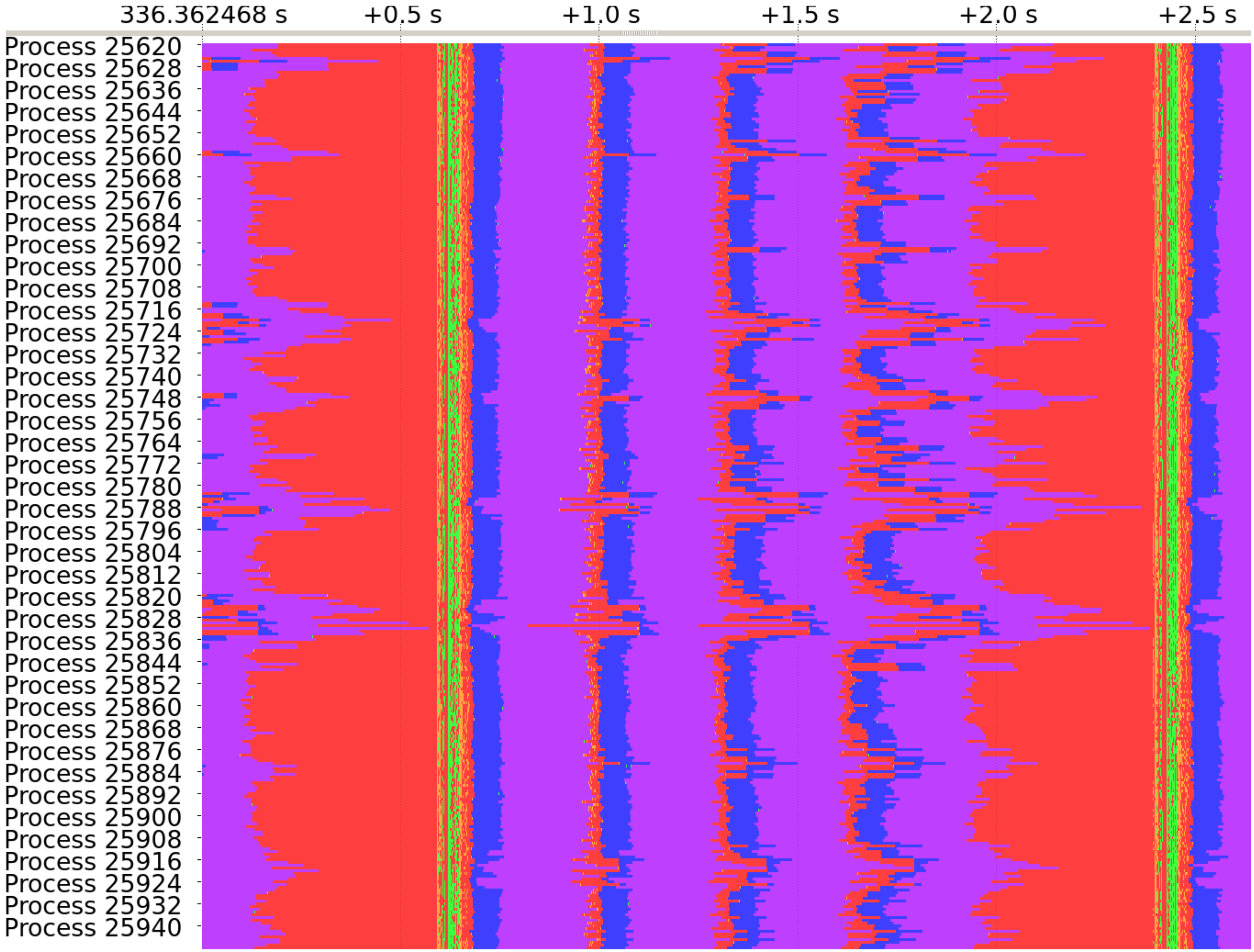


COSMO-SPECS+FD4: Space-filling Curve vs. Graph Part.

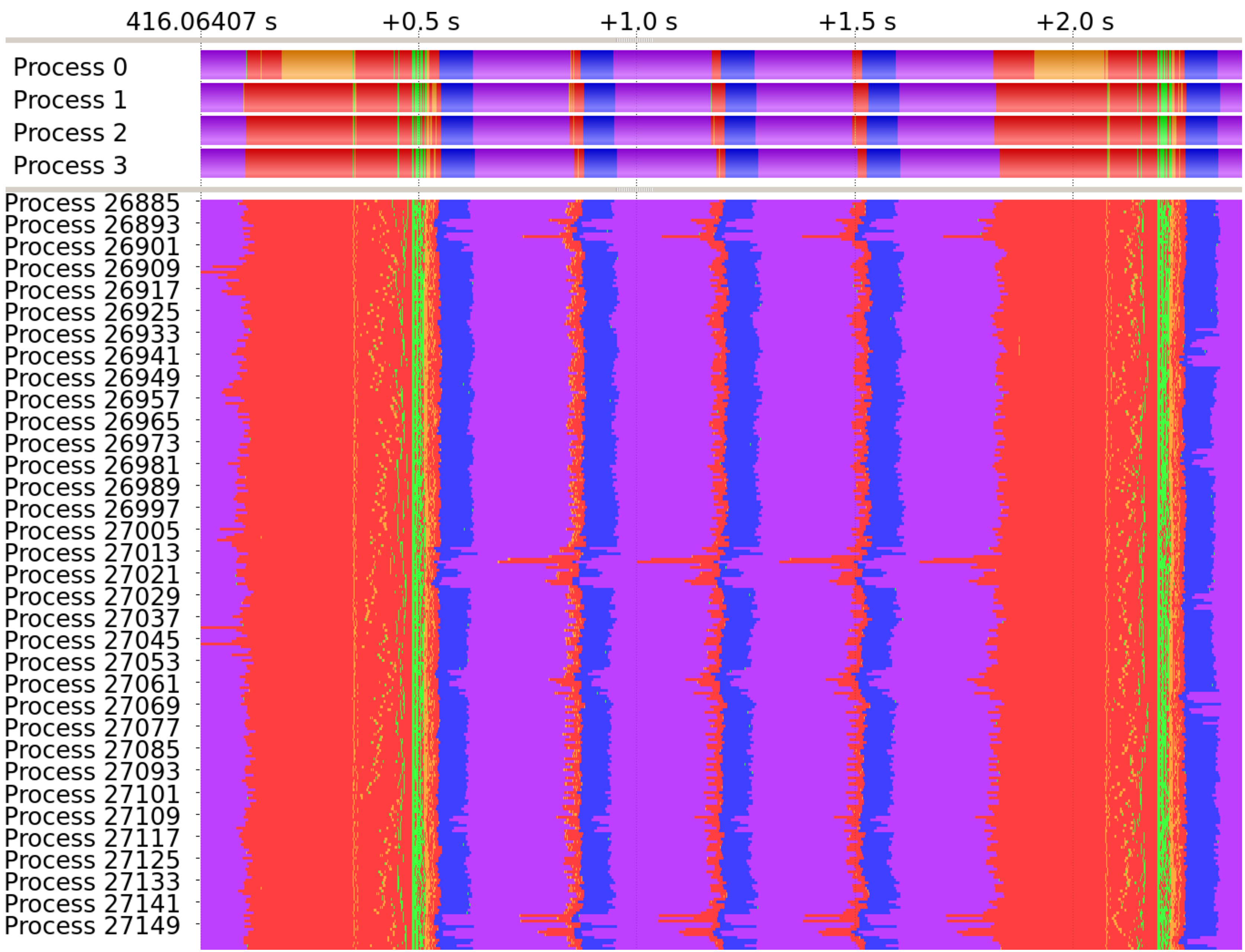


* due to local communication pattern that leads to less network usage & contention

COSMO-SPECS+FD4: SFC Partitioning with Heuristic



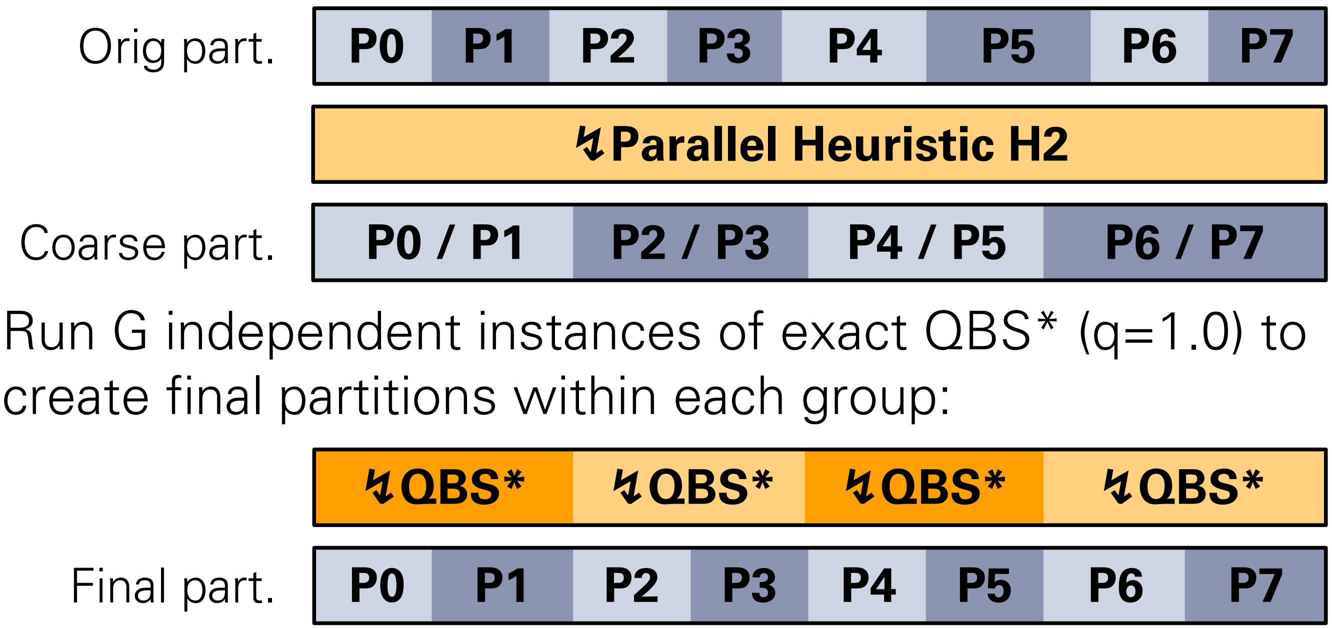
COSMO-SPECS+FD4: SFC Partitioning with Exact Method



Scalable High-Quality 1D Partitioning: Algorithm HIER*

Large scale applications require a fully parallel method, i.e. without gathering all task weights

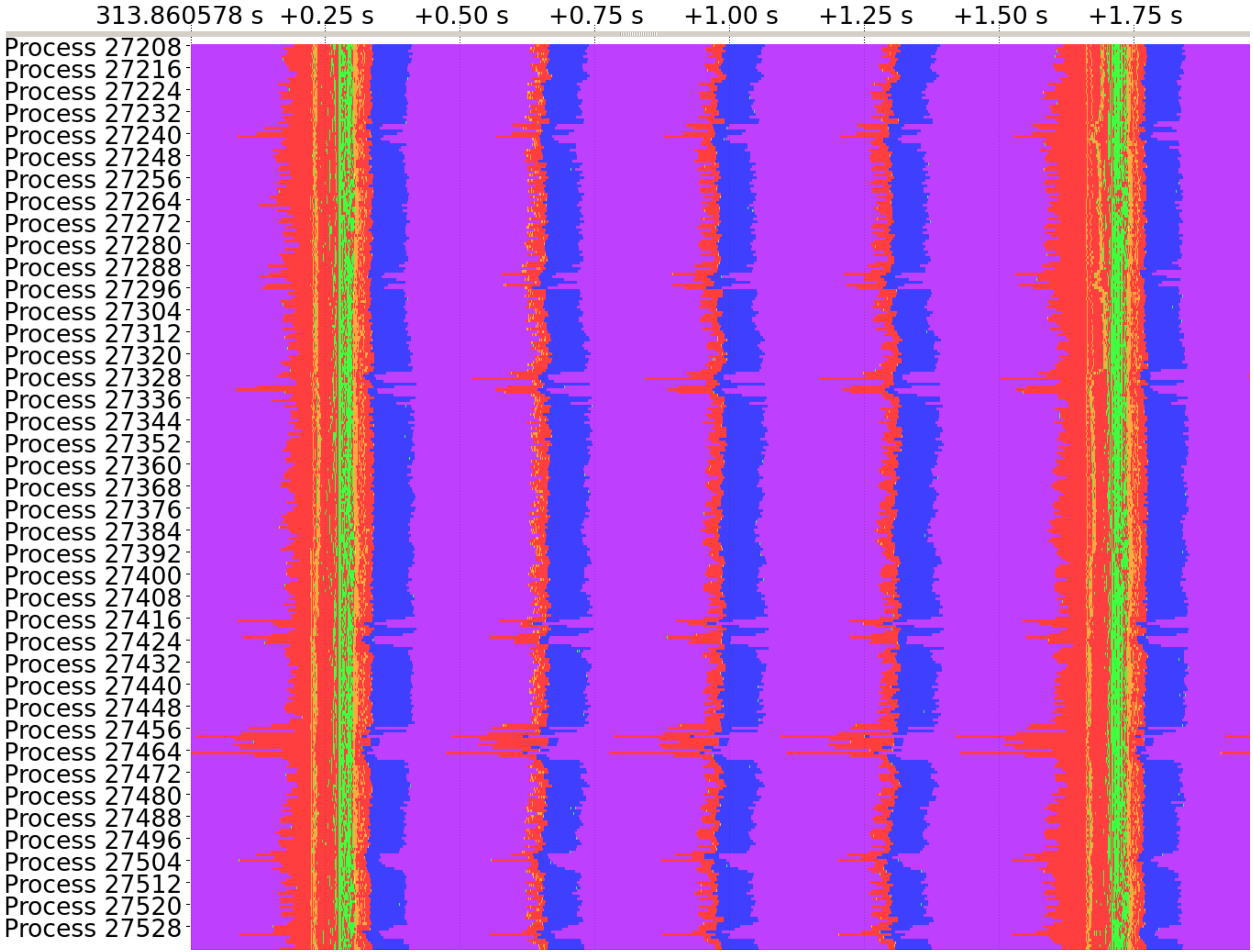
- Run parallel H2 to create G < P coarse partitions:



- Run G independent instances of exact QBS* (q=1.0) to create final partitions within each group:
- Parameter G allows trade-off between scalability (high G → heuristic dominates) and load balance (small G → exact method dominates)

H2 nearly optimal if $w_{max} << W_N / P$: Miguet, Pierson, *Heuristics for 1D rectilinear partitioning as a low cost and high quality answer to dynamic load balancing*, LNCS, vol. 1225, 1997, pp. 550-564.

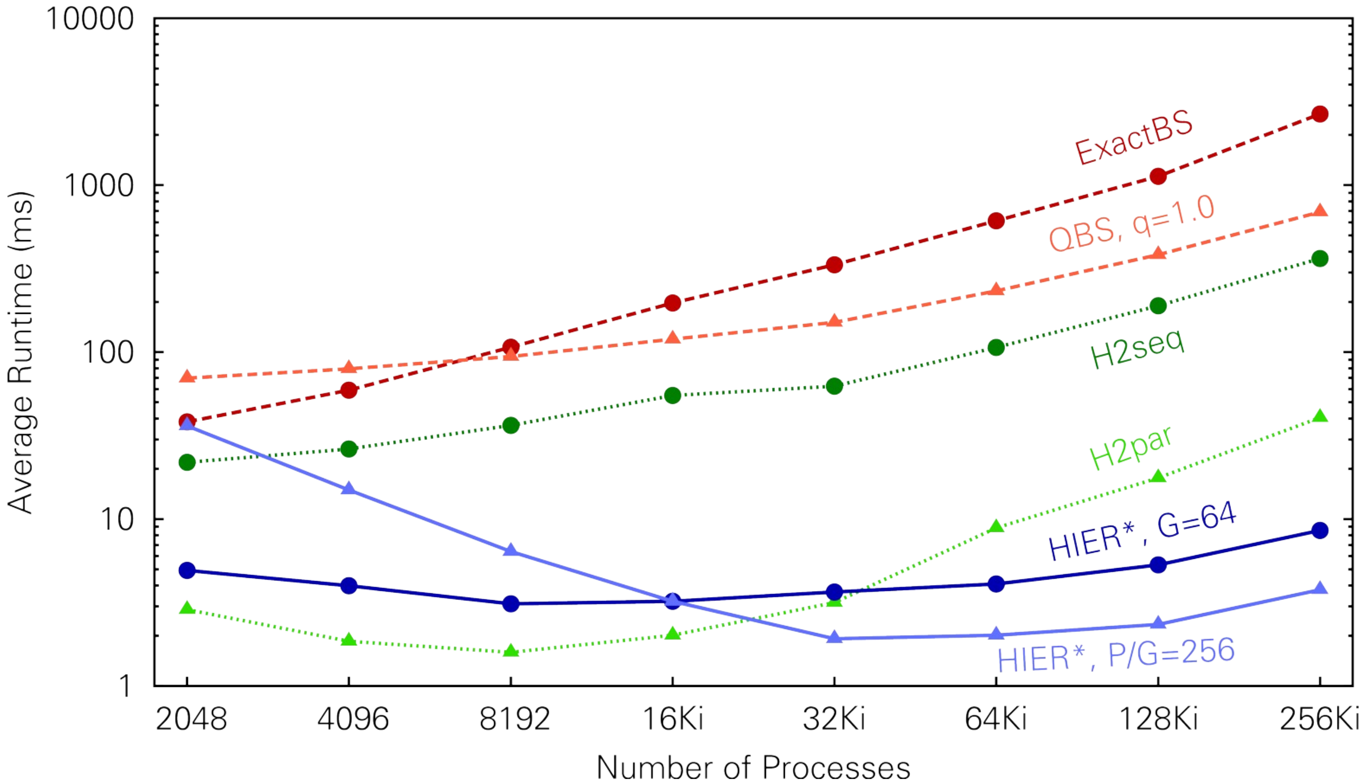
COSMO-SPECS+FD4: SFC Partitioning with Hier. Method



COSMO-SPECS+FD4: Comparison of Partitioning Time

- ExactBS: exact method, but slow and serial
- H2: fast heuristic, but may result in poor load balance
- HIER*: hierarchical algorithm implemented in FD4, achieves nearly optimal load balance

Lieber, Nagel, *Scalable High-Quality 1D Partitioning*, HPCS 2014, pp. 112-119, 2014



ExactBS: 2668 ms

QBS: 692 ms

H2seq: 363 ms

H2par: 40.5 ms

$HIER^*_{G=64}$: 8.55 ms

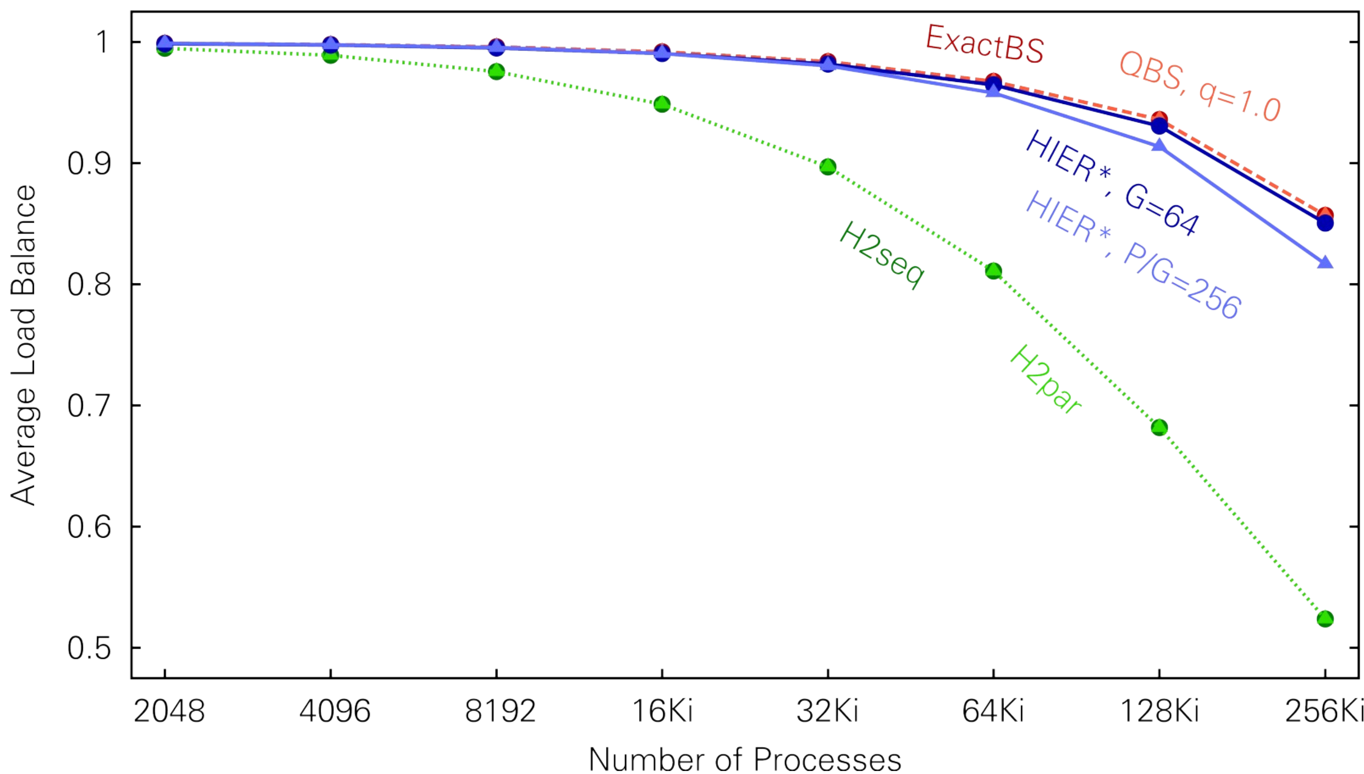
$HIER^*_{P/G=256}$: 3.77 ms

Balancing 1 357 824 objects, IBM Blue Gene/Q

COSMO-SPECS+FD4: Comparison of Load Balance

- ExactBS: exact method, but slow and serial
- H2: fast heuristic, but may result in poor load balance
- HIER*: hierarchical algorithm implemented in FD4, achieves nearly optimal load balance

Lieber, Nagel, *Scalable High-Quality 1D Partitioning*, HPCS 2014, pp. 112-119, 2014



HIER*, G=64 achieves 99.2% of optimal load balance

Balancing 1 357 824 objects, IBM Blue Gene/Q

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Conclusion

- Load balancing is important for many HPC applications
- Will get more important in future
  - Models get more complicated → load variations
  - Hardware gets more complicated → capacity variations
- Quest for high-quality and highly scalable dynamic load balancing methods
  - We will see more hierarchical and fully distributed methods
- Application developers need better support
  - Use (domain-specific) frameworks?
  - Replace (much too static) MPI by new runtime?
  - Get help from OS?

Thank you very much for your attention!

Acknowledgments

Verena Grützun, Ralf Wolke,
Oswald Knoth, Martin Simmel,
René Widera, Matthias Jurenz,
Matthias Müller, Wolfgang E. Nagel

lrz Leibniz Supercomputing Centre of the Bavarian Academy of Sciences and Humanities

VAMPIR www.vampir.eu

TROPOS Leibniz Institute for Tropospheric Research

www.tropos.de

DWD COSMO CONSORTIUM FOR SMALL SCALE MODELING

www.cosmo-model.org

PIConGPU

HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

picongpu.hzdr.de

Funding

DFG Deutsche Forschungsgemeinschaft

cfaed CENTER FOR ADVANCING ELECTRONICS DRESDEN

Europa fördert Sachsen. ESF Europäischer Sozialfonds

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