universität innsbruck

FZ HPC

On using modern C++ and nested recursive task parallelism for HPC applications with AllScale

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From Performance Prediction to Compilers and Distributed Computing

- Superb and Vienna Fortran Compiler [SFB Aurora; Apart Working Group]
  - Parameter based Performance Prediction Tool (P^3T) for HPF
  - Scalea (instrumentation, monitoring, performance analysis) by Hong-Linh Truong (now Aalto University) for Vienna Fortran
  - Zenturio (automatic experiment generation for large scale analysis) by Radu Prodan (Klagenfurt University) for Vienna Fortran

Fortran

- Askalon (application development and runtime for the Grid and the Cloud) [8 EU projects]
  - performance predicton for scientific workflows (Farrukh Nadeem, King Abdulaziz University)
  - performance prediction for services and tasks for clouds (Thanh-Phuong Pham, Helsinky University)
  - scheduling and resource management

C, Java, Python

more Compilers and runtime system

- Insieme C/C++ compiler (Allscale EU project)
  - Cilk, OpenMP
  - auto-tuning for multiple parameters
  - runtime optimization
  - performance prediction (distance to finish task)

C/C++

- Allscale API, compiler and runtime system (Allscale EU project)
  - high-level C++ domain specific language
  - productivity (hide MPI)
  - sophisticated compiler analysis
  - recursive task parallelism

C++

- Celerity API and runtime system for GPU clusters based on SYCL (FETHPC LIGATE)
  - Productivity versus performance
  - API research to hide MPI
  - focus on asynchronous tasks
  - runtime optimization and scheduling

SYCL

more Distributed Systems

- Apollo (application development and runtime for the edge-cloud continuum)
  - scientific workflows
  - programming paradigms, scheduling, resource management
  - semi-automatic serverless function generation

YAML. serverless functions C, C++, Java, Python, …

- Apache Flink
  - data pipelines and big data
  - real-time latency intensive stream/batch applications
  - targeting edge-cloud
  - ensemble scheduling and resource management

Java, Python, Scala

Performance models and analysis:

- simple analytical models and real-time measurements
- more complex models based on ML

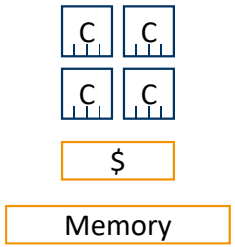
AllScale – A H2020 Success Story

- Horizon 2020 funded project and marked "Success Story"
- Coordinated by Thomas Fahringer, Distributed and Parallel Systems Group and Research Center HPC, Department of Computer Science
- 5 Partners
  - Friedrich-Alexander University Erlangen-Nürnberg
  - IBM Ireland
  - KTH Stockholm
  - Numeca, Brussels
  - Queen's University Belfast

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 671603

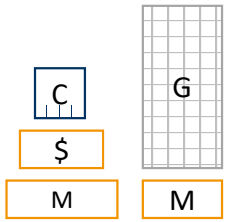
Parallel Architectures

Multicore



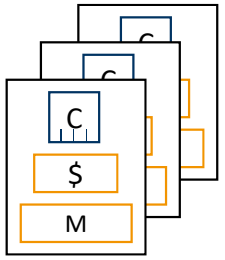
OpenMP/Cilk

Accelerators



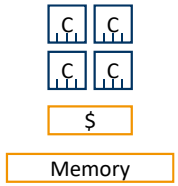
SYCL/OpenCL/CUDA

Clusters

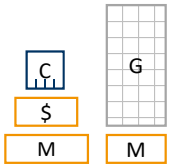


MPI/PGAS

Real World Architectures



OpenMP/Cilk



SYCL/OpenCL/CUDA

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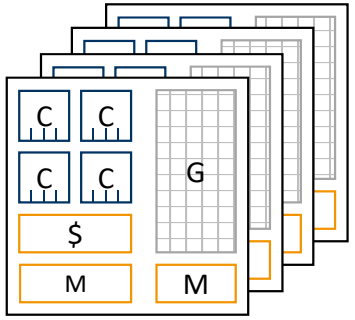
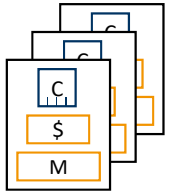
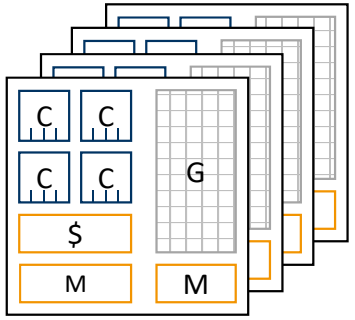




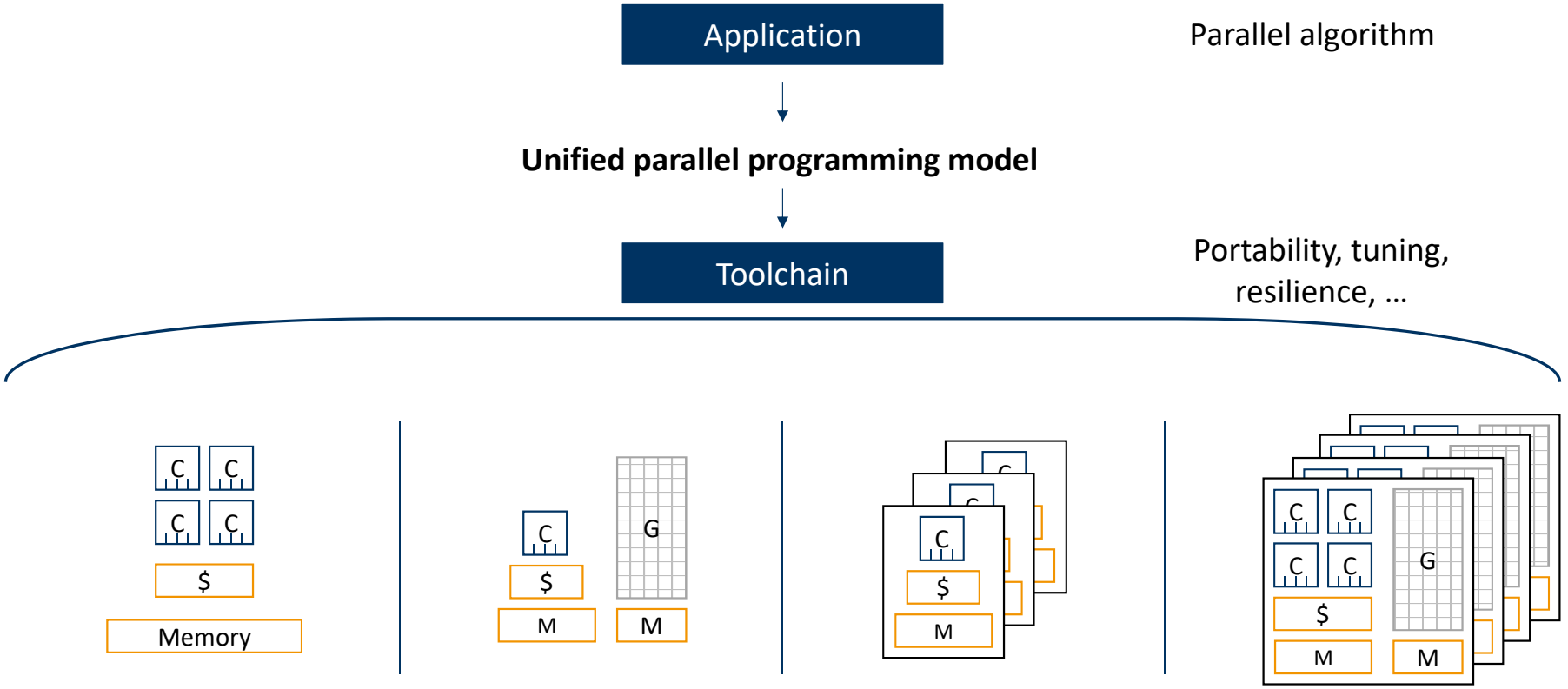
MPI/PGAS

Hybrid Programming Models for Heterogeneous Parallel Architectures

- Issues
  - Hard-coded problem decomposition
  - Lack of coordination among runtime systems
- No built-in support for
  - Portability
  - Auto-tuning
  - Load balancing
  - Monitoring
  - Resilience
  - …

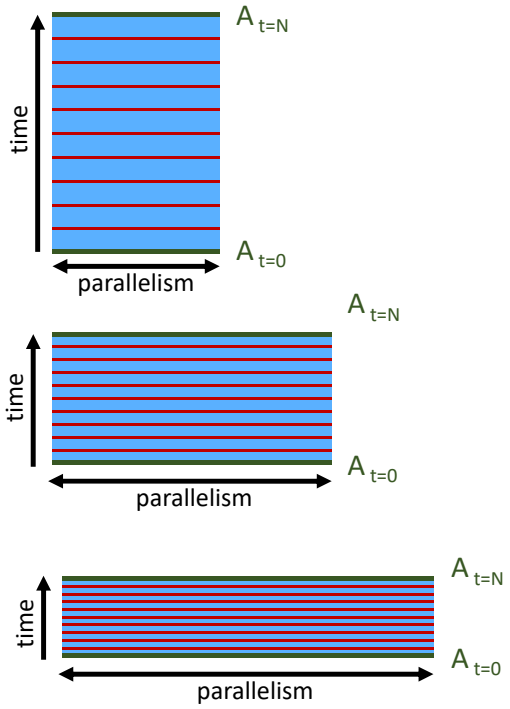


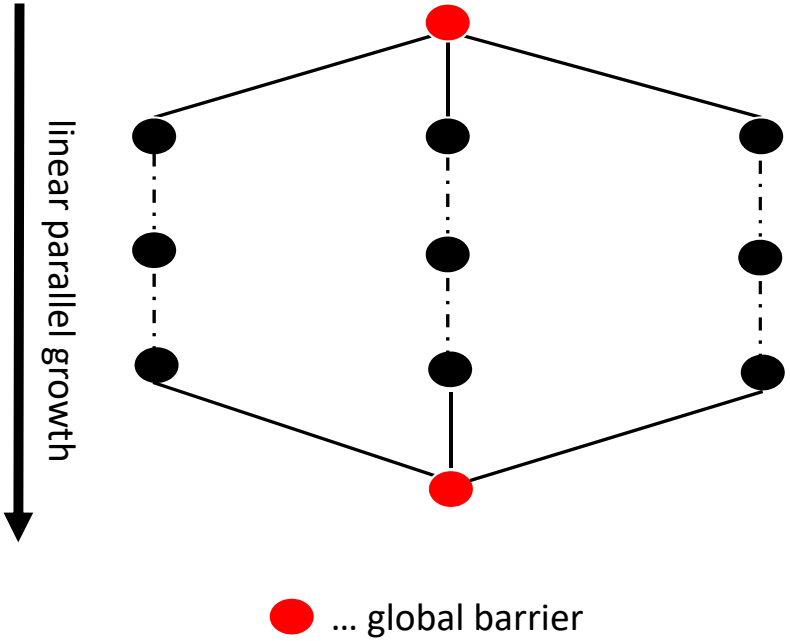
AllScale Vision



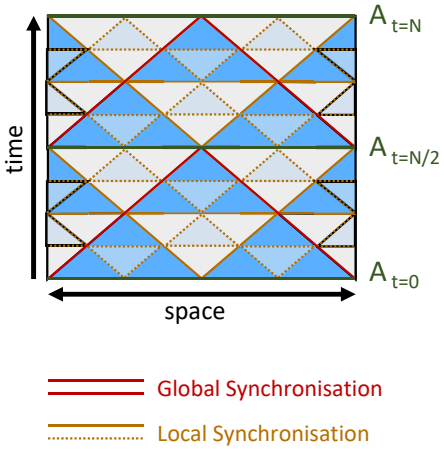
Conventional Flat Parallelism

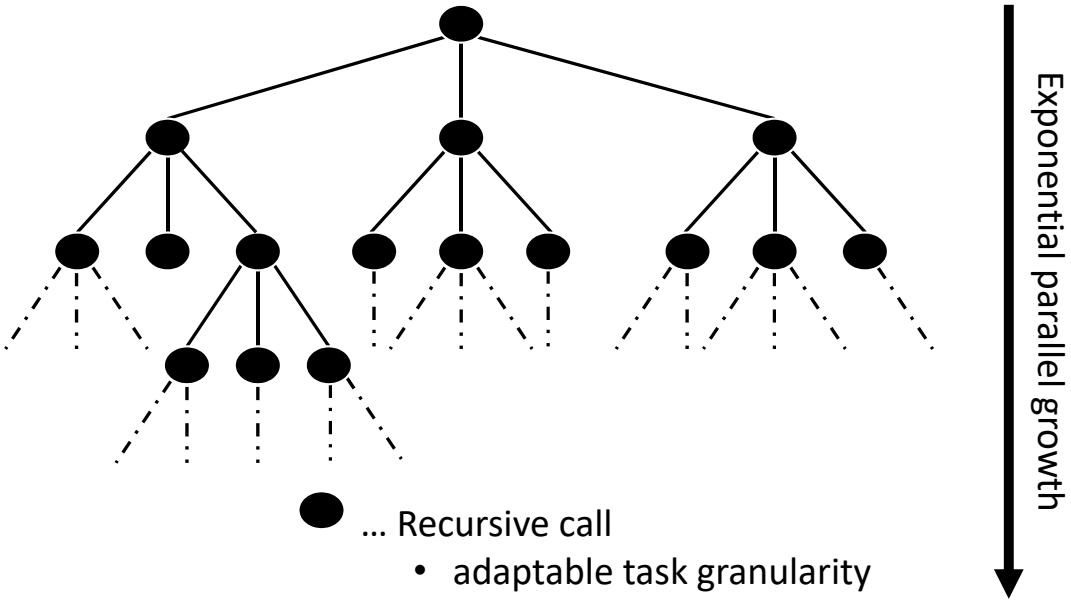
How to map flat parallelism to a hierarchical parallel architecture?
Complex handling of errors – global operations





Recursive Parallelism





… Recursive call

- adaptable task granularity
- multiversioning for tasks
- maps naturally to multiple levels of HW parallelism
- resilience

Recursive Task Parallelism Potential

- Branch and bound algorithms
- Place and Route algorithms
- SAT or SMT Solvers, Datalog Engines or similar reasoners
- Combinatorial optimization problems
- Stencil codes, in any number of dimensions
- Dense algebra operations
- N-body simulation
- Rendering

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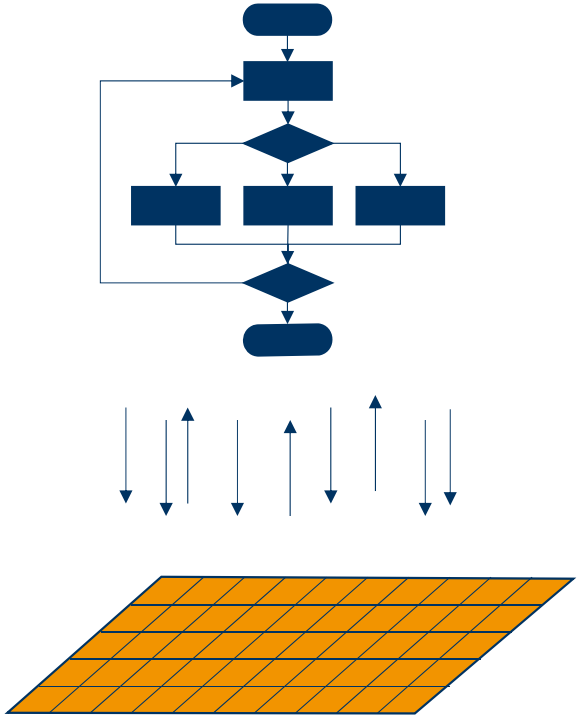
Serial Work and Data

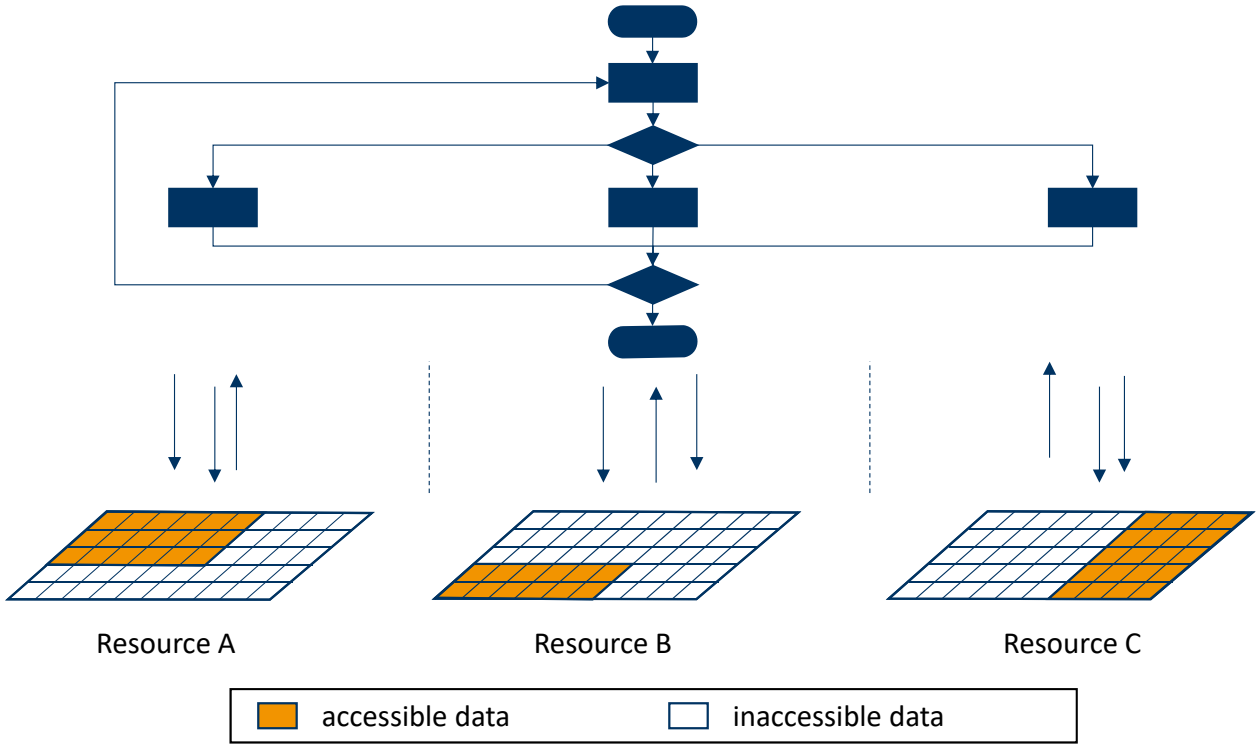
Algorithms
manipulate the
state of
data structures



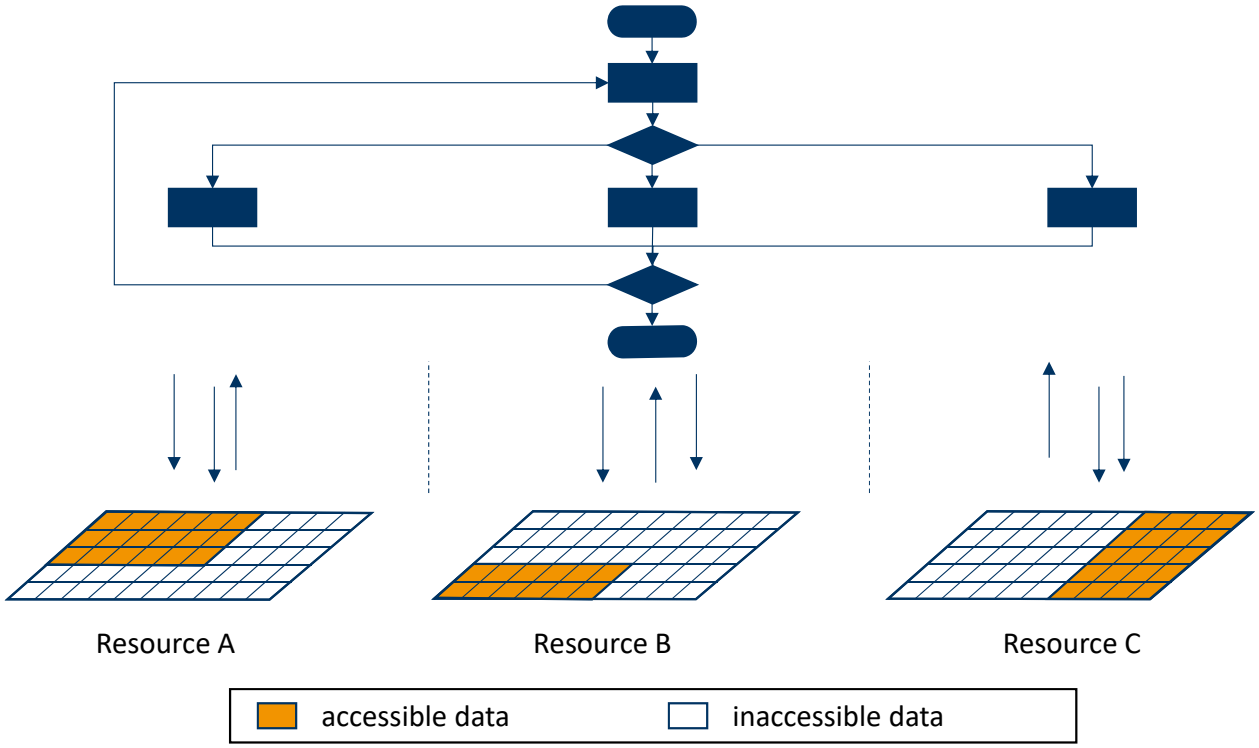
explicitly expressed
in program code

the **implicit** effect
of program code

Parallel Work and Data



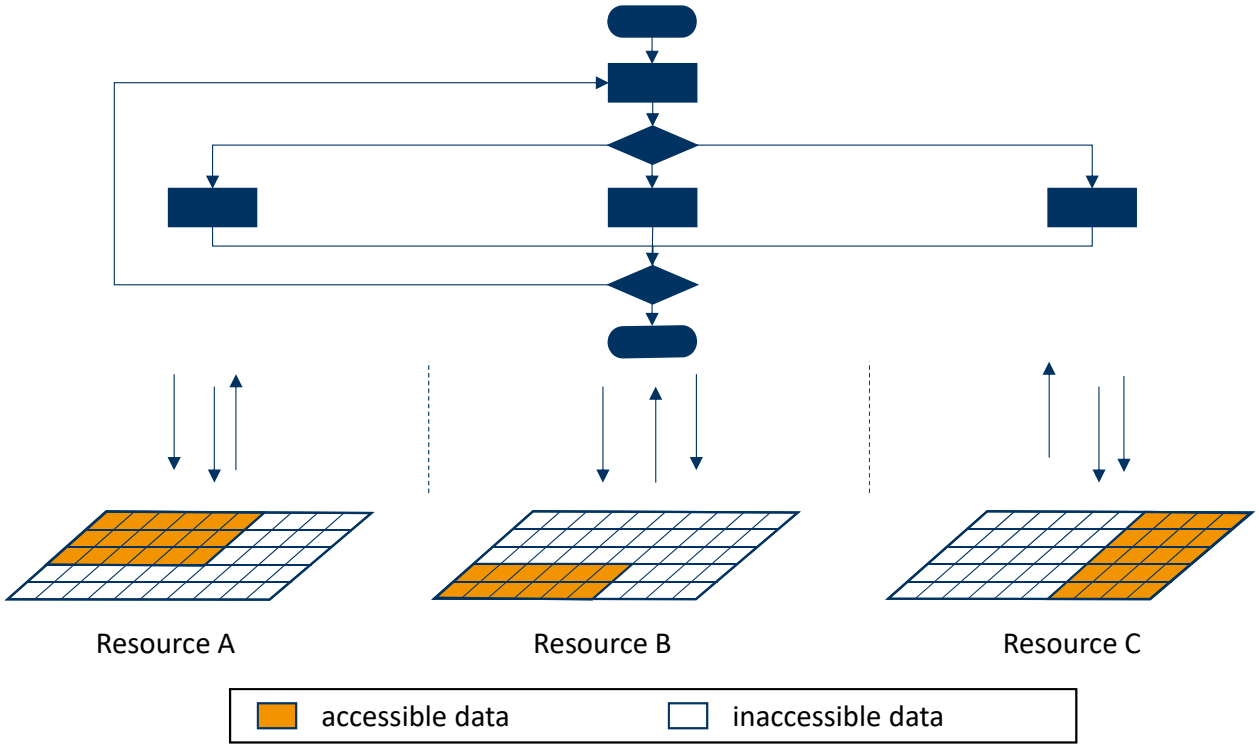
Parallel Work and Data



decomposition of **workload** is main focus of e.g. MPI, OpenMP, Cilk, OpenCL, SYCL, CUDA,…

data structure decomposition and management **left to the user**

Parallel Work and Data

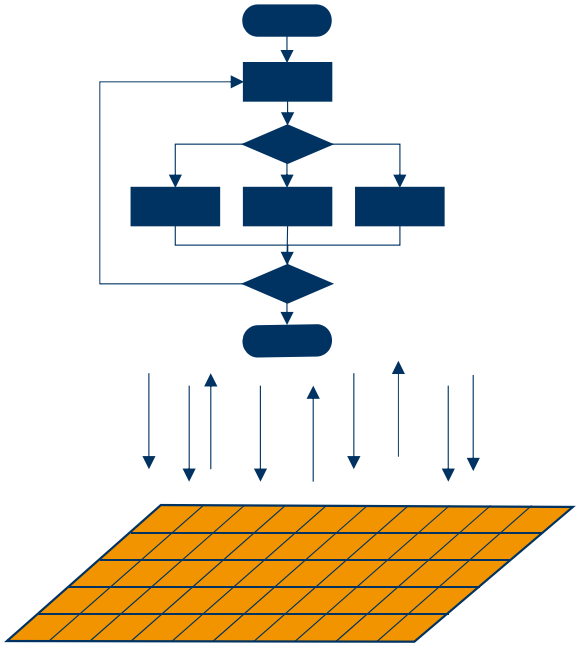


Desired:
advanced system features and services including

- performance **portability**
- inter-node **load balancing**
- **dynamic resource utilization**
- **resilience** to node failures

For those, **runtime systems** require **control** over **distribution** of **work and data**

AllScale User DSL/API Design



application

Operators:

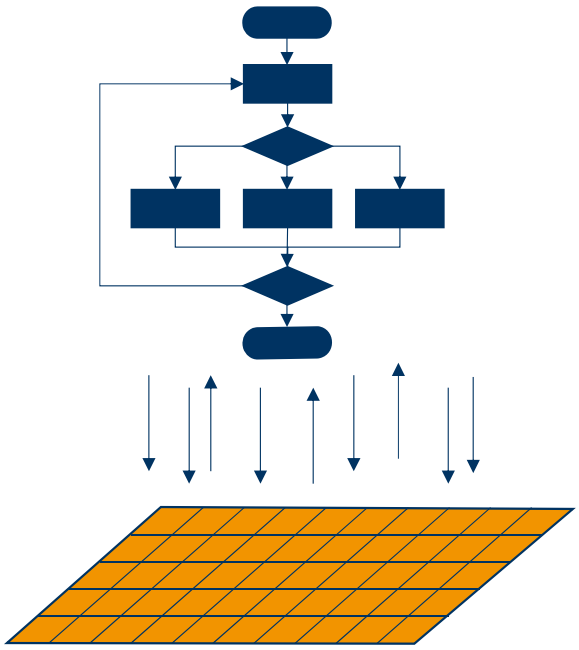
- parallel loops
- parallel reduction
- map-reduce
- stencils
- V-cycles
- brand and bound, linear algebra, …

Data Structures:

- multi-dimensional grids
- adaptive grids
- maps
- trees
- hierarchical meshes
- …

parallel constructs

AllScale's Approach



application

Operators:

- parallel loops (pfor)
- parallel reduction
- map-reduce
- stencils
- V-cycles
- branch and bound, …

higher order parallel primitive

Data Structures:

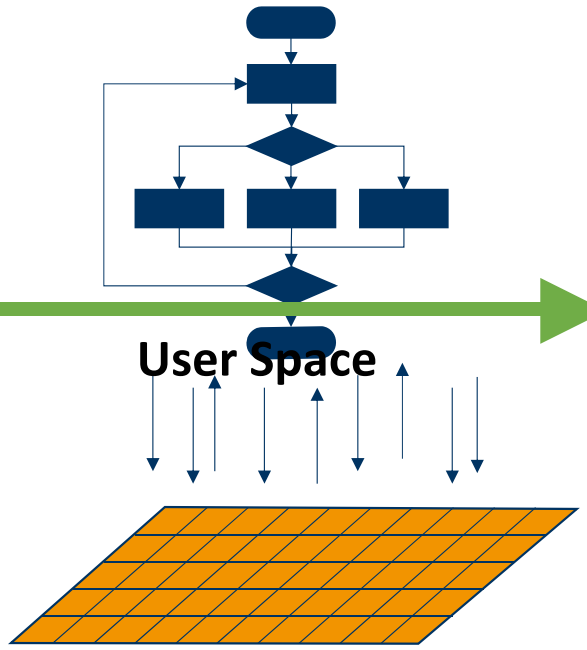
- multi-dimensional grids
- adaptive grids
- maps
- trees
- hierarchical meshes
- …

generalized abstract data structure

parallel constructs

primitives for parallel construct

AllScale's Approach



User Space

application

Operators:

- parallel loops
- parallel reduction
- map-reduce
- stencils
- V-cycles
- …

higher order parallel primitive

Toolchain

Data Structures:

- multi-dimensional grids
- adaptive grids
- maps
- trees
- hierarchical meshes
- …

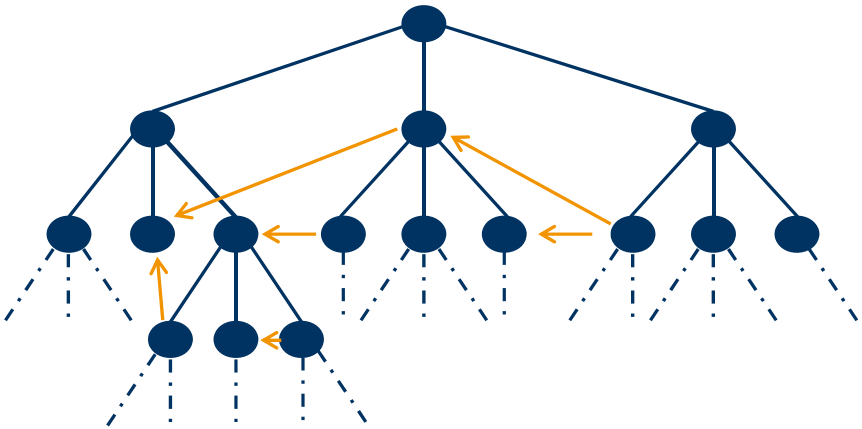
generalized abstract data structure

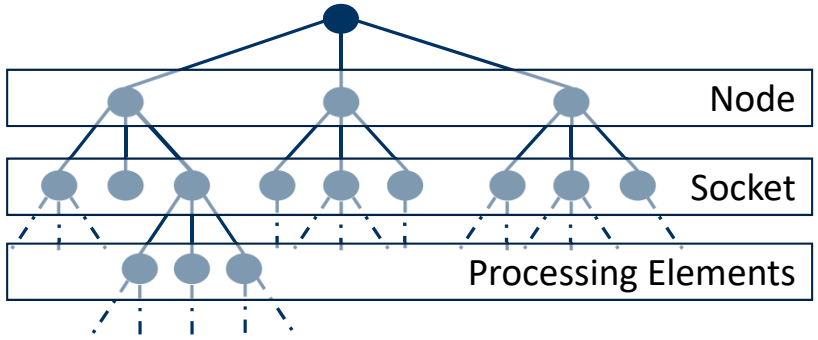
parallel constructs

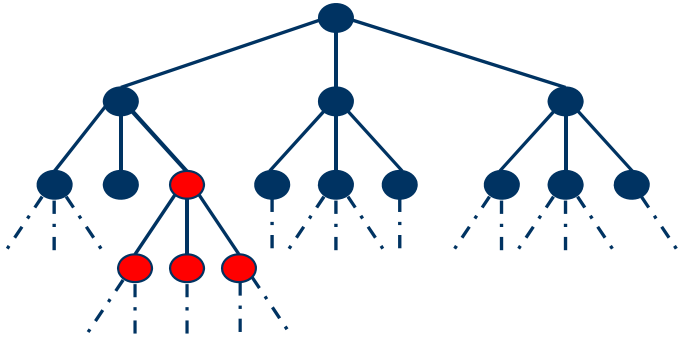
primitives for parallel construct

Work Flow Construct (Implicit Task Parallelism): AllScale Core API

- **prec** – a **higher order function** to
  - express recursive task-based parallelism
  - support fine-grained, hierarchical dependencies

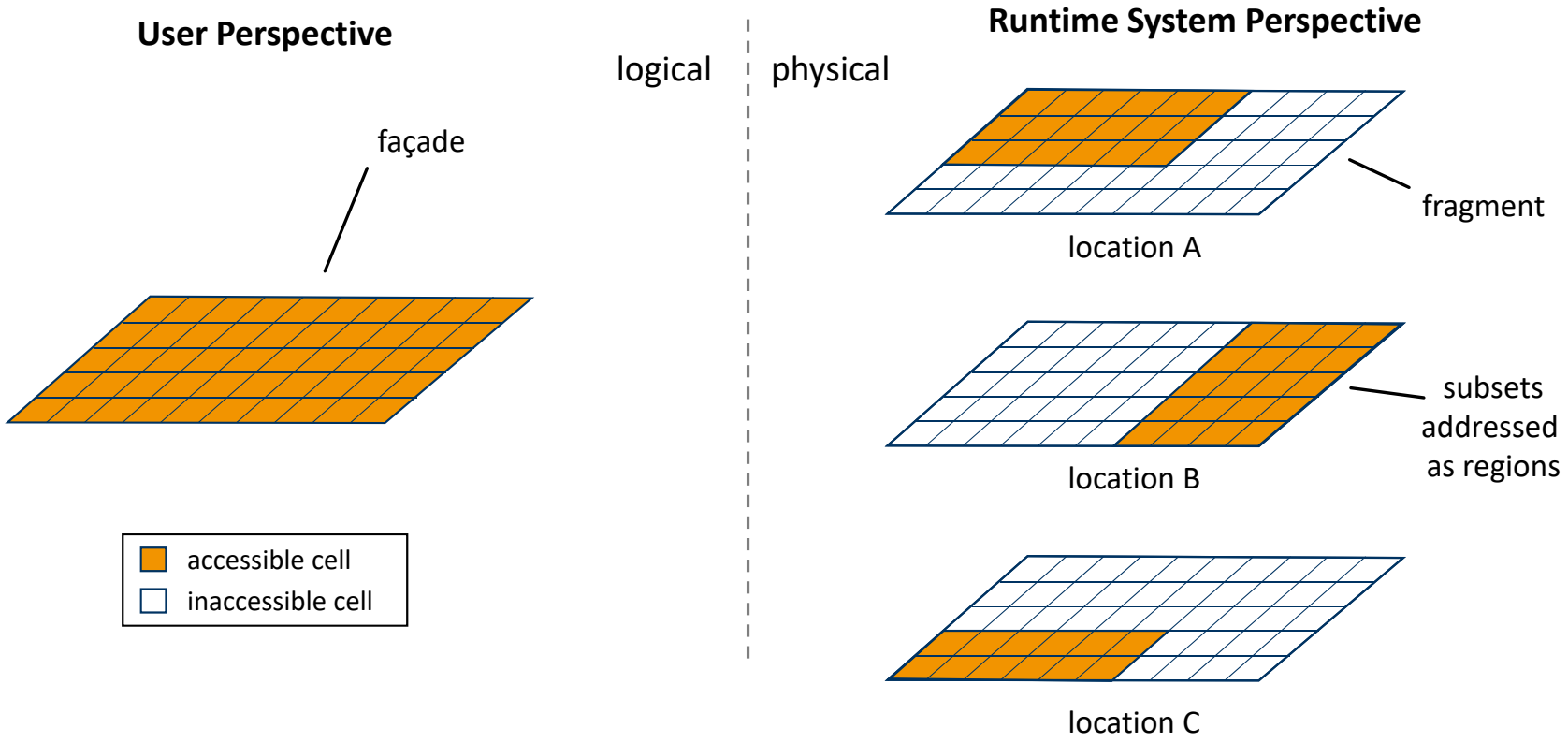




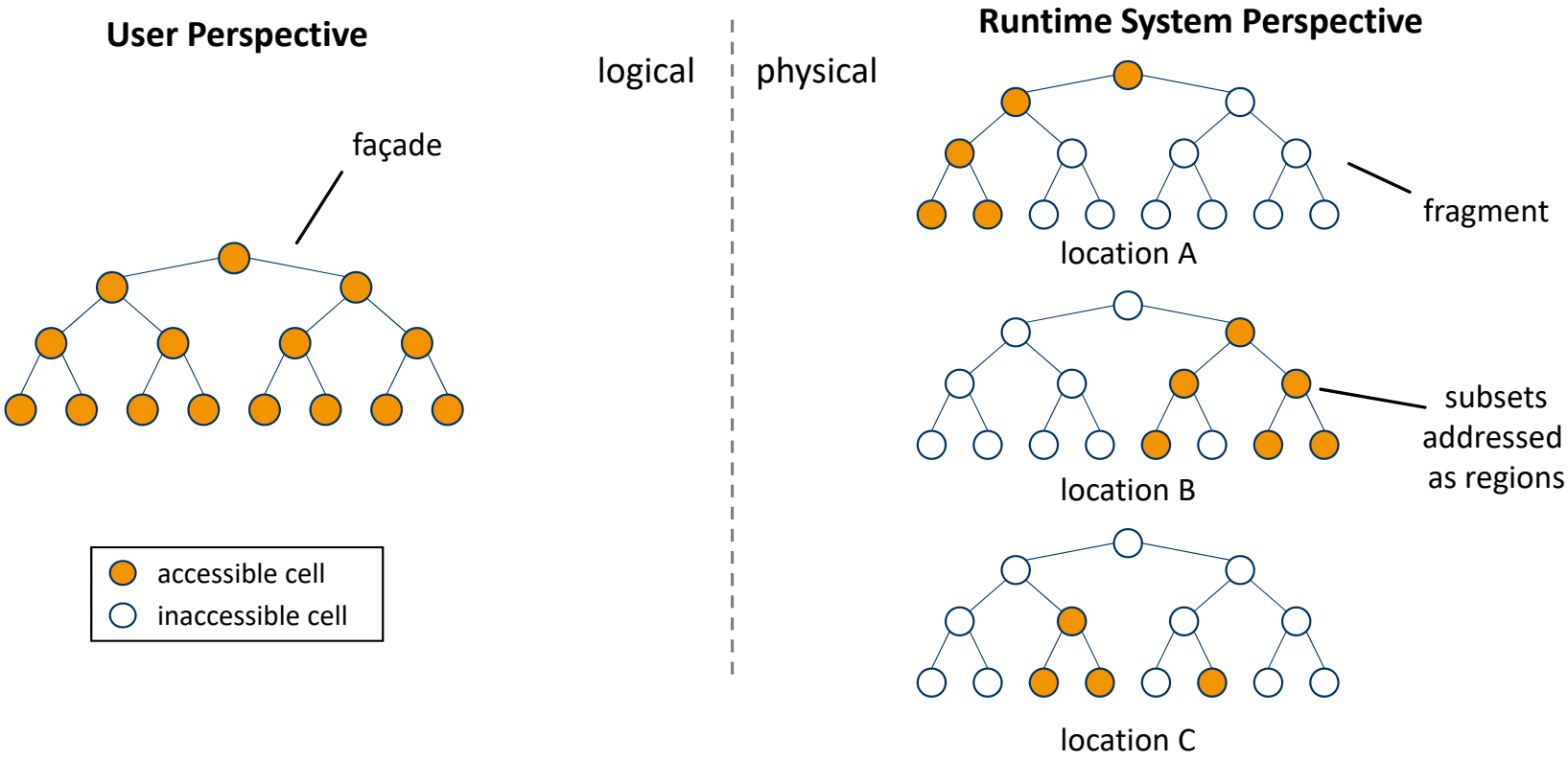


… recursive task — … task hierarchy ← … fine grained dependencies … failed task

Data Items


User Perspective
logical
physical
Runtime System Perspective
façade
fragment
location A
subsets
addressed
as regions
location B
location C
accessible cell
inaccessible cell

Data Items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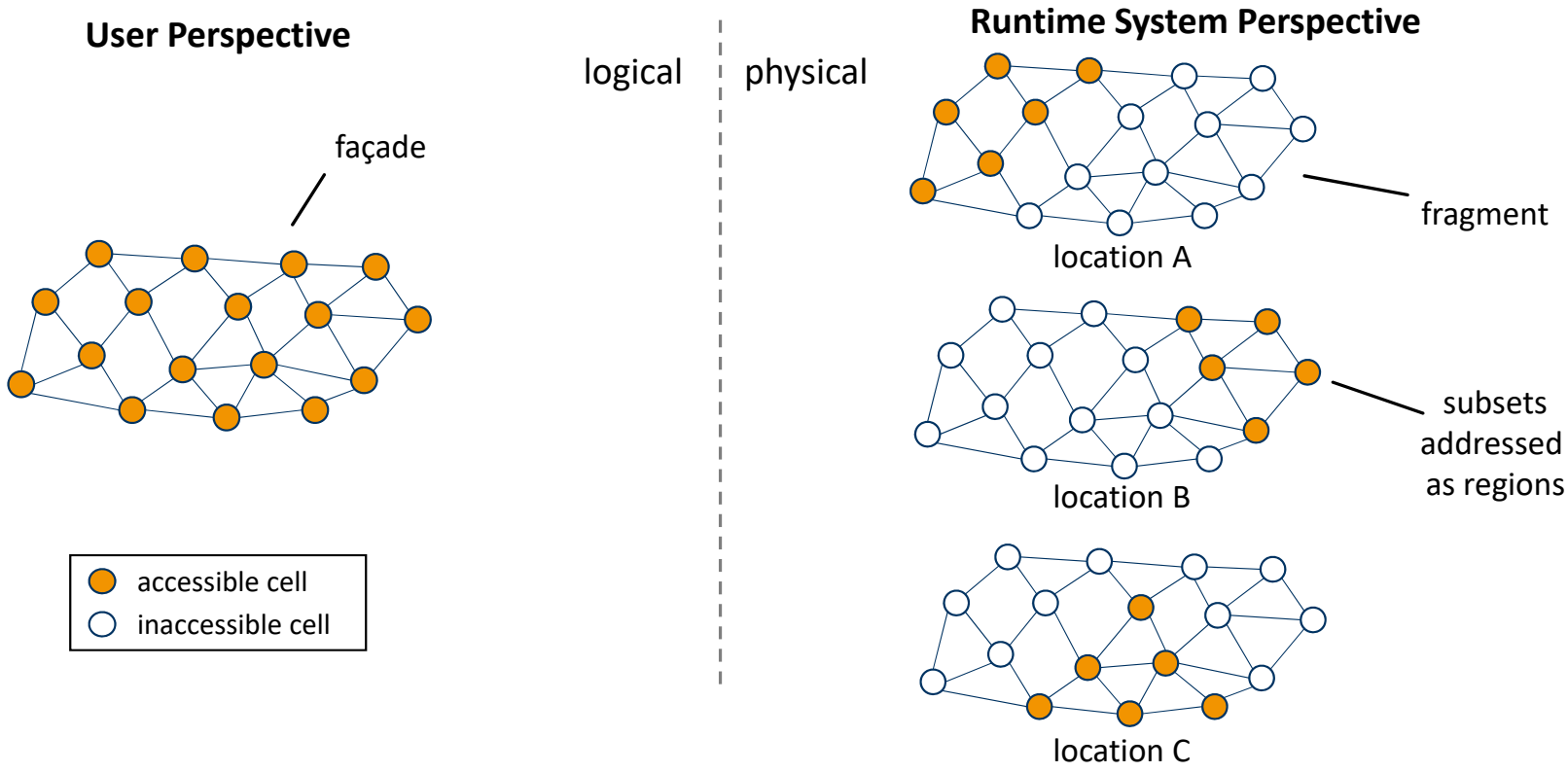
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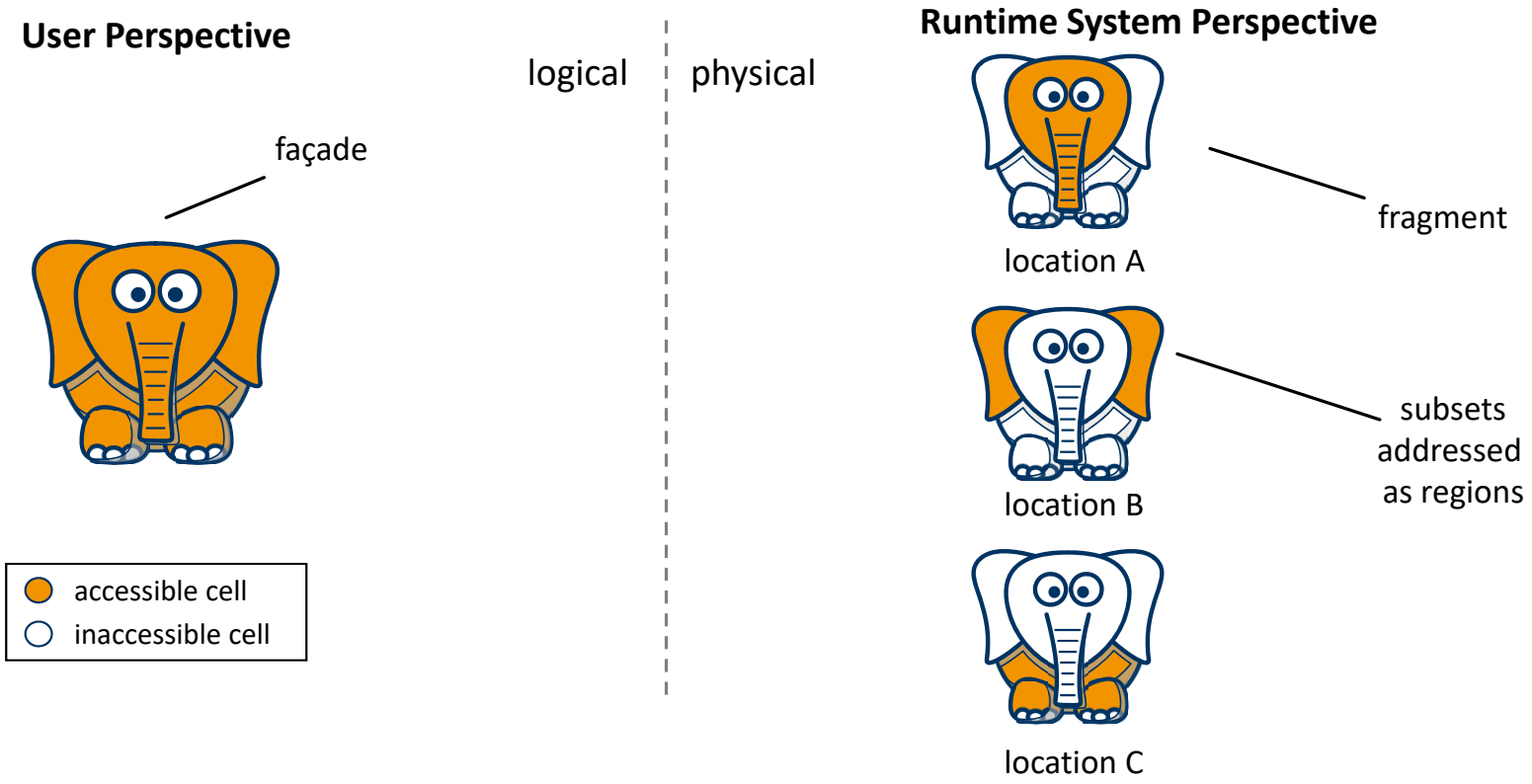
User Perspective
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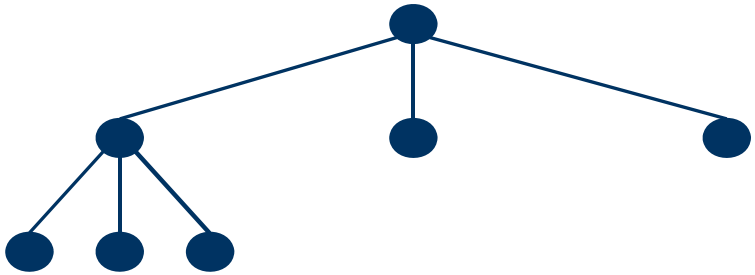
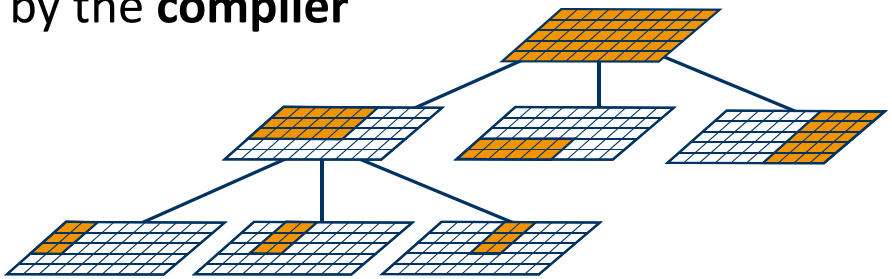
Work and Data Link



recursive work load
decomposition defined
by **algorithm**

automatically deduced
by the **compiler**

data dependencies
of tasks to be managed
by the **runtime system**



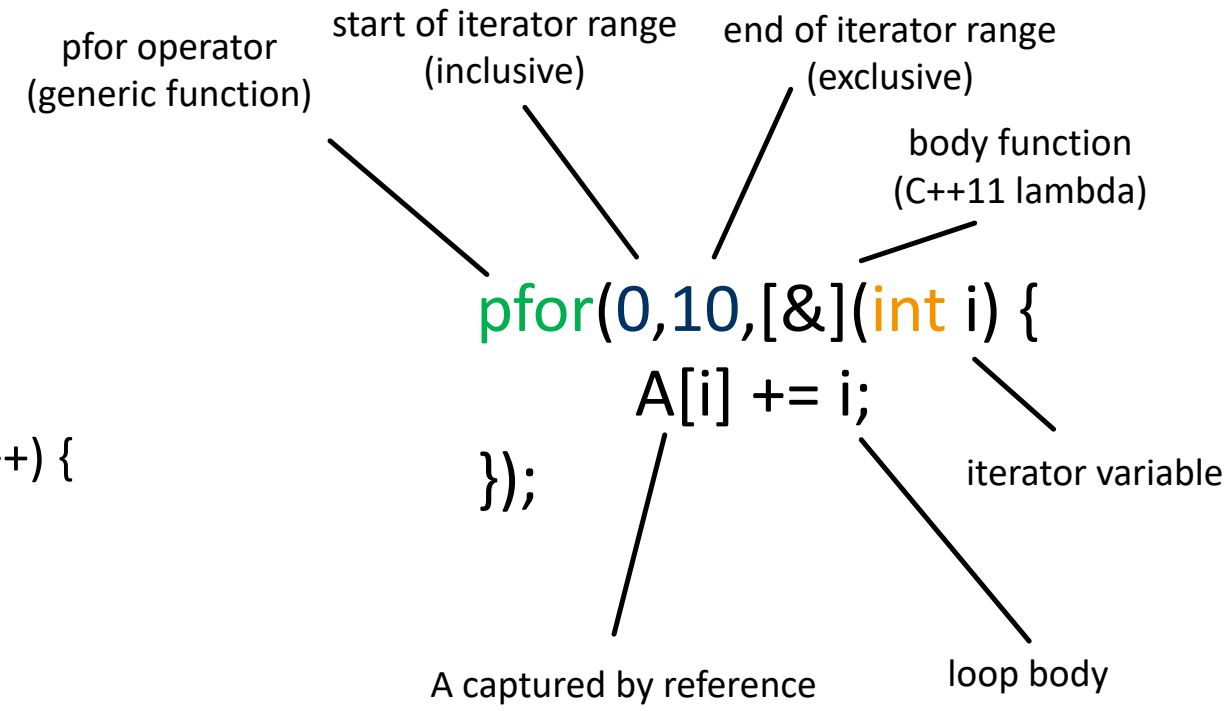
A Simple Loop

```
for (int i = 0; i < 10; i++) {
        A[i] += i;
}
```

Increments the first 10 elements of array A with values 0-9.

A Simple Parallel Loop

```
int rank, size;
MPI_Com_rank(COM,&rank)
MPI_Com_size(COM,&size)
int p = 10/size;
MPI_Scatter(A,…)
for (int i = p*rank; i < p*rank+p; i++) {
        A[i] += i;
}
MPI_Gather(A,…)
```



Increments the first 10 elements of array A with values 0-9 in parallel.

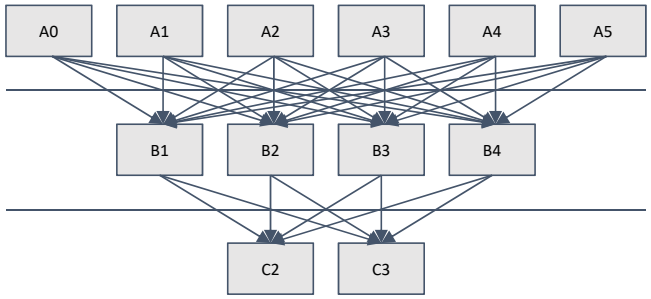
Pfor in Allscale

- Use it just like regular parallel loops:

```
pfor(0…6) a[i] = f(...);

pfor(1…5) b[i] = f(a[i-1],a[i],a[i+1])

pfor(2…4) c[i] = f(b[i-1],b[i],b[i+1])
```

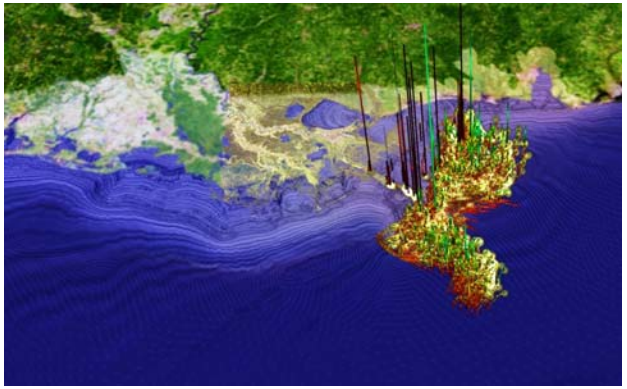


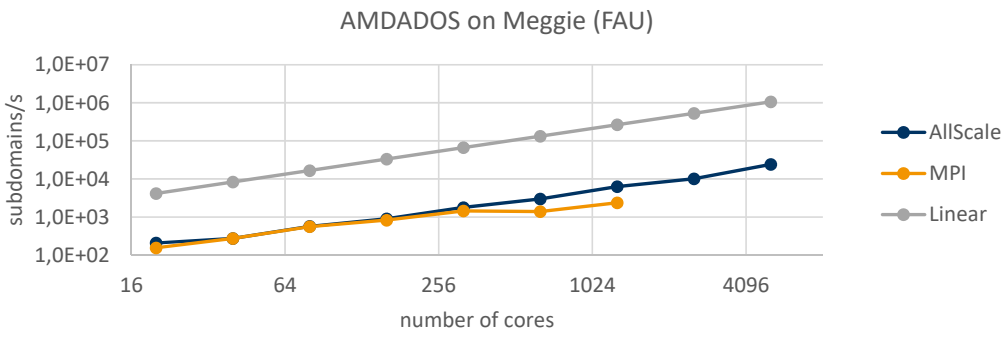
- Each of these spawns a decomposable recursive task processing the given range

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 671603

AMDADOS

- FetHPC H2020 project AllScale
- Oil spill simulation, developed with IBM Ireland
- Stencil and kalman filter for assimilating sensor data
- AllScale exceeds performance of MPI reference implementation

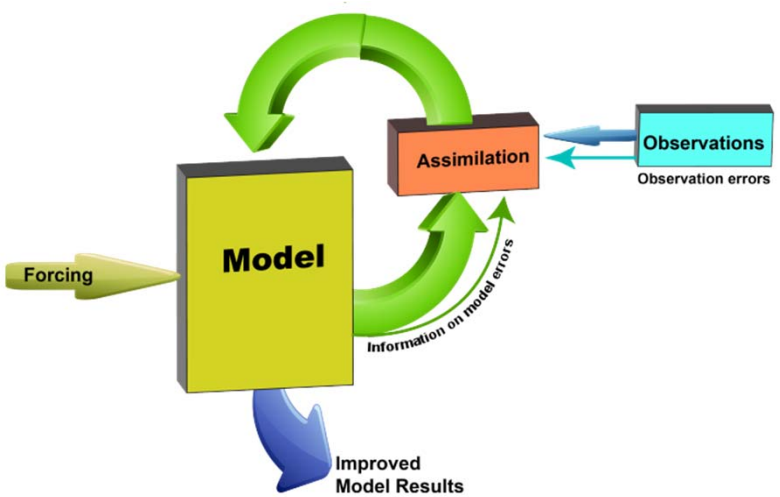




Sources: https://www.chemistryworld.com/features/oil-spill-cleanup/3008990.article, Marcel Ritter (UIBK)

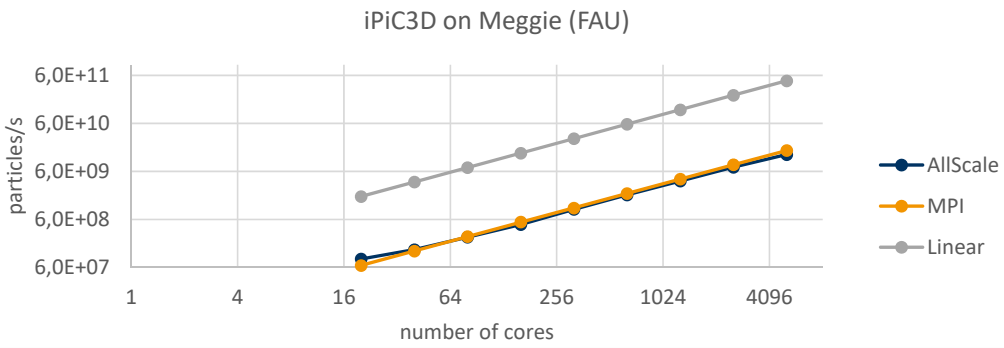
AMDADOS

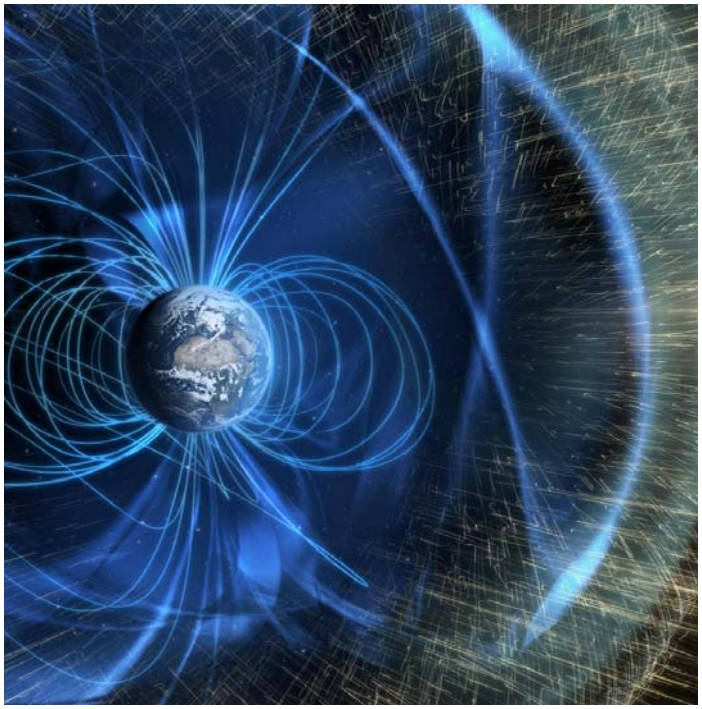
- Goal: simulate oil spill in real time using advection diffusion model with data assimilation
- Data assimilation introduces large load imbalance
  - Assimilation increases computational load by a factor in the order of 10^2
- Stencil operator + adaptive mesh data item
  - Spatio-temporal parallelization
  - Refinements at observations with 3 levels of refinement



iPiC3D

- FetHPC H2020 project AllScale
- Space weather prediction, developed with KTH Stockholm
- Particle-in-Cell simulation
- Productivity improvement compared to MPI reference implementation





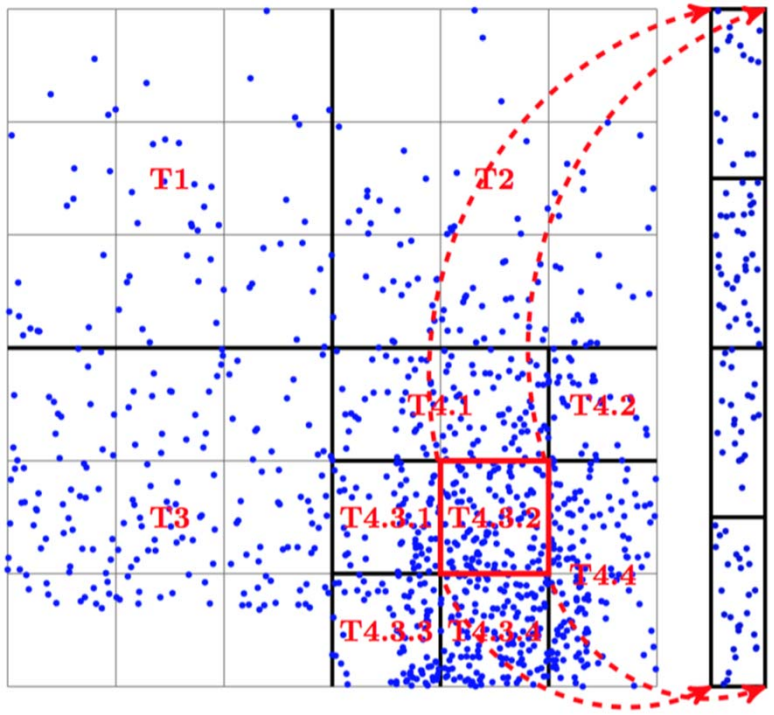
Source:
https://twitter.com/maven2mars/status/984440044659159040

iPiC3D

- Goal: Collision-less plasma simulation

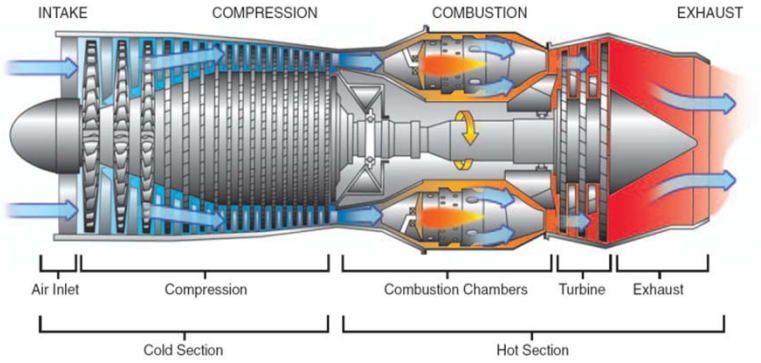
$$\frac{\partial f_s}{\partial \boldsymbol{t}} + \boldsymbol{v} \cdot \frac{\partial f_s}{\partial \boldsymbol{x}} + \frac{q_s}{m_s}\left(\boldsymbol{E} + \frac{\boldsymbol{v} \times \boldsymbol{B}}{c}\right) \cdot \frac{\partial f_s}{\partial \boldsymbol{v}} = 0$$

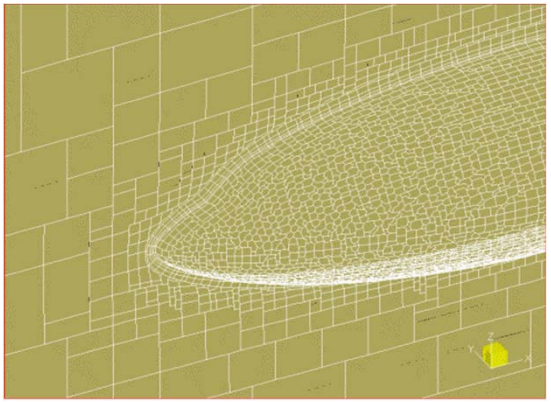
- Compute equation of motion for charged particles and solve Maxwell's equations in turns
- Highly dynamic load imbalance due to varying particle densities
- Nested pfor operators + multiple grids



FINE/Open

- Goal: perform scalable CFD simulations for various use cases (e.g. aircraft)
- Complex configurations with several hundreds of million of points.
  - Irregular data structure
  - Many elements: cells, faces, nodes, ...
  - Even more properties: velocity, pressure, …
- V-cycle and pfor operators + unstructured multi-level mesh

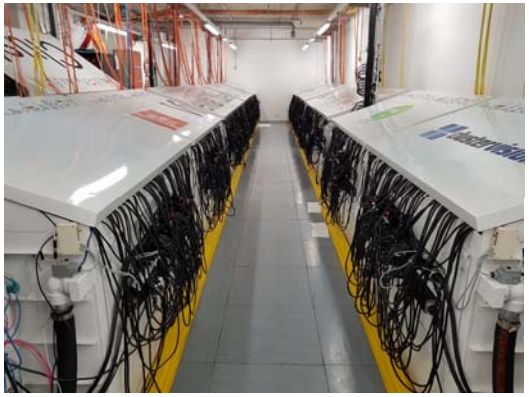




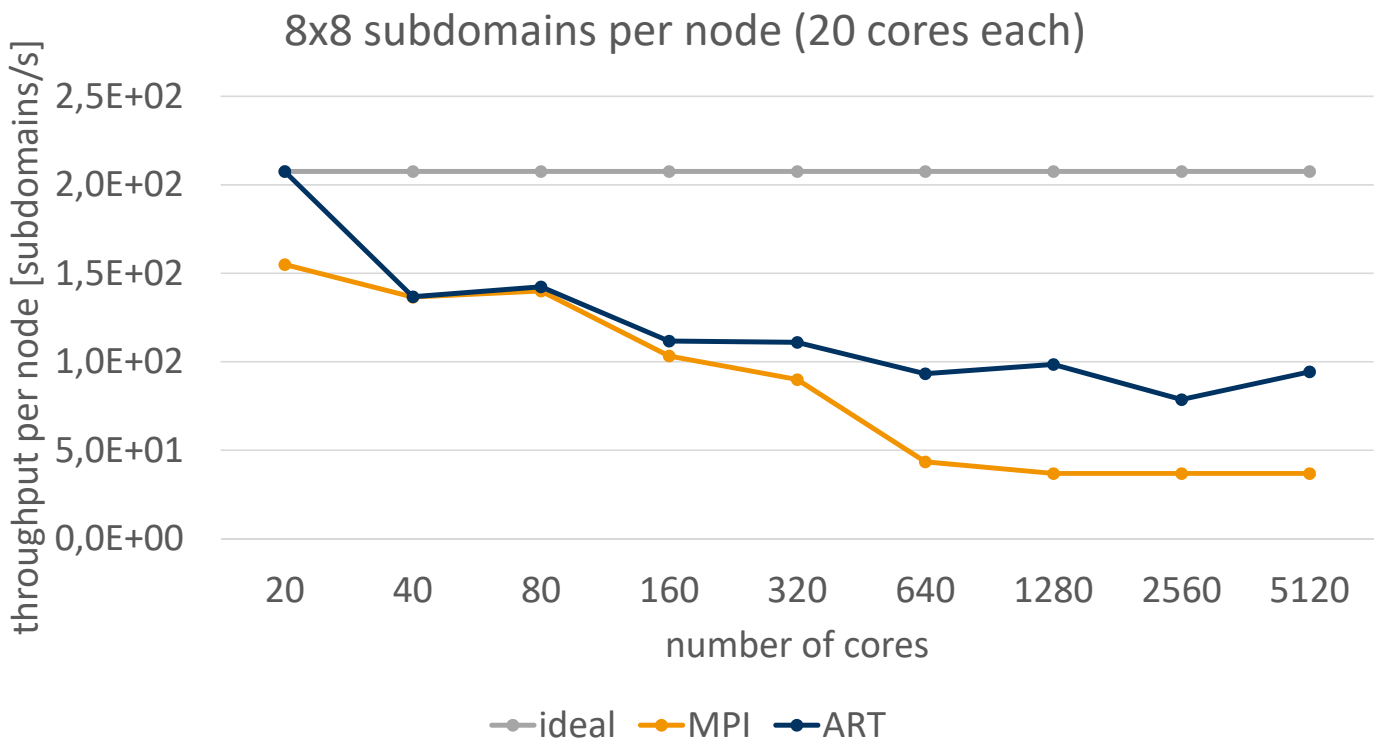
Experimental Target Systems

- Meggie (FAU)
  - 728 nodes
  - 2x Intel Xeon E5-2630 v4 (10 cores) each
  - 14,560 cores in total
  - Intel OmniPath

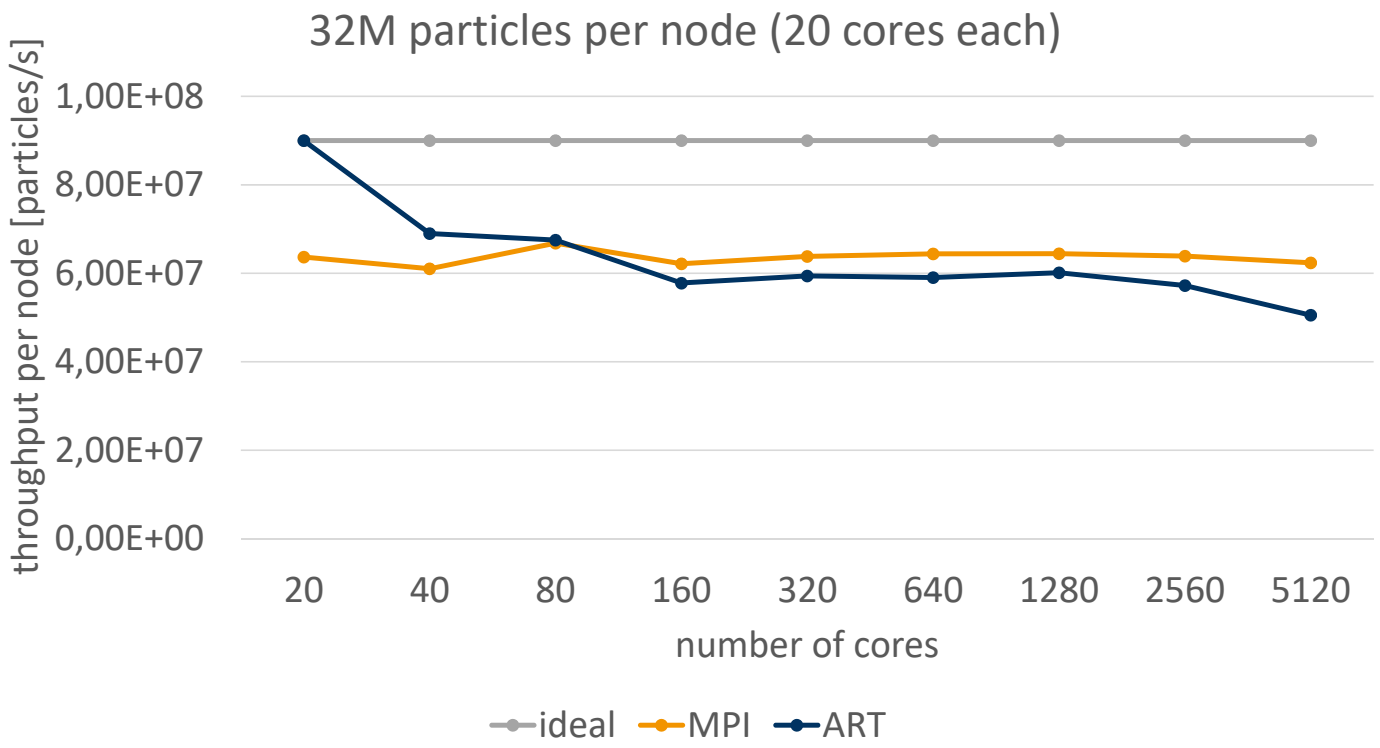
- VSC-3 (UIBK)
  - 2020 nodes
  - 2x Intel Xeon E5-2650 v2 (8 cores) each
  - 32,320 cores in total
  - QDR-80 dual-link InfiniBand



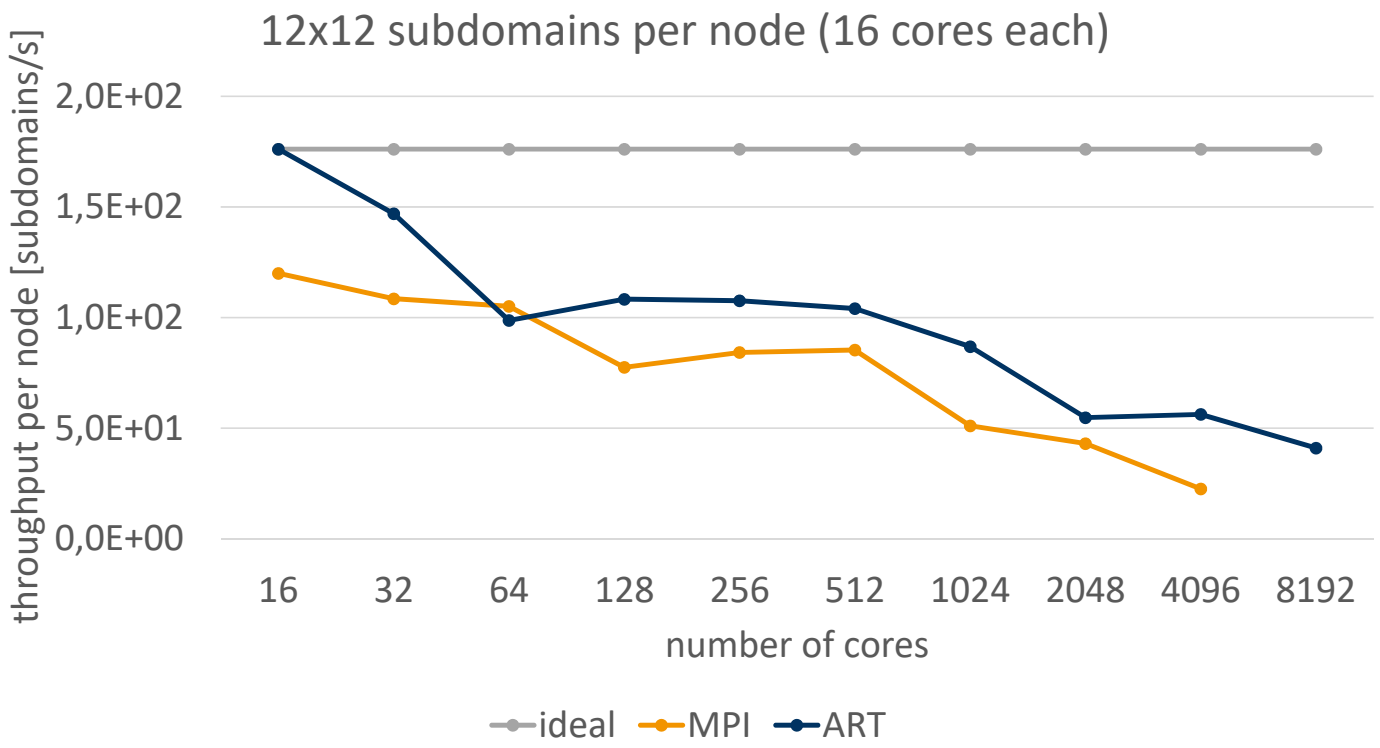
AMDADOS on Meggie



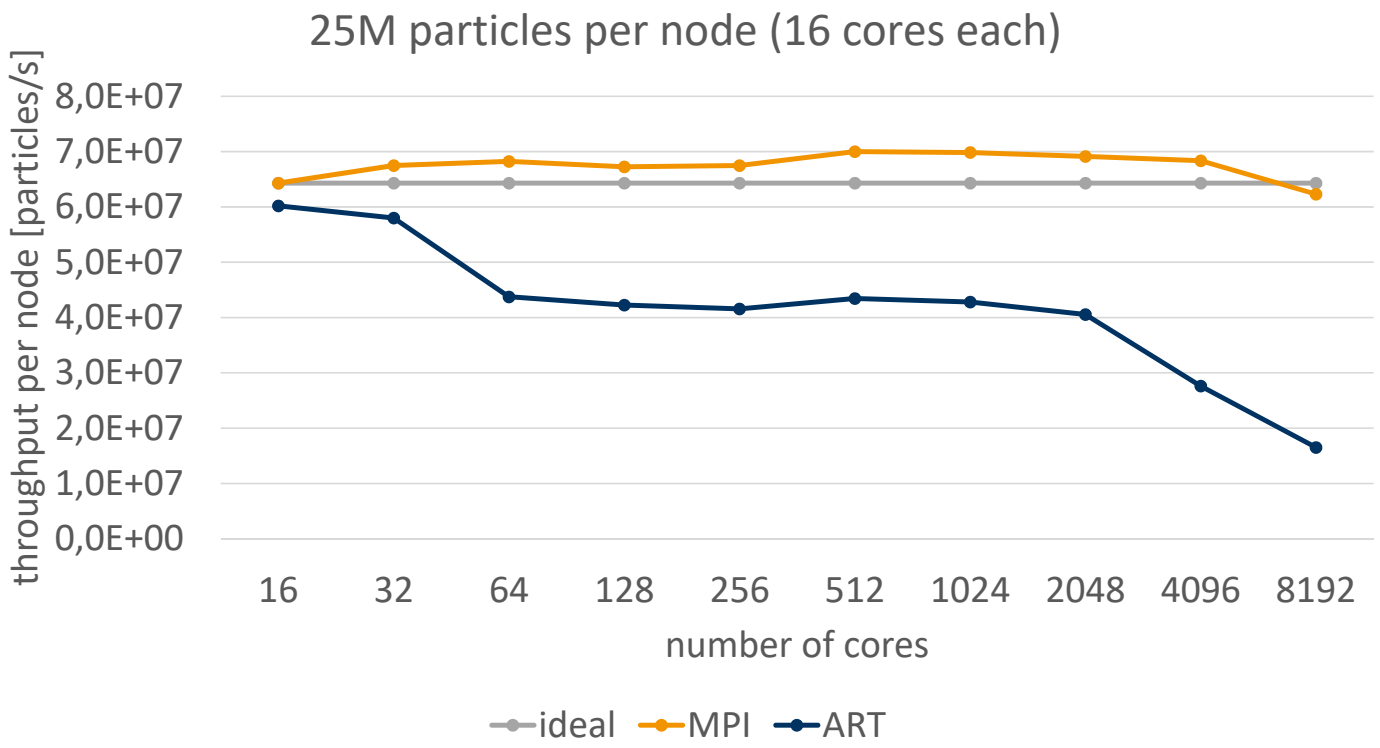
iPiC3D on Meggie



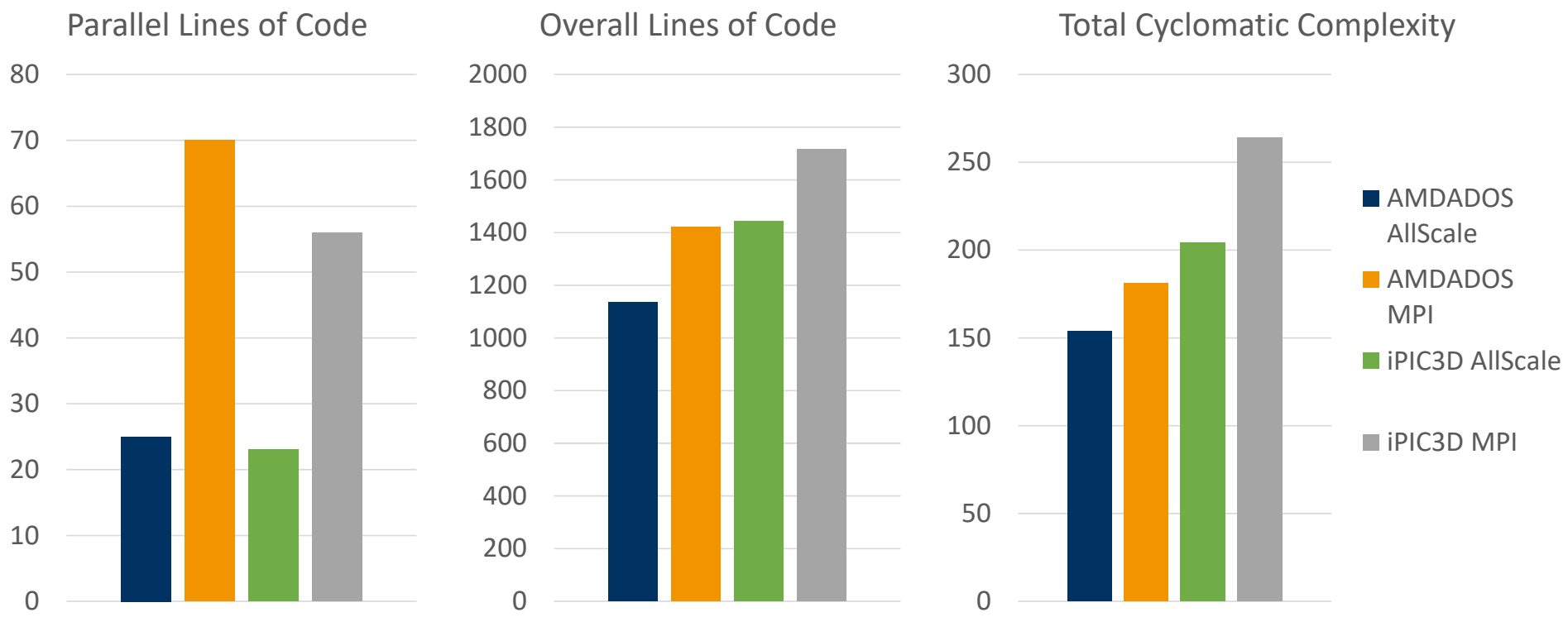
AMDADOS on VSC-3



iPiC3D on VSC-3



Productivity Evaluation



Practical Experience: Benefits and Challenges of AllScale

- Higher-order primites for parallelism and data structures to improve productivity and performance.
- Implicit task parallelism
- Data management out of the box
- No explicit communication and data management
- Automated object serialization
- Implicit intra- and inter-node load balancing
- No need to deal with MPI+X
- Preserve structure of mathematical equations in the application

- Requires advanced C++ knowledge
- Longer compile times (but once for multiple runs)
- No support for external libraries that employ non-AllScale parallelism
- no support for accelerators so far